



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 PM UTC

PDB ID : 3C2W / pdb_00003c2w
Title : Crystal structure of the photosensory core domain of *P. aeruginosa* bacterio-
phytochrome PaBphP in the Pfr state
Authors : Yang, X.; Kuk, J.; Moffat, K.
Deposited on : 2008-01-25
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

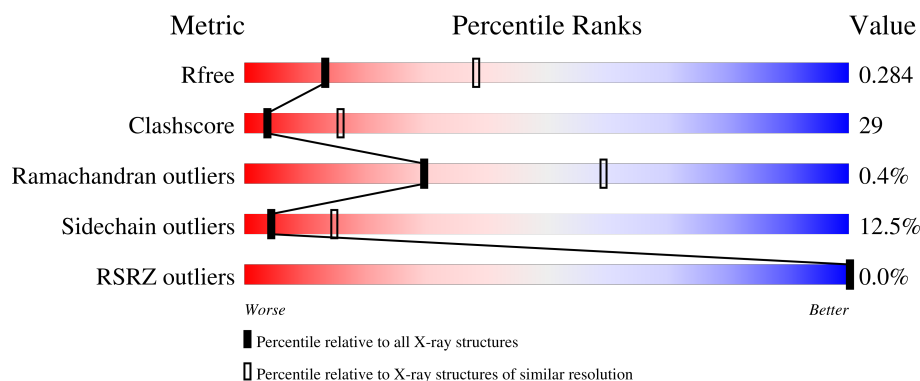
1 Overall quality at a glance

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	505	
1	B	505	
1	C	505	
1	D	505	
1	E	505	

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Mol	Chain	Length	Quality of chain
1	F	505	48%37%8%7%
1	G	505	43%43%10%5%
1	H	505	48%41%7%5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30494 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3782	2382	681	700	19			
1	B	468	Total	C	N	O	S	0	0	0
			3693	2322	663	689	19			
1	C	482	Total	C	N	O	S	0	0	0
			3812	2398	688	707	19			
1	D	478	Total	C	N	O	S	0	0	0
			3788	2383	683	703	19			
1	E	471	Total	C	N	O	S	0	0	0
			3725	2344	673	689	19			
1	F	469	Total	C	N	O	S	0	0	0
			3704	2331	664	690	19			
1	G	482	Total	C	N	O	S	0	1	0
			3816	2401	688	707	20			
1	H	480	Total	C	N	O	S	0	0	0
			3800	2392	686	703	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP Q9HWR3
A	499	GLU	-	expression tag	UNP Q9HWR3
A	500	HIS	-	expression tag	UNP Q9HWR3
A	501	HIS	-	expression tag	UNP Q9HWR3
A	502	HIS	-	expression tag	UNP Q9HWR3
A	503	HIS	-	expression tag	UNP Q9HWR3
A	504	HIS	-	expression tag	UNP Q9HWR3
A	505	HIS	-	expression tag	UNP Q9HWR3
B	498	LEU	-	expression tag	UNP Q9HWR3
B	499	GLU	-	expression tag	UNP Q9HWR3
B	500	HIS	-	expression tag	UNP Q9HWR3
B	501	HIS	-	expression tag	UNP Q9HWR3
B	502	HIS	-	expression tag	UNP Q9HWR3

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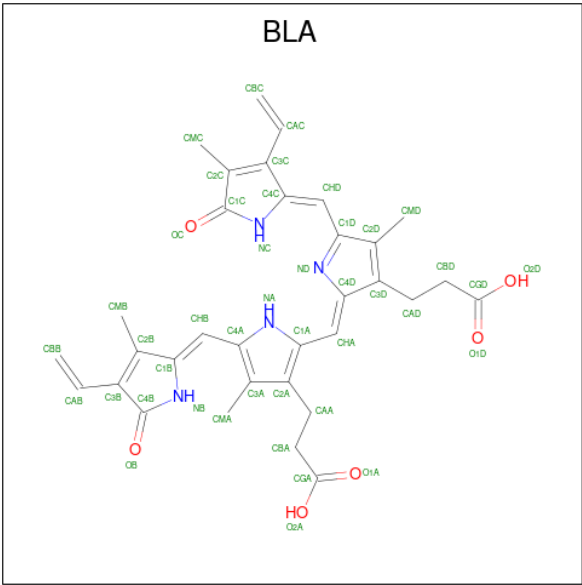
Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3
C	498	LEU	-	expression tag	UNP Q9HWR3
C	499	GLU	-	expression tag	UNP Q9HWR3
C	500	HIS	-	expression tag	UNP Q9HWR3
C	501	HIS	-	expression tag	UNP Q9HWR3
C	502	HIS	-	expression tag	UNP Q9HWR3
C	503	HIS	-	expression tag	UNP Q9HWR3
C	504	HIS	-	expression tag	UNP Q9HWR3
C	505	HIS	-	expression tag	UNP Q9HWR3
D	498	LEU	-	expression tag	UNP Q9HWR3
D	499	GLU	-	expression tag	UNP Q9HWR3
D	500	HIS	-	expression tag	UNP Q9HWR3
D	501	HIS	-	expression tag	UNP Q9HWR3
D	502	HIS	-	expression tag	UNP Q9HWR3
D	503	HIS	-	expression tag	UNP Q9HWR3
D	504	HIS	-	expression tag	UNP Q9HWR3
D	505	HIS	-	expression tag	UNP Q9HWR3
E	498	LEU	-	expression tag	UNP Q9HWR3
E	499	GLU	-	expression tag	UNP Q9HWR3
E	500	HIS	-	expression tag	UNP Q9HWR3
E	501	HIS	-	expression tag	UNP Q9HWR3
E	502	HIS	-	expression tag	UNP Q9HWR3
E	503	HIS	-	expression tag	UNP Q9HWR3
E	504	HIS	-	expression tag	UNP Q9HWR3
E	505	HIS	-	expression tag	UNP Q9HWR3
F	498	LEU	-	expression tag	UNP Q9HWR3
F	499	GLU	-	expression tag	UNP Q9HWR3
F	500	HIS	-	expression tag	UNP Q9HWR3
F	501	HIS	-	expression tag	UNP Q9HWR3
F	502	HIS	-	expression tag	UNP Q9HWR3
F	503	HIS	-	expression tag	UNP Q9HWR3
F	504	HIS	-	expression tag	UNP Q9HWR3
F	505	HIS	-	expression tag	UNP Q9HWR3
G	498	LEU	-	expression tag	UNP Q9HWR3
G	499	GLU	-	expression tag	UNP Q9HWR3
G	500	HIS	-	expression tag	UNP Q9HWR3
G	501	HIS	-	expression tag	UNP Q9HWR3
G	502	HIS	-	expression tag	UNP Q9HWR3
G	503	HIS	-	expression tag	UNP Q9HWR3
G	504	HIS	-	expression tag	UNP Q9HWR3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	505	HIS	-	expression tag	UNP Q9HWR3
H	498	LEU	-	expression tag	UNP Q9HWR3
H	499	GLU	-	expression tag	UNP Q9HWR3
H	500	HIS	-	expression tag	UNP Q9HWR3
H	501	HIS	-	expression tag	UNP Q9HWR3
H	502	HIS	-	expression tag	UNP Q9HWR3
H	503	HIS	-	expression tag	UNP Q9HWR3
H	504	HIS	-	expression tag	UNP Q9HWR3
H	505	HIS	-	expression tag	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: C₃₃H₃₄N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		
2	E	1	Total	C	N	O	0	0
			43	33	4	6		
2	F	1	Total	C	N	O	0	0
			43	33	4	6		
2	G	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			43	33	4	6		

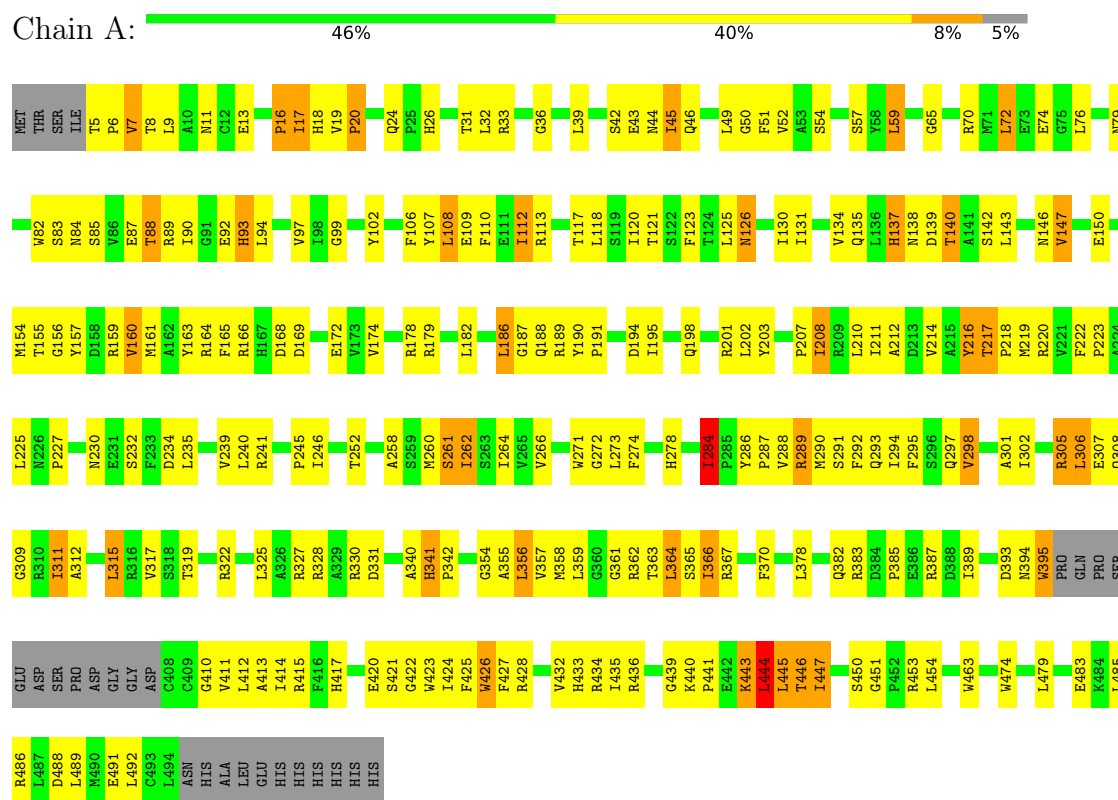
- Molecule 3 is water.

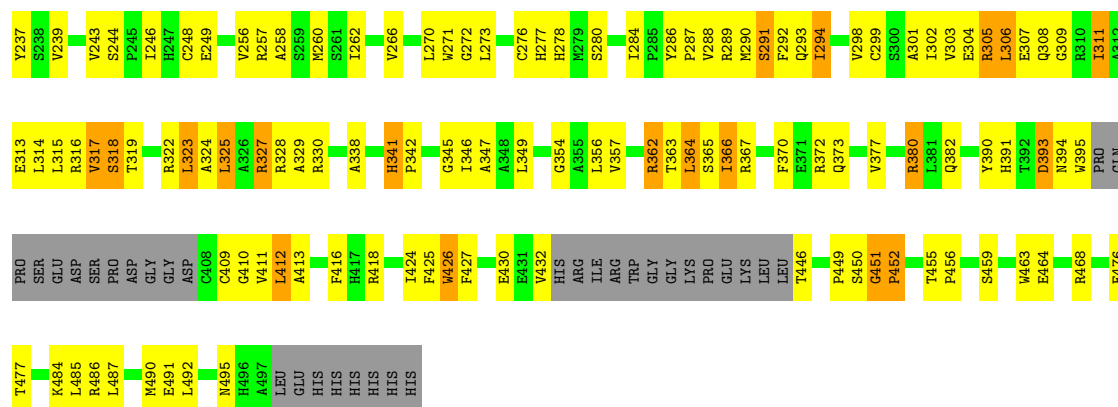
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	2	Total	O	0	0
			2	2		
3	C	6	Total	O	0	0
			6	6		
3	D	3	Total	O	0	0
			3	3		
3	E	1	Total	O	0	0
			1	1		
3	F	2	Total	O	0	0
			2	2		
3	G	7	Total	O	0	0
			7	7		
3	H	2	Total	O	0	0
			2	2		

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.

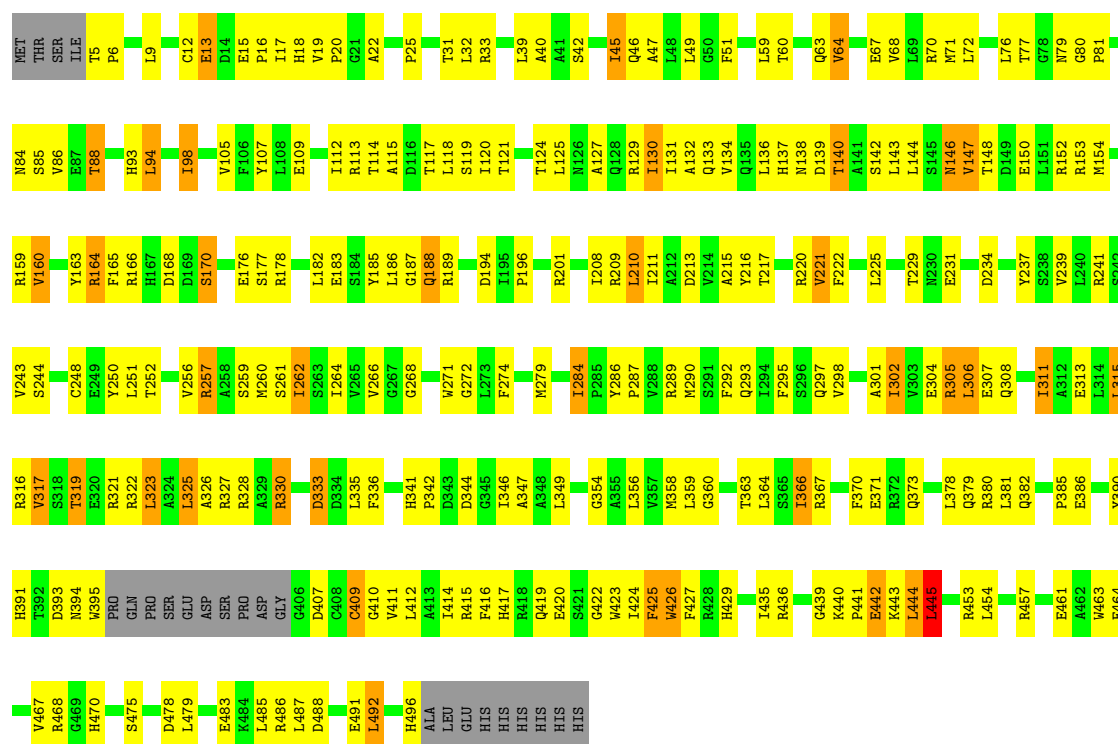
• Molecule 1: Bacteriophytochrome





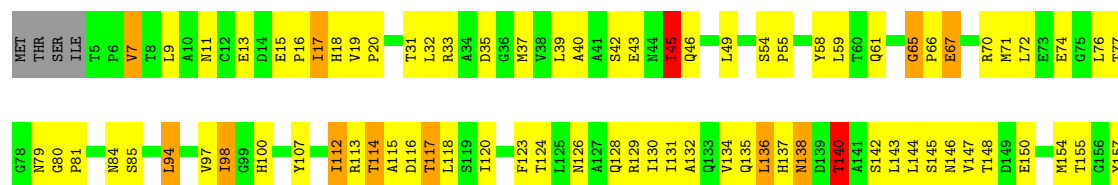
• Molecule 1: Bacteriophytochrome

Chain C: 46% 42% 7% 5%

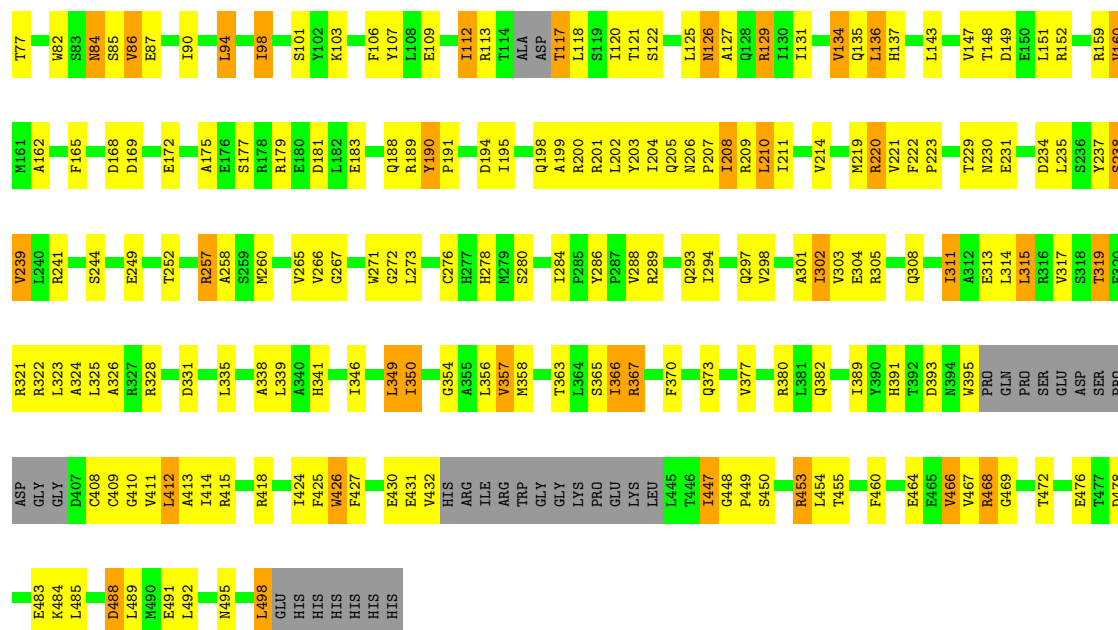


• Molecule 1: Bacteriophytochrome

Chain D: 47% 41% 7% 5%

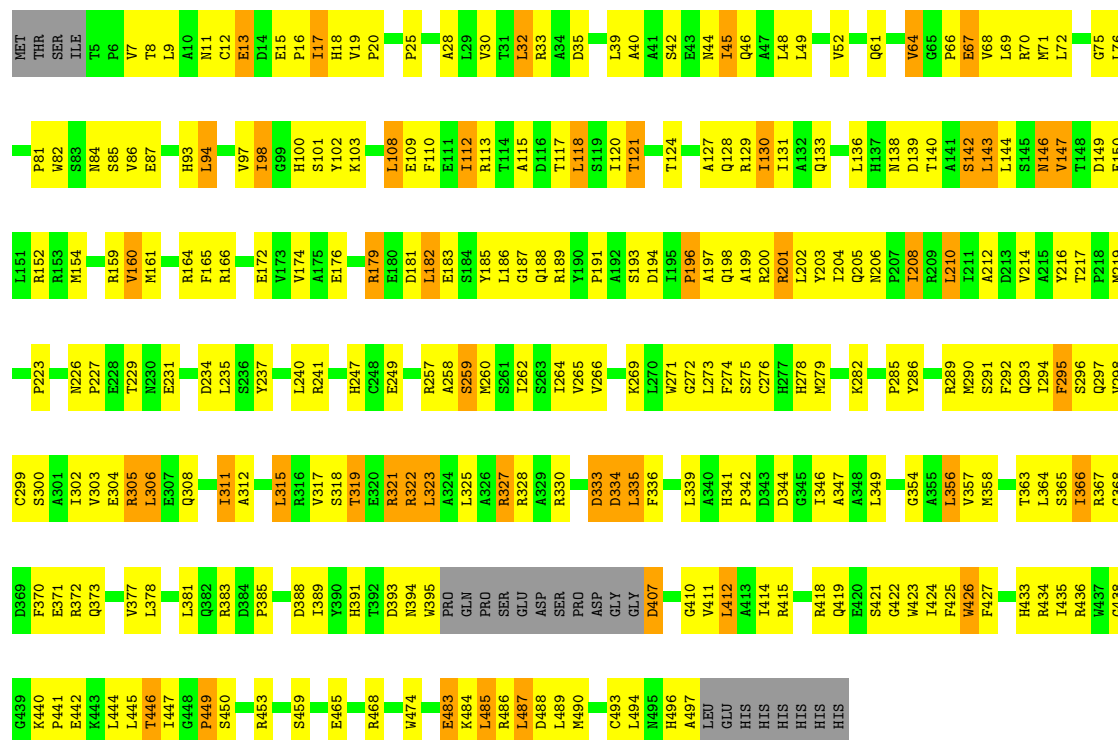






• Molecule 1: Bacteriophytochrome

Chain G: 43% 43% 10% 5%



• Molecule 1: Bacteriophytochrome

Chain H: 48% 41% 7% 5%

H496	ALA	F416	G337	R257	A162	S85	MET
LEU	Q419	A338	A339	A258	Y163	T88	THR
GLU	L339	L339	L339	S259	R164	R89	SER
HIS	G422	A340	A341	M260	F165	I90	ILE
HIS	G423	H341	G342	S261	G171	H83	T5
HIS	I424	P342	I346	I262	E172	L94	P6
HIS	F425	L349	L349	S263	R178	V7	V7
HIS	W426	L349	L349	I264	R179	F95	T8
HIS	F427	L349	L349	V265	R179	D96	
HIS	R428	L349	L349	V266	E180	V97	N11
					D181	I98	E15
					L273	P16	P16
					F274	I17	I17
					S275	H18	H18
					C276	V19	V19
					W437	P20	P20
					G438	G21	G21
					G439	A22	A22
					K440	P25	P25
					P441	I112	I112
					E442	R113	R113
					L445	T114	L29
					T446	A115	V30
					I447	I120	T31
					G448	T121	L32
					P449	S122	R33
					L454	F123	A34
					R457	T124	M37
					F460	L125	A41
					E461	N126	S42
					A462	A127	I45
					W463	Q128	Q46
					E464	I130	I45
					R468	I131	Q46
					T472	V134	L49
					S475	Q135	G50
					W476	L136	F51
					T477	H137	V52
					D478	M138	A53
					I481	L143	Q83
					A482	V147	V84
					E483	T148	G65
					K484	D149	P66
					L485	E150	E67
					D488	L151	V68
					L489	R152	E74
					M490	L76	G75
					E491	R153	L76
					L492	M154	T77
						Y157	G78
						D158	N79
						R159	G80
						V160	S83
						M161	N84

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.42Å 164.25Å 434.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	72.1 (15.00-2.90) 71.5 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.283 0.218 , 0.284	Depositor DCC
R_{free} test set	4546 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30494	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: BLA

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	0.42	2/3866 (0.1%)	0.93	19/5247 (0.4%)
1	B	0.35	0/3773	0.88	10/5122 (0.2%)
1	C	0.45	4/3897 (0.1%)	0.89	9/5289 (0.2%)
1	D	0.34	0/3871	0.88	14/5253 (0.3%)
1	E	0.35	0/3806	0.84	5/5163 (0.1%)
1	F	0.35	0/3783	0.85	12/5134 (0.2%)
1	G	0.49	7/3904 (0.2%)	0.89	3/5299 (0.1%)
1	H	0.34	0/3885	0.83	6/5273 (0.1%)
All	All	0.39	13/30785 (0.0%)	0.87	78/41780 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	G	0	1
All	All	1	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	334	ASP	N-CA	8.40	1.55	1.45
1	G	334	ASP	CA-CB	6.76	1.65	1.53
1	G	333	ASP	CA-C	6.61	1.62	1.52
1	G	333	ASP	CA-CB	6.19	1.62	1.53
1	C	444	LEU	CA-C	6.06	1.60	1.52
1	C	333	ASP	N-CA	5.75	1.53	1.46
1	G	196	PRO	CA-C	5.67	1.58	1.52
1	C	445	LEU	N-CA	5.60	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	LEU	CA-CB	5.42	1.62	1.53
1	A	445	LEU	N-CA	5.42	1.53	1.46
1	G	334	ASP	C-O	-5.15	1.17	1.23
1	C	442	GLU	CA-C	5.14	1.59	1.52
1	G	197	ALA	CA-CB	5.14	1.61	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	333	ASP	N-CA-C	10.88	130.25	113.72
1	B	451	GLY	CA-C-N	9.88	132.19	119.84
1	B	451	GLY	C-N-CA	9.88	132.19	119.84
1	A	444	LEU	CB-CA-C	9.77	129.87	110.42
1	B	118	LEU	N-CA-C	-9.39	102.40	114.04
1	C	333	ASP	N-CA-C	8.75	129.44	110.80
1	A	444	LEU	N-CA-CB	7.87	123.79	110.49
1	A	445	LEU	N-CA-CB	7.26	122.76	110.49
1	F	498	LEU	CB-CG-CD2	-7.24	88.97	110.70
1	B	341	HIS	CA-C-N	7.03	126.55	119.24
1	B	341	HIS	C-N-CA	7.03	126.55	119.24
1	C	115	ALA	N-CA-C	6.79	117.60	108.23
1	F	341	HIS	CA-C-N	6.72	125.96	118.97
1	F	341	HIS	C-N-CA	6.72	125.96	118.97
1	E	226	ASN	CA-C-N	6.64	128.14	119.84
1	E	226	ASN	C-N-CA	6.64	128.14	119.84
1	H	195	ILE	CA-C-N	-6.50	111.72	119.84
1	H	195	ILE	C-N-CA	-6.50	111.72	119.84
1	H	64	VAL	N-CA-C	6.41	117.51	112.12
1	D	206	ASN	CA-C-N	6.34	125.76	118.85
1	D	206	ASN	C-N-CA	6.34	125.76	118.85
1	D	45	ILE	N-CA-C	6.31	116.46	110.53
1	H	442	GLU	N-CA-C	-6.28	105.26	113.17
1	G	196	PRO	CA-C-O	-6.19	114.51	122.13
1	C	441	PRO	CA-C-N	6.04	133.07	121.54
1	C	441	PRO	C-N-CA	6.04	133.07	121.54
1	A	451	GLY	CA-C-N	6.03	125.73	119.64
1	A	451	GLY	C-N-CA	6.03	125.73	119.64
1	C	170	SER	N-CA-C	-6.00	102.79	110.53
1	F	409	CYS	N-CA-C	5.99	120.43	113.18
1	F	448	GLY	CA-C-N	5.99	126.10	119.87
1	F	448	GLY	C-N-CA	5.99	126.10	119.87
1	A	445	LEU	N-CA-C	-5.97	98.07	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	THR	N-CA-C	5.92	117.73	111.28
1	D	341	HIS	CA-C-N	5.87	127.18	119.84
1	D	341	HIS	C-N-CA	5.87	127.18	119.84
1	A	217	THR	CA-C-N	5.86	126.77	119.98
1	A	217	THR	C-N-CA	5.86	126.77	119.98
1	C	441	PRO	N-CA-C	5.79	120.17	111.14
1	F	65	GLY	CA-C-N	5.72	125.19	119.24
1	F	65	GLY	C-N-CA	5.72	125.19	119.24
1	C	442	GLU	N-CA-C	5.70	122.94	110.80
1	A	306	LEU	N-CA-C	-5.66	105.87	112.89
1	A	446	THR	N-CA-C	-5.64	100.05	109.24
1	B	90	ILE	N-CA-C	-5.56	99.77	108.95
1	E	127	ALA	N-CA-C	-5.45	106.63	113.28
1	E	195	ILE	CA-C-N	5.45	125.35	119.85
1	E	195	ILE	C-N-CA	5.45	125.35	119.85
1	F	190	TYR	CA-C-N	5.43	125.42	119.89
1	F	190	TYR	C-N-CA	5.43	125.42	119.89
1	F	195	ILE	CA-C-N	5.42	126.61	119.84
1	F	195	ILE	C-N-CA	5.42	126.61	119.84
1	D	65	GLY	CA-C-N	5.41	125.11	119.64
1	D	65	GLY	C-N-CA	5.41	125.11	119.64
1	D	332	ALA	N-CA-C	-5.40	99.30	110.80
1	A	284	ILE	CA-C-N	5.35	125.36	119.90
1	A	284	ILE	C-N-CA	5.35	125.36	119.90
1	C	284	ILE	N-CA-C	5.33	113.70	107.89
1	A	341	HIS	CA-C-N	5.31	124.94	119.05
1	A	341	HIS	C-N-CA	5.31	124.94	119.05
1	B	103	LYS	CB-CA-C	-5.30	110.49	116.63
1	A	195	ILE	CA-C-N	5.29	126.45	119.84
1	A	195	ILE	C-N-CA	5.29	126.45	119.84
1	G	334	ASP	CB-CA-C	5.28	119.04	109.37
1	D	368	GLY	N-CA-C	5.25	117.97	110.46
1	D	418	ARG	N-CA-C	5.25	117.08	111.36
1	B	306	LEU	N-CA-C	-5.17	106.13	112.90
1	A	65	GLY	CA-C-N	5.15	126.28	119.84
1	A	65	GLY	C-N-CA	5.15	126.28	119.84
1	B	291	SER	N-CA-C	-5.10	107.23	113.50
1	H	65	GLY	CA-C-N	5.08	124.39	118.85
1	H	65	GLY	C-N-CA	5.08	124.39	118.85
1	B	294	ILE	N-CA-C	-5.07	108.35	113.47
1	D	455	THR	CA-C-N	5.03	124.69	119.56
1	D	455	THR	C-N-CA	5.03	124.69	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	THR	N-CA-CB	-5.02	102.25	110.43
1	D	296	SER	N-CA-C	-5.02	106.99	113.01
1	C	79	ASN	N-CA-C	5.01	116.43	111.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	444	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	443	LYS	Peptide
1	A	444	LEU	Mainchain,Peptide
1	G	333	ASP	Peptide

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	3782	0	3730	242	1
1	B	3693	0	3626	216	0
1	C	3812	0	3750	214	1
1	D	3788	0	3723	228	0
1	E	3725	0	3662	232	0
1	F	3704	0	3642	221	0
1	G	3816	0	3757	259	0
1	H	3800	0	3743	211	0
2	A	43	0	31	6	0
2	B	43	0	31	4	0
2	C	43	0	30	9	0
2	D	43	0	30	8	0
2	E	43	0	31	6	0
2	F	43	0	31	4	0
2	G	43	0	31	10	0
2	H	43	0	30	9	0
3	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	6	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	7	0	0	2	0
3	H	2	0	0	0	0
All	All	30494	0	29878	1733	1

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 29.

All (1733) 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)
1:C:153:ARG:CD	1:F:498:LEU:HD21	1.25	1.57
1:C:153:ARG:HD3	1:F:498:LEU:CD2	1.13	1.56
1:C:153:ARG:NH1	1:F:498:LEU:HD11	1.41	1.35
1:C:257:ARG:HG2	1:C:257:ARG:HH11	1.04	1.13
1:E:48:LEU:HD11	1:E:93:HIS:HD2	1.16	1.05
1:A:444:LEU:CD1	1:A:447:ILE:HD11	1.88	1.03
1:D:42:SER:HB3	1:D:221:VAL:HG12	1.40	1.02
1:A:444:LEU:HD12	1:A:447:ILE:CD1	1.90	1.02
1:C:153:ARG:NH1	1:F:498:LEU:CD1	2.23	1.02
1:A:444:LEU:HD12	1:A:447:ILE:HD11	1.06	1.02
1:G:347:ALA:HB2	1:G:366:ILE:HD11	1.42	0.99
1:D:412:LEU:HB3	1:D:426:TRP:HD1	1.28	0.99
1:E:305:ARG:HA	1:E:308:GLN:HG2	1.46	0.98
1:F:87:GLU:HB3	1:F:113:ARG:NH1	1.79	0.97
2:B:900:BLA:HMB2	2:B:900:BLA:HMA2	1.46	0.97
1:G:179:ARG:HG2	1:G:179:ARG:HH11	1.26	0.96
2:H:900:BLA:HMA2	2:H:900:BLA:HMB2	1.47	0.96
2:C:900:BLA:HMA2	2:C:900:BLA:HMB2	1.45	0.96
1:A:364:LEU:HD21	1:G:435:ILE:HG22	1.45	0.94
1:E:140:THR:HG22	1:E:306:LEU:HB3	1.50	0.94
1:A:417:HIS:CD2	1:A:420:GLU:HB2	2.02	0.94
1:A:417:HIS:HD2	1:A:420:GLU:HB2	1.33	0.94
1:E:260:MET:HE3	1:E:289:ARG:HG2	1.50	0.94
1:E:394:ASN:HD21	1:E:470:HIS:CD2	1.86	0.94
2:G:900:BLA:HMA2	2:G:900:BLA:HMB2	1.50	0.93
1:A:125:LEU:HD11	1:B:83:SER:HB3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:LEU:HD21	1:D:363:THR:HG23	1.51	0.92
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.03	0.92
2:D:900:BLA:HMA2	2:D:900:BLA:HMB2	1.51	0.92
2:A:900:BLA:HMA2	2:A:900:BLA:HMB2	1.49	0.92
1:B:356:LEU:HD23	1:B:365:SER:HB3	1.52	0.91
1:B:327:ARG:HG3	1:B:327:ARG:HH11	1.35	0.91
1:C:45:ILE:HD12	1:C:46:GLN:H	1.34	0.91
1:A:130:ILE:HD11	1:A:150:GLU:HG2	1.53	0.91
1:F:266:VAL:HG22	1:F:271:TRP:HB2	1.51	0.91
1:H:79:ASN:HD22	1:H:80:GLY:H	1.19	0.91
1:C:264:ILE:HB	1:C:272:GLY:O	1.70	0.91
2:F:900:BLA:HMA2	2:F:900:BLA:HMB2	1.50	0.91
1:B:210:LEU:HD12	1:B:289:ARG:HD3	1.50	0.91
1:A:327:ARG:HA	1:B:330:ARG:NH1	1.85	0.91
1:G:112:ILE:HD13	1:G:112:ILE:H	1.35	0.90
1:H:220:ARG:HE	1:H:222:PHE:HZ	1.13	0.89
1:H:21:GLY:O	1:H:221:VAL:HG22	1.72	0.89
1:C:257:ARG:HH11	1:C:257:ARG:CG	1.86	0.89
1:D:210:LEU:HD12	1:D:289:ARG:HD3	1.53	0.88
1:B:130:ILE:HD13	1:B:130:ILE:H	1.35	0.88
1:E:48:LEU:HD11	1:E:93:HIS:CD2	2.06	0.88
1:H:220:ARG:NE	1:H:222:PHE:HZ	1.70	0.87
1:G:20:PRO:HD2	1:G:235:LEU:HD12	1.57	0.87
1:G:165:PHE:HD1	1:G:272:GLY:HA2	1.37	0.87
1:C:305:ARG:HA	1:C:308:GLN:HG2	1.57	0.87
1:D:19:VAL:HG12	1:D:234:ASP:HA	1.55	0.87
1:C:257:ARG:HG2	1:C:257:ARG:NH1	1.83	0.86
1:C:304:GLU:HG2	1:D:135:GLN:HE22	1.39	0.86
1:G:33:ARG:HB3	1:G:39:LEU:HD11	1.57	0.86
1:C:153:ARG:NE	1:F:498:LEU:HD21	1.91	0.86
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.41	0.85
1:C:153:ARG:HH12	1:F:498:LEU:HD11	1.42	0.85
1:C:215:ALA:HB3	1:C:257:ARG:HH12	1.41	0.85
1:A:45:ILE:HD12	1:A:46:GLN:H	1.42	0.85
1:E:306:LEU:HD11	1:F:305:ARG:NH2	1.92	0.84
1:A:252:THR:O	1:A:445:LEU:HD21	1.78	0.84
1:G:139:ASP:HB2	1:G:142:SER:HB2	1.60	0.83
1:A:436:ARG:O	1:G:364:LEU:HA	1.78	0.83
1:G:336:PHE:HB3	1:G:364:LEU:HD21	1.58	0.83
1:D:112:ILE:HD13	1:D:112:ILE:H	1.42	0.83
1:E:380:ARG:HB2	1:E:380:ARG:HH11	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:ARG:O	1:E:453:ARG:HD3	1.79	0.82
1:D:134:VAL:HG21	1:D:143:LEU:HD23	1.62	0.82
1:E:319:THR:HG22	1:E:322:ARG:HH21	1.44	0.82
1:C:153:ARG:CD	1:F:498:LEU:CD2	2.10	0.81
1:F:220:ARG:HG3	1:F:220:ARG:HH11	1.43	0.81
1:C:153:ARG:HH11	1:F:498:LEU:CD1	1.93	0.81
1:G:266:VAL:HG22	1:G:271:TRP:HB2	1.62	0.81
1:D:258:ALA:HB3	1:D:278:HIS:HB3	1.60	0.81
1:A:20:PRO:HD2	1:A:235:LEU:HD12	1.61	0.81
1:C:323:LEU:HA	1:D:323:LEU:HD12	1.63	0.80
1:D:147:VAL:HG11	1:D:295:PHE:CZ	2.16	0.80
1:C:330:ARG:HH21	1:C:496:HIS:HB3	1.44	0.80
1:B:305:ARG:HA	1:B:308:GLN:HG2	1.62	0.80
1:G:356:LEU:HB3	1:G:425:PHE:HB2	1.62	0.80
1:D:358:MET:HE3	1:D:423:TRP:HB2	1.62	0.80
1:G:8:THR:H	1:G:11:ASN:HB2	1.46	0.79
1:H:112:ILE:H	1:H:112:ILE:HD13	1.47	0.79
1:F:33:ARG:HB3	1:F:39:LEU:HD11	1.65	0.79
1:F:117:THR:O	1:F:118:LEU:HD23	1.81	0.79
1:A:434:ARG:HG2	1:A:435:ILE:HG23	1.61	0.79
1:A:441:PRO:HB3	1:A:443:LYS:CE	2.12	0.79
1:E:21:GLY:HA2	1:E:233:PHE:CZ	2.18	0.79
1:B:327:ARG:HH11	1:B:327:ARG:CG	1.96	0.79
1:B:162:ALA:HB3	1:B:175:ALA:HB3	1.64	0.79
1:C:153:ARG:HH11	1:F:498:LEU:HD11	1.43	0.79
1:C:196:PRO:HG3	2:C:900:BLA:HAC	1.63	0.79
1:A:341:HIS:CD2	1:A:342:PRO:HD2	2.17	0.78
1:C:124:THR:HA	1:D:294:ILE:HD11	1.65	0.78
1:D:412:LEU:HB3	1:D:426:TRP:CD1	2.17	0.78
1:H:42:SER:O	1:H:45:ILE:HG13	1.84	0.78
1:B:418:ARG:HB3	1:H:201:ARG:HH22	1.49	0.78
1:F:339:LEU:HD13	1:F:357:VAL:HG21	1.65	0.77
1:C:443:LYS:O	1:C:444:LEU:C	2.24	0.77
1:H:20:PRO:HD2	1:H:235:LEU:HD12	1.64	0.77
1:A:308:GLN:HA	1:A:311:ILE:HD12	1.67	0.77
2:G:900:BLA:HMC3	2:G:900:BLA:HBC1	1.66	0.77
1:F:94:LEU:HD23	1:F:113:ARG:NH1	2.00	0.77
1:G:196:PRO:HD2	1:G:199:ALA:HB3	1.66	0.77
1:G:201:ARG:HG2	1:G:201:ARG:HH11	1.50	0.77
1:D:9:LEU:HD21	1:D:450:SER:HB2	1.66	0.77
1:B:61:GLN:HA	1:B:69:LEU:CD1	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:ILE:HD11	1:G:274:PHE:CE1	2.21	0.76
1:D:147:VAL:HG11	1:D:295:PHE:HZ	1.50	0.76
1:G:434:ARG:CZ	1:G:435:ILE:HD11	2.15	0.76
1:F:86:VAL:HG12	1:F:87:GLU:H	1.49	0.76
1:E:162:ALA:HB3	1:E:175:ALA:HB3	1.68	0.75
1:G:336:PHE:HD2	1:G:364:LEU:CD2	1.99	0.75
1:C:153:ARG:HD3	1:F:498:LEU:HD22	1.59	0.75
1:E:139:ASP:OD1	1:E:142:SER:HB2	1.85	0.75
1:H:7:VAL:HA	1:H:11:ASN:HD22	1.52	0.75
1:A:363:THR:HB	1:G:438:GLY:HA3	1.68	0.74
1:C:72:LEU:O	1:C:76:LEU:HD13	1.86	0.74
1:H:394:ASN:O	1:H:395:TRP:HB2	1.88	0.74
1:H:286:TYR:HB3	1:H:287:PRO:HD3	1.69	0.74
1:D:214:VAL:HB	1:D:257:ARG:HA	1.69	0.74
1:H:258:ALA:HB3	1:H:278:HIS:HB3	1.70	0.74
1:G:165:PHE:CD1	1:G:272:GLY:HA2	2.21	0.73
1:G:434:ARG:NE	1:G:435:ILE:HD11	2.02	0.73
1:B:208:ILE:HD13	1:B:208:ILE:H	1.53	0.73
1:D:45:ILE:HD12	1:D:46:GLN:H	1.53	0.73
1:B:324:ALA:HA	1:B:327:ARG:HD2	1.71	0.73
1:C:51:PHE:CG	1:C:63:GLN:HB2	2.24	0.73
2:E:900:BLA:HMB2	2:E:900:BLA:HMA2	1.69	0.73
1:A:72:LEU:O	1:A:76:LEU:HD13	1.89	0.73
1:C:215:ALA:HB3	1:C:257:ARG:HH22	1.53	0.73
1:C:391:HIS:HA	1:C:411:VAL:O	1.87	0.73
1:E:164:ARG:O	1:E:171:GLY:HA2	1.88	0.73
1:F:210:LEU:HD12	1:F:289:ARG:HD3	1.71	0.72
1:A:284:ILE:HG22	1:A:289:ARG:HG3	1.71	0.72
1:C:215:ALA:CB	1:C:257:ARG:HH12	2.01	0.72
1:D:148:THR:HG23	1:D:160:VAL:HG22	1.72	0.72
1:E:328:ARG:HH12	1:E:344:ASP:HB2	1.54	0.72
1:F:29:LEU:HD12	1:F:109:GLU:HG2	1.71	0.72
1:G:194:ASP:HB3	2:G:900:BLA:HHB	1.70	0.72
1:E:45:ILE:O	1:E:49:LEU:HB2	1.88	0.72
1:B:208:ILE:HD12	1:B:293:GLN:HG3	1.72	0.72
1:H:214:VAL:HB	1:H:257:ARG:HA	1.72	0.72
1:C:45:ILE:HD12	1:C:46:GLN:N	2.04	0.71
1:F:258:ALA:HB3	1:F:278:HIS:HB3	1.71	0.71
1:F:468:ARG:CZ	1:F:468:ARG:HA	2.21	0.71
1:G:18:HIS:C	1:G:20:PRO:HD3	2.15	0.71
1:F:325:LEU:HD12	1:F:326:ALA:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ARG:HD2	1:C:177:SER:OG	1.91	0.71
1:F:162:ALA:HB3	1:F:175:ALA:HB3	1.73	0.71
1:D:113:ARG:NH2	1:D:117:THR:HG23	2.05	0.70
1:G:45:ILE:HD12	1:G:46:GLN:N	2.06	0.70
1:G:336:PHE:HD2	1:G:364:LEU:HD23	1.56	0.70
1:A:264:ILE:HD11	1:A:274:PHE:CE1	2.25	0.70
1:F:380:ARG:HH11	1:F:380:ARG:HB2	1.56	0.70
1:F:24:GLN:HE22	1:F:211:ILE:HA	1.57	0.70
1:E:20:PRO:HD2	1:E:235:LEU:HD12	1.72	0.70
1:H:484:LYS:O	1:H:488:ASP:HB2	1.91	0.70
1:A:7:VAL:HG21	1:A:245:PRO:HG2	1.73	0.70
1:A:208:ILE:HD12	1:A:293:GLN:HE21	1.57	0.70
1:A:210:LEU:HD23	1:A:211:ILE:N	2.05	0.70
1:D:33:ARG:HB3	1:D:39:LEU:HD11	1.72	0.70
1:F:45:ILE:HD12	1:F:46:GLN:N	2.05	0.70
1:C:153:ARG:HD3	1:F:498:LEU:HD23	1.57	0.70
1:C:187:GLY:HA3	1:C:435:ILE:HD12	1.72	0.70
1:G:179:ARG:HH11	1:G:179:ARG:CG	2.03	0.70
1:G:383:ARG:O	1:G:385:PRO:HD3	1.90	0.70
1:B:200:ARG:HD3	1:H:386:GLU:OE2	1.91	0.70
1:G:414:ILE:HD12	1:G:486:ARG:HB2	1.74	0.70
1:B:346:ILE:O	1:B:426:TRP:HZ3	1.75	0.69
1:D:394:ASN:O	1:D:395:TRP:HB3	1.92	0.69
1:F:380:ARG:HB2	1:F:380:ARG:NH1	2.06	0.69
1:A:17:ILE:H	1:A:17:ILE:HD12	1.57	0.69
1:D:346:ILE:O	1:D:426:TRP:HZ3	1.75	0.69
1:A:159:ARG:HD3	1:A:161:MET:SD	2.32	0.69
1:B:220:ARG:HE	1:B:222:PHE:HZ	1.41	0.69
1:A:305:ARG:HA	1:A:308:GLN:HG2	1.75	0.69
1:G:67:GLU:HA	1:G:70:ARG:HD2	1.74	0.69
1:B:249:GLU:OE2	1:B:450:SER:HB2	1.92	0.69
1:G:327:ARG:HH11	1:H:491:GLU:HG2	1.57	0.69
1:B:258:ALA:HB3	1:B:278:HIS:HB3	1.74	0.69
1:F:220:ARG:CZ	1:F:222:PHE:HZ	2.05	0.68
1:F:366:ILE:HD13	1:F:366:ILE:H	1.58	0.68
1:C:335:LEU:HD21	1:C:492:LEU:HD23	1.75	0.68
1:F:491:GLU:O	1:F:495:ASN:HB2	1.93	0.68
1:A:130:ILE:CD1	1:A:150:GLU:HG2	2.23	0.68
1:A:414:ILE:HD12	1:A:486:ARG:HB2	1.76	0.68
1:E:89:ARG:HH21	1:E:94:LEU:HG	1.58	0.68
1:F:408:CYS:SG	1:F:427:PHE:HB3	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:GLN:HG2	1:G:52:VAL:HG22	1.75	0.68
1:B:410:GLY:O	1:B:427:PHE:HA	1.94	0.68
1:F:134:VAL:HG23	1:F:143:LEU:HD11	1.76	0.67
1:D:373:GLN:NE2	1:D:395:TRP:HE1	1.93	0.67
1:H:49:LEU:HB3	1:H:63:GLN:NE2	2.09	0.67
1:A:415:ARG:HB2	1:A:423:TRP:CZ3	2.30	0.67
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.28	0.67
1:C:134:VAL:CG1	1:C:302:ILE:HG12	2.24	0.67
1:C:215:ALA:HB3	1:C:257:ARG:NH1	2.09	0.67
1:C:317:VAL:O	1:C:321:ARG:HG2	1.94	0.67
1:B:8:THR:H	1:B:11:ASN:HB3	1.60	0.67
1:A:87:GLU:HG2	1:A:113:ARG:HH22	1.60	0.67
1:E:143:LEU:C	1:E:143:LEU:HD12	2.18	0.67
1:E:260:MET:CE	1:E:289:ARG:HG2	2.24	0.67
1:F:15:GLU:HG2	1:F:17:ILE:HG23	1.75	0.67
1:F:424:ILE:HD11	1:F:489:LEU:HD12	1.77	0.67
1:G:201:ARG:HH11	1:G:201:ARG:CG	2.08	0.67
1:G:327:ARG:NH1	1:H:491:GLU:HG2	2.10	0.66
1:A:439:GLY:O	1:A:441:PRO:HD3	1.95	0.66
1:B:39:LEU:HD22	1:B:227:PRO:HG2	1.75	0.66
1:E:152:ARG:HH21	1:E:179:ARG:HG2	1.59	0.66
1:H:84:ASN:ND2	1:H:85:SER:H	1.92	0.66
1:H:208:ILE:HD13	1:H:208:ILE:H	1.60	0.66
1:B:328:ARG:HB3	1:B:338:ALA:HB2	1.76	0.66
1:G:118:LEU:HD23	1:G:118:LEU:H	1.60	0.66
1:D:213:ASP:O	1:D:216:TYR:HB3	1.95	0.66
1:F:87:GLU:HB3	1:F:113:ARG:CZ	2.25	0.66
1:D:98:ILE:HG21	1:D:286:TYR:CD1	2.31	0.66
1:D:113:ARG:HH22	1:D:117:THR:HG23	1.60	0.66
1:F:214:VAL:HB	1:F:257:ARG:HA	1.78	0.66
1:E:194:ASP:HB3	2:E:900:BLA:HHB	1.77	0.66
1:A:150:GLU:O	1:A:154:MET:HG3	1.95	0.66
1:A:383:ARG:C	1:A:385:PRO:HD3	2.21	0.66
1:C:208:ILE:HD12	1:C:289:ARG:O	1.96	0.66
1:C:330:ARG:O	1:C:330:ARG:HD3	1.96	0.66
1:H:260:MET:HE2	1:H:289:ARG:HG2	1.78	0.66
1:C:266:VAL:HG22	1:C:271:TRP:HB2	1.78	0.65
1:C:394:ASN:O	1:C:395:TRP:HB2	1.95	0.65
1:G:322:ARG:HD2	1:G:488:ASP:OD2	1.96	0.65
1:D:366:ILE:O	1:D:367:ARG:HB2	1.96	0.65
1:G:305:ARG:HA	1:G:308:GLN:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:ASN:O	1:G:395:TRP:HB2	1.96	0.65
1:A:117:THR:HG22	1:A:118:LEU:N	2.10	0.65
1:H:182:LEU:HD21	1:H:279:MET:HE3	1.79	0.65
1:B:139:ASP:HB2	1:B:142:SER:HB2	1.78	0.65
1:E:308:GLN:HA	1:E:311:ILE:HD12	1.79	0.65
1:A:443:LYS:CB	1:A:444:LEU:HD22	2.27	0.65
1:B:147:VAL:O	1:B:151:LEU:HG	1.96	0.65
1:A:220:ARG:HG3	1:A:220:ARG:NH1	2.11	0.65
1:F:7:VAL:HA	1:F:11:ASN:HD22	1.62	0.65
1:H:387:ARG:HB3	1:H:387:ARG:HH11	1.61	0.65
1:E:21:GLY:HA2	1:E:233:PHE:HZ	1.59	0.64
1:A:45:ILE:CD1	1:A:46:GLN:H	2.10	0.64
1:D:299:CYS:O	1:D:303:VAL:HB	1.96	0.64
1:D:391:HIS:HB3	1:D:412:LEU:HD23	1.79	0.64
1:F:121:THR:O	1:F:125:LEU:HB2	1.96	0.64
1:G:139:ASP:HB2	1:G:142:SER:H	1.62	0.64
1:H:328:ARG:HD3	1:H:341:HIS:CE1	2.32	0.64
1:A:383:ARG:O	1:A:385:PRO:HD3	1.96	0.64
1:A:426:TRP:N	1:A:426:TRP:CD1	2.65	0.64
1:E:135:GLN:HE22	1:F:305:ARG:NH1	1.95	0.64
1:A:441:PRO:HB3	1:A:443:LYS:NZ	2.13	0.64
1:D:184:SER:HB3	1:D:437:TRP:CZ2	2.33	0.64
1:B:327:ARG:HG3	1:B:327:ARG:NH1	2.03	0.64
1:H:412:LEU:HB3	1:H:426:TRP:HD1	1.61	0.64
1:B:214:VAL:HB	1:B:257:ARG:HA	1.80	0.64
1:H:49:LEU:HB3	1:H:63:GLN:HE22	1.61	0.64
1:E:134:VAL:HG21	1:E:143:LEU:CB	2.28	0.64
1:F:112:ILE:HD13	1:F:112:ILE:H	1.62	0.64
1:C:381:LEU:HD21	1:C:390:TYR:CD1	2.33	0.64
2:D:900:BLA:HMD3	2:D:900:BLA:HBD2	1.80	0.64
1:F:94:LEU:CD2	1:F:113:ARG:HD3	2.28	0.64
1:F:94:LEU:HD22	1:F:113:ARG:HD3	1.80	0.64
1:F:172:GLU:HG3	1:F:189:ARG:HD3	1.80	0.64
1:G:318:SER:O	1:G:322:ARG:HB2	1.97	0.64
1:D:434:ARG:NH2	1:H:340:ALA:O	2.31	0.64
1:E:143:LEU:O	1:E:147:VAL:HG13	1.98	0.64
1:E:356:LEU:HD13	1:E:357:VAL:N	2.13	0.64
1:F:45:ILE:HD12	1:F:46:GLN:H	1.62	0.64
1:D:147:VAL:HG21	1:D:295:PHE:CZ	2.32	0.64
1:E:410:GLY:O	1:E:427:PHE:HA	1.97	0.64
1:H:8:THR:H	1:H:11:ASN:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:ASN:HD22	1:H:80:GLY:N	1.95	0.64
1:B:380:ARG:HB2	1:B:380:ARG:HH11	1.63	0.63
1:C:304:GLU:HG2	1:D:135:GLN:NE2	2.11	0.63
1:C:319:THR:HA	1:C:322:ARG:HB2	1.80	0.63
1:E:305:ARG:HB3	1:E:308:GLN:HE21	1.62	0.63
1:G:265:VAL:O	1:G:300:SER:HB3	1.98	0.63
1:H:94:LEU:HD21	1:H:113:ARG:HG2	1.80	0.63
1:F:220:ARG:HH11	1:F:220:ARG:CG	2.12	0.63
1:F:389:ILE:HD11	1:F:483:GLU:OE2	1.99	0.63
1:G:262:ILE:HD12	1:G:292:PHE:HB3	1.80	0.63
1:B:137:HIS:CD2	1:B:146:ASN:HD22	2.16	0.63
1:C:84:ASN:ND2	1:C:85:SER:H	1.97	0.63
1:F:201:ARG:HG3	1:F:205:GLN:HE21	1.64	0.63
1:F:319:THR:HG22	1:F:322:ARG:HH21	1.64	0.63
1:H:394:ASN:O	1:H:395:TRP:CB	2.47	0.63
1:H:412:LEU:HB3	1:H:426:TRP:CD1	2.34	0.63
1:C:60:THR:H	1:C:63:GLN:HE21	1.46	0.63
1:E:18:HIS:C	1:E:20:PRO:HD3	2.24	0.63
1:G:311:ILE:O	1:G:315:LEU:HB2	1.99	0.63
1:H:18:HIS:C	1:H:20:PRO:HD3	2.23	0.63
1:B:143:LEU:O	1:B:147:VAL:HG22	1.98	0.63
1:C:176:GLU:OE1	1:C:178:ARG:HD3	1.99	0.63
1:G:143:LEU:O	1:G:147:VAL:HG13	1.99	0.63
1:C:152:ARG:HB2	1:C:160:VAL:CG1	2.29	0.62
1:E:317:VAL:O	1:E:321:ARG:HD2	1.99	0.62
1:A:319:THR:HG22	1:A:322:ARG:HH21	1.64	0.62
1:F:168:ASP:O	1:F:169:ASP:HB2	1.98	0.62
1:C:80:GLY:O	1:C:81:PRO:C	2.42	0.62
1:G:138:ASN:HA	1:H:305:ARG:HH22	1.64	0.62
1:A:59:LEU:H	1:A:59:LEU:HD22	1.64	0.62
1:A:355:ALA:HB3	1:A:366:ILE:HG13	1.81	0.62
1:E:417:HIS:HD2	1:E:420:GLU:HB2	1.65	0.62
1:H:366:ILE:O	1:H:367:ARG:HB2	1.99	0.62
1:C:440:LYS:HG2	1:E:361:GLY:HA3	1.81	0.62
1:G:229:THR:HG23	1:G:231:GLU:H	1.63	0.62
1:B:323:LEU:HD23	1:B:323:LEU:C	2.24	0.62
1:E:164:ARG:HH12	1:E:166:ARG:HE	1.48	0.62
1:E:464:GLU:O	1:E:468:ARG:HG2	1.99	0.62
1:G:131:ILE:HD11	1:H:297:GLN:HB2	1.82	0.62
1:A:294:ILE:O	1:A:298:VAL:HG23	1.99	0.62
1:A:415:ARG:HB2	1:A:423:TRP:CH2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:HA	1:B:69:LEU:HD11	1.80	0.62
1:G:247:HIS:CD2	2:G:900:BLA:HBD1	2.35	0.62
1:C:17:ILE:HD12	1:C:244:SER:HB2	1.82	0.61
1:C:182:LEU:HD13	1:C:279:MET:HE3	1.81	0.61
1:E:380:ARG:HB2	1:E:380:ARG:NH1	2.15	0.61
1:C:359:LEU:HD12	1:C:360:GLY:H	1.65	0.61
1:H:31:THR:HG22	1:H:107:TYR:CD1	2.35	0.61
1:A:130:ILE:HD11	1:A:150:GLU:CG	2.28	0.61
1:A:138:ASN:HD22	1:A:138:ASN:N	1.99	0.61
1:A:164:ARG:NH1	1:A:166:ARG:HH21	1.98	0.61
1:E:322:ARG:HD2	1:E:488:ASP:OD1	2.00	0.61
1:G:410:GLY:O	1:G:427:PHE:HA	2.00	0.61
1:D:301:ALA:O	1:D:305:ARG:HG2	2.01	0.61
1:G:295:PHE:CE1	1:G:299[B]:CYS:SG	2.94	0.61
1:D:16:PRO:HB3	1:D:18:HIS:CE1	2.35	0.61
1:F:468:ARG:HA	1:F:468:ARG:NH1	2.15	0.61
1:G:336:PHE:CD2	1:G:364:LEU:CD2	2.83	0.61
1:H:324:ALA:O	1:H:328:ARG:HB2	2.01	0.61
1:D:358:MET:HE1	1:D:378:LEU:HD11	1.82	0.61
1:E:433:HIS:HD2	1:E:436:ARG:HG2	1.64	0.61
1:G:445:LEU:O	1:G:446:THR:HG22	2.00	0.61
1:H:333:ASP:HB2	1:H:496:HIS:CD2	2.36	0.61
1:H:433:HIS:HD2	1:H:436:ARG:HG2	1.65	0.61
1:A:356:LEU:HD13	1:A:357:VAL:N	2.15	0.61
1:C:196:PRO:CG	2:C:900:BLA:HAC	2.29	0.61
1:E:19:VAL:HG12	1:E:233:PHE:O	2.00	0.61
1:G:33:ARG:HB3	1:G:39:LEU:CD1	2.31	0.61
1:C:220:ARG:HE	1:C:222:PHE:HZ	1.47	0.61
1:C:354:GLY:HA3	1:C:370:PHE:CE1	2.36	0.61
1:F:117:THR:O	1:F:117:THR:CG2	2.48	0.61
1:G:16:PRO:HB3	1:G:18:HIS:HE1	1.65	0.61
1:C:426:TRP:N	1:C:426:TRP:CD1	2.68	0.61
1:F:18:HIS:C	1:F:20:PRO:HD3	2.25	0.61
1:G:179:ARG:HG2	1:G:179:ARG:NH1	2.07	0.61
1:H:210:LEU:HD12	1:H:289:ARG:HE	1.64	0.61
1:A:17:ILE:O	1:A:241:ARG:HD2	1.99	0.61
1:B:51:PHE:HB2	1:B:63:GLN:OE1	2.00	0.61
1:C:328:ARG:HH12	1:C:344:ASP:HB2	1.64	0.61
1:A:322:ARG:HD2	1:A:488:ASP:OD1	2.01	0.60
1:D:7:VAL:HG12	1:D:11:ASN:HD22	1.65	0.60
1:G:328:ARG:HH12	1:G:344:ASP:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:LEU:HD11	1:G:489:LEU:HD22	1.82	0.60
1:G:425:PHE:HB3	1:G:427:PHE:CE1	2.36	0.60
1:E:307:GLU:O	1:E:311:ILE:HG23	2.01	0.60
1:F:179:ARG:NH1	1:F:181:ASP:HB3	2.17	0.60
2:G:900:BLA:HBC1	2:G:900:BLA:CMC	2.30	0.60
1:H:172:GLU:HB2	1:H:189:ARG:HD3	1.83	0.60
1:A:208:ILE:H	1:A:208:ILE:HD13	1.66	0.60
1:A:42:SER:O	1:A:45:ILE:HG13	2.01	0.60
1:D:434:ARG:NH1	1:D:435:ILE:HD13	2.17	0.60
1:A:298:VAL:HG13	1:B:298:VAL:HG13	1.83	0.60
1:G:493:CYS:HA	1:G:496:HIS:HD2	1.65	0.60
1:H:264:ILE:HD11	1:H:274:PHE:CE1	2.37	0.60
1:B:24:GLN:HE22	1:B:211:ILE:HA	1.65	0.60
1:D:145:SER:HA	1:D:175:ALA:HB1	1.84	0.60
1:E:85:SER:HB2	1:E:98:ILE:HG22	1.82	0.60
1:B:31:THR:HG22	1:B:107:TYR:HD1	1.66	0.60
1:B:418:ARG:HB3	1:H:201:ARG:NH2	2.15	0.60
1:C:51:PHE:CD2	1:C:63:GLN:HB2	2.36	0.60
2:C:900:BLA:HMA2	2:C:900:BLA:CMB	2.25	0.60
1:G:113:ARG:HG2	1:G:115:ALA:O	2.01	0.60
1:A:364:LEU:HD21	1:G:435:ILE:CG2	2.26	0.59
1:D:350:ILE:HG23	1:D:351:PRO:HD2	1.84	0.59
1:G:258:ALA:HB1	3:G:903:HOH:O	2.02	0.59
1:B:412:LEU:HB3	1:B:426:TRP:HD1	1.67	0.59
1:E:19:VAL:HG23	1:E:19:VAL:O	2.01	0.59
1:E:112:ILE:H	1:E:112:ILE:HD13	1.66	0.59
1:G:191:PRO:HB2	1:G:193:SER:H	1.67	0.59
1:C:163:TYR:CE1	2:C:900:BLA:HMA3	2.37	0.59
1:H:220:ARG:HB2	1:H:222:PHE:CZ	2.36	0.59
1:D:322:ARG:NH2	1:D:484:LYS:HB3	2.17	0.59
1:E:356:LEU:HB3	1:E:425:PHE:HB2	1.84	0.59
1:G:72:LEU:O	1:G:72:LEU:HD13	2.02	0.59
1:A:134:VAL:HG21	1:A:143:LEU:HD13	1.83	0.59
1:C:209:ARG:NH1	2:C:900:BLA:O1D	2.36	0.59
1:F:321:ARG:HG3	1:F:349:LEU:HD22	1.84	0.59
1:A:59:LEU:HD22	1:A:59:LEU:N	2.16	0.59
1:B:311:ILE:O	1:B:315:LEU:HG	2.02	0.59
1:C:215:ALA:HB3	1:C:257:ARG:NH2	2.17	0.59
1:D:274:PHE:CE1	1:D:295:PHE:CE2	2.91	0.59
1:F:19:VAL:N	1:F:20:PRO:HD3	2.16	0.59
1:F:324:ALA:HB1	1:F:328:ARG:HH22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:416:PHE:HE1	1:H:424:ILE:HG13	1.66	0.59
1:A:188:GLN:HG3	1:A:189:ARG:N	2.18	0.59
1:G:264:ILE:HB	1:G:272:GLY:O	2.03	0.59
2:H:900:BLA:HMA2	2:H:900:BLA:CMB	2.29	0.59
1:A:443:LYS:HB2	1:A:444:LEU:HD22	1.85	0.59
1:E:412:LEU:O	1:E:426:TRP:HD1	1.84	0.59
1:F:59:LEU:HD13	1:F:59:LEU:H	1.68	0.59
1:G:275:SER:OG	2:G:900:BLA:O2A	2.21	0.59
1:G:295:PHE:CZ	1:G:299[B]:CYS:SG	2.95	0.59
1:B:354:GLY:HA3	1:B:370:PHE:CZ	2.38	0.59
1:G:302:ILE:HG13	1:H:305:ARG:HG3	1.84	0.59
1:A:262:ILE:CD1	1:A:292:PHE:HB3	2.33	0.59
1:C:260:MET:HE1	1:C:292:PHE:HD2	1.68	0.59
1:D:373:GLN:HE22	1:D:395:TRP:NE1	2.00	0.59
1:D:410:GLY:O	1:D:427:PHE:HA	2.03	0.59
1:G:108:LEU:HD12	1:G:110:PHE:CZ	2.39	0.58
1:C:127:ALA:O	1:C:131:ILE:HG12	2.03	0.58
1:G:71:MET:SD	1:G:86:VAL:HG23	2.43	0.58
1:H:79:ASN:ND2	1:H:80:GLY:H	1.96	0.58
1:F:136:LEU:O	1:F:136:LEU:HD23	2.03	0.58
2:G:900:BLA:HMA3	2:G:900:BLA:HBA2	1.85	0.58
1:H:346:ILE:O	1:H:426:TRP:HZ3	1.86	0.58
1:B:495:ASN:O	1:B:495:ASN:OD1	2.21	0.58
1:C:129:ARG:HE	1:C:154:MET:HG2	1.68	0.58
1:D:266:VAL:HG23	1:D:266:VAL:O	2.04	0.58
1:F:346:ILE:HD11	1:F:366:ILE:HD11	1.85	0.58
1:H:134:VAL:HG13	1:H:143:LEU:HB2	1.85	0.58
1:A:82:TRP:HE3	1:A:83:SER:O	1.86	0.58
1:A:131:ILE:O	1:A:135:GLN:HB2	2.04	0.58
1:A:143:LEU:O	1:A:147:VAL:HG13	2.04	0.58
1:D:286:TYR:HB3	1:D:287:PRO:HD3	1.84	0.58
1:E:48:LEU:HD12	1:E:48:LEU:O	2.03	0.58
1:F:239:VAL:HG11	1:F:289:ARG:NH2	2.19	0.58
1:G:201:ARG:HG2	1:G:205:GLN:NE2	2.18	0.58
1:H:138:ASN:HD22	1:H:138:ASN:N	2.02	0.58
1:H:220:ARG:NE	1:H:222:PHE:CZ	2.62	0.58
1:A:359:LEU:HA	1:A:421:SER:O	2.04	0.58
2:B:900:BLA:HBB1	2:B:900:BLA:OB	2.03	0.58
1:C:185:TYR:O	1:C:188:GLN:HB2	2.04	0.58
1:A:446:THR:CG2	1:A:446:THR:O	2.51	0.58
1:B:19:VAL:H	1:B:20:PRO:HD3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASP:O	1:B:116:ASP:OD2	2.22	0.58
1:B:266:VAL:HG23	1:B:266:VAL:O	2.02	0.58
1:B:299:CYS:O	1:B:303:VAL:HG23	2.03	0.58
1:E:433:HIS:CD2	1:E:436:ARG:HG2	2.38	0.58
1:G:131:ILE:HG22	1:G:295:PHE:HB2	1.84	0.58
1:H:51:PHE:CG	1:H:52:VAL:N	2.72	0.58
1:B:391:HIS:HA	1:B:411:VAL:O	2.03	0.58
1:D:430:GLU:HG2	1:D:431:GLU:N	2.19	0.58
1:E:385:PRO:O	1:E:386:GLU:HB2	2.04	0.58
1:G:336:PHE:CD2	1:G:364:LEU:HD23	2.39	0.58
1:D:339:LEU:CD1	1:D:357:VAL:HG21	2.34	0.57
1:D:373:GLN:HE22	1:D:395:TRP:HE1	1.53	0.57
1:F:373:GLN:O	1:F:377:VAL:HG23	2.05	0.57
1:H:488:ASP:O	1:H:492:LEU:HD13	2.04	0.57
1:D:43:GLU:HA	1:D:45:ILE:HG13	1.86	0.57
1:E:415:ARG:HD3	1:E:423:TRP:CZ2	2.39	0.57
1:A:18:HIS:C	1:A:20:PRO:HD3	2.29	0.57
1:B:45:ILE:HD13	1:B:52:VAL:HA	1.85	0.57
1:C:420:GLU:OE2	1:G:81:PRO:HG3	2.05	0.57
1:F:206:ASN:HD21	1:F:237:TYR:HA	1.68	0.57
1:A:117:THR:HG23	1:A:287:PRO:HG2	1.87	0.57
1:D:138:ASN:HD22	1:D:138:ASN:N	2.01	0.57
1:D:433:HIS:CE1	1:D:460:PHE:HE1	2.23	0.57
1:G:117:THR:O	1:G:118:LEU:C	2.46	0.57
1:C:201:ARG:HD3	1:G:385:PRO:HB3	1.85	0.57
1:C:378:LEU:HD11	1:C:423:TRP:CE2	2.39	0.57
1:D:222:PHE:HA	1:D:223:PRO:C	2.27	0.57
1:E:134:VAL:HG22	1:E:134:VAL:O	2.04	0.57
1:B:17:ILE:HG21	1:B:244:SER:HB2	1.87	0.57
1:B:19:VAL:N	1:B:20:PRO:HD3	2.19	0.57
1:B:94:LEU:O	1:B:113:ARG:HB3	2.04	0.57
1:B:256:VAL:HG11	1:B:277:HIS:CD2	2.40	0.57
1:D:17:ILE:O	1:D:241:ARG:HD2	2.05	0.57
1:D:46:GLN:HA	1:D:49:LEU:O	2.05	0.57
1:G:143:LEU:C	1:G:143:LEU:HD12	2.30	0.57
1:H:84:ASN:HD22	1:H:85:SER:H	1.52	0.57
1:G:356:LEU:HD13	1:G:357:VAL:N	2.20	0.57
1:B:28:ALA:HB2	1:B:48:LEU:HD22	1.86	0.57
1:B:122:SER:O	1:B:126:ASN:HB2	2.04	0.57
1:C:327:ARG:HH11	1:D:491:GLU:HG2	1.70	0.57
1:E:135:GLN:NE2	1:F:305:ARG:NH1	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ALA:HB1	1:B:367:ARG:HH21	1.70	0.57
1:D:126:ASN:O	1:D:130:ILE:HG23	2.05	0.57
1:D:250:TYR:CZ	1:D:454:LEU:O	2.58	0.57
1:D:373:GLN:O	1:D:377:VAL:HG23	2.05	0.57
1:F:17:ILE:HG21	1:F:244:SER:HB2	1.86	0.57
1:G:164:ARG:HG3	1:G:174:VAL:HG21	1.87	0.57
1:A:356:LEU:HB3	1:A:425:PHE:HB2	1.87	0.57
1:A:361:GLY:O	1:G:440:LYS:HB2	2.05	0.57
1:C:98:ILE:HG12	1:C:109:GLU:HB2	1.86	0.57
1:E:48:LEU:CD1	1:E:93:HIS:HD2	2.03	0.57
1:E:490:MET:O	1:E:494:LEU:HD23	2.05	0.57
1:C:260:MET:HE1	1:C:292:PHE:CD2	2.40	0.56
1:F:305:ARG:HD2	1:F:305:ARG:N	2.20	0.56
1:H:213:ASP:O	1:H:216:TYR:HB3	2.05	0.56
1:A:441:PRO:HB3	1:A:443:LYS:HE3	1.85	0.56
1:D:294:ILE:O	1:D:298:VAL:HG23	2.05	0.56
1:E:135:GLN:NE2	1:E:135:GLN:HA	2.16	0.56
1:E:202:LEU:HD13	1:E:241:ARG:NH2	2.20	0.56
1:F:301:ALA:O	1:F:304:GLU:HB3	2.05	0.56
1:F:366:ILE:HD13	1:F:366:ILE:N	2.20	0.56
1:H:31:THR:C	1:H:32:LEU:HD12	2.30	0.56
1:H:321:ARG:HD3	1:H:349:LEU:HD22	1.85	0.56
1:A:305:ARG:HB3	1:A:308:GLN:NE2	2.20	0.56
1:B:364:LEU:O	1:B:364:LEU:HD23	2.05	0.56
1:C:262:ILE:HD12	1:C:292:PHE:HB3	1.87	0.56
1:D:341:HIS:CG	1:D:342:PRO:HD2	2.40	0.56
1:E:48:LEU:CD1	1:E:93:HIS:CD2	2.85	0.56
1:F:339:LEU:HD22	1:F:346:ILE:HG23	1.86	0.56
1:F:425:PHE:HB3	1:F:427:PHE:CE1	2.40	0.56
1:A:33:ARG:HB3	1:A:39:LEU:HD11	1.88	0.56
1:A:70:ARG:O	1:A:74:GLU:HG2	2.06	0.56
1:D:19:VAL:HG23	1:D:19:VAL:O	2.06	0.56
1:G:118:LEU:O	1:G:121:THR:HG22	2.04	0.56
1:C:186:LEU:HD23	1:C:187:GLY:N	2.20	0.56
1:G:98:ILE:HG21	1:G:286:TYR:CE1	2.40	0.56
1:H:114:THR:HG22	1:H:115:ALA:H	1.70	0.56
1:E:134:VAL:HG21	1:E:143:LEU:HB3	1.85	0.56
1:A:8:THR:H	1:A:11:ASN:HB3	1.69	0.56
1:A:354:GLY:HA3	1:A:370:PHE:CZ	2.41	0.56
1:D:356:LEU:HB3	1:D:425:PHE:HB2	1.87	0.56
1:E:330:ARG:NH1	1:E:333:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ILE:HD12	1:E:486:ARG:HB2	1.87	0.56
1:D:238:SER:HB3	1:D:241:ARG:HB2	1.88	0.56
1:E:408:CYS:SG	1:E:427:PHE:HB3	2.46	0.56
1:C:134:VAL:HG13	1:C:302:ILE:HG21	1.87	0.56
1:B:302:ILE:O	1:B:306:LEU:HB2	2.06	0.56
1:D:136:LEU:HD11	1:G:490:MET:HE3	1.88	0.56
1:D:250:TYR:O	1:D:253:ASN:HB2	2.05	0.56
1:G:336:PHE:HD2	1:G:364:LEU:HD21	1.71	0.56
1:H:52:VAL:HG22	1:H:53:ALA:H	1.71	0.56
1:H:159:ARG:HG2	1:H:160:VAL:N	2.20	0.56
1:B:85:SER:HB2	1:B:98:ILE:HG22	1.87	0.55
1:E:434:ARG:HD2	1:E:435:ILE:HG23	1.89	0.55
1:F:260:MET:O	1:F:276:CYS:HB2	2.06	0.55
1:H:325:LEU:HD21	1:H:339:LEU:HD23	1.87	0.55
1:B:213:ASP:O	1:B:216:TYR:HB3	2.05	0.55
1:G:258:ALA:HB3	1:G:278:HIS:HB3	1.87	0.55
1:G:426:TRP:N	1:G:426:TRP:CD1	2.74	0.55
1:A:123:PHE:CZ	1:A:291:SER:HB2	2.41	0.55
2:A:900:BLA:HMA2	2:A:900:BLA:CMB	2.31	0.55
1:D:494:LEU:HD23	1:E:133:GLN:HG2	1.88	0.55
1:G:378:LEU:HD11	1:G:425:PHE:HZ	1.72	0.55
1:A:54:SER:O	1:A:57:SER:HB3	2.06	0.55
1:B:29:LEU:HD12	1:B:108:LEU:O	2.06	0.55
1:E:318:SER:O	1:E:322:ARG:HB2	2.07	0.55
1:E:394:ASN:ND2	1:E:470:HIS:CD2	2.68	0.55
1:E:17:ILE:H	1:E:17:ILE:HD12	1.71	0.55
1:E:120:ILE:CG1	1:F:120:ILE:HD13	2.36	0.55
1:E:133:GLN:HB3	1:E:146:ASN:OD1	2.06	0.55
1:F:208:ILE:H	1:F:208:ILE:HD13	1.70	0.55
1:H:51:PHE:CE2	1:H:52:VAL:HG12	2.42	0.55
1:H:112:ILE:HG12	1:H:112:ILE:O	2.06	0.55
1:H:295:PHE:HA	1:H:298:VAL:HG12	1.88	0.55
1:A:311:ILE:O	1:A:315:LEU:HB2	2.06	0.55
1:A:378:LEU:O	1:A:382:GLN:HG2	2.07	0.55
1:E:30:VAL:HG12	1:E:32:LEU:CD1	2.36	0.55
1:F:8:THR:H	1:F:11:ASN:ND2	2.03	0.55
1:G:82:TRP:O	1:G:100:HIS:HA	2.07	0.55
1:H:130:ILE:HG12	1:H:147:VAL:HG13	1.87	0.55
1:H:339:LEU:HD13	1:H:357:VAL:HG21	1.89	0.55
1:E:256:VAL:CG1	1:E:277:HIS:HB3	2.37	0.55
1:E:389:ILE:HD11	1:E:483:GLU:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:PHE:HA	1:H:223:PRO:C	2.30	0.55
1:A:447:ILE:HD13	1:A:447:ILE:N	2.21	0.55
1:C:131:ILE:HG22	1:C:295:PHE:HD1	1.70	0.55
2:B:900:BLA:HMB2	2:B:900:BLA:CMA	2.31	0.55
1:C:133:GLN:O	1:C:137:HIS:HD2	1.89	0.55
1:C:416:PHE:HE1	1:C:424:ILE:HG13	1.72	0.55
1:D:325:LEU:HD12	1:D:326:ALA:N	2.21	0.55
1:F:356:LEU:HD23	1:F:365:SER:HB3	1.87	0.55
1:G:423:TRP:HB3	1:G:425:PHE:CE1	2.42	0.55
1:A:290:MET:HB3	1:B:124:THR:OG1	2.05	0.55
1:G:17:ILE:H	1:G:17:ILE:HD12	1.72	0.55
2:G:900:BLA:HBB1	2:G:900:BLA:OB	2.07	0.55
1:B:61:GLN:HA	1:B:69:LEU:HD13	1.88	0.54
1:D:340:ALA:O	1:H:434:ARG:NH2	2.39	0.54
1:E:159:ARG:HG2	1:E:160:VAL:N	2.22	0.54
1:F:31:THR:HG22	1:F:107:TYR:CD1	2.41	0.54
1:F:266:VAL:O	1:F:266:VAL:HG23	2.07	0.54
1:G:64:VAL:CG1	1:G:68:VAL:HG11	2.37	0.54
1:G:412:LEU:HB3	1:G:426:TRP:CD1	2.42	0.54
1:H:266:VAL:HG23	1:H:266:VAL:O	2.08	0.54
1:D:322:ARG:HD3	1:D:488:ASP:OD1	2.08	0.54
1:G:40:ALA:HB2	1:G:223:PRO:HD2	1.88	0.54
1:G:285:PRO:HG3	3:G:907:HOH:O	2.06	0.54
1:G:493:CYS:HA	1:G:496:HIS:CD2	2.42	0.54
2:G:900:BLA:HMA2	2:G:900:BLA:CMB	2.32	0.54
1:A:46:GLN:HB2	1:A:52:VAL:HG22	1.88	0.54
1:C:488:ASP:O	1:C:491:GLU:HB3	2.07	0.54
1:E:325:LEU:O	1:E:325:LEU:HD22	2.07	0.54
1:G:179:ARG:HH12	1:G:181:ASP:HB2	1.72	0.54
1:A:121:THR:CG2	1:B:85:SER:OG	2.54	0.54
1:C:40:ALA:HB1	1:C:222:PHE:O	2.07	0.54
1:C:475:SER:HB2	1:C:478:ASP:H	1.73	0.54
1:D:208:ILE:H	1:D:208:ILE:HD13	1.73	0.54
1:F:148:THR:HG23	1:F:160:VAL:HG22	1.89	0.54
1:G:198:GLN:O	1:G:198:GLN:HG3	2.08	0.54
1:B:51:PHE:HD2	1:B:63:GLN:HG3	1.71	0.54
1:D:351:PRO:HB2	1:D:428:ARG:HH21	1.72	0.54
1:E:113:ARG:HH12	1:E:285:PRO:HB3	1.72	0.54
1:E:330:ARG:HD2	1:F:331:ASP:OD2	2.07	0.54
1:G:201:ARG:CG	1:G:201:ARG:NH1	2.70	0.54
1:G:311:ILE:HD13	1:G:312:ALA:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:GLY:HA3	1:A:370:PHE:CE1	2.42	0.54
1:B:19:VAL:N	1:B:20:PRO:CD	2.70	0.54
1:B:313:GLU:O	1:B:317:VAL:HG13	2.08	0.54
1:D:411:VAL:HG13	1:D:427:PHE:CE2	2.43	0.54
1:F:323:LEU:O	1:F:323:LEU:HD23	2.07	0.54
1:G:133:GLN:HB3	1:G:147:VAL:HG12	1.90	0.54
1:C:268:GLY:HA2	1:G:418:ARG:NH2	2.23	0.54
1:D:460:PHE:HE2	1:D:464:GLU:OE1	1.91	0.54
1:E:316:ARG:HH21	1:E:317:VAL:HG12	1.73	0.54
1:H:286:TYR:O	1:H:290:MET:HG2	2.07	0.54
1:A:491:GLU:HG3	1:A:492:LEU:N	2.22	0.54
1:E:40:ALA:HB2	1:E:223:PRO:HD2	1.90	0.54
1:E:173:VAL:O	1:E:186:LEU:HD23	2.08	0.54
1:A:165:PHE:CD1	1:A:272:GLY:HA2	2.42	0.54
1:A:364:LEU:HD23	1:G:436:ARG:O	2.07	0.54
1:B:54:SER:O	1:B:57:SER:HB3	2.08	0.54
1:B:346:ILE:O	1:B:426:TRP:CZ3	2.59	0.54
1:E:134:VAL:HG21	1:E:143:LEU:HB2	1.89	0.54
1:F:118:LEU:O	1:F:122:SER:CB	2.56	0.54
1:G:423:TRP:HB3	1:G:425:PHE:HE1	1.72	0.54
1:A:330:ARG:HH21	1:B:327:ARG:HB2	1.73	0.54
1:C:125:LEU:O	1:C:125:LEU:HD23	2.08	0.54
1:F:391:HIS:HB3	1:F:412:LEU:HD23	1.88	0.54
1:A:137:HIS:C	1:A:138:ASN:HD22	2.16	0.53
1:B:67:GLU:CD	1:B:67:GLU:H	2.16	0.53
1:C:139:ASP:HB3	1:C:142:SER:HB2	1.89	0.53
1:D:288:VAL:O	1:D:291:SER:HB2	2.08	0.53
1:E:335:LEU:C	1:E:337:GLY:N	2.66	0.53
1:G:327:ARG:O	1:G:327:ARG:HG2	2.08	0.53
1:G:412:LEU:HD12	1:G:474:TRP:CE3	2.43	0.53
1:C:341:HIS:ND1	1:C:342:PRO:HD2	2.23	0.53
1:D:434:ARG:HH12	1:D:435:ILE:HD13	1.73	0.53
1:A:19:VAL:HG23	1:A:19:VAL:O	2.08	0.53
1:B:260:MET:HE1	1:B:292:PHE:CD2	2.44	0.53
1:H:439:GLY:O	1:H:440:LYS:C	2.50	0.53
1:A:50:GLY:O	1:A:51:PHE:HB3	2.09	0.53
1:A:82:TRP:CE3	1:A:83:SER:O	2.62	0.53
1:A:208:ILE:HA	1:A:261:SER:O	2.08	0.53
1:C:194:ASP:HB3	2:C:900:BLA:HBB	1.90	0.53
1:D:415:ARG:HB2	1:D:423:TRP:CE2	2.43	0.53
1:E:172:GLU:HG2	1:E:173:VAL:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:LEU:O	1:F:76:LEU:HD13	2.08	0.53
1:G:202:LEU:O	1:G:206:ASN:HB2	2.08	0.53
1:H:229:THR:HG23	1:H:231:GLU:H	1.74	0.53
1:A:32:LEU:CD2	1:A:72:LEU:HD11	2.38	0.53
1:A:302:ILE:HD12	1:B:302:ILE:HD11	1.90	0.53
1:C:114:THR:HG22	1:C:114:THR:O	2.09	0.53
1:D:143:LEU:HD12	1:D:144:LEU:N	2.23	0.53
1:E:105:VAL:HG12	1:E:106:PHE:N	2.24	0.53
1:E:128:GLN:HG2	1:F:297:GLN:CD	2.34	0.53
1:F:317:VAL:O	1:F:321:ARG:HD2	2.07	0.53
1:F:412:LEU:HB3	1:F:426:TRP:CD1	2.43	0.53
1:H:135:GLN:N	1:H:135:GLN:HE21	2.06	0.53
1:A:72:LEU:HD13	1:A:76:LEU:HD13	1.89	0.53
1:C:94:LEU:CD1	1:C:94:LEU:H	2.21	0.53
1:F:188:GLN:NE2	1:F:460:PHE:HB2	2.23	0.53
1:F:412:LEU:O	1:F:426:TRP:HD1	1.92	0.53
1:G:297:GLN:HB3	1:H:131:ILE:HD11	1.91	0.53
1:H:46:GLN:HG2	1:H:52:VAL:HA	1.90	0.53
1:A:382:GLN:NE2	1:A:382:GLN:HA	2.24	0.53
1:A:414:ILE:HG12	1:A:424:ILE:HB	1.91	0.53
1:C:415:ARG:HD3	1:C:423:TRP:CZ2	2.43	0.53
1:E:354:GLY:HA3	1:E:370:PHE:CE1	2.44	0.53
1:F:314:LEU:O	1:F:317:VAL:HG22	2.09	0.53
1:H:410:GLY:O	1:H:427:PHE:HA	2.08	0.53
1:B:325:LEU:HD13	1:B:325:LEU:C	2.33	0.53
1:D:40:ALA:CB	1:D:223:PRO:HD2	2.39	0.53
1:D:84:ASN:HD22	1:D:85:SER:H	1.55	0.53
1:E:120:ILE:HD11	1:F:120:ILE:HD13	1.90	0.53
1:E:294:ILE:HD11	1:F:127:ALA:HB3	1.91	0.53
1:F:239:VAL:HG11	1:F:289:ARG:HH21	1.74	0.53
1:H:149:ASP:HB3	1:H:153:ARG:HH22	1.74	0.53
1:B:31:THR:C	1:B:32:LEU:HD12	2.33	0.53
1:B:205:GLN:NE2	1:B:237:TYR:HE2	2.07	0.53
1:E:301:ALA:HB2	1:F:135:GLN:HG2	1.90	0.53
1:G:273:LEU:C	1:G:273:LEU:HD12	2.34	0.53
1:H:358:MET:HG3	1:H:363:THR:CG2	2.39	0.53
1:A:327:ARG:HA	1:B:330:ARG:HH12	1.72	0.52
1:B:63:GLN:O	1:B:63:GLN:HG2	2.09	0.52
1:B:315:LEU:O	1:B:319:THR:HG23	2.08	0.52
1:C:385:PRO:HB3	1:G:201:ARG:HG3	1.90	0.52
1:D:243:VAL:HG12	1:D:244:SER:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:TYR:CE1	1:D:454:LEU:O	2.62	0.52
1:D:416:PHE:O	1:D:490:MET:HG2	2.09	0.52
1:E:222:PHE:HA	1:E:223:PRO:C	2.32	0.52
1:E:365:SER:HB2	1:E:368:GLY:O	2.09	0.52
1:G:138:ASN:HA	1:H:305:ARG:NH2	2.22	0.52
1:C:25:PRO:HD3	1:C:216:TYR:HD2	1.74	0.52
1:D:194:ASP:O	1:D:196:PRO:HD3	2.08	0.52
1:F:322:ARG:NH1	1:F:484:LYS:HB3	2.23	0.52
1:F:356:LEU:HB3	1:F:425:PHE:HB2	1.91	0.52
1:G:487:LEU:HA	1:G:490:MET:HE2	1.91	0.52
1:H:315:LEU:O	1:H:318:SER:HB3	2.09	0.52
1:A:88:THR:HG23	1:A:90:ILE:HG13	1.90	0.52
1:A:307:GLU:C	1:A:309:GLY:H	2.17	0.52
1:C:213:ASP:O	1:C:216:TYR:HB3	2.09	0.52
1:E:148:THR:HG23	1:E:160:VAL:HG22	1.92	0.52
1:G:377:VAL:HG21	1:G:411:VAL:HG11	1.90	0.52
1:H:191:PRO:HG3	1:H:463:TRP:HB2	1.91	0.52
1:D:162:ALA:O	1:D:174:VAL:HG22	2.10	0.52
1:E:31:THR:HG22	1:E:107:TYR:CD1	2.44	0.52
1:E:31:THR:HG22	1:E:107:TYR:HD1	1.74	0.52
1:F:134:VAL:HG22	1:F:302:ILE:HG21	1.91	0.52
1:F:278:HIS:HD2	1:F:280:SER:O	1.93	0.52
1:G:72:LEU:HD13	1:G:76:LEU:HD13	1.90	0.52
1:G:389:ILE:HD11	1:G:483:GLU:HG2	1.90	0.52
1:A:258:ALA:HB3	1:A:278:HIS:HB3	1.92	0.52
1:B:94:LEU:O	1:B:94:LEU:HD13	2.09	0.52
1:C:31:THR:O	1:C:32:LEU:HD12	2.09	0.52
1:C:140:THR:HG21	1:C:307:GLU:OE2	2.09	0.52
1:E:140:THR:CA	1:E:306:LEU:HD23	2.40	0.52
1:E:304:GLU:HG2	1:E:305:ARG:NH1	2.25	0.52
1:F:149:ASP:OD1	1:F:177:SER:HB3	2.10	0.52
1:F:266:VAL:CG2	1:F:271:TRP:HB2	2.31	0.52
1:B:412:LEU:HB3	1:B:426:TRP:CD1	2.44	0.52
1:D:142:SER:O	1:D:146:ASN:HB2	2.10	0.52
1:D:358:MET:CE	1:D:423:TRP:HB2	2.35	0.52
1:G:64:VAL:HG12	1:G:68:VAL:HG11	1.91	0.52
1:G:294:ILE:O	1:G:298:VAL:HG23	2.10	0.52
1:D:325:LEU:HD22	1:D:339:LEU:HD23	1.91	0.52
1:D:394:ASN:O	1:D:395:TRP:CB	2.57	0.52
1:F:94:LEU:HD22	1:F:113:ARG:HB2	1.91	0.52
1:F:391:HIS:HA	1:F:411:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:LEU:HD12	1:H:108:LEU:O	2.10	0.52
1:H:353:ASP:O	1:H:367:ARG:HD2	2.09	0.52
1:B:325:LEU:O	1:B:325:LEU:HD22	2.09	0.52
1:F:131:ILE:C	1:F:131:ILE:HD12	2.35	0.52
1:F:447:ILE:HD13	1:F:447:ILE:N	2.25	0.52
1:G:325:LEU:O	1:G:325:LEU:HD22	2.09	0.52
1:H:310:ARG:O	1:H:314:LEU:HD23	2.09	0.52
1:H:346:ILE:O	1:H:426:TRP:CZ3	2.62	0.52
1:H:358:MET:HG3	1:H:363:THR:HG22	1.92	0.52
1:A:85:SER:HB2	1:A:286:TYR:CE2	2.45	0.52
1:B:202:LEU:O	1:B:206:ASN:HB2	2.10	0.52
1:B:125:LEU:O	1:B:125:LEU:HD12	2.10	0.52
1:C:239:VAL:HG11	1:C:289:ARG:NH2	2.25	0.52
1:C:457:ARG:O	1:C:461:GLU:HG3	2.10	0.52
1:E:283:LEU:HD23	1:E:283:LEU:C	2.35	0.52
1:G:16:PRO:HB3	1:G:18:HIS:CE1	2.44	0.52
1:G:124:THR:HG21	1:H:291:SER:HA	1.91	0.52
1:H:152:ARG:HB2	1:H:160:VAL:CG1	2.40	0.52
1:A:18:HIS:O	1:A:20:PRO:HD3	2.09	0.51
1:B:130:ILE:H	1:B:130:ILE:CD1	2.14	0.51
1:C:19:VAL:HG12	1:C:234:ASP:HA	1.91	0.51
1:C:366:ILE:O	1:C:367:ARG:HB2	2.09	0.51
1:C:439:GLY:HA3	1:E:361:GLY:O	2.09	0.51
1:D:13:GLU:OE1	1:D:196:PRO:HB3	2.10	0.51
1:E:384:ASP:HB3	1:E:387:ARG:HB2	1.92	0.51
1:C:323:LEU:CA	1:D:323:LEU:HD12	2.38	0.51
1:D:356:LEU:HD21	1:D:363:THR:CG2	2.34	0.51
1:D:434:ARG:O	1:H:366:ILE:HA	2.10	0.51
1:E:105:VAL:HG12	1:E:106:PHE:H	1.74	0.51
1:F:86:VAL:HG12	1:F:87:GLU:N	2.23	0.51
1:G:42:SER:O	1:G:45:ILE:HG13	2.11	0.51
1:H:18:HIS:ND1	1:H:198:GLN:HG2	2.25	0.51
1:D:214:VAL:HB	1:D:257:ARG:CA	2.40	0.51
2:D:900:BLA:OB	2:D:900:BLA:HBB1	2.10	0.51
1:E:32:LEU:HD23	1:E:72:LEU:HD21	1.93	0.51
1:H:371:GLU:HG3	1:H:372:ARG:N	2.25	0.51
1:H:416:PHE:O	1:H:490:MET:HG2	2.11	0.51
1:C:425:PHE:CD1	1:C:425:PHE:N	2.78	0.51
1:D:32:LEU:HD21	1:D:59:LEU:CD2	2.40	0.51
1:D:162:ALA:HB3	1:D:175:ALA:HB3	1.92	0.51
1:E:98:ILE:HD11	1:E:239:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:SER:HA	1:G:276:CYS:O	2.10	0.51
1:A:126:ASN:OD1	1:A:154:MET:HE3	2.09	0.51
1:A:443:LYS:HB2	1:A:444:LEU:CD2	2.41	0.51
1:B:16:PRO:O	1:B:20:PRO:HD3	2.10	0.51
1:B:127:ALA:HA	1:B:130:ILE:HD11	1.92	0.51
1:C:71:MET:SD	1:C:86:VAL:HG23	2.51	0.51
1:C:147:VAL:HA	1:C:150:GLU:HB3	1.92	0.51
1:C:435:ILE:HG22	1:E:364:LEU:CD2	2.41	0.51
1:F:202:LEU:O	1:F:206:ASN:HB2	2.11	0.51
1:G:319:THR:HG22	1:G:322:ARG:HH21	1.76	0.51
1:G:445:LEU:O	1:G:446:THR:CG2	2.59	0.51
1:A:159:ARG:HG2	1:A:160:VAL:N	2.25	0.51
1:A:387:ARG:HD2	1:A:389:ILE:O	2.11	0.51
1:B:205:GLN:NE2	1:B:237:TYR:CE2	2.78	0.51
1:B:301:ALA:O	1:B:305:ARG:HD2	2.10	0.51
1:E:412:LEU:O	1:E:426:TRP:CD1	2.63	0.51
1:D:94:LEU:HD22	1:D:113:ARG:HB3	1.93	0.51
1:E:46:GLN:HA	1:E:49:LEU:O	2.11	0.51
1:F:94:LEU:HD23	1:F:113:ARG:HH11	1.76	0.51
1:A:121:THR:HG21	1:B:85:SER:N	2.26	0.51
1:B:464:GLU:O	1:B:468:ARG:HG3	2.11	0.51
1:C:150:GLU:O	1:C:153:ARG:HB2	2.10	0.51
1:E:195:ILE:HG22	1:E:200:ARG:HB2	1.92	0.51
1:G:336:PHE:CD2	1:G:364:LEU:HD21	2.45	0.51
1:G:358:MET:O	1:G:422:GLY:HA2	2.11	0.51
1:H:51:PHE:CZ	1:H:52:VAL:HG12	2.46	0.51
1:A:139:ASP:HB2	1:A:142:SER:HB2	1.93	0.51
1:B:416:PHE:O	1:B:490:MET:HG2	2.11	0.51
2:B:900:BLA:HMA2	2:B:900:BLA:CMB	2.30	0.51
1:E:335:LEU:C	1:E:337:GLY:H	2.17	0.51
1:F:18:HIS:CD2	1:F:19:VAL:HG13	2.46	0.51
1:A:130:ILE:HD12	1:A:295:PHE:CZ	2.45	0.51
1:A:210:LEU:HD12	1:A:289:ARG:HD3	1.92	0.51
1:A:366:ILE:HG22	1:G:435:ILE:HD13	1.93	0.51
1:A:443:LYS:HB3	1:A:444:LEU:HD22	1.92	0.51
1:B:328:ARG:CB	1:B:338:ALA:HB2	2.40	0.51
1:C:164:ARG:HB3	1:C:164:ARG:HH11	1.76	0.51
1:D:415:ARG:HB2	1:D:423:TRP:CZ2	2.46	0.51
1:D:430:GLU:HG3	1:D:469:GLY:H	1.74	0.51
1:E:70:ARG:O	1:E:74:GLU:HG3	2.11	0.51
1:H:22:ALA:HA	1:H:220:ARG:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HG22	1:A:118:LEU:H	1.74	0.50
1:B:117:THR:O	1:B:118:LEU:HD23	2.10	0.50
1:A:9:LEU:HD21	1:A:450:SER:HB3	1.93	0.50
1:D:45:ILE:HD12	1:D:46:GLN:N	2.22	0.50
1:E:256:VAL:HG11	1:E:277:HIS:HB3	1.92	0.50
1:G:249:GLU:OE1	1:G:449:PRO:HD2	2.11	0.50
1:A:7:VAL:HA	1:A:11:ASN:HD22	1.77	0.50
1:A:356:LEU:CD2	1:A:365:SER:HB2	2.42	0.50
1:C:153:ARG:CZ	1:F:498:LEU:HD21	2.41	0.50
1:E:25:PRO:HD3	1:E:216:TYR:HD2	1.77	0.50
1:F:322:ARG:CZ	1:F:484:LYS:HB3	2.42	0.50
1:G:290:MET:HE3	1:H:124:THR:HG21	1.93	0.50
1:H:17:ILE:CG2	1:H:244:SER:HB2	2.41	0.50
1:A:97:VAL:HG22	1:A:110:PHE:CD2	2.45	0.50
1:B:14:ASP:HA	1:H:383:ARG:HH12	1.77	0.50
1:B:68:VAL:HG13	1:B:97:VAL:HG11	1.93	0.50
1:B:191:PRO:HD3	1:B:459:SER:O	2.12	0.50
1:C:130:ILE:HG23	1:C:295:PHE:CD1	2.47	0.50
1:C:301:ALA:O	1:C:304:GLU:HB3	2.12	0.50
1:C:336:PHE:CE1	1:C:359:LEU:HB3	2.47	0.50
1:D:214:VAL:CB	1:D:257:ARG:HA	2.41	0.50
1:E:264:ILE:HB	1:E:272:GLY:O	2.11	0.50
1:E:384:ASP:CG	1:E:387:ARG:HG3	2.37	0.50
2:F:900:BLA:HMB2	2:F:900:BLA:CMA	2.34	0.50
1:G:30:VAL:HG12	1:G:32:LEU:CD1	2.42	0.50
1:G:75:GLY:HA2	1:G:82:TRP:CD1	2.45	0.50
1:G:212:ALA:HA	1:G:282:LYS:O	2.11	0.50
1:H:121:THR:O	1:H:125:LEU:HD13	2.12	0.50
1:A:203:TYR:OH	2:A:900:BLA:HAA1	2.12	0.50
1:B:51:PHE:CD2	1:B:63:GLN:HG3	2.47	0.50
1:D:211:ILE:HB	1:D:259:SER:HB3	1.93	0.50
1:D:273:LEU:C	1:D:273:LEU:HD12	2.37	0.50
1:D:391:HIS:HA	1:D:411:VAL:O	2.11	0.50
1:E:383:ARG:C	1:E:385:PRO:HD3	2.36	0.50
1:E:426:TRP:CD1	1:E:426:TRP:N	2.79	0.50
1:F:147:VAL:O	1:F:151:LEU:HG	2.11	0.50
1:G:394:ASN:O	1:G:395:TRP:CB	2.58	0.50
1:H:209:ARG:HH12	2:H:900:BLA:CGD	2.24	0.50
2:H:900:BLA:CMC	2:H:900:BLA:HBC1	2.41	0.50
1:B:380:ARG:HB2	1:B:380:ARG:NH1	2.26	0.50
1:C:464:GLU:O	1:C:468:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ASN:HD22	1:D:85:SER:N	2.09	0.50
1:D:274:PHE:CE1	1:D:295:PHE:HE2	2.27	0.50
1:D:351:PRO:HB2	1:D:428:ARG:NH2	2.26	0.50
1:E:283:LEU:HD23	1:E:284:ILE:N	2.27	0.50
1:G:388:ASP:HB3	1:G:486:ARG:HE	1.77	0.50
1:A:87:GLU:CG	1:A:113:ARG:HH22	2.23	0.50
1:A:165:PHE:CE1	1:A:272:GLY:HA2	2.46	0.50
1:B:19:VAL:HB	1:B:232:SER:HB3	1.94	0.50
1:B:382:GLN:O	1:H:197:ALA:HB1	2.11	0.50
1:C:313:GLU:OE1	1:C:316:ARG:NH1	2.45	0.50
1:G:102:TYR:HE2	1:G:234:ASP:CG	2.19	0.50
1:C:326:ALA:HB2	1:D:327:ARG:NH2	2.27	0.50
1:C:346:ILE:O	1:C:426:TRP:HZ3	1.94	0.50
1:F:120:ILE:O	1:F:120:ILE:HG22	2.12	0.50
1:H:454:LEU:N	1:H:454:LEU:HD23	2.26	0.50
1:B:98:ILE:HG21	1:B:286:TYR:CE1	2.47	0.50
1:D:264:ILE:HB	1:D:272:GLY:O	2.12	0.50
1:D:383:ARG:O	1:D:385:PRO:HD3	2.12	0.50
1:E:140:THR:HA	1:E:306:LEU:HD23	1.93	0.50
1:E:146:ASN:HD22	1:E:146:ASN:C	2.20	0.50
1:E:187:GLY:HA3	1:E:435:ILE:HG13	1.93	0.50
1:E:304:GLU:HG2	1:E:305:ARG:CZ	2.41	0.50
2:E:900:BLA:HBB1	2:E:900:BLA:OB	2.10	0.50
1:F:98:ILE:HG21	1:F:286:TYR:CD1	2.47	0.50
1:G:336:PHE:CD1	1:G:336:PHE:N	2.79	0.50
1:H:457:ARG:O	1:H:461:GLU:HG2	2.11	0.50
2:A:900:BLA:HMB2	2:A:900:BLA:CMA	2.33	0.49
1:C:31:THR:C	1:C:32:LEU:HD12	2.37	0.49
1:D:72:LEU:O	1:D:76:LEU:HD13	2.12	0.49
1:D:220:ARG:HE	1:D:222:PHE:HZ	1.59	0.49
1:E:163:TYR:HA	1:E:172:GLU:O	2.12	0.49
1:E:164:ARG:NH1	1:E:166:ARG:HE	2.10	0.49
1:A:210:LEU:CD1	1:A:289:ARG:HD3	2.42	0.49
1:A:315:LEU:HD12	1:B:316:ARG:HD2	1.92	0.49
1:C:423:TRP:HB3	1:C:425:PHE:CE1	2.47	0.49
1:F:414:ILE:HD11	1:F:424:ILE:HD12	1.92	0.49
1:G:330:ARG:NH1	1:H:327:ARG:HB3	2.26	0.49
1:H:112:ILE:H	1:H:112:ILE:CD1	2.22	0.49
1:C:142:SER:O	1:C:146:ASN:HB2	2.13	0.49
1:D:302:ILE:O	1:D:306:LEU:HB2	2.12	0.49
1:E:113:ARG:NH1	1:E:285:PRO:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:ASN:HA	1:E:409:CYS:HB2	1.93	0.49
1:F:58:TYR:CZ	1:F:59:LEU:HD11	2.47	0.49
1:G:118:LEU:HD23	1:G:118:LEU:N	2.27	0.49
1:A:147:VAL:HG22	1:A:274:PHE:CE2	2.47	0.49
1:B:94:LEU:HD21	1:B:113:ARG:HG2	1.93	0.49
1:C:284:ILE:HG22	1:C:289:ARG:HG3	1.94	0.49
1:D:43:GLU:C	1:D:45:ILE:H	2.20	0.49
1:D:59:LEU:HD22	1:D:59:LEU:N	2.26	0.49
1:E:260:MET:CE	1:E:289:ARG:CG	2.91	0.49
1:F:34:ALA:O	1:F:76:LEU:HG	2.12	0.49
1:H:90:ILE:HD12	1:H:95:PHE:HB2	1.94	0.49
1:C:144:LEU:HD11	1:C:271:TRP:CZ3	2.47	0.49
1:D:94:LEU:CD2	1:D:113:ARG:HB3	2.42	0.49
1:D:187:GLY:HA3	1:D:435:ILE:HG13	1.94	0.49
1:F:315:LEU:O	1:F:319:THR:HG23	2.13	0.49
2:F:900:BLA:HMA2	2:F:900:BLA:CMB	2.34	0.49
1:H:262:ILE:O	1:H:273:LEU:HB2	2.11	0.49
1:A:305:ARG:HH21	1:B:138:ASN:HD22	1.61	0.49
1:B:37:MET:HB2	1:B:58:TYR:CZ	2.48	0.49
1:B:172:GLU:HG3	1:B:189:ARG:HD3	1.93	0.49
1:C:94:LEU:HD22	1:C:113:ARG:HB3	1.95	0.49
1:C:133:GLN:O	1:C:137:HIS:CD2	2.65	0.49
1:C:327:ARG:NH1	1:D:491:GLU:HG2	2.28	0.49
1:E:366:ILE:O	1:E:367:ARG:HB2	2.13	0.49
1:H:138:ASN:N	1:H:138:ASN:ND2	2.58	0.49
1:C:330:ARG:HH21	1:C:496:HIS:CB	2.21	0.49
1:E:22:ALA:HA	1:E:220:ARG:HA	1.94	0.49
1:G:354:GLY:HA3	1:G:370:PHE:CE1	2.47	0.49
1:A:92:GLU:OE1	1:A:93:HIS:CD2	2.65	0.49
1:A:262:ILE:HD11	1:A:292:PHE:HB3	1.95	0.49
1:C:239:VAL:O	1:C:239:VAL:HG12	2.13	0.49
1:G:46:GLN:HE21	1:G:52:VAL:HG21	1.77	0.49
1:H:20:PRO:HG2	1:H:241:ARG:HG3	1.95	0.49
1:A:157:TYR:HD2	1:A:278:HIS:HB2	1.78	0.49
1:A:485:LEU:O	1:A:489:LEU:HG	2.12	0.49
1:C:379:GLN:HA	1:C:382:GLN:HG2	1.94	0.49
1:D:304:GLU:O	1:D:308:GLN:HG2	2.12	0.49
1:E:29:LEU:HD23	1:E:221:VAL:HG11	1.95	0.49
1:C:136:LEU:HB2	1:C:137:HIS:CD2	2.47	0.49
1:E:42:SER:HA	1:E:221:VAL:HA	1.95	0.49
1:G:389:ILE:CD1	1:G:483:GLU:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HA	1:A:306:LEU:HD23	1.94	0.48
1:A:168:ASP:O	1:A:169:ASP:HB2	2.12	0.48
1:B:31:THR:HG22	1:B:107:TYR:CD1	2.47	0.48
1:B:430:GLU:O	1:B:432:VAL:HG23	2.13	0.48
2:C:900:BLA:HMB2	2:C:900:BLA:CMA	2.31	0.48
1:E:136:LEU:HB2	1:E:137:HIS:CD2	2.48	0.48
1:E:341:HIS:ND1	1:E:342:PRO:HD2	2.29	0.48
1:A:252:THR:O	1:A:445:LEU:CD2	2.57	0.48
1:A:446:THR:O	1:A:446:THR:HG23	2.12	0.48
1:F:31:THR:HG22	1:F:107:TYR:HD1	1.78	0.48
1:F:229:THR:HG23	1:F:231:GLU:H	1.78	0.48
1:G:120:ILE:HA	1:H:120:ILE:HD11	1.94	0.48
1:B:143:LEU:O	1:B:143:LEU:HD12	2.14	0.48
1:B:318:SER:O	1:B:322:ARG:HB2	2.13	0.48
1:B:329:ALA:HB3	1:B:492:LEU:HD21	1.96	0.48
1:C:152:ARG:HB2	1:C:160:VAL:HG13	1.95	0.48
1:D:168:ASP:O	1:D:169:ASP:HB2	2.12	0.48
1:A:302:ILE:O	1:A:306:LEU:HB2	2.13	0.48
1:B:98:ILE:HG21	1:B:286:TYR:CD1	2.48	0.48
1:B:324:ALA:HA	1:B:327:ARG:CD	2.43	0.48
1:B:362:ARG:H	1:B:362:ARG:HD2	1.77	0.48
1:C:18:HIS:C	1:C:20:PRO:HD3	2.37	0.48
1:C:221:VAL:CG2	1:C:221:VAL:O	2.61	0.48
1:C:321:ARG:O	1:C:325:LEU:HB2	2.14	0.48
1:C:358:MET:O	1:C:422:GLY:HA2	2.13	0.48
1:C:410:GLY:O	1:C:427:PHE:HA	2.13	0.48
1:D:294:ILE:O	1:D:294:ILE:HG22	2.14	0.48
1:E:121:THR:O	1:E:125:LEU:HB2	2.12	0.48
1:G:25:PRO:HD3	1:G:216:TYR:HD2	1.78	0.48
1:G:139:ASP:CB	1:G:142:SER:HB2	2.37	0.48
1:H:349:LEU:HD12	1:H:481:ILE:HG21	1.95	0.48
1:A:366:ILE:O	1:A:367:ARG:HB2	2.14	0.48
1:C:208:ILE:CD1	1:C:289:ARG:O	2.62	0.48
2:C:900:BLA:OB	2:C:900:BLA:HBB1	2.14	0.48
1:A:44:ASN:CG	1:A:219:MET:HG2	2.39	0.48
1:B:157:TYR:CD2	1:B:276:CYS:HB3	2.49	0.48
1:B:390:TYR:O	1:B:412:LEU:HD23	2.13	0.48
1:E:299:CYS:O	1:E:303:VAL:HB	2.14	0.48
1:E:315:LEU:O	1:E:319:THR:HG23	2.14	0.48
1:E:325:LEU:HD13	1:E:325:LEU:C	2.39	0.48
1:G:140:THR:HB	1:G:306:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:ALA:HB1	1:H:45:ILE:HG21	1.96	0.48
1:H:74:GLU:HA	1:H:77:THR:HB	1.94	0.48
1:A:72:LEU:HD13	1:A:76:LEU:CD1	2.43	0.48
1:D:305:ARG:N	1:D:305:ARG:HD2	2.28	0.48
1:E:266:VAL:HG22	1:E:271:TRP:HB2	1.95	0.48
1:E:455:THR:HB	1:E:456:PRO:HD2	1.95	0.48
1:G:172:GLU:HG3	1:G:189:ARG:HD2	1.96	0.48
1:H:42:SER:HA	1:H:221:VAL:HA	1.95	0.48
1:A:20:PRO:HG2	1:A:241:ARG:HG3	1.94	0.48
1:A:222:PHE:HA	1:A:223:PRO:C	2.39	0.48
2:A:900:BLA:OB	2:A:900:BLA:HBB1	2.13	0.48
1:C:264:ILE:HD11	1:C:274:PHE:CE1	2.49	0.48
1:D:325:LEU:HA	1:D:328:ARG:HB3	1.95	0.48
1:A:117:THR:CG2	1:A:118:LEU:N	2.76	0.48
1:C:143:LEU:O	1:C:147:VAL:HG13	2.14	0.48
1:C:407:ASP:OD1	1:C:407:ASP:N	2.47	0.48
1:D:123:PHE:O	1:D:123:PHE:CG	2.67	0.48
1:E:178:ARG:HD2	1:E:183:GLU:O	2.14	0.48
1:F:98:ILE:HG13	1:F:109:GLU:HB2	1.96	0.48
1:F:346:ILE:HD13	1:F:357:VAL:HG23	1.94	0.48
1:F:468:ARG:HA	1:F:468:ARG:NE	2.26	0.48
2:F:900:BLA:OB	2:F:900:BLA:HBB1	2.13	0.48
1:G:112:ILE:HD13	1:G:112:ILE:N	2.17	0.48
1:G:124:THR:O	1:G:128:GLN:HG3	2.14	0.48
1:G:317:VAL:O	1:G:321:ARG:HB3	2.14	0.48
1:B:286:TYR:HB3	1:B:287:PRO:HD3	1.95	0.48
1:C:211:ILE:HD13	1:C:243:VAL:HG21	1.95	0.48
1:E:292:PHE:C	1:E:294:ILE:H	2.21	0.48
1:G:82:TRP:H	1:G:101:SER:HB3	1.78	0.48
1:A:159:ARG:CG	1:A:160:VAL:N	2.77	0.47
1:B:126:ASN:HD22	1:B:288:VAL:HG22	1.79	0.47
1:C:347:ALA:CB	1:C:366:ILE:HD11	2.44	0.47
1:D:17:ILE:H	1:D:17:ILE:HD12	1.79	0.47
1:E:412:LEU:HB3	1:E:426:TRP:CD1	2.49	0.47
1:G:319:THR:O	1:G:323:LEU:HB2	2.14	0.47
1:A:106:PHE:HE2	1:A:108:LEU:HD23	1.79	0.47
1:A:330:ARG:NH2	1:B:327:ARG:HB2	2.28	0.47
1:B:207:PRO:HB2	1:B:293:GLN:HG3	1.96	0.47
1:B:222:PHE:HA	1:B:223:PRO:C	2.39	0.47
1:E:308:GLN:HA	1:E:311:ILE:CD1	2.43	0.47
1:G:377:VAL:O	1:G:381:LEU:HG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:VAL:HG22	1:H:53:ALA:N	2.29	0.47
2:H:900:BLA:HBC1	2:H:900:BLA:HMC3	1.97	0.47
1:A:139:ASP:HB2	1:A:142:SER:CB	2.44	0.47
1:A:157:TYR:CD2	1:A:278:HIS:HB2	2.49	0.47
1:B:15:GLU:HA	1:B:16:PRO:HD3	1.76	0.47
1:B:127:ALA:HB2	1:B:291:SER:OG	2.15	0.47
1:B:134:VAL:HG13	1:B:302:ILE:HG12	1.96	0.47
1:D:114:THR:HG22	1:D:115:ALA:H	1.79	0.47
1:E:42:SER:O	1:E:45:ILE:HG13	2.14	0.47
1:G:129:ARG:HH21	1:G:154:MET:HG2	1.78	0.47
1:H:152:ARG:HB2	1:H:160:VAL:HG12	1.96	0.47
1:A:288:VAL:C	1:A:290:MET:N	2.71	0.47
1:C:46:GLN:HA	1:C:51:PHE:O	2.14	0.47
1:D:273:LEU:HD12	1:D:273:LEU:O	2.13	0.47
1:E:250:TYR:N	1:E:454:LEU:HD21	2.29	0.47
1:G:85:SER:HB2	1:G:98:ILE:HG22	1.96	0.47
1:G:179:ARG:CG	1:G:179:ARG:NH1	2.69	0.47
1:H:313:GLU:O	1:H:317:VAL:HG22	2.14	0.47
1:H:336:PHE:CD2	1:H:364:LEU:HD22	2.48	0.47
1:H:352:CYS:O	1:H:367:ARG:NH2	2.48	0.47
1:D:159:ARG:HG2	1:D:160:VAL:N	2.29	0.47
1:H:211:ILE:HD12	1:H:259:SER:HB3	1.96	0.47
1:H:353:ASP:HA	1:H:367:ARG:NH1	2.30	0.47
1:H:440:LYS:O	1:H:441:PRO:C	2.58	0.47
1:H:442:GLU:O	1:H:442:GLU:HG3	2.13	0.47
1:A:266:VAL:HG21	1:A:271:TRP:CD1	2.50	0.47
1:B:32:LEU:HD12	1:B:32:LEU:N	2.30	0.47
1:B:319:THR:HG22	1:B:322:ARG:NH2	2.30	0.47
1:D:37:MET:HB2	1:D:58:TYR:CZ	2.49	0.47
1:D:71:MET:HE1	1:D:97:VAL:HG12	1.96	0.47
1:E:278:HIS:CE1	1:E:282:LYS:HD2	2.50	0.47
1:E:462:ALA:O	1:E:466:VAL:HG23	2.14	0.47
1:G:335:LEU:HD12	1:G:339:LEU:HD11	1.95	0.47
1:H:7:VAL:HA	1:H:11:ASN:ND2	2.24	0.47
1:H:415:ARG:HA	1:H:422:GLY:O	2.15	0.47
1:H:433:HIS:CD2	1:H:436:ARG:HG2	2.46	0.47
1:B:324:ALA:HB1	1:B:328:ARG:NH2	2.30	0.47
1:B:394:ASN:O	1:B:395:TRP:HB2	2.14	0.47
1:B:455:THR:HB	1:B:456:PRO:HD2	1.97	0.47
1:C:414:ILE:HD12	1:C:486:ARG:HB2	1.96	0.47
1:D:61:GLN:NE2	1:D:66:PRO:HG3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:HIS:CD2	1:D:107:TYR:HB2	2.50	0.47
1:D:207:PRO:HG2	1:D:293:GLN:NE2	2.29	0.47
1:D:289:ARG:O	1:D:292:PHE:HD2	1.97	0.47
1:D:436:ARG:HG3	1:H:369:ASP:OD1	2.14	0.47
2:D:900:BLA:HMA2	2:D:900:BLA:CMB	2.33	0.47
1:E:54:SER:O	1:E:55:PRO:C	2.56	0.47
1:E:59:LEU:HD23	1:E:59:LEU:H	1.79	0.47
1:E:189:ARG:HH21	1:E:189:ARG:HB3	1.79	0.47
1:F:118:LEU:O	1:F:122:SER:HB2	2.15	0.47
1:H:355:ALA:HB3	1:H:366:ILE:HG13	1.96	0.47
1:A:26:HIS:O	1:A:112:ILE:HG12	2.15	0.47
1:B:214:VAL:C	1:B:216:TYR:H	2.21	0.47
1:B:266:VAL:HG22	1:B:271:TRP:HB2	1.97	0.47
1:B:393:ASP:HA	1:B:409:CYS:O	2.15	0.47
1:E:356:LEU:CD2	1:E:365:SER:HB3	2.45	0.47
1:F:249:GLU:CD	1:F:449:PRO:HD2	2.40	0.47
1:G:103:LYS:HD3	1:G:103:LYS:HA	1.66	0.47
1:A:121:THR:HG22	1:B:286:TYR:OH	2.15	0.47
1:A:410:GLY:O	1:A:427:PHE:HA	2.15	0.47
1:A:445:LEU:HG	1:A:446:THR:H	1.80	0.47
1:E:40:ALA:CB	1:E:223:PRO:HD2	2.44	0.47
1:E:128:GLN:HG2	1:F:297:GLN:OE1	2.14	0.47
1:F:431:GLU:O	1:F:432:VAL:C	2.57	0.47
1:G:67:GLU:CD	1:G:67:GLU:H	2.23	0.47
1:G:315:LEU:O	1:G:318:SER:HB2	2.15	0.47
1:G:378:LEU:CD1	1:G:425:PHE:HZ	2.27	0.47
1:H:94:LEU:O	1:H:94:LEU:HD13	2.14	0.47
1:H:149:ASP:HB3	1:H:153:ARG:NH2	2.30	0.47
1:C:208:ILE:HD11	1:C:293:GLN:N	2.30	0.47
1:D:79:ASN:H	1:D:79:ASN:HD22	1.62	0.47
1:D:326:ALA:C	1:D:328:ARG:H	2.23	0.47
1:F:430:GLU:HB3	1:F:468:ARG:NH1	2.30	0.47
1:G:322:ARG:NH2	1:G:484:LYS:HD3	2.30	0.47
1:D:19:VAL:HG12	1:D:233:PHE:O	2.15	0.46
1:D:339:LEU:HD13	1:D:357:VAL:HG21	1.97	0.46
1:E:315:LEU:HD22	1:E:315:LEU:HA	1.72	0.46
1:F:350:ILE:HD13	1:F:478:ASP:HB3	1.96	0.46
1:F:412:LEU:HB3	1:F:426:TRP:HD1	1.80	0.46
1:G:412:LEU:HB3	1:G:426:TRP:HD1	1.78	0.46
1:C:130:ILE:O	1:C:130:ILE:HD13	2.14	0.46
1:C:417:HIS:HD2	1:C:420:GLU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:ILE:CG2	1:G:296:SER:HB2	2.45	0.46
1:H:319:THR:HA	1:H:322:ARG:HB2	1.98	0.46
1:D:356:LEU:HD23	1:D:365:SER:HA	1.96	0.46
1:E:64:VAL:HG12	1:E:68:VAL:HG11	1.98	0.46
2:E:900:BLA:CMC	2:E:900:BLA:HBC1	2.46	0.46
1:F:311:ILE:C	1:F:313:GLU:H	2.23	0.46
1:G:48:LEU:HD11	1:G:112:ILE:HD12	1.97	0.46
1:G:68:VAL:HG13	1:G:97:VAL:HG11	1.96	0.46
1:G:109:GLU:HG2	1:G:240:LEU:HD12	1.98	0.46
1:A:102:TYR:HE2	1:A:234:ASP:OD2	1.98	0.46
1:B:237:TYR:OH	1:H:419:GLN:HG2	2.15	0.46
1:C:138:ASN:ND2	1:D:305:ARG:HH22	2.14	0.46
1:D:31:THR:C	1:D:32:LEU:HD12	2.40	0.46
1:D:134:VAL:CG2	1:D:143:LEU:HD23	2.41	0.46
1:E:305:ARG:CA	1:E:308:GLN:HG2	2.32	0.46
1:F:118:LEU:O	1:F:122:SER:HB3	2.15	0.46
1:F:354:GLY:HA3	1:F:370:PHE:CZ	2.50	0.46
1:G:260:MET:HE1	1:G:292:PHE:CD2	2.51	0.46
1:A:178:ARG:NH2	1:G:334:ASP:OD2	2.48	0.46
1:A:436:ARG:O	1:G:364:LEU:CA	2.55	0.46
1:B:18:HIS:CD2	1:B:19:VAL:HG13	2.50	0.46
1:B:168:ASP:O	1:B:169:ASP:HB2	2.16	0.46
1:C:467:VAL:O	1:C:468:ARG:C	2.58	0.46
1:D:362:ARG:HH12	1:H:178:ARG:HH22	1.61	0.46
1:F:29:LEU:CD1	1:F:109:GLU:HG2	2.44	0.46
1:G:336:PHE:H	1:G:336:PHE:HD1	1.58	0.46
1:H:278:HIS:HD2	1:H:280:SER:O	1.97	0.46
1:A:16:PRO:HB2	1:A:19:VAL:HG22	1.97	0.46
1:C:121:THR:HG23	1:D:287:PRO:HB3	1.98	0.46
1:D:391:HIS:HB3	1:D:412:LEU:CD2	2.46	0.46
1:E:278:HIS:ND1	1:E:282:LYS:HD2	2.30	0.46
1:F:71:MET:HG2	1:F:82:TRP:CZ2	2.51	0.46
1:F:159:ARG:NH1	1:F:183:GLU:O	2.48	0.46
1:F:207:PRO:HG2	1:F:293:GLN:HG3	1.97	0.46
1:F:311:ILE:C	1:F:313:GLU:N	2.74	0.46
1:F:466:VAL:HG12	1:F:467:VAL:HG13	1.98	0.46
1:G:143:LEU:HD12	1:G:144:LEU:N	2.31	0.46
1:A:108:LEU:HD22	1:A:108:LEU:HA	1.70	0.46
1:A:214:VAL:O	1:A:214:VAL:HG12	2.16	0.46
1:A:319:THR:HG22	1:A:322:ARG:NH2	2.31	0.46
1:D:339:LEU:O	1:D:346:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:900:BLA:HMB2	2:D:900:BLA:CMA	2.35	0.46
1:E:103:LYS:HD2	1:E:103:LYS:HA	1.63	0.46
1:G:214:VAL:C	1:G:216:TYR:H	2.24	0.46
1:H:33:ARG:HG2	1:H:37:MET:HB3	1.97	0.46
1:H:130:ILE:HG12	1:H:147:VAL:CG1	2.45	0.46
1:D:71:MET:O	1:D:74:GLU:HG2	2.15	0.46
1:D:460:PHE:C	1:D:460:PHE:CD2	2.94	0.46
1:E:172:GLU:HB2	1:E:189:ARG:HD3	1.98	0.46
1:E:292:PHE:C	1:E:294:ILE:N	2.70	0.46
1:F:44:ASN:OD1	1:F:219:MET:HG2	2.16	0.46
1:A:109:GLU:HG2	1:A:240:LEU:HD12	1.98	0.46
1:B:94:LEU:C	1:B:94:LEU:HD22	2.41	0.46
1:C:94:LEU:H	1:C:94:LEU:HD13	1.80	0.46
1:C:119:SER:O	1:D:120:ILE:HD11	2.15	0.46
1:G:129:ARG:NH2	1:G:154:MET:HG2	2.31	0.46
1:G:465:GLU:HG2	1:G:468:ARG:HH21	1.80	0.46
1:H:103:LYS:HD2	1:H:103:LYS:HA	1.76	0.46
1:A:89:ARG:HG3	1:A:94:LEU:HA	1.98	0.46
1:A:140:THR:HG21	1:A:307:GLU:OE2	2.16	0.46
1:B:11:ASN:O	1:B:11:ASN:ND2	2.49	0.46
1:C:262:ILE:CD1	1:C:292:PHE:HB3	2.46	0.46
1:D:339:LEU:HD12	1:D:357:VAL:HG21	1.98	0.46
1:D:358:MET:O	1:D:422:GLY:HA2	2.16	0.46
1:E:82:TRP:O	1:E:100:HIS:HA	2.16	0.46
1:E:120:ILE:HG13	1:F:120:ILE:HD13	1.98	0.46
1:E:130:ILE:HG23	1:E:147:VAL:HG12	1.98	0.46
1:E:142:SER:O	1:E:146:ASN:HB2	2.16	0.46
1:E:294:ILE:O	1:E:298:VAL:HG23	2.16	0.46
1:E:389:ILE:HG22	1:E:390:TYR:N	2.31	0.46
1:F:101:SER:HB2	1:F:106:PHE:CE2	2.51	0.46
1:F:485:LEU:HD13	1:F:485:LEU:O	2.15	0.46
1:G:199:ALA:O	1:G:203:TYR:CD1	2.69	0.46
1:A:108:LEU:HD12	1:A:110:PHE:CZ	2.52	0.45
1:B:38:VAL:O	1:B:55:PRO:HA	2.16	0.45
1:E:7:VAL:HG11	1:E:15:GLU:HG3	1.97	0.45
1:F:44:ASN:CG	1:F:219:MET:HG2	2.41	0.45
1:G:98:ILE:HG21	1:G:286:TYR:CZ	2.51	0.45
1:G:308:GLN:HA	1:G:311:ILE:HD12	1.98	0.45
1:G:485:LEU:HD23	1:G:485:LEU:HA	1.79	0.45
1:H:464:GLU:O	1:H:468:ARG:HB2	2.16	0.45
1:A:32:LEU:HD23	1:A:72:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:THR:CG2	1:B:306:LEU:HB3	2.46	0.45
1:F:126:ASN:OD1	1:F:288:VAL:HG13	2.16	0.45
1:G:13:GLU:H	1:G:13:GLU:HG3	1.49	0.45
1:H:354:GLY:HA3	1:H:370:PHE:CE2	2.51	0.45
1:C:189:ARG:HH21	1:C:463:TRP:NE1	2.14	0.45
1:C:286:TYR:N	1:C:287:PRO:CD	2.79	0.45
1:D:364:LEU:HD23	1:D:364:LEU:HA	1.72	0.45
1:E:123:PHE:CD2	1:E:123:PHE:C	2.94	0.45
1:F:235:LEU:O	1:F:238:SER:HB3	2.17	0.45
1:A:331:ASP:CG	1:B:495:ASN:HD21	2.25	0.45
1:C:119:SER:C	1:D:120:ILE:HD11	2.42	0.45
1:C:165:PHE:HD1	1:C:272:GLY:HA2	1.82	0.45
1:F:271:TRP:CE3	1:F:303:VAL:HG11	2.52	0.45
1:A:217:THR:HA	1:A:218:PRO:HD3	1.72	0.45
1:C:60:THR:N	1:C:63:GLN:HE21	2.14	0.45
1:E:210:LEU:C	1:E:210:LEU:HD23	2.42	0.45
1:F:19:VAL:HG12	1:F:234:ASP:HA	1.97	0.45
1:F:179:ARG:HH11	1:F:181:ASP:HB3	1.82	0.45
1:G:133:GLN:CB	1:G:147:VAL:HG12	2.47	0.45
1:G:186:LEU:HD23	1:G:187:GLY:N	2.31	0.45
1:G:311:ILE:HD13	1:G:311:ILE:C	2.42	0.45
1:H:410:GLY:HA3	1:H:428:ARG:HB2	1.98	0.45
1:A:417:HIS:NE2	1:A:420:GLU:OE1	2.49	0.45
1:B:201:ARG:HA	1:B:201:ARG:HD3	1.75	0.45
1:D:325:LEU:HD12	1:D:325:LEU:C	2.42	0.45
1:F:366:ILE:H	1:F:366:ILE:CD1	2.23	0.45
1:G:159:ARG:NH1	1:G:183:GLU:O	2.49	0.45
1:G:266:VAL:HG23	1:G:266:VAL:O	2.16	0.45
1:H:288:VAL:O	1:H:291:SER:HB3	2.15	0.45
1:A:45:ILE:HD12	1:A:46:GLN:N	2.22	0.45
1:B:24:GLN:NE2	1:B:211:ILE:HG23	2.31	0.45
1:B:173:VAL:HG12	1:B:186:LEU:HD23	1.99	0.45
1:B:315:LEU:HD21	1:B:477:THR:HG23	1.99	0.45
1:C:237:TYR:OH	1:G:419:GLN:HG2	2.16	0.45
1:E:43:GLU:HB3	1:E:222:PHE:HE2	1.80	0.45
1:E:140:THR:CG2	1:E:306:LEU:HB3	2.35	0.45
1:G:249:GLU:OE2	1:G:450:SER:HB2	2.17	0.45
1:H:152:ARG:HG3	1:H:157:TYR:O	2.16	0.45
1:C:25:PRO:HD3	1:C:216:TYR:CD2	2.52	0.45
1:C:336:PHE:HE1	1:C:359:LEU:HB3	1.81	0.45
1:C:443:LYS:O	1:C:445:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:PRO:O	1:D:70:ARG:HB2	2.16	0.45
1:D:181:ASP:OD1	1:D:181:ASP:N	2.41	0.45
1:E:135:GLN:OE1	1:F:305:ARG:CZ	2.65	0.45
1:F:204:ILE:HG23	1:F:265:VAL:HG21	1.98	0.45
1:G:179:ARG:NH1	1:G:181:ASP:HB2	2.32	0.45
1:G:187:GLY:O	1:G:433:HIS:HE1	1.99	0.45
1:H:416:PHE:CE1	1:H:424:ILE:HG13	2.48	0.45
1:H:475:SER:HB3	1:H:478:ASP:H	1.81	0.45
1:B:164:ARG:HG3	1:B:174:VAL:HG21	1.98	0.45
1:C:183:GLU:HG2	1:C:443:LYS:HE3	1.99	0.45
1:C:290:MET:HE3	1:D:124:THR:HG21	1.99	0.45
1:D:18:HIS:C	1:D:20:PRO:HD3	2.41	0.45
1:D:251:LEU:HD23	1:D:251:LEU:HA	1.81	0.45
1:F:214:VAL:CG1	1:F:252:THR:HG23	2.47	0.45
1:G:391:HIS:HA	1:G:411:VAL:O	2.17	0.45
1:G:424:ILE:HD11	1:G:489:LEU:HD11	1.98	0.45
1:H:278:HIS:CD2	1:H:280:SER:O	2.69	0.45
1:H:336:PHE:HD2	1:H:364:LEU:HD22	1.82	0.45
1:H:356:LEU:HD12	1:H:425:PHE:CD1	2.52	0.45
1:A:84:ASN:HB2	1:A:99:GLY:O	2.16	0.45
1:A:327:ARG:HH11	1:A:328:ARG:HE	1.65	0.45
1:B:68:VAL:CG1	1:B:97:VAL:HG11	2.46	0.45
1:C:435:ILE:HG22	1:E:364:LEU:HD22	1.98	0.45
1:D:197:ALA:HB1	1:F:382:GLN:O	2.16	0.45
1:F:415:ARG:CZ	1:F:418:ARG:HG2	2.47	0.45
1:F:426:TRP:CD1	1:F:426:TRP:N	2.85	0.45
1:G:493:CYS:O	1:G:496:HIS:CD2	2.70	0.45
1:H:127:ALA:C	1:H:129:ARG:H	2.25	0.45
1:H:323:LEU:C	1:H:323:LEU:HD23	2.42	0.45
1:B:341:HIS:O	1:B:345:GLY:HA3	2.17	0.44
1:C:64:VAL:CG1	1:C:68:VAL:HB	2.47	0.44
1:C:134:VAL:HG12	1:C:302:ILE:HG12	1.99	0.44
1:F:200:ARG:O	1:F:204:ILE:HG13	2.17	0.44
1:F:424:ILE:HD11	1:F:489:LEU:CD1	2.44	0.44
2:H:900:BLA:HBB1	2:H:900:BLA:OB	2.16	0.44
1:A:24:GLN:HE22	1:A:212:ALA:H	1.64	0.44
1:A:363:THR:HB	1:G:438:GLY:CA	2.45	0.44
1:B:150:GLU:O	1:B:154:MET:HG3	2.17	0.44
1:C:20:PRO:HG2	1:C:241:ARG:HG3	1.98	0.44
1:C:243:VAL:HB	1:C:248:CYS:SG	2.57	0.44
1:E:135:GLN:NE2	1:E:135:GLN:CA	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ARG:CG	1:E:160:VAL:N	2.80	0.44
1:F:328:ARG:HD2	1:F:338:ALA:HA	1.99	0.44
1:F:356:LEU:C	1:F:356:LEU:HD13	2.42	0.44
1:H:162:ALA:HA	1:H:273:LEU:O	2.18	0.44
1:H:328:ARG:HD3	1:H:341:HIS:ND1	2.32	0.44
1:A:331:ASP:OD2	1:B:495:ASN:ND2	2.50	0.44
1:B:164:ARG:HB3	1:B:164:ARG:NH1	2.32	0.44
1:B:202:LEU:C	1:B:204:ILE:H	2.23	0.44
1:B:327:ARG:HH11	1:B:327:ARG:CB	2.30	0.44
1:D:98:ILE:HG21	1:D:286:TYR:CE1	2.52	0.44
1:D:346:ILE:O	1:D:426:TRP:CZ3	2.63	0.44
1:E:249:GLU:C	1:E:454:LEU:HD21	2.42	0.44
1:H:319:THR:HG22	1:H:322:ARG:HH21	1.83	0.44
1:H:356:LEU:HB3	1:H:425:PHE:HB2	1.99	0.44
1:A:202:LEU:HD13	1:A:241:ARG:NH2	2.32	0.44
1:A:246:ILE:HG23	1:A:454:LEU:HD21	2.00	0.44
1:B:164:ARG:O	1:B:171:GLY:HA2	2.17	0.44
1:B:373:GLN:O	1:B:377:VAL:HG23	2.18	0.44
1:B:411:VAL:HG22	1:B:427:PHE:CE2	2.52	0.44
1:C:302:ILE:HG23	1:C:306:LEU:HD22	1.98	0.44
1:G:161:MET:HG2	1:G:176:GLU:HG3	2.00	0.44
1:A:307:GLU:C	1:A:309:GLY:N	2.74	0.44
1:A:434:ARG:O	1:G:366:ILE:HA	2.18	0.44
1:C:215:ALA:HB3	1:C:257:ARG:CZ	2.47	0.44
1:E:286:TYR:HB3	1:E:287:PRO:HD3	1.99	0.44
1:F:305:ARG:HA	1:F:308:GLN:HG2	2.00	0.44
1:G:127:ALA:HB2	1:G:291:SER:OG	2.17	0.44
1:H:46:GLN:CG	1:H:52:VAL:HA	2.47	0.44
1:A:24:GLN:HG2	1:A:216:TYR:HE2	1.81	0.44
1:A:394:ASN:O	1:A:395:TRP:CD1	2.71	0.44
1:C:153:ARG:HD3	1:F:498:LEU:HD21	0.45	0.44
1:D:98:ILE:HG21	1:D:286:TYR:CG	2.52	0.44
1:D:208:ILE:HG22	1:D:262:ILE:CD1	2.48	0.44
1:E:59:LEU:HD12	1:E:69:LEU:HD13	1.98	0.44
1:E:140:THR:HG22	1:E:306:LEU:CB	2.34	0.44
1:E:195:ILE:CG2	1:E:200:ARG:HB2	2.47	0.44
1:F:24:GLN:NE2	1:F:211:ILE:HA	2.27	0.44
1:G:17:ILE:O	1:G:241:ARG:HD2	2.18	0.44
1:G:154:MET:HE1	1:G:292:PHE:HE1	1.82	0.44
1:G:201:ARG:HG2	1:G:205:GLN:HE21	1.83	0.44
1:A:164:ARG:HH12	1:A:166:ARG:HH21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:O	1:A:227:PRO:HD3	2.18	0.44
1:A:301:ALA:HB2	1:B:135:GLN:HG2	2.00	0.44
1:B:136:LEU:HB2	1:B:137:HIS:ND1	2.33	0.44
1:B:451:GLY:HA2	1:B:452:PRO:HD3	1.65	0.44
1:C:189:ARG:NH2	1:C:463:TRP:HE1	2.15	0.44
1:D:206:ASN:HA	1:D:207:PRO:HD3	1.76	0.44
1:D:324:ALA:O	1:D:328:ARG:HB2	2.18	0.44
1:D:366:ILE:HG23	1:H:435:ILE:HG22	2.00	0.44
1:E:120:ILE:CD1	1:F:120:ILE:HD13	2.48	0.44
1:E:130:ILE:HD11	1:E:150:GLU:HB2	1.99	0.44
1:E:273:LEU:C	1:E:273:LEU:HD12	2.43	0.44
1:H:314:LEU:O	1:H:318:SER:HB2	2.18	0.44
1:A:297:GLN:HA	1:B:135:GLN:NE2	2.32	0.44
1:A:305:ARG:HB3	1:A:308:GLN:HE21	1.82	0.44
1:B:305:ARG:HE	1:B:305:ARG:HB3	1.67	0.44
1:C:13:GLU:H	1:C:13:GLU:HG3	1.44	0.44
1:C:19:VAL:HG23	1:C:19:VAL:O	2.18	0.44
1:C:297:GLN:NE2	1:D:128:GLN:NE2	2.66	0.44
1:D:129:ARG:NH2	1:G:497:ALA:CB	2.80	0.44
1:D:195:ILE:HA	1:D:196:PRO:HD3	1.74	0.44
1:E:188:GLN:HE22	1:E:460:PHE:HB2	1.83	0.44
1:E:225:LEU:HD22	1:E:225:LEU:N	2.32	0.44
1:E:311:ILE:HB	1:E:477:THR:HG21	1.99	0.44
1:G:306:LEU:HD12	1:G:306:LEU:HA	1.71	0.44
1:A:216:TYR:CD1	1:A:216:TYR:C	2.95	0.44
1:C:210:LEU:HD12	1:C:289:ARG:HD3	2.00	0.44
1:D:42:SER:O	1:D:45:ILE:HG23	2.17	0.44
1:E:98:ILE:CD1	1:E:239:VAL:HG21	2.48	0.44
1:E:306:LEU:HD11	1:F:305:ARG:CZ	2.47	0.44
1:F:199:ALA:O	1:F:203:TYR:HD1	2.01	0.44
1:F:201:ARG:CG	1:F:205:GLN:HE21	2.30	0.44
1:F:313:GLU:O	1:F:317:VAL:HG13	2.18	0.44
1:G:45:ILE:O	1:G:49:LEU:HB2	2.17	0.44
1:G:131:ILE:HD11	1:H:297:GLN:CB	2.46	0.44
1:G:191:PRO:C	1:G:193:SER:H	2.26	0.44
1:G:273:LEU:HD12	1:G:273:LEU:O	2.18	0.44
1:H:93:HIS:CD2	1:H:93:HIS:H	2.35	0.44
1:H:244:SER:HB3	2:H:900:BLA:HMD2	2.00	0.44
1:A:155:THR:OG1	1:A:156:GLY:N	2.50	0.43
1:C:315:LEU:O	1:C:319:THR:HG23	2.17	0.43
1:D:154:MET:HE2	1:D:154:MET:HB3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:GLU:H	1:F:67:GLU:CD	2.24	0.43
1:F:117:THR:O	1:F:117:THR:HG22	2.18	0.43
1:F:413:ALA:HB2	1:F:425:PHE:CE2	2.53	0.43
1:H:34:ALA:O	1:H:76:LEU:HD23	2.18	0.43
1:H:121:THR:O	1:H:121:THR:HG22	2.18	0.43
1:A:298:VAL:HG12	1:A:302:ILE:HD13	2.00	0.43
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.79	0.43
1:B:210:LEU:HD23	1:B:211:ILE:N	2.33	0.43
1:C:306:LEU:HA	1:C:306:LEU:HD12	1.54	0.43
1:C:419:GLN:HG3	1:G:237:TYR:CZ	2.53	0.43
1:D:131:ILE:O	1:D:134:VAL:HG12	2.18	0.43
1:E:140:THR:N	1:E:306:LEU:HD23	2.33	0.43
1:E:182:LEU:HD13	1:E:279:MET:CE	2.49	0.43
1:E:297:GLN:HB2	1:F:131:ILE:HD11	2.00	0.43
1:F:69:LEU:O	1:F:73:GLU:HB2	2.19	0.43
1:A:358:MET:O	1:A:422:GLY:HA2	2.18	0.43
1:E:128:GLN:HE21	1:F:297:GLN:CG	2.31	0.43
1:F:220:ARG:NE	1:F:222:PHE:HZ	2.17	0.43
1:G:19:VAL:N	1:G:20:PRO:HD3	2.33	0.43
1:H:85:SER:HB2	1:H:98:ILE:HG22	2.00	0.43
1:A:340:ALA:O	1:A:341:HIS:C	2.61	0.43
1:C:5:THR:HA	1:C:6:PRO:HD3	1.81	0.43
1:C:22:ALA:HA	1:C:221:VAL:HG13	1.99	0.43
1:C:488:ASP:HB3	1:D:327:ARG:NH2	2.33	0.43
1:D:414:ILE:HG13	1:D:414:ILE:O	2.18	0.43
1:E:394:ASN:HD21	1:E:470:HIS:CG	2.33	0.43
1:E:412:LEU:HD12	1:E:474:TRP:CE3	2.53	0.43
1:H:260:MET:HE2	1:H:289:ARG:CG	2.45	0.43
1:A:142:SER:O	1:A:146:ASN:CG	2.62	0.43
1:A:163:TYR:CG	1:A:190:TYR:OH	2.68	0.43
1:B:24:GLN:HA	1:B:25:PRO:HD3	1.89	0.43
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.84	0.43
1:B:413:ALA:HA	1:B:424:ILE:O	2.18	0.43
1:D:15:GLU:HA	1:D:16:PRO:HD3	1.79	0.43
1:D:273:LEU:C	1:D:273:LEU:CD1	2.92	0.43
1:F:71:MET:HG2	1:F:82:TRP:HZ2	1.83	0.43
1:F:87:GLU:OE1	1:F:113:ARG:NH2	2.51	0.43
1:G:130:ILE:O	1:G:130:ILE:HD13	2.18	0.43
1:G:185:TYR:O	1:G:188:GLN:HB3	2.17	0.43
1:G:415:ARG:HD3	1:G:423:TRP:CZ2	2.53	0.43
1:H:17:ILE:HG21	1:H:244:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:HIS:O	1:C:20:PRO:HD3	2.18	0.43
1:D:32:LEU:HD21	1:D:59:LEU:HD21	2.00	0.43
1:D:65:GLY:HA2	1:D:66:PRO:HD3	1.81	0.43
1:D:187:GLY:HA3	1:D:435:ILE:CD1	2.49	0.43
1:D:353:ASP:O	1:D:367:ARG:HD3	2.19	0.43
1:G:346:ILE:O	1:G:426:TRP:CZ3	2.72	0.43
2:H:900:BLA:HMB2	2:H:900:BLA:CMA	2.33	0.43
1:A:45:ILE:HG22	1:A:49:LEU:HD12	2.00	0.43
1:A:179:ARG:H	1:A:182:LEU:HD12	1.83	0.43
1:D:15:GLU:OE2	1:D:245:PRO:HD2	2.19	0.43
1:D:416:PHE:CE1	1:D:422:GLY:C	2.96	0.43
1:E:33:ARG:HG2	1:E:37:MET:HB3	1.99	0.43
1:E:158:ASP:OD1	1:E:278:HIS:CE1	2.72	0.43
1:F:190:TYR:HA	1:F:191:PRO:HD3	1.83	0.43
1:H:250:TYR:O	1:H:250:TYR:HD1	2.02	0.43
1:A:208:ILE:H	1:A:208:ILE:CD1	2.29	0.43
1:B:125:LEU:HD12	1:B:125:LEU:C	2.44	0.43
1:B:130:ILE:HG12	1:B:131:ILE:N	2.33	0.43
1:D:243:VAL:CG1	1:D:244:SER:N	2.82	0.43
1:E:24:GLN:HA	1:E:25:PRO:HD3	1.82	0.43
1:E:201:ARG:NH1	1:E:205:GLN:HG3	2.34	0.43
1:F:44:ASN:HB3	1:F:219:MET:SD	2.58	0.43
1:G:86:VAL:HG12	1:G:87:GLU:N	2.34	0.43
1:G:133:GLN:HE21	1:G:150:GLU:HB2	1.82	0.43
1:G:407:ASP:OD2	1:G:407:ASP:N	2.51	0.43
1:H:25:PRO:HD3	1:H:216:TYR:HD2	1.83	0.43
1:A:130:ILE:CG1	1:A:150:GLU:HG2	2.48	0.43
1:A:305:ARG:HB3	1:A:305:ARG:HE	1.73	0.43
1:B:42:SER:O	1:B:45:ILE:HG13	2.19	0.43
1:B:164:ARG:HB3	1:B:164:ARG:CZ	2.49	0.43
1:B:346:ILE:HD13	1:B:357:VAL:HG23	1.99	0.43
1:B:486:ARG:HH11	1:B:487:LEU:HD12	1.84	0.43
1:E:55:PRO:HG3	1:E:223:PRO:HD3	1.99	0.43
1:F:152:ARG:HD3	1:F:177:SER:O	2.19	0.43
1:F:203:TYR:HD2	1:F:273:LEU:CD2	2.32	0.43
1:G:424:ILE:HD12	1:G:485:LEU:HD13	1.99	0.43
1:G:441:PRO:O	1:G:442:GLU:C	2.59	0.43
1:H:328:ARG:HB3	1:H:338:ALA:HB1	2.01	0.43
1:A:85:SER:HB2	1:A:286:TYR:HE2	1.81	0.43
1:A:441:PRO:HB3	1:A:443:LYS:CD	2.48	0.43
1:C:134:VAL:HG11	1:C:302:ILE:HG12	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ALA:HB2	1:D:223:PRO:HD2	2.01	0.43
1:G:15:GLU:HA	1:G:16:PRO:HD3	1.75	0.43
1:G:152:ARG:HB2	1:G:160:VAL:CG1	2.49	0.43
1:G:210:LEU:HD23	1:G:259:SER:O	2.19	0.43
1:A:5:THR:HA	1:A:6:PRO:HD2	1.86	0.42
1:B:65:GLY:O	1:B:69:LEU:HD12	2.19	0.42
1:B:157:TYR:CE1	1:B:284:ILE:HD11	2.54	0.42
1:B:324:ALA:HB1	1:B:328:ARG:HH21	1.83	0.42
1:C:371:GLU:O	1:C:371:GLU:HG2	2.19	0.42
1:D:239:VAL:HG12	1:D:289:ARG:HH12	1.84	0.42
1:D:317:VAL:HG23	1:D:318:SER:N	2.34	0.42
1:E:475:SER:OG	1:E:478:ASP:CG	2.61	0.42
1:G:214:VAL:HG23	1:G:257:ARG:O	2.19	0.42
1:G:349:LEU:CD1	1:G:485:LEU:HG	2.49	0.42
1:D:161:MET:O	1:D:274:PHE:HA	2.19	0.42
1:F:87:GLU:HB3	1:F:113:ARG:HH12	1.73	0.42
1:B:278:HIS:HD2	1:B:280:SER:O	2.03	0.42
1:C:33:ARG:HB3	1:C:39:LEU:HD11	2.00	0.42
1:D:113:ARG:HH11	1:D:285:PRO:HB3	1.85	0.42
1:D:171:GLY:O	1:D:189:ARG:HA	2.19	0.42
1:D:479:LEU:O	1:D:483:GLU:HB2	2.19	0.42
1:F:17:ILE:O	1:F:241:ARG:HD2	2.20	0.42
1:F:209:ARG:O	1:F:260:MET:HA	2.20	0.42
1:F:222:PHE:HA	1:F:223:PRO:C	2.44	0.42
1:G:440:LYS:HB3	1:G:440:LYS:HE3	1.85	0.42
1:H:15:GLU:HA	1:H:16:PRO:HD3	1.81	0.42
1:H:179:ARG:HD2	1:H:181:ASP:OD2	2.19	0.42
1:A:194:ASP:HB3	2:A:900:BLA:HHB	2.00	0.42
1:A:327:ARG:HH11	1:A:328:ARG:NE	2.18	0.42
1:A:330:ARG:CD	1:B:330:ARG:HB2	2.49	0.42
1:B:71:MET:SD	1:B:86:VAL:HG23	2.59	0.42
1:C:31:THR:HG22	1:C:107:TYR:CD1	2.54	0.42
1:D:9:LEU:HD22	1:D:9:LEU:N	2.35	0.42
1:D:210:LEU:HD23	1:D:211:ILE:N	2.34	0.42
1:D:361:GLY:O	1:H:440:LYS:HD3	2.18	0.42
1:E:72:LEU:O	1:E:76:LEU:HD13	2.19	0.42
1:E:217:THR:HA	1:E:218:PRO:HD3	1.83	0.42
1:E:305:ARG:HB3	1:E:305:ARG:HE	1.66	0.42
1:F:49:LEU:CD1	1:F:63:GLN:HE21	2.33	0.42
1:F:367:ARG:HA	1:F:367:ARG:HD3	1.61	0.42
1:H:191:PRO:HG3	1:H:463:TRP:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ALA:O	1:C:136:LEU:HG	2.18	0.42
1:C:251:LEU:HD22	1:C:256:VAL:CG1	2.49	0.42
1:C:301:ALA:O	1:C:305:ARG:HD2	2.19	0.42
1:D:80:GLY:O	1:D:81:PRO:C	2.61	0.42
1:E:118:LEU:HD23	1:E:118:LEU:HA	1.91	0.42
1:E:172:GLU:HA	1:E:188:GLN:O	2.20	0.42
1:E:214:VAL:C	1:E:216:TYR:H	2.28	0.42
1:H:435:ILE:HG13	1:H:435:ILE:O	2.19	0.42
1:A:92:GLU:HG3	1:A:93:HIS:N	2.35	0.42
1:B:165:PHE:CD1	1:B:272:GLY:HA2	2.54	0.42
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.83	0.42
1:C:15:GLU:HA	1:C:16:PRO:HD3	1.77	0.42
1:C:183:GLU:H	1:C:443:LYS:HE3	1.84	0.42
1:D:19:VAL:CG1	1:D:234:ASP:HA	2.38	0.42
1:E:43:GLU:HB3	1:E:222:PHE:CE2	2.55	0.42
1:F:9:LEU:HD21	1:F:450:SER:HB2	2.02	0.42
1:F:103:LYS:HD3	1:F:103:LYS:HA	1.70	0.42
1:F:464:GLU:O	1:F:468:ARG:HG2	2.20	0.42
1:F:488:ASP:O	1:F:492:LEU:HD13	2.20	0.42
1:G:322:ARG:NH1	1:G:484:LYS:HB3	2.35	0.42
1:G:335:LEU:HD22	1:G:335:LEU:HA	1.78	0.42
1:A:286:TYR:N	1:A:287:PRO:CD	2.83	0.42
1:A:311:ILE:HD13	1:A:312:ALA:N	2.35	0.42
1:D:186:LEU:HD23	1:D:186:LEU:C	2.44	0.42
1:D:433:HIS:NE2	1:D:460:PHE:HE1	2.18	0.42
1:E:80:GLY:O	1:E:81:PRO:C	2.60	0.42
1:E:288:VAL:HG12	1:E:292:PHE:CE2	2.55	0.42
1:G:139:ASP:HB2	1:G:142:SER:CB	2.42	0.42
1:G:210:LEU:HD12	1:G:289:ARG:HD3	2.01	0.42
1:G:434:ARG:NH2	1:G:435:ILE:HD11	2.33	0.42
1:H:122:SER:O	1:H:126:ASN:HB2	2.20	0.42
1:H:150:GLU:O	1:H:154:MET:HG3	2.19	0.42
1:A:36:GLY:HA2	1:A:76:LEU:HD21	2.01	0.42
1:A:143:LEU:HD22	1:A:302:ILE:CG2	2.49	0.42
1:D:140:THR:HB	1:D:306:LEU:HD23	2.02	0.42
1:D:278:HIS:HD2	1:D:280:SER:O	2.02	0.42
1:F:165:PHE:CD1	1:F:272:GLY:HA2	2.55	0.42
1:G:9:LEU:H	1:G:9:LEU:HD22	1.85	0.42
1:H:83:SER:HA	1:H:99:GLY:O	2.20	0.42
1:H:249:GLU:OE1	1:H:449:PRO:HD2	2.19	0.42
1:H:292:PHE:C	1:H:294:ILE:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ASP:O	1:D:367:ARG:CD	2.68	0.42
1:E:19:VAL:HG12	1:E:234:ASP:HA	2.02	0.42
1:E:90:ILE:HD11	1:E:97:VAL:HG21	2.00	0.42
1:E:166:ARG:NH2	1:E:172:GLU:OE1	2.53	0.42
1:F:18:HIS:CG	1:F:198:GLN:NE2	2.88	0.42
1:F:127:ALA:C	1:F:129:ARG:N	2.78	0.42
1:G:305:ARG:CA	1:G:308:GLN:HG2	2.49	0.42
1:G:347:ALA:HB2	1:G:366:ILE:CD1	2.31	0.42
1:H:25:PRO:HD3	1:H:216:TYR:CD2	2.54	0.42
1:H:127:ALA:C	1:H:129:ARG:N	2.78	0.42
1:H:135:GLN:N	1:H:135:GLN:NE2	2.68	0.42
1:A:59:LEU:H	1:A:59:LEU:CD2	2.31	0.42
1:A:288:VAL:C	1:A:290:MET:H	2.27	0.42
1:B:322:ARG:HH22	1:B:484:LYS:HD2	1.85	0.42
1:B:356:LEU:HD13	1:B:357:VAL:N	2.35	0.42
1:C:45:ILE:CD1	1:C:46:GLN:N	2.79	0.42
1:C:59:LEU:HD12	1:C:64:VAL:HG21	2.02	0.42
1:D:54:SER:HA	1:D:55:PRO:HD3	1.90	0.42
1:E:220:ARG:HB2	1:E:222:PHE:CZ	2.54	0.42
1:G:39:LEU:O	1:G:223:PRO:HD2	2.20	0.42
1:G:139:ASP:HB2	1:G:142:SER:N	2.33	0.42
1:G:226:ASN:HA	1:G:227:PRO:HD3	1.88	0.42
1:H:17:ILE:H	1:H:17:ILE:HG13	1.64	0.42
1:H:208:ILE:HG13	1:H:289:ARG:HD2	2.00	0.42
1:A:305:ARG:HH21	1:B:138:ASN:ND2	2.18	0.41
1:A:428:ARG:NH2	1:A:474:TRP:CE3	2.75	0.41
1:B:356:LEU:HB3	1:B:425:PHE:HB2	2.02	0.41
1:D:19:VAL:N	1:D:20:PRO:HD3	2.35	0.41
1:D:201:ARG:O	1:D:201:ARG:HD3	2.19	0.41
1:D:264:ILE:HD11	1:D:274:PHE:CE1	2.55	0.41
1:E:346:ILE:O	1:E:426:TRP:HZ3	2.03	0.41
1:E:453:ARG:O	1:E:453:ARG:CD	2.62	0.41
2:E:900:BLA:HBC1	2:E:900:BLA:HMC3	2.02	0.41
1:G:44:ASN:HB3	1:G:219:MET:HG2	2.01	0.41
1:G:182:LEU:HD13	1:G:279:MET:CE	2.50	0.41
1:H:126:ASN:HD22	1:H:126:ASN:HA	1.55	0.41
1:H:165:PHE:CE1	1:H:272:GLY:HA2	2.54	0.41
1:H:366:ILE:H	1:H:366:ILE:HG12	1.62	0.41
1:B:49:LEU:HD22	1:B:90:ILE:CD1	2.50	0.41
1:E:124:THR:HG23	1:F:294:ILE:HD12	2.02	0.41
1:E:414:ILE:HG21	1:E:482:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ALA:C	1:F:129:ARG:H	2.28	0.41
1:F:410:GLY:O	1:F:427:PHE:HA	2.19	0.41
1:G:262:ILE:CD1	1:G:292:PHE:HB3	2.50	0.41
1:H:207:PRO:HB3	1:H:293:GLN:HG3	2.01	0.41
1:A:382:GLN:HA	1:A:382:GLN:HE21	1.84	0.41
1:B:59:LEU:N	1:B:59:LEU:HD22	2.36	0.41
1:B:112:ILE:HD13	1:B:112:ILE:N	2.34	0.41
1:B:157:TYR:CG	1:B:276:CYS:HB3	2.56	0.41
1:B:290:MET:HE3	1:B:290:MET:HB3	1.81	0.41
1:B:366:ILE:O	1:B:367:ARG:HB2	2.20	0.41
1:C:117:THR:O	1:C:118:LEU:C	2.63	0.41
1:C:386:GLU:HG2	1:G:269:LYS:HA	2.02	0.41
1:C:419:GLN:HG3	1:G:237:TYR:OH	2.20	0.41
1:D:7:VAL:HG11	1:D:15:GLU:HB2	2.02	0.41
1:D:7:VAL:HG11	1:D:15:GLU:HG3	2.02	0.41
1:E:143:LEU:HD13	1:E:147:VAL:HG11	2.02	0.41
1:E:155:THR:HG22	1:E:292:PHE:CZ	2.55	0.41
1:E:354:GLY:HA3	1:E:370:PHE:HE1	1.86	0.41
1:F:84:ASN:ND2	1:F:85:SER:H	2.17	0.41
1:F:265:VAL:HG12	1:F:267:GLY:O	2.21	0.41
1:G:446:THR:C	1:G:447:ILE:HD13	2.45	0.41
1:H:339:LEU:O	1:H:346:ILE:HG12	2.19	0.41
1:A:186:LEU:HD22	1:A:187:GLY:N	2.35	0.41
1:A:210:LEU:HD23	1:A:211:ILE:C	2.45	0.41
1:B:208:ILE:H	1:B:208:ILE:CD1	2.27	0.41
1:C:67:GLU:HA	1:C:70:ARG:HB2	2.03	0.41
1:C:86:VAL:HG12	1:C:88:THR:HG22	2.02	0.41
1:D:150:GLU:OE2	1:D:154:MET:HG3	2.20	0.41
1:E:335:LEU:O	1:E:337:GLY:N	2.54	0.41
1:F:49:LEU:HD22	1:F:90:ILE:CG2	2.51	0.41
1:F:74:GLU:HA	1:F:77:THR:OG1	2.21	0.41
1:F:194:ASP:OD2	1:F:453:ARG:NH2	2.54	0.41
1:F:454:LEU:O	1:F:455:THR:HG23	2.20	0.41
1:G:160:VAL:HA	1:G:275:SER:O	2.20	0.41
1:H:260:MET:HB3	1:H:276:CYS:HB2	2.01	0.41
1:A:330:ARG:HD3	1:B:330:ARG:CB	2.51	0.41
1:B:95:PHE:CD2	1:B:112:ILE:HA	2.56	0.41
1:B:208:ILE:HD12	1:B:293:GLN:CG	2.47	0.41
1:C:229:THR:HG23	1:C:231:GLU:H	1.85	0.41
1:C:347:ALA:HB3	1:C:366:ILE:HD11	2.03	0.41
1:D:67:GLU:CD	1:D:67:GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:SER:O	1:D:478:ASP:HB2	2.20	0.41
1:G:28:ALA:CB	1:G:48:LEU:HD23	2.50	0.41
1:H:68:VAL:HG21	1:H:88:THR:HG21	2.02	0.41
1:H:112:ILE:HD13	1:H:112:ILE:N	2.25	0.41
1:H:165:PHE:CD1	1:H:272:GLY:HA2	2.56	0.41
1:H:433:HIS:CE1	1:H:460:PHE:HE1	2.39	0.41
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.71	0.41
1:A:433:HIS:HD2	1:A:436:ARG:HG2	1.86	0.41
1:B:45:ILE:O	1:B:49:LEU:HB2	2.20	0.41
1:B:59:LEU:HB3	1:B:69:LEU:HD21	2.02	0.41
1:B:62:GLU:OE1	1:B:62:GLU:HA	2.20	0.41
1:C:257:ARG:CG	1:C:257:ARG:NH1	2.57	0.41
1:F:30:VAL:HG12	1:F:32:LEU:CD1	2.51	0.41
1:F:98:ILE:HG21	1:F:286:TYR:CE1	2.55	0.41
1:F:468:ARG:HH11	1:F:469:GLY:H	1.68	0.41
1:G:8:THR:O	1:G:12:CYS:N	2.53	0.41
1:G:142:SER:O	1:G:146:ASN:HB2	2.20	0.41
1:G:200:ARG:O	1:G:204:ILE:HG13	2.20	0.41
1:G:341:HIS:HA	1:G:342:PRO:HD3	1.93	0.41
1:A:43:GLU:HG3	1:A:222:PHE:HE2	1.86	0.41
1:A:106:PHE:CD2	1:A:107:TYR:N	2.88	0.41
1:B:19:VAL:HG12	1:B:233:PHE:O	2.21	0.41
1:C:159:ARG:NH1	1:C:183:GLU:O	2.54	0.41
1:D:275:SER:OG	2:D:900:BLA:CGA	2.68	0.41
1:F:117:THR:O	1:F:117:THR:HG23	2.20	0.41
1:F:126:ASN:HD22	1:F:126:ASN:HA	1.54	0.41
1:G:45:ILE:HG13	1:G:45:ILE:H	1.70	0.41
1:H:199:ALA:O	1:H:203:TYR:CD1	2.73	0.41
1:A:159:ARG:HD3	1:A:161:MET:CG	2.51	0.41
1:A:189:ARG:NH2	1:A:463:TRP:NE1	2.69	0.41
1:A:315:LEU:HD22	1:A:315:LEU:HA	1.74	0.41
1:A:411:VAL:HG22	1:A:427:PHE:CD2	2.56	0.41
1:C:32:LEU:O	1:C:105:VAL:HG13	2.21	0.41
1:C:208:ILE:HA	1:C:261:SER:O	2.20	0.41
1:C:308:GLN:O	1:C:311:ILE:HD13	2.21	0.41
1:D:45:ILE:HG13	1:D:45:ILE:H	1.57	0.41
1:E:158:ASP:OD2	1:E:279:MET:HG2	2.21	0.41
1:G:124:THR:CG2	1:H:291:SER:HA	2.51	0.41
1:G:249:GLU:CD	1:G:449:PRO:HD2	2.46	0.41
1:G:412:LEU:O	1:G:426:TRP:HD1	2.04	0.41
1:H:18:HIS:HB3	1:H:202:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:ARG:O	1:H:171:GLY:HA2	2.19	0.41
1:A:7:VAL:CG2	1:A:245:PRO:HG2	2.47	0.41
1:A:190:TYR:HA	1:A:191:PRO:HD3	1.86	0.41
1:A:261:SER:HB2	1:A:273:LEU:HD13	2.02	0.41
1:A:307:GLU:O	1:A:311:ILE:HG23	2.21	0.41
1:A:415:ARG:HD3	1:A:423:TRP:CE2	2.51	0.41
1:B:90:ILE:HD12	1:B:95:PHE:CD1	2.55	0.41
1:B:127:ALA:O	1:B:131:ILE:HG13	2.21	0.41
1:B:262:ILE:CD1	1:B:292:PHE:HB3	2.50	0.41
1:B:314:LEU:O	1:B:318:SER:HB2	2.20	0.41
1:B:382:GLN:O	1:H:197:ALA:CB	2.68	0.41
1:C:137:HIS:O	1:D:305:ARG:NH2	2.54	0.41
1:C:302:ILE:O	1:C:306:LEU:HB2	2.20	0.41
1:C:306:LEU:HD11	1:D:305:ARG:HH21	1.85	0.41
1:D:349:LEU:HD11	1:D:481:ILE:CG2	2.51	0.41
1:E:313:GLU:O	1:E:317:VAL:HG13	2.20	0.41
1:F:94:LEU:HD22	1:F:94:LEU:C	2.46	0.41
1:F:220:ARG:CG	1:F:220:ARG:NH1	2.75	0.41
1:G:247:HIS:CD2	2:G:900:BLA:CBD	3.03	0.41
1:A:163:TYR:HA	1:A:172:GLU:O	2.21	0.41
1:C:194:ASP:OD2	1:C:453:ARG:NH2	2.51	0.41
1:E:186:LEU:CD2	1:E:187:GLY:N	2.84	0.41
1:E:194:ASP:HB3	2:E:900:BLA:CHB	2.48	0.41
1:F:214:VAL:HG12	1:F:252:THR:CG2	2.50	0.41
1:G:84:ASN:ND2	1:G:85:SER:H	2.19	0.41
1:A:362:ARG:HG3	1:G:441:PRO:HG2	2.03	0.40
1:A:366:ILE:H	1:A:366:ILE:HG12	1.72	0.40
1:B:95:PHE:HE2	1:B:112:ILE:HG22	1.86	0.40
1:B:243:VAL:HB	1:B:248:CYS:SG	2.61	0.40
1:B:266:VAL:O	1:B:266:VAL:CG2	2.68	0.40
1:C:166:ARG:HA	1:C:166:ARG:HD3	1.88	0.40
1:C:168:ASP:OD2	1:C:170:SER:HB3	2.21	0.40
1:C:467:VAL:O	1:C:470:HIS:N	2.49	0.40
1:D:431:GLU:HG3	1:D:467:VAL:HB	2.02	0.40
1:E:169:ASP:HB3	1:E:200:ARG:CZ	2.51	0.40
1:F:63:GLN:O	1:F:90:ILE:HG23	2.21	0.40
1:F:356:LEU:HD11	1:F:358:MET:HG3	2.03	0.40
1:G:35:ASP:OD1	1:G:35:ASP:C	2.64	0.40
1:H:107:TYR:O	1:H:108:LEU:HD22	2.21	0.40
1:H:201:ARG:HA	1:H:201:ARG:HD2	1.90	0.40
1:H:339:LEU:HD23	1:H:339:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:387:ARG:NH1	1:H:389:ILE:O	2.54	0.40
1:A:389:ILE:HD11	1:A:483:GLU:HG2	2.02	0.40
1:A:486:ARG:O	1:A:486:ARG:HG2	2.22	0.40
1:C:42:SER:HA	1:C:221:VAL:HA	2.03	0.40
1:C:250:TYR:CD2	1:C:454:LEU:O	2.74	0.40
1:D:132:ALA:O	1:D:136:LEU:HD23	2.21	0.40
1:D:157:TYR:CD2	1:D:278:HIS:HB2	2.57	0.40
1:D:217:THR:HG23	1:D:217:THR:O	2.20	0.40
1:E:51:PHE:CD1	1:E:63:GLN:HB3	2.56	0.40
1:E:120:ILE:HG13	1:F:120:ILE:CD1	2.52	0.40
1:F:162:ALA:CB	1:F:175:ALA:HB3	2.48	0.40
1:G:7:VAL:HG11	1:G:15:GLU:OE2	2.21	0.40
1:G:208:ILE:HD12	1:G:293:GLN:HE21	1.86	0.40
1:G:365:SER:OG	1:G:368:GLY:O	2.37	0.40
1:G:371:GLU:O	1:G:372:ARG:C	2.64	0.40
1:A:94:LEU:HD21	1:A:113:ARG:HH11	1.87	0.40
1:A:378:LEU:O	1:A:378:LEU:HD23	2.21	0.40
1:B:32:LEU:HD21	1:B:59:LEU:CD2	2.52	0.40
1:B:136:LEU:HB2	1:B:137:HIS:CE1	2.56	0.40
1:B:191:PRO:HG3	1:B:463:TRP:N	2.37	0.40
1:B:430:GLU:OE2	1:B:468:ARG:HA	2.21	0.40
1:C:427:PHE:N	1:C:427:PHE:CD1	2.89	0.40
1:D:155:THR:O	1:D:282:LYS:HE2	2.21	0.40
1:D:316:ARG:HE	1:D:316:ARG:HB3	1.69	0.40
1:D:344:ASP:OD1	1:D:344:ASP:N	2.54	0.40
1:E:29:LEU:HD12	1:E:108:LEU:O	2.21	0.40
1:E:168:ASP:OD2	1:E:170:SER:HB3	2.21	0.40
1:F:377:VAL:HA	1:F:395:TRP:CH2	2.56	0.40
1:G:69:LEU:O	1:G:70:ARG:C	2.64	0.40
1:G:164:ARG:HH11	1:G:166:ARG:HH21	1.70	0.40
1:H:148:THR:HG23	1:H:160:VAL:O	2.21	0.40
1:H:208:ILE:HG22	1:H:262:ILE:HD13	2.03	0.40
1:H:209:ARG:NH1	2:H:900:BLA:CGD	2.85	0.40
1:H:416:PHE:HE1	1:H:424:ILE:CG1	2.33	0.40
1:H:481:ILE:O	1:H:482:ALA:C	2.64	0.40
1:A:117:THR:CG2	1:A:118:LEU:H	2.34	0.40
1:A:413:ALA:HA	1:A:424:ILE:O	2.21	0.40
1:B:5:THR:N	1:B:6:PRO:HD3	2.37	0.40
1:B:152:ARG:NH2	1:B:179:ARG:HB2	2.36	0.40
1:B:307:GLU:C	1:B:309:GLY:N	2.80	0.40
1:D:13:GLU:OE2	2:D:900:BLA:HBC1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:SER:HA	1:D:221:VAL:HA	2.02	0.40
1:E:297:GLN:HB2	1:F:131:ILE:CD1	2.51	0.40
1:F:42:SER:HA	1:F:221:VAL:HA	2.04	0.40
1:F:209:ARG:HA	1:F:209:ARG:HD2	1.91	0.40
1:G:94:LEU:HD22	1:G:94:LEU:C	2.46	0.40
1:A:121:THR:HG21	1:B:85:SER:OG	2.22	0.40
1:A:240:LEU:O	1:A:241:ARG:C	2.64	0.40
1:B:98:ILE:HG13	1:B:109:GLU:HB2	2.03	0.40
1:B:262:ILE:HD12	1:B:292:PHE:HB3	2.04	0.40
1:C:366:ILE:HA	1:E:434:ARG:O	2.22	0.40
1:C:395:TRP:HB3	1:C:409:CYS:HA	2.04	0.40
1:D:118:LEU:HD13	1:D:118:LEU:HA	1.96	0.40
1:D:209:ARG:NH1	2:D:900:BLA:O1D	2.53	0.40
1:E:89:ARG:HB2	1:E:94:LEU:HD23	2.03	0.40
1:E:129:ARG:O	1:E:133:GLN:HB2	2.22	0.40
1:E:157:TYR:CD2	1:E:278:HIS:HB2	2.56	0.40
1:E:189:ARG:HB3	1:E:189:ARG:NH2	2.35	0.40
1:E:391:HIS:HA	1:E:411:VAL:O	2.21	0.40
1:F:19:VAL:N	1:F:20:PRO:CD	2.82	0.40
1:F:24:GLN:HA	1:F:25:PRO:HD3	1.95	0.40
1:G:72:LEU:HD13	1:G:72:LEU:C	2.45	0.40
1:G:305:ARG:HG3	1:H:305:ARG:HB2	2.03	0.40
1:H:17:ILE:HG22	1:H:244:SER:HB2	2.04	0.40
1:H:19:VAL:N	1:H:20:PRO:HD3	2.36	0.40
1:H:96:ASP:HB2	1:H:111:GLU:HB3	2.02	0.40
1:H:187:GLY:HA3	1:H:435:ILE:CG1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:O	1:C:47:ALA:O[7_445]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	474/505 (94%)	428 (90%)	42 (9%)	4 (1%)	16	44
1	B	462/505 (92%)	434 (94%)	25 (5%)	3 (1%)	21	51
1	C	478/505 (95%)	439 (92%)	37 (8%)	2 (0%)	30	59
1	D	472/505 (94%)	443 (94%)	29 (6%)	0	100	100
1	E	463/505 (92%)	425 (92%)	36 (8%)	2 (0%)	30	59
1	F	461/505 (91%)	433 (94%)	28 (6%)	0	100	100
1	G	479/505 (95%)	443 (92%)	33 (7%)	3 (1%)	21	51
1	H	476/505 (94%)	427 (90%)	47 (10%)	2 (0%)	30	59
All	All	3765/4040 (93%)	3472 (92%)	277 (7%)	16 (0%)	30	59

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	ASP
1	C	442	GLU
1	A	289	ARG
1	E	333	ASP
1	H	196	PRO
1	A	20	PRO
1	E	267	GLY
1	G	421	SER
1	H	342	PRO
1	B	452	PRO
1	B	19	VAL
1	B	449	PRO
1	G	66	PRO
1	G	449	PRO
1	A	16	PRO
1	A	207	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	407/431 (94%)	359 (88%)	48 (12%)	5	17
1	B	398/431 (92%)	350 (88%)	48 (12%)	5	16
1	C	410/431 (95%)	350 (85%)	60 (15%)	3	10
1	D	408/431 (95%)	365 (90%)	43 (10%)	6	22
1	E	400/431 (93%)	353 (88%)	47 (12%)	5	17
1	F	400/431 (93%)	348 (87%)	52 (13%)	4	13
1	G	411/431 (95%)	352 (86%)	59 (14%)	3	11
1	H	409/431 (95%)	362 (88%)	47 (12%)	5	18
All	All	3243/3448 (94%)	2839 (88%)	404 (12%)	4	15

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	GLU
1	A	17	ILE
1	A	31	THR
1	A	45	ILE
1	A	59	LEU
1	A	72	LEU
1	A	88	THR
1	A	93	HIS
1	A	108	LEU
1	A	112	ILE
1	A	120	ILE
1	A	126	ASN
1	A	137	HIS
1	A	140	THR
1	A	147	VAL
1	A	160	VAL
1	A	174	VAL
1	A	186	LEU
1	A	198	GLN
1	A	201	ARG
1	A	208	ILE
1	A	216	TYR
1	A	230	ASN
1	A	232	SER
1	A	239	VAL
1	A	260	MET

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Mol	Chain	Res	Type
1	A	261	SER
1	A	262	ILE
1	A	284	ILE
1	A	298	VAL
1	A	305	ARG
1	A	311	ILE
1	A	315	LEU
1	A	317	VAL
1	A	325	LEU
1	A	356	LEU
1	A	364	LEU
1	A	366	ILE
1	A	393	ASP
1	A	395	TRP
1	A	412	LEU
1	A	426	TRP
1	A	432	VAL
1	A	440	LYS
1	A	447	ILE
1	A	453	ARG
1	A	479	LEU
1	B	11	ASN
1	B	13	GLU
1	B	32	LEU
1	B	45	ILE
1	B	67	GLU
1	B	77	THR
1	B	94	LEU
1	B	112	ILE
1	B	114	THR
1	B	116	ASP
1	B	117	THR
1	B	119	SER
1	B	125	LEU
1	B	130	ILE
1	B	134	VAL
1	B	142	SER
1	B	160	VAL
1	B	177	SER
1	B	181	ASP
1	B	201	ARG
1	B	204	ILE

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Mol	Chain	Res	Type
1	B	208	ILE
1	B	239	VAL
1	B	246	ILE
1	B	273	LEU
1	B	294	ILE
1	B	304	GLU
1	B	305	ARG
1	B	311	ILE
1	B	317	VAL
1	B	318	SER
1	B	323	LEU
1	B	325	LEU
1	B	327	ARG
1	B	349	LEU
1	B	362	ARG
1	B	363	THR
1	B	364	LEU
1	B	366	ILE
1	B	372	ARG
1	B	380	ARG
1	B	393	ASP
1	B	412	LEU
1	B	426	TRP
1	B	446	THR
1	B	476	GLU
1	B	485	LEU
1	B	491	GLU
1	C	9	LEU
1	C	12	CYS
1	C	13	GLU
1	C	45	ILE
1	C	49	LEU
1	C	64	VAL
1	C	77	THR
1	C	88	THR
1	C	93	HIS
1	C	94	LEU
1	C	98	ILE
1	C	112	ILE
1	C	120	ILE
1	C	130	ILE
1	C	140	THR

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	147	VAL
1	C	148	THR
1	C	160	VAL
1	C	164	ARG
1	C	188	GLN
1	C	210	LEU
1	C	217	THR
1	C	221	VAL
1	C	225	LEU
1	C	252	THR
1	C	257	ARG
1	C	259	SER
1	C	262	ILE
1	C	298	VAL
1	C	302	ILE
1	C	305	ARG
1	C	306	LEU
1	C	311	ILE
1	C	315	LEU
1	C	317	VAL
1	C	319	THR
1	C	323	LEU
1	C	325	LEU
1	C	330	ARG
1	C	349	LEU
1	C	356	LEU
1	C	363	THR
1	C	364	LEU
1	C	366	ILE
1	C	373	GLN
1	C	380	ARG
1	C	393	ASP
1	C	409	CYS
1	C	412	LEU
1	C	425	PHE
1	C	426	TRP
1	C	429	HIS
1	C	436	ARG
1	C	445	LEU
1	C	479	LEU
1	C	483	GLU

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Mol	Chain	Res	Type
1	C	485	LEU
1	C	487	LEU
1	C	492	LEU
1	D	7	VAL
1	D	17	ILE
1	D	35	ASP
1	D	45	ILE
1	D	67	GLU
1	D	77	THR
1	D	94	LEU
1	D	98	ILE
1	D	112	ILE
1	D	114	THR
1	D	116	ASP
1	D	117	THR
1	D	136	LEU
1	D	137	HIS
1	D	138	ASN
1	D	140	THR
1	D	160	VAL
1	D	173	VAL
1	D	195	ILE
1	D	201	ARG
1	D	208	ILE
1	D	210	LEU
1	D	239	VAL
1	D	273	LEU
1	D	303	VAL
1	D	311	ILE
1	D	316	ARG
1	D	344	ASP
1	D	349	LEU
1	D	363	THR
1	D	364	LEU
1	D	366	ILE
1	D	384	ASP
1	D	393	ASP
1	D	395	TRP
1	D	411	VAL
1	D	412	LEU
1	D	435	ILE
1	D	444	LEU

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Mol	Chain	Res	Type
1	D	446	THR
1	D	483	GLU
1	D	485	LEU
1	D	494	LEU
1	E	17	ILE
1	E	59	LEU
1	E	64	VAL
1	E	69	LEU
1	E	84	ASN
1	E	86	VAL
1	E	103	LYS
1	E	104	GLU
1	E	108	LEU
1	E	112	ILE
1	E	135	GLN
1	E	140	THR
1	E	143	LEU
1	E	154	MET
1	E	160	VAL
1	E	179	ARG
1	E	182	LEU
1	E	186	LEU
1	E	208	ILE
1	E	229	THR
1	E	294	ILE
1	E	302	ILE
1	E	304	GLU
1	E	305	ARG
1	E	311	ILE
1	E	314	LEU
1	E	315	LEU
1	E	317	VAL
1	E	322	ARG
1	E	325	LEU
1	E	330	ARG
1	E	346	ILE
1	E	349	LEU
1	E	356	LEU
1	E	364	LEU
1	E	378	LEU
1	E	380	ARG
1	E	381	LEU

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Mol	Chain	Res	Type
1	E	393	ASP
1	E	394	ASN
1	E	412	LEU
1	E	426	TRP
1	E	434	ARG
1	E	447	ILE
1	E	450	SER
1	E	483	GLU
1	E	485	LEU
1	F	8	THR
1	F	11	ASN
1	F	13	GLU
1	F	17	ILE
1	F	45	ILE
1	F	59	LEU
1	F	61	GLN
1	F	64	VAL
1	F	67	GLU
1	F	76	LEU
1	F	84	ASN
1	F	86	VAL
1	F	94	LEU
1	F	98	ILE
1	F	112	ILE
1	F	117	THR
1	F	126	ASN
1	F	129	ARG
1	F	134	VAL
1	F	136	LEU
1	F	137	HIS
1	F	160	VAL
1	F	208	ILE
1	F	210	LEU
1	F	220	ARG
1	F	230	ASN
1	F	238	SER
1	F	239	VAL
1	F	257	ARG
1	F	284	ILE
1	F	298	VAL
1	F	302	ILE
1	F	311	ILE

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Mol	Chain	Res	Type
1	F	315	LEU
1	F	319	THR
1	F	335	LEU
1	F	349	LEU
1	F	350	ILE
1	F	357	VAL
1	F	363	THR
1	F	366	ILE
1	F	367	ARG
1	F	393	ASP
1	F	412	LEU
1	F	426	TRP
1	F	447	ILE
1	F	453	ARG
1	F	466	VAL
1	F	468	ARG
1	F	472	THR
1	F	476	GLU
1	F	488	ASP
1	G	13	GLU
1	G	17	ILE
1	G	32	LEU
1	G	45	ILE
1	G	61	GLN
1	G	64	VAL
1	G	67	GLU
1	G	93	HIS
1	G	94	LEU
1	G	98	ILE
1	G	108	LEU
1	G	112	ILE
1	G	118	LEU
1	G	121	THR
1	G	130	ILE
1	G	136	LEU
1	G	142	SER
1	G	143	LEU
1	G	146	ASN
1	G	147	VAL
1	G	149	ASP
1	G	160	VAL
1	G	179	ARG

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Mol	Chain	Res	Type
1	G	182	LEU
1	G	201	ARG
1	G	208	ILE
1	G	210	LEU
1	G	217	THR
1	G	259	SER
1	G	295	PHE
1	G	303	VAL
1	G	304	GLU
1	G	305	ARG
1	G	306	LEU
1	G	311	ILE
1	G	315	LEU
1	G	319	THR
1	G	321	ARG
1	G	322	ARG
1	G	323	LEU
1	G	327	ARG
1	G	335	LEU
1	G	356	LEU
1	G	363	THR
1	G	366	ILE
1	G	367	ARG
1	G	373	GLN
1	G	393	ASP
1	G	407	ASP
1	G	412	LEU
1	G	426	TRP
1	G	444	LEU
1	G	446	THR
1	G	453	ARG
1	G	459	SER
1	G	483	GLU
1	G	485	LEU
1	G	487	LEU
1	G	494	LEU
1	H	17	ILE
1	H	64	VAL
1	H	67	GLU
1	H	68	VAL
1	H	77	THR
1	H	93	HIS

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Mol	Chain	Res	Type
1	H	94	LEU
1	H	112	ILE
1	H	114	THR
1	H	120	ILE
1	H	126	ASN
1	H	130	ILE
1	H	134	VAL
1	H	135	GLN
1	H	136	LEU
1	H	137	HIS
1	H	138	ASN
1	H	160	VAL
1	H	181	ASP
1	H	183	GLU
1	H	208	ILE
1	H	210	LEU
1	H	221	VAL
1	H	230	ASN
1	H	260	MET
1	H	273	LEU
1	H	294	ILE
1	H	306	LEU
1	H	314	LEU
1	H	315	LEU
1	H	322	ARG
1	H	341	HIS
1	H	349	LEU
1	H	357	VAL
1	H	366	ILE
1	H	378	LEU
1	H	387	ARG
1	H	412	LEU
1	H	437	TRP
1	H	445	LEU
1	H	446	THR
1	H	447	ILE
1	H	454	LEU
1	H	472	THR
1	H	477	THR
1	H	483	GLU
1	H	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	24	GLN
1	A	93	HIS
1	A	128	GLN
1	A	137	HIS
1	A	138	ASN
1	A	146	ASN
1	A	198	GLN
1	A	205	GLN
1	A	230	ASN
1	A	293	GLN
1	A	297	GLN
1	A	382	GLN
1	A	394	ASN
1	A	433	HIS
1	A	470	HIS
1	B	11	ASN
1	B	24	GLN
1	B	26	HIS
1	B	128	GLN
1	B	138	ASN
1	B	146	ASN
1	B	198	GLN
1	B	205	GLN
1	B	206	ASN
1	B	230	ASN
1	B	277	HIS
1	B	278	HIS
1	B	293	GLN
1	B	308	GLN
1	B	341	HIS
1	B	373	GLN
1	B	495	ASN
1	C	24	GLN
1	C	63	GLN
1	C	84	ASN
1	C	93	HIS
1	C	100	HIS
1	C	128	GLN
1	C	133	GLN
1	C	137	HIS
1	C	138	ASN

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Mol	Chain	Res	Type
1	C	205	GLN
1	C	230	ASN
1	C	293	GLN
1	C	394	ASN
1	C	417	HIS
1	C	495	ASN
1	C	496	HIS
1	D	11	ASN
1	D	24	GLN
1	D	61	GLN
1	D	79	ASN
1	D	84	ASN
1	D	100	HIS
1	D	126	ASN
1	D	128	GLN
1	D	135	GLN
1	D	138	ASN
1	D	226	ASN
1	D	230	ASN
1	D	293	GLN
1	D	373	GLN
1	E	84	ASN
1	E	93	HIS
1	E	128	GLN
1	E	138	ASN
1	E	188	GLN
1	E	230	ASN
1	E	293	GLN
1	E	308	GLN
1	E	391	HIS
1	E	394	ASN
1	E	417	HIS
1	E	433	HIS
1	E	470	HIS
1	F	11	ASN
1	F	24	GLN
1	F	26	HIS
1	F	63	GLN
1	F	84	ASN
1	F	100	HIS
1	F	126	ASN
1	F	128	GLN

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Mol	Chain	Res	Type
1	F	133	GLN
1	F	138	ASN
1	F	146	ASN
1	F	205	GLN
1	F	206	ASN
1	F	230	ASN
1	F	293	GLN
1	F	394	ASN
1	F	417	HIS
1	G	24	GLN
1	G	46	GLN
1	G	84	ASN
1	G	126	ASN
1	G	230	ASN
1	G	247	HIS
1	G	293	GLN
1	G	373	GLN
1	G	394	ASN
1	G	417	HIS
1	G	429	HIS
1	G	433	HIS
1	G	496	HIS
1	H	11	ASN
1	H	24	GLN
1	H	61	GLN
1	H	63	GLN
1	H	79	ASN
1	H	84	ASN
1	H	93	HIS
1	H	100	HIS
1	H	126	ASN
1	H	133	GLN
1	H	135	GLN
1	H	137	HIS
1	H	138	ASN
1	H	146	ASN
1	H	230	ASN
1	H	277	HIS
1	H	278	HIS
1	H	391	HIS
1	H	394	ASN
1	H	433	HIS

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Mol	Chain	Res	Type
1	H	496	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	BLA	D	900	1	46,46,46	2.74	17 (36%)	66,67,67	1.87	17 (25%)
2	BLA	H	900	1	46,46,46	2.61	17 (36%)	66,67,67	1.86	16 (24%)
2	BLA	E	900	1	46,46,46	2.89	19 (41%)	66,67,67	1.79	17 (25%)
2	BLA	B	900	1	46,46,46	2.74	18 (39%)	66,67,67	1.83	21 (31%)
2	BLA	C	900	1	46,46,46	2.98	17 (36%)	66,67,67	1.95	20 (30%)
2	BLA	G	900	1	46,46,46	2.67	16 (34%)	66,67,67	1.77	16 (24%)
2	BLA	F	900	1	46,46,46	2.62	16 (34%)	66,67,67	1.84	20 (30%)
2	BLA	A	900	1	46,46,46	2.65	17 (36%)	66,67,67	1.80	15 (22%)

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	BLA	D	900	1	-	8/26/74/74	0/4/4/4
2	BLA	H	900	1	-	9/26/74/74	0/4/4/4
2	BLA	E	900	1	-	11/26/74/74	0/4/4/4
2	BLA	B	900	1	-	8/26/74/74	0/4/4/4
2	BLA	C	900	1	-	10/26/74/74	0/4/4/4
2	BLA	G	900	1	-	8/26/74/74	0/4/4/4
2	BLA	F	900	1	-	8/26/74/74	0/4/4/4
2	BLA	A	900	1	-	9/26/74/74	0/4/4/4

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	BLA	C4D-C3D	-8.43	1.32	1.45
2	H	900	BLA	CHB-C1B	7.04	1.54	1.37
2	G	900	BLA	CHB-C1B	6.99	1.54	1.37
2	E	900	BLA	C4D-C3D	-6.92	1.34	1.45
2	D	900	BLA	CHB-C1B	6.92	1.54	1.37
2	E	900	BLA	CHB-C1B	6.86	1.54	1.37
2	B	900	BLA	CHB-C1B	6.85	1.54	1.37
2	D	900	BLA	CHB-C4A	6.77	1.55	1.40
2	F	900	BLA	CHB-C1B	6.73	1.54	1.37
2	A	900	BLA	CHB-C1B	6.70	1.53	1.37
2	C	900	BLA	CHB-C1B	6.60	1.53	1.37
2	C	900	BLA	CHB-C4A	6.46	1.55	1.40
2	F	900	BLA	CHD-C4C	6.45	1.53	1.37
2	A	900	BLA	CHD-C4C	6.43	1.53	1.37
2	E	900	BLA	CHB-C4A	6.40	1.54	1.40
2	H	900	BLA	CHB-C4A	6.36	1.54	1.40
2	G	900	BLA	CHB-C4A	6.26	1.54	1.40
2	D	900	BLA	CHD-C4C	6.24	1.52	1.37
2	B	900	BLA	CHD-C4C	6.23	1.52	1.37
2	E	900	BLA	CHD-C4C	6.18	1.52	1.37
2	G	900	BLA	CHD-C4C	6.15	1.52	1.37
2	H	900	BLA	CHD-C4C	6.15	1.52	1.37
2	F	900	BLA	CHB-C4A	6.07	1.54	1.40
2	B	900	BLA	CHB-C4A	6.07	1.54	1.40
2	A	900	BLA	CHB-C4A	6.02	1.54	1.40
2	G	900	BLA	CHD-C1D	5.84	1.54	1.40
2	A	900	BLA	CHD-C1D	5.80	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CHD-C1D	5.72	1.53	1.40
2	E	900	BLA	CHD-C1D	5.72	1.53	1.40
2	C	900	BLA	CHD-C4C	5.68	1.51	1.37
2	F	900	BLA	CHD-C1D	5.67	1.53	1.40
2	D	900	BLA	CHD-C1D	5.62	1.53	1.40
2	B	900	BLA	C4D-C3D	-5.40	1.37	1.45
2	D	900	BLA	C4D-C3D	-5.27	1.37	1.45
2	C	900	BLA	CHD-C1D	5.19	1.52	1.40
2	H	900	BLA	CHD-C1D	5.11	1.52	1.40
2	E	900	BLA	CBC-CAC	4.95	1.54	1.30
2	C	900	BLA	CBC-CAC	4.94	1.54	1.30
2	F	900	BLA	CBC-CAC	4.90	1.53	1.30
2	B	900	BLA	CBC-CAC	4.88	1.53	1.30
2	C	900	BLA	C1D-C2D	-4.87	1.35	1.45
2	A	900	BLA	CBC-CAC	4.83	1.53	1.30
2	G	900	BLA	CBC-CAC	4.82	1.53	1.30
2	C	900	BLA	C1A-NA	-4.79	1.29	1.37
2	H	900	BLA	CBC-CAC	4.78	1.53	1.30
2	D	900	BLA	CBC-CAC	4.77	1.53	1.30
2	G	900	BLA	C4D-C3D	-4.35	1.38	1.45
2	C	900	BLA	C1C-C2C	-4.15	1.38	1.48
2	E	900	BLA	C1D-C2D	-4.15	1.36	1.45
2	A	900	BLA	C4D-C3D	-4.10	1.39	1.45
2	G	900	BLA	C1C-C2C	-4.03	1.38	1.48
2	F	900	BLA	C1C-C2C	-4.02	1.38	1.48
2	E	900	BLA	C1A-NA	-4.02	1.31	1.37
2	H	900	BLA	C1C-C2C	-3.93	1.38	1.48
2	E	900	BLA	C1C-C2C	-3.91	1.38	1.48
2	B	900	BLA	C1C-C2C	-3.88	1.38	1.48
2	B	900	BLA	C1D-C2D	-3.88	1.37	1.45
2	D	900	BLA	C1D-C2D	-3.85	1.37	1.45
2	D	900	BLA	C1C-C2C	-3.85	1.38	1.48
2	A	900	BLA	C1C-C2C	-3.73	1.39	1.48
2	H	900	BLA	C4D-C3D	-3.72	1.39	1.45
2	H	900	BLA	C1D-C2D	-3.59	1.38	1.45
2	G	900	BLA	C1D-C2D	-3.55	1.38	1.45
2	A	900	BLA	C1D-C2D	-3.55	1.38	1.45
2	B	900	BLA	C1A-NA	-3.53	1.31	1.37
2	F	900	BLA	CAB-C3B	-3.53	1.38	1.47
2	C	900	BLA	C4D-ND	-3.41	1.31	1.38
2	F	900	BLA	C1D-C2D	-3.38	1.38	1.45
2	H	900	BLA	C3C-C4C	-3.27	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	900	BLA	C4D-C3D	-3.26	1.40	1.45
2	A	900	BLA	CAB-C3B	-3.21	1.38	1.47
2	F	900	BLA	C3C-C4C	-3.20	1.39	1.45
2	A	900	BLA	C3C-C4C	-3.13	1.40	1.45
2	C	900	BLA	CAB-C3B	-3.12	1.39	1.47
2	G	900	BLA	CAB-C3B	-3.07	1.39	1.47
2	D	900	BLA	C3C-C4C	-3.07	1.40	1.45
2	H	900	BLA	CAB-C3B	-3.07	1.39	1.47
2	B	900	BLA	C3C-C4C	-3.06	1.40	1.45
2	D	900	BLA	CAB-C3B	-3.04	1.39	1.47
2	D	900	BLA	C1A-NA	-3.04	1.32	1.37
2	E	900	BLA	C3C-C4C	-3.03	1.40	1.45
2	E	900	BLA	CAB-C3B	-2.92	1.39	1.47
2	B	900	BLA	CAB-C3B	-2.91	1.39	1.47
2	C	900	BLA	C4C-NC	-2.89	1.32	1.37
2	C	900	BLA	C3C-C4C	-2.87	1.40	1.45
2	G	900	BLA	C3C-C4C	-2.85	1.40	1.45
2	E	900	BLA	CAC-C3C	2.82	1.54	1.47
2	G	900	BLA	CAC-C3C	2.81	1.54	1.47
2	B	900	BLA	C1B-C2B	-2.77	1.40	1.45
2	E	900	BLA	C1B-C2B	-2.76	1.40	1.45
2	A	900	BLA	C1A-NA	-2.75	1.33	1.37
2	D	900	BLA	C1B-C2B	-2.70	1.40	1.45
2	C	900	BLA	CAC-C3C	2.70	1.54	1.47
2	G	900	BLA	C1B-C2B	-2.69	1.40	1.45
2	E	900	BLA	C4D-ND	-2.68	1.32	1.38
2	C	900	BLA	C1B-C2B	-2.66	1.40	1.45
2	F	900	BLA	C1B-C2B	-2.65	1.40	1.45
2	A	900	BLA	C4A-NA	-2.64	1.33	1.37
2	H	900	BLA	CAC-C3C	2.61	1.54	1.47
2	A	900	BLA	C1B-C2B	-2.60	1.40	1.45
2	F	900	BLA	CAC-C3C	2.56	1.54	1.47
2	B	900	BLA	CAC-C3C	2.56	1.54	1.47
2	G	900	BLA	C1A-NA	-2.55	1.33	1.37
2	F	900	BLA	C4A-NA	-2.55	1.33	1.37
2	A	900	BLA	CAC-C3C	2.51	1.54	1.47
2	H	900	BLA	C1B-C2B	-2.48	1.40	1.45
2	D	900	BLA	C4D-ND	-2.48	1.33	1.38
2	H	900	BLA	C4A-NA	-2.47	1.33	1.37
2	B	900	BLA	C4D-ND	-2.36	1.33	1.38
2	E	900	BLA	C4C-NC	-2.33	1.33	1.37
2	D	900	BLA	CAC-C3C	2.31	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C4D-ND	-2.31	1.33	1.38
2	H	900	BLA	C4D-ND	-2.28	1.33	1.38
2	G	900	BLA	C4A-NA	-2.26	1.34	1.37
2	E	900	BLA	C4A-NA	-2.24	1.34	1.37
2	D	900	BLA	C4C-NC	-2.21	1.34	1.37
2	H	900	BLA	C4C-NC	-2.20	1.34	1.37
2	E	900	BLA	C1B-NB	-2.20	1.34	1.37
2	H	900	BLA	C3B-C4B	-2.20	1.38	1.47
2	B	900	BLA	C3B-C4B	-2.19	1.38	1.47
2	D	900	BLA	C4A-NA	-2.18	1.34	1.37
2	B	900	BLA	C4A-NA	-2.16	1.34	1.37
2	G	900	BLA	C3B-C4B	-2.14	1.38	1.47
2	F	900	BLA	C1A-NA	-2.13	1.34	1.37
2	C	900	BLA	C3B-C4B	-2.13	1.38	1.47
2	F	900	BLA	C4C-NC	-2.11	1.34	1.37
2	F	900	BLA	C3B-C4B	-2.11	1.38	1.47
2	D	900	BLA	C3B-C4B	-2.08	1.38	1.47
2	A	900	BLA	C3B-C4B	-2.07	1.38	1.47
2	E	900	BLA	C3B-C4B	-2.07	1.38	1.47
2	H	900	BLA	C1A-NA	-2.07	1.34	1.37
2	B	900	BLA	C4C-NC	-2.07	1.34	1.37
2	E	900	BLA	C1C-NC	-2.05	1.33	1.38
2	G	900	BLA	C4C-NC	-2.05	1.34	1.37
2	A	900	BLA	C4C-NC	-2.04	1.34	1.37
2	B	900	BLA	C4B-NB	-2.03	1.33	1.38
2	C	900	BLA	CMA-C3A	2.03	1.54	1.50

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	900	BLA	C4C-CHD-C1D	-6.40	112.34	128.06
2	D	900	BLA	C4C-CHD-C1D	-6.03	113.24	128.06
2	F	900	BLA	C4C-CHD-C1D	-5.90	113.57	128.06
2	B	900	BLA	C4C-CHD-C1D	-5.70	114.05	128.06
2	E	900	BLA	C4C-CHD-C1D	-5.59	114.34	128.06
2	G	900	BLA	C4C-CHD-C1D	-5.19	115.30	128.06
2	C	900	BLA	C1A-CHA-C4D	-5.08	117.12	128.22
2	C	900	BLA	CAD-C3D-C4D	4.88	133.58	125.02
2	A	900	BLA	C4C-CHD-C1D	-4.73	116.44	128.06
2	G	900	BLA	C1A-CHA-C4D	-4.66	118.04	128.22
2	D	900	BLA	C1A-CHA-C4D	-4.60	118.17	128.22
2	A	900	BLA	C1A-CHA-C4D	-4.54	118.31	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	BLA	C1A-CHA-C4D	-4.41	118.58	128.22
2	H	900	BLA	C1A-CHA-C4D	-4.32	118.78	128.22
2	D	900	BLA	C4A-CHB-C1B	-4.30	118.45	130.82
2	C	900	BLA	C4C-CHD-C1D	-4.22	117.70	128.06
2	F	900	BLA	C1A-CHA-C4D	-4.21	119.02	128.22
2	C	900	BLA	C4A-CHB-C1B	-4.16	118.85	130.82
2	H	900	BLA	CMB-C2B-C1B	4.16	129.22	124.16
2	E	900	BLA	C4A-CHB-C1B	-4.15	118.86	130.82
2	A	900	BLA	C4A-CHB-C1B	-4.09	119.06	130.82
2	B	900	BLA	C1A-CHA-C4D	-4.01	119.47	128.22
2	H	900	BLA	C4A-CHB-C1B	-3.97	119.40	130.82
2	C	900	BLA	CAD-C3D-C2D	-3.89	120.59	127.87
2	A	900	BLA	CMB-C2B-C1B	3.85	128.84	124.16
2	G	900	BLA	C4A-CHB-C1B	-3.74	120.07	130.82
2	B	900	BLA	C4A-CHB-C1B	-3.73	120.09	130.82
2	F	900	BLA	C4A-CHB-C1B	-3.68	120.22	130.82
2	G	900	BLA	CHA-C4D-ND	3.60	132.15	124.60
2	C	900	BLA	CMB-C2B-C1B	3.56	128.49	124.16
2	E	900	BLA	CAD-C3D-C4D	3.52	131.20	125.02
2	H	900	BLA	CHA-C4D-ND	3.49	131.92	124.60
2	C	900	BLA	CHD-C1D-ND	3.47	132.46	124.95
2	F	900	BLA	CMB-C2B-C1B	3.38	128.27	124.16
2	C	900	BLA	CHA-C1A-C2A	-3.37	119.98	127.22
2	B	900	BLA	CAD-C3D-C4D	3.36	130.92	125.02
2	D	900	BLA	CMB-C2B-C1B	3.27	128.13	124.16
2	D	900	BLA	CBC-CAC-C3C	-3.21	111.47	127.53
2	F	900	BLA	CHA-C4D-ND	3.19	131.29	124.60
2	G	900	BLA	CMB-C2B-C1B	3.19	128.03	124.16
2	D	900	BLA	CHA-C1A-C2A	-3.17	120.41	127.22
2	E	900	BLA	CHA-C1A-C2A	-3.15	120.45	127.22
2	A	900	BLA	CHA-C4D-ND	3.08	131.07	124.60
2	F	900	BLA	CAD-C3D-C4D	3.04	130.35	125.02
2	D	900	BLA	CAD-C3D-C4D	3.02	130.32	125.02
2	F	900	BLA	CHA-C1A-C2A	-2.97	120.84	127.22
2	B	900	BLA	CMB-C2B-C1B	2.95	127.74	124.16
2	B	900	BLA	CHA-C1A-C2A	-2.88	121.02	127.22
2	E	900	BLA	CMB-C2B-C1B	2.86	127.64	124.16
2	B	900	BLA	CBC-CAC-C3C	-2.86	113.25	127.53
2	A	900	BLA	CMC-C2C-C1C	2.80	127.06	121.21
2	A	900	BLA	CBC-CAC-C3C	-2.78	113.64	127.53
2	A	900	BLA	CAD-C3D-C4D	2.78	129.90	125.02
2	H	900	BLA	CHA-C1A-C2A	-2.73	121.34	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	BLA	C1A-C2A-C3A	-2.72	104.45	107.62
2	F	900	BLA	CBC-CAC-C3C	-2.72	113.94	127.53
2	C	900	BLA	CBC-CAC-C3C	-2.67	114.17	127.53
2	G	900	BLA	CHA-C4D-C3D	-2.67	119.23	125.40
2	A	900	BLA	CHD-C1D-ND	2.67	130.71	124.95
2	D	900	BLA	CMC-C2C-C1C	2.67	126.78	121.21
2	G	900	BLA	CHD-C1D-ND	2.65	130.68	124.95
2	G	900	BLA	CHA-C1A-C2A	-2.64	121.55	127.22
2	E	900	BLA	CAD-C3D-C2D	-2.63	122.94	127.87
2	B	900	BLA	CHA-C4D-ND	2.62	130.09	124.60
2	D	900	BLA	CHA-C4D-ND	2.58	130.01	124.60
2	H	900	BLA	CBC-CAC-C3C	-2.58	114.65	127.53
2	C	900	BLA	CHA-C1A-NA	2.55	131.06	125.29
2	H	900	BLA	CAD-C3D-C4D	2.54	129.48	125.02
2	C	900	BLA	C2D-C1D-ND	-2.52	105.08	110.58
2	C	900	BLA	O1D-CGD-CBD	-2.51	115.13	123.09
2	F	900	BLA	CBD-CAD-C3D	-2.49	105.65	112.53
2	F	900	BLA	CHD-C1D-ND	2.48	130.32	124.95
2	E	900	BLA	CBC-CAC-C3C	-2.46	115.24	127.53
2	G	900	BLA	CBC-CAC-C3C	-2.45	115.27	127.53
2	C	900	BLA	CHB-C1B-NB	-2.45	120.84	126.06
2	H	900	BLA	C4D-ND-C1D	2.42	110.96	106.52
2	A	900	BLA	C1D-C2D-C3D	2.42	109.22	106.48
2	G	900	BLA	C1A-C2A-C3A	-2.41	104.82	107.62
2	B	900	BLA	CAD-C3D-C2D	-2.40	123.36	127.87
2	H	900	BLA	CHB-C1B-C2B	2.40	131.76	126.97
2	A	900	BLA	C4D-ND-C1D	2.40	110.92	106.52
2	D	900	BLA	CHA-C1A-NA	2.40	130.71	125.29
2	B	900	BLA	CHD-C1D-ND	2.39	130.11	124.95
2	F	900	BLA	CHB-C4A-C3A	2.38	133.37	127.53
2	C	900	BLA	C1A-C2A-C3A	-2.37	104.86	107.62
2	A	900	BLA	CHA-C1A-C2A	-2.37	122.13	127.22
2	C	900	BLA	C3B-C4B-NB	2.32	109.05	106.13
2	C	900	BLA	CHB-C1B-C2B	2.31	131.59	126.97
2	B	900	BLA	C3B-C4B-NB	2.31	109.03	106.13
2	F	900	BLA	O1D-CGD-CBD	-2.31	115.78	123.09
2	D	900	BLA	C3B-C4B-NB	2.29	109.00	106.13
2	B	900	BLA	C1D-C2D-C3D	2.27	109.06	106.48
2	E	900	BLA	C3C-C4C-NC	2.26	110.33	106.64
2	B	900	BLA	CHA-C1A-NA	2.26	130.39	125.29
2	A	900	BLA	CHB-C1B-NB	-2.24	121.28	126.06
2	H	900	BLA	CHA-C1A-NA	2.24	130.35	125.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	BLA	C1D-C2D-C3D	2.23	109.01	106.48
2	B	900	BLA	CMC-C2C-C1C	2.23	125.88	121.21
2	B	900	BLA	CHB-C1B-C2B	2.22	131.40	126.97
2	E	900	BLA	C3B-C4B-NB	2.22	108.92	106.13
2	H	900	BLA	CHA-C4D-C3D	-2.21	120.30	125.40
2	E	900	BLA	CHA-C4D-ND	2.20	129.22	124.60
2	E	900	BLA	CHA-C1A-NA	2.19	130.24	125.29
2	B	900	BLA	CHB-C1B-NB	-2.19	121.39	126.06
2	D	900	BLA	CAD-C3D-C2D	-2.19	123.77	127.87
2	D	900	BLA	C1A-C2A-C3A	-2.18	105.08	107.62
2	F	900	BLA	C1D-C2D-C3D	2.17	108.94	106.48
2	D	900	BLA	C4D-ND-C1D	2.17	110.49	106.52
2	B	900	BLA	C1A-C2A-C3A	-2.16	105.11	107.62
2	G	900	BLA	C1D-C2D-C3D	2.13	108.90	106.48
2	H	900	BLA	O1D-CGD-CBD	-2.12	116.37	123.09
2	H	900	BLA	CHB-C1B-NB	-2.12	121.55	126.06
2	H	900	BLA	CHD-C1D-ND	2.11	129.52	124.95
2	B	900	BLA	O1D-CGD-CBD	-2.10	116.43	123.09
2	A	900	BLA	O1D-CGD-CBD	-2.10	116.44	123.09
2	B	900	BLA	CHB-C4A-C3A	2.10	132.67	127.53
2	G	900	BLA	CAD-C3D-C4D	2.10	128.70	125.02
2	F	900	BLA	C4D-ND-C1D	2.10	110.36	106.52
2	G	900	BLA	C4C-NC-C1C	-2.08	108.10	110.66
2	F	900	BLA	CHA-C1A-NA	2.08	130.00	125.29
2	D	900	BLA	O1D-CGD-CBD	-2.08	116.49	123.09
2	C	900	BLA	C3C-C4C-NC	2.08	110.03	106.64
2	G	900	BLA	C3B-C4B-NB	2.07	108.74	106.13
2	E	900	BLA	O1D-CGD-CBD	-2.07	116.52	123.09
2	F	900	BLA	CAD-C3D-C2D	-2.07	123.98	127.87
2	C	900	BLA	C3A-C4A-NA	-2.07	104.61	107.43
2	F	900	BLA	C1A-C2A-C3A	-2.07	105.21	107.62
2	D	900	BLA	O1A-CGA-CBA	-2.06	116.55	123.09
2	D	900	BLA	C1D-C2D-C3D	2.06	108.81	106.48
2	G	900	BLA	C3C-C4C-NC	2.06	109.99	106.64
2	H	900	BLA	CMB-C2B-C3B	-2.06	123.45	128.43
2	A	900	BLA	CHA-C4D-C3D	-2.04	120.68	125.40
2	F	900	BLA	CHB-C4A-NA	-2.04	120.68	125.29
2	B	900	BLA	C4D-ND-C1D	2.03	110.25	106.52
2	E	900	BLA	CHD-C1D-ND	2.03	129.33	124.95
2	C	900	BLA	C4D-ND-C1D	2.02	110.22	106.52
2	B	900	BLA	C2D-C1D-ND	-2.02	106.18	110.58
2	E	900	BLA	C2D-C1D-ND	-2.01	106.18	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	900	BLA	CBA-CAA-C2A	2.01	118.10	112.53
2	G	900	BLA	O1D-CGD-CBD	-2.01	116.72	123.09
2	E	900	BLA	C4C-NC-C1C	-2.01	108.19	110.66
2	F	900	BLA	CHA-C4D-C3D	-2.01	120.76	125.40

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NB-C1B-CHB-C4A
2	A	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	NB-C1B-CHB-C4A
2	C	900	BLA	C2B-C1B-CHB-C4A
2	D	900	BLA	NB-C1B-CHB-C4A
2	D	900	BLA	C2B-C1B-CHB-C4A
2	E	900	BLA	NB-C1B-CHB-C4A
2	E	900	BLA	C2B-C1B-CHB-C4A
2	F	900	BLA	NB-C1B-CHB-C4A
2	F	900	BLA	C2B-C1B-CHB-C4A
2	G	900	BLA	C3A-C2A-CAA-CBA
2	G	900	BLA	NB-C1B-CHB-C4A
2	G	900	BLA	C2B-C1B-CHB-C4A
2	H	900	BLA	NB-C1B-CHB-C4A
2	H	900	BLA	C2B-C1B-CHB-C4A
2	A	900	BLA	NA-C4A-CHB-C1B
2	C	900	BLA	NA-C4A-CHB-C1B
2	G	900	BLA	NA-C4A-CHB-C1B
2	G	900	BLA	C1A-C2A-CAA-CBA
2	B	900	BLA	NA-C4A-CHB-C1B
2	F	900	BLA	NA-C4A-CHB-C1B
2	H	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	C	900	BLA	C3A-C4A-CHB-C1B
2	D	900	BLA	C3A-C4A-CHB-C1B
2	F	900	BLA	C3A-C4A-CHB-C1B
2	G	900	BLA	C3A-C4A-CHB-C1B
2	H	900	BLA	C3A-C4A-CHB-C1B
2	D	900	BLA	NA-C4A-CHB-C1B
2	E	900	BLA	NA-C4A-CHB-C1B

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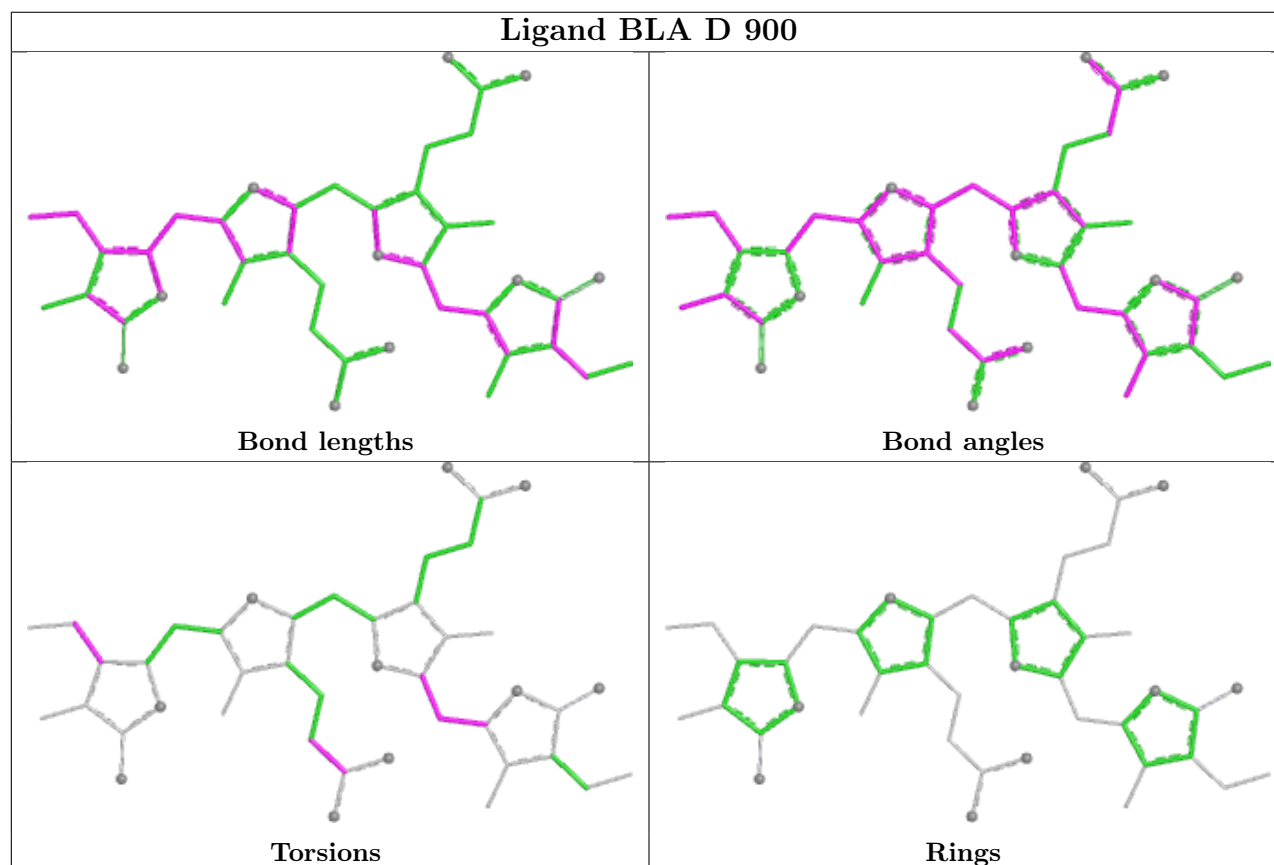
Mol	Chain	Res	Type	Atoms
2	E	900	BLA	C3A-C4A-CHB-C1B
2	C	900	BLA	NC-C4C-CHD-C1D
2	D	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAD-CBD-CGD-O1D
2	D	900	BLA	CAD-CBD-CGD-O2D
2	E	900	BLA	CAD-CBD-CGD-O2D
2	C	900	BLA	C3C-C4C-CHD-C1D
2	E	900	BLA	C4D-C3D-CAD-CBD
2	E	900	BLA	CAD-CBD-CGD-O1D
2	E	900	BLA	C2D-C3D-CAD-CBD
2	H	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAA-CBA-CGA-O1A
2	H	900	BLA	CAD-CBD-CGD-O1D
2	D	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAA-CBA-CGA-O2A
2	C	900	BLA	CAD-CBD-CGD-O2D
2	C	900	BLA	CAD-CBD-CGD-O1D
2	E	900	BLA	ND-C1D-CHD-C4C
2	B	900	BLA	CAD-CBD-CGD-O1D
2	G	900	BLA	CAD-CBD-CGD-O2D
2	D	900	BLA	C4C-C3C-CAC-CBC
2	F	900	BLA	CAD-CBD-CGD-O1D
2	F	900	BLA	CAD-CBD-CGD-O2D
2	H	900	BLA	C2D-C3D-CAD-CBD
2	E	900	BLA	CAA-CBA-CGA-O1A
2	G	900	BLA	CAD-CBD-CGD-O1D
2	H	900	BLA	CAA-CBA-CGA-O1A
2	C	900	BLA	CAA-CBA-CGA-O1A
2	F	900	BLA	CAA-CBA-CGA-O1A
2	C	900	BLA	CAA-CBA-CGA-O2A
2	E	900	BLA	CAA-CBA-CGA-O2A
2	H	900	BLA	CAA-CBA-CGA-O2A
2	B	900	BLA	CAA-CBA-CGA-O1A
2	F	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	C2C-C3C-CAC-CBC
2	B	900	BLA	CAA-CBA-CGA-O2A

There are no ring outliers.

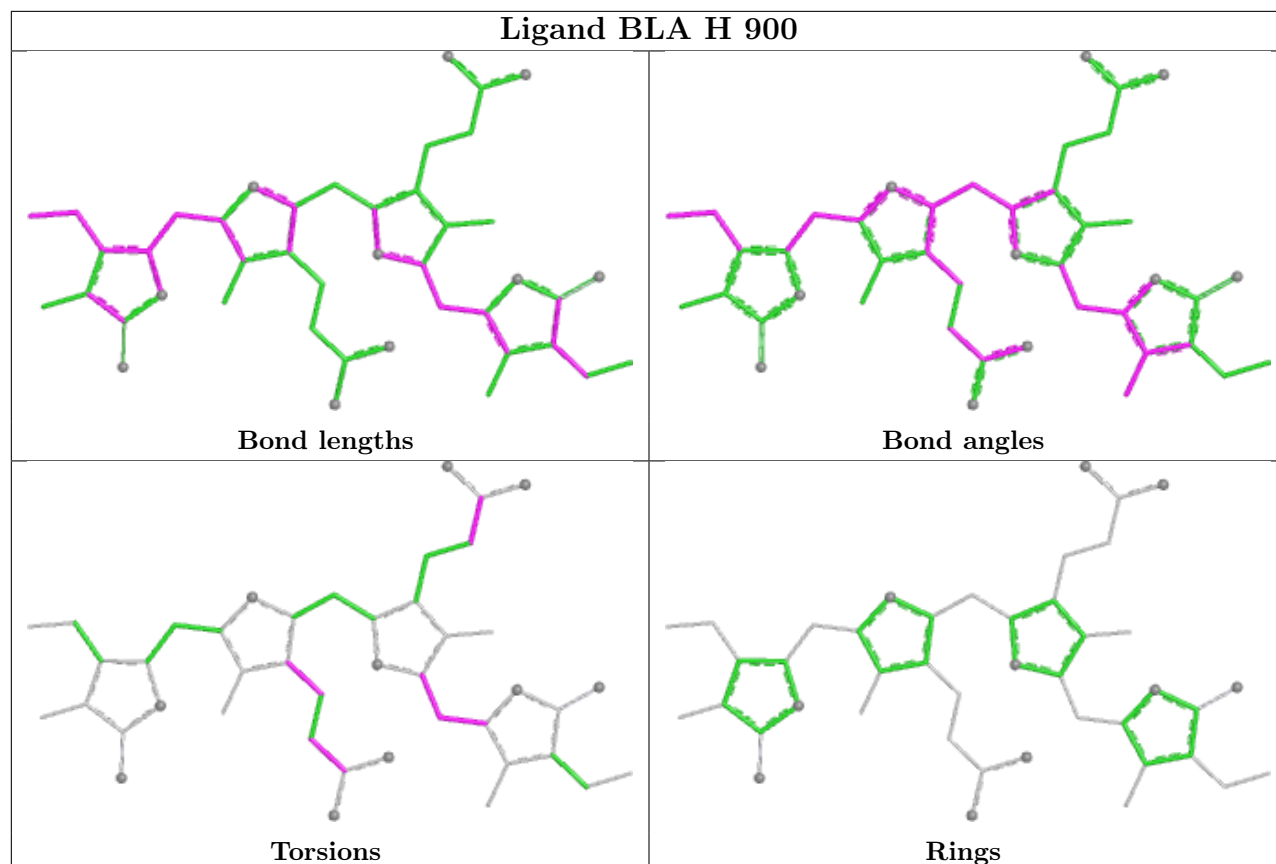
8 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	BLA	8	0
2	H	900	BLA	9	0
2	E	900	BLA	6	0
2	B	900	BLA	4	0
2	C	900	BLA	9	0
2	G	900	BLA	10	0
2	F	900	BLA	4	0
2	A	900	BLA	6	0

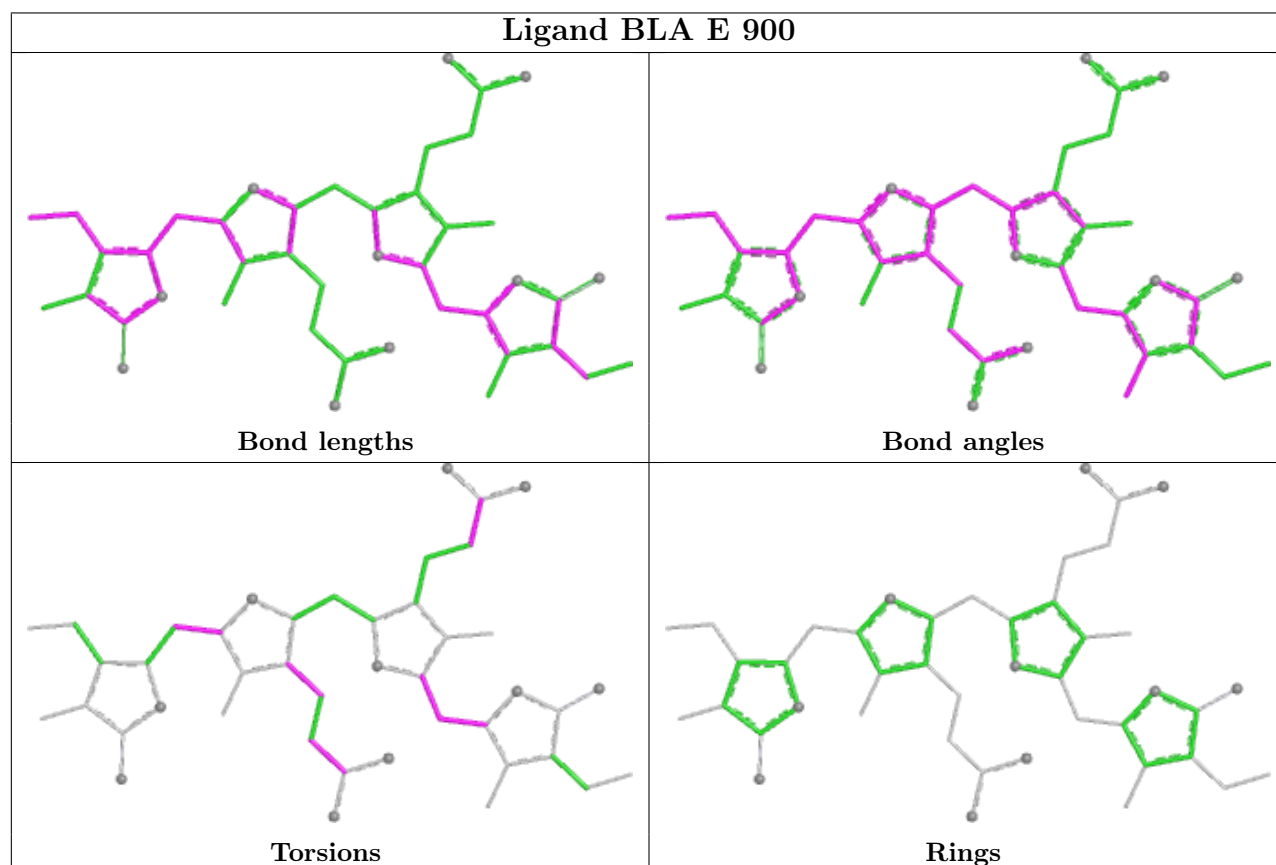
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



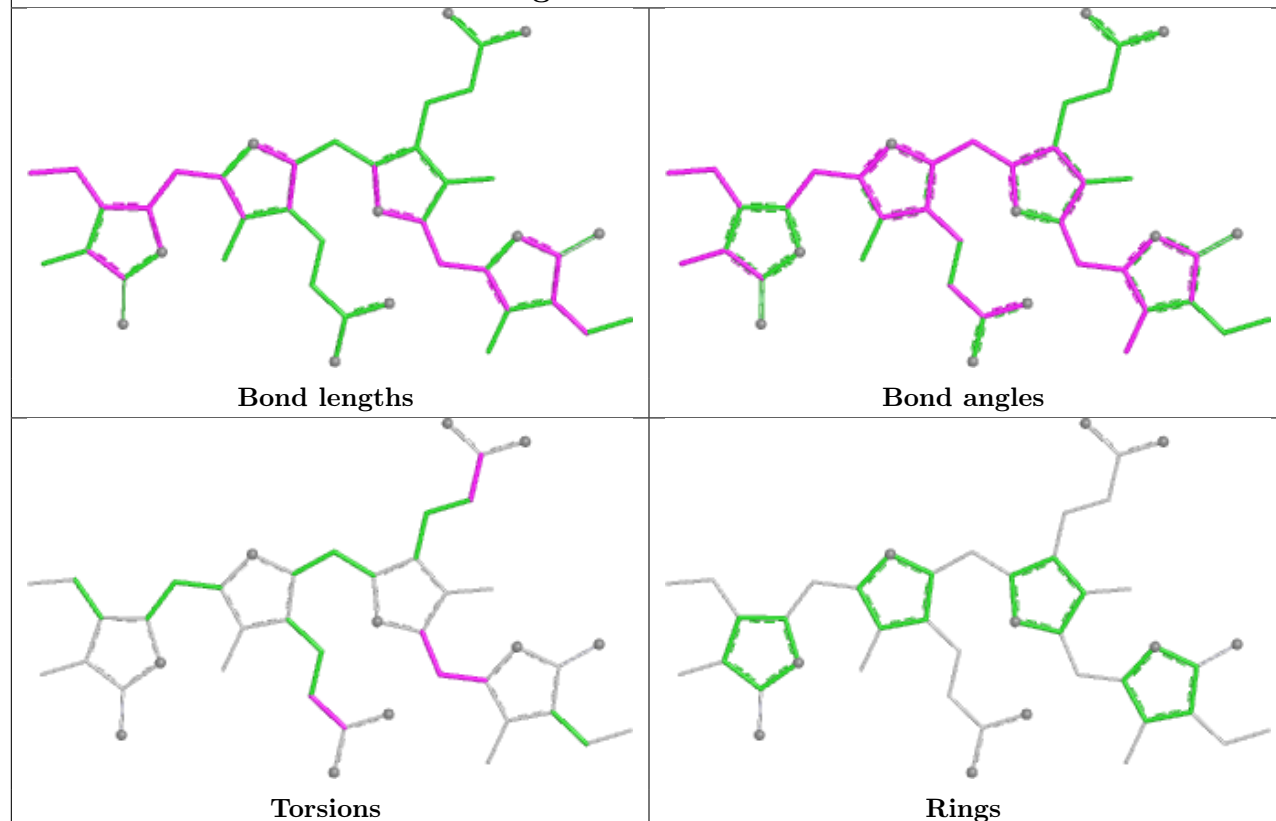
Ligand BLA H 900



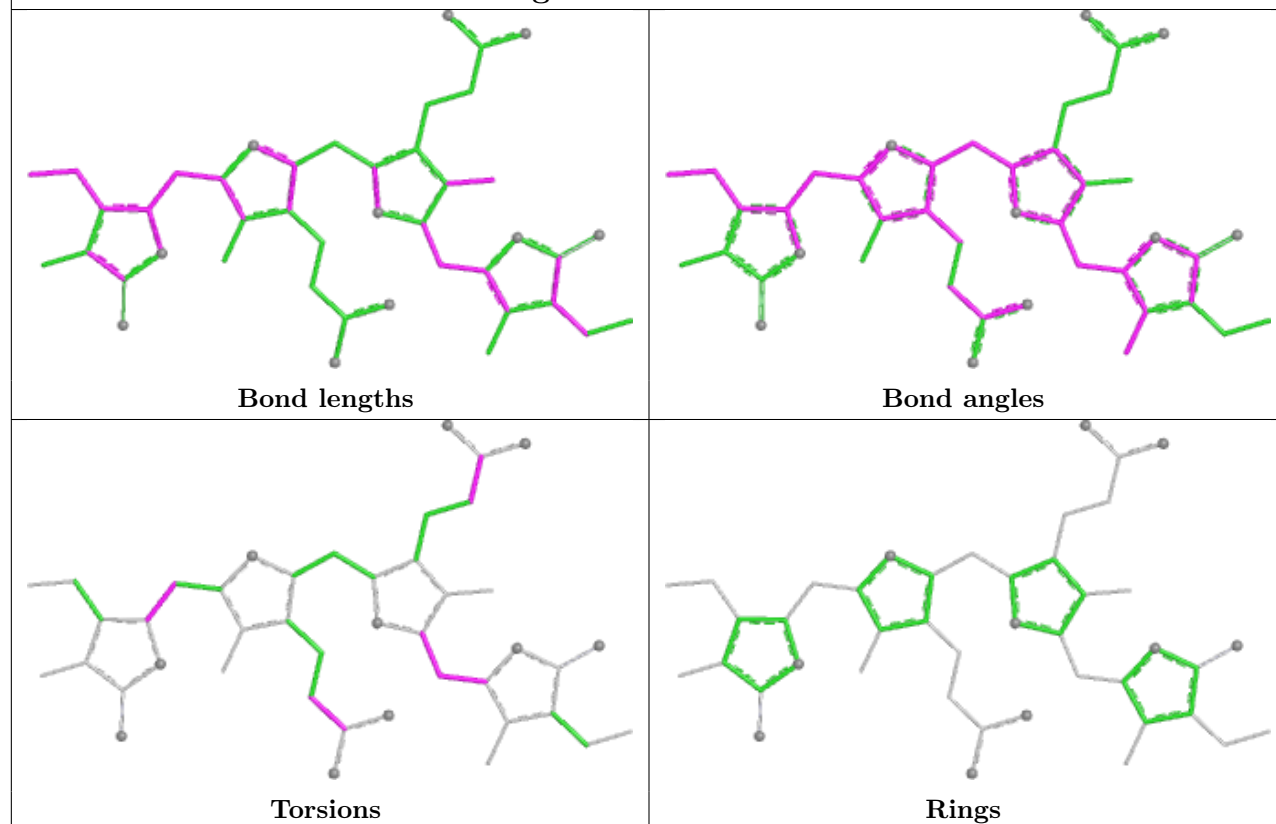
Ligand BLA E 900



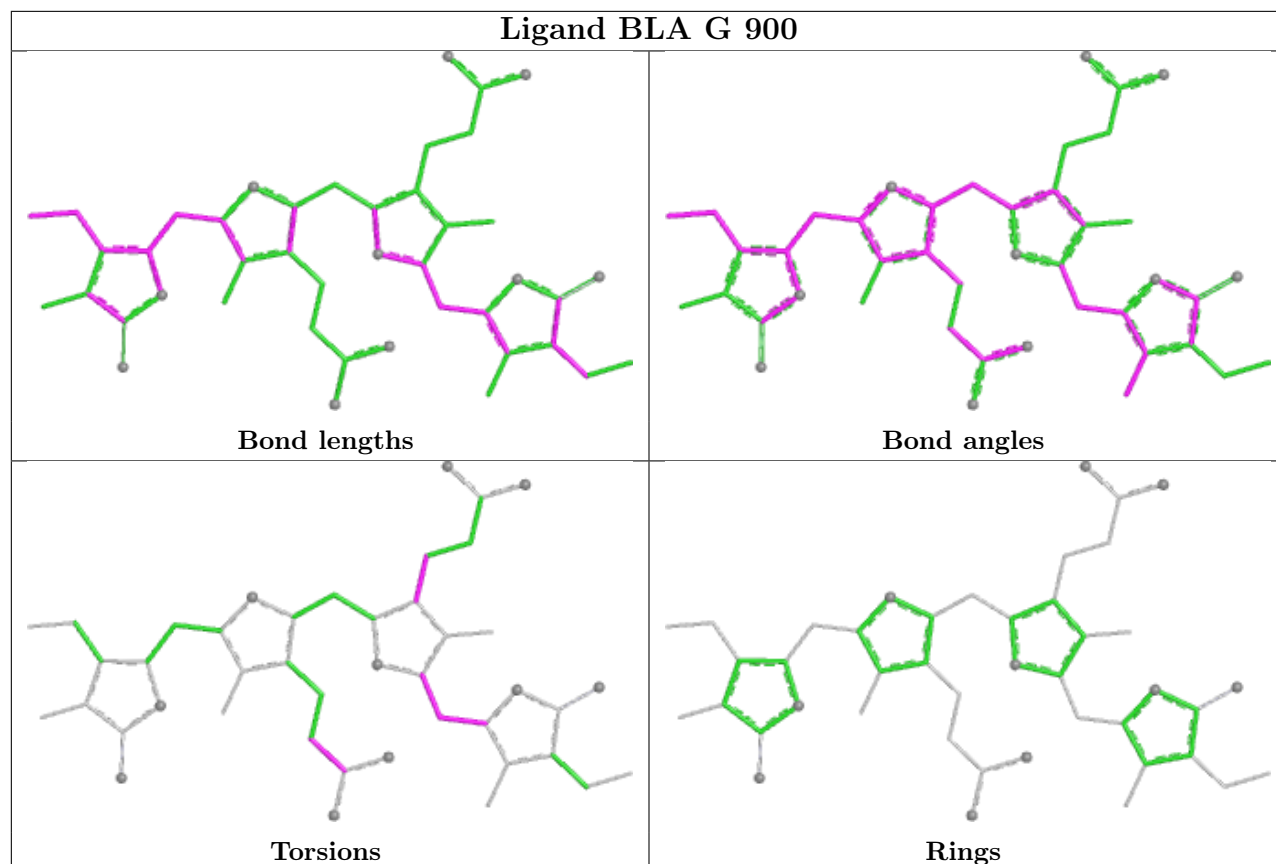
Ligand BLA B 900



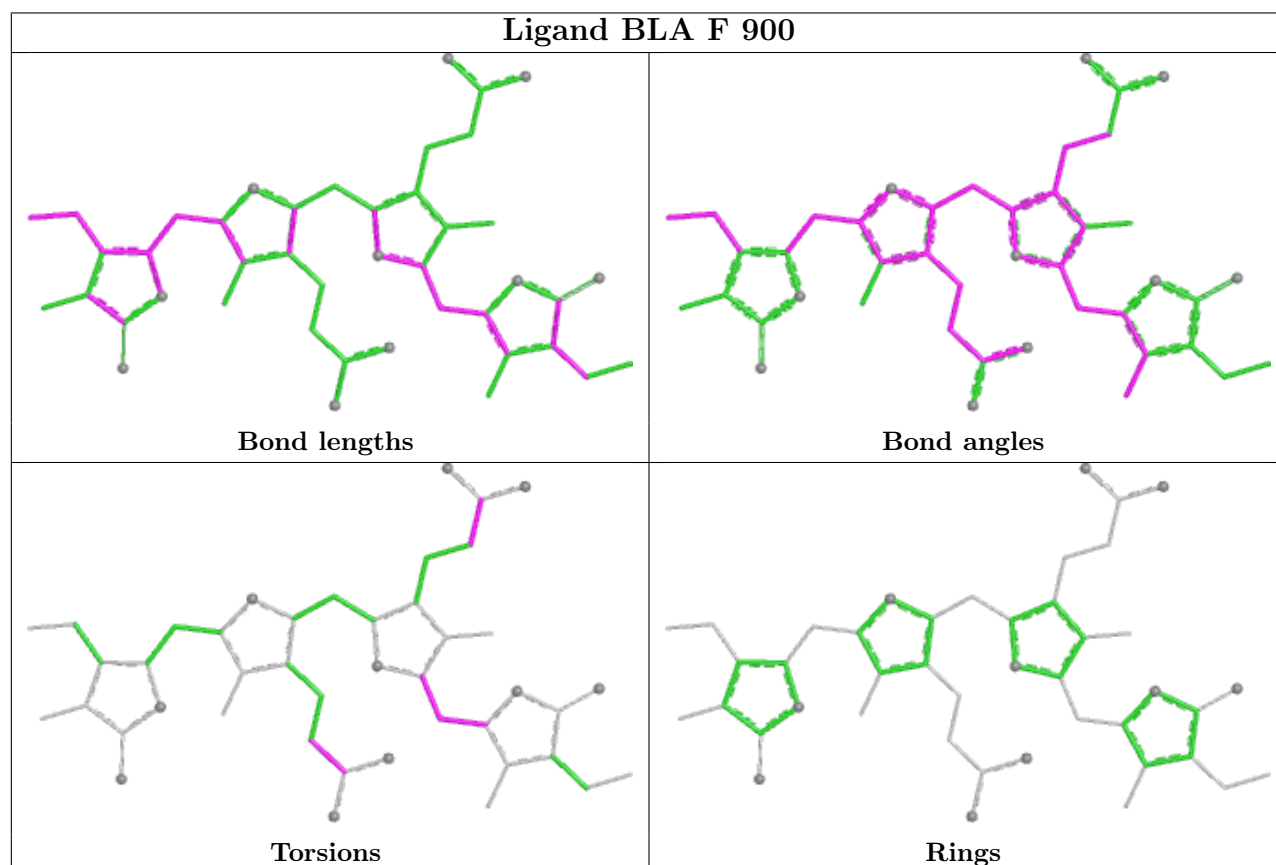
Ligand BLA C 900

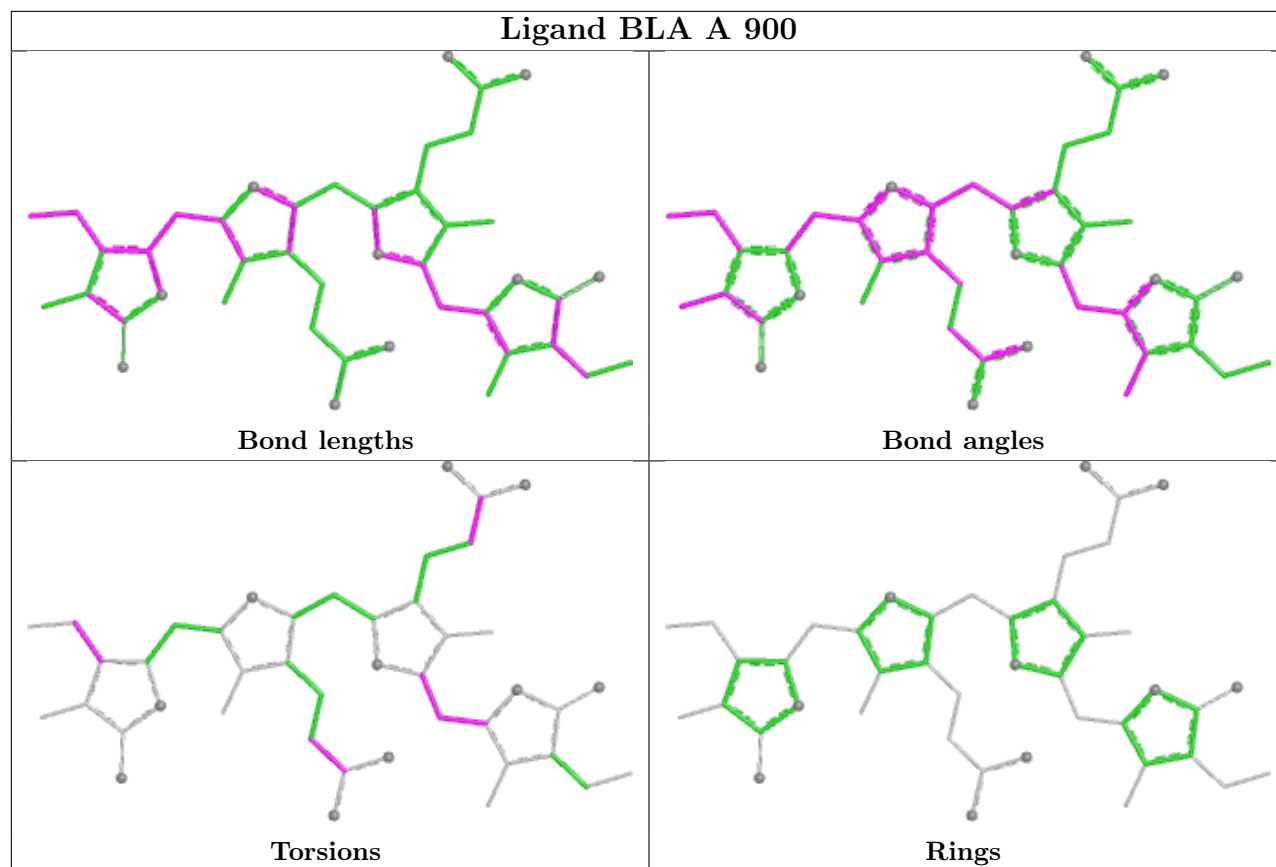


Ligand BLA G 900



Ligand BLA F 900





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	478/505 (94%)	-0.63	0 100 100	67, 98, 155, 233	0
1	B	468/505 (92%)	-0.57	0 100 100	74, 129, 188, 243	0
1	C	482/505 (95%)	-0.72	0 100 100	66, 99, 148, 206	0
1	D	478/505 (94%)	-0.47	1 (0%) 91 89	83, 139, 194, 239	0
1	E	471/505 (93%)	-0.54	0 100 100	87, 139, 186, 225	0
1	F	469/505 (92%)	-0.52	0 100 100	80, 124, 203, 282	0
1	G	482/505 (95%)	-0.66	0 100 100	58, 103, 152, 217	1 (0%)
1	H	480/505 (95%)	-0.47	0 100 100	84, 139, 214, 274	0
All	All	3808/4040 (94%)	-0.57	1 (0%) 100 100	58, 122, 191, 282	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	395	TRP	2.4

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 [i](#)

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,

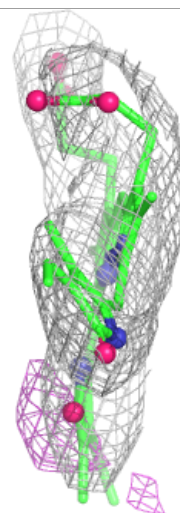
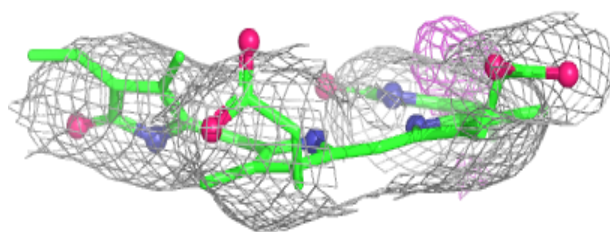
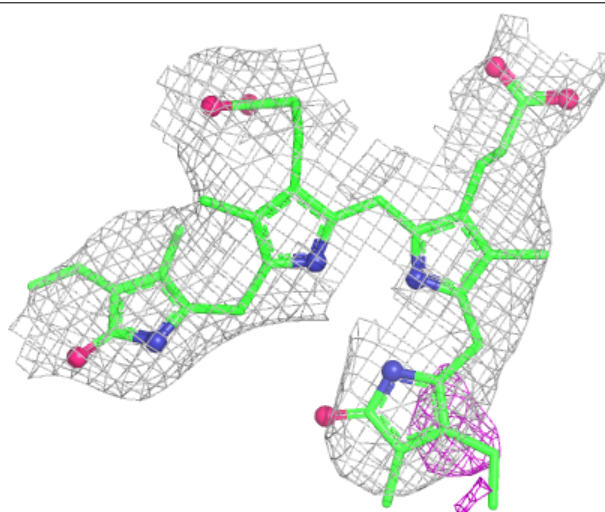
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	H	900	43/43	0.92	0.08	79,121,140,148	0
2	BLA	E	900	43/43	0.93	0.08	100,144,164,174	0
2	BLA	D	900	43/43	0.93	0.07	99,123,140,148	0
2	BLA	F	900	43/43	0.94	0.07	74,102,118,132	0
2	BLA	A	900	43/43	0.95	0.07	60,83,113,119	0
2	BLA	G	900	43/43	0.95	0.07	67,93,104,128	0
2	BLA	B	900	43/43	0.95	0.07	105,121,135,145	0
2	BLA	C	900	43/43	0.96	0.07	64,88,102,108	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.

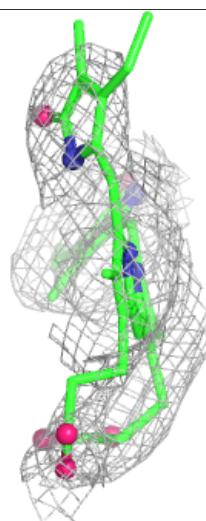
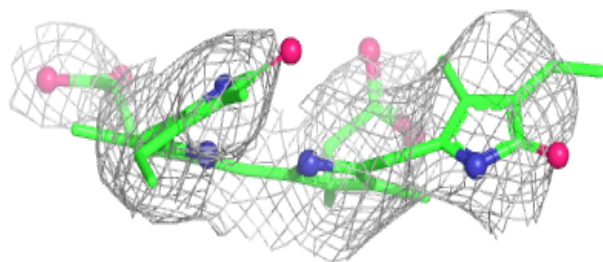
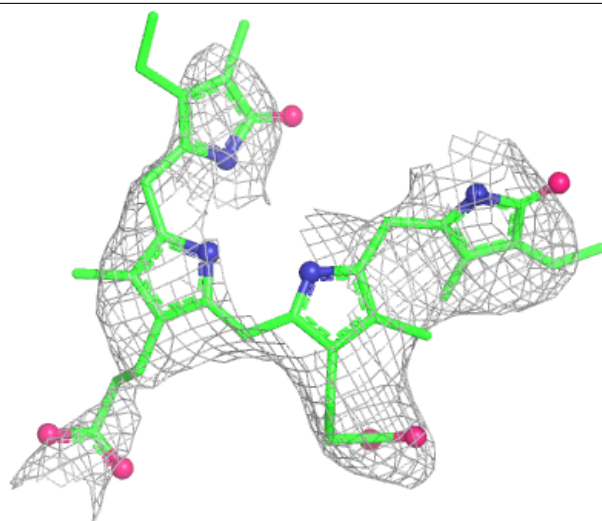
Electron density around BLA H 900:

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



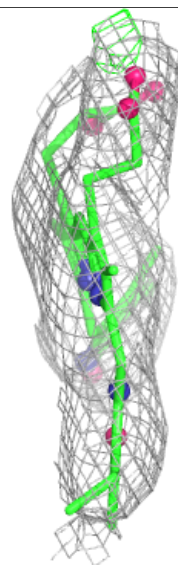
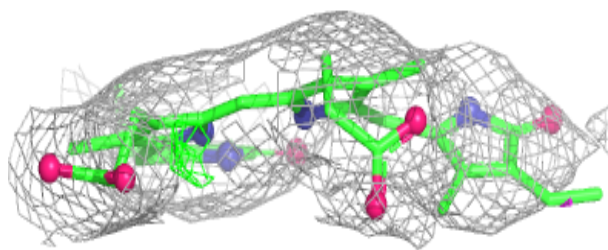
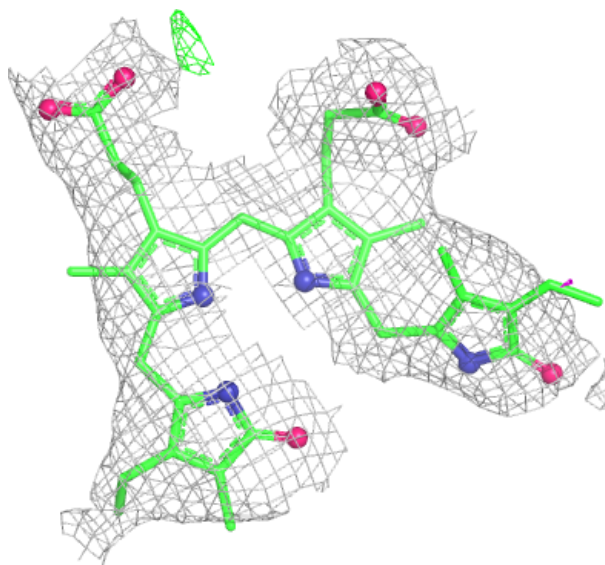
Electron density around BLA E 900:

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



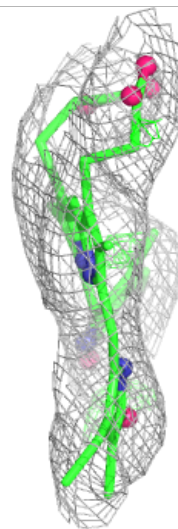
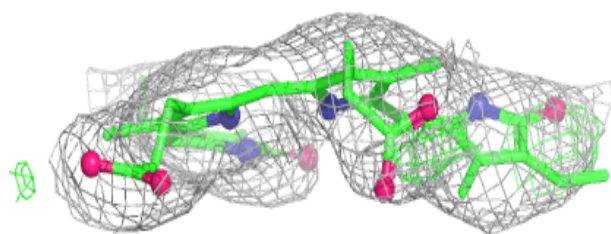
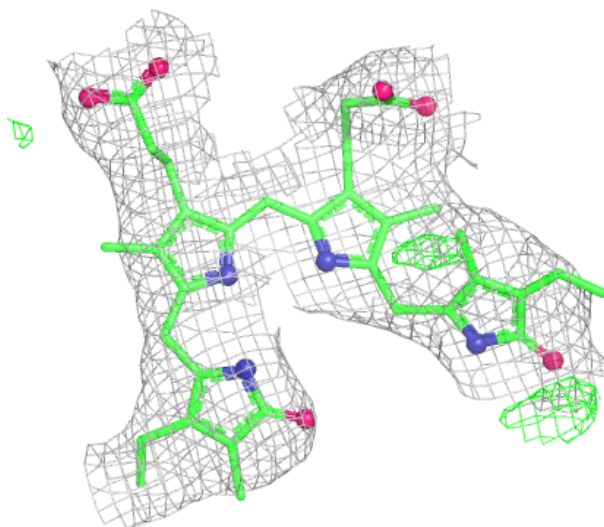
Electron density around BLA D 900:

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



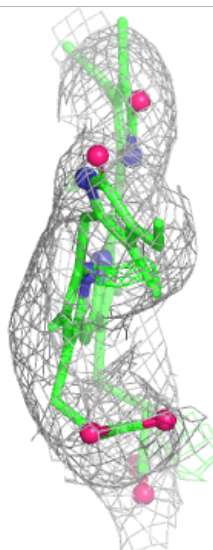
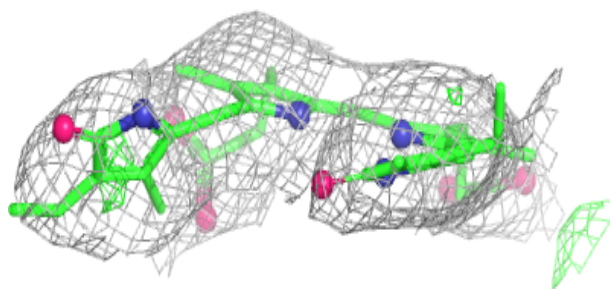
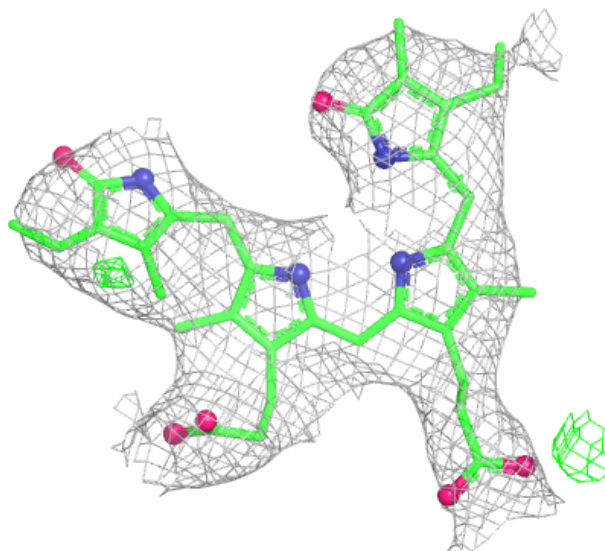
Electron density around BLA F 900:

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



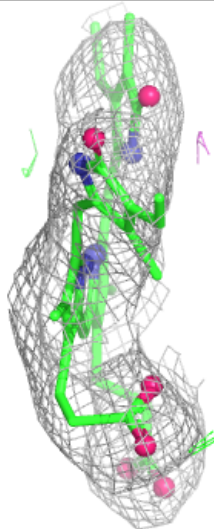
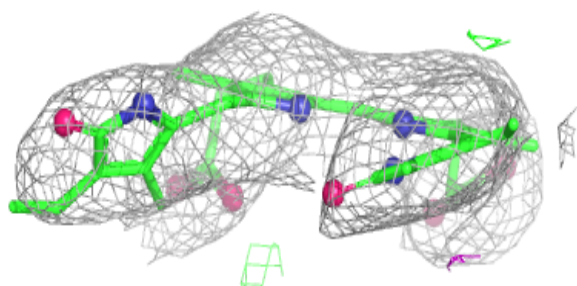
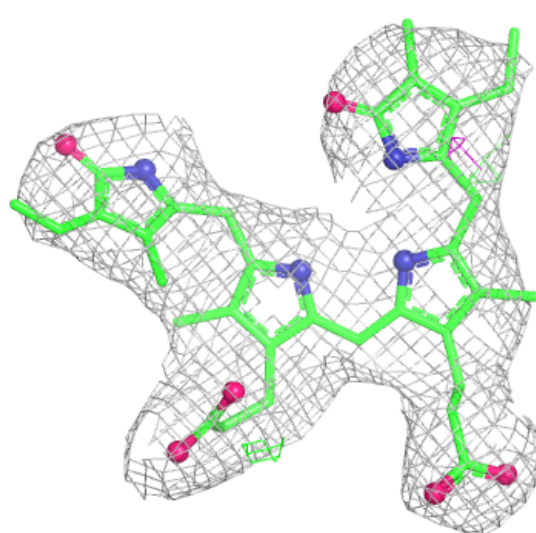
Electron density around BLA A 900:

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



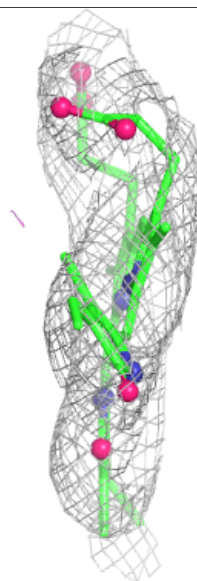
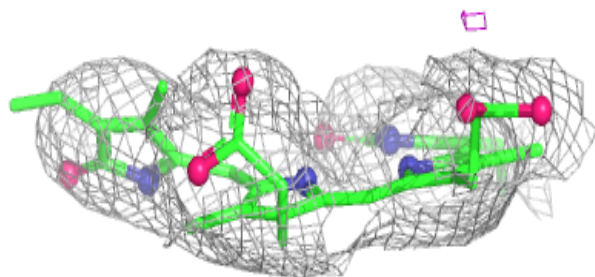
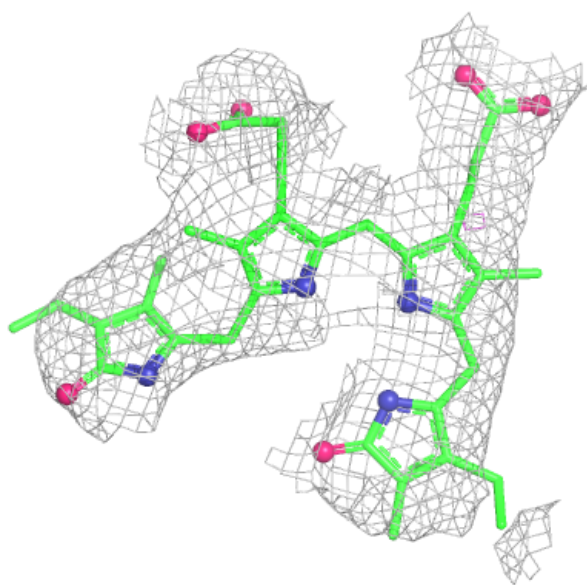
Electron density around BLA G 900:

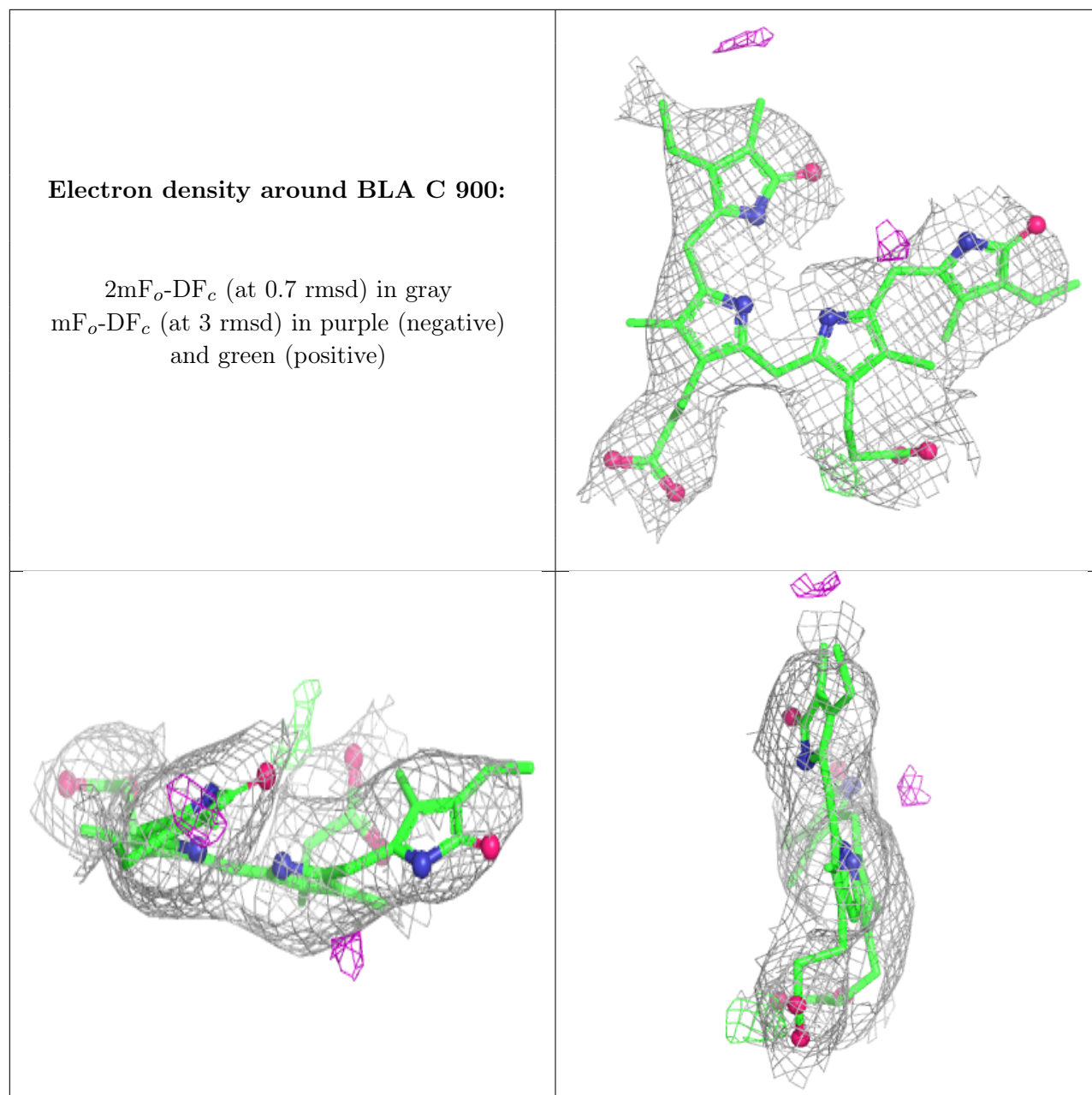
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLA B 900:

$2mF_o-DF_c$ (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.