



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 02:18 AM UTC

PDB ID : 3A2C / pdb_00003a2c
Title : Crystal structure of a pyrazolopyrimidine inhibitor complex bound to MAP-KAP Kinase-2 (MK2)
Authors : Fujino, A.; Takimoto-Kamimura, M.
Deposited on : 2009-05-12
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

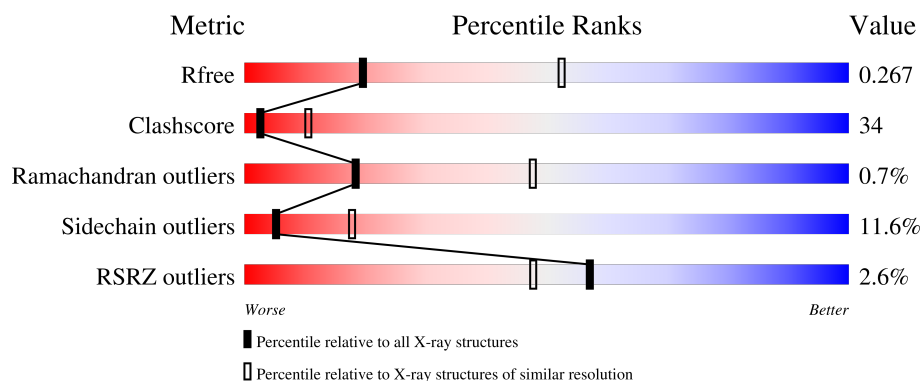
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	324	
1	B	324	
1	C	324	
1	D	324	
1	E	324	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	324	
1	G	324	
1	H	324	
1	I	324	
1	J	324	
1	K	324	
1	L	324	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PDY	C	2	-	-	X	-
2	PDY	E	1	-	-	X	-
2	PDY	E	2	-	-	X	-
2	PDY	F	2	-	-	X	-
2	PDY	G	1	-	-	X	-
2	PDY	G	2	-	-	X	-
2	PDY	H	1	-	-	X	-
2	PDY	H	2	-	-	X	-
2	PDY	I	1	-	-	X	-
2	PDY	I	2	-	-	X	-
2	PDY	J	1	-	-	X	-
2	PDY	K	1	-	-	X	-
2	PDY	K	2	-	-	X	-
2	PDY	L	1	-	-	X	-
2	PDY	L	2	-	-	X	-

2 Entry composition

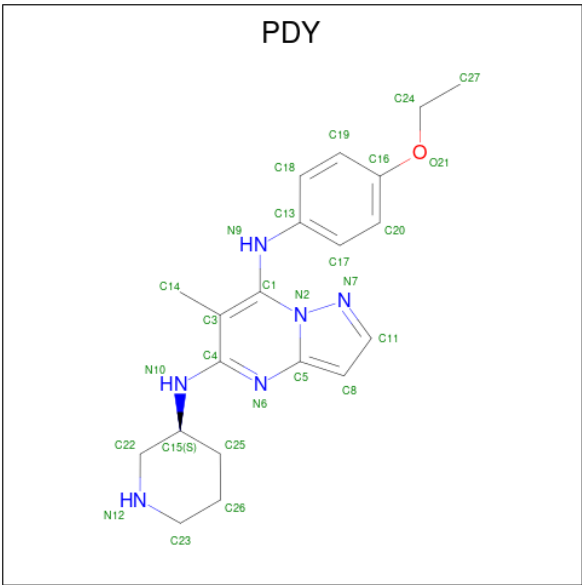
There are 3 unique types of molecules in this entry. The entry contains 27440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2218	1415	384	402	17			
1	B	277	Total	C	N	O	S	0	0	0
			2240	1426	388	409	17			
1	C	273	Total	C	N	O	S	0	0	0
			2207	1409	380	401	17			
1	D	277	Total	C	N	O	S	0	0	0
			2244	1430	389	408	17			
1	E	276	Total	C	N	O	S	0	0	0
			2234	1425	385	407	17			
1	F	287	Total	C	N	O	S	0	0	0
			2316	1476	401	422	17			
1	G	273	Total	C	N	O	S	0	0	0
			2210	1411	381	401	17			
1	H	275	Total	C	N	O	S	0	0	0
			2226	1421	385	403	17			
1	I	275	Total	C	N	O	S	0	0	0
			2225	1420	384	404	17			
1	J	275	Total	C	N	O	S	0	0	0
			2225	1420	384	404	17			
1	K	273	Total	C	N	O	S	0	0	0
			2208	1409	381	401	17			
1	L	276	Total	C	N	O	S	0	0	0
			2234	1425	385	407	17			

- Molecule 2 is N 7 -(4-ethoxyphenyl)-6-methyl-N 5 -[(3S)-piperidin-3-yl]pyrazolo[1,5-a]pyrimidine-5,7-diamine (CCD ID: PDY) (formula: C₂₀H₂₆N₆O).



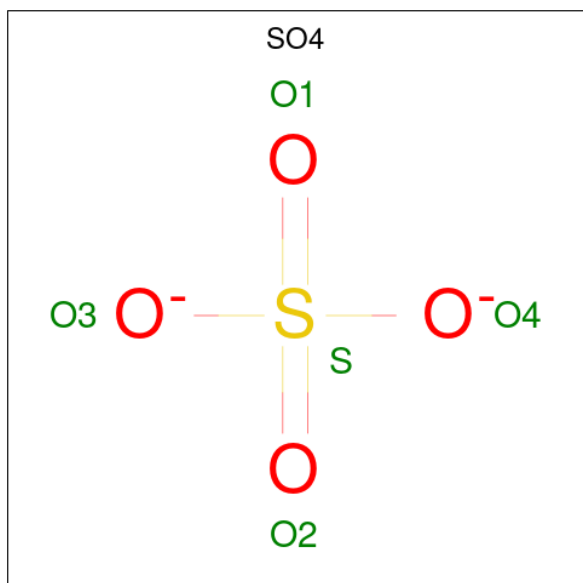
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		
2	D	1	Total	C	N	O	0	0
			27	20	6	1		
2	D	1	Total	C	N	O	0	0
			27	20	6	1		
2	E	1	Total	C	N	O	0	0
			27	20	6	1		
2	E	1	Total	C	N	O	0	0
			27	20	6	1		
2	F	1	Total	C	N	O	0	0
			27	20	6	1		
2	F	1	Total	C	N	O	0	0
			27	20	6	1		
2	G	1	Total	C	N	O	0	0
			27	20	6	1		
2	G	1	Total	C	N	O	0	0
			27	20	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			27	20	6	1		
2	H	1	Total	C	N	O	0	0
			27	20	6	1		
2	I	1	Total	C	N	O	0	0
			27	20	6	1		
2	I	1	Total	C	N	O	0	0
			27	20	6	1		
2	J	1	Total	C	N	O	0	0
			27	20	6	1		
2	J	1	Total	C	N	O	0	0
			27	20	6	1		
2	K	1	Total	C	N	O	0	0
			27	20	6	1		
2	K	1	Total	C	N	O	0	0
			27	20	6	1		
2	L	1	Total	C	N	O	0	0
			27	20	6	1		
2	L	1	Total	C	N	O	0	0
			27	20	6	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

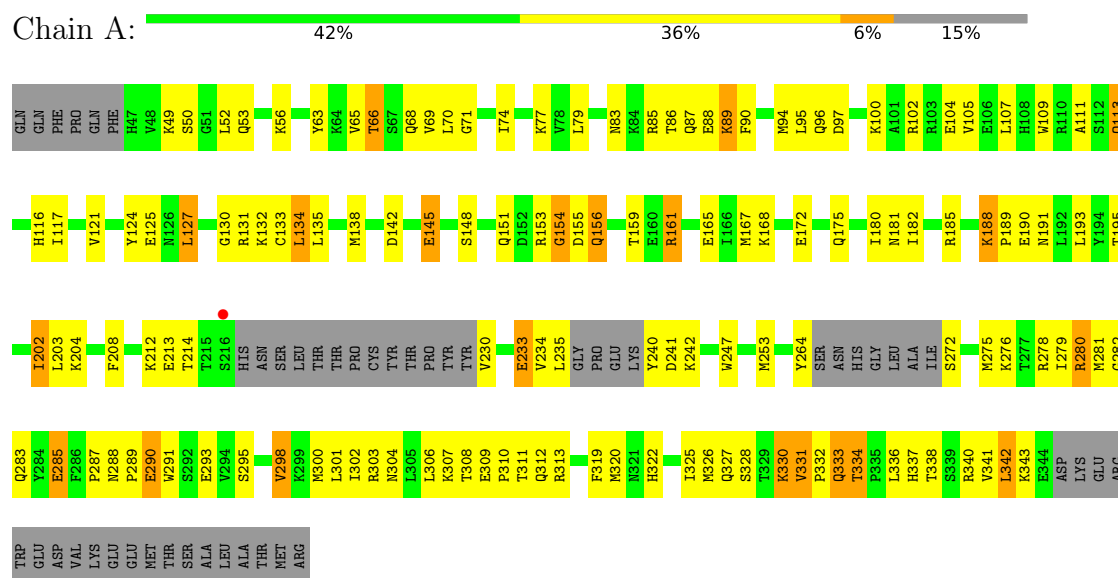


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	O S	0	0
			5	4 1		

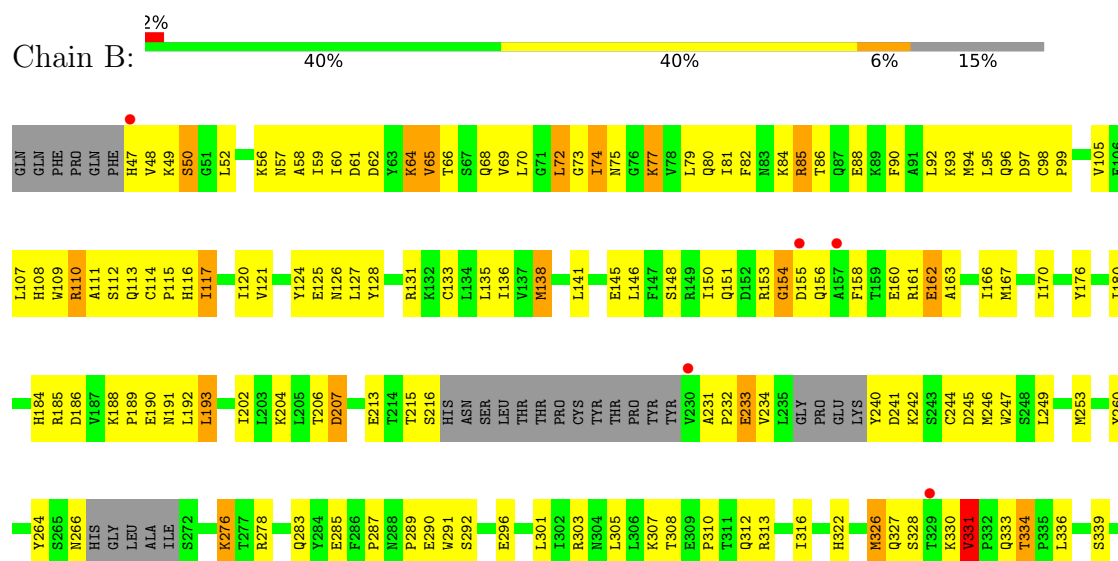
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MAP kinase-activated protein kinase 2

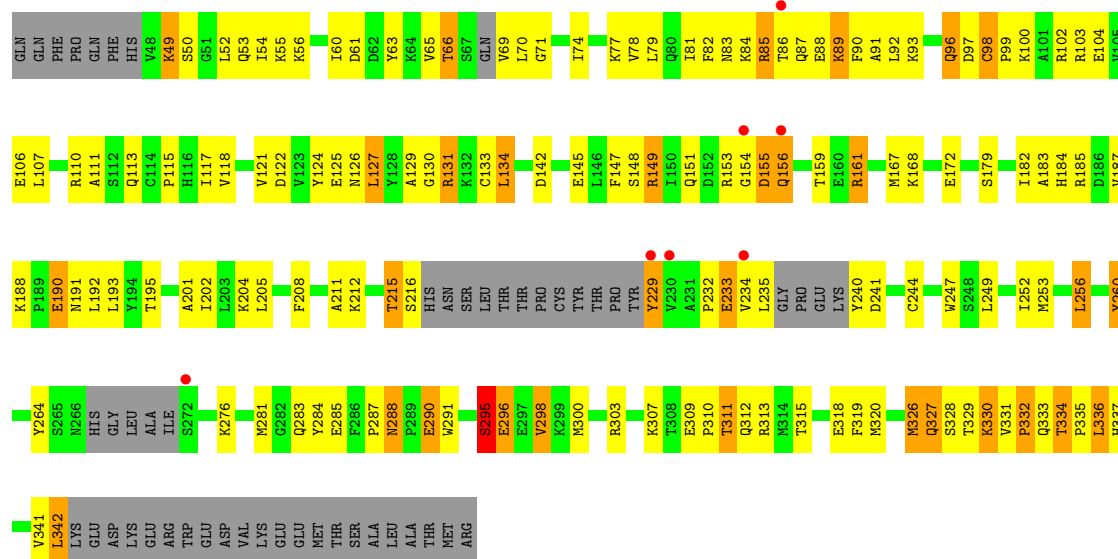


• Molecule 1: MAP kinase-activated protein kinase 2

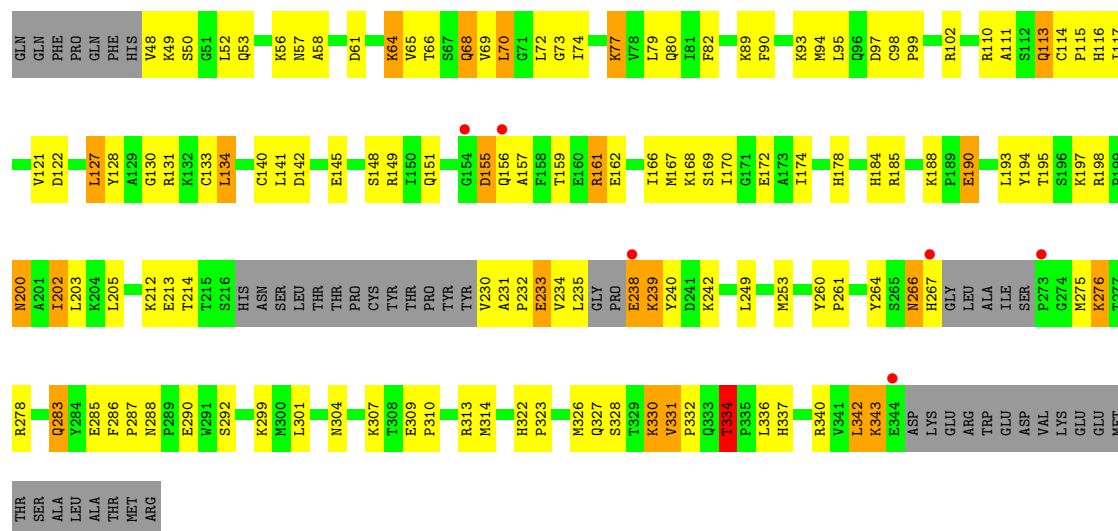
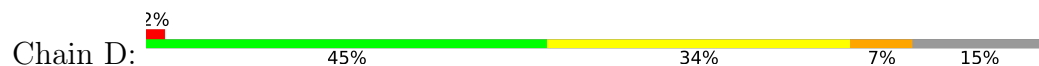


L342 K343 E344 D345 LYS GLU ARG TRP GLU ASP VAL LYS GLU GLU MET THR SER ALA LEU ALA THR MET ARG

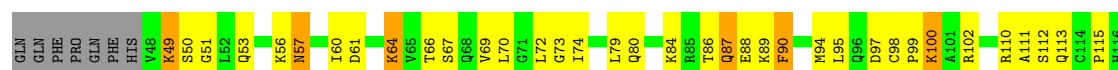
• Molecule 1: MAP kinase-activated protein kinase 2

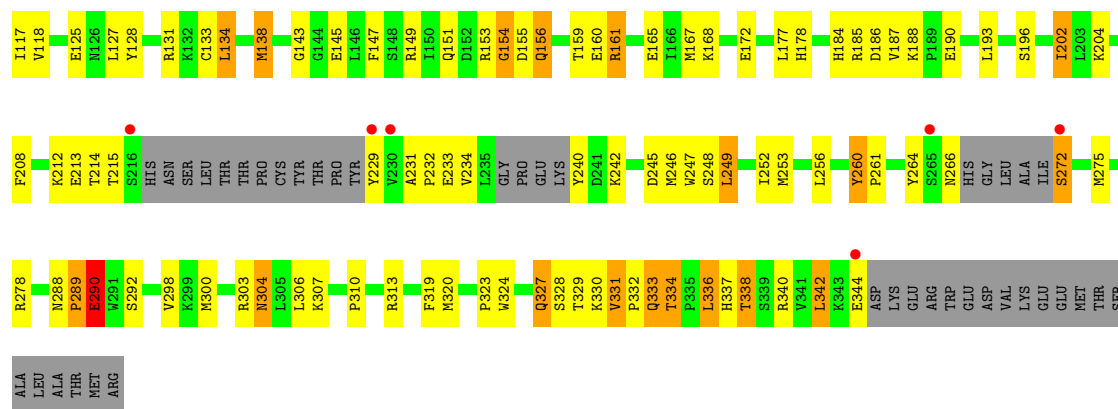


• Molecule 1: MAP kinase-activated protein kinase 2

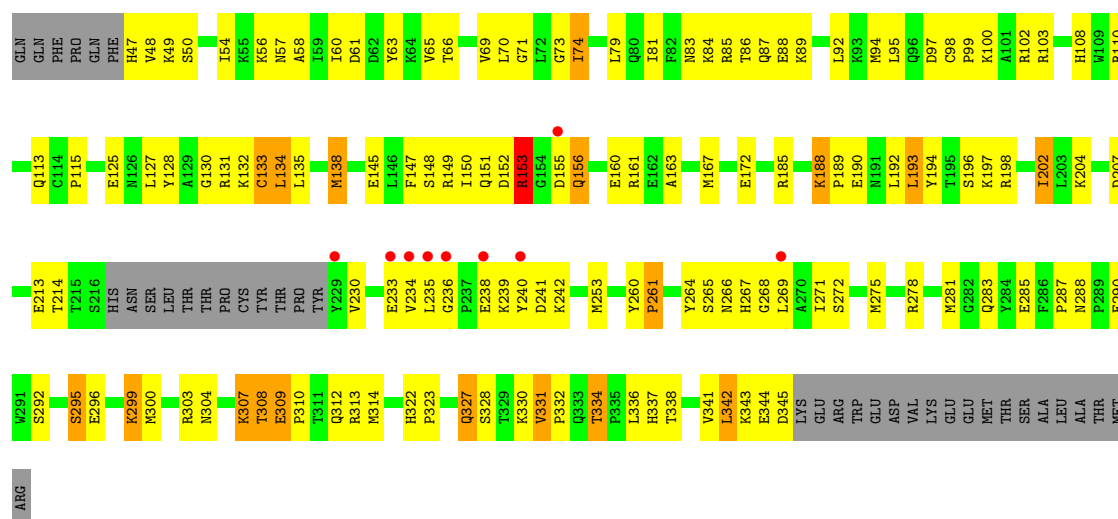


• Molecule 1: MAP kinase-activated protein kinase 2

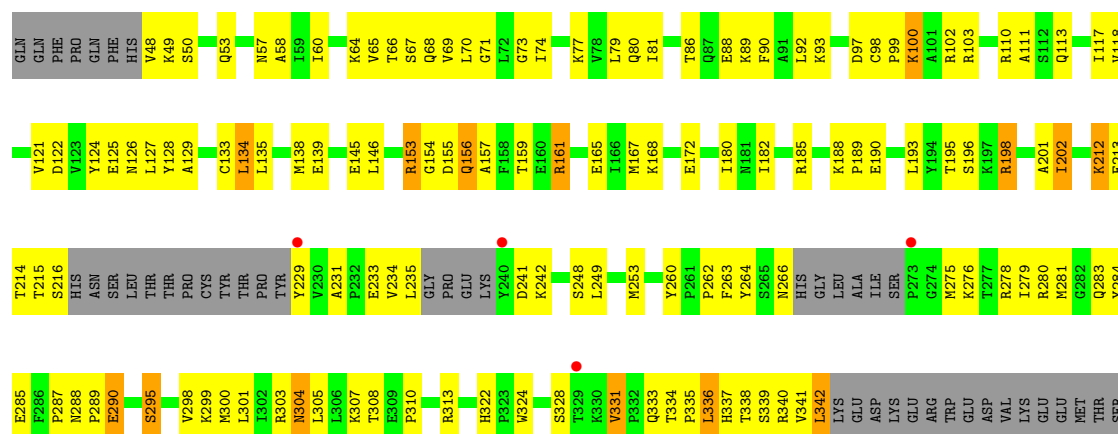
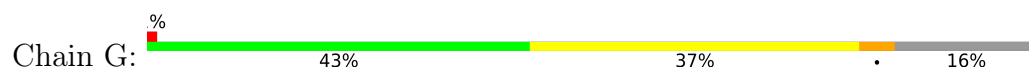




- Molecule 1: MAP kinase-activated protein kinase 2

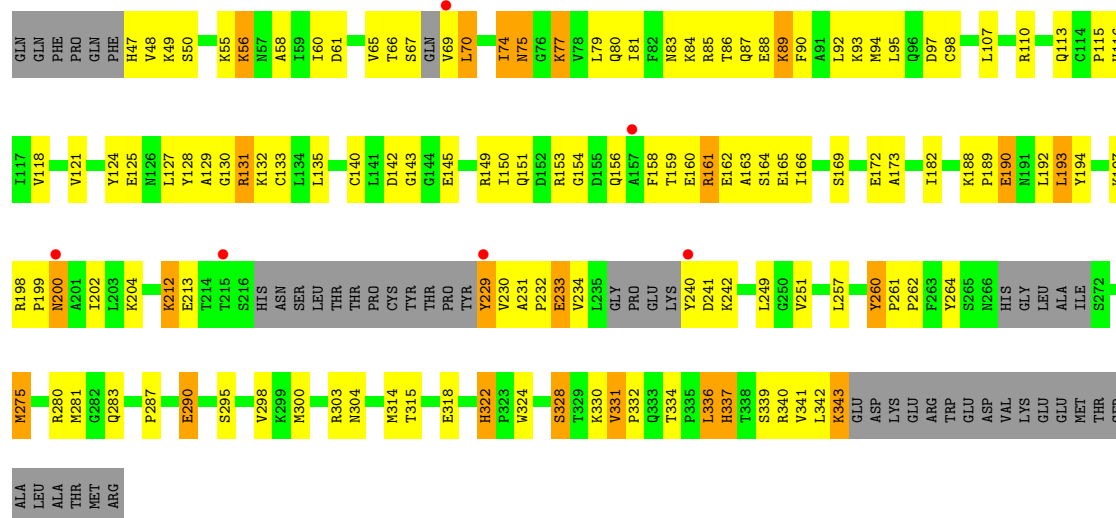
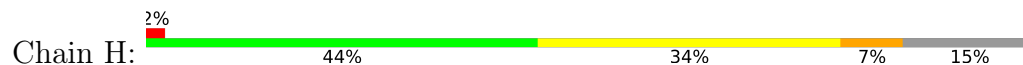


- Molecule 1: MAP kinase-activated protein kinase 2

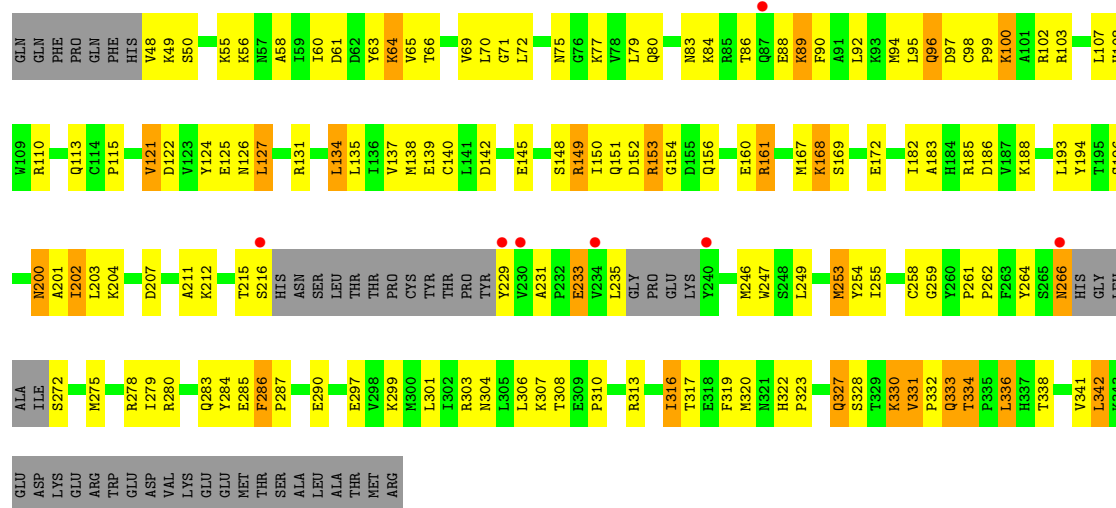


ALA
LEU
ALA
THR
MET
ARG

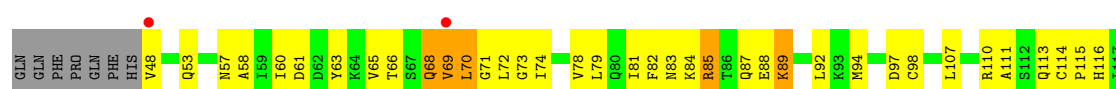
• Molecule 1: MAP kinase-activated protein kinase 2

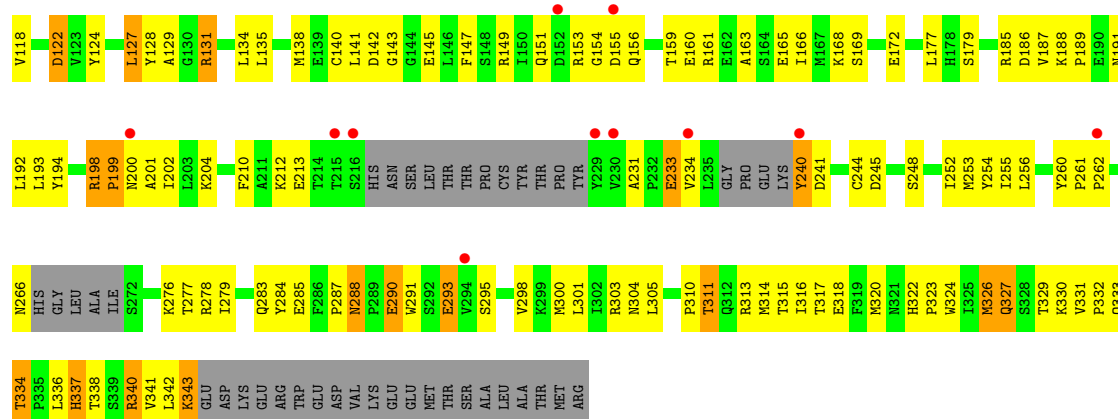


• Molecule 1: MAP kinase-activated protein kinase 2

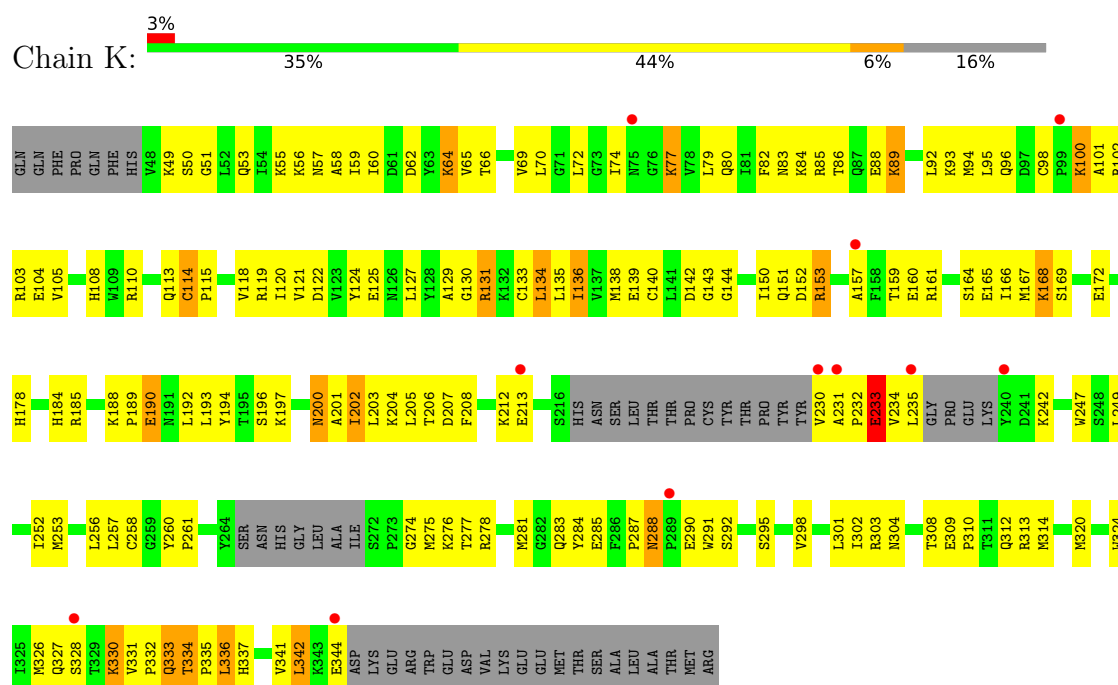


• Molecule 1: MAP kinase-activated protein kinase 2

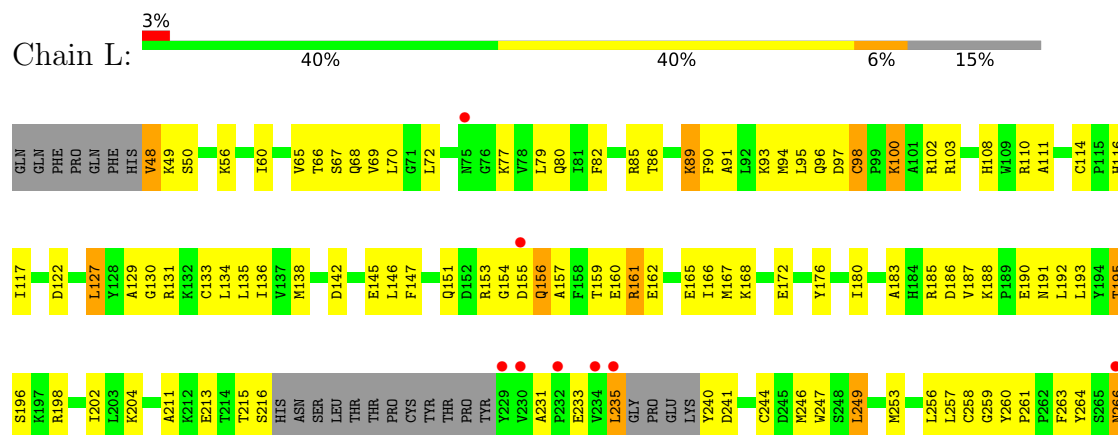


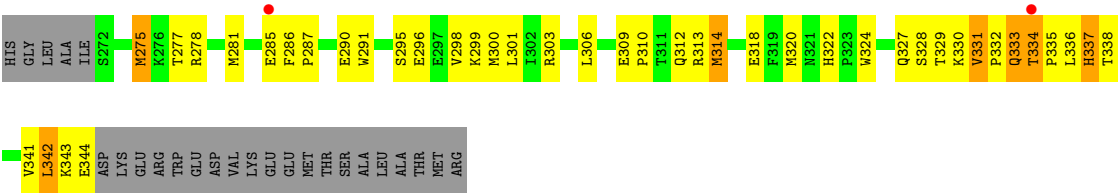


• Molecule 1: MAP kinase-activated protein kinase 2



• Molecule 1: MAP kinase-activated protein kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.16Å 180.96Å 216.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.90) 99.4 (19.99-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.91Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.288 , 0.335 0.213 , 0.267	Depositor DCC
R_{free} test set	6091 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27440	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PDY, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/2262	0.87	3/3048 (0.1%)
1	B	0.50	0/2284	0.85	2/3078 (0.1%)
1	C	0.46	0/2250	0.82	3/3032 (0.1%)
1	D	0.50	0/2288	0.82	2/3081 (0.1%)
1	E	0.52	0/2278	0.89	8/3070 (0.3%)
1	F	0.54	0/2365	0.88	6/3191 (0.2%)
1	G	0.47	0/2254	0.81	2/3038 (0.1%)
1	H	0.47	0/2270	0.86	7/3058 (0.2%)
1	I	0.51	0/2269	0.80	2/3058 (0.1%)
1	J	0.39	0/2269	0.75	0/3058
1	K	0.42	0/2251	0.80	3/3033 (0.1%)
1	L	0.41	0/2278	0.82	2/3070 (0.1%)
All	All	0.48	0/27318	0.83	40/36815 (0.1%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	TYR	CA-C-N	8.05	125.45	119.66
1	C	260	TYR	C-N-CA	8.05	125.45	119.66
1	F	240	TYR	N-CA-C	7.11	119.21	109.11
1	C	296	GLU	N-CA-C	-6.72	105.23	113.50
1	B	331	VAL	CA-C-N	6.52	126.50	119.78
1	B	331	VAL	C-N-CA	6.52	126.50	119.78
1	H	260	TYR	CA-C-N	6.20	124.19	119.66
1	H	260	TYR	C-N-CA	6.20	124.19	119.66
1	K	114	CYS	CA-C-N	6.02	125.57	119.19
1	K	114	CYS	C-N-CA	6.02	125.57	119.19
1	I	286	PHE	CA-C-N	5.98	125.92	119.76
1	I	286	PHE	C-N-CA	5.98	125.92	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	331	VAL	CA-C-N	5.67	125.63	119.78
1	H	331	VAL	C-N-CA	5.67	125.63	119.78
1	A	290	GLU	N-CA-C	5.58	118.30	111.82
1	D	334	THR	CA-C-N	5.55	125.56	119.90
1	D	334	THR	C-N-CA	5.55	125.56	119.90
1	F	261	PRO	CA-C-N	5.53	125.06	119.19
1	F	261	PRO	C-N-CA	5.53	125.06	119.19
1	E	264	TYR	N-CA-C	5.50	115.64	107.88
1	H	322	HIS	CA-C-N	5.45	125.54	119.32
1	H	322	HIS	C-N-CA	5.45	125.54	119.32
1	E	290	GLU	N-CA-C	5.43	118.70	111.75
1	E	272	SER	CA-C-N	-5.40	113.34	119.28
1	E	272	SER	C-N-CA	-5.40	113.34	119.28
1	G	331	VAL	CA-C-N	5.38	125.28	119.85
1	G	331	VAL	C-N-CA	5.38	125.28	119.85
1	E	260	TYR	CA-C-N	5.37	125.91	120.38
1	E	260	TYR	C-N-CA	5.37	125.91	120.38
1	F	236	GLY	CA-C-N	5.36	125.26	119.85
1	F	236	GLY	C-N-CA	5.36	125.26	119.85
1	A	272	SER	CA-C-N	5.35	124.69	118.85
1	A	272	SER	C-N-CA	5.35	124.69	118.85
1	E	90	PHE	N-CA-C	5.29	116.32	108.86
1	K	136	ILE	N-CA-C	5.26	114.88	106.88
1	L	331	VAL	CA-C-N	5.19	125.47	119.92
1	L	331	VAL	C-N-CA	5.19	125.47	119.92
1	H	241	ASP	N-CA-C	5.16	116.90	111.28
1	F	133	CYS	N-CA-C	5.09	116.99	108.99
1	E	338	THR	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2218	0	2255	143	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2240	0	2270	159	0
1	C	2207	0	2240	165	0
1	D	2244	0	2281	122	0
1	E	2234	0	2268	138	0
1	F	2316	0	2347	132	0
1	G	2210	0	2245	132	0
1	H	2226	0	2260	165	0
1	I	2225	0	2262	155	0
1	J	2225	0	2262	180	0
1	K	2208	0	2248	169	0
1	L	2234	0	2268	163	0
2	A	54	0	52	8	0
2	B	54	0	52	15	0
2	C	54	0	52	17	0
2	D	54	0	52	13	0
2	E	54	0	52	23	0
2	F	54	0	52	15	0
2	G	54	0	52	20	0
2	H	54	0	51	40	0
2	I	54	0	52	37	0
2	J	54	0	52	16	0
2	K	54	0	52	25	0
2	L	54	0	52	22	0
3	F	5	0	0	1	0
All	All	27440	0	27829	1879	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1879) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:PDY:H18	2:L:2:PDY:C14	1.53	1.38
1:H:264:TYR:CZ	2:H:2:PDY:H20	1.61	1.32
1:I:264:TYR:CG	2:I:2:PDY:H17	1.65	1.32
2:D:2:PDY:H18	2:D:2:PDY:C14	1.60	1.29
2:J:1:PDY:C14	2:J:1:PDY:H18	1.60	1.29
2:D:2:PDY:H18	2:D:2:PDY:H14A	1.22	1.18
2:I:2:PDY:C18	2:I:2:PDY:H14	1.74	1.17
1:H:264:TYR:CE2	2:H:2:PDY:H20	1.79	1.16
1:D:66:THR:HG22	1:D:68:GLN:H	1.06	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2:PDY:H14A	2:J:2:PDY:H18	1.25	1.15
1:C:202:ILE:HD11	1:C:204:LYS:HE2	1.26	1.14
1:I:264:TYR:CB	2:I:2:PDY:H17	1.77	1.13
2:J:1:PDY:H18	2:J:1:PDY:H14A	1.14	1.12
2:H:1:PDY:C14	2:H:1:PDY:H18	1.80	1.10
1:E:70:LEU:HA	1:E:94:MET:HE1	1.32	1.10
2:I:1:PDY:H18	2:I:1:PDY:H14A	1.29	1.10
2:H:1:PDY:H18	2:H:1:PDY:H14A	1.26	1.10
2:L:1:PDY:H27A	2:L:1:PDY:H19	1.13	1.08
1:L:66:THR:HG23	1:L:69:VAL:H	1.10	1.07
2:K:1:PDY:H18	2:K:1:PDY:C14	1.83	1.07
2:K:1:PDY:H18	2:K:1:PDY:H14A	1.35	1.06
1:I:264:TYR:CG	2:I:2:PDY:C17	2.38	1.06
1:F:73:GLY:HA3	1:F:94:MET:HE3	1.37	1.05
1:G:100:LYS:HA	1:G:100:LYS:HE3	1.36	1.05
1:H:264:TYR:CE1	2:H:2:PDY:H20	1.90	1.05
1:G:185:ARG:HH21	1:G:212:LYS:HG3	0.95	1.04
2:L:2:PDY:H18	2:L:2:PDY:H14	1.05	1.04
2:I:1:PDY:H18	2:I:1:PDY:C14	1.88	1.04
2:L:2:PDY:C14	2:L:2:PDY:C18	2.35	1.03
2:J:2:PDY:H18	2:J:2:PDY:C14	1.88	1.03
2:H:2:PDY:H18	2:H:2:PDY:H14	1.35	1.03
2:J:1:PDY:C14	2:J:1:PDY:C18	2.36	1.03
1:H:264:TYR:CG	2:H:2:PDY:C17	2.42	1.02
2:K:1:PDY:C14	2:K:1:PDY:C18	2.37	1.02
2:I:2:PDY:C18	2:I:2:PDY:C14	2.37	1.02
2:I:2:PDY:H14	2:I:2:PDY:H18	1.05	1.01
2:K:2:PDY:C14	2:K:2:PDY:C18	2.39	1.01
2:K:2:PDY:C18	2:K:2:PDY:H14A	1.90	1.00
2:E:2:PDY:C18	2:E:2:PDY:H14A	1.91	1.00
1:H:264:TYR:CD2	2:H:2:PDY:H17	1.95	1.00
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.43	1.00
2:H:1:PDY:H14A	2:H:1:PDY:C18	1.92	1.00
2:H:1:PDY:C14	2:H:1:PDY:C18	2.39	1.00
1:I:264:TYR:CD2	2:I:2:PDY:H17	1.97	1.00
1:L:69:VAL:HG13	1:L:79:LEU:HD13	1.44	1.00
1:H:264:TYR:CG	2:H:2:PDY:H17	1.97	0.99
2:K:1:PDY:H14A	2:K:1:PDY:C18	1.91	0.99
2:F:2:PDY:H18	2:F:2:PDY:H14A	1.44	0.98
1:K:230:VAL:HG22	1:K:231:ALA:H	1.27	0.98
1:L:111:ALA:HB1	1:L:117:ILE:HD13	1.42	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:264:TYR:HB2	2:I:2:PDY:H17	1.45	0.98
2:E:2:PDY:C18	2:E:2:PDY:C14	2.41	0.98
2:F:2:PDY:H14A	2:F:2:PDY:C18	1.95	0.97
2:I:1:PDY:C14	2:I:1:PDY:C18	2.42	0.97
1:B:202:ILE:HD11	1:B:204:LYS:HE2	1.43	0.97
2:G:1:PDY:C18	2:G:1:PDY:C14	2.41	0.97
2:D:1:PDY:H18	2:D:1:PDY:H14A	1.46	0.97
1:C:69:VAL:HB	1:C:79:LEU:HD13	1.47	0.97
2:E:1:PDY:C14	2:E:1:PDY:C18	2.43	0.96
1:G:328:SER:O	1:G:331:VAL:HG12	1.65	0.96
1:D:49:LYS:HD2	1:D:113:GLN:HG2	1.45	0.96
1:G:185:ARG:NH2	1:G:212:LYS:HG3	1.81	0.96
2:I:2:PDY:C14	2:I:2:PDY:H18	1.94	0.95
2:G:1:PDY:H14A	2:G:1:PDY:H18	1.48	0.95
1:K:80:GLN:NE2	2:K:1:PDY:H24A	1.82	0.94
2:F:2:PDY:H18	2:F:2:PDY:C14	1.97	0.94
2:F:2:PDY:C18	2:F:2:PDY:C14	2.46	0.94
1:I:70:LEU:HA	1:I:94:MET:HE1	1.50	0.94
1:K:70:LEU:HD23	1:K:94:MET:HE1	1.48	0.94
2:L:1:PDY:H27A	2:L:1:PDY:C19	1.98	0.94
2:E:1:PDY:C18	2:E:1:PDY:H14A	1.97	0.94
2:E:1:PDY:H14A	2:E:1:PDY:H18	1.46	0.94
2:H:2:PDY:H18	2:H:2:PDY:C14	1.97	0.94
1:H:264:TYR:CE1	2:H:2:PDY:C20	2.51	0.93
2:G:1:PDY:C18	2:G:1:PDY:H14A	1.97	0.93
1:B:161:ARG:HH21	1:B:333:GLN:HE21	0.93	0.93
1:J:313:ARG:HH22	1:K:233:GLU:HG2	1.32	0.93
2:L:2:PDY:H18	2:L:2:PDY:H14A	1.51	0.93
1:K:49:LYS:HD3	1:K:50:SER:H	1.31	0.93
2:B:2:PDY:C18	2:B:2:PDY:H14A	2.00	0.92
2:F:1:PDY:C14	2:F:1:PDY:C18	2.47	0.92
2:E:1:PDY:C14	2:E:1:PDY:H18	1.99	0.92
2:D:2:PDY:H18	2:D:2:PDY:H14	1.50	0.92
2:G:2:PDY:C18	2:G:2:PDY:H14A	2.00	0.92
1:D:266:ASN:HD22	1:D:266:ASN:H	1.10	0.91
2:J:2:PDY:H14A	2:J:2:PDY:C18	2.01	0.91
2:L:1:PDY:H19	2:L:1:PDY:C27	2.00	0.91
2:G:2:PDY:C18	2:G:2:PDY:C14	2.49	0.91
2:D:1:PDY:H18	2:D:1:PDY:C14	2.01	0.91
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.51	0.91
1:H:69:VAL:HG23	1:H:79:LEU:HD13	1.52	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:GLN:NE2	1:E:156:GLN:H	1.69	0.90
1:E:73:GLY:HA3	1:E:94:MET:HE3	1.53	0.90
1:I:49:LYS:HG3	1:I:50:SER:H	1.37	0.90
1:J:156:GLN:HE21	1:J:340:ARG:HD2	1.37	0.89
1:H:264:TYR:CD1	2:H:2:PDY:C20	2.56	0.89
2:D:1:PDY:C14	2:D:1:PDY:C18	2.51	0.89
2:F:1:PDY:C18	2:F:1:PDY:H14A	2.03	0.88
2:G:1:PDY:C14	2:G:1:PDY:H18	2.02	0.88
1:H:129:ALA:HB3	1:H:131:ARG:HD3	1.52	0.88
1:D:66:THR:HG22	1:D:68:GLN:N	1.87	0.88
2:L:2:PDY:H14	2:L:2:PDY:C18	1.99	0.88
2:J:1:PDY:H14A	2:J:1:PDY:C18	1.99	0.88
1:F:70:LEU:HA	1:F:94:MET:HE1	1.54	0.88
2:I:1:PDY:H14A	2:I:1:PDY:C18	2.03	0.88
1:L:264:TYR:HB2	2:L:2:PDY:H17	1.56	0.88
2:B:2:PDY:C18	2:B:2:PDY:C14	2.52	0.87
1:H:264:TYR:CZ	2:H:2:PDY:C20	2.55	0.87
2:D:1:PDY:H14A	2:D:1:PDY:C18	2.04	0.87
1:H:188:LYS:HG3	1:H:190:GLU:HG2	1.56	0.87
2:F:1:PDY:H14A	2:F:1:PDY:H18	1.56	0.87
1:C:295:SER:HB2	1:C:298:VAL:HG23	1.54	0.86
1:B:85:ARG:HD2	1:B:86:THR:HG23	1.56	0.86
2:C:1:PDY:H18	2:C:1:PDY:H14A	1.54	0.86
2:F:1:PDY:C14	2:F:1:PDY:H18	2.04	0.86
1:J:69:VAL:HG23	1:J:79:LEU:HD12	1.57	0.86
1:E:80:GLN:NE2	1:E:89:LYS:HD3	1.88	0.86
1:L:151:GLN:HB3	1:L:342:LEU:HD23	1.56	0.86
1:D:266:ASN:HD22	1:D:266:ASN:N	1.73	0.86
1:G:69:VAL:HB	1:G:79:LEU:HD13	1.58	0.86
1:B:161:ARG:NH2	1:B:333:GLN:HE21	1.73	0.86
1:H:264:TYR:CD2	2:H:2:PDY:C17	2.59	0.86
1:H:332:PRO:HB2	1:H:334:THR:HG23	1.56	0.86
2:J:2:PDY:C14	2:J:2:PDY:C18	2.53	0.86
1:F:74:ILE:HD13	1:F:74:ILE:H	1.39	0.85
1:B:94:MET:HG2	1:B:135:LEU:HD23	1.58	0.85
1:B:77:LYS:HZ2	1:B:77:LYS:HB3	1.41	0.85
1:C:100:LYS:HE3	1:C:103:ARG:HH22	1.39	0.85
1:F:100:LYS:HG3	1:F:103:ARG:NH2	1.91	0.85
1:G:231:ALA:HB3	1:G:234:VAL:HG23	1.57	0.85
1:B:184:HIS:HD2	1:B:186:ASP:H	1.22	0.85
1:D:266:ASN:H	1:D:266:ASN:ND2	1.70	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:TYR:OH	1:H:242:LYS:HD2	1.77	0.84
2:H:1:PDY:H18	2:H:1:PDY:C3	2.05	0.84
1:E:49:LYS:HD2	1:E:50:SER:H	1.42	0.84
2:F:2:PDY:H18	2:F:2:PDY:C3	2.05	0.84
1:G:67:SER:HA	1:G:70:LEU:HD23	1.57	0.84
2:K:1:PDY:H18	2:K:1:PDY:C3	1.99	0.84
1:C:153:ARG:O	1:C:155:ASP:HA	1.77	0.84
2:D:2:PDY:C14	2:D:2:PDY:C18	2.52	0.84
1:I:266:ASN:ND2	1:I:266:ASN:H	1.72	0.84
1:H:80:GLN:HE21	1:H:89:LYS:HG3	1.43	0.84
1:F:65:VAL:HG11	1:F:70:LEU:HD13	1.59	0.84
1:E:327:GLN:HB2	1:E:330:LYS:HZ2	1.42	0.84
1:I:125:GLU:C	1:I:126:ASN:HD22	1.86	0.83
1:J:159:THR:HG22	1:J:161:ARG:H	1.42	0.83
2:F:1:PDY:H18	2:F:1:PDY:C3	2.09	0.83
1:A:49:LYS:HG3	1:A:113:GLN:OE1	1.79	0.83
1:G:301:LEU:HD13	1:G:322:HIS:CD2	2.13	0.83
2:J:1:PDY:H18	2:J:1:PDY:C3	2.09	0.83
1:A:185:ARG:NH2	1:A:212:LYS:HE2	1.92	0.82
1:I:264:TYR:CD2	2:I:2:PDY:C17	2.62	0.82
1:L:159:THR:HG22	1:L:161:ARG:H	1.44	0.82
1:I:115:PRO:O	1:I:204:LYS:HE2	1.79	0.82
1:I:264:TYR:CE1	2:I:2:PDY:H20	2.14	0.82
2:C:1:PDY:C14	2:C:1:PDY:C18	2.58	0.82
1:I:264:TYR:CZ	2:I:2:PDY:H20	2.15	0.81
1:I:278:ARG:HG2	1:I:283:GLN:HB2	1.59	0.81
2:C:1:PDY:H18	2:C:1:PDY:C14	2.09	0.81
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.61	0.81
1:L:66:THR:HG23	1:L:69:VAL:N	1.94	0.81
2:L:2:PDY:C18	2:L:2:PDY:H14A	2.06	0.81
1:E:156:GLN:H	1:E:156:GLN:HE21	1.27	0.81
1:K:62:ASP:HA	1:K:85:ARG:HH21	1.46	0.81
1:F:95:LEU:O	1:F:133:CYS:HB2	1.80	0.81
1:E:188:LYS:HZ2	1:E:190:GLU:HG2	1.43	0.81
1:K:80:GLN:NE2	2:K:1:PDY:C24	2.43	0.81
1:K:96:GLN:HE22	1:K:131:ARG:HE	1.28	0.80
2:B:2:PDY:C3	2:B:2:PDY:H18	2.10	0.80
1:B:161:ARG:HH21	1:B:333:GLN:NE2	1.78	0.80
2:B:2:PDY:H14A	2:B:2:PDY:H18	1.62	0.80
2:K:2:PDY:C3	2:K:2:PDY:H18	2.10	0.80
1:L:155:ASP:HA	1:L:156:GLN:C	2.07	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:HIS:HE1	1:I:138:MET:HE3	1.47	0.80
1:K:83:ASN:HB3	1:K:86:THR:HB	1.64	0.80
1:L:337:HIS:O	1:L:341:VAL:HG23	1.80	0.80
1:C:83:ASN:HD21	1:C:85:ARG:HD2	1.47	0.79
1:I:69:VAL:HA	1:I:79:LEU:HD22	1.63	0.79
1:K:49:LYS:HD3	1:K:50:SER:N	1.95	0.79
1:J:276:LYS:HG3	1:K:235:LEU:HD12	1.64	0.79
1:K:115:PRO:O	1:K:204:LYS:HE2	1.82	0.79
2:K:2:PDY:H14A	2:K:2:PDY:H18	1.64	0.79
1:H:80:GLN:NE2	1:H:89:LYS:HG3	1.97	0.79
1:A:156:GLN:NE2	1:A:156:GLN:H	1.80	0.78
2:C:2:PDY:H14A	2:C:2:PDY:C18	2.13	0.78
1:F:86:THR:HG22	1:F:88:GLU:H	1.46	0.78
1:G:80:GLN:HB2	2:G:1:PDY:H24A	1.65	0.78
2:C:2:PDY:C18	2:C:2:PDY:C14	2.62	0.78
1:D:185:ARG:HH21	1:D:212:LYS:HG3	1.48	0.78
1:H:322:HIS:HD2	1:H:324:TRP:H	1.32	0.78
1:K:70:LEU:HA	1:K:94:MET:HE1	1.66	0.78
2:K:2:PDY:C14	2:K:2:PDY:H18	2.12	0.78
1:H:264:TYR:CD2	2:H:2:PDY:H20	2.19	0.78
1:F:100:LYS:HG3	1:F:103:ARG:HH21	1.48	0.78
1:L:69:VAL:HG13	1:L:79:LEU:CD1	2.13	0.78
2:B:2:PDY:C14	2:B:2:PDY:H18	2.13	0.78
1:K:94:MET:HG2	1:K:135:LEU:HD23	1.67	0.77
1:F:73:GLY:HA3	1:F:94:MET:CE	2.15	0.77
2:H:2:PDY:C14	2:H:2:PDY:C18	2.62	0.77
1:E:69:VAL:HB	1:E:79:LEU:HD13	1.65	0.77
1:J:156:GLN:NE2	1:J:340:ARG:HD2	1.99	0.77
1:J:115:PRO:O	1:J:204:LYS:HE2	1.85	0.77
1:H:264:TYR:CG	2:H:2:PDY:C20	2.67	0.77
1:I:264:TYR:CB	2:I:2:PDY:C17	2.61	0.76
1:K:95:LEU:O	1:K:133:CYS:HB2	1.85	0.76
1:J:72:LEU:HB2	1:J:79:LEU:HD11	1.66	0.76
1:A:327:GLN:NE2	1:A:330:LYS:HD3	2.01	0.76
2:E:1:PDY:H18	2:E:1:PDY:C3	2.15	0.76
2:B:1:PDY:C18	2:B:1:PDY:C14	2.64	0.76
1:E:202:ILE:HD11	1:E:204:LYS:HE2	1.68	0.76
1:D:167:MET:HE2	1:D:253:MET:HE3	1.67	0.76
1:H:49:LYS:HG3	1:H:113:GLN:NE2	2.01	0.76
1:B:73:GLY:HA3	1:B:94:MET:SD	2.26	0.75
1:C:66:THR:OG1	1:C:69:VAL:HG13	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:TYR:O	1:H:131:ARG:HG2	1.85	0.75
1:B:266:ASN:CG	1:B:278:ARG:HH22	1.94	0.75
1:K:98:CYS:HB2	1:K:101:ALA:H	1.52	0.75
1:G:185:ARG:HH21	1:G:212:LYS:CG	1.89	0.75
1:K:70:LEU:HD23	1:K:94:MET:CE	2.17	0.75
1:L:66:THR:HG22	1:L:69:VAL:HG23	1.69	0.75
1:B:48:VAL:HB	1:L:70:LEU:HD21	1.69	0.74
1:E:80:GLN:HE21	1:E:89:LYS:HD3	1.47	0.74
2:G:2:PDY:C3	2:G:2:PDY:H18	2.16	0.74
1:J:198:ARG:NH1	1:J:200:ASN:H	1.85	0.74
1:A:156:GLN:H	1:A:156:GLN:HE21	1.33	0.74
1:J:161:ARG:HD2	1:J:329:THR:HA	1.69	0.74
1:D:66:THR:CG2	1:D:68:GLN:H	1.95	0.74
1:G:304:ASN:O	1:G:307:LYS:HG2	1.88	0.74
1:G:80:GLN:OE1	1:G:89:LYS:HD2	1.87	0.74
1:I:49:LYS:HG3	1:I:50:SER:N	2.01	0.74
1:H:188:LYS:HE2	1:H:190:GLU:HG3	1.70	0.74
1:K:185:ARG:HH21	1:K:212:LYS:HG3	1.50	0.74
1:C:100:LYS:HE3	1:C:103:ARG:NH2	2.03	0.73
2:C:1:PDY:H14A	2:C:1:PDY:C18	2.17	0.73
1:L:49:LYS:HD2	1:L:50:SER:H	1.53	0.73
1:D:337:HIS:HA	1:D:340:ARG:NH1	2.02	0.73
1:A:49:LYS:HE2	1:A:113:GLN:HG2	1.71	0.73
1:G:100:LYS:HE2	1:G:103:ARG:CZ	2.18	0.73
1:L:95:LEU:O	1:L:133:CYS:HB2	1.88	0.73
1:I:98:CYS:HB2	1:I:99:PRO:HD2	1.70	0.73
1:K:167:MET:HE2	1:K:253:MET:HE3	1.68	0.73
1:F:81:ILE:HD13	1:F:92:LEU:HB2	1.69	0.73
1:I:100:LYS:HD2	1:I:103:ARG:HH21	1.53	0.73
1:K:167:MET:HG3	1:K:253:MET:HE2	1.69	0.73
1:G:161:ARG:O	1:G:165:GLU:HG3	1.88	0.73
1:F:47:HIS:CD2	1:G:67:SER:HB3	2.24	0.72
1:H:264:TYR:CE2	2:H:2:PDY:C20	2.67	0.72
1:B:285:GLU:HG3	1:B:287:PRO:HD3	1.70	0.72
1:D:49:LYS:CD	1:D:113:GLN:HG2	2.19	0.72
1:B:72:LEU:HB3	1:B:77:LYS:HG3	1.71	0.72
1:G:66:THR:O	1:G:69:VAL:HG22	1.90	0.72
1:I:264:TYR:CG	2:I:2:PDY:C20	2.72	0.72
1:D:190:GLU:CD	1:D:190:GLU:H	1.97	0.72
1:F:278:ARG:HG2	1:F:283:GLN:HB2	1.68	0.72
2:J:1:PDY:C18	2:J:1:PDY:H14	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:GLU:OE1	1:G:190:GLU:N	2.22	0.72
1:J:118:VAL:HG21	1:J:138:MET:HE2	1.71	0.72
1:G:260:TYR:HB2	2:G:2:PDY:H19	1.72	0.72
1:K:328:SER:O	1:K:331:VAL:HG22	1.89	0.72
2:I:1:PDY:C18	2:I:1:PDY:H14	2.19	0.72
1:J:159:THR:CG2	1:J:333:GLN:HA	2.20	0.72
1:J:327:GLN:HG2	1:J:330:LYS:HD3	1.70	0.72
1:H:61:ASP:O	1:H:84:LYS:HD2	1.90	0.72
1:H:261:PRO:HD3	2:H:2:PDY:H25	1.71	0.71
1:H:264:TYR:CD2	2:H:2:PDY:C20	2.72	0.71
1:F:71:GLY:HA2	1:F:74:ILE:HD11	1.72	0.71
1:F:185:ARG:HD3	1:F:241:ASP:HB3	1.71	0.71
1:B:185:ARG:HD3	1:B:241:ASP:HB3	1.72	0.71
1:J:231:ALA:O	1:J:234:VAL:HG12	1.90	0.71
2:D:1:PDY:H18	2:D:1:PDY:C3	2.19	0.71
1:A:264:TYR:O	1:A:275:MET:HG3	1.91	0.71
1:A:49:LYS:HE2	1:A:113:GLN:CD	2.16	0.70
1:D:66:THR:HB	1:D:69:VAL:HG23	1.71	0.70
1:I:97:ASP:OD2	1:I:102:ARG:NH2	2.22	0.70
1:I:264:TYR:CD1	2:I:2:PDY:H20	2.25	0.70
1:D:69:VAL:HG13	1:D:79:LEU:HD13	1.72	0.70
1:F:196:SER:OG	1:F:198:ARG:HB2	1.92	0.70
1:I:140:CYS:SG	2:I:1:PDY:H17	2.32	0.70
1:L:159:THR:HG21	1:L:161:ARG:HB3	1.73	0.70
1:K:288:ASN:OD1	1:K:292:SER:HB3	1.91	0.70
1:A:71:GLY:O	1:A:74:ILE:HG22	1.91	0.70
1:A:70:LEU:HD13	1:G:48:VAL:HG23	1.73	0.70
2:B:1:PDY:C18	2:B:1:PDY:H14A	2.22	0.70
1:F:327:GLN:HE21	1:F:330:LYS:HD2	1.57	0.70
1:K:96:GLN:HE22	1:K:131:ARG:NE	1.90	0.70
1:B:97:ASP:H	1:B:133:CYS:HA	1.56	0.69
1:E:86:THR:HG21	1:E:88:GLU:CD	2.17	0.69
1:E:185:ARG:HE	1:E:212:LYS:HG3	1.55	0.69
1:E:327:GLN:HB2	1:E:330:LYS:NZ	2.06	0.69
1:I:264:TYR:CE2	2:I:2:PDY:H20	2.28	0.69
1:A:66:THR:H	1:A:69:VAL:CG2	2.06	0.69
1:F:150:ILE:O	1:F:153:ARG:HG2	1.92	0.69
1:C:185:ARG:CZ	1:C:212:LYS:HD2	2.21	0.69
1:F:97:ASP:H	1:F:133:CYS:HA	1.58	0.69
1:G:49:LYS:HD2	1:G:113:GLN:OE1	1.92	0.69
1:K:89:LYS:HD2	1:K:89:LYS:H	1.55	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:LEU:HA	1:L:94:MET:CE	2.23	0.69
1:L:246:MET:HA	1:L:246:MET:HE3	1.74	0.69
1:A:66:THR:H	1:A:69:VAL:HG22	1.57	0.69
1:A:304:ASN:O	1:A:307:LYS:HG2	1.93	0.69
1:B:68:GLN:NE2	1:F:267:HIS:HB3	2.08	0.69
1:C:327:GLN:NE2	1:C:330:LYS:HZ2	1.91	0.69
1:L:70:LEU:HA	1:L:94:MET:HE1	1.74	0.69
1:A:309:GLU:CD	1:C:311:THR:HG22	2.17	0.68
1:L:257:LEU:HD11	1:L:298:VAL:HG11	1.74	0.68
1:B:141:LEU:HD13	1:B:193:LEU:HB2	1.74	0.68
1:E:145:GLU:HG2	1:E:193:LEU:CD2	2.23	0.68
1:A:145:GLU:HG3	1:A:193:LEU:CD2	2.24	0.68
1:C:88:GLU:HG2	1:C:89:LYS:N	2.07	0.68
1:I:328:SER:O	1:I:331:VAL:HG13	1.94	0.68
1:E:333:GLN:HE21	1:E:333:GLN:HA	1.58	0.68
1:H:322:HIS:CD2	1:H:324:TRP:H	2.12	0.68
1:C:161:ARG:NH1	1:C:331:VAL:O	2.27	0.68
1:J:145:GLU:HG2	1:J:193:LEU:CD2	2.24	0.67
1:J:332:PRO:HB2	1:J:334:THR:HG22	1.75	0.67
1:K:80:GLN:HE21	2:K:1:PDY:C24	2.05	0.67
1:H:231:ALA:HB3	1:H:234:VAL:HG23	1.75	0.67
1:I:327:GLN:HE21	1:I:330:LYS:NZ	1.92	0.67
1:L:66:THR:CG2	1:L:69:VAL:H	1.99	0.67
2:G:1:PDY:H18	2:G:1:PDY:C3	2.22	0.67
2:G:2:PDY:H14A	2:G:2:PDY:H18	1.74	0.67
1:F:272:SER:HB3	1:F:275:MET:HB2	1.77	0.67
1:H:65:VAL:HG11	1:H:70:LEU:HD13	1.75	0.67
1:E:60:ILE:HD12	1:E:61:ASP:N	2.10	0.67
1:E:188:LYS:NZ	1:E:190:GLU:HG2	2.09	0.67
1:K:166:ILE:O	1:K:169:SER:HB3	1.94	0.67
1:L:129:ALA:O	1:L:131:ARG:HG3	1.94	0.67
1:B:231:ALA:HB1	1:B:233:GLU:HG3	1.77	0.67
1:I:284:TYR:OH	1:I:303:ARG:HG2	1.94	0.67
1:G:69:VAL:HB	1:G:79:LEU:CD1	2.24	0.67
1:G:80:GLN:CB	2:G:1:PDY:H24A	2.24	0.67
1:G:260:TYR:CB	2:G:2:PDY:H19	2.25	0.67
1:J:145:GLU:HG2	1:J:193:LEU:HD21	1.77	0.67
1:J:329:THR:C	1:J:331:VAL:H	2.00	0.67
1:L:153:ARG:HB2	1:L:156:GLN:HG2	1.76	0.67
1:L:202:ILE:HD11	1:L:204:LYS:HE2	1.76	0.67
1:A:49:LYS:HE2	1:A:113:GLN:CG	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ILE:HD11	1:F:204:LYS:HE2	1.76	0.67
1:L:70:LEU:HG	1:L:94:MET:HE1	1.77	0.67
1:G:66:THR:HG23	1:G:69:VAL:HG13	1.76	0.67
1:C:188:LYS:HG3	1:C:190:GLU:HG2	1.76	0.66
1:K:89:LYS:H	1:K:89:LYS:CD	2.08	0.66
1:A:328:SER:O	1:A:331:VAL:HG13	1.95	0.66
1:I:186:ASP:OD1	1:I:188:LYS:HE3	1.95	0.66
2:J:2:PDY:H18	2:J:2:PDY:C3	2.23	0.66
1:J:198:ARG:HH11	1:J:198:ARG:HG3	1.60	0.66
1:L:167:MET:HG3	1:L:253:MET:HG3	1.77	0.66
1:G:71:GLY:O	1:G:74:ILE:HG22	1.95	0.66
1:C:55:LYS:HD3	1:C:124:TYR:CE2	2.30	0.66
1:C:287:PRO:O	1:C:291:TRP:HB2	1.95	0.66
2:E:2:PDY:C3	2:E:2:PDY:H18	2.25	0.66
1:I:148:SER:HA	1:I:151:GLN:HG2	1.76	0.66
1:G:161:ARG:HD3	1:G:331:VAL:O	1.95	0.66
1:J:72:LEU:HB2	1:J:79:LEU:CD1	2.26	0.66
1:J:198:ARG:HH11	1:J:200:ASN:H	1.42	0.66
1:J:337:HIS:O	1:J:341:VAL:HG23	1.96	0.66
1:C:147:PHE:HE2	1:C:256:LEU:HD23	1.60	0.66
1:D:233:GLU:HG2	1:E:310:PRO:HG3	1.76	0.66
1:L:66:THR:CG2	1:L:69:VAL:HG23	2.24	0.66
1:B:81:ILE:HD13	1:B:92:LEU:HB2	1.77	0.66
1:E:118:VAL:HG11	1:E:138:MET:HE2	1.78	0.66
1:G:229:TYR:HD1	1:H:251:VAL:HG11	1.61	0.66
2:G:2:PDY:C14	2:G:2:PDY:H18	2.23	0.66
1:I:72:LEU:HB2	1:I:79:LEU:HD21	1.77	0.66
1:E:70:LEU:CA	1:E:94:MET:HE1	2.20	0.65
1:K:105:VAL:HG22	1:K:136:ILE:HD11	1.77	0.65
1:L:97:ASP:H	1:L:133:CYS:HA	1.60	0.65
1:L:161:ARG:HD3	1:L:331:VAL:O	1.95	0.65
1:F:230:VAL:HG21	1:F:235:LEU:HD21	1.78	0.65
2:G:2:PDY:C18	2:G:2:PDY:C3	2.73	0.65
1:H:56:LYS:HE2	1:H:125:GLU:HB3	1.77	0.65
2:H:2:PDY:H14	2:H:2:PDY:C18	2.20	0.65
1:K:121:VAL:HG12	1:K:122:ASP:OD1	1.96	0.65
1:E:110:ARG:O	1:E:113:GLN:HG3	1.97	0.65
1:J:185:ARG:NE	1:J:212:LYS:HG3	2.11	0.65
1:F:296:GLU:OE2	1:F:300:MET:HG2	1.96	0.65
1:A:102:ARG:NH2	1:A:125:GLU:OE1	2.29	0.65
1:B:107:LEU:HD21	1:B:213:GLU:HG3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ARG:HA	1:E:331:VAL:CG2	2.27	0.65
1:I:94:MET:O	1:I:95:LEU:HD23	1.97	0.65
1:K:83:ASN:CB	1:K:86:THR:HB	2.27	0.65
1:L:264:TYR:HB2	2:L:2:PDY:C17	2.26	0.65
1:L:314:MET:HG3	1:L:318:GLU:HB2	1.78	0.65
2:L:1:PDY:C18	2:L:1:PDY:C14	2.75	0.65
1:I:307:LYS:HB2	1:I:313:ARG:HG3	1.79	0.65
1:K:72:LEU:HD12	1:K:77:LYS:HD2	1.78	0.65
1:D:327:GLN:HB3	1:D:330:LYS:HD2	1.78	0.64
1:J:83:ASN:HD21	1:J:85:ARG:HH11	1.43	0.64
1:J:168:LYS:O	1:J:172:GLU:HG3	1.97	0.64
1:K:62:ASP:HA	1:K:85:ARG:NH2	2.10	0.64
1:K:114:CYS:SG	1:K:115:PRO:HD2	2.36	0.64
1:F:296:GLU:OE2	1:F:303:ARG:NH2	2.30	0.64
1:H:83:ASN:HB3	1:H:86:THR:HB	1.80	0.64
1:A:153:ARG:O	1:A:154:GLY:O	2.15	0.64
1:C:60:ILE:C	1:C:60:ILE:HD12	2.23	0.64
2:C:2:PDY:C3	2:C:2:PDY:H18	2.26	0.64
1:B:188:LYS:HD2	1:B:190:GLU:HB2	1.80	0.64
1:E:327:GLN:CB	1:E:330:LYS:HZ2	2.08	0.64
2:E:2:PDY:C14	2:E:2:PDY:H18	2.28	0.64
1:I:60:ILE:HG22	1:I:65:VAL:HB	1.79	0.64
1:I:150:ILE:O	1:I:153:ARG:HG3	1.98	0.64
1:B:69:VAL:O	1:B:73:GLY:N	2.28	0.64
1:A:310:PRO:HG3	1:C:233:GLU:HG2	1.80	0.64
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.78	0.64
1:F:49:LYS:HG3	1:G:127:LEU:HD23	1.79	0.64
1:H:161:ARG:HD3	1:H:331:VAL:O	1.98	0.64
1:I:264:TYR:CD2	2:I:2:PDY:C20	2.81	0.64
1:K:96:GLN:NE2	1:K:131:ARG:HE	1.94	0.64
1:J:83:ASN:ND2	1:J:85:ARG:HH11	1.96	0.64
1:L:155:ASP:CA	1:L:156:GLN:C	2.70	0.64
1:D:195:THR:HG23	1:D:202:ILE:O	1.98	0.64
1:H:188:LYS:HE2	1:H:190:GLU:CG	2.26	0.64
1:H:264:TYR:CB	2:H:2:PDY:H17	2.27	0.64
1:D:330:LYS:O	1:D:330:LYS:HG2	1.97	0.64
1:H:86:THR:HG22	1:H:88:GLU:HB2	1.80	0.64
1:H:315:THR:OG1	1:H:318:GLU:HG3	1.98	0.64
1:J:310:PRO:HB3	1:K:233:GLU:OE1	1.98	0.64
1:D:167:MET:HG3	1:D:253:MET:HE2	1.78	0.63
1:H:107:LEU:HD21	1:H:213:GLU:HG3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:LYS:HG3	1:I:235:LEU:HD22	1.80	0.63
1:H:74:ILE:O	1:H:74:ILE:HD13	1.97	0.63
1:I:280:ARG:NH2	1:J:131:ARG:HH12	1.95	0.63
1:D:230:VAL:HG11	1:D:235:LEU:HD21	1.80	0.63
1:F:100:LYS:HZ2	1:F:103:ARG:HH22	1.46	0.63
1:J:69:VAL:HG23	1:J:79:LEU:CD1	2.28	0.63
1:J:143:GLY:O	1:J:149:ARG:HD3	1.98	0.63
2:E:2:PDY:H14A	2:E:2:PDY:H18	1.76	0.63
2:E:2:PDY:C14	2:E:2:PDY:C13	2.76	0.63
1:B:188:LYS:HD2	1:B:190:GLU:OE1	1.98	0.63
1:C:315:THR:OG1	1:C:318:GLU:HG3	1.99	0.63
1:A:333:GLN:HA	1:A:333:GLN:HE21	1.63	0.63
1:J:149:ARG:HG3	1:J:194:TYR:CD2	2.34	0.63
1:B:69:VAL:HG23	1:B:70:LEU:N	2.12	0.63
1:C:185:ARG:NH2	1:C:212:LYS:HD2	2.14	0.63
1:D:64:LYS:HA	1:D:64:LYS:HE3	1.79	0.63
1:E:70:LEU:HA	1:E:94:MET:CE	2.20	0.63
1:F:65:VAL:CG1	1:F:70:LEU:HD13	2.28	0.63
1:G:337:HIS:O	1:G:341:VAL:HG23	1.99	0.63
1:H:159:THR:OG1	1:H:162:GLU:HG3	1.99	0.63
1:L:72:LEU:HD23	1:L:77:LYS:HD3	1.81	0.63
1:L:114:CYS:HB2	1:L:176:TYR:CD2	2.34	0.63
1:L:266:ASN:HB2	1:L:278:ARG:NH2	2.14	0.63
1:A:285:GLU:C	1:A:287:PRO:HD3	2.24	0.63
1:G:290:GLU:HA	1:G:337:HIS:CD2	2.34	0.63
1:J:304:ASN:OD1	1:J:314:MET:HB2	1.99	0.63
2:A:1:PDY:C18	2:A:1:PDY:C14	2.77	0.62
1:I:83:ASN:HB3	1:I:86:THR:O	1.99	0.62
1:J:288:ASN:HD22	1:J:288:ASN:N	1.96	0.62
1:A:151:GLN:O	1:A:343:LYS:HE2	2.00	0.62
1:E:88:GLU:HG3	1:E:90:PHE:HE1	1.63	0.62
1:K:190:GLU:H	1:K:190:GLU:CD	2.06	0.62
1:A:66:THR:HG23	1:A:68:GLN:H	1.64	0.62
1:F:156:GLN:HA	1:F:156:GLN:HE21	1.64	0.62
1:A:307:LYS:HB2	1:A:313:ARG:HG3	1.81	0.62
1:G:153:ARG:HG3	1:G:157:ALA:HB3	1.81	0.62
1:E:60:ILE:HD12	1:E:60:ILE:C	2.25	0.62
1:B:109:TRP:O	1:B:112:SER:HB2	1.99	0.62
1:I:264:TYR:CD1	2:I:2:PDY:C20	2.83	0.62
1:G:97:ASP:HB2	1:G:133:CYS:HA	1.81	0.62
1:J:198:ARG:NH1	1:J:198:ARG:HG3	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ARG:HD3	1:D:331:VAL:O	1.99	0.62
1:E:161:ARG:HA	1:E:331:VAL:HG21	1.82	0.62
1:L:258:CYS:O	1:L:341:VAL:HG21	1.99	0.62
1:C:85:ARG:O	1:C:85:ARG:HG2	2.00	0.61
2:D:2:PDY:H14A	2:D:2:PDY:C18	2.15	0.61
1:H:70:LEU:HD12	1:H:94:MET:SD	2.39	0.61
1:L:70:LEU:CG	1:L:94:MET:HE1	2.30	0.61
1:I:100:LYS:HD2	1:I:103:ARG:NH2	2.14	0.61
1:C:290:GLU:HA	1:C:337:HIS:CD2	2.35	0.61
1:E:49:LYS:HD2	1:E:50:SER:N	2.15	0.61
1:E:214:THR:HG21	1:E:242:LYS:HG3	1.82	0.61
1:H:304:ASN:OD1	1:H:314:MET:HB2	1.97	0.61
1:L:69:VAL:CG1	1:L:79:LEU:HD13	2.27	0.61
1:J:233:GLU:HG2	1:L:310:PRO:HG3	1.81	0.61
1:K:92:LEU:HD12	1:K:93:LYS:N	2.15	0.61
1:J:60:ILE:HD12	1:J:61:ASP:N	2.16	0.61
1:L:77:LYS:HE3	1:L:79:LEU:HD23	1.81	0.61
1:A:327:GLN:CD	1:A:330:LYS:HD3	2.25	0.61
1:I:49:LYS:CG	1:I:50:SER:H	2.11	0.61
1:I:266:ASN:HD21	1:I:272:SER:CB	2.14	0.61
1:K:129:ALA:C	1:K:131:ARG:H	2.09	0.61
1:E:66:THR:HG23	1:E:69:VAL:H	1.66	0.61
1:E:338:THR:HG22	1:E:342:LEU:HD23	1.83	0.61
1:H:229:TYR:HD1	1:H:230:VAL:H	1.49	0.61
1:I:196:SER:O	1:I:201:ALA:HB2	2.01	0.61
1:L:85:ARG:O	1:L:85:ARG:HD2	2.01	0.61
1:D:231:ALA:HB1	1:D:233:GLU:OE2	2.00	0.61
1:E:304:ASN:C	1:E:304:ASN:OD1	2.43	0.61
1:H:69:VAL:CG2	1:H:79:LEU:HD13	2.29	0.61
1:I:231:ALA:HB1	1:I:233:GLU:OE2	2.00	0.61
1:C:264:TYR:CZ	2:C:2:PDY:H24	2.36	0.61
1:D:327:GLN:CB	1:D:330:LYS:HD2	2.29	0.61
1:F:110:ARG:HH22	1:F:213:GLU:CD	2.09	0.61
1:C:65:VAL:CG1	1:C:70:LEU:HD11	2.31	0.61
1:E:80:GLN:OE1	2:E:1:PDY:H24A	2.01	0.61
1:F:156:GLN:HE21	1:F:156:GLN:CA	2.13	0.61
1:J:288:ASN:HD22	1:J:288:ASN:H	1.47	0.61
1:D:69:VAL:CG1	1:D:79:LEU:HD13	2.31	0.60
1:G:278:ARG:HG2	1:G:283:GLN:HG3	1.82	0.60
1:G:289:PRO:HG2	1:G:290:GLU:OE2	2.01	0.60
1:J:276:LYS:HG3	1:K:235:LEU:CD1	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:310:PRO:HA	1:J:313:ARG:HG3	1.80	0.60
1:K:66:THR:O	1:K:69:VAL:HG22	2.01	0.60
1:K:143:GLY:HA3	1:K:194:TYR:HB2	1.82	0.60
1:L:235:LEU:N	1:L:235:LEU:HD12	2.16	0.60
1:D:77:LYS:NZ	1:D:77:LYS:HB3	2.16	0.60
2:D:2:PDY:H14	2:D:2:PDY:C18	2.26	0.60
1:H:154:GLY:HA2	1:H:156:GLN:N	2.15	0.60
1:H:264:TYR:HB2	2:H:2:PDY:H17	1.83	0.60
1:H:342:LEU:O	1:H:343:LYS:HD2	2.01	0.60
1:C:49:LYS:HD2	1:C:50:SER:N	2.15	0.60
1:I:108:HIS:CE1	1:I:138:MET:HE3	2.34	0.60
1:D:82:PHE:CE1	1:D:89:LYS:HB3	2.36	0.60
1:F:161:ARG:HA	1:F:331:VAL:CG2	2.32	0.60
1:A:127:LEU:HD23	1:G:113:GLN:OE1	2.02	0.60
1:A:327:GLN:HG2	1:A:330:LYS:HG2	1.82	0.60
1:B:48:VAL:HG11	1:L:60:ILE:HG23	1.84	0.60
1:D:290:GLU:CD	1:D:290:GLU:H	2.10	0.60
1:I:264:TYR:HB2	2:I:2:PDY:C17	2.25	0.60
1:J:278:ARG:HG2	1:J:283:GLN:HB2	1.83	0.60
1:K:80:GLN:HE21	2:K:1:PDY:H24A	1.63	0.60
2:H:2:PDY:C18	2:H:2:PDY:H14A	2.32	0.60
1:K:188:LYS:HG3	1:K:190:GLU:HG2	1.84	0.60
1:L:187:VAL:O	1:L:187:VAL:HG12	2.02	0.60
1:B:160:GLU:HB3	1:B:334:THR:HG23	1.83	0.60
1:B:266:ASN:OD1	1:B:266:ASN:O	2.19	0.60
1:C:327:GLN:HE21	1:C:330:LYS:CE	2.14	0.60
1:H:140:CYS:SG	2:H:1:PDY:H17	2.42	0.60
1:J:66:THR:O	1:J:69:VAL:HG13	2.02	0.60
1:K:202:ILE:HD12	1:K:203:LEU:N	2.16	0.60
2:L:1:PDY:H18	2:L:1:PDY:H14A	1.83	0.60
1:A:233:GLU:OE2	1:B:313:ARG:NH1	2.34	0.59
1:C:81:ILE:HD13	1:C:92:LEU:HB2	1.84	0.59
1:E:64:LYS:HD2	1:E:84:LYS:HE2	1.84	0.59
1:E:153:ARG:O	1:E:154:GLY:O	2.19	0.59
1:K:92:LEU:HD12	1:K:93:LYS:H	1.66	0.59
1:K:298:VAL:HG22	1:K:324:TRP:CD1	2.37	0.59
1:F:188:LYS:HD3	1:F:190:GLU:OE1	2.01	0.59
1:H:143:GLY:HA2	1:H:197:LYS:HD2	1.84	0.59
1:I:280:ARG:HH22	1:J:131:ARG:HH12	1.49	0.59
1:J:60:ILE:HD12	1:J:60:ILE:C	2.26	0.59
1:B:49:LYS:HD3	1:B:113:GLN:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ARG:HD2	1:E:328:SER:O	2.01	0.59
1:F:304:ASN:CG	1:F:314:MET:HB2	2.26	0.59
1:I:80:GLN:OE1	1:I:89:LYS:HG3	2.02	0.59
1:J:66:THR:HG23	1:J:68:GLN:HB2	1.83	0.59
1:J:124:TYR:HB2	1:J:135:LEU:HB2	1.84	0.59
1:L:257:LEU:CD1	1:L:298:VAL:HG11	2.31	0.59
1:A:66:THR:HG23	1:A:68:GLN:N	2.17	0.59
1:A:280:ARG:HH11	1:C:235:LEU:HD13	1.67	0.59
2:C:2:PDY:H14A	2:C:2:PDY:H18	1.83	0.59
1:E:110:ARG:HH22	1:E:213:GLU:CD	2.09	0.59
1:L:202:ILE:CD1	1:L:204:LYS:HE2	2.31	0.59
1:A:161:ARG:HD3	1:A:331:VAL:O	2.02	0.59
1:E:128:TYR:HD1	1:L:48:VAL:HG23	1.67	0.59
1:J:329:THR:C	1:J:331:VAL:N	2.60	0.59
1:K:284:TYR:OH	1:K:303:ARG:HA	2.03	0.59
1:L:151:GLN:HB3	1:L:342:LEU:CD2	2.30	0.59
1:A:52:LEU:O	1:F:56:LYS:HD2	2.02	0.59
1:A:70:LEU:HD13	1:G:48:VAL:CG2	2.32	0.59
1:B:70:LEU:HD23	1:B:128:TYR:CE1	2.38	0.59
1:E:86:THR:HB	1:E:88:GLU:HG2	1.85	0.59
1:F:234:VAL:HG12	1:F:235:LEU:HD23	1.85	0.59
1:I:55:LYS:HD3	1:I:124:TYR:CZ	2.38	0.59
1:I:327:GLN:HB3	1:I:330:LYS:HG2	1.85	0.59
1:K:281:MET:HB2	1:K:283:GLN:HG3	1.85	0.59
1:L:168:LYS:O	1:L:172:GLU:HG3	2.02	0.59
1:D:72:LEU:HD22	1:D:77:LYS:HE3	1.85	0.59
1:H:200:ASN:HD22	1:H:200:ASN:N	2.00	0.59
1:G:77:LYS:HB3	1:G:79:LEU:HD21	1.85	0.59
1:K:200:ASN:N	1:K:200:ASN:OD1	2.34	0.59
1:K:309:GLU:HB3	1:K:312:GLN:HG3	1.85	0.59
2:E:2:PDY:C18	2:E:2:PDY:C3	2.75	0.59
1:F:295:SER:O	1:F:299:LYS:HD3	2.03	0.59
1:G:100:LYS:HA	1:G:100:LYS:CE	2.20	0.59
1:G:190:GLU:H	1:G:190:GLU:CD	2.10	0.59
1:H:337:HIS:HA	1:H:340:ARG:NH1	2.17	0.59
1:L:159:THR:HG22	1:L:161:ARG:N	2.16	0.59
1:A:50:SER:HB2	1:F:57:ASN:HA	1.85	0.58
1:A:190:GLU:CD	1:A:190:GLU:H	2.11	0.58
1:E:49:LYS:CD	1:E:50:SER:H	2.12	0.58
1:E:111:ALA:HB1	1:E:117:ILE:HD13	1.85	0.58
1:F:151:GLN:HG3	1:F:152:ASP:N	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:264:TYR:HB2	2:I:2:PDY:HN9	1.68	0.58
1:A:188:LYS:HD2	1:A:191:ASN:ND2	2.18	0.58
1:C:55:LYS:HD3	1:C:124:TYR:CZ	2.38	0.58
1:F:87:GLN:HA	1:F:87:GLN:OE1	2.03	0.58
1:I:58:ALA:HA	1:I:126:ASN:OD1	2.03	0.58
2:I:2:PDY:C18	2:I:2:PDY:H14A	2.32	0.58
1:B:49:LYS:CD	1:B:113:GLN:HG2	2.33	0.58
1:B:66:THR:OG1	1:B:69:VAL:HG13	2.02	0.58
1:B:74:ILE:HD12	1:B:75:ASN:N	2.18	0.58
1:B:192:LEU:C	1:B:193:LEU:HD23	2.28	0.58
1:C:129:ALA:HB3	1:C:131:ARG:HE	1.68	0.58
1:G:90:PHE:CE2	1:G:121:VAL:HG21	2.39	0.58
1:A:278:ARG:HA	1:A:283:GLN:HG2	1.85	0.58
1:B:60:ILE:C	1:B:60:ILE:HD12	2.28	0.58
1:B:70:LEU:HD23	1:B:128:TYR:HE1	1.68	0.58
2:B:1:PDY:C3	2:B:1:PDY:H18	2.33	0.58
1:C:88:GLU:HG2	1:C:89:LYS:H	1.69	0.58
1:E:88:GLU:HG3	1:E:90:PHE:CE1	2.38	0.58
1:F:151:GLN:O	1:F:343:LYS:HE3	2.03	0.58
1:J:97:ASP:O	1:J:98:CYS:HB3	2.03	0.58
1:K:66:THR:H	1:K:69:VAL:CG2	2.16	0.58
1:L:93:LYS:HG2	1:L:136:ILE:HB	1.84	0.58
1:H:202:ILE:HD11	1:H:204:LYS:NZ	2.18	0.58
1:I:64:LYS:HD2	1:I:84:LYS:HE3	1.86	0.58
1:I:167:MET:HE2	1:I:253:MET:HG3	1.85	0.58
1:I:264:TYR:CD2	2:I:2:PDY:H20	2.39	0.58
1:J:159:THR:HG22	1:J:161:ARG:N	2.16	0.58
1:B:328:SER:O	1:B:331:VAL:HG13	2.03	0.58
1:E:57:ASN:H	1:E:57:ASN:HD22	1.51	0.58
1:K:290:GLU:HA	1:K:337:HIS:HD2	1.68	0.58
1:K:295:SER:OG	1:K:298:VAL:HG23	2.04	0.58
1:B:77:LYS:HB3	1:B:77:LYS:NZ	2.18	0.58
1:C:161:ARG:NH1	1:C:333:GLN:HG2	2.18	0.58
1:D:77:LYS:NZ	1:D:79:LEU:HD21	2.17	0.58
1:F:66:THR:O	1:F:70:LEU:HB2	2.04	0.58
1:H:264:TYR:CD1	2:H:2:PDY:H20	2.27	0.58
1:B:184:HIS:HD2	1:B:186:ASP:N	1.98	0.58
1:G:264:TYR:O	1:G:275:MET:HG3	2.04	0.58
1:I:140:CYS:SG	2:I:1:PDY:C17	2.92	0.58
1:G:285:GLU:C	1:G:287:PRO:HD3	2.29	0.58
1:G:307:LYS:HB2	1:G:313:ARG:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:GLY:C	1:I:156:GLN:H	2.12	0.58
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.68	0.57
1:G:264:TYR:C	1:G:264:TYR:CD2	2.82	0.57
1:I:58:ALA:O	1:I:61:ASP:HB2	2.04	0.57
1:J:288:ASN:N	1:J:288:ASN:ND2	2.52	0.57
1:J:322:HIS:ND1	1:J:323:PRO:HD2	2.19	0.57
1:A:195:THR:HG23	1:A:202:ILE:O	2.04	0.57
1:B:49:LYS:HD3	1:B:113:GLN:CG	2.34	0.57
1:B:74:ILE:HG23	1:B:94:MET:HE2	1.86	0.57
1:D:214:THR:O	1:D:238:GLU:HB3	2.04	0.57
1:E:156:GLN:HE21	1:E:156:GLN:N	2.01	0.57
1:C:185:ARG:HD3	1:C:241:ASP:CG	2.29	0.57
1:E:229:TYR:OH	1:F:188:LYS:HE2	2.03	0.57
1:F:70:LEU:HD12	1:F:94:MET:CE	2.34	0.57
1:H:110:ARG:HH22	1:H:213:GLU:CD	2.12	0.57
1:I:215:THR:OG1	1:I:216:SER:N	2.37	0.57
1:L:48:VAL:O	1:L:48:VAL:HG12	2.02	0.57
1:A:295:SER:OG	1:A:298:VAL:HG23	2.04	0.57
1:B:108:HIS:CG	1:B:120:ILE:HD11	2.40	0.57
2:C:2:PDY:C14	2:C:2:PDY:H18	2.33	0.57
1:J:300:MET:SD	1:J:303:ARG:HD2	2.44	0.57
1:C:54:ILE:HG21	1:C:125:GLU:HB2	1.85	0.57
1:C:65:VAL:HG12	1:C:70:LEU:HD11	1.87	0.57
1:J:66:THR:CG2	1:J:68:GLN:HB2	2.33	0.57
1:C:97:ASP:H	1:C:133:CYS:HA	1.70	0.57
1:G:300:MET:SD	1:G:303:ARG:NH2	2.75	0.57
1:I:275:MET:O	1:I:279:ILE:HG13	2.05	0.57
1:J:147:PHE:HB3	1:J:342:LEU:HD21	1.86	0.57
1:J:156:GLN:HG3	1:J:340:ARG:HH11	1.69	0.57
1:B:108:HIS:HE1	1:B:138:MET:CE	2.16	0.57
1:F:264:TYR:CZ	2:F:2:PDY:H24	2.40	0.57
1:H:240:TYR:CE1	1:H:242:LYS:HB2	2.40	0.57
1:I:200:ASN:HD22	1:I:200:ASN:N	2.03	0.57
1:J:74:ILE:N	1:J:94:MET:HE3	2.19	0.57
1:K:288:ASN:H	1:K:288:ASN:HD22	1.52	0.57
1:D:49:LYS:HD2	1:D:113:GLN:CG	2.28	0.57
1:D:58:ALA:O	1:D:61:ASP:HB2	2.05	0.57
1:F:260:TYR:OH	1:F:287:PRO:HG2	2.05	0.57
1:J:140:CYS:SG	2:J:1:PDY:H17	2.45	0.57
1:K:102:ARG:HG3	1:K:134:LEU:HD21	1.87	0.57
1:D:110:ARG:HH22	1:D:213:GLU:CD	2.12	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ARG:HA	1:D:283:GLN:HG3	1.86	0.57
1:G:189:PRO:HG2	1:G:190:GLU:OE1	2.04	0.57
1:I:264:TYR:CG	2:I:2:PDY:H20	2.39	0.57
1:K:66:THR:H	1:K:69:VAL:HG22	1.69	0.57
2:B:1:PDY:H14A	2:B:1:PDY:H18	1.87	0.56
1:L:49:LYS:CD	1:L:50:SER:H	2.18	0.56
1:L:110:ARG:HH22	1:L:213:GLU:CD	2.12	0.56
1:C:264:TYR:OH	2:C:2:PDY:H24	2.04	0.56
1:C:295:SER:CB	1:C:298:VAL:HG23	2.29	0.56
1:D:155:ASP:CG	1:D:156:GLN:H	2.12	0.56
1:E:202:ILE:CD1	1:E:204:LYS:HE2	2.34	0.56
1:J:187:VAL:HG12	1:J:187:VAL:O	2.04	0.56
1:J:278:ARG:CG	1:J:283:GLN:HE21	2.18	0.56
2:B:1:PDY:C14	2:B:1:PDY:H18	2.35	0.56
1:C:63:TYR:O	1:C:65:VAL:HG23	2.04	0.56
1:E:66:THR:HG22	1:E:69:VAL:HG13	1.85	0.56
1:E:161:ARG:HB3	1:E:333:GLN:NE2	2.20	0.56
1:E:184:HIS:HD2	1:E:186:ASP:H	1.53	0.56
1:G:310:PRO:HG3	1:I:233:GLU:HG2	1.87	0.56
1:I:121:VAL:HB	1:I:137:VAL:HG12	1.87	0.56
1:L:155:ASP:HA	1:L:157:ALA:N	2.20	0.56
1:B:108:HIS:HE1	1:B:138:MET:HE3	1.70	0.56
1:D:202:ILE:HD12	1:D:203:LEU:N	2.20	0.56
1:K:60:ILE:C	1:K:60:ILE:HD12	2.30	0.56
1:C:327:GLN:HB2	1:C:330:LYS:HZ3	1.70	0.56
1:F:288:ASN:OD1	1:F:292:SER:HB3	2.05	0.56
1:G:167:MET:HE2	1:G:253:MET:HB2	1.87	0.56
1:G:188:LYS:HB2	1:G:189:PRO:HD2	1.87	0.56
1:F:100:LYS:NZ	1:F:103:ARG:HH22	2.04	0.56
1:F:281:MET:HB2	1:F:283:GLN:HG3	1.88	0.56
1:K:119:ARG:HB3	1:K:139:GLU:OE1	2.06	0.56
2:L:1:PDY:C18	2:L:1:PDY:H14A	2.34	0.56
1:A:276:LYS:HD3	1:A:280:ARG:HH12	1.70	0.56
2:A:1:PDY:C18	2:A:1:PDY:H14A	2.35	0.56
1:B:60:ILE:HD12	1:B:61:ASP:N	2.21	0.56
1:F:69:VAL:HB	1:F:79:LEU:HD13	1.87	0.56
1:H:328:SER:O	1:H:331:VAL:HG22	2.05	0.56
1:G:196:SER:OG	1:G:198:ARG:HG2	2.06	0.56
1:I:69:VAL:CA	1:I:79:LEU:HD22	2.34	0.56
1:A:63:TYR:HE1	1:A:124:TYR:HH	1.53	0.56
1:B:232:PRO:HD3	1:C:247:TRP:CZ2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:HB3	1:C:310:PRO:HG3	1.88	0.56
1:C:188:LYS:HE3	1:C:191:ASN:HD21	1.70	0.56
1:E:260:TYR:HE2	1:E:290:GLU:OE1	1.88	0.56
1:F:338:THR:O	1:F:342:LEU:HB2	2.05	0.56
1:I:107:LEU:HD22	1:I:182:ILE:CD1	2.36	0.56
1:I:266:ASN:H	1:I:266:ASN:HD22	1.53	0.56
1:J:66:THR:CG2	1:J:69:VAL:HG12	2.36	0.56
1:J:71:GLY:O	1:J:74:ILE:HG22	2.06	0.56
2:E:2:PDY:C13	2:E:2:PDY:H14	2.36	0.56
1:H:66:THR:O	1:H:70:LEU:HB2	2.06	0.56
1:K:92:LEU:HD21	1:K:94:MET:HE2	1.88	0.56
1:E:300:MET:SD	1:E:303:ARG:NE	2.70	0.55
1:H:295:SER:OG	1:H:298:VAL:HG23	2.07	0.55
1:H:341:VAL:C	1:H:343:LYS:H	2.14	0.55
1:I:185:ARG:HH21	1:I:212:LYS:HG3	1.72	0.55
1:J:110:ARG:HH22	1:J:213:GLU:CD	2.14	0.55
1:L:49:LYS:HD2	1:L:50:SER:N	2.20	0.55
1:L:327:GLN:NE2	1:L:330:LYS:HD3	2.21	0.55
1:F:261:PRO:HD3	2:F:2:PDY:H25	1.87	0.55
1:H:300:MET:SD	1:H:303:ARG:NE	2.77	0.55
1:J:118:VAL:HG21	2:J:1:PDY:H11	1.88	0.55
1:A:175:GLN:NE2	1:A:320:MET:HG3	2.20	0.55
1:B:184:HIS:HE1	1:B:206:THR:O	1.89	0.55
1:C:83:ASN:ND2	1:C:86:THR:HB	2.22	0.55
1:E:97:ASP:HB2	1:E:134:LEU:HD13	1.87	0.55
1:G:338:THR:O	1:G:342:LEU:HB2	2.06	0.55
1:H:257:LEU:HD11	1:H:298:VAL:HG11	1.88	0.55
1:I:322:HIS:ND1	1:I:323:PRO:HD2	2.20	0.55
1:L:97:ASP:O	1:L:98:CYS:HB3	2.05	0.55
1:C:82:PHE:HA	1:C:88:GLU:O	2.06	0.55
1:D:167:MET:HE2	1:D:253:MET:HB2	1.89	0.55
1:E:66:THR:O	1:E:69:VAL:HG22	2.05	0.55
1:F:304:ASN:OD1	1:F:314:MET:HB2	2.06	0.55
1:H:48:VAL:HG13	1:H:48:VAL:O	2.07	0.55
1:L:300:MET:SD	1:L:303:ARG:NH2	2.75	0.55
1:A:280:ARG:HH11	1:C:235:LEU:CD1	2.20	0.55
1:G:86:THR:C	1:G:88:GLU:H	2.14	0.55
1:G:97:ASP:OD2	1:G:102:ARG:NH2	2.37	0.55
1:B:296:GLU:OE2	1:B:303:ARG:NH2	2.39	0.55
1:C:252:ILE:O	1:C:256:LEU:HB2	2.07	0.55
1:G:195:THR:HG23	1:G:202:ILE:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:254:TYR:CG	1:J:262:PRO:HG3	2.42	0.55
1:F:60:ILE:HD12	1:F:60:ILE:C	2.31	0.55
2:G:1:PDY:C18	2:G:1:PDY:H14	2.34	0.55
1:B:108:HIS:CE1	1:B:138:MET:HE3	2.42	0.55
1:C:307:LYS:HD2	1:C:312:GLN:OE1	2.06	0.55
1:K:82:PHE:HA	1:K:88:GLU:O	2.07	0.55
1:K:258:CYS:HB3	1:K:291:TRP:NE1	2.22	0.55
1:A:69:VAL:HB	1:A:79:LEU:CD1	2.37	0.55
1:D:184:HIS:CD2	1:D:205:LEU:HD21	2.42	0.55
1:K:110:ARG:HH22	1:K:213:GLU:CD	2.15	0.55
1:L:147:PHE:HE2	1:L:256:LEU:HD23	1.71	0.55
1:C:264:TYR:CE1	2:C:2:PDY:H24A	2.42	0.55
2:C:2:PDY:C18	2:C:2:PDY:C3	2.84	0.55
1:J:159:THR:HG23	1:J:333:GLN:HA	1.89	0.55
1:L:94:MET:O	1:L:95:LEU:HD23	2.06	0.55
1:A:167:MET:HE2	1:A:253:MET:HE2	1.89	0.54
1:B:206:THR:OG1	1:B:207:ASP:OD2	2.21	0.54
1:E:111:ALA:HB1	1:E:117:ILE:CD1	2.38	0.54
1:F:202:ILE:CD1	1:F:204:LYS:HE2	2.37	0.54
1:B:125:GLU:C	1:B:126:ASN:HD22	2.15	0.54
1:C:153:ARG:HB2	1:C:156:GLN:HE22	1.72	0.54
1:G:49:LYS:HD2	1:G:113:GLN:CD	2.33	0.54
1:G:80:GLN:CD	1:G:89:LYS:HD2	2.31	0.54
1:J:116:HIS:CE1	1:J:169:SER:OG	2.60	0.54
1:J:287:PRO:O	1:J:291:TRP:HB2	2.06	0.54
1:B:58:ALA:O	1:B:61:ASP:HB2	2.08	0.54
1:B:155:ASP:HA	1:B:343:LYS:NZ	2.22	0.54
1:B:158:PHE:CE1	1:B:162:GLU:HB3	2.43	0.54
1:C:130:GLY:O	1:J:110:ARG:HD3	2.06	0.54
1:H:264:TYR:CD1	2:H:2:PDY:C17	2.89	0.54
1:J:73:GLY:C	1:J:94:MET:HE3	2.32	0.54
1:L:202:ILE:HD11	1:L:204:LYS:CE	2.36	0.54
1:K:230:VAL:HG22	1:K:231:ALA:N	2.07	0.54
1:L:142:ASP:N	1:L:195:THR:O	2.41	0.54
1:C:66:THR:HG1	1:C:69:VAL:N	2.06	0.54
1:E:178:HIS:HE1	1:E:245:ASP:OD2	1.91	0.54
1:H:233:GLU:HG2	1:I:310:PRO:HG3	1.90	0.54
1:J:327:GLN:HB3	1:J:330:LYS:HG2	1.90	0.54
1:K:150:ILE:O	1:K:153:ARG:HG3	2.07	0.54
2:K:2:PDY:C14	2:K:2:PDY:C13	2.86	0.54
1:A:332:PRO:CB	1:A:334:THR:HG22	2.30	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:MET:SD	1:C:303:ARG:NE	2.80	0.54
1:E:145:GLU:HG2	1:E:193:LEU:HD21	1.90	0.54
1:I:72:LEU:CB	1:I:79:LEU:HD21	2.37	0.54
1:K:260:TYR:HB2	2:K:2:PDY:H19	1.90	0.54
1:A:66:THR:O	1:A:69:VAL:HG22	2.07	0.54
1:A:159:THR:OG1	1:A:333:GLN:NE2	2.41	0.54
1:C:161:ARG:HD3	1:C:331:VAL:HG13	1.90	0.54
1:C:327:GLN:HB3	1:C:330:LYS:HG3	1.90	0.54
1:F:214:THR:HG21	1:F:242:LYS:HE3	1.88	0.54
1:H:90:PHE:HE2	1:H:121:VAL:HG21	1.71	0.54
1:H:198:ARG:HG2	1:H:199:PRO:HD2	1.89	0.54
1:H:264:TYR:CB	2:H:2:PDY:C17	2.85	0.54
1:J:298:VAL:HG22	1:J:324:TRP:CD1	2.42	0.54
1:K:260:TYR:OH	1:K:287:PRO:HG2	2.07	0.54
1:L:235:LEU:HD12	1:L:235:LEU:H	1.73	0.54
1:B:167:MET:HE2	1:B:253:MET:HB2	1.89	0.54
1:I:202:ILE:HD11	1:I:204:LYS:HG2	1.89	0.54
1:K:261:PRO:HD3	2:K:2:PDY:H25	1.90	0.54
1:A:188:LYS:HE2	1:A:190:GLU:HB2	1.90	0.54
1:H:81:ILE:HD13	1:H:92:LEU:HB2	1.89	0.54
1:I:253:MET:HE1	1:I:301:LEU:CD2	2.38	0.54
1:J:66:THR:HG22	1:J:69:VAL:HG12	1.89	0.54
1:K:49:LYS:HB3	1:K:113:GLN:NE2	2.23	0.54
1:L:147:PHE:CE2	1:L:256:LEU:HD23	2.43	0.54
1:H:97:ASP:OD1	1:H:98:CYS:N	2.41	0.53
1:I:92:LEU:HD21	1:I:94:MET:HE2	1.89	0.53
1:A:290:GLU:CD	1:A:290:GLU:H	2.16	0.53
1:B:146:LEU:HD11	1:B:166:ILE:HD13	1.89	0.53
1:D:188:LYS:HG3	1:D:190:GLU:HG2	1.91	0.53
1:J:63:TYR:O	1:J:84:LYS:HE3	2.08	0.53
1:J:118:VAL:CG2	1:J:138:MET:HE2	2.37	0.53
1:J:159:THR:HG21	1:J:333:GLN:HG2	1.90	0.53
1:L:146:LEU:HD11	1:L:166:ILE:HD13	1.89	0.53
1:A:161:ARG:HD2	1:A:328:SER:O	2.09	0.53
2:C:1:PDY:H18	2:C:1:PDY:C3	2.39	0.53
1:J:278:ARG:HG3	1:J:283:GLN:HE21	1.73	0.53
1:A:49:LYS:HG3	1:A:113:GLN:CD	2.33	0.53
1:E:69:VAL:CB	1:E:79:LEU:HD13	2.38	0.53
1:H:150:ILE:O	1:H:153:ARG:HG2	2.08	0.53
1:K:80:GLN:NE2	2:K:1:PDY:H24	2.22	0.53
1:K:309:GLU:OE2	1:K:310:PRO:HD2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:CYS:HB2	1:D:99:PRO:CD	2.39	0.53
1:H:151:GLN:NE2	1:H:342:LEU:O	2.42	0.53
1:K:332:PRO:HB2	1:K:334:THR:CG2	2.26	0.53
1:L:159:THR:HB	1:L:162:GLU:HG3	1.90	0.53
1:A:288:ASN:HB3	1:A:289:PRO:HA	1.90	0.53
1:F:108:HIS:HE1	1:F:138:MET:HE2	1.73	0.53
1:H:69:VAL:HG13	1:H:70:LEU:H	1.74	0.53
1:A:214:THR:HG21	1:A:242:LYS:HE3	1.90	0.53
1:B:155:ASP:N	1:B:156:GLN:OE1	2.41	0.53
1:C:60:ILE:HD12	1:C:61:ASP:N	2.24	0.53
1:K:234:VAL:HG12	1:K:234:VAL:O	2.09	0.53
1:B:247:TRP:HB2	1:B:313:ARG:NH1	2.24	0.53
1:E:275:MET:HA	1:E:278:ARG:HH11	1.74	0.53
1:E:332:PRO:HB2	1:E:334:THR:HG22	1.89	0.53
1:J:276:LYS:CG	1:K:235:LEU:HD12	2.38	0.53
1:K:89:LYS:CD	1:K:89:LYS:N	2.72	0.53
2:K:1:PDY:C18	2:K:1:PDY:H14	2.36	0.53
1:L:260:TYR:OH	1:L:287:PRO:HG2	2.09	0.53
1:A:52:LEU:C	1:F:56:LYS:HD2	2.34	0.53
1:E:87:GLN:N	1:E:87:GLN:NE2	2.57	0.53
1:H:212:LYS:HD3	1:H:213:GLU:N	2.23	0.53
1:J:185:ARG:CZ	1:J:212:LYS:HG3	2.38	0.53
1:J:198:ARG:HH11	1:J:198:ARG:CG	2.22	0.53
1:K:95:LEU:O	1:K:133:CYS:CB	2.56	0.53
1:C:125:GLU:C	1:C:126:ASN:HD22	2.17	0.52
1:C:148:SER:HA	1:C:151:GLN:HB3	1.91	0.52
1:I:70:LEU:HD23	1:I:94:MET:CE	2.38	0.52
1:J:156:GLN:HG3	1:J:340:ARG:NH1	2.23	0.52
1:J:255:ILE:HG12	1:J:261:PRO:HA	1.91	0.52
1:A:107:LEU:HD21	1:A:213:GLU:HG3	1.90	0.52
1:C:284:TYR:C	1:C:285:GLU:HG2	2.34	0.52
1:D:328:SER:O	1:D:331:VAL:HG13	2.08	0.52
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.91	0.52
1:H:115:PRO:O	1:H:204:LYS:NZ	2.40	0.52
1:H:154:GLY:HA2	1:H:156:GLN:H	1.75	0.52
1:C:78:VAL:CG1	1:C:91:ALA:HB1	2.38	0.52
1:K:178:HIS:CE1	1:K:242:LYS:HG2	2.45	0.52
1:C:129:ALA:HB3	1:C:131:ARG:NE	2.25	0.52
1:E:80:GLN:OE1	2:E:1:PDY:C24	2.58	0.52
1:H:67:SER:C	1:H:69:VAL:N	2.67	0.52
1:I:338:THR:O	1:I:342:LEU:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:ASP:O	1:J:244:CYS:HB3	2.10	0.52
1:L:241:ASP:O	1:L:244:CYS:HB3	2.09	0.52
1:A:278:ARG:O	1:A:282:GLY:N	2.43	0.52
1:A:285:GLU:O	1:A:287:PRO:HD3	2.09	0.52
1:C:260:TYR:OH	1:C:290:GLU:HG3	2.09	0.52
1:I:160:GLU:HA	1:I:336:LEU:HD21	1.91	0.52
1:J:198:ARG:HH11	1:J:200:ASN:N	2.07	0.52
1:K:129:ALA:O	1:K:131:ARG:N	2.42	0.52
1:E:161:ARG:HD3	1:E:331:VAL:O	2.09	0.52
1:J:276:LYS:HA	1:J:279:ILE:HD12	1.92	0.52
1:K:104:GLU:HG3	1:K:208:PHE:O	2.10	0.52
1:K:140:CYS:SG	2:K:1:PDY:H17	2.50	0.52
1:E:160:GLU:HA	1:E:336:LEU:HD21	1.91	0.52
1:K:70:LEU:HA	1:K:94:MET:CE	2.38	0.52
1:B:290:GLU:HB2	1:B:291:TRP:CD1	2.44	0.52
1:F:304:ASN:OD1	1:F:304:ASN:C	2.53	0.52
1:H:154:GLY:CA	1:H:156:GLN:H	2.23	0.52
1:C:149:ARG:NH2	1:C:201:ALA:HB3	2.25	0.52
1:D:73:GLY:HA3	1:D:94:MET:SD	2.50	0.52
1:D:286:PHE:CD1	1:D:299:LYS:HG2	2.44	0.52
1:F:70:LEU:HD12	1:F:94:MET:SD	2.50	0.52
1:K:332:PRO:CB	1:K:334:THR:HG22	2.27	0.52
1:B:47:HIS:HD2	1:L:70:LEU:HD22	1.73	0.51
1:D:49:LYS:HG2	1:D:50:SER:N	2.25	0.51
1:D:130:GLY:O	1:I:110:ARG:NH1	2.41	0.51
1:E:185:ARG:NE	1:E:212:LYS:HG3	2.25	0.51
1:G:69:VAL:CB	1:G:79:LEU:HD13	2.34	0.51
1:G:214:THR:HG21	1:G:242:LYS:HG3	1.91	0.51
1:L:159:THR:HG22	1:L:160:GLU:N	2.25	0.51
1:C:183:ALA:O	1:C:211:ALA:HA	2.09	0.51
2:I:1:PDY:H18	2:I:1:PDY:C3	2.38	0.51
1:J:70:LEU:HA	1:J:94:MET:HE1	1.92	0.51
1:K:108:HIS:CG	1:K:120:ILE:HD11	2.45	0.51
1:B:189:PRO:HD2	1:B:190:GLU:OE1	2.10	0.51
1:B:339:SER:O	1:B:343:LYS:HG3	2.10	0.51
1:C:167:MET:HE2	1:C:253:MET:HE3	1.93	0.51
1:D:195:THR:HG21	1:D:202:ILE:HG23	1.92	0.51
1:E:98:CYS:HB2	1:E:99:PRO:HD2	1.91	0.51
1:I:151:GLN:C	1:I:153:ARG:H	2.18	0.51
1:J:332:PRO:HB2	1:J:334:THR:CG2	2.41	0.51
1:F:190:GLU:CD	1:F:190:GLU:H	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:TYR:HB2	2:F:2:PDY:H19	1.92	0.51
1:K:337:HIS:O	1:K:341:VAL:HG23	2.10	0.51
1:G:154:GLY:O	1:G:155:ASP:C	2.54	0.51
1:I:202:ILE:HD11	1:I:204:LYS:CG	2.40	0.51
1:J:141:LEU:CD1	1:J:193:LEU:HB2	2.40	0.51
1:J:331:VAL:HG23	1:J:332:PRO:HD2	1.91	0.51
1:G:73:GLY:CA	1:G:79:LEU:HD11	2.40	0.51
1:G:156:GLN:HE22	1:G:340:ARG:NH1	2.09	0.51
1:K:164:SER:HB2	1:K:324:TRP:CZ2	2.46	0.51
1:L:261:PRO:HB2	1:L:263:PHE:O	2.11	0.51
1:C:284:TYR:O	1:C:285:GLU:HG2	2.11	0.51
1:C:327:GLN:C	1:C:329:THR:H	2.17	0.51
1:D:48:VAL:O	1:D:48:VAL:HG13	2.09	0.51
1:F:161:ARG:HD3	1:F:331:VAL:O	2.09	0.51
1:F:214:THR:HG21	1:F:242:LYS:HG3	1.93	0.51
1:I:168:LYS:O	1:I:172:GLU:HG3	2.10	0.51
1:K:232:PRO:C	1:K:234:VAL:H	2.17	0.51
2:A:2:PDY:C17	2:A:2:PDY:H14A	2.41	0.51
1:J:73:GLY:O	1:J:94:MET:HB2	2.10	0.51
1:J:185:ARG:NH2	1:J:212:LYS:HE2	2.26	0.51
1:K:188:LYS:NZ	1:K:190:GLU:HG3	2.25	0.51
1:A:168:LYS:HB2	1:A:325:ILE:HG23	1.93	0.51
1:A:275:MET:HE3	1:A:279:ILE:HD11	1.93	0.51
1:B:66:THR:O	1:B:69:VAL:HG22	2.10	0.51
1:B:69:VAL:HG23	1:B:70:LEU:H	1.74	0.51
1:C:102:ARG:NH2	1:C:134:LEU:HD11	2.26	0.51
1:D:110:ARG:O	1:D:113:GLN:HG3	2.11	0.51
1:E:115:PRO:O	1:E:202:ILE:HD11	2.11	0.51
1:E:260:TYR:HB2	2:E:2:PDY:H19	1.92	0.51
1:F:271:ILE:HG23	1:F:275:MET:HE2	1.92	0.51
1:G:284:TYR:OH	1:G:303:ARG:HG2	2.11	0.51
1:I:100:LYS:CD	1:I:103:ARG:HH21	2.22	0.51
1:J:110:ARG:O	1:J:113:GLN:HG2	2.11	0.51
1:A:185:ARG:NE	1:A:212:LYS:HG3	2.26	0.51
1:B:155:ASP:HA	1:B:343:LYS:HZ1	1.76	0.51
1:C:234:VAL:O	1:C:234:VAL:HG22	2.11	0.51
1:F:307:LYS:HG2	1:F:312:GLN:HB3	1.92	0.51
1:G:231:ALA:HB1	1:G:233:GLU:OE2	2.11	0.51
1:B:184:HIS:CD2	1:B:186:ASP:H	2.14	0.50
1:E:328:SER:C	1:E:330:LYS:H	2.18	0.50
1:F:149:ARG:HG3	1:F:194:TYR:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:ASN:N	1:H:200:ASN:ND2	2.59	0.50
1:K:167:MET:HG3	1:K:253:MET:CE	2.39	0.50
1:A:50:SER:HB2	1:F:56:LYS:O	2.11	0.50
1:A:111:ALA:HB1	1:A:117:ILE:HD13	1.93	0.50
1:A:235:LEU:HD11	1:B:276:LYS:HE2	1.92	0.50
1:F:192:LEU:C	1:F:193:LEU:HD23	2.35	0.50
1:J:81:ILE:HD13	1:J:92:LEU:HB2	1.92	0.50
1:J:202:ILE:HD11	1:J:204:LYS:HE3	1.92	0.50
1:L:80:GLN:HB2	2:L:1:PDY:H24A	1.92	0.50
1:L:97:ASP:N	1:L:133:CYS:HA	2.26	0.50
1:L:159:THR:CG2	1:L:161:ARG:HB3	2.40	0.50
1:B:69:VAL:CG2	1:B:70:LEU:N	2.73	0.50
1:B:153:ARG:O	1:B:154:GLY:C	2.54	0.50
1:D:239:LYS:O	1:D:240:TYR:HB2	2.11	0.50
1:E:260:TYR:HB2	1:E:261:PRO:HD2	1.92	0.50
1:G:234:VAL:O	1:G:234:VAL:HG12	2.11	0.50
1:H:304:ASN:CG	1:H:314:MET:HE3	2.36	0.50
1:J:185:ARG:CZ	1:J:212:LYS:HE2	2.41	0.50
1:L:264:TYR:CD2	2:L:2:PDY:H20	2.47	0.50
1:B:111:ALA:HB1	1:B:117:ILE:HD12	1.93	0.50
1:B:161:ARG:HD3	1:B:331:VAL:O	2.11	0.50
1:C:107:LEU:HD22	1:C:182:ILE:HG12	1.93	0.50
1:H:264:TYR:CG	2:H:2:PDY:H20	2.42	0.50
1:I:70:LEU:HD23	1:I:94:MET:HE1	1.92	0.50
1:L:190:GLU:OE1	1:L:190:GLU:N	2.38	0.50
1:A:153:ARG:O	1:A:154:GLY:C	2.54	0.50
1:D:97:ASP:H	1:D:133:CYS:HA	1.76	0.50
1:F:56:LYS:HE3	1:F:125:GLU:CD	2.36	0.50
1:J:114:CYS:SG	1:J:116:HIS:HB2	2.52	0.50
1:J:147:PHE:HE2	1:J:256:LEU:HD23	1.76	0.50
1:K:164:SER:HA	1:K:324:TRP:CH2	2.46	0.50
2:K:2:PDY:H14A	2:K:2:PDY:C19	2.41	0.50
1:L:66:THR:HG22	1:L:69:VAL:CG2	2.38	0.50
1:B:52:LEU:HD22	1:B:105:VAL:HG12	1.93	0.50
1:C:202:ILE:CD1	1:C:204:LYS:HE2	2.18	0.50
1:J:192:LEU:O	1:J:193:LEU:HD23	2.11	0.50
1:J:287:PRO:HD2	1:J:291:TRP:CD1	2.46	0.50
1:K:288:ASN:N	1:K:288:ASN:ND2	2.59	0.50
1:F:69:VAL:HG23	1:F:70:LEU:N	2.26	0.50
1:K:108:HIS:CD2	1:K:120:ILE:HD11	2.47	0.50
1:L:264:TYR:CB	2:L:2:PDY:C17	2.88	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:O	1:B:153:ARG:HG2	2.12	0.50
1:B:266:ASN:CG	1:B:278:ARG:NH2	2.68	0.50
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.47	0.50
1:G:161:ARG:NH1	1:G:333:GLN:HG3	2.26	0.50
1:H:290:GLU:H	1:H:290:GLU:CD	2.20	0.50
1:H:341:VAL:O	1:H:343:LYS:N	2.37	0.50
1:J:198:ARG:HG3	1:J:199:PRO:N	2.27	0.50
1:L:161:ARG:NH1	1:L:333:GLN:HG2	2.27	0.50
1:B:66:THR:O	1:B:70:LEU:HD13	2.12	0.50
1:D:232:PRO:HD2	1:D:233:GLU:OE2	2.11	0.50
2:E:1:PDY:C18	2:E:1:PDY:H14	2.39	0.50
1:J:293:GLU:OE2	1:J:293:GLU:HA	2.10	0.50
1:A:313:ARG:NH1	1:C:233:GLU:OE1	2.44	0.49
1:B:145:GLU:O	1:B:148:SER:HB3	2.12	0.49
1:E:288:ASN:HA	1:E:289:PRO:C	2.36	0.49
1:K:62:ASP:CA	1:K:85:ARG:HH21	2.22	0.49
1:L:247:TRP:HZ3	1:L:306:LEU:O	1.95	0.49
1:A:276:LYS:HG3	1:C:235:LEU:HD11	1.94	0.49
2:B:1:PDY:C18	2:B:1:PDY:C3	2.88	0.49
1:C:127:LEU:O	1:J:48:VAL:HA	2.11	0.49
1:D:151:GLN:HB3	1:D:342:LEU:HB3	1.94	0.49
1:G:180:ILE:HD11	1:G:182:ILE:HD12	1.94	0.49
1:L:260:TYR:OH	1:L:290:GLU:HG3	2.12	0.49
1:B:190:GLU:CD	1:B:190:GLU:N	2.70	0.49
1:E:214:THR:O	1:E:215:THR:HB	2.11	0.49
1:F:332:PRO:HB2	1:F:334:THR:HG22	1.93	0.49
1:G:235:LEU:HD12	1:H:280:ARG:HG3	1.93	0.49
2:H:1:PDY:C18	2:H:1:PDY:C3	2.73	0.49
2:L:1:PDY:C14	2:L:1:PDY:H18	2.40	0.49
1:A:161:ARG:O	1:A:165:GLU:HG3	2.12	0.49
1:A:328:SER:O	1:A:331:VAL:CG1	2.61	0.49
1:B:57:ASN:ND2	1:B:57:ASN:H	2.08	0.49
1:B:232:PRO:HD3	1:C:247:TRP:CH2	2.47	0.49
1:C:168:LYS:O	1:C:172:GLU:HG3	2.12	0.49
1:C:296:GLU:OE2	1:C:303:ARG:NH2	2.42	0.49
1:D:145:GLU:HG2	1:D:193:LEU:CD2	2.43	0.49
1:C:184:HIS:CD2	1:C:205:LEU:HD21	2.47	0.49
1:H:190:GLU:H	1:H:190:GLU:CD	2.21	0.49
1:H:337:HIS:O	1:H:340:ARG:HG3	2.12	0.49
2:J:1:PDY:C18	2:J:1:PDY:C3	2.81	0.49
1:K:178:HIS:ND1	1:K:242:LYS:HG2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:VAL:O	1:B:234:VAL:HG12	2.13	0.49
1:C:327:GLN:CB	1:C:330:LYS:HZ3	2.26	0.49
1:E:159:THR:OG1	1:E:333:GLN:NE2	2.46	0.49
1:H:342:LEU:C	1:H:343:LYS:HD2	2.37	0.49
1:I:66:THR:OG1	1:I:69:VAL:HG23	2.12	0.49
1:I:161:ARG:HD3	1:I:331:VAL:O	2.13	0.49
1:L:154:GLY:C	1:L:156:GLN:HB3	2.37	0.49
1:A:309:GLU:CG	1:C:311:THR:HG22	2.43	0.49
1:A:338:THR:HG22	1:A:342:LEU:CD2	2.42	0.49
1:D:66:THR:HB	1:D:69:VAL:CG2	2.40	0.49
1:D:266:ASN:N	1:D:266:ASN:ND2	2.40	0.49
1:I:330:LYS:HG3	1:I:330:LYS:O	2.13	0.49
1:J:89:LYS:HZ2	1:J:140:CYS:HB3	1.78	0.49
1:A:235:LEU:CD1	1:B:276:LYS:HE2	2.42	0.49
1:B:69:VAL:CG2	1:B:70:LEU:H	2.26	0.49
1:C:104:GLU:HG3	1:C:208:PHE:C	2.37	0.49
1:D:239:LYS:HG2	1:D:240:TYR:CD1	2.48	0.49
1:G:124:TYR:HB2	1:G:135:LEU:HB2	1.95	0.49
1:I:107:LEU:HD22	1:I:182:ILE:HD13	1.93	0.49
1:I:172:GLU:HG2	1:I:320:MET:HE1	1.93	0.49
1:J:198:ARG:HG2	1:J:201:ALA:N	2.27	0.49
1:K:247:TRP:HB2	1:K:313:ARG:NH1	2.28	0.49
1:L:266:ASN:HB2	1:L:278:ARG:HH22	1.77	0.49
1:A:97:ASP:HB3	1:A:132:LYS:O	2.13	0.49
1:A:280:ARG:NH1	1:C:235:LEU:HD13	2.28	0.49
1:B:202:ILE:CD1	1:B:204:LYS:HE2	2.30	0.49
1:C:110:ARG:HD2	1:H:130:GLY:O	2.13	0.49
1:F:145:GLU:HG2	1:F:193:LEU:HD22	1.95	0.49
1:K:66:THR:OG1	1:K:69:VAL:HG13	2.12	0.49
1:K:160:GLU:HB3	1:K:336:LEU:HD11	1.95	0.49
1:A:304:ASN:OD1	1:A:304:ASN:C	2.56	0.49
1:C:264:TYR:CE1	2:C:2:PDY:C24	2.96	0.49
1:D:65:VAL:CG1	1:D:70:LEU:HD13	2.42	0.49
1:E:70:LEU:HD23	1:E:94:MET:CE	2.43	0.49
1:F:83:ASN:OD1	1:F:84:LYS:N	2.46	0.49
1:G:58:ALA:HB1	1:G:60:ILE:HG13	1.94	0.49
1:K:118:VAL:HG11	1:K:206:THR:HG22	1.94	0.49
1:K:274:GLY:O	1:K:278:ARG:HG3	2.12	0.49
1:A:116:HIS:O	1:A:204:LYS:HA	2.12	0.48
1:B:190:GLU:CD	1:B:190:GLU:H	2.20	0.48
1:C:161:ARG:HB2	1:C:332:PRO:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LYS:HZ2	1:D:79:LEU:HD21	1.75	0.48
1:G:153:ARG:HB3	1:G:339:SER:OG	2.13	0.48
2:G:2:PDY:C14	2:G:2:PDY:C13	2.90	0.48
1:H:129:ALA:CB	1:H:131:ARG:HD3	2.34	0.48
1:I:264:TYR:CZ	2:I:2:PDY:H24	2.48	0.48
1:K:188:LYS:NZ	1:K:190:GLU:CG	2.75	0.48
1:L:116:HIS:O	1:L:204:LYS:HA	2.12	0.48
1:D:162:GLU:O	1:D:166:ILE:HG13	2.13	0.48
1:E:332:PRO:HG2	1:E:334:THR:CG2	2.43	0.48
1:F:148:SER:HA	1:F:151:GLN:HG2	1.96	0.48
1:G:66:THR:HG23	1:G:68:GLN:HG2	1.95	0.48
1:G:188:LYS:HD3	1:I:229:TYR:CE1	2.48	0.48
1:I:69:VAL:HG13	1:I:79:LEU:CB	2.43	0.48
1:I:108:HIS:HE1	1:I:138:MET:CE	2.23	0.48
1:K:105:VAL:HG21	1:K:134:LEU:HD23	1.95	0.48
1:L:77:LYS:HE3	1:L:79:LEU:CD2	2.42	0.48
1:L:331:VAL:HG23	1:L:332:PRO:HD2	1.95	0.48
1:B:52:LEU:CD2	1:B:105:VAL:HG12	2.43	0.48
1:B:65:VAL:HG12	1:B:70:LEU:CD1	2.43	0.48
1:D:74:ILE:HG13	1:D:128:TYR:CE2	2.48	0.48
1:D:151:GLN:HE21	1:D:343:LYS:HA	1.77	0.48
1:F:70:LEU:O	1:F:74:ILE:HD13	2.14	0.48
1:G:66:THR:HG21	1:G:68:GLN:OE1	2.13	0.48
1:G:264:TYR:C	1:G:264:TYR:HD2	2.21	0.48
1:H:69:VAL:HG13	1:H:70:LEU:N	2.28	0.48
1:J:73:GLY:N	1:J:79:LEU:HD11	2.29	0.48
1:K:56:LYS:NZ	1:K:125:GLU:OE1	2.46	0.48
1:L:295:SER:OG	1:L:298:VAL:HG23	2.13	0.48
1:L:301:LEU:HD13	1:L:322:HIS:CD2	2.48	0.48
1:A:233:GLU:HG2	1:B:310:PRO:HD3	1.95	0.48
1:B:48:VAL:HB	1:L:70:LEU:CD2	2.42	0.48
1:C:52:LEU:HG	1:C:53:GLN:N	2.28	0.48
1:E:298:VAL:HG22	1:E:324:TRP:NE1	2.28	0.48
1:G:290:GLU:OE2	1:G:337:HIS:HD2	1.96	0.48
1:G:295:SER:O	1:G:299:LYS:HG3	2.13	0.48
1:H:86:THR:C	1:H:88:GLU:H	2.19	0.48
1:J:83:ASN:O	1:J:87:GLN:HA	2.13	0.48
1:L:108:HIS:HE1	1:L:138:MET:HE3	1.78	0.48
1:C:192:LEU:C	1:C:193:LEU:HD23	2.38	0.48
1:E:66:THR:CG2	1:E:69:VAL:HG13	2.44	0.48
1:E:232:PRO:C	1:E:234:VAL:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:THR:HG23	1:G:216:SER:N	2.29	0.48
1:K:70:LEU:O	1:K:74:ILE:HG12	2.13	0.48
1:A:230:VAL:O	1:A:230:VAL:HG13	2.14	0.48
1:B:260:TYR:OH	1:B:290:GLU:HG3	2.13	0.48
1:C:190:GLU:H	1:C:190:GLU:CD	2.21	0.48
1:G:145:GLU:HG2	1:G:193:LEU:HD21	1.94	0.48
1:G:264:TYR:C	1:G:275:MET:HG3	2.38	0.48
1:H:116:HIS:HB3	1:H:173:ALA:HB2	1.95	0.48
1:J:69:VAL:HA	1:J:79:LEU:HD13	1.95	0.48
1:B:49:LYS:HG3	1:B:50:SER:N	2.28	0.48
1:B:114:CYS:HB2	1:B:176:TYR:CD2	2.49	0.48
1:C:167:MET:HG3	1:C:253:MET:HE2	1.95	0.48
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.96	0.48
1:J:311:THR:HG22	1:L:309:GLU:CD	2.38	0.48
1:J:340:ARG:O	1:J:343:LYS:HD3	2.14	0.48
1:A:85:ARG:HG2	1:A:85:ARG:NH1	2.28	0.48
1:B:242:LYS:O	1:B:245:ASP:HB2	2.13	0.48
1:D:157:ALA:O	1:D:159:THR:HG23	2.13	0.48
1:E:323:PRO:HA	1:E:327:GLN:NE2	2.28	0.48
1:F:86:THR:HG22	1:F:87:GLN:N	2.29	0.48
1:F:149:ARG:NH1	1:F:196:SER:O	2.44	0.48
1:H:66:THR:H	1:H:69:VAL:CG1	2.26	0.48
1:H:77:LYS:HD3	1:H:79:LEU:HD21	1.96	0.48
1:H:110:ARG:HD3	1:J:127:LEU:HD11	1.96	0.48
1:H:129:ALA:C	1:H:131:ARG:H	2.20	0.48
1:H:164:SER:HB3	1:H:328:SER:HB3	1.95	0.48
1:H:337:HIS:CG	1:H:340:ARG:NH1	2.82	0.48
1:I:83:ASN:OD1	1:I:84:LYS:N	2.47	0.48
1:I:285:GLU:C	1:I:287:PRO:HD3	2.39	0.48
1:J:65:VAL:HG12	1:J:70:LEU:HD22	1.96	0.48
1:J:159:THR:HG23	1:J:333:GLN:CA	2.42	0.48
1:J:326:MET:HA	1:J:326:MET:HE3	1.95	0.48
1:K:327:GLN:HG2	1:K:330:LYS:NZ	2.29	0.48
1:B:80:GLN:CD	2:B:1:PDY:H24A	2.39	0.48
1:B:85:ARG:HD2	1:B:86:THR:CG2	2.38	0.48
1:B:110:ARG:NH2	1:B:213:GLU:OE2	2.47	0.48
1:G:60:ILE:C	1:G:60:ILE:HD12	2.39	0.48
1:I:56:LYS:O	1:K:51:GLY:N	2.44	0.48
1:J:57:ASN:H	1:J:57:ASN:HD22	1.61	0.48
1:K:161:ARG:NH2	1:K:333:GLN:HG3	2.29	0.48
1:L:82:PHE:CE1	1:L:89:LYS:HB2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ALA:HB1	1:B:233:GLU:CG	2.43	0.48
1:B:289:PRO:O	1:B:290:GLU:C	2.57	0.48
1:G:156:GLN:HG3	1:G:335:PRO:CB	2.44	0.48
1:I:172:GLU:HG2	1:I:320:MET:CE	2.44	0.48
1:J:311:THR:O	1:L:312:GLN:NE2	2.47	0.48
1:K:159:THR:C	1:K:161:ARG:H	2.22	0.48
1:C:253:MET:HE1	1:C:319:PHE:CE1	2.48	0.47
1:H:55:LYS:HD3	1:H:124:TYR:CE2	2.49	0.47
1:H:154:GLY:C	1:H:156:GLN:H	2.22	0.47
1:I:261:PRO:HG3	2:I:2:PDY:H25	1.95	0.47
1:K:56:LYS:NZ	1:K:125:GLU:CD	2.71	0.47
1:B:64:LYS:HE3	1:B:84:LYS:HE3	1.96	0.47
1:C:106:GLU:OE2	1:H:132:LYS:HE2	2.13	0.47
1:C:300:MET:SD	1:C:303:ARG:NH2	2.86	0.47
1:E:97:ASP:H	1:E:133:CYS:HA	1.80	0.47
1:H:125:GLU:OE2	1:H:132:LYS:HE3	2.14	0.47
1:I:149:ARG:HG3	1:I:194:TYR:CD2	2.49	0.47
1:I:207:ASP:OD2	2:I:1:PDY:N12	2.43	0.47
1:B:59:ILE:HG13	1:B:124:TYR:CE1	2.50	0.47
1:B:330:LYS:O	1:B:330:LYS:HG3	2.14	0.47
2:E:2:PDY:H14A	2:E:2:PDY:C19	2.40	0.47
1:L:296:GLU:O	1:L:300:MET:HB2	2.14	0.47
1:B:266:ASN:OD1	1:B:266:ASN:C	2.56	0.47
1:B:326:MET:O	1:B:326:MET:HG3	2.14	0.47
1:D:70:LEU:HD21	1:I:48:VAL:HG11	1.95	0.47
1:F:48:VAL:O	1:F:48:VAL:HG13	2.13	0.47
1:G:73:GLY:N	1:G:79:LEU:HD11	2.29	0.47
1:G:118:VAL:HG23	1:G:139:GLU:HG2	1.96	0.47
1:G:185:ARG:HD3	1:G:241:ASP:OD2	2.14	0.47
1:I:86:THR:C	1:I:88:GLU:H	2.22	0.47
1:J:83:ASN:OD1	1:J:85:ARG:N	2.46	0.47
1:K:172:GLU:HG3	1:K:320:MET:HE1	1.96	0.47
2:K:1:PDY:H24	2:K:1:PDY:H20	1.43	0.47
1:L:70:LEU:HD12	1:L:94:MET:HE1	1.96	0.47
1:B:278:ARG:HG2	1:B:283:GLN:HG3	1.95	0.47
1:C:327:GLN:NE2	1:C:330:LYS:NZ	2.61	0.47
1:E:56:LYS:O	1:L:50:SER:HB2	2.15	0.47
1:F:160:GLU:O	1:F:163:ALA:HB3	2.14	0.47
1:F:235:LEU:HD23	1:F:235:LEU:N	2.29	0.47
1:G:90:PHE:HE2	1:G:121:VAL:HG21	1.77	0.47
1:G:231:ALA:HB3	1:G:234:VAL:CG2	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:GLU:O	1:H:166:ILE:HG13	2.15	0.47
1:I:254:TYR:CD1	1:I:262:PRO:HD3	2.48	0.47
1:L:70:LEU:CD1	1:L:94:MET:HE1	2.44	0.47
1:A:66:THR:HG22	1:A:69:VAL:HG13	1.96	0.47
1:B:82:PHE:HA	1:B:88:GLU:O	2.15	0.47
1:C:60:ILE:O	1:C:84:LYS:HE3	2.15	0.47
1:D:276:LYS:HB2	1:D:276:LYS:HE3	1.45	0.47
1:E:231:ALA:HB1	1:E:233:GLU:CD	2.39	0.47
1:F:272:SER:HB3	1:F:275:MET:H	1.79	0.47
1:G:49:LYS:HG2	1:G:50:SER:N	2.30	0.47
1:G:69:VAL:HG23	1:G:70:LEU:N	2.30	0.47
1:G:198:ARG:HG3	1:G:201:ALA:N	2.30	0.47
2:G:1:PDY:C14	2:G:1:PDY:C13	2.92	0.47
1:H:340:ARG:HG3	1:H:341:VAL:H	1.80	0.47
1:I:168:LYS:O	1:I:168:LYS:HG3	2.14	0.47
1:J:336:LEU:C	1:J:338:THR:H	2.23	0.47
1:A:185:ARG:HE	1:A:212:LYS:HG3	1.79	0.47
1:C:327:GLN:HG2	1:C:330:LYS:HD3	1.97	0.47
1:D:266:ASN:ND2	1:D:267:HIS:HD2	2.11	0.47
1:E:86:THR:O	1:E:87:GLN:HB2	2.13	0.47
1:F:86:THR:HG22	1:F:88:GLU:N	2.23	0.47
1:G:145:GLU:HG2	1:G:193:LEU:CD2	2.45	0.47
2:H:1:PDY:C18	2:H:1:PDY:H14	2.38	0.47
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.50	0.47
1:F:322:HIS:ND1	1:F:323:PRO:HD2	2.30	0.47
1:K:288:ASN:H	1:K:288:ASN:ND2	2.11	0.47
1:L:161:ARG:O	1:L:165:GLU:HG3	2.15	0.47
1:A:185:ARG:HD3	1:A:241:ASP:HB3	1.97	0.47
1:C:129:ALA:O	1:C:131:ARG:HD3	2.14	0.47
1:C:154:GLY:HA2	1:C:155:ASP:HB3	1.97	0.47
1:C:330:LYS:NZ	1:C:330:LYS:HB2	2.28	0.47
1:D:307:LYS:HB2	1:D:313:ARG:HG3	1.97	0.47
1:G:102:ARG:HH22	1:G:125:GLU:CD	2.23	0.47
1:G:281:MET:HE3	1:I:317:THR:OG1	2.15	0.47
1:I:307:LYS:HB2	1:I:313:ARG:CG	2.45	0.47
1:J:70:LEU:HA	1:J:94:MET:CE	2.44	0.47
1:A:276:LYS:CG	1:C:235:LEU:HD11	2.45	0.47
2:A:2:PDY:H14A	2:A:2:PDY:H17	1.97	0.47
1:B:166:ILE:O	1:B:170:ILE:HG13	2.15	0.47
1:D:140:CYS:SG	2:D:1:PDY:H17	2.55	0.47
1:E:310:PRO:O	1:E:313:ARG:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:GLU:O	1:G:146:LEU:C	2.57	0.47
1:G:229:TYR:CD1	1:H:251:VAL:HG11	2.47	0.47
1:L:89:LYS:HE2	1:L:142:ASP:OD2	2.15	0.47
1:L:215:THR:HG23	1:L:216:SER:N	2.29	0.47
1:E:261:PRO:HD3	2:E:2:PDY:H22A	1.97	0.46
1:F:156:GLN:CA	1:F:156:GLN:NE2	2.76	0.46
1:H:199:PRO:HG2	1:H:200:ASN:HD22	1.80	0.46
1:I:124:TYR:HB2	1:I:135:LEU:HB2	1.97	0.46
1:J:116:HIS:HE1	1:J:169:SER:OG	1.97	0.46
1:J:327:GLN:HG2	1:J:330:LYS:CD	2.41	0.46
1:B:233:GLU:OE2	1:C:313:ARG:NH1	2.44	0.46
1:D:151:GLN:NE2	1:D:343:LYS:HA	2.31	0.46
1:D:301:LEU:CD1	1:D:314:MET:HE1	2.45	0.46
1:E:72:LEU:HB3	1:E:79:LEU:HD11	1.98	0.46
1:E:102:ARG:NH2	1:E:125:GLU:OE1	2.49	0.46
1:G:262:PRO:HG2	1:G:263:PHE:CD1	2.50	0.46
1:L:183:ALA:O	1:L:211:ALA:HA	2.15	0.46
1:A:86:THR:O	1:A:86:THR:HG22	2.14	0.46
1:A:327:GLN:HG2	1:A:330:LYS:HD3	1.97	0.46
2:A:2:PDY:C17	2:A:2:PDY:C14	2.93	0.46
2:C:1:PDY:C18	2:C:1:PDY:H14	2.42	0.46
1:F:266:ASN:C	1:F:268:GLY:N	2.73	0.46
1:G:138:MET:HE3	1:G:138:MET:HB2	1.87	0.46
1:I:55:LYS:HD3	1:I:124:TYR:CE2	2.49	0.46
1:I:167:MET:HG3	1:I:253:MET:HG2	1.97	0.46
1:K:59:ILE:HA	1:K:124:TYR:CE2	2.51	0.46
1:K:185:ARG:NH2	1:K:212:LYS:HG3	2.25	0.46
1:D:80:GLN:HB2	2:D:1:PDY:H24A	1.97	0.46
1:E:187:VAL:HG12	1:E:252:ILE:HD11	1.97	0.46
1:H:322:HIS:HD2	1:H:324:TRP:N	2.06	0.46
1:I:202:ILE:HD12	1:I:203:LEU:N	2.30	0.46
1:J:252:ILE:C	1:J:254:TYR:H	2.23	0.46
1:K:72:LEU:HB3	1:K:77:LYS:HB3	1.96	0.46
1:K:77:LYS:HB3	1:K:79:LEU:HD21	1.98	0.46
1:K:257:LEU:HD11	1:K:298:VAL:HG11	1.98	0.46
1:K:281:MET:CB	1:K:283:GLN:HG3	2.45	0.46
1:A:180:ILE:HG22	1:F:130:GLY:HA3	1.97	0.46
1:A:331:VAL:HG23	1:A:332:PRO:HD2	1.97	0.46
1:F:98:CYS:HB2	1:F:99:PRO:CD	2.45	0.46
1:H:135:LEU:HD12	1:H:135:LEU:N	2.30	0.46
1:J:57:ASN:H	1:J:57:ASN:ND2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:70:LEU:O	1:J:94:MET:HE1	2.16	0.46
1:L:286:PHE:CE1	1:L:299:LYS:HB3	2.51	0.46
1:C:70:LEU:HD12	1:C:70:LEU:N	2.30	0.46
1:C:153:ARG:HD3	1:C:156:GLN:NE2	2.30	0.46
1:H:160:GLU:O	1:H:163:ALA:HB3	2.16	0.46
1:H:304:ASN:OD1	1:H:314:MET:HE3	2.15	0.46
1:H:337:HIS:HA	1:H:340:ARG:HH11	1.79	0.46
1:I:286:PHE:CB	1:I:299:LYS:HE2	2.46	0.46
2:A:1:PDY:H14A	2:A:1:PDY:H18	1.96	0.46
1:B:74:ILE:HG23	1:B:94:MET:CE	2.46	0.46
1:C:187:VAL:HG22	1:C:205:LEU:HD11	1.98	0.46
1:D:288:ASN:OD1	1:D:292:SER:HB3	2.16	0.46
1:E:161:ARG:O	1:E:165:GLU:HG3	2.15	0.46
1:G:65:VAL:HG12	1:G:70:LEU:CD2	2.46	0.46
1:I:327:GLN:HE21	1:I:330:LYS:HZ1	1.60	0.46
1:J:314:MET:CG	1:J:318:GLU:HB2	2.46	0.46
1:K:197:LYS:HD2	1:K:197:LYS:HA	1.77	0.46
1:L:79:LEU:O	1:L:91:ALA:HA	2.16	0.46
1:L:97:ASP:CG	1:L:102:ARG:HH21	2.24	0.46
1:C:70:LEU:N	1:C:70:LEU:CD1	2.79	0.46
1:F:147:PHE:HE1	1:F:189:PRO:HG3	1.80	0.46
1:G:275:MET:HE3	1:G:279:ILE:HD11	1.98	0.46
1:H:118:VAL:HG21	2:H:1:PDY:H11	1.97	0.46
1:H:251:VAL:HG13	1:H:262:PRO:HD2	1.97	0.46
1:K:121:VAL:C	1:K:122:ASP:OD1	2.59	0.46
1:A:202:ILE:HD12	1:A:203:LEU:N	2.31	0.46
1:B:95:LEU:O	1:B:133:CYS:HB2	2.16	0.46
1:B:188:LYS:NZ	1:B:190:GLU:HB2	2.31	0.46
1:D:66:THR:HG21	1:D:68:GLN:CG	2.46	0.46
1:D:233:GLU:HG2	1:E:310:PRO:CG	2.43	0.46
1:F:70:LEU:CA	1:F:94:MET:HE1	2.37	0.46
1:I:327:GLN:HE21	1:I:330:LYS:HZ2	1.61	0.46
1:J:122:ASP:N	1:J:122:ASP:OD1	2.47	0.46
1:J:166:ILE:O	1:J:169:SER:HB3	2.15	0.46
1:L:264:TYR:CB	2:L:2:PDY:H17	2.34	0.46
1:C:241:ASP:O	1:C:244:CYS:HB3	2.16	0.46
1:F:147:PHE:CD1	1:F:189:PRO:HB3	2.51	0.46
1:F:310:PRO:O	1:F:313:ARG:HB2	2.16	0.46
1:H:275:MET:HE3	1:H:275:MET:HB3	1.71	0.46
1:J:155:ASP:OD2	1:J:340:ARG:HG3	2.16	0.46
1:K:55:LYS:HE2	1:K:57:ASN:HD21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:HG2	1:A:334:THR:CG2	2.47	0.45
1:B:156:GLN:OE1	1:B:156:GLN:N	2.49	0.45
1:C:121:VAL:O	1:C:122:ASP:HB3	2.16	0.45
1:C:215:THR:HG23	1:C:216:SER:N	2.30	0.45
1:G:125:GLU:O	1:G:126:ASN:ND2	2.43	0.45
1:I:97:ASP:HB2	1:I:134:LEU:HD13	1.98	0.45
1:J:48:VAL:O	1:J:48:VAL:HG13	2.16	0.45
1:L:336:LEU:C	1:L:338:THR:H	2.23	0.45
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.46	0.45
1:C:145:GLU:HG2	1:C:193:LEU:CD2	2.47	0.45
1:C:327:GLN:O	1:C:329:THR:N	2.43	0.45
1:E:128:TYR:CD1	1:L:48:VAL:HG23	2.49	0.45
1:I:183:ALA:O	1:I:211:ALA:HA	2.16	0.45
1:J:153:ARG:O	1:J:154:GLY:C	2.59	0.45
1:K:80:GLN:HE21	2:K:1:PDY:H24	1.80	0.45
1:C:83:ASN:HD22	1:C:86:THR:HB	1.82	0.45
1:C:188:LYS:HE3	1:C:191:ASN:ND2	2.31	0.45
1:E:338:THR:HG22	1:E:342:LEU:CD2	2.46	0.45
1:H:202:ILE:HD11	1:H:204:LYS:HE2	1.98	0.45
1:I:185:ARG:NH2	1:I:212:LYS:HG3	2.32	0.45
1:I:286:PHE:HB3	1:I:299:LYS:HE2	1.98	0.45
1:B:160:GLU:O	1:B:163:ALA:HB3	2.17	0.45
1:D:66:THR:HG21	1:D:68:GLN:HG3	1.97	0.45
1:D:322:HIS:ND1	1:D:323:PRO:HD2	2.31	0.45
1:E:66:THR:HG22	1:E:69:VAL:HG22	1.99	0.45
1:G:264:TYR:CE1	2:G:2:PDY:H24A	2.52	0.45
1:I:77:LYS:HD3	1:I:77:LYS:HA	1.79	0.45
1:J:186:ASP:OD1	1:J:188:LYS:HE3	2.16	0.45
1:J:278:ARG:HG3	1:J:283:GLN:NE2	2.31	0.45
1:A:52:LEU:HD21	1:A:105:VAL:HG12	1.98	0.45
1:A:185:ARG:NH2	1:A:212:LYS:HG3	2.31	0.45
1:A:298:VAL:O	1:A:302:ILE:HG13	2.16	0.45
1:B:151:GLN:HB2	1:B:342:LEU:HB3	1.99	0.45
1:C:309:GLU:HB3	1:C:312:GLN:HG3	1.98	0.45
1:D:97:ASP:OD1	1:D:102:ARG:NE	2.42	0.45
1:D:97:ASP:HA	1:D:134:LEU:HD22	1.99	0.45
1:D:111:ALA:HB1	1:D:117:ILE:HD13	1.98	0.45
1:D:301:LEU:HD13	1:D:314:MET:HE1	1.98	0.45
1:H:67:SER:O	1:H:69:VAL:N	2.49	0.45
1:K:64:LYS:HE2	1:K:84:LYS:HZ2	1.82	0.45
1:L:188:LYS:HE2	1:L:190:GLU:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD21	1:A:105:VAL:CG1	2.46	0.45
1:A:69:VAL:HB	1:A:79:LEU:HD12	1.98	0.45
1:E:188:LYS:NZ	1:E:190:GLU:CG	2.79	0.45
1:H:94:MET:O	1:H:95:LEU:HD23	2.17	0.45
1:I:69:VAL:HG13	1:I:79:LEU:HD22	1.98	0.45
1:K:160:GLU:O	1:K:160:GLU:HG3	2.17	0.45
1:L:100:LYS:O	1:L:103:ARG:HB3	2.17	0.45
1:L:159:THR:HB	1:L:162:GLU:H	1.81	0.45
1:L:161:ARG:HD2	1:L:328:SER:O	2.16	0.45
1:L:231:ALA:HB1	1:L:233:GLU:OE2	2.17	0.45
1:L:298:VAL:HG22	1:L:324:TRP:CD1	2.52	0.45
1:A:65:VAL:HG12	1:A:70:LEU:HG	1.97	0.45
1:D:188:LYS:NZ	1:D:190:GLU:HG3	2.32	0.45
1:E:253:MET:HE1	1:E:319:PHE:HE1	1.82	0.45
1:F:260:TYR:CB	2:F:2:PDY:H19	2.47	0.45
1:H:233:GLU:H	1:H:233:GLU:HG3	1.35	0.45
1:J:240:TYR:HD2	1:J:240:TYR:HA	1.68	0.45
1:J:316:ILE:HG23	1:J:317:THR:N	2.31	0.45
1:K:232:PRO:C	1:K:234:VAL:N	2.73	0.45
1:K:310:PRO:HB3	1:L:233:GLU:OE1	2.17	0.45
1:L:249:LEU:HD12	1:L:249:LEU:HA	1.76	0.45
1:A:300:MET:SD	1:A:303:ARG:NH2	2.79	0.45
1:B:124:TYR:HB2	1:B:135:LEU:HB2	1.98	0.45
1:C:49:LYS:HB2	1:C:113:GLN:NE2	2.32	0.45
1:C:161:ARG:NH1	1:C:333:GLN:CG	2.80	0.45
1:G:118:VAL:HG21	2:G:1:PDY:H11	1.99	0.45
1:G:188:LYS:HB3	1:I:229:TYR:CD1	2.52	0.45
1:H:49:LYS:HB2	1:J:127:LEU:HB2	1.97	0.45
1:J:155:ASP:CG	1:J:156:GLN:HE22	2.25	0.45
1:K:313:ARG:HH22	1:L:233:GLU:CD	2.25	0.45
1:B:70:LEU:O	1:B:74:ILE:HG13	2.16	0.45
1:B:327:GLN:NE2	1:B:330:LYS:NZ	2.65	0.45
1:C:60:ILE:C	1:C:60:ILE:CD1	2.90	0.45
1:C:327:GLN:HB2	1:C:330:LYS:NZ	2.32	0.45
1:F:265:SER:HB3	1:F:268:GLY:HA2	1.98	0.45
1:H:158:PHE:HZ	1:H:166:ILE:HD12	1.82	0.45
1:H:298:VAL:HG22	1:H:324:TRP:CD1	2.52	0.45
1:A:309:GLU:HG2	1:C:311:THR:HG22	1.98	0.45
1:C:229:TYR:N	1:C:229:TYR:CD2	2.85	0.45
1:D:57:ASN:ND2	1:D:57:ASN:H	2.14	0.45
1:D:178:HIS:CG	1:D:242:LYS:HG2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:VAL:HG23	1:F:234:VAL:HG11	1.97	0.45
1:G:215:THR:OG1	1:G:216:SER:N	2.50	0.45
1:G:305:LEU:O	1:G:313:ARG:HD3	2.16	0.45
1:H:90:PHE:CE2	1:H:121:VAL:HG21	2.51	0.45
2:I:1:PDY:C14	2:I:1:PDY:C13	2.95	0.45
1:J:160:GLU:O	1:J:163:ALA:HB3	2.16	0.45
1:L:155:ASP:O	1:L:155:ASP:CG	2.60	0.45
1:L:344:GLU:OE1	1:L:344:GLU:N	2.50	0.45
1:C:145:GLU:HG2	1:C:193:LEU:HD22	1.99	0.44
1:D:167:MET:HE2	1:D:253:MET:CE	2.42	0.44
1:E:95:LEU:O	1:E:133:CYS:HB2	2.16	0.44
1:F:125:GLU:OE2	1:F:132:LYS:HD2	2.17	0.44
1:A:88:GLU:HG2	1:A:89:LYS:N	2.31	0.44
1:C:233:GLU:H	1:C:233:GLU:HG3	1.47	0.44
1:E:80:GLN:CD	2:E:1:PDY:H24A	2.41	0.44
1:E:100:LYS:HE2	1:E:100:LYS:HB2	1.84	0.44
1:E:155:ASP:OD2	1:E:155:ASP:N	2.49	0.44
1:E:213:GLU:HB3	1:E:215:THR:HG22	2.00	0.44
1:F:49:LYS:HD3	1:F:113:GLN:HG2	1.99	0.44
1:F:343:LYS:C	1:F:345:ASP:H	2.25	0.44
1:H:202:ILE:HD11	1:H:204:LYS:CE	2.47	0.44
1:H:342:LEU:HD12	1:H:342:LEU:HA	1.84	0.44
1:I:145:GLU:HG2	1:I:193:LEU:CD2	2.47	0.44
1:J:338:THR:O	1:J:342:LEU:HB2	2.17	0.44
1:L:259:GLY:HA3	1:L:341:VAL:HG11	1.98	0.44
1:A:69:VAL:HB	1:A:79:LEU:HD13	1.98	0.44
1:A:161:ARG:HB3	1:A:333:GLN:NE2	2.31	0.44
2:A:2:PDY:H17	2:A:2:PDY:C3	2.47	0.44
1:E:275:MET:HA	1:E:278:ARG:NH1	2.31	0.44
1:L:258:CYS:HB3	1:L:291:TRP:CZ2	2.52	0.44
2:L:2:PDY:H20	2:L:2:PDY:H24A	1.72	0.44
1:C:71:GLY:O	1:C:74:ILE:HG22	2.18	0.44
1:C:331:VAL:HG23	1:C:332:PRO:HD2	2.00	0.44
1:D:113:GLN:O	1:D:115:PRO:HD3	2.17	0.44
1:D:264:TYR:C	1:D:275:MET:HG3	2.42	0.44
1:G:161:ARG:NH1	1:G:331:VAL:O	2.46	0.44
1:H:192:LEU:C	1:H:193:LEU:HD23	2.42	0.44
1:H:332:PRO:HB2	1:H:334:THR:CG2	2.38	0.44
1:I:246:MET:HE1	1:I:316:ILE:HA	1.99	0.44
1:J:188:LYS:HB2	1:J:189:PRO:CD	2.48	0.44
1:J:254:TYR:CD1	1:J:262:PRO:HG3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:327:GLN:C	1:J:329:THR:H	2.26	0.44
1:K:161:ARG:O	1:K:165:GLU:HG3	2.18	0.44
1:K:188:LYS:HB2	1:K:189:PRO:HD2	1.99	0.44
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.85	0.44
1:A:188:LYS:HB2	1:A:189:PRO:HD2	1.99	0.44
1:A:311:THR:O	1:B:312:GLN:NE2	2.50	0.44
1:C:147:PHE:O	1:C:151:GLN:N	2.50	0.44
1:D:198:ARG:HB3	1:D:200:ASN:OD1	2.18	0.44
1:G:111:ALA:O	1:G:117:ILE:HG13	2.17	0.44
1:G:213:GLU:C	1:G:215:THR:H	2.25	0.44
1:H:97:ASP:H	1:H:133:CYS:HA	1.81	0.44
1:H:233:GLU:OE2	1:I:313:ARG:NH1	2.41	0.44
1:J:58:ALA:O	1:J:61:ASP:OD2	2.36	0.44
1:K:56:LYS:HZ1	1:K:125:GLU:CD	2.26	0.44
1:K:188:LYS:HZ2	1:K:190:GLU:CG	2.30	0.44
1:K:202:ILE:HD12	1:K:203:LEU:H	1.82	0.44
1:B:327:GLN:HE22	1:B:330:LYS:HZ2	1.66	0.44
2:B:2:PDY:C14	2:B:2:PDY:C13	2.95	0.44
1:C:159:THR:C	1:C:336:LEU:HD22	2.42	0.44
1:E:118:VAL:CG1	1:E:138:MET:HE2	2.46	0.44
1:J:311:THR:HG22	1:L:309:GLU:CG	2.48	0.44
1:J:313:ARG:NH2	1:K:233:GLU:HG2	2.14	0.44
1:K:96:GLN:HE22	1:K:131:ARG:CD	2.30	0.44
1:A:97:ASP:H	1:A:133:CYS:HA	1.80	0.44
1:D:185:ARG:HH21	1:D:212:LYS:CG	2.24	0.44
1:E:145:GLU:HG2	1:E:193:LEU:HD23	1.99	0.44
1:F:49:LYS:HB2	1:F:113:GLN:NE2	2.32	0.44
1:H:65:VAL:CG1	1:H:70:LEU:HD13	2.45	0.44
1:K:276:LYS:HE3	1:K:276:LYS:HB2	1.73	0.44
1:K:302:ILE:C	1:K:304:ASN:N	2.75	0.44
1:L:196:SER:C	1:L:198:ARG:H	2.26	0.44
1:A:97:ASP:OD2	1:A:102:ARG:NH2	2.33	0.44
1:B:58:ALA:HB1	1:B:60:ILE:HG13	2.00	0.44
1:D:148:SER:HA	1:D:151:GLN:HG2	2.00	0.44
1:D:309:GLU:OE2	1:D:310:PRO:HD2	2.18	0.44
1:E:112:SER:O	1:E:113:GLN:C	2.60	0.44
1:F:233:GLU:HG2	1:F:234:VAL:N	2.33	0.44
1:G:81:ILE:HD13	1:G:92:LEU:HB2	1.99	0.44
1:H:158:PHE:O	1:H:336:LEU:HB2	2.17	0.44
1:H:200:ASN:HD22	1:H:200:ASN:H	1.63	0.44
1:I:285:GLU:O	1:I:287:PRO:HD3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:304:ASN:O	1:I:307:LYS:HG2	2.18	0.44
1:K:103:ARG:NH1	1:K:212:LYS:HE2	2.33	0.44
1:K:165:GLU:O	1:K:168:LYS:HB3	2.17	0.44
1:L:336:LEU:HD22	1:L:336:LEU:N	2.32	0.44
1:B:80:GLN:NE2	2:B:1:PDY:H24A	2.32	0.44
1:E:168:LYS:HG3	1:E:320:MET:HE1	1.98	0.44
1:E:229:TYR:CE1	1:F:188:LYS:HG2	2.53	0.44
1:F:97:ASP:HA	1:F:134:LEU:HD22	2.00	0.44
1:G:185:ARG:NH2	1:G:212:LYS:HE2	2.32	0.44
1:H:161:ARG:O	1:H:165:GLU:HG3	2.17	0.44
1:H:264:TYR:HB2	2:H:2:PDY:C17	2.47	0.44
1:I:121:VAL:HB	1:I:137:VAL:O	2.17	0.44
1:L:108:HIS:CE1	1:L:138:MET:HE3	2.53	0.44
1:L:145:GLU:HG2	1:L:193:LEU:CD2	2.48	0.44
1:A:233:GLU:H	1:A:233:GLU:HG3	1.50	0.43
1:C:65:VAL:HG12	1:C:70:LEU:CD1	2.48	0.43
1:C:90:PHE:CE2	1:C:121:VAL:HG21	2.53	0.43
1:D:70:LEU:HD21	1:I:48:VAL:CG1	2.48	0.43
1:D:161:ARG:HA	1:D:331:VAL:CG2	2.48	0.43
1:D:230:VAL:CG2	1:D:234:VAL:HB	2.47	0.43
1:F:308:THR:HG22	1:F:309:GLU:N	2.33	0.43
1:G:288:ASN:HB3	1:G:289:PRO:HA	1.99	0.43
1:G:328:SER:C	1:G:331:VAL:HG12	2.40	0.43
1:K:167:MET:SD	1:K:256:LEU:HD12	2.58	0.43
1:K:334:THR:HA	1:K:335:PRO:HD3	1.76	0.43
1:L:275:MET:HE2	1:L:275:MET:HB3	1.83	0.43
1:A:190:GLU:CD	1:A:190:GLU:N	2.76	0.43
1:F:234:VAL:C	1:F:235:LEU:HD23	2.44	0.43
1:I:89:LYS:NZ	1:I:142:ASP:OD2	2.48	0.43
1:J:192:LEU:HD11	1:J:252:ILE:HD13	1.99	0.43
1:K:253:MET:HE3	1:K:253:MET:HB2	1.91	0.43
1:L:188:LYS:HD2	1:L:190:GLU:CD	2.44	0.43
1:D:155:ASP:OD1	1:D:156:GLN:HG2	2.18	0.43
1:E:337:HIS:CG	1:E:340:ARG:NH2	2.86	0.43
1:G:70:LEU:H	1:G:70:LEU:HD22	1.83	0.43
1:K:309:GLU:CD	1:K:310:PRO:HD2	2.43	0.43
1:L:215:THR:OG1	1:L:216:SER:N	2.50	0.43
1:L:341:VAL:C	1:L:343:LYS:H	2.26	0.43
1:A:83:ASN:O	1:A:87:GLN:N	2.51	0.43
1:A:130:GLY:O	1:G:110:ARG:HD2	2.17	0.43
1:C:235:LEU:HD13	1:C:235:LEU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:O	1:D:133:CYS:HB2	2.18	0.43
1:D:95:LEU:O	1:D:134:LEU:N	2.48	0.43
1:D:260:TYR:OH	1:D:287:PRO:HG2	2.17	0.43
1:G:337:HIS:ND1	1:G:340:ARG:NH1	2.66	0.43
1:I:98:CYS:HB2	1:I:99:PRO:CD	2.45	0.43
1:L:93:LYS:HB2	1:L:93:LYS:HE3	1.76	0.43
1:A:135:LEU:HD12	1:A:135:LEU:N	2.33	0.43
1:B:56:LYS:O	1:E:50:SER:HB2	2.19	0.43
1:C:96:GLN:HE21	1:C:96:GLN:HB3	1.59	0.43
1:C:260:TYR:HD2	1:C:341:VAL:HG11	1.83	0.43
1:D:57:ASN:H	1:D:57:ASN:HD22	1.66	0.43
1:E:149:ARG:NH1	1:E:196:SER:O	2.51	0.43
1:G:98:CYS:HB2	1:G:99:PRO:CD	2.48	0.43
1:G:278:ARG:HA	1:G:283:GLN:HG2	1.99	0.43
1:J:141:LEU:HD13	1:J:193:LEU:HB2	2.00	0.43
1:L:192:LEU:C	1:L:193:LEU:HD23	2.44	0.43
1:B:264:TYR:CZ	2:B:2:PDY:H24	2.53	0.43
1:C:115:PRO:C	1:C:117:ILE:H	2.27	0.43
1:D:230:VAL:HG22	1:D:234:VAL:HB	1.99	0.43
1:E:249:LEU:HD12	1:E:249:LEU:HA	1.71	0.43
1:J:48:VAL:O	1:J:48:VAL:HG22	2.18	0.43
1:K:58:ALA:HB1	1:K:60:ILE:HG13	2.00	0.43
1:L:94:MET:HE2	1:L:135:LEU:CD2	2.49	0.43
1:L:342:LEU:N	1:L:342:LEU:CD1	2.82	0.43
1:A:253:MET:HE1	1:A:319:PHE:HE1	1.83	0.43
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.54	0.43
1:A:337:HIS:ND1	1:A:340:ARG:NH2	2.67	0.43
1:E:246:MET:HB3	1:E:246:MET:HE3	1.75	0.43
1:E:337:HIS:CD2	1:E:340:ARG:HH21	2.36	0.43
2:E:1:PDY:H24	2:E:1:PDY:H20	1.57	0.43
1:F:81:ILE:CD1	1:F:92:LEU:HB2	2.45	0.43
1:H:149:ARG:HG3	1:H:194:TYR:CD2	2.54	0.43
1:I:255:ILE:O	1:I:259:GLY:N	2.46	0.43
1:J:107:LEU:HD21	1:J:213:GLU:HG2	2.00	0.43
1:K:230:VAL:HG13	1:K:231:ALA:N	2.33	0.43
1:K:344:GLU:O	1:K:344:GLU:HG2	2.18	0.43
1:A:63:TYR:HE1	1:A:124:TYR:OH	2.02	0.43
1:B:180:ILE:HG21	1:L:130:GLY:HA3	2.01	0.43
1:B:215:THR:HG22	1:B:216:SER:N	2.33	0.43
1:B:246:MET:CE	1:B:316:ILE:HA	2.49	0.43
2:C:2:PDY:C14	2:C:2:PDY:C13	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ARG:HD2	1:D:200:ASN:OD1	2.19	0.43
1:F:54:ILE:HD13	1:F:102:ARG:NH1	2.34	0.43
1:G:298:VAL:HG22	1:G:324:TRP:CD1	2.54	0.43
1:I:80:GLN:HE21	1:I:80:GLN:HB3	1.61	0.43
1:J:78:VAL:O	1:J:79:LEU:HD23	2.19	0.43
1:J:111:ALA:HB2	1:J:177:LEU:HD21	2.01	0.43
1:J:160:GLU:HG2	1:J:331:VAL:CG2	2.49	0.43
1:J:341:VAL:O	1:J:343:LYS:N	2.47	0.43
1:K:184:HIS:CD2	1:K:205:LEU:HD21	2.54	0.43
1:K:230:VAL:CG2	1:K:231:ALA:H	2.09	0.43
1:A:156:GLN:NE2	1:A:156:GLN:N	2.58	0.43
1:C:111:ALA:HB1	1:C:117:ILE:HD13	2.01	0.43
1:C:121:VAL:O	1:C:122:ASP:CB	2.67	0.43
1:C:172:GLU:HG2	1:C:320:MET:CE	2.49	0.43
1:C:307:LYS:O	1:C:313:ARG:NE	2.50	0.43
1:C:307:LYS:O	1:C:313:ARG:NH2	2.46	0.43
1:D:134:LEU:HD12	1:D:134:LEU:HA	1.87	0.43
1:E:70:LEU:HA	1:E:70:LEU:HD23	1.89	0.43
1:G:69:VAL:O	1:G:70:LEU:C	2.62	0.43
1:H:337:HIS:CG	1:H:340:ARG:HH11	2.37	0.43
1:H:340:ARG:O	1:H:343:LYS:HD3	2.19	0.43
1:I:160:GLU:CA	1:I:336:LEU:HD21	2.49	0.43
1:J:336:LEU:HD22	1:J:336:LEU:N	2.34	0.43
1:B:96:GLN:O	1:B:97:ASP:C	2.62	0.43
1:C:88:GLU:CG	1:C:89:LYS:N	2.79	0.43
1:C:288:ASN:ND2	1:C:288:ASN:N	2.66	0.43
1:D:114:CYS:HB3	1:D:117:ILE:HD12	2.01	0.43
1:E:156:GLN:NE2	1:E:156:GLN:N	2.51	0.43
1:G:156:GLN:O	1:G:335:PRO:HB3	2.19	0.43
1:I:96:GLN:OE1	1:I:131:ARG:HD2	2.19	0.43
1:I:247:TRP:HZ3	1:I:306:LEU:O	2.02	0.43
1:J:252:ILE:C	1:J:254:TYR:N	2.75	0.43
1:K:102:ARG:NH2	1:K:125:GLU:OE1	2.51	0.43
1:K:142:ASP:C	1:K:144:GLY:N	2.76	0.43
1:A:185:ARG:CZ	1:A:212:LYS:HE2	2.49	0.42
1:B:327:GLN:NE2	1:B:330:LYS:HZ2	2.17	0.42
1:D:90:PHE:CE2	1:D:121:VAL:HG21	2.53	0.42
1:D:285:GLU:HB2	1:D:287:PRO:HD3	2.01	0.42
1:E:340:ARG:O	1:E:344:GLU:HG3	2.19	0.42
1:G:156:GLN:HG3	1:G:335:PRO:HB2	2.01	0.42
1:H:189:PRO:HD2	1:H:190:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:VAL:HA	1:I:79:LEU:CD2	2.42	0.42
1:J:186:ASP:HB2	1:J:210:PHE:HD2	1.83	0.42
1:L:80:GLN:CB	2:L:1:PDY:H24A	2.49	0.42
1:L:80:GLN:HA	1:L:90:PHE:O	2.19	0.42
1:L:127:LEU:HD12	1:L:127:LEU:HA	1.85	0.42
1:D:149:ARG:NH1	1:D:197:LYS:HA	2.34	0.42
1:F:49:LYS:NZ	1:F:113:GLN:HG3	2.34	0.42
1:F:327:GLN:O	1:F:328:SER:C	2.62	0.42
1:G:71:GLY:C	1:G:74:ILE:HG22	2.43	0.42
1:H:66:THR:OG1	1:H:69:VAL:HG12	2.20	0.42
1:H:140:CYS:SG	2:H:1:PDY:C17	3.07	0.42
1:K:157:ALA:HB1	1:K:335:PRO:HB3	2.01	0.42
1:L:329:THR:C	1:L:331:VAL:H	2.27	0.42
1:A:247:TRP:CZ2	1:C:232:PRO:HD3	2.54	0.42
1:B:188:LYS:HE3	1:B:191:ASN:ND2	2.35	0.42
1:D:233:GLU:CD	1:E:313:ARG:HH12	2.27	0.42
1:E:97:ASP:OD2	1:E:102:ARG:NH2	2.34	0.42
1:E:187:VAL:HG12	1:E:252:ILE:CD1	2.49	0.42
1:E:332:PRO:HG2	1:E:334:THR:HG22	2.00	0.42
1:H:331:VAL:HB	1:H:332:PRO:HD2	2.01	0.42
2:H:1:PDY:H20	2:H:1:PDY:H24	1.40	0.42
1:J:305:LEU:O	1:J:313:ARG:HD3	2.20	0.42
1:L:68:GLN:O	1:L:72:LEU:HD13	2.19	0.42
1:A:234:VAL:O	1:A:234:VAL:HG12	2.19	0.42
1:A:287:PRO:O	1:A:291:TRP:HB2	2.18	0.42
1:A:327:GLN:CG	1:A:330:LYS:HD3	2.50	0.42
1:B:77:LYS:NZ	1:B:79:LEU:HD23	2.33	0.42
1:F:115:PRO:O	1:F:202:ILE:HD11	2.19	0.42
1:H:151:GLN:HA	1:H:339:SER:OG	2.19	0.42
1:K:72:LEU:HB2	1:K:79:LEU:HD11	2.01	0.42
1:L:176:TYR:O	1:L:180:ILE:HG12	2.20	0.42
1:L:259:GLY:HA3	1:L:341:VAL:CG1	2.49	0.42
1:B:56:LYS:O	1:E:51:GLY:N	2.46	0.42
1:C:98:CYS:SG	1:C:99:PRO:HD2	2.60	0.42
1:C:125:GLU:O	1:C:126:ASN:ND2	2.42	0.42
1:D:77:LYS:HB3	1:D:77:LYS:HZ2	1.84	0.42
2:E:1:PDY:C14	2:E:1:PDY:C13	2.96	0.42
1:F:278:ARG:NH2	3:F:3:SO4:O2	2.53	0.42
1:G:159:THR:C	1:G:336:LEU:HD21	2.45	0.42
1:H:50:SER:O	1:J:127:LEU:HD23	2.19	0.42
1:I:161:ARG:NH2	1:I:333:GLN:CD	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:66:THR:HG23	1:J:69:VAL:H	1.84	0.42
1:A:104:GLU:HG3	1:A:208:PHE:C	2.44	0.42
1:B:108:HIS:HD2	1:B:108:HIS:O	2.03	0.42
1:E:154:GLY:HA2	1:E:155:ASP:HA	1.72	0.42
1:F:49:LYS:CG	1:G:127:LEU:HB2	2.49	0.42
1:F:307:LYS:HG2	1:F:312:GLN:CB	2.49	0.42
1:H:161:ARG:HA	1:H:331:VAL:CG2	2.50	0.42
1:K:98:CYS:C	1:K:100:LYS:N	2.74	0.42
1:K:310:PRO:HG3	1:L:233:GLU:HG2	2.02	0.42
1:B:65:VAL:HG12	1:B:69:VAL:CG2	2.49	0.42
1:D:52:LEU:O	1:K:56:LYS:HE3	2.19	0.42
1:I:60:ILE:HA	1:I:63:TYR:O	2.19	0.42
1:J:161:ARG:CZ	1:J:333:GLN:HG3	2.50	0.42
1:L:343:LYS:N	1:L:344:GLU:OE1	2.53	0.42
1:B:327:GLN:O	1:B:328:SER:C	2.61	0.42
1:C:153:ARG:O	1:C:153:ARG:HG3	2.19	0.42
1:C:327:GLN:HE21	1:C:330:LYS:HE3	1.82	0.42
1:F:238:GLU:O	1:F:239:LYS:C	2.62	0.42
1:F:304:ASN:ND2	1:F:314:MET:HB2	2.35	0.42
1:H:116:HIS:CE1	1:H:169:SER:HB2	2.55	0.42
1:I:341:VAL:O	1:I:342:LEU:C	2.63	0.42
1:J:189:PRO:C	1:J:191:ASN:H	2.26	0.42
1:J:233:GLU:OE2	1:L:313:ARG:NH1	2.53	0.42
1:K:77:LYS:HG2	1:K:79:LEU:CD2	2.49	0.42
2:K:2:PDY:C13	2:K:2:PDY:H14	2.50	0.42
1:B:116:HIS:O	1:B:204:LYS:HA	2.20	0.42
1:C:142:ASP:N	1:C:195:THR:O	2.49	0.42
1:E:143:GLY:O	1:E:149:ARG:HD3	2.19	0.42
1:F:49:LYS:O	1:G:127:LEU:N	2.52	0.42
1:F:300:MET:SD	1:F:303:ARG:NE	2.91	0.42
1:J:128:TYR:O	1:J:129:ALA:HB3	2.19	0.42
1:J:261:PRO:HD3	2:J:2:PDY:H25	2.02	0.42
1:J:327:GLN:HG2	1:J:330:LYS:CG	2.50	0.42
1:K:65:VAL:HG12	1:K:70:LEU:HG	2.00	0.42
1:B:62:ASP:OD2	1:B:62:ASP:N	2.53	0.42
1:B:113:GLN:HE21	1:B:113:GLN:HB3	1.55	0.42
1:D:127:LEU:HD12	1:D:127:LEU:HA	1.91	0.42
1:D:240:TYR:CD1	1:D:240:TYR:N	2.88	0.42
1:E:60:ILE:C	1:E:60:ILE:CD1	2.92	0.42
1:F:58:ALA:O	1:F:61:ASP:HB2	2.20	0.42
1:F:128:TYR:CD2	1:F:128:TYR:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:ASP:HA	1:G:134:LEU:HD22	2.02	0.42
1:H:75:ASN:HD22	1:H:75:ASN:HA	1.66	0.42
1:H:260:TYR:OH	1:H:287:PRO:HG2	2.20	0.42
1:J:233:GLU:CG	1:L:310:PRO:HG3	2.50	0.42
1:K:69:VAL:HG23	1:K:70:LEU:N	2.35	0.42
1:A:52:LEU:HB2	1:A:109:TRP:CD1	2.55	0.41
1:B:241:ASP:O	1:B:244:CYS:HB3	2.19	0.41
1:B:344:GLU:O	1:B:345:ASP:CG	2.63	0.41
1:C:147:PHE:CE2	1:C:256:LEU:HD23	2.47	0.41
1:C:229:TYR:N	1:C:229:TYR:HD2	2.17	0.41
1:E:247:TRP:HZ3	1:E:306:LEU:O	2.03	0.41
1:F:156:GLN:NE2	1:F:156:GLN:N	2.67	0.41
1:J:143:GLY:CA	1:J:149:ARG:NH1	2.83	0.41
1:K:66:THR:N	1:K:69:VAL:HG22	2.33	0.41
1:K:194:TYR:CZ	1:K:203:LEU:HD13	2.55	0.41
1:L:195:THR:OG1	1:L:196:SER:N	2.53	0.41
1:A:113:GLN:HE21	1:A:113:GLN:HB3	1.62	0.41
1:B:105:VAL:HG22	1:B:136:ILE:HD11	2.02	0.41
1:C:50:SER:HB2	1:H:58:ALA:N	2.35	0.41
1:C:253:MET:HE1	1:C:319:PHE:HE1	1.83	0.41
1:E:304:ASN:HA	1:E:307:LYS:HG3	2.01	0.41
1:H:142:ASP:O	1:H:197:LYS:HE3	2.20	0.41
1:I:148:SER:O	1:I:152:ASP:HB2	2.20	0.41
1:I:322:HIS:HA	1:I:323:PRO:HD3	1.94	0.41
1:C:92:LEU:HD12	1:C:93:LYS:H	1.86	0.41
1:E:245:ASP:O	1:E:248:SER:HB2	2.21	0.41
1:F:268:GLY:HA2	1:F:269:LEU:HA	1.70	0.41
1:G:125:GLU:C	1:G:126:ASN:HD22	2.27	0.41
1:H:154:GLY:O	1:H:156:GLN:NE2	2.53	0.41
1:J:141:LEU:HD12	1:J:193:LEU:HB2	2.00	0.41
1:J:188:LYS:HB2	1:J:189:PRO:HD2	2.03	0.41
1:K:275:MET:C	1:K:277:THR:N	2.76	0.41
1:B:246:MET:HE1	1:B:316:ILE:HA	2.03	0.41
1:C:104:GLU:HG3	1:C:208:PHE:O	2.21	0.41
1:D:65:VAL:HG12	1:D:70:LEU:HD13	2.00	0.41
1:D:190:GLU:CD	1:D:190:GLU:N	2.73	0.41
1:E:97:ASP:OD1	1:E:97:ASP:C	2.63	0.41
1:E:147:PHE:HE2	1:E:256:LEU:HD23	1.85	0.41
1:J:172:GLU:HG2	1:J:320:MET:CE	2.51	0.41
1:J:337:HIS:ND1	1:J:337:HIS:N	2.68	0.41
1:K:143:GLY:HA3	1:K:194:TYR:CB	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:LEU:HD11	1:K:252:ILE:HD13	2.02	0.41
1:L:108:HIS:HE1	1:L:138:MET:CE	2.33	0.41
1:B:115:PRO:O	1:B:204:LYS:HD3	2.21	0.41
1:C:127:LEU:HD12	1:C:127:LEU:HA	1.87	0.41
1:C:185:ARG:HH21	1:C:212:LYS:HG3	1.85	0.41
1:G:57:ASN:O	1:G:58:ALA:C	2.63	0.41
1:I:167:MET:HG3	1:I:253:MET:CG	2.49	0.41
1:I:253:MET:HE3	1:I:319:PHE:HE1	1.84	0.41
1:I:258:CYS:HB2	1:I:290:GLU:HG3	2.03	0.41
1:K:260:TYR:CB	2:K:2:PDY:H19	2.50	0.41
1:K:275:MET:O	1:K:278:ARG:N	2.53	0.41
1:L:95:LEU:O	1:L:133:CYS:CB	2.63	0.41
1:L:114:CYS:HB3	1:L:117:ILE:HD12	2.03	0.41
1:B:85:ARG:HH11	1:B:86:THR:HG21	1.84	0.41
1:B:307:LYS:HD3	1:B:307:LYS:HA	1.83	0.41
1:C:188:LYS:HG2	1:C:191:ASN:ND2	2.35	0.41
1:F:49:LYS:HB3	1:G:127:LEU:HB2	2.01	0.41
1:F:60:ILE:HA	1:F:63:TYR:O	2.21	0.41
1:F:167:MET:HE2	1:F:253:MET:HB2	2.02	0.41
1:F:337:HIS:O	1:F:341:VAL:HG23	2.20	0.41
1:H:133:CYS:SG	1:H:135:LEU:HD11	2.60	0.41
1:H:143:GLY:HA2	1:H:197:LYS:CD	2.50	0.41
1:H:340:ARG:O	1:H:343:LYS:HG2	2.20	0.41
1:I:71:GLY:O	1:I:75:ASN:HB2	2.20	0.41
2:I:1:PDY:H14	2:I:1:PDY:C13	2.50	0.41
1:J:260:TYR:OH	1:J:290:GLU:HG3	2.20	0.41
1:J:284:TYR:CD2	1:J:284:TYR:C	2.98	0.41
1:J:322:HIS:ND1	1:J:323:PRO:CD	2.83	0.41
1:K:118:VAL:CG1	1:K:206:THR:HG22	2.51	0.41
1:A:107:LEU:HD22	1:A:182:ILE:HG12	2.02	0.41
1:B:188:LYS:CD	1:B:190:GLU:HB2	2.50	0.41
1:C:71:GLY:C	1:C:74:ILE:HG22	2.46	0.41
1:D:141:LEU:HD13	1:D:193:LEU:HB2	2.03	0.41
1:D:170:ILE:O	1:D:174:ILE:HG12	2.20	0.41
1:E:86:THR:C	1:E:87:GLN:HE21	2.29	0.41
1:E:159:THR:C	1:E:336:LEU:HD22	2.46	0.41
1:E:167:MET:SD	1:E:256:LEU:HD12	2.61	0.41
1:H:314:MET:HG3	1:H:318:GLU:HB2	2.03	0.41
1:I:65:VAL:HG11	1:I:70:LEU:HD21	2.03	0.41
1:I:127:LEU:HD12	1:I:127:LEU:HA	1.87	0.41
1:J:245:ASP:O	1:J:248:SER:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:LEU:HD12	1:L:94:MET:CE	2.51	0.41
1:L:161:ARG:CZ	1:L:333:GLN:NE2	2.84	0.41
1:L:185:ARG:HD3	1:L:241:ASP:OD2	2.20	0.41
1:A:281:MET:HE2	1:C:179:SER:HB3	2.02	0.41
1:C:83:ASN:OD1	1:C:84:LYS:N	2.53	0.41
1:H:231:ALA:HB1	1:H:232:PRO:HD2	2.02	0.41
1:H:337:HIS:CB	1:H:340:ARG:HH11	2.34	0.41
1:I:100:LYS:HG3	1:I:103:ARG:HH21	1.85	0.41
1:J:107:LEU:HD21	1:J:213:GLU:CG	2.50	0.41
1:J:315:THR:OG1	1:J:318:GLU:HG3	2.20	0.41
1:K:151:GLN:HG3	1:K:152:ASP:N	2.36	0.41
1:A:66:THR:HG22	1:A:69:VAL:H	1.86	0.41
1:A:233:GLU:OE2	1:B:313:ARG:CZ	2.69	0.41
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.56	0.41
1:B:301:LEU:HD22	1:B:322:HIS:CE1	2.56	0.41
1:C:65:VAL:HG11	1:C:70:LEU:HD11	2.00	0.41
1:E:177:LEU:HD21	1:E:208:PHE:HE2	1.86	0.41
1:E:212:LYS:HB3	1:E:212:LYS:HE3	1.83	0.41
1:E:328:SER:HA	1:E:331:VAL:HG13	2.03	0.41
1:F:185:ARG:HD3	1:F:241:ASP:CB	2.47	0.41
1:F:233:GLU:C	1:F:235:LEU:N	2.77	0.41
1:F:233:GLU:O	1:F:234:VAL:C	2.63	0.41
1:F:304:ASN:OD1	1:F:304:ASN:O	2.37	0.41
2:F:2:PDY:C14	2:F:2:PDY:C13	2.98	0.41
1:H:85:ARG:O	1:H:86:THR:C	2.64	0.41
1:H:107:LEU:HD22	1:H:182:ILE:CD1	2.51	0.41
1:H:145:GLU:HG2	1:H:193:LEU:HD22	2.03	0.41
1:H:233:GLU:CG	1:I:310:PRO:HG3	2.51	0.41
1:H:281:MET:HB2	1:H:283:GLN:HG3	2.02	0.41
1:I:86:THR:C	1:I:88:GLU:N	2.78	0.41
1:I:90:PHE:CE2	1:I:121:VAL:HG21	2.55	0.41
1:I:139:GLU:O	1:I:139:GLU:HG3	2.20	0.41
1:J:111:ALA:CB	1:J:177:LEU:HD21	2.51	0.41
1:J:301:LEU:HD12	1:J:301:LEU:O	2.20	0.41
1:L:309:GLU:OE2	1:L:310:PRO:HD2	2.21	0.41
1:A:233:GLU:OE2	1:B:310:PRO:HB3	2.21	0.41
1:A:341:VAL:O	1:A:342:LEU:C	2.63	0.41
1:B:52:LEU:HB2	1:B:109:TRP:CG	2.57	0.41
1:C:281:MET:C	1:C:283:GLN:N	2.79	0.41
1:C:332:PRO:HB2	1:C:334:THR:HG22	2.03	0.41
1:G:74:ILE:HG12	1:G:74:ILE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:TYR:O	1:G:129:ALA:C	2.64	0.41
1:J:82:PHE:HA	1:J:88:GLU:O	2.21	0.41
1:K:49:LYS:CD	1:K:50:SER:N	2.78	0.41
1:L:264:TYR:CG	2:L:2:PDY:C17	3.04	0.41
1:L:266:ASN:CB	1:L:278:ARG:NH2	2.82	0.41
1:A:233:GLU:OE2	1:B:313:ARG:NH2	2.54	0.40
1:A:313:ARG:HH22	1:C:233:GLU:CG	2.33	0.40
1:C:86:THR:O	1:C:87:GLN:CB	2.68	0.40
1:C:118:VAL:O	1:C:118:VAL:HG13	2.20	0.40
1:C:151:GLN:NE2	1:C:342:LEU:O	2.54	0.40
1:D:155:ASP:CG	1:D:156:GLN:N	2.78	0.40
1:D:233:GLU:CD	1:E:313:ARG:HH22	2.28	0.40
1:E:69:VAL:HB	1:E:79:LEU:CD1	2.45	0.40
1:E:327:GLN:CD	1:E:330:LYS:NZ	2.79	0.40
1:F:281:MET:CB	1:F:283:GLN:HG3	2.51	0.40
1:F:327:GLN:HG2	1:F:330:LYS:HD2	2.02	0.40
1:H:86:THR:C	1:H:88:GLU:N	2.79	0.40
1:K:151:GLN:HB3	1:K:342:LEU:HB3	2.02	0.40
1:K:190:GLU:CD	1:K:190:GLU:N	2.78	0.40
1:L:186:ASP:O	1:L:191:ASN:ND2	2.53	0.40
1:A:95:LEU:O	1:A:133:CYS:HB2	2.21	0.40
1:A:145:GLU:HG3	1:A:193:LEU:HD23	2.02	0.40
1:A:181:ASN:HD22	1:A:214:THR:HG1	1.68	0.40
1:C:334:THR:HA	1:C:335:PRO:HD3	1.92	0.40
1:F:271:ILE:HD13	1:F:275:MET:HE1	2.04	0.40
1:H:85:ARG:O	1:H:87:GLN:N	2.55	0.40
1:I:264:TYR:CE2	2:I:2:PDY:C20	2.99	0.40
1:I:266:ASN:ND2	1:I:266:ASN:N	2.49	0.40
1:A:327:GLN:OE1	1:A:330:LYS:NZ	2.53	0.40
2:A:1:PDY:C14	2:A:1:PDY:H18	2.49	0.40
1:B:64:LYS:CE	1:B:84:LYS:HE3	2.51	0.40
1:D:149:ARG:HG3	1:D:194:TYR:CD2	2.57	0.40
2:E:1:PDY:C18	2:E:1:PDY:C3	2.78	0.40
1:F:156:GLN:HE21	1:F:156:GLN:N	2.20	0.40
1:G:66:THR:C	1:G:68:GLN:N	2.80	0.40
1:I:80:GLN:OE1	1:I:89:LYS:NZ	2.41	0.40
1:J:60:ILE:C	1:J:60:ILE:CD1	2.93	0.40
1:J:331:VAL:CG2	1:J:332:PRO:HD2	2.51	0.40
2:J:2:PDY:C18	2:J:2:PDY:C3	2.90	0.40
1:K:142:ASP:C	1:K:144:GLY:H	2.29	0.40
1:K:196:SER:H	1:K:201:ALA:HB1	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:334:THR:HA	1:L:335:PRO:HD3	1.87	0.40
1:A:77:LYS:HB3	1:A:79:LEU:HD21	2.04	0.40
1:B:65:VAL:HG12	1:B:69:VAL:HG21	2.03	0.40
1:B:92:LEU:HD12	1:B:93:LYS:N	2.35	0.40
1:B:156:GLN:N	1:B:156:GLN:CD	2.79	0.40
1:D:48:VAL:O	1:D:48:VAL:CG1	2.68	0.40
1:F:271:ILE:CD1	1:F:275:MET:HE1	2.51	0.40
1:H:80:GLN:OE1	2:H:1:PDY:H24A	2.21	0.40
1:H:341:VAL:C	1:H:343:LYS:N	2.77	0.40
1:J:179:SER:HA	1:L:281:MET:SD	2.61	0.40
1:J:314:MET:HG3	1:J:318:GLU:OE1	2.21	0.40
1:K:330:LYS:HG3	1:K:330:LYS:O	2.21	0.40
1:L:277:THR:O	1:L:281:MET:HG2	2.21	0.40
1:L:285:GLU:C	1:L:287:PRO:HD3	2.46	0.40
1:A:151:GLN:HE21	1:A:342:LEU:C	2.30	0.40
1:A:247:TRP:HZ3	1:A:306:LEU:O	2.05	0.40
1:B:85:ARG:HH11	1:B:86:THR:CG2	2.34	0.40
1:B:253:MET:CE	1:B:305:LEU:HD12	2.52	0.40
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.56	0.40
1:C:281:MET:HB3	1:C:283:GLN:HG3	2.03	0.40
1:D:253:MET:HE3	1:D:253:MET:HB2	1.73	0.40
1:E:127:LEU:HD23	1:L:50:SER:O	2.22	0.40
1:H:193:LEU:HD11	2:H:1:PDY:H22A	2.04	0.40
1:L:86:THR:O	1:L:86:THR:HG22	2.21	0.40
1:L:331:VAL:CG2	1:L:332:PRO:HD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	266/324 (82%)	251 (94%)	14 (5%)	1 (0%)	30 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/324 (83%)	252 (94%)	15 (6%)	2 (1%)	18	48
1	C	263/324 (81%)	237 (90%)	21 (8%)	5 (2%)	6	23
1	D	269/324 (83%)	249 (93%)	19 (7%)	1 (0%)	30	59
1	E	268/324 (83%)	249 (93%)	16 (6%)	3 (1%)	11	36
1	F	283/324 (87%)	262 (93%)	19 (7%)	2 (1%)	18	48
1	G	265/324 (82%)	240 (91%)	24 (9%)	1 (0%)	30	59
1	H	265/324 (82%)	242 (91%)	23 (9%)	0	100	100
1	I	267/324 (82%)	251 (94%)	16 (6%)	0	100	100
1	J	267/324 (82%)	231 (86%)	34 (13%)	2 (1%)	18	48
1	K	265/324 (82%)	238 (90%)	24 (9%)	3 (1%)	11	36
1	L	268/324 (83%)	241 (90%)	24 (9%)	3 (1%)	11	36
All	All	3215/3888 (83%)	2943 (92%)	249 (8%)	23 (1%)	18	48

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	154	GLY
1	A	154	GLY
1	C	328	SER
1	G	295	SER
1	L	156	GLN
1	C	66	THR
1	C	295	SER
1	C	332	PRO
1	F	153	ARG
1	J	85	ARG
1	J	199	PRO
1	K	207	ASP
1	D	155	ASP
1	E	329	THR
1	F	207	ASP
1	K	233	GLU
1	L	195	THR
1	B	154	GLY
1	B	207	ASP
1	C	326	MET
1	K	130	GLY
1	L	98	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	289	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/293 (85%)	212 (86%)	36 (14%)	3	10
1	B	251/293 (86%)	225 (90%)	26 (10%)	7	23
1	C	247/293 (84%)	214 (87%)	33 (13%)	4	12
1	D	251/293 (86%)	217 (86%)	34 (14%)	4	12
1	E	250/293 (85%)	221 (88%)	29 (12%)	5	18
1	F	258/293 (88%)	228 (88%)	30 (12%)	5	18
1	G	247/293 (84%)	223 (90%)	24 (10%)	8	25
1	H	249/293 (85%)	222 (89%)	27 (11%)	6	21
1	I	249/293 (85%)	219 (88%)	30 (12%)	5	16
1	J	249/293 (85%)	219 (88%)	30 (12%)	5	16
1	K	247/293 (84%)	219 (89%)	28 (11%)	5	19
1	L	250/293 (85%)	228 (91%)	22 (9%)	9	29
All	All	2996/3516 (85%)	2647 (88%)	349 (12%)	5	18

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	56	LYS
1	A	66	THR
1	A	89	LYS
1	A	94	MET
1	A	96	GLN
1	A	100	LYS
1	A	113	GLN
1	A	127	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	131	ARG
1	A	134	LEU
1	A	138	MET
1	A	142	ASP
1	A	145	GLU
1	A	148	SER
1	A	155	ASP
1	A	156	GLN
1	A	161	ARG
1	A	172	GLU
1	A	188	LYS
1	A	202	ILE
1	A	233	GLU
1	A	240	TYR
1	A	280	ARG
1	A	285	GLU
1	A	293	GLU
1	A	298	VAL
1	A	308	THR
1	A	312	GLN
1	A	326	MET
1	A	330	LYS
1	A	331	VAL
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	342	LEU
1	B	50	SER
1	B	64	LYS
1	B	65	VAL
1	B	72	LEU
1	B	74	ILE
1	B	77	LYS
1	B	85	ARG
1	B	110	ARG
1	B	117	ILE
1	B	127	LEU
1	B	131	ARG
1	B	138	MET
1	B	162	GLU
1	B	193	LEU
1	B	233	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	240	TYR
1	B	249	LEU
1	B	276	LYS
1	B	292	SER
1	B	308	THR
1	B	326	MET
1	B	331	VAL
1	B	334	THR
1	B	336	LEU
1	B	342	LEU
1	B	344	GLU
1	C	49	LYS
1	C	56	LYS
1	C	77	LYS
1	C	85	ARG
1	C	89	LYS
1	C	96	GLN
1	C	98	CYS
1	C	127	LEU
1	C	131	ARG
1	C	134	LEU
1	C	149	ARG
1	C	155	ASP
1	C	156	GLN
1	C	161	ARG
1	C	190	GLU
1	C	215	THR
1	C	229	TYR
1	C	233	GLU
1	C	240	TYR
1	C	249	LEU
1	C	256	LEU
1	C	276	LYS
1	C	288	ASN
1	C	290	GLU
1	C	295	SER
1	C	298	VAL
1	C	311	THR
1	C	326	MET
1	C	327	GLN
1	C	330	LYS
1	C	334	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	336	LEU
1	C	342	LEU
1	D	53	GLN
1	D	56	LYS
1	D	64	LYS
1	D	68	GLN
1	D	70	LEU
1	D	77	LYS
1	D	93	LYS
1	D	113	GLN
1	D	122	ASP
1	D	127	LEU
1	D	131	ARG
1	D	134	LEU
1	D	142	ASP
1	D	161	ARG
1	D	168	LYS
1	D	172	GLU
1	D	190	GLU
1	D	200	ASN
1	D	202	ILE
1	D	233	GLU
1	D	238	GLU
1	D	239	LYS
1	D	249	LEU
1	D	266	ASN
1	D	276	LYS
1	D	283	GLN
1	D	304	ASN
1	D	326	MET
1	D	330	LYS
1	D	331	VAL
1	D	334	THR
1	D	336	LEU
1	D	342	LEU
1	D	343	LYS
1	E	49	LYS
1	E	53	GLN
1	E	57	ASN
1	E	64	LYS
1	E	67	SER
1	E	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	87	GLN
1	E	100	LYS
1	E	131	ARG
1	E	134	LEU
1	E	138	MET
1	E	151	GLN
1	E	156	GLN
1	E	161	ARG
1	E	172	GLU
1	E	202	ILE
1	E	240	TYR
1	E	249	LEU
1	E	266	ASN
1	E	272	SER
1	E	290	GLU
1	E	292	SER
1	E	304	ASN
1	E	327	GLN
1	E	331	VAL
1	E	333	GLN
1	E	334	THR
1	E	336	LEU
1	E	342	LEU
1	F	50	SER
1	F	74	ILE
1	F	85	ARG
1	F	89	LYS
1	F	127	LEU
1	F	131	ARG
1	F	134	LEU
1	F	135	LEU
1	F	138	MET
1	F	153	ARG
1	F	155	ASP
1	F	156	GLN
1	F	172	GLU
1	F	188	LYS
1	F	193	LEU
1	F	197	LYS
1	F	202	ILE
1	F	285	GLU
1	F	290	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	295	SER
1	F	299	LYS
1	F	307	LYS
1	F	308	THR
1	F	309	GLU
1	F	327	GLN
1	F	331	VAL
1	F	334	THR
1	F	336	LEU
1	F	342	LEU
1	F	344	GLU
1	G	53	GLN
1	G	64	LYS
1	G	93	LYS
1	G	100	LYS
1	G	122	ASP
1	G	134	LEU
1	G	153	ARG
1	G	156	GLN
1	G	161	ARG
1	G	168	LYS
1	G	172	GLU
1	G	198	ARG
1	G	202	ILE
1	G	212	LYS
1	G	248	SER
1	G	249	LEU
1	G	266	ASN
1	G	280	ARG
1	G	290	GLU
1	G	304	ASN
1	G	308	THR
1	G	334	THR
1	G	336	LEU
1	G	342	LEU
1	H	47	HIS
1	H	56	LYS
1	H	60	ILE
1	H	70	LEU
1	H	74	ILE
1	H	75	ASN
1	H	77	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	89	LYS
1	H	93	LYS
1	H	127	LEU
1	H	131	ARG
1	H	161	ARG
1	H	172	GLU
1	H	190	GLU
1	H	193	LEU
1	H	200	ASN
1	H	212	LYS
1	H	229	TYR
1	H	233	GLU
1	H	249	LEU
1	H	275	MET
1	H	290	GLU
1	H	328	SER
1	H	330	LYS
1	H	336	LEU
1	H	337	HIS
1	H	343	LYS
1	I	64	LYS
1	I	89	LYS
1	I	96	GLN
1	I	100	LYS
1	I	113	GLN
1	I	121	VAL
1	I	122	ASP
1	I	127	LEU
1	I	134	LEU
1	I	149	ARG
1	I	153	ARG
1	I	161	ARG
1	I	168	LYS
1	I	169	SER
1	I	200	ASN
1	I	202	ILE
1	I	233	GLU
1	I	249	LEU
1	I	253	MET
1	I	266	ASN
1	I	297	GLU
1	I	308	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	316	ILE
1	I	327	GLN
1	I	330	LYS
1	I	331	VAL
1	I	333	GLN
1	I	334	THR
1	I	336	LEU
1	I	342	LEU
1	J	53	GLN
1	J	68	GLN
1	J	69	VAL
1	J	70	LEU
1	J	89	LYS
1	J	122	ASP
1	J	127	LEU
1	J	131	ARG
1	J	134	LEU
1	J	142	ASP
1	J	151	GLN
1	J	165	GLU
1	J	198	ARG
1	J	233	GLU
1	J	240	TYR
1	J	253	MET
1	J	266	ASN
1	J	277	THR
1	J	285	GLU
1	J	288	ASN
1	J	290	GLU
1	J	293	GLU
1	J	295	SER
1	J	311	THR
1	J	326	MET
1	J	327	GLN
1	J	334	THR
1	J	337	HIS
1	J	340	ARG
1	J	343	LYS
1	K	53	GLN
1	K	64	LYS
1	K	77	LYS
1	K	89	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	100	LYS
1	K	127	LEU
1	K	131	ARG
1	K	134	LEU
1	K	138	MET
1	K	153	ARG
1	K	168	LYS
1	K	190	GLU
1	K	193	LEU
1	K	200	ASN
1	K	202	ILE
1	K	233	GLU
1	K	249	LEU
1	K	285	GLU
1	K	288	ASN
1	K	301	LEU
1	K	308	THR
1	K	314	MET
1	K	326	MET
1	K	330	LYS
1	K	333	GLN
1	K	334	THR
1	K	336	LEU
1	K	342	LEU
1	L	48	VAL
1	L	56	LYS
1	L	65	VAL
1	L	67	SER
1	L	89	LYS
1	L	96	GLN
1	L	100	LYS
1	L	122	ASP
1	L	127	LEU
1	L	134	LEU
1	L	161	ARG
1	L	235	LEU
1	L	240	TYR
1	L	249	LEU
1	L	266	ASN
1	L	275	MET
1	L	314	MET
1	L	320	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	333	GLN
1	L	334	THR
1	L	337	HIS
1	L	342	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	57	ASN
1	A	68	GLN
1	A	80	GLN
1	A	87	GLN
1	A	116	HIS
1	A	151	GLN
1	A	156	GLN
1	A	175	GLN
1	A	181	ASN
1	A	333	GLN
1	B	47	HIS
1	B	57	ASN
1	B	108	HIS
1	B	181	ASN
1	B	184	HIS
1	B	327	GLN
1	B	333	GLN
1	C	53	GLN
1	C	57	ASN
1	C	75	ASN
1	C	113	GLN
1	C	116	HIS
1	C	151	GLN
1	C	156	GLN
1	C	175	GLN
1	C	191	ASN
1	C	200	ASN
1	C	283	GLN
1	C	288	ASN
1	C	327	GLN
1	C	337	HIS
1	D	53	GLN
1	D	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	68	GLN
1	D	87	GLN
1	D	96	GLN
1	D	151	GLN
1	D	156	GLN
1	D	175	GLN
1	D	266	ASN
1	D	267	HIS
1	E	53	GLN
1	E	57	ASN
1	E	80	GLN
1	E	87	GLN
1	E	116	HIS
1	E	151	GLN
1	E	156	GLN
1	E	178	HIS
1	E	181	ASN
1	E	184	HIS
1	E	321	ASN
1	E	327	GLN
1	E	333	GLN
1	E	337	HIS
1	F	68	GLN
1	F	108	HIS
1	F	126	ASN
1	F	156	GLN
1	F	175	GLN
1	F	181	ASN
1	F	283	GLN
1	F	327	GLN
1	G	53	GLN
1	G	57	ASN
1	G	87	GLN
1	G	96	GLN
1	G	108	HIS
1	G	116	HIS
1	G	126	ASN
1	G	156	GLN
1	G	175	GLN
1	G	266	ASN
1	G	304	ASN
1	G	333	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	53	GLN
1	H	57	ASN
1	H	75	ASN
1	H	80	GLN
1	H	108	HIS
1	H	113	GLN
1	H	116	HIS
1	H	151	GLN
1	H	175	GLN
1	H	181	ASN
1	H	200	ASN
1	H	322	HIS
1	H	333	GLN
1	I	108	HIS
1	I	126	ASN
1	I	151	GLN
1	I	181	ASN
1	I	200	ASN
1	I	266	ASN
1	I	304	ASN
1	I	321	ASN
1	I	327	GLN
1	I	333	GLN
1	J	57	ASN
1	J	68	GLN
1	J	87	GLN
1	J	116	HIS
1	J	126	ASN
1	J	151	GLN
1	J	156	GLN
1	J	191	ASN
1	J	283	GLN
1	J	288	ASN
1	J	327	GLN
1	K	53	GLN
1	K	57	ASN
1	K	80	GLN
1	K	87	GLN
1	K	96	GLN
1	K	116	HIS
1	K	151	GLN
1	K	175	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	304	ASN
1	K	327	GLN
1	K	333	GLN
1	K	337	HIS
1	L	68	GLN
1	L	87	GLN
1	L	96	GLN
1	L	108	HIS
1	L	113	GLN
1	L	181	ASN
1	L	321	ASN
1	L	327	GLN
1	L	333	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PDY	E	1	-	29,30,30	2.65	5 (17%)	28,41,41	2.97	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PDY	I	2	-	29,30,30	2.61	6 (20%)	28,41,41	3.12	15 (53%)
2	PDY	L	1	-	29,30,30	2.66	5 (17%)	28,41,41	3.07	7 (25%)
3	SO4	F	3	-	4,4,4	0.34	0	6,6,6	0.14	0
2	PDY	J	2	-	29,30,30	2.65	5 (17%)	28,41,41	2.88	6 (21%)
2	PDY	C	2	-	29,30,30	2.64	6 (20%)	28,41,41	2.93	4 (14%)
2	PDY	F	1	-	29,30,30	2.65	5 (17%)	28,41,41	3.11	8 (28%)
2	PDY	G	2	-	29,30,30	2.64	6 (20%)	28,41,41	2.86	6 (21%)
2	PDY	J	1	-	29,30,30	2.65	5 (17%)	28,41,41	2.81	6 (21%)
2	PDY	K	2	-	29,30,30	2.64	6 (20%)	28,41,41	3.02	8 (28%)
2	PDY	A	2	-	29,30,30	2.64	5 (17%)	28,41,41	2.82	7 (25%)
2	PDY	L	2	-	29,30,30	2.62	5 (17%)	28,41,41	2.65	7 (25%)
2	PDY	E	2	-	29,30,30	2.64	6 (20%)	28,41,41	2.93	6 (21%)
2	PDY	K	1	-	29,30,30	2.64	5 (17%)	28,41,41	2.92	7 (25%)
2	PDY	F	2	-	29,30,30	2.66	5 (17%)	28,41,41	3.02	7 (25%)
2	PDY	C	1	-	29,30,30	2.65	5 (17%)	28,41,41	3.06	8 (28%)
2	PDY	B	2	-	29,30,30	2.66	6 (20%)	28,41,41	3.03	6 (21%)
2	PDY	D	1	-	29,30,30	2.66	5 (17%)	28,41,41	3.01	7 (25%)
2	PDY	B	1	-	29,30,30	2.65	5 (17%)	28,41,41	3.03	5 (17%)
2	PDY	I	1	-	29,30,30	2.65	5 (17%)	28,41,41	3.04	6 (21%)
2	PDY	H	2	-	29,30,30	2.68	6 (20%)	28,41,41	3.35	14 (50%)
2	PDY	G	1	-	29,30,30	2.66	6 (20%)	28,41,41	3.05	7 (25%)
2	PDY	D	2	-	29,30,30	2.61	5 (17%)	28,41,41	2.69	5 (17%)
2	PDY	H	1	-	29,30,30	2.67	6 (20%)	28,41,41	3.11	8 (28%)
2	PDY	A	1	-	29,30,30	2.66	5 (17%)	28,41,41	3.07	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PDY	E	1	-	-	5/11/19/19	0/4/4/4
2	PDY	I	2	-	-	2/11/19/19	0/4/4/4
2	PDY	L	1	-	-	5/11/19/19	0/4/4/4
2	PDY	J	2	-	-	4/11/19/19	0/4/4/4
2	PDY	C	2	-	-	4/11/19/19	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PDY	F	1	-	-	5/11/19/19	0/4/4/4
2	PDY	G	2	-	-	4/11/19/19	0/4/4/4
2	PDY	J	1	-	-	2/11/19/19	0/4/4/4
2	PDY	K	2	-	-	5/11/19/19	0/4/4/4
2	PDY	A	2	-	-	4/11/19/19	0/4/4/4
2	PDY	L	2	-	-	2/11/19/19	0/4/4/4
2	PDY	E	2	-	-	4/11/19/19	0/4/4/4
2	PDY	K	1	-	-	3/11/19/19	0/4/4/4
2	PDY	F	2	-	-	4/11/19/19	0/4/4/4
2	PDY	C	1	-	-	2/11/19/19	0/4/4/4
2	PDY	B	2	-	-	4/11/19/19	0/4/4/4
2	PDY	D	1	-	-	3/11/19/19	0/4/4/4
2	PDY	B	1	-	-	2/11/19/19	0/4/4/4
2	PDY	I	1	-	-	2/11/19/19	0/4/4/4
2	PDY	H	2	-	-	1/11/19/19	0/4/4/4
2	PDY	G	1	-	-	5/11/19/19	0/4/4/4
2	PDY	D	2	-	-	3/11/19/19	0/4/4/4
2	PDY	H	1	-	-	3/11/19/19	0/4/4/4
2	PDY	A	1	-	-	4/11/19/19	0/4/4/4

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	PDY	N2-N7	-8.83	1.23	1.37
2	H	2	PDY	N2-N7	-8.73	1.23	1.37
2	D	1	PDY	N2-N7	-8.69	1.23	1.37
2	F	2	PDY	N2-N7	-8.68	1.23	1.37
2	B	2	PDY	N2-N7	-8.66	1.23	1.37
2	J	1	PDY	N2-N7	-8.64	1.23	1.37
2	H	1	PDY	N2-N7	-8.64	1.23	1.37
2	B	1	PDY	N2-N7	-8.62	1.23	1.37
2	F	1	PDY	N2-N7	-8.61	1.23	1.37
2	A	1	PDY	N2-N7	-8.61	1.23	1.37
2	C	1	PDY	N2-N7	-8.60	1.23	1.37
2	E	1	PDY	N2-N7	-8.60	1.23	1.37
2	I	1	PDY	N2-N7	-8.60	1.23	1.37
2	G	1	PDY	N2-N7	-8.60	1.23	1.37
2	L	1	PDY	N2-N7	-8.58	1.23	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	PDY	N2-N7	-8.57	1.23	1.37
2	J	2	PDY	N2-N7	-8.57	1.23	1.37
2	C	2	PDY	N2-N7	-8.57	1.23	1.37
2	K	2	PDY	N2-N7	-8.55	1.23	1.37
2	G	2	PDY	N2-N7	-8.54	1.23	1.37
2	E	2	PDY	N2-N7	-8.49	1.23	1.37
2	L	2	PDY	N2-N7	-8.38	1.24	1.37
2	I	2	PDY	N2-N7	-8.37	1.24	1.37
2	D	2	PDY	N2-N7	-8.33	1.24	1.37
2	L	2	PDY	C8-C11	7.41	1.53	1.39
2	I	2	PDY	C8-C11	7.39	1.53	1.39
2	D	2	PDY	C8-C11	7.38	1.53	1.39
2	H	2	PDY	C8-C11	7.35	1.53	1.39
2	L	1	PDY	C8-C11	7.32	1.53	1.39
2	J	1	PDY	C8-C11	7.31	1.53	1.39
2	I	1	PDY	C8-C11	7.30	1.53	1.39
2	E	2	PDY	C8-C11	7.30	1.53	1.39
2	J	2	PDY	C8-C11	7.30	1.53	1.39
2	H	1	PDY	C8-C11	7.29	1.53	1.39
2	F	1	PDY	C8-C11	7.29	1.53	1.39
2	D	1	PDY	C8-C11	7.28	1.53	1.39
2	A	1	PDY	C8-C11	7.28	1.53	1.39
2	G	1	PDY	C8-C11	7.28	1.53	1.39
2	B	1	PDY	C8-C11	7.27	1.53	1.39
2	C	2	PDY	C8-C11	7.27	1.53	1.39
2	F	2	PDY	C8-C11	7.26	1.53	1.39
2	K	1	PDY	C8-C11	7.26	1.53	1.39
2	A	2	PDY	C8-C11	7.26	1.53	1.39
2	G	2	PDY	C8-C11	7.26	1.53	1.39
2	K	2	PDY	C8-C11	7.26	1.53	1.39
2	B	2	PDY	C8-C11	7.25	1.53	1.39
2	C	1	PDY	C8-C11	7.24	1.53	1.39
2	E	1	PDY	C8-C11	7.24	1.53	1.39
2	E	2	PDY	C11-N7	5.93	1.47	1.33
2	K	2	PDY	C11-N7	5.90	1.47	1.33
2	L	1	PDY	C11-N7	5.90	1.47	1.33
2	H	2	PDY	C11-N7	5.90	1.47	1.33
2	G	1	PDY	C11-N7	5.88	1.47	1.33
2	C	2	PDY	C11-N7	5.88	1.47	1.33
2	G	2	PDY	C11-N7	5.87	1.47	1.33
2	B	1	PDY	C11-N7	5.86	1.47	1.33
2	B	2	PDY	C11-N7	5.85	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	PDY	C11-N7	5.85	1.47	1.33
2	A	1	PDY	C11-N7	5.85	1.47	1.33
2	E	1	PDY	C11-N7	5.84	1.47	1.33
2	D	1	PDY	C11-N7	5.84	1.47	1.33
2	F	1	PDY	C11-N7	5.84	1.47	1.33
2	J	2	PDY	C11-N7	5.83	1.47	1.33
2	C	1	PDY	C11-N7	5.83	1.47	1.33
2	I	1	PDY	C11-N7	5.82	1.47	1.33
2	I	2	PDY	C11-N7	5.80	1.47	1.33
2	J	1	PDY	C11-N7	5.80	1.47	1.33
2	K	1	PDY	C11-N7	5.79	1.47	1.33
2	D	2	PDY	C11-N7	5.79	1.47	1.33
2	L	2	PDY	C11-N7	5.79	1.47	1.33
2	H	1	PDY	C11-N7	5.79	1.47	1.33
2	A	2	PDY	C11-N7	5.75	1.47	1.33
2	H	1	PDY	C13-N9	-4.43	1.32	1.41
2	F	1	PDY	C13-N9	-4.32	1.32	1.41
2	K	1	PDY	C13-N9	-4.30	1.33	1.41
2	E	1	PDY	C13-N9	-4.29	1.33	1.41
2	A	1	PDY	C13-N9	-4.26	1.33	1.41
2	B	1	PDY	C13-N9	-4.21	1.33	1.41
2	I	1	PDY	C13-N9	-4.21	1.33	1.41
2	F	2	PDY	C13-N9	-4.20	1.33	1.41
2	D	1	PDY	C13-N9	-4.20	1.33	1.41
2	L	1	PDY	C13-N9	-4.19	1.33	1.41
2	G	1	PDY	C13-N9	-4.18	1.33	1.41
2	B	2	PDY	C13-N9	-4.16	1.33	1.41
2	J	1	PDY	C13-N9	-4.16	1.33	1.41
2	J	2	PDY	C13-N9	-4.15	1.33	1.41
2	C	1	PDY	C13-N9	-4.15	1.33	1.41
2	G	2	PDY	C13-N9	-4.09	1.33	1.41
2	A	2	PDY	C13-N9	-4.07	1.33	1.41
2	K	2	PDY	C13-N9	-4.03	1.33	1.41
2	C	2	PDY	C13-N9	-4.01	1.33	1.41
2	L	2	PDY	C13-N9	-3.95	1.33	1.41
2	H	2	PDY	C13-N9	-3.94	1.33	1.41
2	E	2	PDY	C13-N9	-3.82	1.33	1.41
2	D	2	PDY	C13-N9	-3.82	1.33	1.41
2	I	2	PDY	C13-N9	-3.79	1.34	1.41
2	I	2	PDY	C8-C5	-2.53	1.33	1.40
2	A	2	PDY	C8-C5	-2.52	1.33	1.40
2	D	2	PDY	C8-C5	-2.50	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	PDY	C8-C5	-2.49	1.33	1.40
2	H	2	PDY	C8-C5	-2.49	1.33	1.40
2	H	1	PDY	C8-C5	-2.49	1.33	1.40
2	B	2	PDY	C8-C5	-2.49	1.33	1.40
2	C	1	PDY	C8-C5	-2.48	1.33	1.40
2	D	1	PDY	C8-C5	-2.48	1.33	1.40
2	K	1	PDY	C8-C5	-2.48	1.33	1.40
2	L	2	PDY	C8-C5	-2.47	1.33	1.40
2	K	2	PDY	C8-C5	-2.47	1.33	1.40
2	E	2	PDY	C8-C5	-2.46	1.33	1.40
2	L	1	PDY	C8-C5	-2.46	1.33	1.40
2	G	2	PDY	C8-C5	-2.46	1.33	1.40
2	F	1	PDY	C8-C5	-2.46	1.33	1.40
2	A	1	PDY	C8-C5	-2.45	1.33	1.40
2	C	2	PDY	C8-C5	-2.45	1.33	1.40
2	F	2	PDY	C8-C5	-2.45	1.33	1.40
2	B	1	PDY	C8-C5	-2.44	1.33	1.40
2	J	1	PDY	C8-C5	-2.44	1.33	1.40
2	E	1	PDY	C8-C5	-2.44	1.33	1.40
2	G	1	PDY	C8-C5	-2.44	1.33	1.40
2	I	1	PDY	C8-C5	-2.44	1.33	1.40
2	E	2	PDY	C1-N2	2.20	1.41	1.36
2	H	2	PDY	C3-C4	-2.15	1.39	1.44
2	H	1	PDY	C3-C4	-2.07	1.39	1.44
2	I	2	PDY	C3-C4	-2.06	1.39	1.44
2	C	2	PDY	C1-N2	2.06	1.41	1.36
2	K	2	PDY	C1-N2	2.06	1.41	1.36
2	G	2	PDY	C1-N2	2.04	1.41	1.36
2	B	2	PDY	C1-N2	2.03	1.41	1.36
2	G	1	PDY	C3-C4	-2.01	1.39	1.44

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	PDY	C11-N7-N2	11.60	112.20	103.26
2	C	2	PDY	C11-N7-N2	11.51	112.12	103.26
2	A	1	PDY	C11-N7-N2	11.49	112.11	103.26
2	D	1	PDY	C11-N7-N2	11.33	111.98	103.26
2	F	1	PDY	C11-N7-N2	11.30	111.97	103.26
2	C	1	PDY	C11-N7-N2	11.23	111.91	103.26
2	G	1	PDY	C11-N7-N2	11.20	111.89	103.26
2	B	2	PDY	C11-N7-N2	11.18	111.87	103.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	PDY	C11-N7-N2	11.16	111.86	103.26
2	L	1	PDY	C11-N7-N2	11.11	111.81	103.26
2	K	2	PDY	C11-N7-N2	10.65	111.47	103.26
2	E	1	PDY	C11-N7-N2	10.65	111.46	103.26
2	I	1	PDY	C11-N7-N2	10.64	111.45	103.26
2	E	2	PDY	C11-N7-N2	10.50	111.35	103.26
2	J	2	PDY	C11-N7-N2	10.48	111.33	103.26
2	J	1	PDY	C11-N7-N2	10.46	111.31	103.26
2	G	2	PDY	C11-N7-N2	10.44	111.30	103.26
2	K	1	PDY	C11-N7-N2	10.39	111.27	103.26
2	H	1	PDY	C11-N7-N2	10.28	111.17	103.26
2	A	2	PDY	C11-N7-N2	9.82	110.83	103.26
2	D	2	PDY	C11-N7-N2	8.97	110.17	103.26
2	F	1	PDY	C8-C11-N7	-8.69	100.08	112.37
2	B	1	PDY	C8-C11-N7	-8.62	100.18	112.37
2	L	1	PDY	C8-C11-N7	-8.57	100.25	112.37
2	C	1	PDY	C8-C11-N7	-8.53	100.30	112.37
2	A	1	PDY	C8-C11-N7	-8.48	100.37	112.37
2	D	1	PDY	C8-C11-N7	-8.39	100.50	112.37
2	H	1	PDY	C8-C11-N7	-8.37	100.53	112.37
2	A	2	PDY	C8-C11-N7	-8.34	100.57	112.37
2	G	1	PDY	C8-C11-N7	-8.30	100.62	112.37
2	C	2	PDY	C8-C11-N7	-8.28	100.65	112.37
2	J	1	PDY	C8-C11-N7	-8.26	100.67	112.37
2	K	1	PDY	C8-C11-N7	-8.25	100.69	112.37
2	B	2	PDY	C8-C11-N7	-8.23	100.73	112.37
2	F	2	PDY	C8-C11-N7	-8.22	100.74	112.37
2	E	1	PDY	C8-C11-N7	-8.21	100.75	112.37
2	I	1	PDY	C8-C11-N7	-8.20	100.76	112.37
2	J	2	PDY	C8-C11-N7	-8.06	100.97	112.37
2	K	2	PDY	C8-C11-N7	-8.04	100.99	112.37
2	E	2	PDY	C8-C11-N7	-8.03	101.01	112.37
2	G	2	PDY	C8-C11-N7	-8.01	101.03	112.37
2	L	2	PDY	C11-N7-N2	7.91	109.35	103.26
2	I	2	PDY	C11-N7-N2	7.72	109.21	103.26
2	D	2	PDY	C8-C11-N7	-7.67	101.51	112.37
2	I	2	PDY	C1-N2-C5	-7.57	117.06	123.31
2	L	2	PDY	C8-C11-N7	-7.39	101.91	112.37
2	I	2	PDY	C8-C11-N7	-7.38	101.93	112.37
2	H	2	PDY	C8-C11-N7	-7.29	102.05	112.37
2	H	2	PDY	C1-N2-C5	-7.24	117.33	123.31
2	H	2	PDY	C11-N7-N2	6.81	108.51	103.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	PDY	C1-N2-C5	-5.60	118.69	123.31
2	E	2	PDY	C1-N2-C5	-5.54	118.73	123.31
2	H	2	PDY	C17-C20-C16	5.46	125.96	119.73
2	H	1	PDY	C24-O21-C16	-5.37	105.36	117.90
2	L	1	PDY	C1-N2-C5	-4.55	119.55	123.31
2	G	2	PDY	C1-N2-C5	-4.53	119.57	123.31
2	B	2	PDY	C15-N10-C4	-4.46	116.16	122.74
2	I	1	PDY	C1-N2-C5	-4.46	119.62	123.31
2	H	2	PDY	N10-C4-N6	-4.44	113.10	119.70
2	K	2	PDY	C1-N2-C5	-4.40	119.68	123.31
2	F	2	PDY	C15-N10-C4	-4.29	116.42	122.74
2	H	2	PDY	C19-C16-C20	-4.29	113.91	120.16
2	H	2	PDY	C13-N9-C1	4.28	137.48	125.17
2	D	2	PDY	C1-N2-C5	-4.14	119.89	123.31
2	K	2	PDY	C15-N10-C4	-4.13	116.66	122.74
2	F	1	PDY	C24-O21-C16	-4.05	108.44	117.90
2	E	1	PDY	C1-N2-C5	-3.99	120.02	123.31
2	K	1	PDY	C1-N2-C5	-3.96	120.04	123.31
2	H	1	PDY	C1-N2-C5	-3.90	120.09	123.31
2	G	1	PDY	C1-N2-C5	-3.83	120.14	123.31
2	I	2	PDY	C22-C15-N10	3.61	114.67	109.98
2	I	1	PDY	N2-C5-N6	-3.53	118.94	121.49
2	C	2	PDY	C1-N2-C5	-3.50	120.42	123.31
2	J	1	PDY	C1-N2-C5	-3.48	120.43	123.31
2	A	1	PDY	C1-N2-C5	-3.47	120.44	123.31
2	J	2	PDY	C1-N2-C5	-3.46	120.45	123.31
2	D	1	PDY	C24-O21-C16	-3.45	109.85	117.90
2	A	2	PDY	C22-C15-N10	3.44	114.46	109.98
2	K	1	PDY	C24-O21-C16	-3.43	109.90	117.90
2	B	1	PDY	C1-N2-C5	-3.43	120.48	123.31
2	B	2	PDY	C1-N2-C5	-3.42	120.49	123.31
2	A	2	PDY	C11-C8-C5	3.39	106.86	104.54
2	C	1	PDY	N2-C5-N6	-3.35	119.07	121.49
2	I	2	PDY	C13-N9-C1	3.32	134.72	125.17
2	H	1	PDY	C11-C8-C5	3.32	106.81	104.54
2	D	1	PDY	C1-N2-C5	-3.29	120.59	123.31
2	H	2	PDY	C17-C13-N9	-3.29	109.38	120.41
2	H	1	PDY	N2-C5-N6	-3.26	119.13	121.49
2	C	1	PDY	C1-N2-C5	-3.26	120.62	123.31
2	C	1	PDY	C22-C15-N10	-3.24	105.76	109.98
2	E	1	PDY	C24-O21-C16	-3.22	110.40	117.90
2	G	1	PDY	C15-N10-C4	-3.21	118.00	122.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PDY	N2-C5-N6	-3.13	119.23	121.49
2	G	1	PDY	N2-C5-N6	-3.12	119.23	121.49
2	H	2	PDY	C24-O21-C16	-3.09	110.69	117.90
2	I	2	PDY	N10-C4-N6	-3.07	115.14	119.70
2	D	2	PDY	C13-N9-C1	3.06	133.98	125.17
2	F	1	PDY	N2-C5-N6	-3.05	119.28	121.49
2	H	2	PDY	C22-C15-N10	3.03	113.92	109.98
2	H	2	PDY	C11-C8-C5	3.02	106.61	104.54
2	I	2	PDY	C15-N10-C4	-3.00	118.31	122.74
2	L	1	PDY	C13-N9-C1	2.99	133.77	125.17
2	L	1	PDY	C11-C8-C5	2.98	106.58	104.54
2	A	1	PDY	C25-C15-N10	-2.97	104.63	110.57
2	B	1	PDY	N2-C5-N6	-2.92	119.38	121.49
2	F	2	PDY	C1-N2-C5	-2.92	120.90	123.31
2	F	1	PDY	C11-C8-C5	2.90	106.52	104.54
2	J	1	PDY	C11-C8-C5	2.90	106.52	104.54
2	G	1	PDY	C25-C15-N10	-2.89	104.79	110.57
2	F	1	PDY	C1-N2-C5	-2.88	120.93	123.31
2	L	1	PDY	N2-C5-N6	-2.87	119.41	121.49
2	L	2	PDY	C11-C8-C5	2.86	106.49	104.54
2	E	1	PDY	N2-C5-N6	-2.85	119.43	121.49
2	L	2	PDY	C13-N9-C1	2.85	133.36	125.17
2	A	2	PDY	C1-N2-C5	-2.84	120.96	123.31
2	B	1	PDY	C11-C8-C5	2.83	106.48	104.54
2	I	2	PDY	C11-C8-C5	2.82	106.47	104.54
2	D	2	PDY	C11-C8-C5	2.80	106.45	104.54
2	I	2	PDY	N2-C5-N6	-2.80	119.47	121.49
2	H	2	PDY	N2-C5-N6	-2.78	119.48	121.49
2	C	1	PDY	C11-C8-C5	2.77	106.44	104.54
2	F	2	PDY	N2-C5-N6	-2.74	119.51	121.49
2	H	2	PDY	C18-C13-N9	2.72	129.56	120.41
2	G	2	PDY	C15-N10-C4	-2.71	118.74	122.74
2	C	2	PDY	C15-N10-C4	-2.67	118.80	122.74
2	I	1	PDY	C11-C8-C5	2.66	106.36	104.54
2	A	1	PDY	C13-N9-C1	2.66	132.81	125.17
2	H	2	PDY	C15-N10-C4	-2.65	118.84	122.74
2	K	1	PDY	C11-C8-C5	2.65	106.35	104.54
2	H	1	PDY	C20-C17-C13	-2.63	117.28	120.30
2	K	2	PDY	C24-O21-C16	-2.62	111.78	117.90
2	E	2	PDY	C1-N2-N7	2.62	129.31	124.82
2	K	1	PDY	N2-C5-N6	-2.56	119.64	121.49
2	D	1	PDY	N2-C5-N6	-2.53	119.66	121.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	PDY	C25-C15-N10	2.53	115.63	110.57
2	I	2	PDY	C20-C17-C13	2.46	123.13	120.30
2	D	1	PDY	C25-C15-N10	-2.45	105.67	110.57
2	C	1	PDY	C15-N10-C4	-2.45	119.12	122.74
2	J	2	PDY	C15-N10-C4	-2.45	119.13	122.74
2	J	1	PDY	N2-C5-N6	-2.44	119.73	121.49
2	D	1	PDY	C11-C8-C5	2.43	106.20	104.54
2	I	2	PDY	C19-C16-C20	-2.42	116.62	120.16
2	J	2	PDY	N2-C5-N6	-2.42	119.74	121.49
2	A	1	PDY	C11-C8-C5	2.41	106.19	104.54
2	E	2	PDY	C11-C8-C5	2.40	106.18	104.54
2	E	1	PDY	C11-C8-C5	2.39	106.17	104.54
2	H	1	PDY	C18-C13-C17	2.36	122.17	119.04
2	B	2	PDY	N2-C5-N6	-2.35	119.79	121.49
2	I	2	PDY	C1-N2-N7	2.34	128.83	124.82
2	I	2	PDY	C17-C13-N9	-2.34	112.57	120.41
2	L	1	PDY	C15-N10-C4	-2.32	119.32	122.74
2	I	2	PDY	C18-C19-C16	2.29	122.35	119.73
2	F	1	PDY	C22-C15-N10	-2.29	107.00	109.98
2	E	1	PDY	C15-N10-C4	-2.28	119.38	122.74
2	B	2	PDY	N10-C4-N6	-2.26	116.34	119.70
2	J	1	PDY	C24-O21-C16	-2.25	112.64	117.90
2	L	2	PDY	C22-C15-N10	2.23	112.88	109.98
2	I	1	PDY	C15-N10-C4	-2.22	119.46	122.74
2	G	2	PDY	C11-C8-C5	2.22	106.06	104.54
2	L	2	PDY	N2-C5-N6	-2.22	119.89	121.49
2	J	2	PDY	C11-C8-C5	2.21	106.05	104.54
2	I	2	PDY	C18-C13-C17	-2.18	116.15	119.04
2	G	1	PDY	C11-C8-C5	2.16	106.02	104.54
2	K	2	PDY	C11-C8-C5	2.15	106.01	104.54
2	A	2	PDY	C18-C13-C17	-2.14	116.20	119.04
2	E	1	PDY	C25-C15-N10	-2.11	106.36	110.57
2	K	2	PDY	C1-N2-N7	2.11	128.43	124.82
2	F	2	PDY	C25-C15-N10	-2.06	106.46	110.57
2	A	2	PDY	C19-C18-C13	2.04	122.65	120.30
2	K	2	PDY	O21-C24-C27	2.03	114.38	108.04
2	G	2	PDY	C1-N2-N7	2.03	128.30	124.82
2	F	1	PDY	C15-N10-C4	-2.02	119.76	122.74
2	K	1	PDY	C20-C17-C13	-2.01	117.98	120.30
2	C	1	PDY	C13-N9-C1	2.01	130.95	125.17
2	F	2	PDY	C11-C8-C5	2.00	105.91	104.54

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	PDY	N2-C1-N9-C13
2	E	1	PDY	N2-C1-N9-C13
2	G	1	PDY	N2-C1-N9-C13
2	H	1	PDY	N2-C1-N9-C13
2	H	2	PDY	C3-C1-N9-C13
2	K	1	PDY	N2-C1-N9-C13
2	L	1	PDY	N2-C1-N9-C13
2	L	2	PDY	C3-C1-N9-C13
2	K	2	PDY	C27-C24-O21-C16
2	F	2	PDY	C20-C16-O21-C24
2	B	2	PDY	C19-C16-O21-C24
2	E	2	PDY	C20-C16-O21-C24
2	E	2	PDY	C19-C16-O21-C24
2	G	1	PDY	C19-C16-O21-C24
2	A	2	PDY	C20-C16-O21-C24
2	B	2	PDY	C20-C16-O21-C24
2	G	1	PDY	C20-C16-O21-C24
2	G	2	PDY	C20-C16-O21-C24
2	F	2	PDY	C19-C16-O21-C24
2	A	2	PDY	C19-C16-O21-C24
2	G	2	PDY	C19-C16-O21-C24
2	C	2	PDY	C19-C16-O21-C24
2	C	2	PDY	C20-C16-O21-C24
2	F	1	PDY	C19-C16-O21-C24
2	K	2	PDY	C19-C16-O21-C24
2	F	1	PDY	C20-C16-O21-C24
2	K	2	PDY	C20-C16-O21-C24
2	J	2	PDY	C20-C16-O21-C24
2	G	1	PDY	C27-C24-O21-C16
2	J	2	PDY	C19-C16-O21-C24
2	A	1	PDY	C19-C16-O21-C24
2	K	1	PDY	C27-C24-O21-C16
2	D	1	PDY	C27-C24-O21-C16
2	A	1	PDY	C20-C16-O21-C24
2	L	1	PDY	C20-C16-O21-C24
2	L	1	PDY	C19-C16-O21-C24
2	L	2	PDY	C27-C24-O21-C16
2	H	1	PDY	C27-C24-O21-C16
2	D	2	PDY	C27-C24-O21-C16
2	L	1	PDY	C27-C24-O21-C16
2	D	2	PDY	C3-C1-N9-C13
2	A	1	PDY	N2-C1-N9-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2	PDY	N2-C1-N9-C13
2	B	1	PDY	N2-C1-N9-C13
2	B	2	PDY	N2-C1-N9-C13
2	C	2	PDY	N2-C1-N9-C13
2	D	1	PDY	N2-C1-N9-C13
2	D	2	PDY	N2-C1-N9-C13
2	E	2	PDY	N2-C1-N9-C13
2	F	1	PDY	N2-C1-N9-C13
2	F	2	PDY	N2-C1-N9-C13
2	G	2	PDY	N2-C1-N9-C13
2	I	1	PDY	N2-C1-N9-C13
2	J	1	PDY	N2-C1-N9-C13
2	J	2	PDY	N2-C1-N9-C13
2	K	2	PDY	N2-C1-N9-C13
2	E	1	PDY	C27-C24-O21-C16
2	I	2	PDY	C20-C16-O21-C24
2	E	1	PDY	C19-C16-O21-C24
2	E	1	PDY	C20-C16-O21-C24
2	A	1	PDY	C3-C1-N9-C13
2	A	2	PDY	C3-C1-N9-C13
2	B	1	PDY	C3-C1-N9-C13
2	B	2	PDY	C3-C1-N9-C13
2	C	1	PDY	C3-C1-N9-C13
2	C	2	PDY	C3-C1-N9-C13
2	D	1	PDY	C3-C1-N9-C13
2	E	1	PDY	C3-C1-N9-C13
2	E	2	PDY	C3-C1-N9-C13
2	F	1	PDY	C3-C1-N9-C13
2	F	2	PDY	C3-C1-N9-C13
2	G	1	PDY	C3-C1-N9-C13
2	G	2	PDY	C3-C1-N9-C13
2	H	1	PDY	C3-C1-N9-C13
2	I	1	PDY	C3-C1-N9-C13
2	I	2	PDY	C3-C1-N9-C13
2	J	1	PDY	C3-C1-N9-C13
2	J	2	PDY	C3-C1-N9-C13
2	K	1	PDY	C3-C1-N9-C13
2	K	2	PDY	C3-C1-N9-C13
2	L	1	PDY	C3-C1-N9-C13
2	F	1	PDY	C27-C24-O21-C16

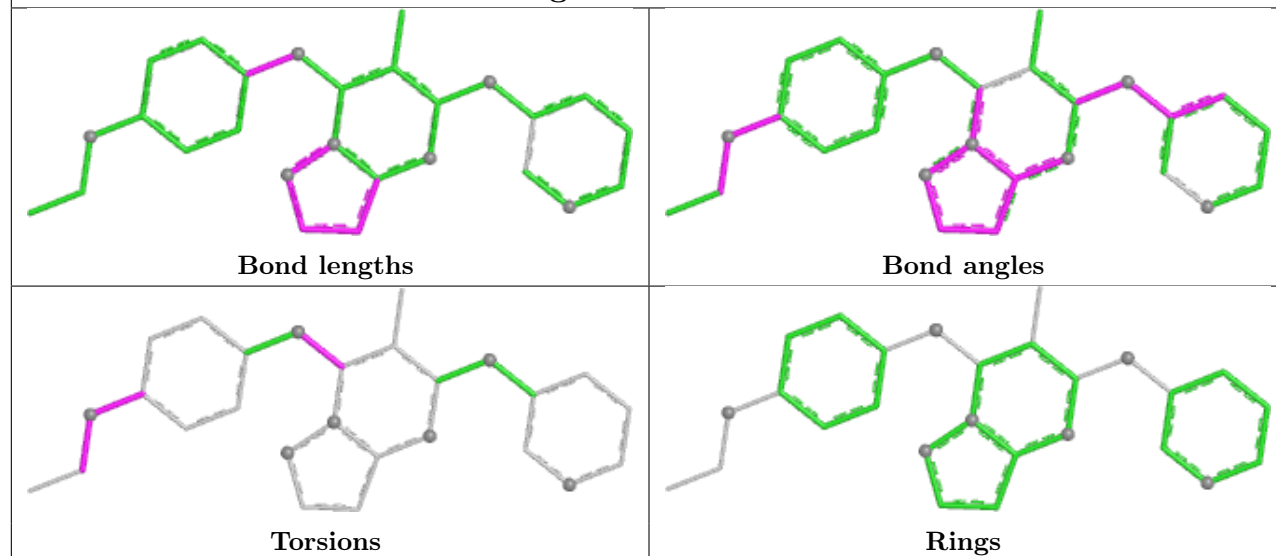
There are no ring outliers.

25 monomers are involved in 252 short contacts:

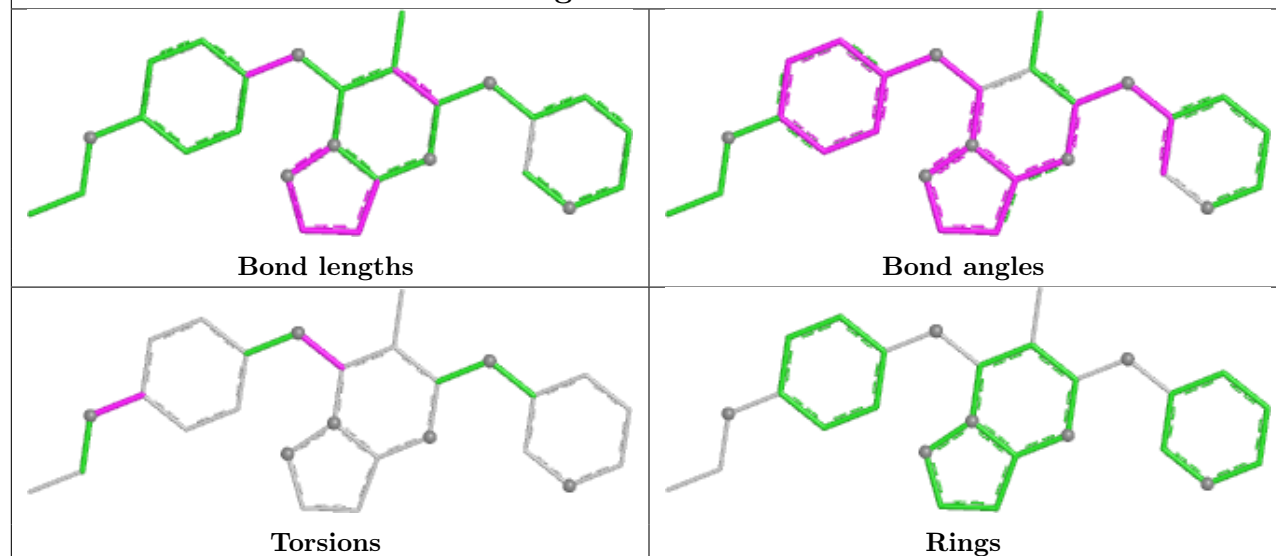
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	PDY	12	0
2	I	2	PDY	26	0
2	L	1	PDY	9	0
3	F	3	SO4	1	0
2	J	2	PDY	7	0
2	C	2	PDY	11	0
2	F	1	PDY	5	0
2	G	2	PDY	10	0
2	J	1	PDY	9	0
2	K	2	PDY	11	0
2	A	2	PDY	4	0
2	L	2	PDY	13	0
2	E	2	PDY	11	0
2	K	1	PDY	14	0
2	F	2	PDY	10	0
2	C	1	PDY	6	0
2	B	2	PDY	7	0
2	D	1	PDY	7	0
2	B	1	PDY	8	0
2	I	1	PDY	11	0
2	H	2	PDY	27	0
2	G	1	PDY	10	0
2	D	2	PDY	6	0
2	H	1	PDY	13	0
2	A	1	PDY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

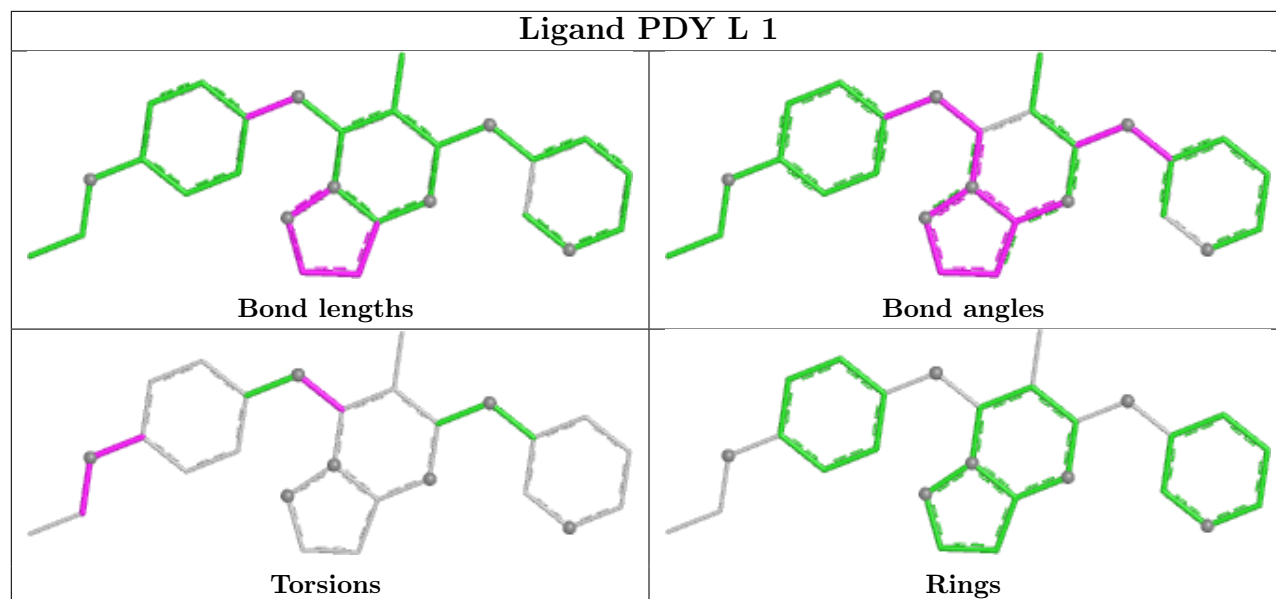
Ligand PDY E 1



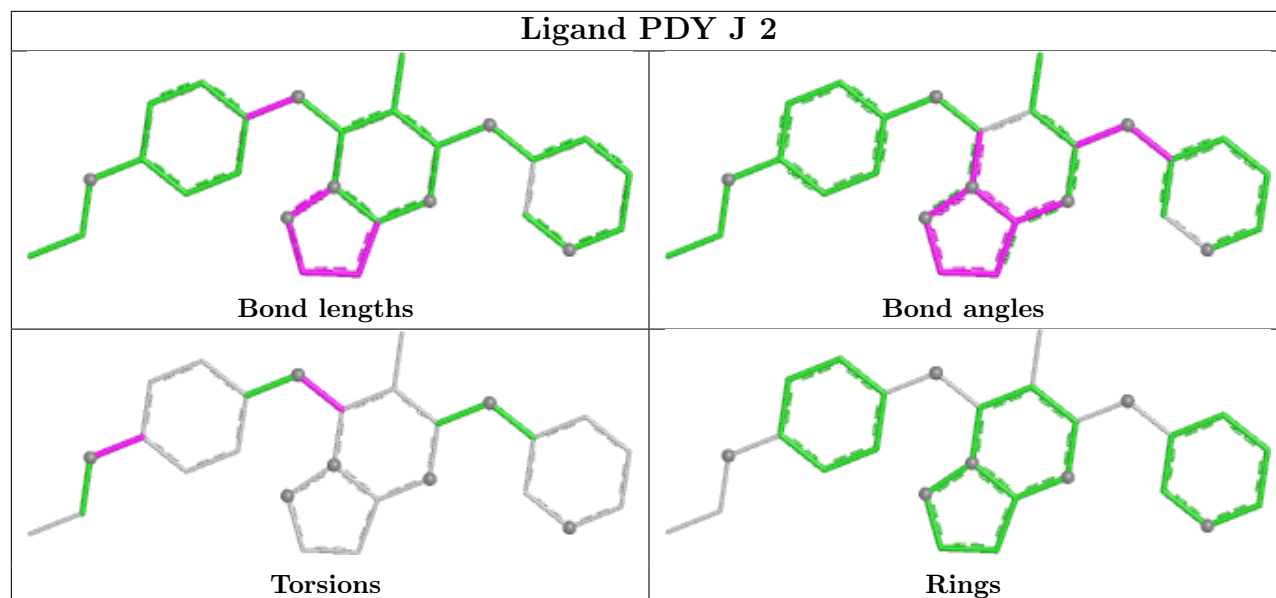
Ligand PDY I 2



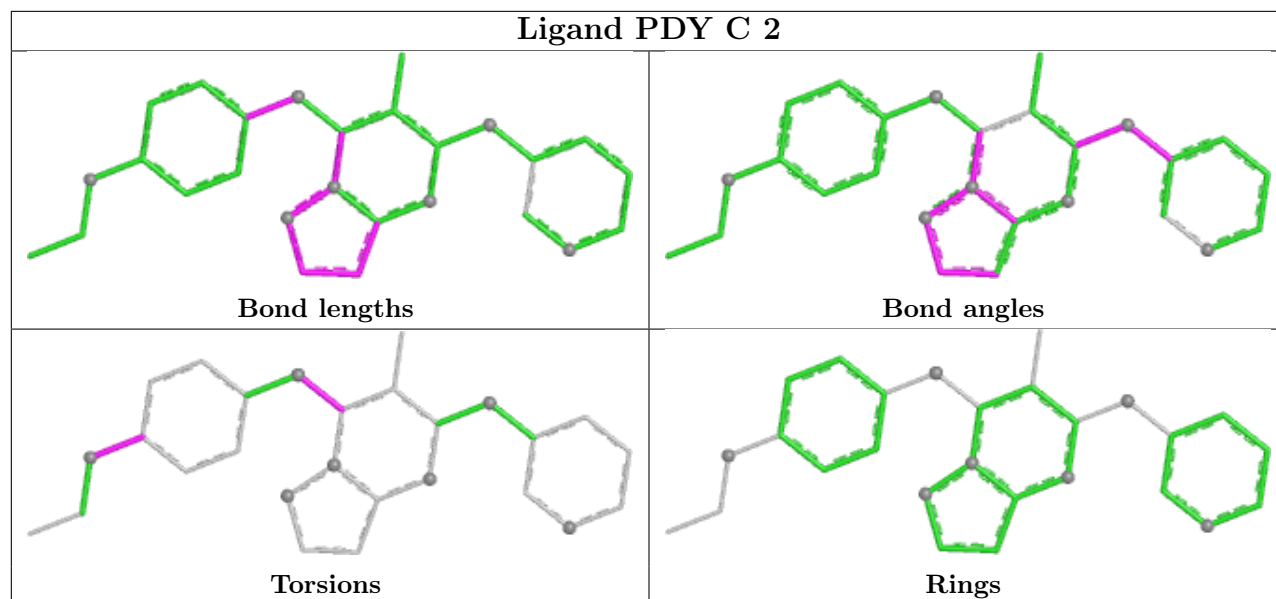
Ligand PDY L 1



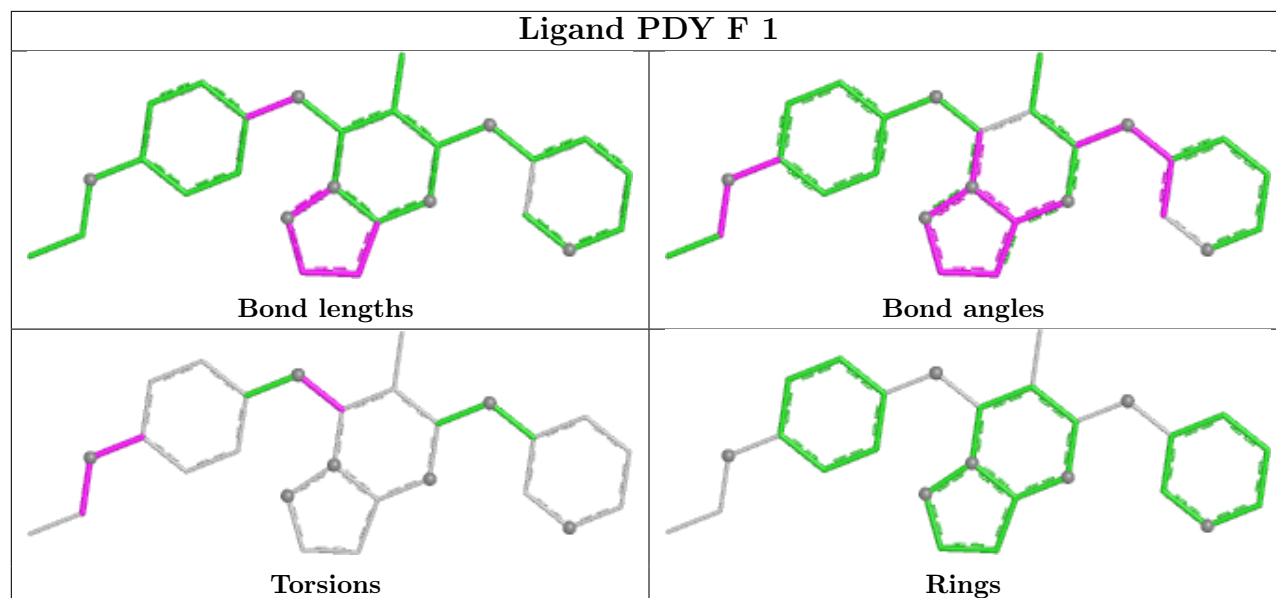
Ligand PDY J 2



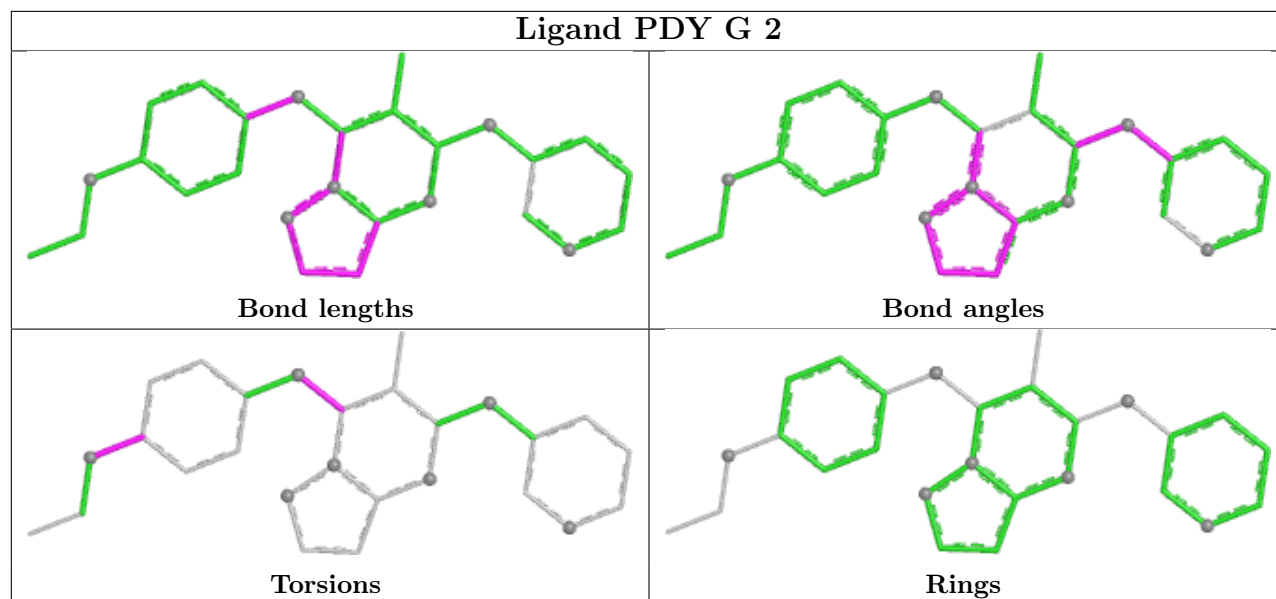
Ligand PDY C 2



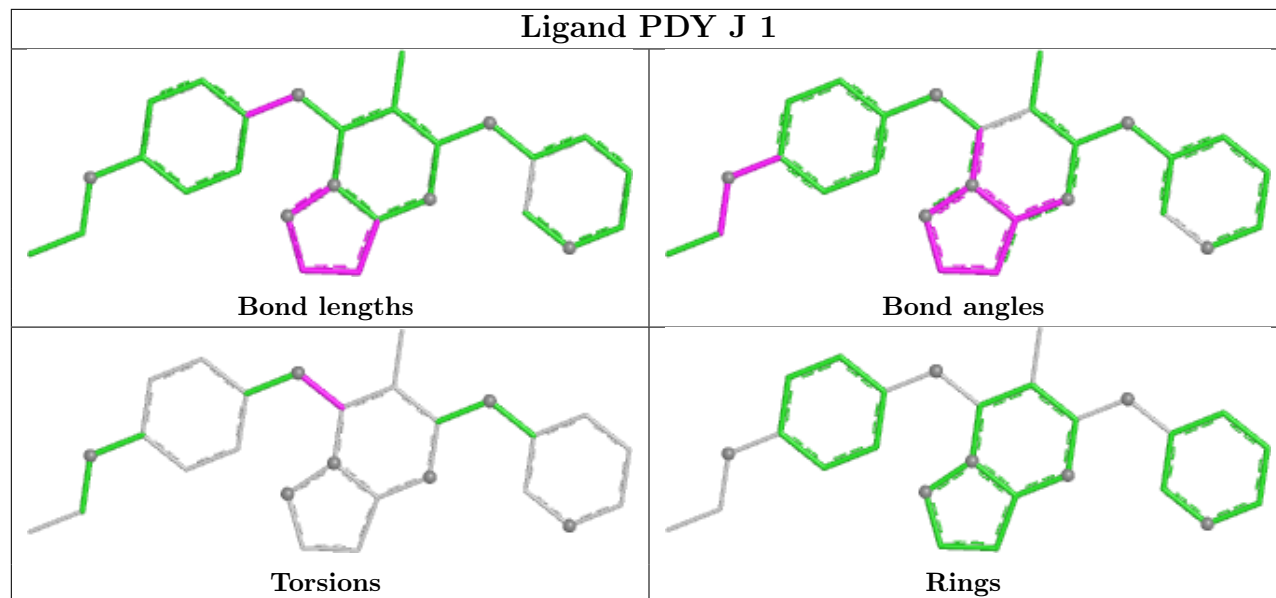
Ligand PDY F 1



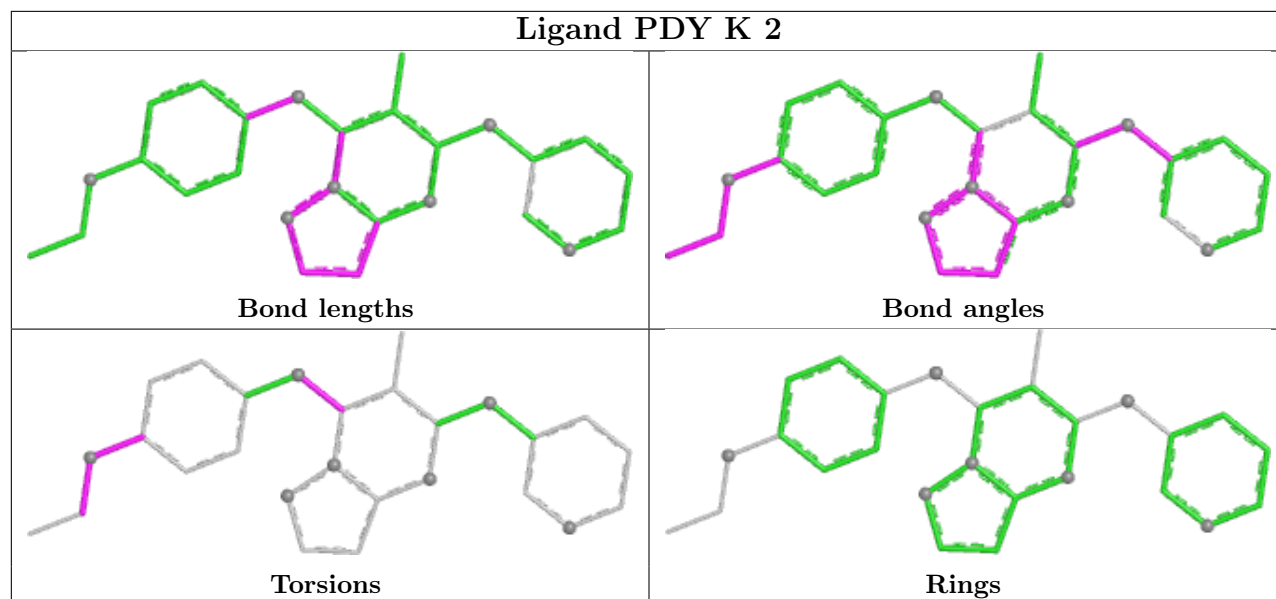
Ligand PDY G 2



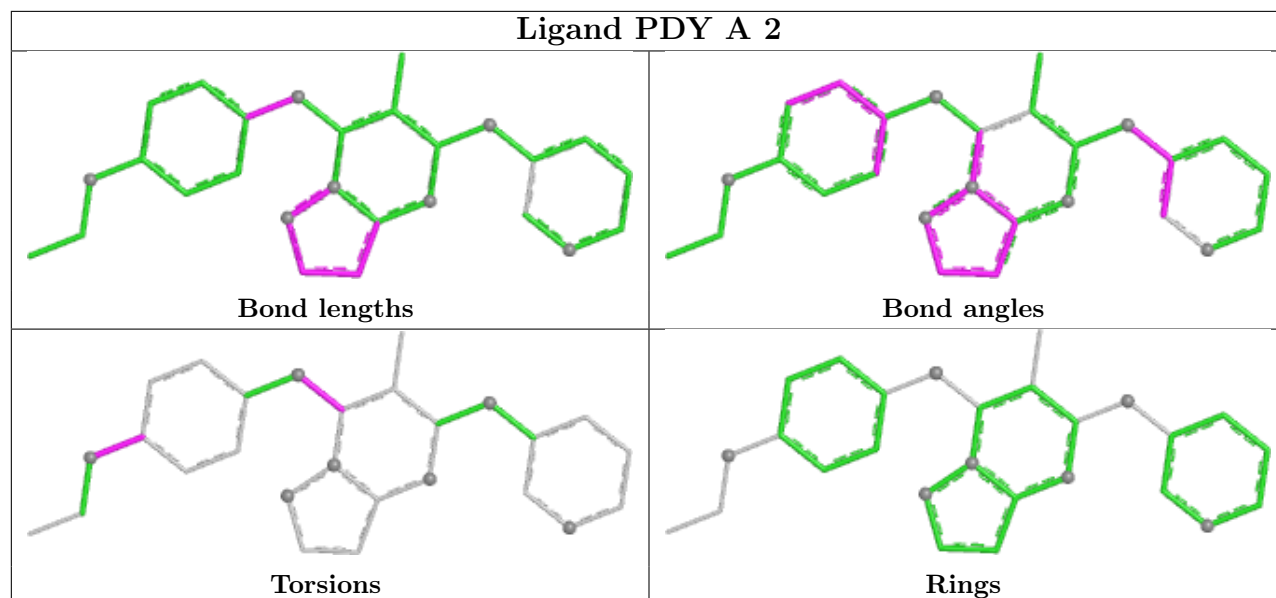
Ligand PDY J 1



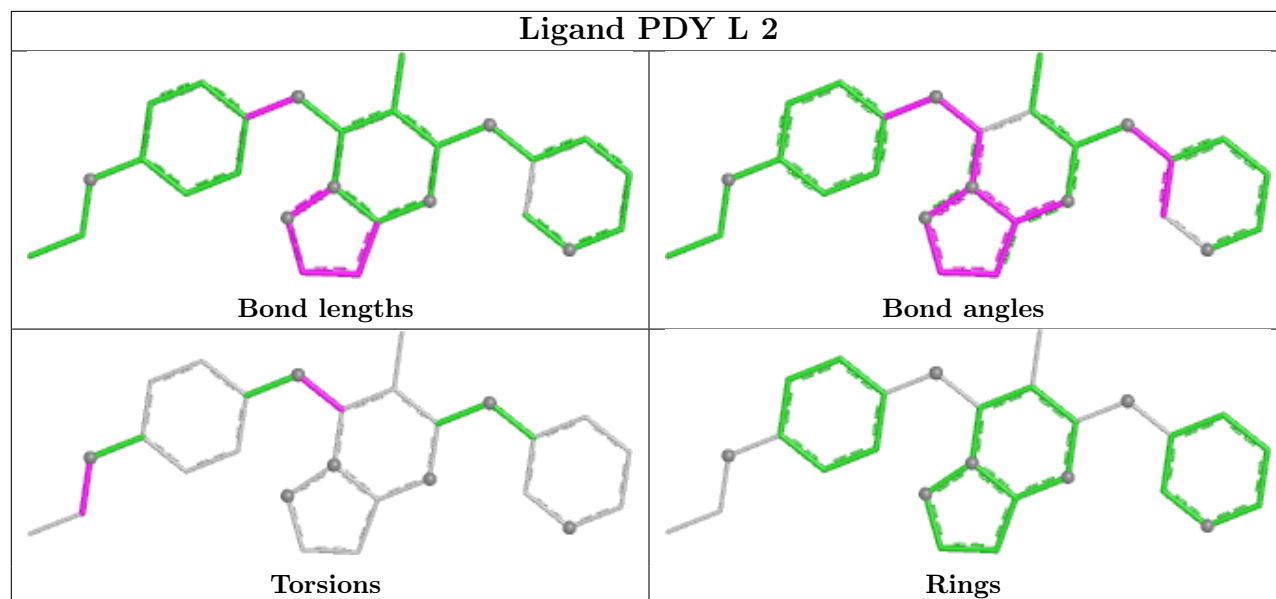
Ligand PDY K 2



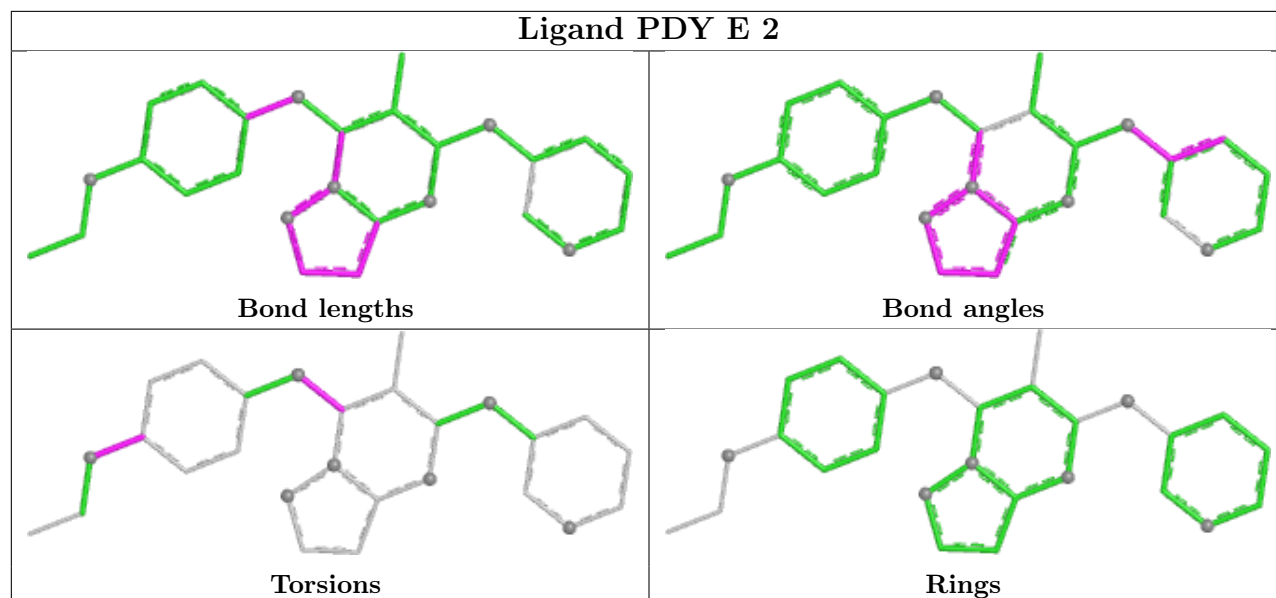
Ligand PDY A 2



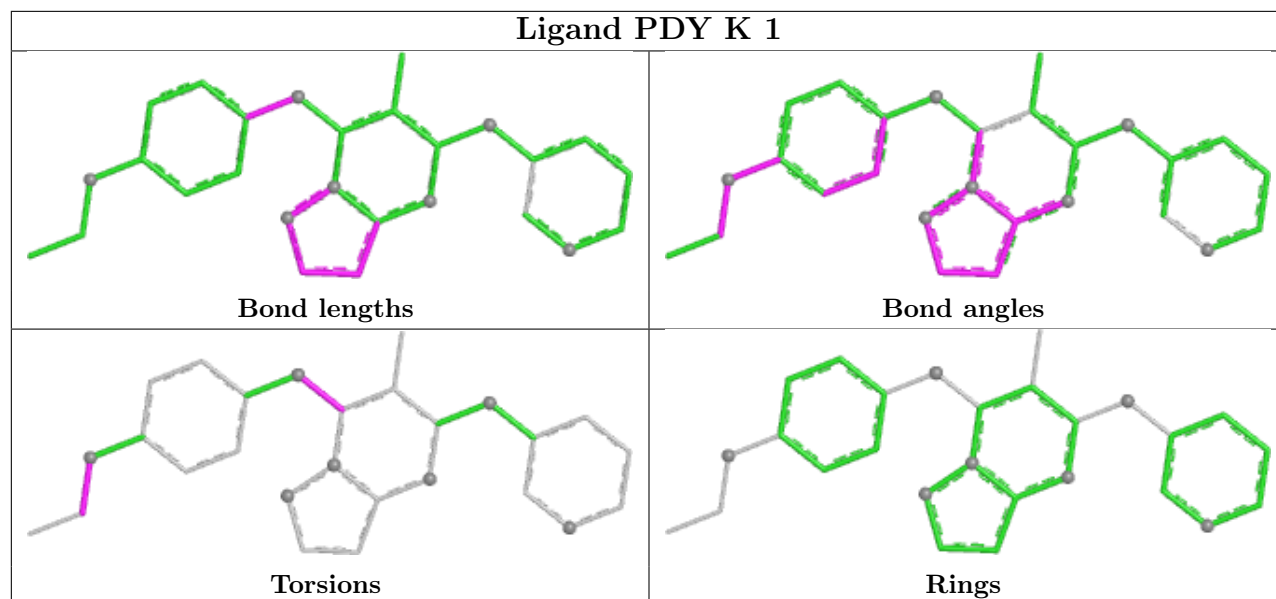
Ligand PDY L 2



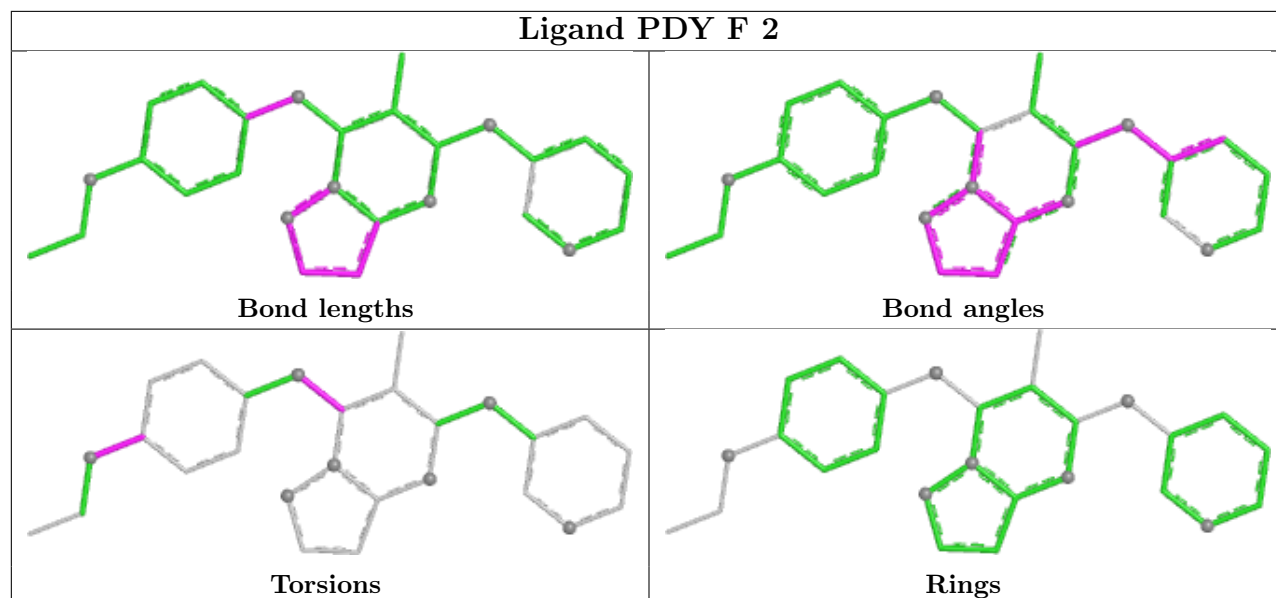
Ligand PDY E 2



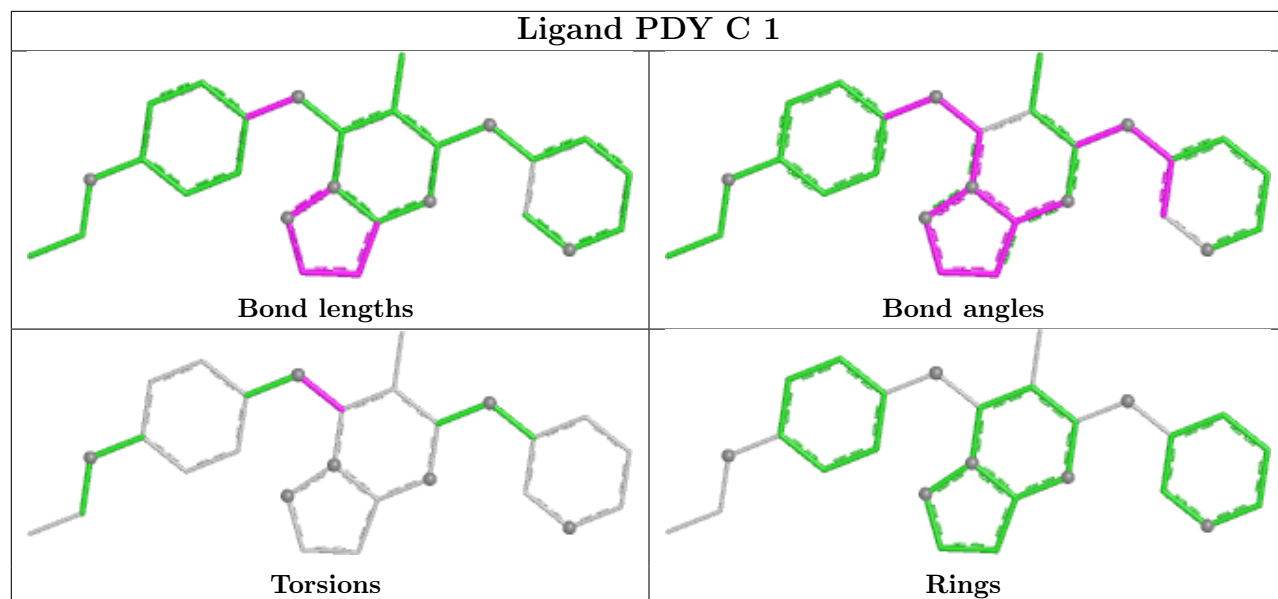
Ligand PDY K 1



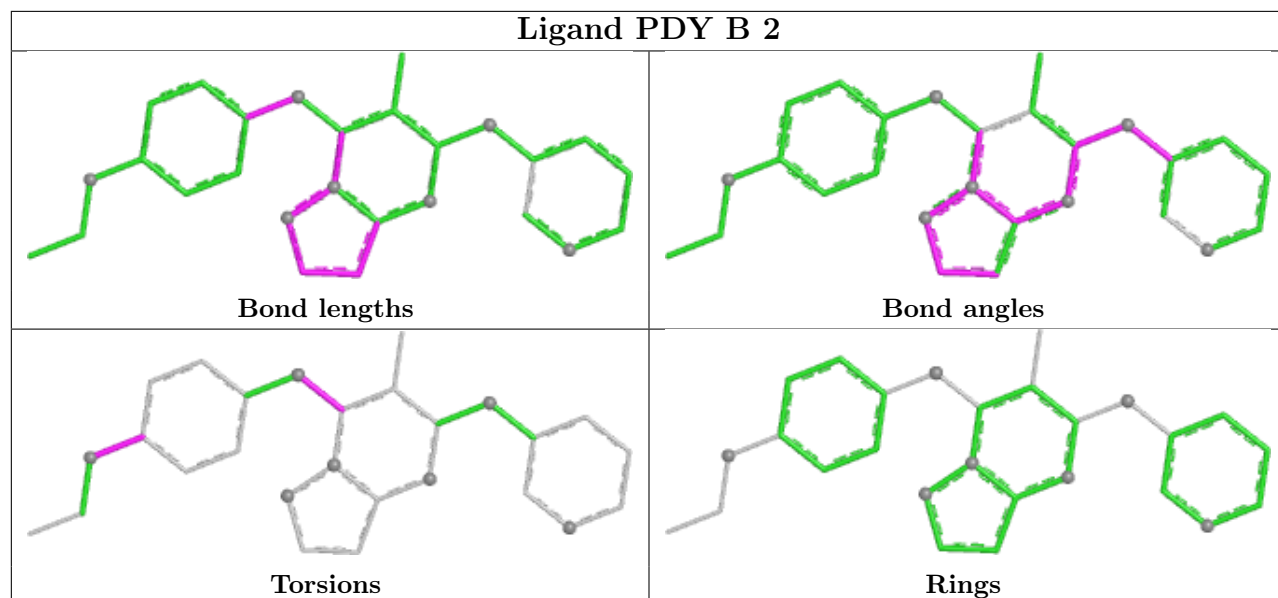
Ligand PDY F 2



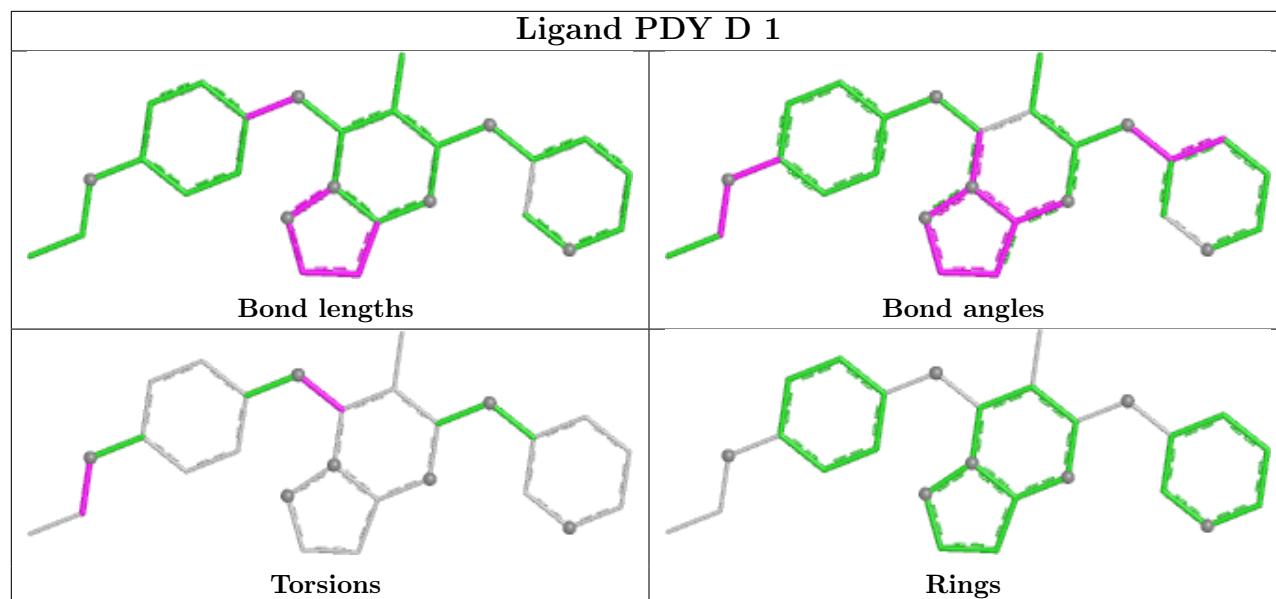
Ligand PDY C 1



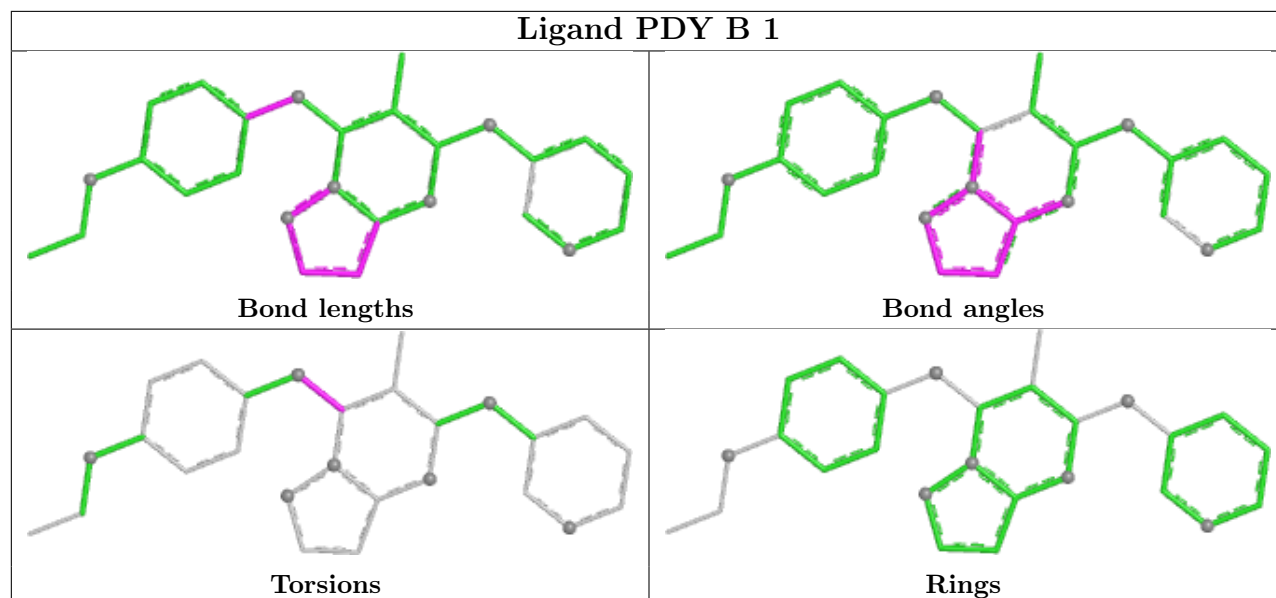
Ligand PDY B 2



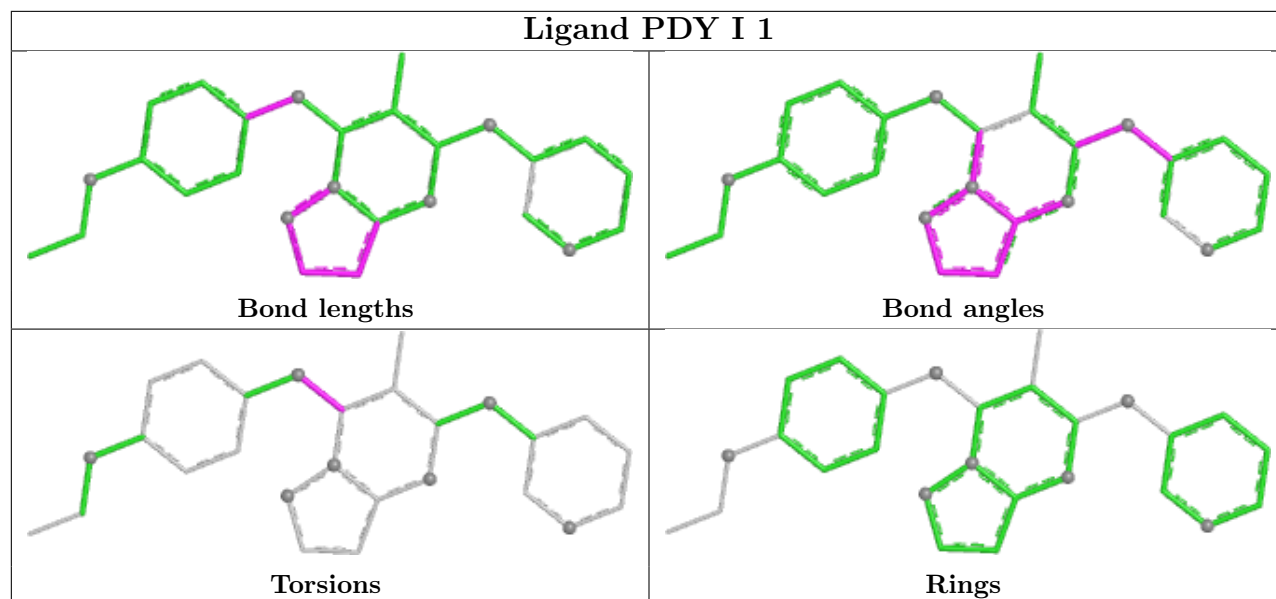
Ligand PDY D 1



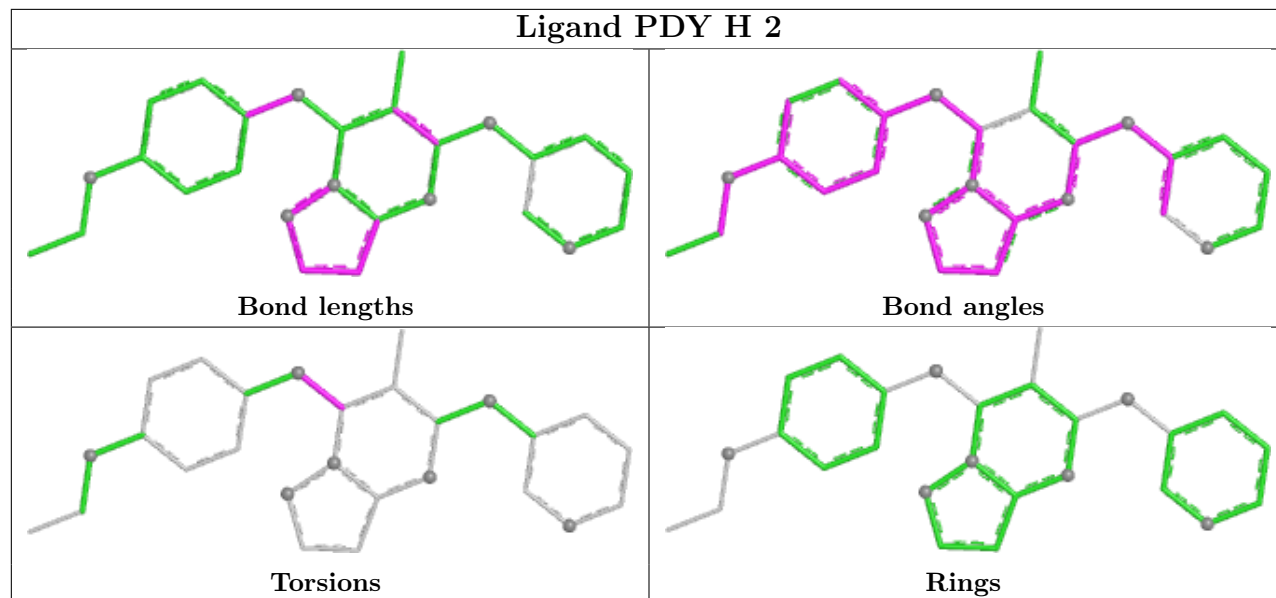
Ligand PDY B 1



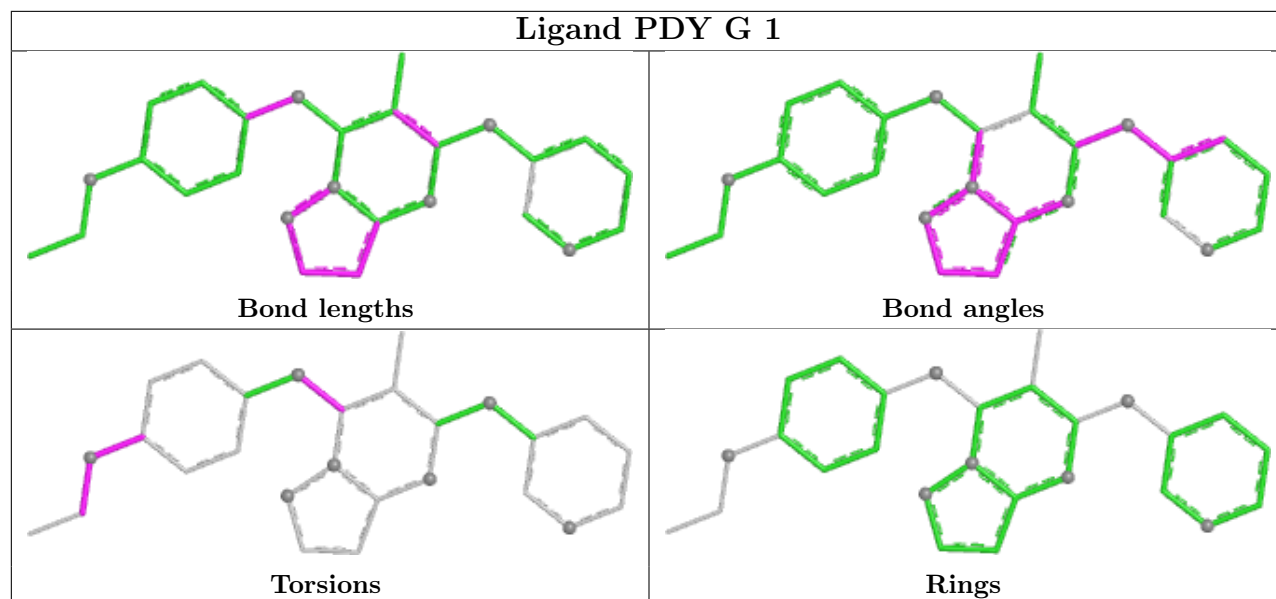
Ligand PDY I 1



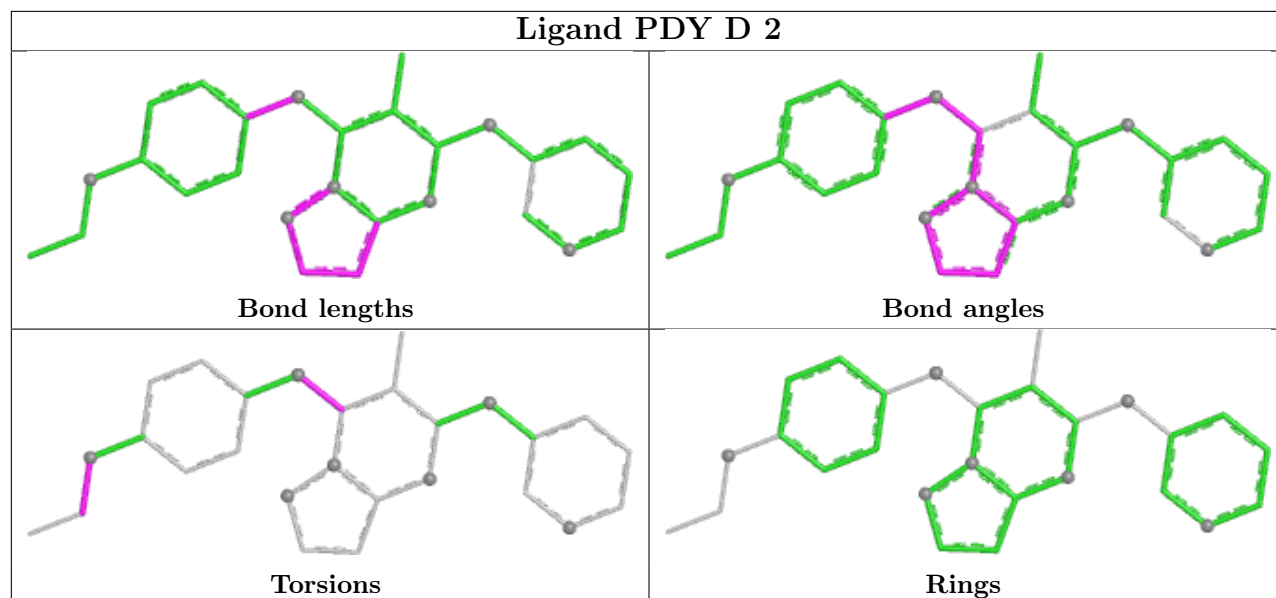
Ligand PDY H 2

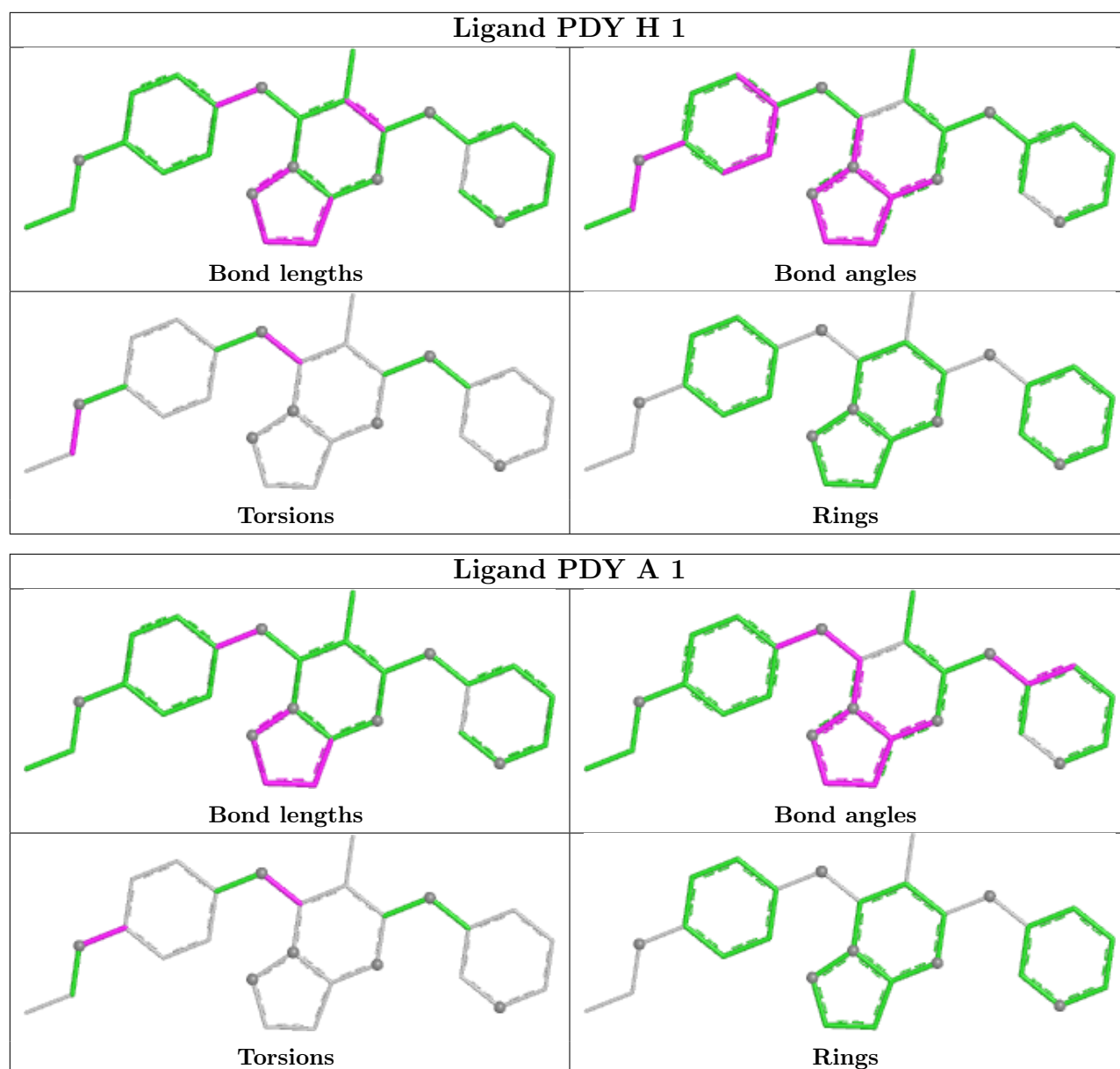


Ligand PDY G 1



Ligand PDY D 2





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/324 (84%)	-0.37	1 (0%) 88 85	8, 24, 56, 81	0
1	B	277/324 (85%)	-0.18	5 (1%) 67 59	7, 29, 71, 80	0
1	C	273/324 (84%)	0.01	7 (2%) 57 48	15, 40, 73, 83	0
1	D	277/324 (85%)	-0.14	6 (2%) 62 53	8, 32, 70, 81	0
1	E	276/324 (85%)	-0.29	6 (2%) 62 53	10, 28, 58, 76	0
1	F	287/324 (88%)	-0.22	9 (3%) 51 42	4, 25, 70, 86	0
1	G	273/324 (84%)	-0.03	4 (1%) 72 64	16, 38, 67, 79	0
1	H	275/324 (84%)	-0.06	6 (2%) 62 53	13, 39, 68, 84	0
1	I	275/324 (84%)	-0.19	7 (2%) 58 48	14, 30, 66, 97	0
1	J	275/324 (84%)	0.28	13 (4%) 36 28	27, 52, 81, 100	0
1	K	273/324 (84%)	0.22	11 (4%) 42 34	25, 49, 76, 98	0
1	L	276/324 (85%)	0.16	10 (3%) 46 38	15, 46, 83, 110	0
All	All	3311/3888 (85%)	-0.07	85 (2%) 57 48	4, 37, 73, 110	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	230	VAL	4.6
1	B	230	VAL	4.5
1	G	273	PRO	4.5
1	C	154	GLY	4.2
1	F	234	VAL	4.2
1	K	240	TYR	4.1
1	I	229	TYR	4.0
1	E	229	TYR	3.8
1	D	344	GLU	3.8
1	F	269	LEU	3.7
1	H	229	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	235	LEU	3.6
1	L	229	TYR	3.5
1	H	215	THR	3.5
1	J	215	THR	3.5
1	H	240	TYR	3.5
1	J	230	VAL	3.4
1	K	157	ALA	3.4
1	J	48	VAL	3.2
1	J	155	ASP	3.2
1	L	235	LEU	3.0
1	J	234	VAL	3.0
1	A	216	SER	3.0
1	C	229	TYR	2.9
1	F	229	TYR	2.9
1	G	229	TYR	2.8
1	J	229	TYR	2.8
1	L	155	ASP	2.8
1	E	344	GLU	2.7
1	B	155	ASP	2.7
1	L	230	VAL	2.7
1	C	86	THR	2.7
1	D	267	HIS	2.7
1	K	230	VAL	2.7
1	B	157	ALA	2.6
1	D	154	GLY	2.6
1	J	152	ASP	2.6
1	F	233	GLU	2.6
1	H	157	ALA	2.6
1	B	47	HIS	2.6
1	C	156	GLN	2.6
1	C	272	SER	2.5
1	C	230	VAL	2.5
1	J	294	VAL	2.5
1	K	344	GLU	2.5
1	H	200	ASN	2.5
1	K	75	ASN	2.5
1	K	235	LEU	2.4
1	L	266	ASN	2.4
1	G	240	TYR	2.4
1	J	69	VAL	2.3
1	D	156	GLN	2.3
1	E	230	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	285	GLU	2.3
1	K	99	PRO	2.3
1	F	240	TYR	2.3
1	I	240	TYR	2.3
1	C	234	VAL	2.3
1	K	289	PRO	2.3
1	J	200	ASN	2.3
1	E	272	SER	2.3
1	I	216	SER	2.3
1	I	234	VAL	2.3
1	I	266	ASN	2.2
1	E	216	SER	2.2
1	L	232	PRO	2.2
1	F	238	GLU	2.2
1	I	87	GLN	2.2
1	E	265	SER	2.2
1	L	334	THR	2.2
1	F	155	ASP	2.1
1	K	213	GLU	2.1
1	K	328	SER	2.1
1	L	75	ASN	2.1
1	B	329	THR	2.1
1	J	262	PRO	2.1
1	K	231	ALA	2.1
1	J	240	TYR	2.1
1	F	236	GLY	2.0
1	D	238	GLU	2.0
1	H	69	VAL	2.0
1	J	216	SER	2.0
1	D	273	PRO	2.0
1	G	329	THR	2.0
1	L	234	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

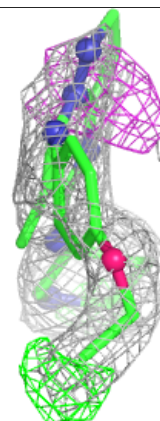
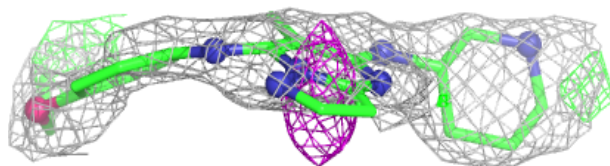
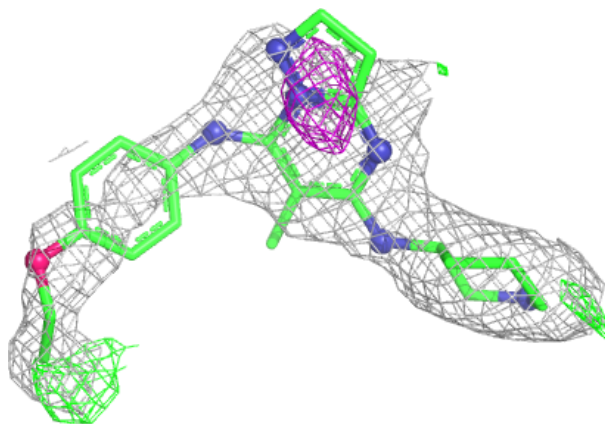
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PDY	D	2	27/27	0.62	0.21	65,74,80,81	0
2	PDY	K	2	27/27	0.69	0.16	61,67,79,80	0
2	PDY	E	2	27/27	0.70	0.18	60,67,69,69	0
2	PDY	I	2	27/27	0.71	0.18	53,61,74,75	0
2	PDY	L	2	27/27	0.72	0.18	71,75,77,77	0
2	PDY	A	2	27/27	0.73	0.17	60,65,69,71	0
2	PDY	G	2	27/27	0.80	0.13	52,56,64,64	0
2	PDY	H	2	27/27	0.81	0.14	52,55,60,60	0
3	SO4	F	3	5/5	0.82	0.12	61,62,64,65	0
2	PDY	J	2	27/27	0.84	0.13	59,62,67,68	0
2	PDY	C	2	27/27	0.87	0.11	48,50,62,63	0
2	PDY	B	2	27/27	0.92	0.09	20,29,34,35	0
2	PDY	C	1	27/27	0.92	0.10	18,32,56,58	0
2	PDY	F	2	27/27	0.94	0.08	20,24,28,29	0
2	PDY	K	1	27/27	0.94	0.09	27,44,54,55	0
2	PDY	I	1	27/27	0.94	0.08	5,19,43,45	0
2	PDY	L	1	27/27	0.94	0.08	30,34,47,50	0
2	PDY	H	1	27/27	0.94	0.09	22,31,54,55	0
2	PDY	J	1	27/27	0.94	0.08	31,39,54,55	0
2	PDY	F	1	27/27	0.95	0.07	5,15,32,34	0
2	PDY	D	1	27/27	0.95	0.08	16,23,43,44	0
2	PDY	G	1	27/27	0.95	0.07	4,20,38,43	0
2	PDY	B	1	27/27	0.96	0.07	6,16,37,38	0
2	PDY	E	1	27/27	0.96	0.07	7,23,37,38	0
2	PDY	A	1	27/27	0.97	0.07	2,11,31,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

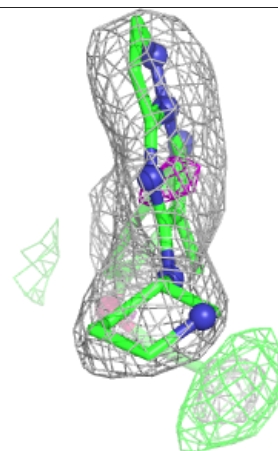
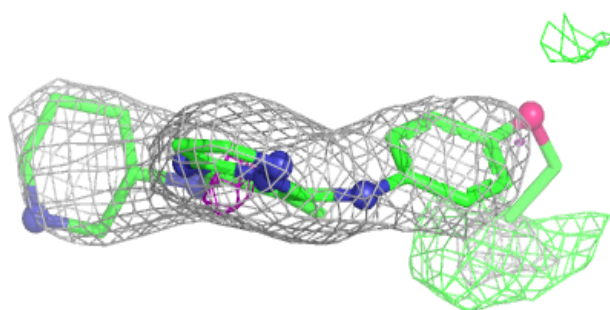
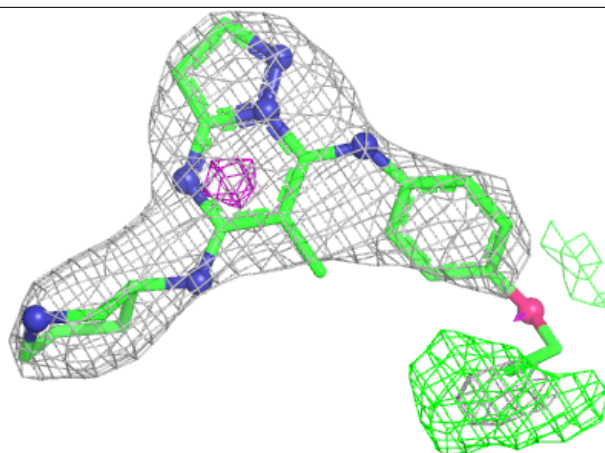
Electron density around PDY D 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

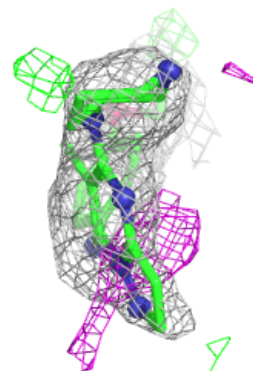
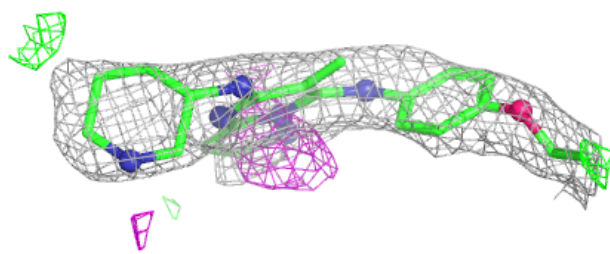
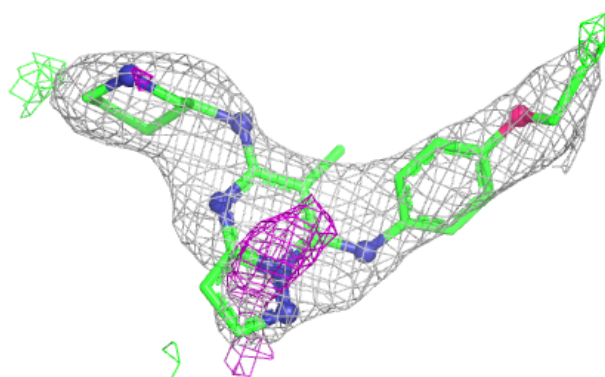


Electron density around PDY K 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

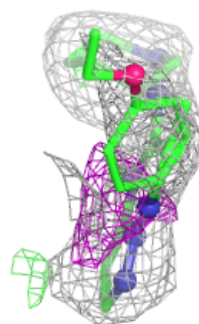
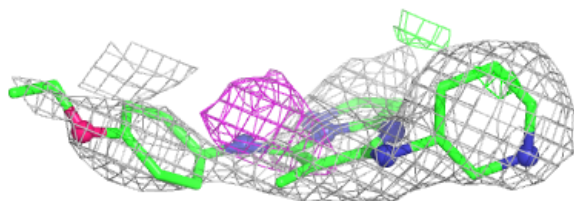
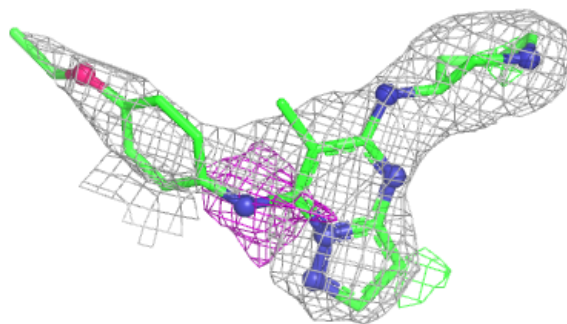
**Electron density around PDY E 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

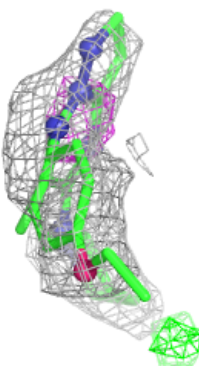
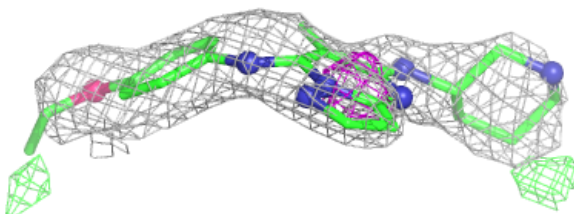
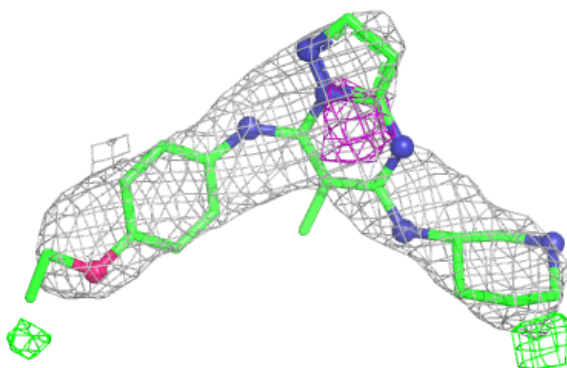


Electron density around PDY I 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

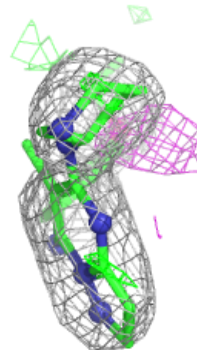
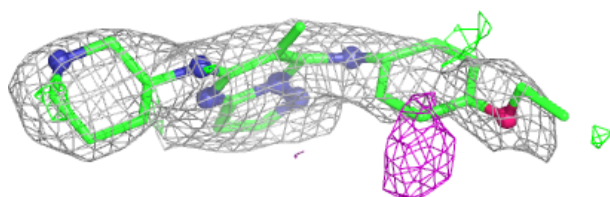
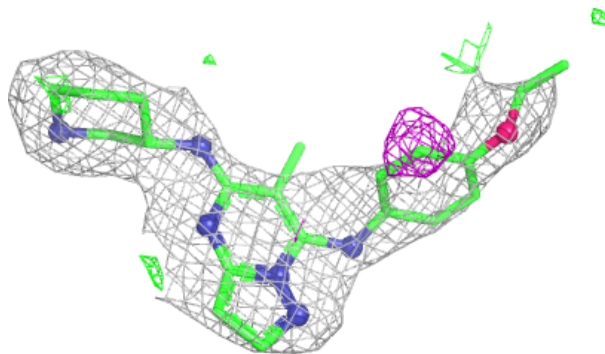
**Electron density around PDY L 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

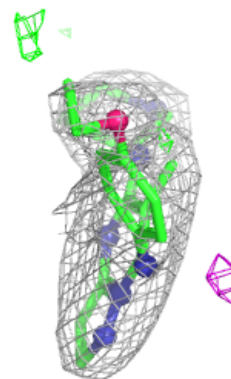
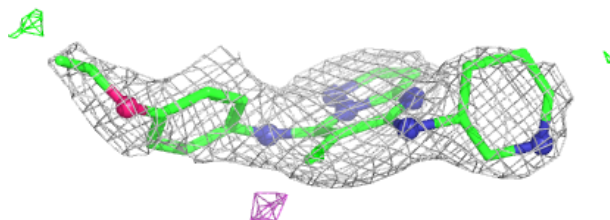
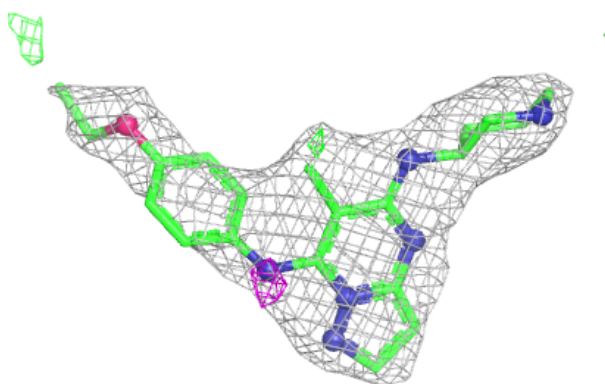


Electron density around PDY A 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

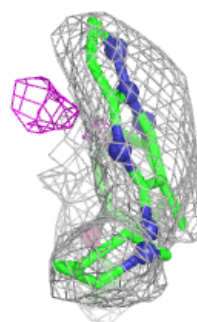
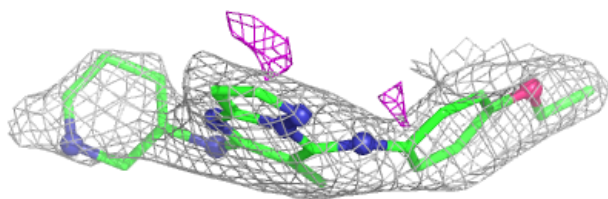
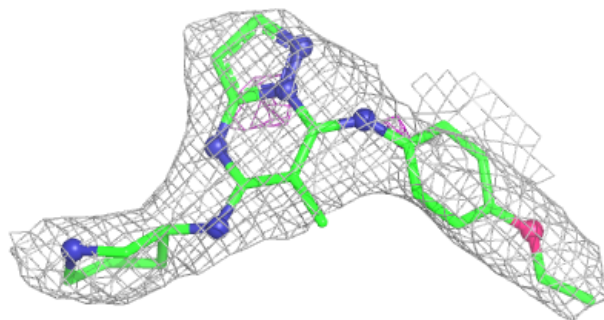
**Electron density around PDY G 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

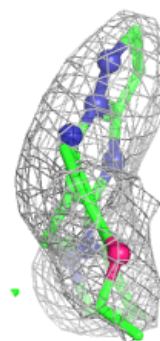
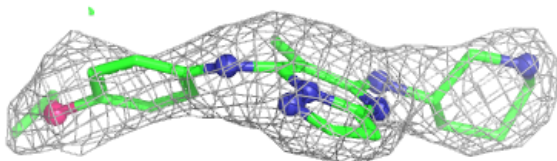
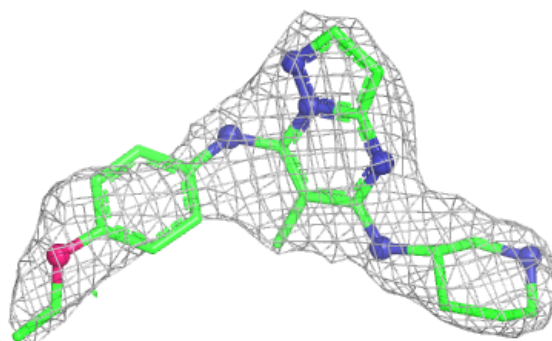


Electron density around PDY H 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

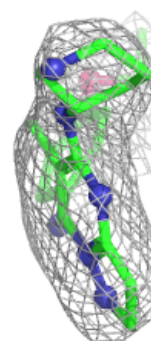
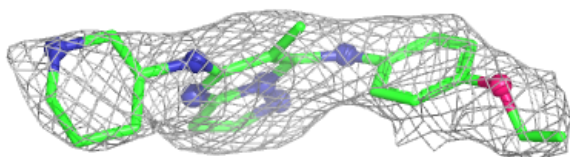
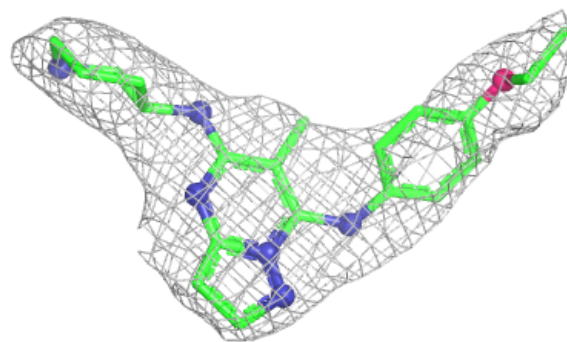
**Electron density around PDY J 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

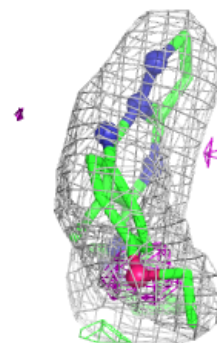
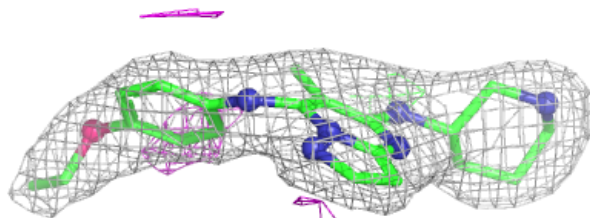
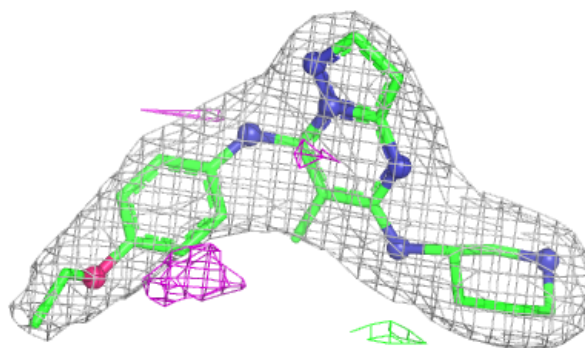


Electron density around PDY C 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

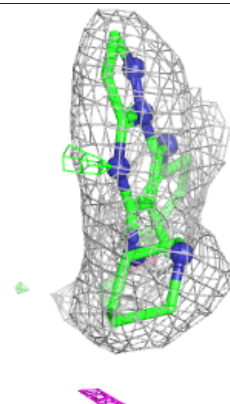
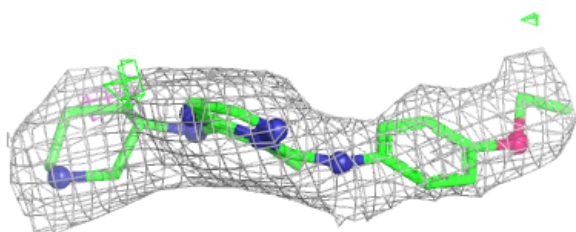
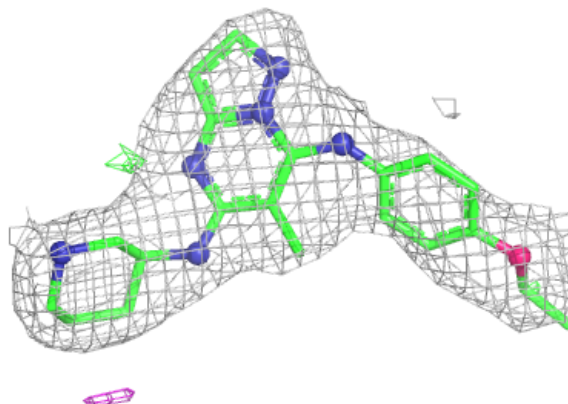
**Electron density around PDY B 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

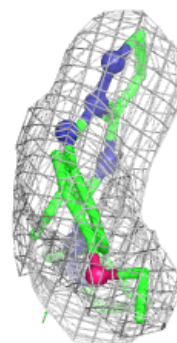
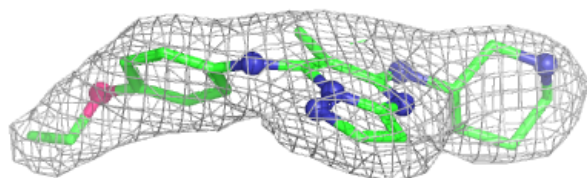
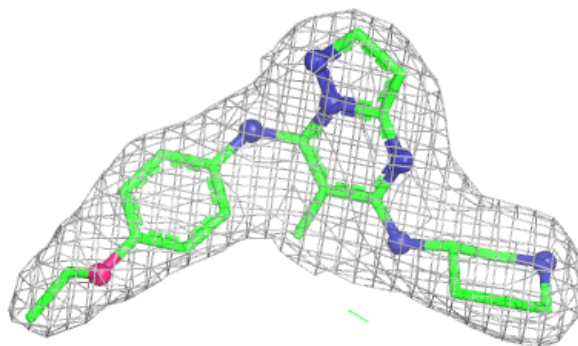


Electron density around PDY C 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

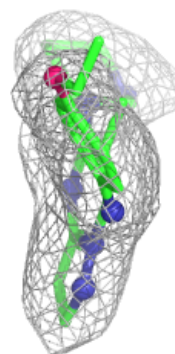
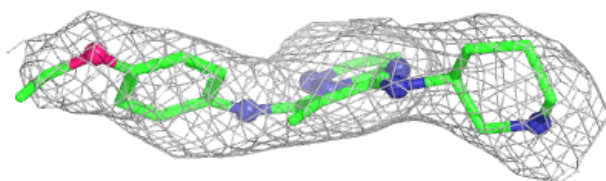
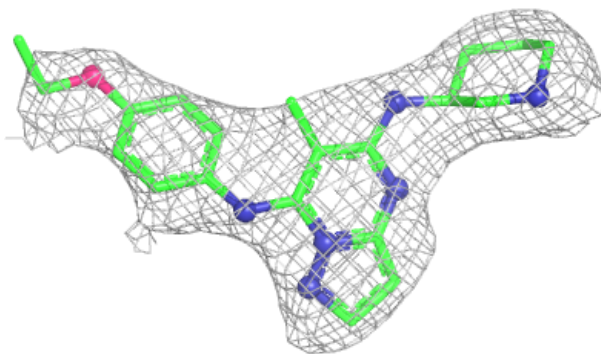
**Electron density around PDY F 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

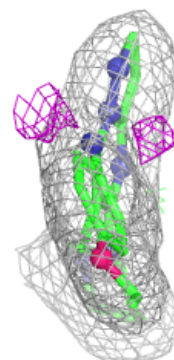
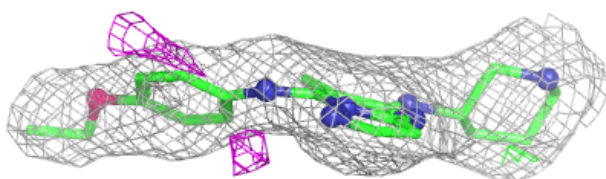
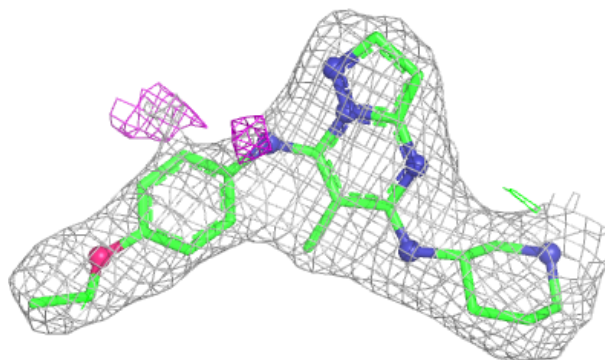


Electron density around PDY K 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

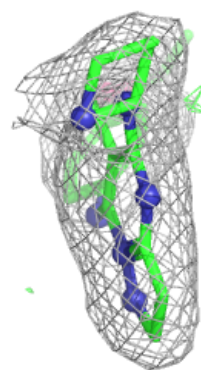
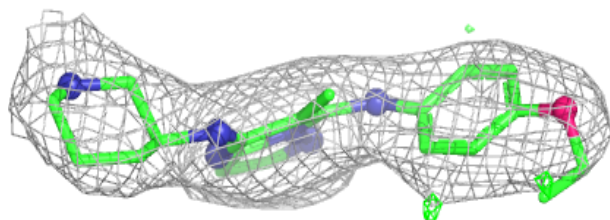
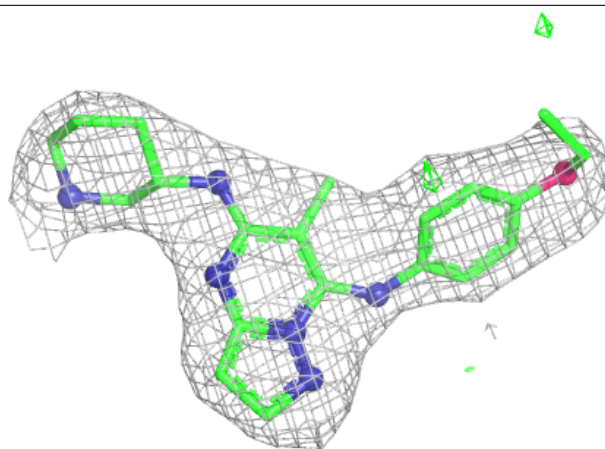
**Electron density around PDY I 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



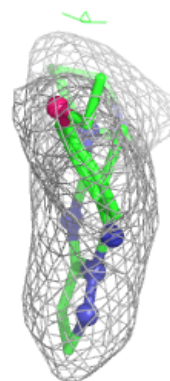
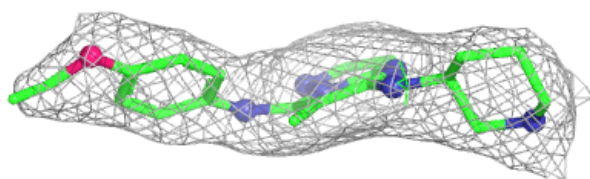
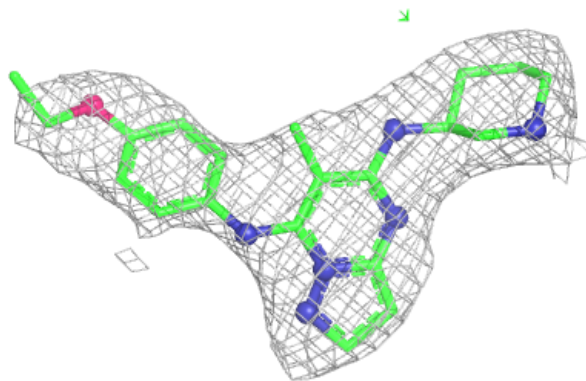
Electron density around PDY L 1:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

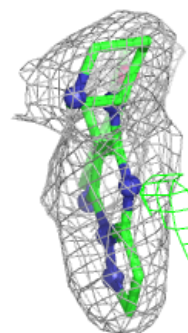
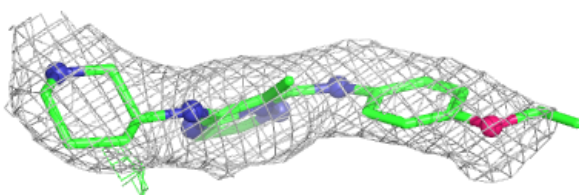
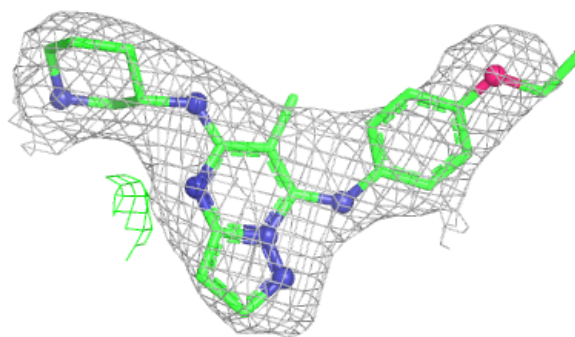


Electron density around PDY H 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

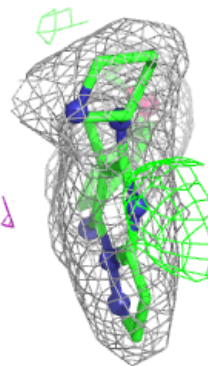
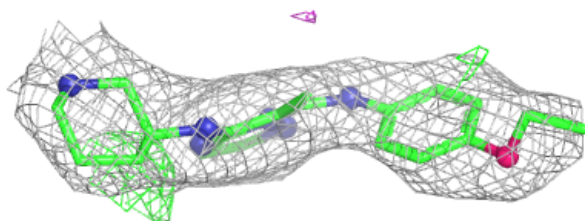
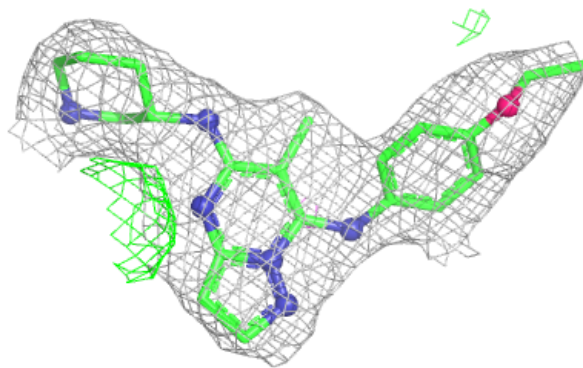
**Electron density around PDY J 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

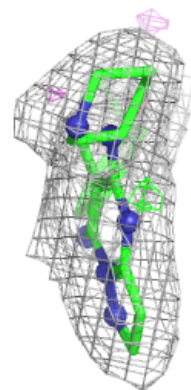
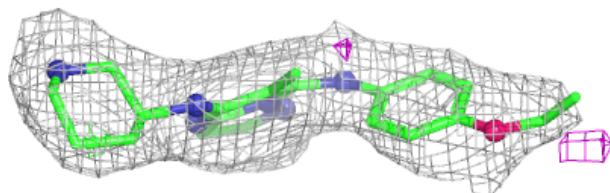
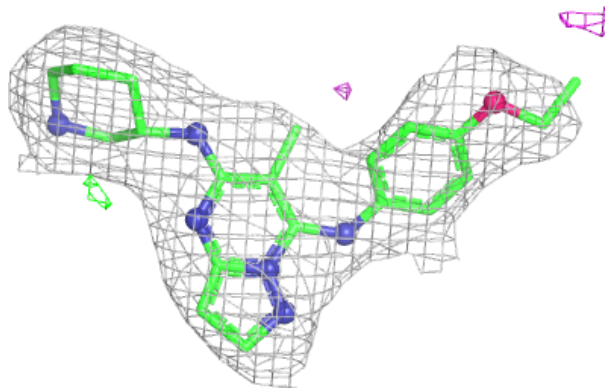


Electron density around PDY F 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

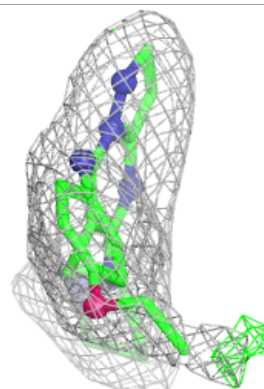
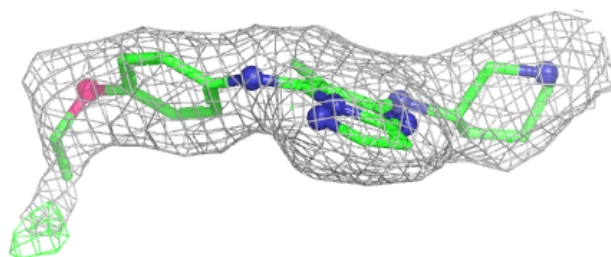
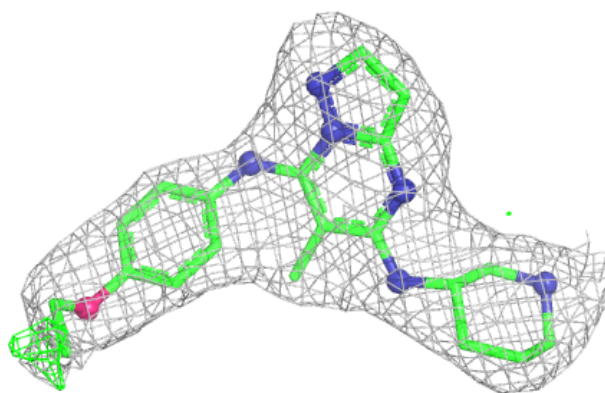
**Electron density around PDY D 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

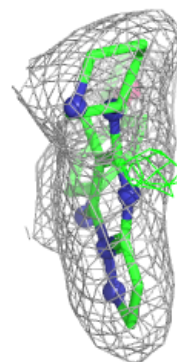
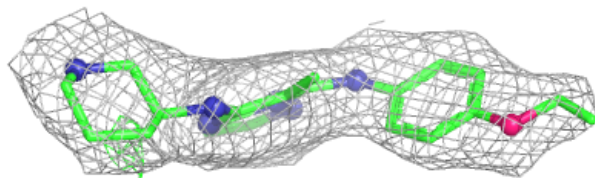
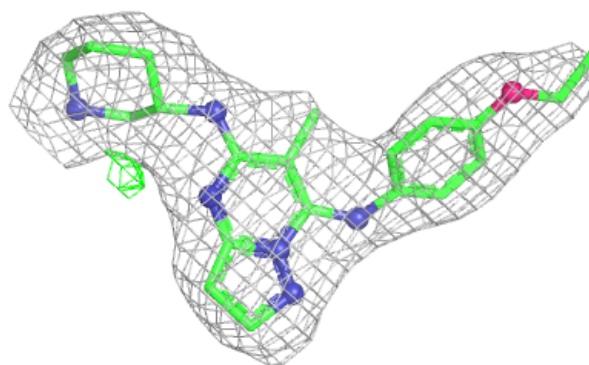


Electron density around PDY G 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

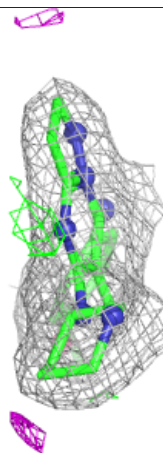
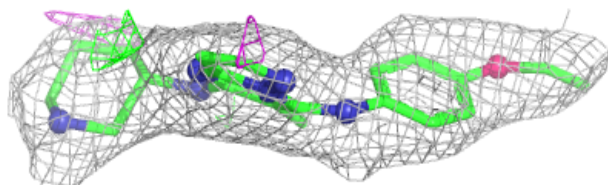
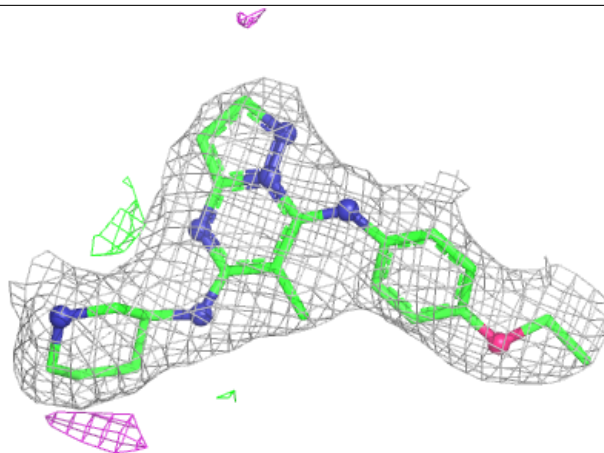
**Electron density around PDY B 1:**

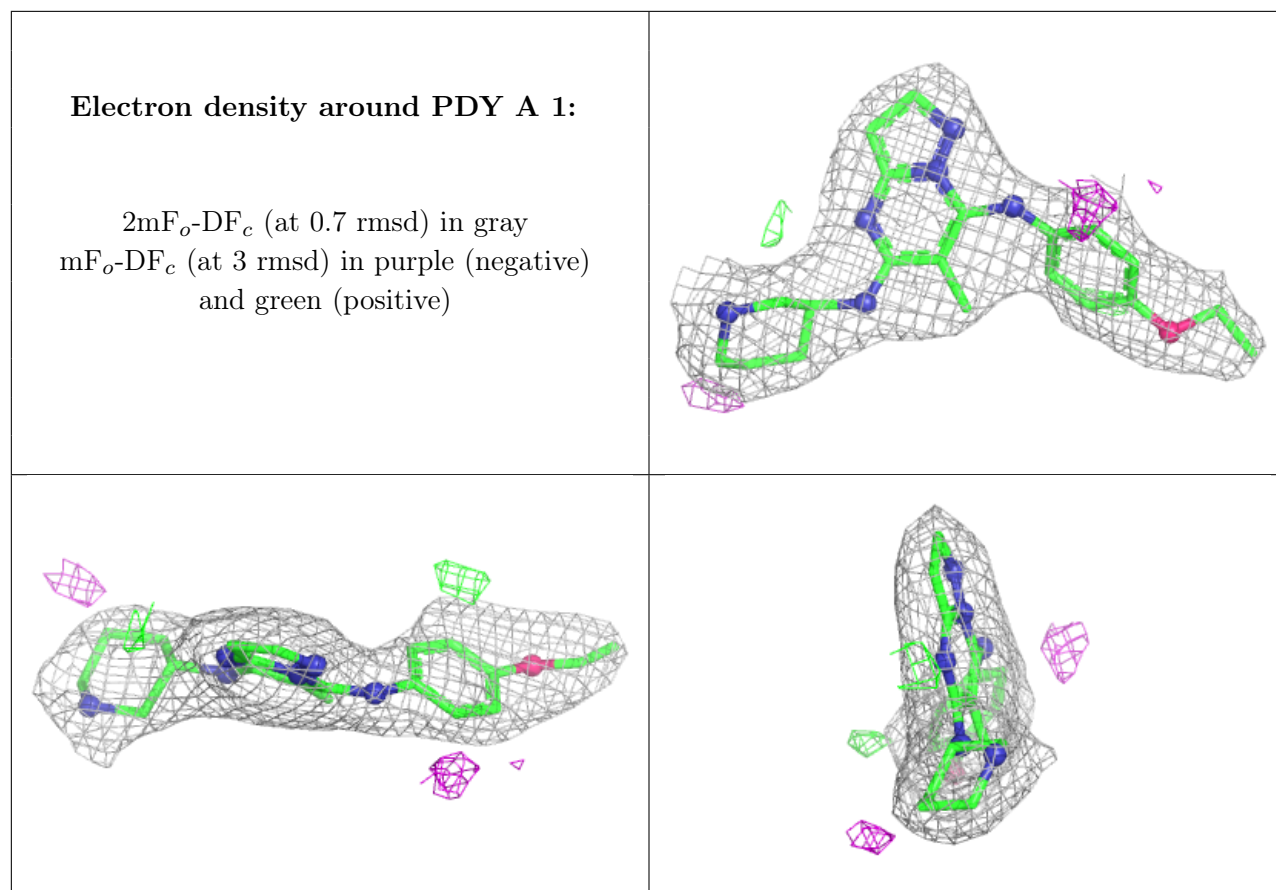
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PDY E 1:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.