



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:13 PM EDT

PDB ID : 4RH7 / pdb_00004rh7
Title : Crystal structure of human cytoplasmic dynein 2 motor domain in complex with ADP.Vi
Authors : Schmidt, H.; Zalyte, R.; Urnavicius, L.; Carter, A.P.
Deposited on : 2014-10-01
Resolution : 3.41 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

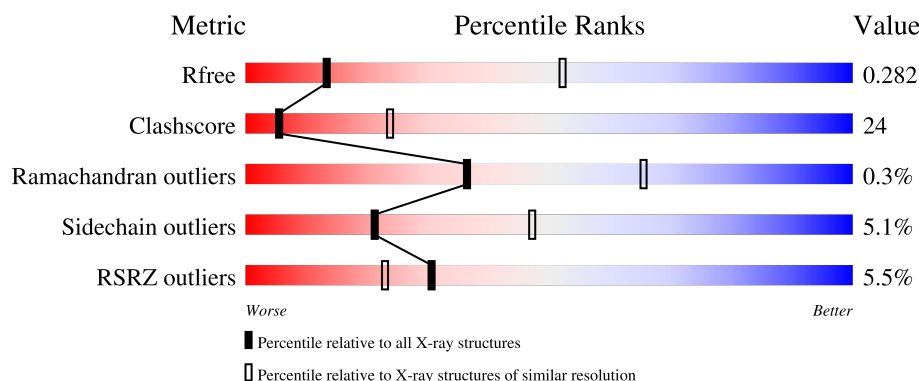
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	3450	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AOV	A	4401	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22816 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.

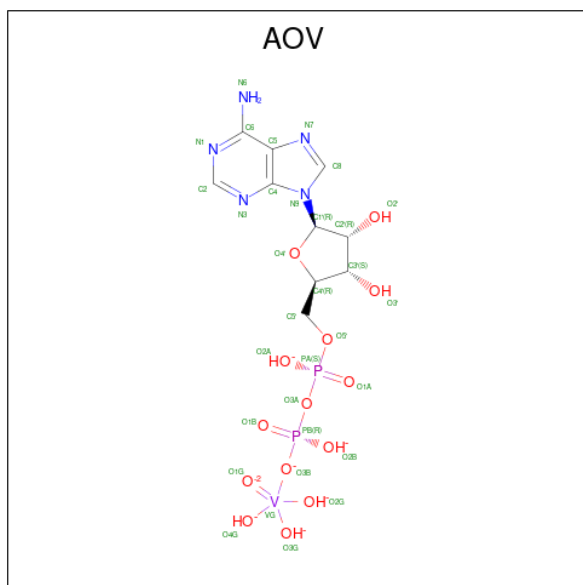
- Molecule 1 is a protein called Green fluorescent protein/Cytoplasmic dynein 2 heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	3005	22697	14414	3922	4263	98	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	GLY	-	linker	UNP Q8NCM8
A	1090	SER	-	linker	UNP Q8NCM8
A	1413	ARG	LYS	variant	UNP Q8NCM8
A	2871	GLN	ARG	variant	UNP Q8NCM8
A	3680	VAL	ALA	variant	UNP Q8NCM8
A	4308	VAL	-	expression tag	UNP Q8NCM8

- Molecule 2 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$).

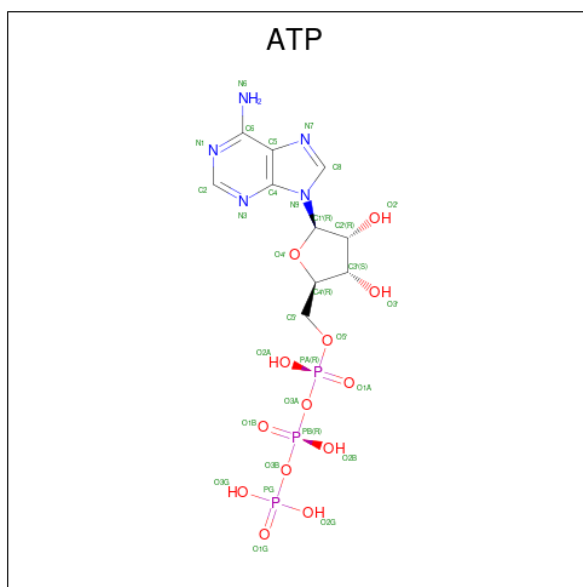


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	
			32	10	5	14	2	1	
									0
									0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

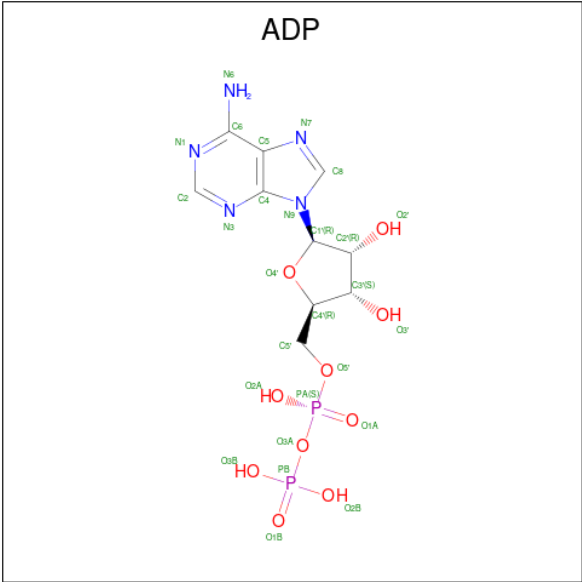
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg		
			2	2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



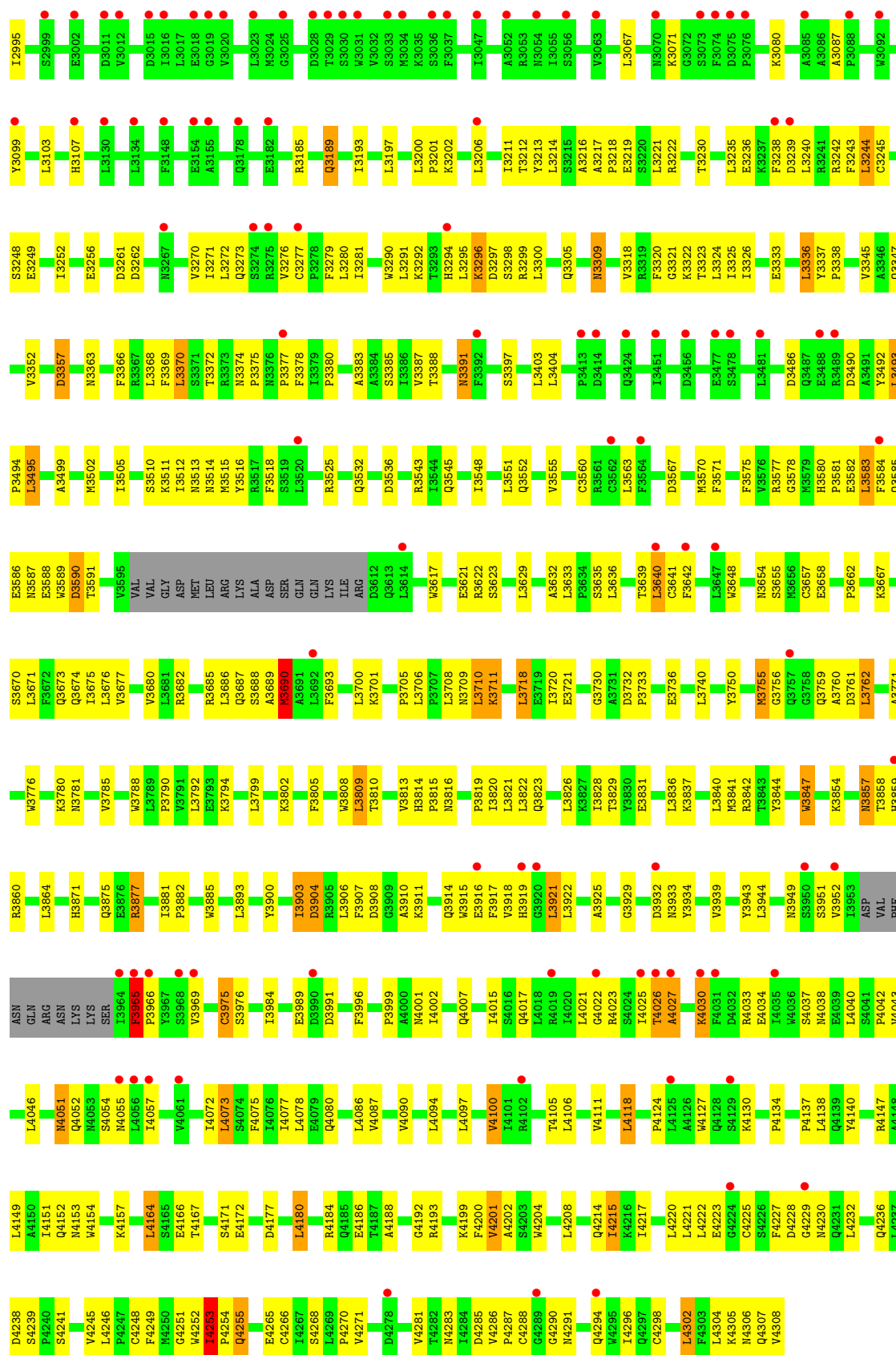
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P		
			31	10	5	13	3	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	136.03Å 487.15Å 276.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.60 – 3.41 56.60 – 3.41	Depositor EDS
% Data completeness (in resolution range)	62.2 (56.60-3.41) 62.4 (56.60-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.285 0.237 , 0.282	Depositor DCC
R_{free} test set	3915 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 110.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: MG, AOV, ATP, ADP

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	0.89	6/23147 (0.0%)	1.10	69/31474 (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	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2769	THR	N-CA	-5.64	1.39	1.46
1	A	2653	LEU	CA-C	-5.24	1.46	1.53
1	A	2053	ILE	N-CA	-5.21	1.39	1.46
1	A	2723	LEU	C-O	-5.20	1.17	1.24
1	A	3710	LEU	CA-C	-5.11	1.46	1.52
1	A	2806	LEU	CA-C	-5.10	1.46	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3297	ASP	N-CA-C	-11.12	100.47	112.93
1	A	3296	LYS	N-CA-C	9.26	122.53	111.33
1	A	2311	THR	N-CA-C	8.95	122.76	109.24
1	A	3949	ASN	N-CA-C	8.31	120.94	108.31
1	A	1398	ARG	N-CA-C	-7.21	103.12	110.97
1	A	2275	PHE	CB-CA-C	-7.16	98.76	110.79
1	A	1792	ASN	CA-C-N	-6.75	113.73	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1792	ASN	C-N-CA	-6.75	113.73	120.21
1	A	4015	ILE	CB-CA-C	-6.70	103.31	111.88
1	A	3857	ASN	N-CA-C	6.65	118.53	111.28
1	A	2432	TYR	CA-C-N	-6.53	113.25	119.85
1	A	2432	TYR	C-N-CA	-6.53	113.25	119.85
1	A	3951	SER	N-CA-C	6.49	119.61	111.24
1	A	2163	VAL	N-CA-C	6.47	117.26	110.72
1	A	2164	VAL	N-CA-C	6.42	116.82	108.35
1	A	4022	GLY	N-CA-C	6.39	120.39	112.73
1	A	3617	TRP	N-CA-C	6.31	119.82	111.75
1	A	4251	GLY	N-CA-C	6.08	118.78	110.69
1	A	2096	THR	N-CA-C	6.04	118.31	108.76
1	A	2239	ALA	N-CA-C	6.04	119.07	108.75
1	A	3809	LEU	N-CA-C	6.00	119.31	108.69
1	A	2764	VAL	N-CA-C	5.92	116.66	110.62
1	A	4253	ILE	CB-CA-C	-5.92	100.59	111.36
1	A	2981	VAL	N-CA-C	5.88	116.92	111.45
1	A	3297	ASP	N-CA-CB	-5.86	102.47	110.56
1	A	2077	THR	N-CA-C	5.86	118.06	108.52
1	A	2275	PHE	N-CA-C	5.85	118.54	111.40
1	A	2238	LEU	CB-CA-C	-5.84	109.82	116.54
1	A	3370	LEU	N-CA-C	5.83	117.71	108.79
1	A	3280	LEU	N-CA-C	5.83	118.22	108.96
1	A	3965	PHE	CA-C-N	-5.78	113.81	119.76
1	A	3965	PHE	C-N-CA	-5.78	113.81	119.76
1	A	3623	SER	N-CA-C	5.76	118.31	111.33
1	A	4255	GLN	N-CA-C	-5.71	102.99	110.53
1	A	3655	SER	N-CA-C	-5.70	102.47	110.50
1	A	2058	ILE	N-CA-C	5.63	116.00	108.11
1	A	2214	HIS	N-CA-C	-5.61	105.07	111.07
1	A	3916	GLU	N-CA-C	5.61	117.84	111.11
1	A	2297	LYS	N-CA-C	-5.59	105.09	111.07
1	A	2355	VAL	N-CA-C	5.55	116.11	108.12
1	A	3710	LEU	CB-CA-C	-5.55	101.42	110.85
1	A	2461	GLY	N-CA-C	-5.52	101.29	111.34
1	A	2661	ARG	N-CA-C	-5.52	105.34	111.36
1	A	3711	LYS	N-CA-C	-5.48	105.46	111.82
1	A	2912	ASP	N-CA-C	5.42	117.19	111.28
1	A	3893	LEU	N-CA-C	-5.38	106.22	112.89
1	A	3975	CYS	N-CA-C	5.31	116.88	111.14
1	A	3107	HIS	CA-C-N	-5.29	113.47	118.97
1	A	3107	HIS	C-N-CA	-5.29	113.47	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2136	GLU	N-CA-C	-5.27	105.53	111.28
1	A	2981	VAL	CB-CA-C	-5.27	105.02	111.92
1	A	1292	ILE	N-CA-C	5.27	116.37	109.21
1	A	2474	VAL	N-CA-C	-5.26	105.25	110.62
1	A	3318	VAL	CB-CA-C	-5.24	104.99	112.22
1	A	1972	ARG	N-CA-C	5.24	118.12	109.85
1	A	1891	ASN	N-CA-C	5.22	116.82	111.03
1	A	2995	ILE	N-CA-C	5.18	115.78	109.30
1	A	3799	LEU	N-CA-C	5.17	117.79	110.50
1	A	2220	PRO	O-C-N	5.17	123.58	121.15
1	A	2126	ILE	CB-CA-C	-5.16	105.18	112.14
1	A	1276	PHE	N-CA-C	5.15	118.12	110.14
1	A	1761	ILE	CB-CA-C	-5.14	105.29	112.02
1	A	1911	THR	N-CA-C	-5.11	103.78	110.53
1	A	3690	MET	N-CA-C	-5.08	105.02	111.11
1	A	2059	ASP	CB-CA-C	-5.07	102.41	110.02
1	A	1900	GLN	N-CA-C	-5.07	105.65	111.07
1	A	2708	VAL	CB-CA-C	-5.06	102.28	110.28
1	A	2193	ILE	CB-CA-C	-5.03	105.45	112.04
1	A	1907	MET	N-CA-C	5.02	118.51	112.38

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	LEU	Peptide
1	A	2247	GLU	Peptide
1	A	2275	PHE	Peptide
1	A	2310	SER	Peptide
1	A	2416	LYS	Peptide
1	A	2659	VAL	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	22697	0	21503	1050	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	0	12	12	0
3	A	2	0	0	0	0
4	A	31	0	12	4	0
5	A	54	0	24	10	0
All	All	22816	0	21551	1051	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1051) 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:A:3581:PRO:HA	1:A:3584:PHE:CE1	1.16	1.63
1:A:2284:LYS:CE	1:A:2401:GLN:HG3	1.33	1.55
1:A:2284:LYS:HE3	1:A:2401:GLN:CG	1.49	1.40
1:A:3291:LEU:O	1:A:3294:HIS:CE1	1.75	1.39
1:A:3581:PRO:CA	1:A:3584:PHE:CE1	2.04	1.38
1:A:2284:LYS:CD	1:A:2353:ARG:HH22	1.37	1.37
1:A:2659:VAL:CG2	1:A:2811:TRP:HE1	1.45	1.30
1:A:2847:VAL:CG1	1:A:2849:PRO:HD2	1.61	1.30
1:A:3291:LEU:O	1:A:3294:HIS:ND1	1.63	1.29
1:A:2284:LYS:HD2	1:A:2353:ARG:NH2	1.47	1.27
1:A:2473:MET:HE2	1:A:2502:TRP:CD2	1.70	1.26
1:A:3238:PHE:HZ	1:A:3243:PHE:CD1	1.51	1.25
1:A:4030:LYS:HG3	1:A:4034:GLU:OE1	1.34	1.21
1:A:2660:GLY:HA3	5:A:4406:ADP:O1A	1.34	1.21
1:A:2592:LEU:HD21	1:A:2707:GLN:OE1	1.37	1.19
1:A:4054:SER:HB3	1:A:4057:ILE:CD1	1.71	1.19
1:A:2284:LYS:HG3	1:A:2401:GLN:OE1	1.38	1.18
1:A:3238:PHE:CZ	1:A:3243:PHE:CD1	2.32	1.18
1:A:4054:SER:CB	1:A:4057:ILE:HD12	1.73	1.17
1:A:1690:PRO:HA	1:A:1798:TYR:OH	1.47	1.15
1:A:2004:LYS:HG3	1:A:2006:TYR:CE1	1.82	1.14
1:A:2659:VAL:CB	1:A:2811:TRP:HE1	1.61	1.13
1:A:2131:ARG:HA	1:A:2138:ARG:NH2	1.66	1.11
1:A:4100:VAL:HG12	1:A:4105:THR:HG21	1.31	1.10
1:A:1716:ASP:CG	1:A:1745:ARG:NH2	2.10	1.09
1:A:4100:VAL:HG12	1:A:4105:THR:CG2	1.83	1.08
1:A:2473:MET:CE	1:A:2502:TRP:CE2	2.14	1.08
1:A:2847:VAL:HG12	1:A:2849:PRO:CD	1.83	1.08
1:A:4171:SER:HB2	1:A:4308:VAL:O	1.54	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2661:ARG:O	1:A:2665:THR:HG23	1.55	1.06
1:A:3581:PRO:HA	1:A:3584:PHE:CZ	1.89	1.06
1:A:4100:VAL:HA	1:A:4105:THR:HG22	1.36	1.06
1:A:1867:ARG:NH1	2:A:4401:AOV:O3B	1.89	1.05
1:A:3580:HIS:O	1:A:3584:PHE:CZ	2.08	1.05
1:A:2659:VAL:CG2	1:A:2811:TRP:NE1	2.20	1.03
1:A:2607:LEU:HD23	1:A:2634:LEU:CD1	1.86	1.03
1:A:3291:LEU:HD12	1:A:3294:HIS:CE1	1.95	1.02
1:A:4100:VAL:HA	1:A:4105:THR:CG2	1.90	1.02
1:A:2607:LEU:CD2	1:A:2634:LEU:HD12	1.89	1.01
1:A:2607:LEU:HD23	1:A:2634:LEU:HD12	1.01	1.01
1:A:2653:LEU:HB3	1:A:2661:ARG:HG2	1.44	1.00
1:A:2473:MET:HE2	1:A:2502:TRP:CE2	1.47	0.98
1:A:2284:LYS:HE3	1:A:2401:GLN:CB	1.93	0.98
1:A:3581:PRO:CA	1:A:3584:PHE:HE1	1.56	0.97
1:A:2284:LYS:CE	1:A:2353:ARG:HH22	1.76	0.96
1:A:2811:TRP:HB2	1:A:2816:MET:CE	1.96	0.96
1:A:2359:LYS:O	1:A:2360:ASP:OD1	1.83	0.96
1:A:2284:LYS:CE	1:A:2401:GLN:CG	2.23	0.96
1:A:2847:VAL:HG12	1:A:2849:PRO:HD2	0.97	0.95
1:A:3511:LYS:NZ	1:A:4021:LEU:O	1.98	0.94
1:A:2284:LYS:HD2	1:A:2353:ARG:HH22	0.79	0.93
1:A:3291:LEU:C	1:A:3294:HIS:CE1	2.46	0.93
1:A:2659:VAL:HG23	1:A:2811:TRP:HE1	1.33	0.93
1:A:4054:SER:HB3	1:A:4057:ILE:HD12	0.94	0.92
1:A:1584:PRO:HB2	1:A:1587:THR:CG2	1.98	0.92
1:A:4100:VAL:CG1	1:A:4105:THR:HG21	1.98	0.92
1:A:4171:SER:CB	1:A:4308:VAL:O	2.16	0.92
1:A:3581:PRO:CB	1:A:3584:PHE:HE1	1.82	0.92
1:A:1896:HIS:CD2	1:A:1929:ILE:HG23	2.05	0.92
1:A:3238:PHE:HZ	1:A:3243:PHE:HD1	0.98	0.91
1:A:1716:ASP:OD2	1:A:1745:ARG:NH2	2.03	0.91
1:A:2847:VAL:CG1	1:A:2849:PRO:CD	2.42	0.91
1:A:2659:VAL:HB	1:A:2811:TRP:HE1	1.33	0.91
1:A:2284:LYS:CD	1:A:2401:GLN:HG3	2.01	0.90
1:A:1662:LEU:HD11	1:A:1697:GLU:HB3	1.54	0.90
1:A:2284:LYS:HE2	1:A:2401:GLN:HG3	1.51	0.90
1:A:1584:PRO:HB2	1:A:1587:THR:HG22	1.55	0.89
1:A:4057:ILE:HD13	1:A:4149:LEU:HD23	1.54	0.89
1:A:2284:LYS:HG3	1:A:2401:GLN:CD	1.97	0.89
1:A:3755:MET:N	1:A:3755:MET:HE2	1.88	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4171:SER:C	1:A:4308:VAL:O	2.16	0.89
1:A:3581:PRO:HA	1:A:3584:PHE:HE1	1.08	0.88
1:A:1674:THR:HG22	1:A:3925:ALA:HA	1.54	0.88
1:A:1716:ASP:OD1	1:A:1745:ARG:NH2	2.06	0.88
1:A:2004:LYS:CG	1:A:2006:TYR:CE1	2.56	0.88
1:A:2659:VAL:HB	1:A:2811:TRP:NE1	1.88	0.88
1:A:1796:LYS:HD3	1:A:1797:GLY:N	1.88	0.87
1:A:1690:PRO:CA	1:A:1798:TYR:OH	2.22	0.87
1:A:2284:LYS:CD	1:A:2353:ARG:NH2	2.19	0.87
1:A:2284:LYS:HE3	1:A:2401:GLN:HG3	0.88	0.87
1:A:2660:GLY:CA	5:A:4406:ADP:O1A	2.22	0.87
1:A:3377:PRO:CB	1:A:3378:PHE:HB2	2.05	0.86
1:A:4100:VAL:CA	1:A:4105:THR:CG2	2.53	0.86
1:A:4030:LYS:HB2	1:A:4034:GLU:HG3	1.57	0.85
1:A:2284:LYS:CE	1:A:2353:ARG:NH2	2.36	0.85
1:A:2660:GLY:O	1:A:2664:ILE:HD13	1.76	0.85
1:A:2592:LEU:CD2	1:A:2707:GLN:OE1	2.24	0.84
1:A:2510:ASP:O	1:A:2522:TYR:OH	1.96	0.83
1:A:2659:VAL:HG23	1:A:2811:TRP:NE1	1.87	0.83
1:A:2284:LYS:HD2	1:A:2353:ARG:CZ	2.07	0.83
1:A:1716:ASP:OD1	1:A:1745:ARG:CZ	2.27	0.82
1:A:2004:LYS:HG3	1:A:2006:TYR:HE1	1.41	0.82
1:A:4057:ILE:HD13	1:A:4149:LEU:CD2	2.09	0.82
1:A:2658:GLY:HA3	1:A:2870:SER:HB3	1.62	0.81
1:A:3291:LEU:HA	1:A:3294:HIS:CE1	2.16	0.81
1:A:2055:ASP:OD1	1:A:2420:ARG:NH2	2.14	0.81
1:A:1716:ASP:OD2	1:A:2065:SER:HA	1.80	0.81
1:A:2811:TRP:HB2	1:A:2816:MET:HE2	1.62	0.81
1:A:4171:SER:CB	1:A:4305:LYS:CB	2.59	0.80
1:A:3291:LEU:C	1:A:3294:HIS:ND1	2.40	0.80
1:A:1554:ALA:HA	1:A:1560:LEU:HD12	1.63	0.80
1:A:2288:ILE:HD11	1:A:2425:VAL:HG21	1.63	0.80
1:A:3238:PHE:CZ	1:A:3243:PHE:HD1	1.85	0.80
1:A:4171:SER:HB3	1:A:4305:LYS:CB	2.12	0.80
1:A:4057:ILE:CD1	1:A:4149:LEU:CD2	2.60	0.80
1:A:3291:LEU:HD12	1:A:3294:HIS:HE1	1.46	0.79
1:A:2575:THR:HG21	1:A:2645:SER:OG	1.80	0.79
1:A:3857:ASN:HB2	1:A:3975:CYS:SG	2.21	0.79
1:A:1715:CYS:SG	1:A:1743:PHE:HA	2.22	0.79
1:A:4100:VAL:CG1	1:A:4105:THR:CG2	2.57	0.79
1:A:3377:PRO:HB2	1:A:3378:PHE:HB2	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3640:LEU:HG	1:A:3642:PHE:CE2	2.18	0.78
1:A:3502:MET:HE1	1:A:3551:LEU:HD12	1.65	0.78
1:A:2263:ILE:HD13	1:A:2441:ILE:HA	1.65	0.78
1:A:3640:LEU:HG	1:A:3642:PHE:CZ	2.20	0.77
1:A:3581:PRO:HA	1:A:3584:PHE:CD1	2.11	0.77
1:A:2811:TRP:HB2	1:A:2816:MET:HE3	1.64	0.77
1:A:1513:GLN:HG3	1:A:1514:LEU:N	2.00	0.76
1:A:2847:VAL:HG13	1:A:2849:PRO:HD2	1.66	0.76
1:A:2658:GLY:HA3	1:A:2870:SER:CB	2.16	0.76
1:A:3512:ILE:HG23	1:A:4021:LEU:CD2	2.16	0.76
1:A:4171:SER:CA	1:A:4308:VAL:O	2.33	0.76
1:A:4304:LEU:HD12	1:A:4305:LYS:N	2.00	0.76
1:A:4030:LYS:CG	1:A:4034:GLU:OE1	2.28	0.75
1:A:2821:GLU:HB2	1:A:2852:LEU:HD13	1.68	0.75
1:A:3291:LEU:CA	1:A:3294:HIS:CE1	2.70	0.75
1:A:2473:MET:HE2	1:A:2502:TRP:CE3	1.91	0.74
1:A:3760:ALA:HA	1:A:3788:TRP:CH2	2.22	0.74
1:A:2810:GLY:O	1:A:2811:TRP:HD1	1.70	0.74
1:A:4208:LEU:O	1:A:4214:GLN:NE2	2.20	0.74
1:A:2685:TYR:HB2	1:A:2718:VAL:HG21	1.68	0.73
1:A:3515:MET:HE1	1:A:3813:VAL:HG13	1.71	0.73
1:A:2135:ALA:HA	1:A:2138:ARG:CB	1.71	0.73
1:A:4057:ILE:CD1	1:A:4152:GLN:HE22	2.01	0.73
1:A:1583:ASP:N	1:A:1584:PRO:HD2	2.02	0.73
1:A:1696:THR:OG1	2:A:4401:AOV:O2B	2.05	0.73
1:A:2659:VAL:CB	1:A:2811:TRP:NE1	2.41	0.73
1:A:1896:HIS:HA	1:A:1929:ILE:HD13	1.69	0.73
1:A:2205:ARG:NH2	1:A:2429:SER:OG	2.20	0.73
1:A:3291:LEU:C	1:A:3294:HIS:HD1	1.95	0.73
1:A:2653:LEU:CB	1:A:2661:ARG:HG2	2.17	0.72
1:A:3587:ASN:OD1	1:A:3590:ASP:OD2	2.07	0.72
1:A:1752:SER:OG	1:A:3755:MET:O	2.06	0.72
1:A:1283:ASP:HB3	1:A:1353:GLU:OE2	1.89	0.72
1:A:1693:THR:HG23	1:A:1817:MET:O	1.89	0.72
1:A:1460:GLY:HA3	1:A:1655:TYR:HD2	1.54	0.72
1:A:2135:ALA:N	1:A:2138:ARG:HG3	1.73	0.71
1:A:1801:ARG:NH1	1:A:2064:GLU:OE1	2.23	0.71
1:A:1279:ILE:HD12	1:A:1293:LYS:HG3	1.71	0.71
1:A:1514:LEU:CD1	1:A:1534:PHE:CE1	2.74	0.71
1:A:1690:PRO:HD2	1:A:1818:SER:HA	1.72	0.71
1:A:2661:ARG:O	1:A:2665:THR:CG2	2.37	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3642:PHE:HA	1:A:3648:TRP:NE1	2.06	0.70
1:A:3881:ILE:HG23	1:A:3882:PRO:HA	1.72	0.70
1:A:3512:ILE:HD12	1:A:3513:ASN:HB2	1.72	0.70
1:A:4100:VAL:HG12	1:A:4105:THR:HG23	1.72	0.70
1:A:2607:LEU:CD2	1:A:2634:LEU:CD1	2.61	0.70
1:A:3966:PRO:HB2	1:A:3969:VAL:HG12	1.73	0.70
1:A:2004:LYS:CG	1:A:2006:TYR:HE1	2.00	0.70
1:A:2658:GLY:CA	1:A:2870:SER:HB3	2.21	0.70
1:A:4100:VAL:CB	1:A:4105:THR:CG2	2.70	0.70
1:A:2135:ALA:HA	1:A:2138:ARG:HB2	1.72	0.69
1:A:2168:LEU:O	1:A:2169:VAL:C	2.34	0.69
1:A:1587:THR:OG1	1:A:1590:GLY:HA3	1.93	0.69
1:A:3847:TRP:HH2	1:A:3900:TYR:HB2	1.56	0.69
1:A:4097:LEU:HD13	1:A:4111:VAL:CG1	2.23	0.69
1:A:2867:ALA:HA	1:A:2871:GLN:OE1	1.93	0.69
1:A:1900:GLN:N	1:A:1900:GLN:OE1	2.22	0.68
1:A:4236:GLN:O	1:A:4239:SER:OG	2.10	0.68
1:A:2274:TYR:CE2	1:A:2428:CYS:HB3	2.28	0.68
1:A:2284:LYS:CG	1:A:2401:GLN:HG3	2.22	0.68
1:A:4057:ILE:HD11	1:A:4152:GLN:HE22	1.57	0.68
1:A:1397:ILE:HD12	1:A:1398:ARG:N	2.09	0.67
1:A:1665:THR:OG1	1:A:1666:PRO:HD2	1.94	0.67
1:A:3762:LEU:C	1:A:3762:LEU:HD12	2.18	0.67
1:A:2719:HIS:ND1	1:A:2720:PRO:HD2	2.09	0.67
1:A:1752:SER:CB	1:A:3755:MET:O	2.43	0.67
1:A:4046:LEU:HD11	1:A:4138:LEU:HD13	1.77	0.67
1:A:4222:LEU:HD23	1:A:4223:GLU:N	2.09	0.67
1:A:1540:CYS:SG	1:A:1599:LEU:HD12	2.35	0.67
1:A:3295:LEU:O	1:A:3298:SER:OG	2.11	0.67
1:A:3837:LYS:HB2	1:A:3984:ILE:HG23	1.75	0.67
1:A:3877:ARG:CZ	1:A:3943:TYR:OH	2.42	0.67
1:A:2131:ARG:HA	1:A:2138:ARG:CZ	2.24	0.67
1:A:1514:LEU:HD12	1:A:1534:PHE:HE1	1.58	0.67
1:A:2390:GLU:O	1:A:2391:ASN:CB	2.43	0.67
1:A:1514:LEU:HD12	1:A:1534:PHE:CE1	2.30	0.66
1:A:2473:MET:HE1	1:A:2502:TRP:CE2	2.12	0.66
1:A:3099:TYR:O	1:A:3103:LEU:N	2.29	0.66
1:A:4154:TRP:NE1	1:A:4172:GLU:OE2	2.28	0.66
1:A:3814:HIS:ND1	1:A:3815:PRO:O	2.21	0.66
1:A:2450:LEU:HD11	1:A:2460:TRP:HB3	1.78	0.66
1:A:2242:VAL:O	1:A:2269:GLN:NE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2284:LYS:HG3	1:A:2401:GLN:CG	2.25	0.66
1:A:2265:THR:HB	1:A:2266:PRO:CD	2.26	0.66
1:A:2518:HIS:N	1:A:2519:PRO:HA	2.10	0.66
1:A:4171:SER:O	1:A:4308:VAL:O	2.13	0.66
1:A:2109:ARG:NH2	2:A:4401:AOV:O3G	2.28	0.66
1:A:2295:CYS:SG	1:A:2430:ILE:HG13	2.35	0.66
1:A:1624:TRP:CD2	1:A:3917:PHE:HB3	2.31	0.66
1:A:3847:TRP:HH2	1:A:3900:TYR:CB	2.09	0.66
1:A:4051:ASN:OD1	1:A:4051:ASN:N	2.29	0.66
1:A:1662:LEU:HD11	1:A:1697:GLU:CB	2.25	0.65
1:A:2135:ALA:H	1:A:2138:ARG:HG3	1.56	0.65
1:A:3374:ASN:ND2	1:A:3377:PRO:HD2	2.10	0.65
1:A:2212:VAL:HA	1:A:2215:TRP:HE3	1.62	0.65
1:A:4030:LYS:HG3	1:A:4034:GLU:CD	2.16	0.65
1:A:4030:LYS:HB2	1:A:4034:GLU:CG	2.25	0.65
1:A:4215:ILE:HB	1:A:4217:ILE:HD11	1.77	0.65
1:A:2816:MET:HB2	1:A:2856:LEU:HD21	1.78	0.65
1:A:2335:CYS:HG	1:A:2347:ARG:C	2.05	0.65
1:A:2292:PRO:O	1:A:2295:CYS:HB2	1.96	0.65
1:A:4307:GLN:HG3	1:A:4307:GLN:O	1.97	0.65
1:A:2131:ARG:CA	1:A:2138:ARG:NH2	2.52	0.65
1:A:1693:THR:CG2	1:A:1817:MET:O	2.44	0.65
1:A:2004:LYS:HE3	1:A:2006:TYR:CZ	2.32	0.65
1:A:4057:ILE:CD1	1:A:4149:LEU:HD22	2.27	0.65
1:A:2354:LEU:HD23	1:A:2355:VAL:N	2.12	0.65
1:A:1696:THR:OG1	1:A:1741:ASP:OD1	2.15	0.64
1:A:2362:ASN:HD21	1:A:2406:MET:HB2	1.62	0.64
1:A:1584:PRO:HB2	1:A:1587:THR:HG21	1.77	0.64
1:A:2651:LEU:HD23	1:A:2653:LEU:HD21	1.78	0.64
1:A:2135:ALA:N	1:A:2138:ARG:CG	2.38	0.64
1:A:2442:TYR:O	1:A:2446:LEU:HB2	1.97	0.64
1:A:2473:MET:CE	1:A:2502:TRP:CD2	2.63	0.64
1:A:2656:ARG:NH1	1:A:2783:ASP:OD1	2.31	0.64
1:A:1938:GLU:N	1:A:1938:GLU:OE2	2.31	0.64
1:A:2653:LEU:HB3	1:A:2661:ARG:CG	2.25	0.63
1:A:3273:GLN:OE1	1:A:3276:VAL:N	2.31	0.63
1:A:4025:ILE:HD12	1:A:4025:ILE:N	2.14	0.63
1:A:1482:GLU:OE1	1:A:1658:ASN:ND2	2.32	0.63
1:A:3871:HIS:NE2	1:A:3875:GLN:OE1	2.32	0.63
1:A:1752:SER:HB3	1:A:3755:MET:O	1.99	0.63
1:A:2261:PRO:O	1:A:2445:TYR:OH	2.08	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ILE:HD12	1:A:1293:LYS:CG	2.28	0.62
1:A:1499:TRP:CZ3	1:A:1503:LEU:HD11	2.34	0.62
1:A:2264:GLN:HA	1:A:2268:MET:HG3	1.80	0.62
1:A:4220:LEU:HB2	1:A:4245:VAL:HG13	1.80	0.62
1:A:2357:TYR:C	1:A:2358:LEU:HD23	2.24	0.62
1:A:3080:LYS:CB	1:A:3087:ALA:HB2	2.30	0.62
1:A:3374:ASN:HB2	1:A:3820:ILE:HD11	1.82	0.62
1:A:1715:CYS:O	1:A:1716:ASP:OD1	2.18	0.62
1:A:3836:LEU:HD23	1:A:3991:ASP:CB	2.30	0.62
1:A:4052:GLN:HA	1:A:4055:ASN:OD1	1.98	0.62
1:A:2660:GLY:HA3	5:A:4406:ADP:PA	2.38	0.62
1:A:2664:ILE:HD12	1:A:2664:ILE:N	2.14	0.62
1:A:2699:GLN:NE2	1:A:2704:GLU:OE1	2.33	0.62
1:A:3511:LYS:CE	1:A:4021:LEU:O	2.48	0.61
1:A:2375:VAL:HA	1:A:2378:LEU:HD12	1.82	0.61
1:A:1472:HIS:ND1	1:A:1490:VAL:O	2.33	0.61
1:A:2239:ALA:O	1:A:2240:THR:HG23	2.00	0.61
1:A:1645:VAL:HG12	1:A:1646:ASP:H	1.66	0.61
1:A:2597:LYS:HB2	1:A:2645:SER:HB3	1.82	0.61
1:A:4057:ILE:HG23	1:A:4152:GLN:OE1	2.01	0.61
1:A:4281:VAL:HG21	1:A:4304:LEU:HD23	1.81	0.61
1:A:3238:PHE:CZ	1:A:3243:PHE:CG	2.86	0.61
1:A:3755:MET:HG3	1:A:3785:VAL:HG21	1.83	0.61
1:A:1509:LYS:NZ	1:A:1512:GLU:OE1	2.34	0.61
1:A:3238:PHE:CZ	1:A:3243:PHE:HB2	2.36	0.61
1:A:3377:PRO:HB2	1:A:3378:PHE:CB	2.29	0.61
1:A:1411:CYS:O	1:A:1414:SER:OG	2.19	0.60
1:A:2517:ASN:CB	1:A:2519:PRO:HB3	2.31	0.60
1:A:4265:GLU:O	1:A:4288:CYS:CB	2.49	0.60
1:A:2265:THR:HB	1:A:2266:PRO:HD2	1.83	0.60
1:A:2517:ASN:HB3	1:A:2519:PRO:HB3	1.82	0.60
1:A:3374:ASN:HD22	1:A:3377:PRO:HD2	1.66	0.60
1:A:3904:ASP:O	1:A:3908:ASP:N	2.34	0.60
1:A:2284:LYS:CG	1:A:2401:GLN:CG	2.79	0.60
1:A:2288:ILE:HD11	1:A:2425:VAL:CG2	2.32	0.60
1:A:3292:LYS:O	1:A:3295:LEU:HB2	2.01	0.60
1:A:2284:LYS:NZ	1:A:2353:ARG:NH2	2.49	0.60
1:A:1795:GLY:HA3	1:A:1798:TYR:HD1	1.66	0.60
1:A:4217:ILE:HD12	1:A:4217:ILE:N	2.17	0.60
1:A:1583:ASP:N	1:A:1584:PRO:CD	2.64	0.60
1:A:2816:MET:CB	1:A:2856:LEU:HD21	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:LEU:HB3	2:A:4401:AOV:C6	2.31	0.59
1:A:3837:LYS:O	1:A:3841:MET:N	2.30	0.59
1:A:2363:LEU:N	1:A:2364:PRO:HD2	2.17	0.59
1:A:2659:VAL:HG22	1:A:2659:VAL:O	2.01	0.59
1:A:3372:THR:HG22	1:A:3374:ASN:H	1.67	0.59
1:A:2548:PHE:HA	1:A:2551:ILE:HD12	1.84	0.59
1:A:3245:CYS:SG	1:A:3249:GLU:HB2	2.43	0.59
1:A:4100:VAL:CA	1:A:4105:THR:HG21	2.30	0.59
1:A:1943:LEU:HA	1:A:1995:ALA:HB2	1.85	0.59
1:A:2011:LYS:NZ	1:A:2367:ASP:OD2	2.33	0.59
1:A:2167:SER:O	1:A:2168:LEU:C	2.43	0.59
1:A:2284:LYS:HD2	1:A:2353:ARG:NH1	2.17	0.59
1:A:4281:VAL:HG21	1:A:4304:LEU:CD2	2.32	0.59
1:A:2135:ALA:CA	1:A:2138:ARG:HB2	2.30	0.59
1:A:2353:ARG:HG2	1:A:2354:LEU:N	2.16	0.59
1:A:2847:VAL:CG1	1:A:2849:PRO:CG	2.80	0.59
1:A:1747:GLU:HB3	1:A:1750:VAL:HG23	1.84	0.59
1:A:3512:ILE:CG2	1:A:4021:LEU:CD2	2.80	0.59
1:A:3844:TYR:HA	1:A:3847:TRP:HB2	1.85	0.58
1:A:3585:GLN:O	1:A:3585:GLN:NE2	2.36	0.58
1:A:4306:ASN:O	1:A:4307:GLN:HB3	2.03	0.58
1:A:2335:CYS:SG	1:A:2347:ARG:O	2.58	0.58
1:A:1554:ALA:CA	1:A:1560:LEU:HD12	2.32	0.58
1:A:3291:LEU:C	1:A:3294:HIS:HE1	2.08	0.58
1:A:3711:LYS:HG2	1:A:3740:LEU:HD13	1.85	0.58
1:A:1973:MET:SD	1:A:2074:ARG:NH1	2.77	0.58
1:A:2162:TYR:HB2	1:A:2199:ASN:O	2.03	0.58
1:A:2185:HIS:CE1	1:A:2189:ILE:HD11	2.39	0.58
1:A:3296:LYS:C	1:A:3298:SER:H	2.10	0.58
1:A:3591:THR:HG21	1:A:3632:ALA:HB1	1.85	0.58
1:A:1584:PRO:CB	1:A:1587:THR:HG22	2.31	0.58
1:A:3781:ASN:H	1:A:3810:THR:HB	1.67	0.58
1:A:1796:LYS:HD3	1:A:1797:GLY:H	1.67	0.58
1:A:2396:GLY:C	1:A:2397:LEU:HD22	2.28	0.58
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.37	0.58
1:A:2676:LEU:O	1:A:2676:LEU:HD23	2.04	0.58
1:A:3877:ARG:NH1	1:A:3943:TYR:OH	2.37	0.58
1:A:1716:ASP:CG	1:A:1745:ARG:HH22	1.97	0.57
1:A:1986:SER:OG	4:A:4403:ATP:O2B	2.16	0.57
1:A:1496:VAL:HA	1:A:1499:TRP:NE1	2.18	0.57
1:A:2625:LEU:HB3	1:A:2627:ILE:HD13	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2858:ILE:O	1:A:2861:SER:OG	2.16	0.57
1:A:2366:LEU:HD11	1:A:2415:HIS:HB3	1.85	0.57
1:A:1437:LEU:CD2	1:A:1441:LEU:HD12	2.34	0.57
1:A:1590:GLY:C	1:A:1591:ILE:HG13	2.29	0.57
1:A:2462:SER:O	1:A:2465:LYS:N	2.37	0.57
1:A:3621:GLU:HG3	1:A:3622:ARG:N	2.19	0.57
1:A:3492:TYR:O	1:A:3495:LEU:HB3	2.05	0.57
1:A:4052:GLN:HA	1:A:4055:ASN:CG	2.29	0.57
1:A:2095:GLU:OE2	4:A:4403:ATP:O3G	2.23	0.57
1:A:3067:LEU:O	1:A:3071:LYS:N	2.38	0.57
1:A:1397:ILE:HD12	1:A:1398:ARG:H	1.69	0.57
1:A:1514:LEU:CD1	1:A:1534:PHE:HE1	2.16	0.57
1:A:2739:TYR:HB3	1:A:2744:LEU:HD21	1.87	0.57
1:A:3525:ARG:NH2	1:A:3721:GLU:OE1	2.38	0.57
1:A:1440:ILE:HD11	1:A:1453:HIS:CG	2.40	0.56
1:A:4220:LEU:HB3	1:A:4302:LEU:HD21	1.84	0.56
1:A:3921:LEU:HD23	1:A:3922:LEU:N	2.19	0.56
1:A:4054:SER:HB3	1:A:4057:ILE:CG1	2.34	0.56
1:A:1534:PHE:HB2	1:A:1539:LEU:HD11	1.86	0.56
1:A:2130:LEU:O	1:A:2138:ARG:NE	2.38	0.56
1:A:2643:VAL:HG11	1:A:2651:LEU:CD1	2.36	0.56
1:A:3245:CYS:SG	1:A:3249:GLU:CB	2.93	0.56
1:A:3499:ALA:HA	1:A:3502:MET:HE3	1.87	0.56
1:A:3640:LEU:HD12	1:A:3642:PHE:CE1	2.40	0.56
1:A:3642:PHE:HA	1:A:3648:TRP:CD1	2.40	0.56
1:A:1908:SER:N	1:A:1964:GLU:OE2	2.39	0.56
1:A:1800:GLY:C	1:A:1801:ARG:HG3	2.29	0.56
1:A:3864:LEU:HD23	1:A:3903:ILE:HD12	1.87	0.56
1:A:4164:LEU:HD13	1:A:4214:GLN:O	2.05	0.56
1:A:4204:TRP:CZ2	1:A:4248:CYS:SG	2.99	0.56
1:A:3249:GLU:N	1:A:3249:GLU:OE1	2.39	0.56
1:A:3577:ARG:O	1:A:3584:PHE:HZ	1.89	0.56
1:A:3580:HIS:O	1:A:3584:PHE:CE2	2.55	0.56
1:A:3591:THR:CG2	1:A:3632:ALA:HB1	2.36	0.56
1:A:1353:GLU:HB3	1:A:1354:PRO:HD3	1.87	0.56
1:A:2565:LEU:HG	1:A:2566:ASP:O	2.06	0.56
1:A:4100:VAL:CB	1:A:4105:THR:HG23	2.35	0.56
1:A:2382:LEU:HD21	1:A:2402:ILE:HD13	1.87	0.55
1:A:2810:GLY:O	1:A:2811:TRP:CD1	2.58	0.55
1:A:1282:GLU:HA	1:A:1287:ARG:O	2.06	0.55
1:A:1813:ARG:HD3	1:A:1814:PRO:HD2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1824:LEU:O	1:A:1828:VAL:HG23	2.06	0.55
1:A:2402:ILE:HD12	1:A:2402:ILE:N	2.21	0.55
1:A:2664:ILE:O	1:A:2668:VAL:HG23	2.05	0.55
1:A:4220:LEU:O	1:A:4221:LEU:HD23	2.06	0.55
1:A:1472:HIS:C	1:A:1473:ILE:HD12	2.31	0.55
1:A:3581:PRO:HB3	1:A:3584:PHE:HE1	1.69	0.55
1:A:1260:ILE:HD12	1:A:1317:TYR:HB2	1.87	0.55
1:A:1667:LEU:HD22	1:A:1819:HIS:O	2.06	0.55
1:A:4137:PRO:O	1:A:4140:TYR:HB3	2.07	0.55
1:A:2536:ARG:HG2	1:A:2545:LEU:HD22	1.88	0.55
1:A:3239:ASP:O	1:A:3242:ARG:HG2	2.06	0.55
1:A:3570:MET:SD	1:A:4017:GLN:HB3	2.47	0.55
1:A:2767:TYR:CE2	1:A:2771:ARG:HD2	2.42	0.55
1:A:3294:HIS:CE1	1:A:3295:LEU:HG	2.42	0.55
1:A:1694:GLY:HA3	2:A:4401:AOV:H8	1.89	0.55
1:A:2592:LEU:HD22	1:A:2645:SER:O	2.05	0.55
1:A:1408:LEU:HA	1:A:1411:CYS:SG	2.46	0.55
1:A:2348:PRO:HB3	1:A:2354:LEU:HB2	1.88	0.55
1:A:2390:GLU:O	1:A:2391:ASN:HB3	2.07	0.55
1:A:3718:LEU:HD13	1:A:3720:ILE:HB	1.89	0.55
1:A:1439:GLU:HB2	1:A:1440:ILE:HD12	1.87	0.55
1:A:1835:PHE:CE2	1:A:1894:GLU:HB3	2.42	0.55
1:A:2659:VAL:HG21	1:A:2811:TRP:NE1	2.20	0.55
1:A:3238:PHE:CE1	1:A:3243:PHE:HB2	2.41	0.55
1:A:1996:LEU:O	1:A:2000:GLY:N	2.36	0.54
1:A:2230:TYR:OH	1:A:2266:PRO:O	2.24	0.54
1:A:3991:ASP:N	1:A:3991:ASP:OD1	2.40	0.54
1:A:4051:ASN:O	1:A:4055:ASN:N	2.40	0.54
1:A:1925:VAL:HG23	1:A:1926:PHE:HD1	1.72	0.54
1:A:1582:GLU:C	1:A:1584:PRO:HD2	2.33	0.54
1:A:1810:GLN:HG3	1:A:3732:ASP:HB2	1.90	0.54
1:A:3658:GLU:OE1	1:A:3658:GLU:N	2.41	0.54
1:A:3922:LEU:C	1:A:3922:LEU:HD13	2.32	0.54
1:A:1711:LEU:HD12	1:A:1731:LEU:HD21	1.89	0.54
1:A:3512:ILE:CG2	1:A:4021:LEU:HD21	2.38	0.54
1:A:2536:ARG:NH1	1:A:2549:ASP:OD2	2.41	0.54
1:A:3587:ASN:OD1	1:A:3590:ASP:CG	2.51	0.54
1:A:4025:ILE:HG22	1:A:4027:ALA:N	2.24	0.54
1:A:1645:VAL:HG12	1:A:1646:ASP:N	2.23	0.53
1:A:2134:PRO:O	1:A:2135:ALA:HB3	2.08	0.53
1:A:3854:LYS:O	1:A:3857:ASN:HB3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:LEU:CD2	1:A:1634:MET:HE1	2.39	0.53
1:A:1663:VAL:CG2	1:A:1829:ILE:HD11	2.38	0.53
1:A:2051:TRP:C	1:A:2052:ILE:HD13	2.34	0.53
1:A:2530:GLU:O	1:A:2531:ALA:C	2.51	0.53
1:A:2579:ARG:C	1:A:2580:HIS:CD2	2.87	0.53
1:A:3750:TYR:HA	1:A:3776:TRP:O	2.08	0.53
1:A:4057:ILE:HD12	1:A:4149:LEU:CD2	2.35	0.53
1:A:2663:THR:OG1	5:A:4406:ADP:H5'1	2.09	0.53
1:A:4051:ASN:O	1:A:4055:ASN:OD1	2.27	0.53
1:A:4308:VAL:O	1:A:4308:VAL:HG12	2.08	0.53
1:A:1879:LEU:HD12	1:A:1897:ILE:HG23	1.90	0.53
1:A:2135:ALA:CA	1:A:2138:ARG:CB	2.56	0.53
1:A:2450:LEU:O	1:A:2453:ASN:O	2.27	0.53
1:A:3740:LEU:HD12	1:A:3740:LEU:O	2.07	0.53
1:A:4030:LYS:HB2	1:A:4034:GLU:CD	2.34	0.53
1:A:4147:ARG:O	1:A:4151:ILE:HG12	2.08	0.53
1:A:4265:GLU:O	1:A:4288:CYS:N	2.35	0.53
1:A:1709:GLN:O	1:A:1709:GLN:HG3	2.09	0.53
1:A:2689:GLN:HG3	1:A:2690:PHE:N	2.24	0.53
1:A:4199:LYS:CD	1:A:4255:GLN:HG2	2.39	0.53
1:A:1376:ARG:O	1:A:1379:MET:HB3	2.08	0.53
1:A:2041:VAL:CG2	1:A:2050:SER:CB	2.87	0.53
1:A:2249:LEU:HB2	1:A:2448:PRO:HG3	1.91	0.53
1:A:2660:GLY:HA2	5:A:4406:ADP:PB	2.49	0.53
1:A:3299:ARG:HH21	1:A:3322:LYS:HD3	1.73	0.53
1:A:3577:ARG:HA	1:A:3584:PHE:HE2	1.72	0.53
1:A:2639:ARG:O	1:A:2642:ARG:HG2	2.09	0.52
1:A:3864:LEU:CD2	1:A:3903:ILE:HG21	2.39	0.52
1:A:1343:ASN:OD1	1:A:1344:HIS:N	2.42	0.52
1:A:1472:HIS:HA	1:A:1490:VAL:O	2.10	0.52
1:A:1624:TRP:CZ2	1:A:3906:LEU:HD13	2.44	0.52
1:A:3212:THR:HG23	1:A:3213:TYR:CD2	2.44	0.52
1:A:3262:ASP:OD1	1:A:3262:ASP:N	2.42	0.52
1:A:1993:ARG:HB2	1:A:2003:VAL:HG11	1.92	0.52
1:A:2004:LYS:HE2	1:A:2006:TYR:OH	2.09	0.52
1:A:2175:GLY:CA	1:A:2196:LEU:HD23	2.39	0.52
1:A:2389:ASP:N	1:A:2393:GLU:O	2.43	0.52
1:A:2848:ASP:N	1:A:2849:PRO:HD2	2.24	0.52
1:A:3296:LYS:HA	1:A:3300:LEU:HD21	1.92	0.52
1:A:4188:ALA:O	1:A:4192:GLY:N	2.42	0.52
1:A:1987:THR:O	1:A:1988:LEU:C	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2208:PHE:O	1:A:2209:THR:C	2.51	0.52
1:A:2650:SER:HB2	1:A:2803:CYS:HB3	1.91	0.52
1:A:3238:PHE:CA	1:A:3242:ARG:HH21	2.23	0.52
1:A:4199:LYS:CE	1:A:4255:GLN:HG2	2.39	0.52
1:A:1691:ALA:HB1	1:A:2105:ALA:HA	1.91	0.52
1:A:1908:SER:HB2	1:A:2113:ILE:HA	1.91	0.52
1:A:3324:LEU:HG	1:A:3325:ILE:N	2.25	0.52
1:A:3675:ILE:HD11	1:A:3693:PHE:HB2	1.92	0.52
1:A:4265:GLU:O	1:A:4288:CYS:HB3	2.09	0.52
1:A:1861:HIS:HB2	1:A:2112:MET:SD	2.50	0.52
1:A:2131:ARG:HA	1:A:2138:ARG:HH22	1.64	0.52
1:A:2254:PHE:O	1:A:2595:HIS:HE1	1.92	0.52
1:A:4046:LEU:CD1	1:A:4138:LEU:HD22	2.40	0.52
1:A:1631:ARG:O	1:A:1642:VAL:HG13	2.10	0.52
1:A:1811:LEU:HD12	1:A:1811:LEU:N	2.25	0.52
1:A:1896:HIS:CD2	1:A:1929:ILE:CG2	2.88	0.52
1:A:2254:PHE:O	1:A:2595:HIS:CE1	2.63	0.52
1:A:2486:VAL:HB	1:A:4106:LEU:HD21	1.91	0.52
1:A:2774:GLN:N	1:A:2774:GLN:OE1	2.42	0.52
1:A:3218:PRO:HD2	1:A:3221:LEU:HD12	1.92	0.52
1:A:3635:SER:O	1:A:3639:THR:HG23	2.09	0.52
1:A:4026:THR:O	1:A:4027:ALA:HB3	2.10	0.52
1:A:4204:TRP:CE2	1:A:4248:CYS:SG	3.03	0.52
1:A:1398:ARG:O	1:A:1402:LEU:HG	2.09	0.52
1:A:1408:LEU:O	1:A:1411:CYS:SG	2.67	0.52
1:A:2577:GLY:HA3	1:A:2602:LEU:HD11	1.92	0.52
1:A:2465:LYS:O	1:A:2468:LEU:HB3	2.10	0.51
1:A:3197:LEU:C	1:A:3197:LEU:HD12	2.35	0.51
1:A:2823:LEU:HD13	1:A:2826:GLU:OE1	2.09	0.51
1:A:3877:ARG:HB2	1:A:3885:TRP:CD1	2.46	0.51
1:A:3965:PHE:HB3	1:A:3966:PRO:CD	2.40	0.51
1:A:1285:GLN:O	1:A:1287:ARG:HG3	2.10	0.51
1:A:2133:GLN:O	1:A:2138:ARG:HD2	2.11	0.51
1:A:3380:PRO:HD2	1:A:3383:ALA:HB3	1.92	0.51
1:A:4100:VAL:CG1	1:A:4105:THR:HG23	2.35	0.51
1:A:1529:VAL:C	1:A:1531:PRO:HD3	2.36	0.51
1:A:2263:ILE:HD11	1:A:2444:ALA:HB3	1.93	0.51
1:A:3640:LEU:CD1	1:A:3648:TRP:CZ2	2.93	0.51
1:A:4052:GLN:HA	1:A:4055:ASN:ND2	2.26	0.51
1:A:1993:ARG:HG3	1:A:1994:ALA:N	2.25	0.51
1:A:3240:LEU:HA	1:A:3243:PHE:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2592:LEU:HD11	1:A:2707:GLN:OE1	2.10	0.51
1:A:3577:ARG:NH2	1:A:3577:ARG:HB3	2.26	0.51
1:A:1628:LYS:HB2	1:A:3917:PHE:CZ	2.46	0.51
1:A:1806:ASP:OD2	1:A:3730:GLY:N	2.43	0.51
1:A:3755:MET:HE2	1:A:3755:MET:CA	2.40	0.51
1:A:2284:LYS:NZ	1:A:2401:GLN:N	2.59	0.51
1:A:2811:TRP:CE2	1:A:2869:PRO:HB3	2.46	0.51
1:A:3325:ILE:HA	1:A:3369:PHE:O	2.11	0.51
1:A:3515:MET:HA	1:A:3822:LEU:HD13	1.93	0.51
1:A:2284:LYS:HZ3	1:A:2400:ILE:C	2.19	0.51
1:A:2847:VAL:HG13	1:A:2849:PRO:CD	2.30	0.50
1:A:3640:LEU:HD12	1:A:3648:TRP:CZ2	2.46	0.50
1:A:1804:LEU:HD12	1:A:1805:PRO:HD2	1.92	0.50
1:A:3586:GLU:O	1:A:3587:ASN:HB3	2.11	0.50
1:A:2187:GLU:HG2	1:A:2191:ASN:OD1	2.11	0.50
1:A:3577:ARG:HB3	1:A:3577:ARG:CZ	2.42	0.50
1:A:1697:GLU:OE2	1:A:2072:ASP:HB3	2.12	0.50
1:A:1973:MET:HG3	1:A:2070:LEU:HD23	1.94	0.50
1:A:1458:PHE:HB3	1:A:1461:ILE:CD1	2.42	0.50
1:A:1695:LYS:NZ	2:A:4401:AOV:O1G	2.44	0.50
1:A:1728:PHE:CZ	1:A:1758:ILE:HD11	2.47	0.50
1:A:1802:GLN:N	1:A:1802:GLN:OE1	2.45	0.50
1:A:2294:GLY:O	1:A:2496:PRO:HG2	2.11	0.50
1:A:3272:LEU:C	1:A:3272:LEU:HD23	2.37	0.50
1:A:3514:ASN:O	1:A:3515:MET:HB2	2.11	0.50
1:A:3685:ARG:O	1:A:3686:LEU:C	2.53	0.50
1:A:3881:ILE:CG2	1:A:3882:PRO:HA	2.41	0.50
1:A:3932:ASP:OD1	1:A:3932:ASP:N	2.45	0.50
1:A:2327:LEU:O	1:A:2328:LEU:C	2.53	0.50
1:A:3910:ALA:O	1:A:3911:LYS:HG3	2.12	0.50
1:A:1337:GLU:O	1:A:1341:ASN:ND2	2.45	0.50
1:A:2004:LYS:CE	1:A:2006:TYR:CZ	2.95	0.50
1:A:3291:LEU:HA	1:A:3294:HIS:ND1	2.27	0.50
1:A:4227:PHE:CD2	1:A:4232:LEU:CD2	2.94	0.50
1:A:1499:TRP:CE3	1:A:1503:LEU:HD11	2.47	0.49
1:A:2078:MET:HG3	1:A:2082:GLU:HB3	1.94	0.49
1:A:2284:LYS:CG	1:A:2401:GLN:OE1	2.33	0.49
1:A:2659:VAL:HG21	1:A:2811:TRP:CD1	2.47	0.49
1:A:4171:SER:HB2	1:A:4305:LYS:CB	2.39	0.49
1:A:1388:VAL:HG13	1:A:1389:THR:N	2.27	0.49
1:A:2318:CYS:HB2	1:A:2360:ASP:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2363:LEU:N	1:A:2363:LEU:HD22	2.27	0.49
1:A:2769:THR:HA	1:A:2772:ILE:HD12	1.94	0.49
1:A:2045:PRO:O	1:A:2048:VAL:HG22	2.13	0.49
1:A:2173:MET:HB3	1:A:2426:ARG:NH1	2.27	0.49
1:A:3580:HIS:C	1:A:3584:PHE:CZ	2.86	0.49
1:A:4038:ASN:O	1:A:4042:PRO:HD3	2.13	0.49
1:A:1825:ILE:O	1:A:1829:ILE:HG12	2.12	0.49
1:A:2362:ASN:HB2	1:A:2363:LEU:HD22	1.94	0.49
1:A:1547:PHE:CE1	1:A:1606:ASN:HB3	2.48	0.49
1:A:1862:TYR:CD2	1:A:1864:TRP:CH2	3.01	0.49
1:A:2473:MET:CE	1:A:2502:TRP:CE3	2.79	0.49
1:A:2512:GLU:OE2	1:A:2579:ARG:HG3	2.12	0.49
1:A:1879:LEU:O	1:A:1882:GLN:N	2.43	0.49
1:A:1896:HIS:O	1:A:1900:GLN:OE1	2.30	0.49
1:A:2284:LYS:CE	1:A:2401:GLN:CA	2.91	0.49
1:A:2683:ARG:NH2	1:A:3305:GLN:O	2.46	0.49
1:A:3674:GLN:O	1:A:3677:VAL:HB	2.13	0.49
1:A:2175:GLY:HA2	1:A:2196:LEU:HD23	1.93	0.49
1:A:2320:ALA:HA	1:A:2364:PRO:HA	1.95	0.49
1:A:3847:TRP:CH2	1:A:3900:TYR:HB2	2.41	0.49
1:A:2223:PHE:CE2	1:A:2224:HIS:HB2	2.47	0.49
1:A:2625:LEU:HD22	1:A:2627:ILE:HD13	1.94	0.49
1:A:3636:LEU:HA	1:A:3639:THR:OG1	2.12	0.49
1:A:4253:ILE:HG22	1:A:4254:PRO:HD2	1.95	0.49
1:A:2819:ILE:HB	1:A:2820:PRO:HD3	1.95	0.49
1:A:3300:LEU:HA	1:A:3323:THR:O	2.13	0.49
1:A:1514:LEU:HD11	1:A:1534:PHE:CE1	2.47	0.48
1:A:1696:THR:HA	1:A:1790:THR:HG21	1.95	0.48
1:A:2274:TYR:HE2	1:A:2428:CYS:HB3	1.76	0.48
1:A:3536:ASP:O	1:A:3543:ARG:NH1	2.46	0.48
1:A:3577:ARG:HA	1:A:3584:PHE:CE2	2.48	0.48
1:A:4171:SER:OG	1:A:4308:VAL:HG12	2.13	0.48
1:A:2000:GLY:O	1:A:2001:LYS:C	2.54	0.48
1:A:2041:VAL:HG21	1:A:2050:SER:CB	2.43	0.48
1:A:2459:ILE:HD12	1:A:2519:PRO:HD2	1.95	0.48
1:A:2749:LEU:N	1:A:2750:PRO:CD	2.76	0.48
1:A:1516:LYS:HD3	1:A:1638:HIS:HB3	1.94	0.48
1:A:1939:LEU:O	1:A:1939:LEU:HD23	2.14	0.48
1:A:2396:GLY:O	1:A:2397:LEU:HD22	2.13	0.48
1:A:4222:LEU:HD22	1:A:4225:CYS:O	2.13	0.48
1:A:1276:PHE:HE1	1:A:1388:VAL:HA	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:ASP:HA	1:A:1289:MET:O	2.13	0.48
1:A:2723:LEU:N	1:A:2723:LEU:HD22	2.29	0.48
1:A:1378:ILE:O	1:A:1382:ILE:HD12	2.13	0.48
1:A:1397:ILE:O	1:A:1398:ARG:C	2.56	0.48
1:A:2529:TYR:O	1:A:2533:ARG:HG2	2.13	0.48
1:A:3291:LEU:O	1:A:3295:LEU:HG	2.14	0.48
1:A:3829:THR:HG22	1:A:3831:GLU:HG3	1.96	0.48
1:A:4043:VAL:HG21	1:A:4118:LEU:CD2	2.44	0.48
1:A:1749:SER:O	1:A:3756:GLY:CA	2.61	0.48
1:A:3374:ASN:HB2	1:A:3820:ILE:CG1	2.44	0.48
1:A:4046:LEU:HD12	1:A:4138:LEU:HD22	1.96	0.48
1:A:1792:ASN:HB3	1:A:1798:TYR:CE2	2.49	0.48
1:A:1795:GLY:HA3	1:A:1798:TYR:CD1	2.48	0.48
1:A:1943:LEU:HA	1:A:1995:ALA:CB	2.44	0.48
1:A:2284:LYS:HD2	1:A:2353:ARG:HH12	1.79	0.48
1:A:2805:VAL:C	1:A:2806:LEU:HD23	2.39	0.48
1:A:3296:LYS:HD2	1:A:3296:LYS:O	2.14	0.48
1:A:3291:LEU:CA	1:A:3294:HIS:ND1	2.75	0.48
1:A:3347:GLN:HG3	1:A:3352:VAL:CG2	2.44	0.48
1:A:3238:PHE:HA	1:A:3242:ARG:HH21	1.79	0.47
1:A:3245:CYS:SG	1:A:3249:GLU:HB3	2.53	0.47
1:A:4188:ALA:HB1	1:A:4193:ARG:O	2.14	0.47
1:A:1472:HIS:HD1	1:A:1490:VAL:C	2.22	0.47
1:A:1716:ASP:OD2	1:A:2065:SER:CA	2.57	0.47
1:A:1879:LEU:HD23	1:A:1879:LEU:N	2.29	0.47
1:A:2168:LEU:O	1:A:2171:THR:OG1	2.26	0.47
1:A:2345:VAL:HG21	1:A:2398:GLU:HB2	1.96	0.47
1:A:2625:LEU:HD22	1:A:2627:ILE:CD1	2.44	0.47
1:A:3219:GLU:N	1:A:3219:GLU:OE1	2.47	0.47
1:A:3238:PHE:N	1:A:3242:ARG:HH21	2.12	0.47
1:A:3256:GLU:OE1	1:A:3290:TRP:NE1	2.47	0.47
1:A:4227:PHE:CD1	1:A:4227:PHE:C	2.92	0.47
1:A:1512:GLU:O	1:A:1516:LYS:NZ	2.47	0.47
1:A:2235:ARG:HB3	1:A:2237:ARG:CG	2.44	0.47
1:A:2459:ILE:O	1:A:2462:SER:OG	2.28	0.47
1:A:2848:ASP:N	1:A:2849:PRO:CD	2.77	0.47
1:A:3629:LEU:HD22	1:A:3680:VAL:HG21	1.95	0.47
1:A:3966:PRO:HB2	1:A:3969:VAL:CG1	2.43	0.47
1:A:4270:PRO:HA	1:A:4283:ASN:HB3	1.97	0.47
1:A:1902:LEU:HD21	1:A:1918:PHE:HZ	1.78	0.47
1:A:2238:LEU:HD22	1:A:2238:LEU:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2114:PHE:C	1:A:2115:LEU:HD12	2.39	0.47
1:A:2230:TYR:N	1:A:2239:ALA:HB1	2.28	0.47
1:A:2632:GLU:OE2	1:A:2812:SER:N	2.48	0.47
1:A:2643:VAL:HG11	1:A:2651:LEU:HD11	1.96	0.47
1:A:2659:VAL:CG2	1:A:2811:TRP:CD1	2.95	0.47
1:A:3640:LEU:CD1	1:A:3642:PHE:CE1	2.96	0.47
1:A:3877:ARG:HH22	1:A:3996:PHE:HA	1.80	0.47
1:A:4072:ILE:HG23	1:A:4073:LEU:N	2.30	0.47
1:A:4077:ILE:O	1:A:4080:GLN:HB3	2.15	0.47
1:A:4288:CYS:SG	1:A:4290:GLY:C	2.97	0.47
1:A:1643:GLN:HG3	1:A:1647:SER:O	2.14	0.47
1:A:1742:GLU:OE2	2:A:4401:AOV:O2G	2.32	0.47
1:A:1855:LEU:C	1:A:1855:LEU:HD12	2.39	0.47
1:A:2495:THR:H	1:A:2498:ILE:HG12	1.80	0.47
1:A:2652:LEU:C	1:A:2652:LEU:HD23	2.40	0.47
1:A:3321:GLY:HA3	1:A:3363:ASN:OD1	2.13	0.47
1:A:4033:ARG:O	1:A:4037:SER:N	2.46	0.47
1:A:1746:LEU:HB3	1:A:1751:LEU:HD21	1.96	0.47
1:A:1792:ASN:OD1	2:A:4401:AOV:O2G	2.32	0.47
1:A:1993:ARG:HB2	1:A:2003:VAL:HG21	1.95	0.47
1:A:1280:ASP:OD1	1:A:1290:LYS:HE3	2.14	0.47
1:A:1815:VAL:HA	1:A:3929:GLY:HA2	1.97	0.47
1:A:2319:SER:N	1:A:2322:THR:OG1	2.42	0.47
1:A:2764:VAL:O	1:A:2767:TYR:HB3	2.14	0.47
1:A:3291:LEU:CD1	1:A:3294:HIS:HE1	2.23	0.47
1:A:1732:VAL:HB	1:A:1781:VAL:HG23	1.96	0.47
1:A:2135:ALA:C	1:A:2138:ARG:H	2.23	0.47
1:A:1440:ILE:HD11	1:A:1453:HIS:CD2	2.49	0.47
1:A:2447:GLU:HB3	1:A:2448:PRO:HD3	1.97	0.47
1:A:2469:LEU:HD22	1:A:2560:TRP:HZ2	1.80	0.47
1:A:2639:ARG:O	1:A:2643:VAL:HG23	2.14	0.47
1:A:2704:GLU:O	1:A:2705:ALA:HB3	2.14	0.47
1:A:3357:ASP:N	1:A:3357:ASP:OD1	2.48	0.47
2:A:4401:AOV:O2B	2:A:4401:AOV:O4G	2.33	0.47
1:A:1508:LYS:O	1:A:1512:GLU:HB2	2.15	0.46
1:A:2004:LYS:CG	1:A:2006:TYR:CZ	2.98	0.46
1:A:2019:LEU:O	1:A:2035:THR:HG21	2.14	0.46
1:A:2076:LEU:HD12	1:A:2077:THR:N	2.31	0.46
1:A:2166:THR:OG1	1:A:2171:THR:HG23	2.15	0.46
1:A:2256:ASN:OD1	1:A:2257:GLY:N	2.48	0.46
1:A:3771:ALA:HA	1:A:3805:PHE:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:SER:HB3	1:A:1496:VAL:HG22	1.96	0.46
1:A:2607:LEU:O	1:A:2610:VAL:N	2.48	0.46
1:A:3337:TYR:N	1:A:3338:PRO:HD2	2.31	0.46
1:A:3560:CYS:HA	1:A:3563:LEU:HG	1.98	0.46
1:A:1534:PHE:CB	1:A:1539:LEU:HD11	2.45	0.46
1:A:1688:TYR:CD1	1:A:1688:TYR:C	2.93	0.46
1:A:2502:TRP:HE1	1:A:2531:ALA:HB2	1.81	0.46
1:A:3864:LEU:HD21	1:A:3903:ILE:HG21	1.97	0.46
1:A:1363:LYS:O	1:A:1366:THR:OG1	2.33	0.46
1:A:2287:PHE:HA	1:A:2426:ARG:O	2.15	0.46
1:A:3347:GLN:HG3	1:A:3352:VAL:HG22	1.96	0.46
1:A:3560:CYS:HB3	1:A:3705:PRO:HG3	1.97	0.46
1:A:2284:LYS:HE3	1:A:2353:ARG:NH2	2.29	0.46
1:A:2664:ILE:N	1:A:2664:ILE:CD1	2.78	0.46
1:A:1518:CYS:HB2	1:A:1534:PHE:CZ	2.51	0.46
1:A:1747:GLU:O	1:A:1750:VAL:HB	2.15	0.46
1:A:3587:ASN:OD1	1:A:3590:ASP:HB2	2.16	0.46
1:A:3780:LYS:HA	1:A:3810:THR:HB	1.96	0.46
1:A:4229:GLY:O	1:A:4230:ASN:HB2	2.16	0.46
1:A:1446:ASN:HB3	1:A:1449:VAL:HB	1.98	0.46
1:A:1624:TRP:HB3	1:A:3917:PHE:CB	2.46	0.46
1:A:1719:ILE:HG22	1:A:1723:SER:HB3	1.96	0.46
1:A:2004:LYS:HG2	1:A:2006:TYR:CE1	2.47	0.46
1:A:2077:THR:HA	1:A:2083:ARG:HG2	1.97	0.46
1:A:2155:TRP:CZ3	1:A:2208:PHE:HB2	2.51	0.46
1:A:2213:PHE:HB3	1:A:2219:SER:HA	1.98	0.46
1:A:3563:LEU:HD11	1:A:3571:PHE:CD2	2.50	0.46
1:A:2041:VAL:HG23	1:A:2050:SER:CB	2.45	0.46
1:A:2360:ASP:HB3	1:A:2363:LEU:HD23	1.97	0.46
1:A:3216:ALA:O	1:A:3391:ASN:ND2	2.48	0.46
1:A:3621:GLU:HG3	1:A:3622:ARG:H	1.81	0.46
1:A:4057:ILE:CG2	1:A:4152:GLN:OE1	2.63	0.46
1:A:2307:GLN:HA	1:A:2307:GLN:OE1	2.16	0.46
1:A:3505:ILE:HG21	1:A:3575:PHE:HA	1.98	0.46
1:A:4177:ASP:O	1:A:4180:LEU:HB2	2.16	0.46
1:A:4199:LYS:HD2	1:A:4255:GLN:HG2	1.96	0.46
1:A:1401:LEU:HA	1:A:1404:ILE:HD12	1.96	0.46
1:A:1499:TRP:HZ3	1:A:1503:LEU:HD11	1.80	0.46
1:A:1982:GLY:HA3	1:A:2169:VAL:HG21	1.98	0.46
1:A:2134:PRO:HB2	1:A:2136:GLU:HG3	1.98	0.46
1:A:2223:PHE:CG	1:A:2224:HIS:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2399:ASN:C	1:A:2400:ILE:HD12	2.41	0.46
1:A:3325:ILE:HG22	1:A:3326:ILE:N	2.30	0.46
1:A:4177:ASP:OD1	1:A:4177:ASP:N	2.49	0.46
1:A:2805:VAL:O	1:A:2806:LEU:HD23	2.17	0.45
1:A:3701:LYS:HE2	1:A:3989:GLU:OE1	2.16	0.45
1:A:1480:GLU:CD	1:A:1480:GLU:H	2.25	0.45
1:A:2130:LEU:HD13	1:A:2142:GLU:HG2	1.97	0.45
1:A:2292:PRO:HG2	1:A:2432:TYR:HE1	1.82	0.45
1:A:2392:LEU:N	1:A:2392:LEU:HD12	2.31	0.45
1:A:3292:LYS:O	1:A:3296:LYS:N	2.49	0.45
1:A:3512:ILE:HG23	1:A:4021:LEU:HD23	1.97	0.45
1:A:3819:PRO:HA	1:A:3822:LEU:HD12	1.98	0.45
1:A:3934:TYR:CD1	1:A:3934:TYR:C	2.93	0.45
1:A:2447:GLU:N	1:A:2448:PRO:CD	2.78	0.45
1:A:2650:SER:O	1:A:2803:CYS:HB2	2.16	0.45
1:A:3299:ARG:NH2	1:A:3320:PHE:O	2.48	0.45
1:A:4090:VAL:HG12	1:A:4094:LEU:HD12	1.97	0.45
1:A:1654:GLU:HB3	1:A:1707:GLY:O	2.17	0.45
1:A:1955:ILE:CG2	1:A:1956:PRO:HD2	2.46	0.45
1:A:2164:VAL:O	1:A:2166:THR:HG23	2.16	0.45
1:A:3261:ASP:OD1	1:A:3262:ASP:N	2.50	0.45
1:A:3721:GLU:HG3	1:A:3826:LEU:HD11	1.98	0.45
1:A:2235:ARG:HB3	1:A:2237:ARG:HG2	1.98	0.45
1:A:2460:TRP:HE1	1:A:2519:PRO:HB2	1.80	0.45
1:A:2593:PRO:HG2	1:A:2597:LYS:HA	1.99	0.45
1:A:2749:LEU:HB3	1:A:2750:PRO:HD3	1.98	0.45
1:A:3279:PHE:HA	1:A:3370:LEU:HD12	1.99	0.45
1:A:4075:PHE:CD1	1:A:4075:PHE:C	2.94	0.45
1:A:4184:ARG:HG3	1:A:4252:TRP:CD2	2.52	0.45
1:A:4227:PHE:HD2	1:A:4232:LEU:CD2	2.28	0.45
1:A:1601:LEU:HD21	1:A:1832:SER:HB3	1.99	0.45
1:A:2296:GLY:C	5:A:4405:ADP:O1A	2.60	0.45
1:A:3577:ARG:O	1:A:3584:PHE:CZ	2.69	0.45
1:A:3710:LEU:CD1	1:A:3736:GLU:CD	2.89	0.45
1:A:4025:ILE:N	1:A:4025:ILE:CD1	2.79	0.45
1:A:4097:LEU:HD13	1:A:4111:VAL:HG12	1.98	0.45
1:A:4288:CYS:HG	1:A:4290:GLY:C	2.24	0.45
1:A:1411:CYS:SG	1:A:1412:GLN:N	2.89	0.45
1:A:1741:ASP:O	1:A:1742:GLU:CB	2.64	0.45
1:A:2495:THR:HB	1:A:2496:PRO:HD2	1.99	0.45
1:A:2870:SER:OG	1:A:3385:SER:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4025:ILE:HG22	1:A:4027:ALA:H	1.81	0.45
1:A:1274:ALA:HB1	1:A:1388:VAL:CG1	2.47	0.45
1:A:1624:TRP:CE3	1:A:3917:PHE:HB3	2.51	0.45
1:A:1663:VAL:N	2:A:4401:AOV:N1	2.64	0.45
1:A:1708:ARG:NH1	1:A:1784:ASN:O	2.49	0.45
1:A:2651:LEU:HD12	1:A:2651:LEU:N	2.32	0.45
1:A:4134:PRO:HG2	1:A:4140:TYR:HA	1.99	0.45
1:A:1381:ASP:O	1:A:1385:ASP:HB3	2.17	0.45
1:A:1906:THR:HG21	1:A:1918:PHE:CZ	2.52	0.45
1:A:2007:THR:HG21	1:A:2384:TYR:CE2	2.52	0.45
1:A:2287:PHE:CD1	1:A:2287:PHE:C	2.95	0.45
1:A:3900:TYR:CD1	1:A:3900:TYR:C	2.95	0.45
1:A:4201:VAL:HG12	1:A:4202:ALA:H	1.81	0.45
1:A:1560:LEU:HD23	1:A:1560:LEU:HA	1.80	0.45
1:A:1787:ILE:O	1:A:1788:PHE:CD1	2.70	0.45
1:A:1820:PRO:O	1:A:1822:ASN:OD1	2.35	0.45
1:A:1907:MET:HA	1:A:1907:MET:HE2	1.99	0.45
1:A:3368:LEU:HD23	1:A:3369:PHE:N	2.32	0.45
1:A:4057:ILE:CD1	1:A:4152:GLN:NE2	2.77	0.45
1:A:1315:SER:O	1:A:1318:TYR:HB3	2.17	0.44
1:A:1372:ASP:OD1	1:A:1376:ARG:NH1	2.49	0.44
1:A:1624:TRP:HD1	1:A:3914:GLN:CD	2.25	0.44
1:A:1749:SER:O	1:A:3756:GLY:HA3	2.17	0.44
1:A:2004:LYS:HG2	1:A:2006:TYR:OH	2.17	0.44
1:A:2041:VAL:HG23	1:A:2050:SER:OG	2.17	0.44
1:A:2134:PRO:C	1:A:2138:ARG:HD2	2.42	0.44
1:A:2303:TYR:CD1	1:A:2303:TYR:C	2.95	0.44
1:A:2382:LEU:CD2	1:A:2402:ILE:HD13	2.47	0.44
1:A:2411:ARG:CB	1:A:2414:ARG:CZ	2.94	0.44
1:A:3200:LEU:N	1:A:3201:PRO:CD	2.80	0.44
1:A:3248:SER:OG	1:A:3249:GLU:OE1	2.27	0.44
1:A:3640:LEU:CG	1:A:3642:PHE:CZ	2.98	0.44
1:A:3708:LEU:O	1:A:3709:ASN:C	2.59	0.44
1:A:3732:ASP:HA	1:A:3733:PRO:HD3	1.81	0.44
1:A:3847:TRP:HH2	1:A:3900:TYR:CG	2.35	0.44
1:A:1547:PHE:O	1:A:1551:VAL:HG23	2.17	0.44
1:A:1550:ASP:O	1:A:1554:ALA:N	2.49	0.44
1:A:2004:LYS:CE	1:A:2006:TYR:OH	2.64	0.44
1:A:2517:ASN:HB3	1:A:2519:PRO:CB	2.47	0.44
1:A:3864:LEU:HD21	1:A:3903:ILE:CG2	2.47	0.44
1:A:4001:ASN:ND2	1:A:4241:SER:HA	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4057:ILE:HG12	1:A:4152:GLN:OE1	2.17	0.44
1:A:4134:PRO:CG	1:A:4140:TYR:HA	2.48	0.44
1:A:1278:LEU:HD12	1:A:1278:LEU:N	2.32	0.44
1:A:1444:SER:CB	1:A:1496:VAL:HG22	2.47	0.44
1:A:1591:ILE:HB	1:A:1592:LEU:HD12	1.98	0.44
1:A:1670:LYS:O	1:A:1671:CYS:C	2.58	0.44
1:A:1671:CYS:O	1:A:1675:LEU:HG	2.16	0.44
1:A:1699:VAL:HG11	1:A:1788:PHE:CD2	2.52	0.44
1:A:1719:ILE:HG13	1:A:2079:PRO:HB3	2.00	0.44
1:A:2213:PHE:HA	1:A:2216:ALA:HB3	1.99	0.44
1:A:2503:VAL:HG13	1:A:2504:LEU:CD1	2.48	0.44
1:A:2711:LEU:O	1:A:2712:LEU:HD23	2.17	0.44
1:A:1862:TYR:CD2	1:A:1864:TRP:HH2	2.36	0.44
1:A:2002:VAL:HG12	1:A:2003:VAL:N	2.30	0.44
1:A:1401:LEU:HB2	1:A:1402:LEU:HD23	2.00	0.44
1:A:1474:THR:O	1:A:1474:THR:HG22	2.16	0.44
1:A:2168:LEU:O	1:A:2171:THR:N	2.50	0.44
1:A:2311:THR:OG1	1:A:2312:GLN:N	2.50	0.44
1:A:2821:GLU:HB2	1:A:2852:LEU:CD1	2.44	0.44
1:A:3193:ILE:HG22	1:A:3197:LEU:HD23	1.99	0.44
1:A:3291:LEU:CA	1:A:3294:HIS:HE1	2.25	0.44
1:A:3577:ARG:HD2	1:A:3589:TRP:CH2	2.53	0.44
1:A:3788:TRP:CD1	1:A:3788:TRP:C	2.95	0.44
1:A:4286:VAL:HG13	1:A:4287:PRO:HD2	2.00	0.44
1:A:4288:CYS:SG	1:A:4290:GLY:CA	3.06	0.44
1:A:1988:LEU:C	1:A:1988:LEU:HD23	2.42	0.44
1:A:2629:LEU:N	1:A:2629:LEU:HD12	2.32	0.44
1:A:2643:VAL:CG1	1:A:2651:LEU:HD11	2.48	0.44
1:A:3755:MET:CG	1:A:3785:VAL:HG21	2.47	0.44
1:A:4040:LEU:HD22	1:A:4118:LEU:HD23	1.99	0.44
1:A:4266:CYS:HB3	1:A:4285:ASP:HB3	1.98	0.44
1:A:1624:TRP:CG	1:A:3917:PHE:HB3	2.52	0.44
1:A:1810:GLN:HG3	1:A:3732:ASP:CB	2.48	0.44
1:A:2730:LEU:HB3	1:A:2802:LYS:HG3	2.00	0.44
1:A:3587:ASN:OD1	1:A:3590:ASP:CB	2.66	0.44
1:A:3654:ASN:O	1:A:3682:ARG:NH1	2.50	0.44
1:A:3965:PHE:CB	1:A:3966:PRO:CD	2.94	0.44
1:A:1276:PHE:CD2	1:A:1292:ILE:HD12	2.53	0.44
1:A:1713:PHE:HB2	1:A:1740:PHE:CD1	2.52	0.44
1:A:2016:TYR:CD1	1:A:2016:TYR:C	2.96	0.44
1:A:2284:LYS:HE3	1:A:2401:GLN:CA	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2717:PHE:CD1	1:A:2723:LEU:HD21	2.53	0.44
1:A:3837:LYS:HB2	1:A:3984:ILE:CG2	2.45	0.44
1:A:3933:ASN:OD1	1:A:3933:ASN:C	2.61	0.44
1:A:4307:GLN:O	1:A:4308:VAL:HG23	2.18	0.44
1:A:1986:SER:HB3	1:A:2095:GLU:CD	2.42	0.43
1:A:2038:ALA:HA	1:A:2041:VAL:HG12	2.00	0.43
1:A:2188:PHE:CD1	1:A:2188:PHE:C	2.96	0.43
1:A:3217:ALA:O	1:A:3222:ARG:NE	2.51	0.43
1:A:3244:LEU:HD22	1:A:3244:LEU:HA	1.85	0.43
1:A:3999:PRO:HG2	1:A:4002:ILE:HG12	2.00	0.43
1:A:4227:PHE:HD2	1:A:4232:LEU:HD21	1.84	0.43
1:A:1506:GLU:OE2	1:A:1510:THR:OG1	2.36	0.43
1:A:2579:ARG:O	1:A:2580:HIS:CD2	2.71	0.43
1:A:1274:ALA:HB1	1:A:1388:VAL:HG11	2.00	0.43
1:A:1500:LEU:HA	1:A:1503:LEU:HG	2.00	0.43
1:A:1699:VAL:CG1	1:A:1788:PHE:CD2	3.01	0.43
1:A:2765:PHE:O	1:A:2768:PHE:HB3	2.18	0.43
1:A:3273:GLN:OE1	1:A:3276:VAL:O	2.36	0.43
1:A:3581:PRO:CA	1:A:3584:PHE:CZ	2.73	0.43
1:A:3802:LYS:O	1:A:3805:PHE:HB3	2.18	0.43
1:A:4202:ALA:HA	1:A:4249:PHE:O	2.19	0.43
1:A:1458:PHE:HB3	1:A:1461:ILE:HD12	1.98	0.43
1:A:1859:GLN:HB2	1:A:1862:TYR:CD2	2.53	0.43
1:A:1973:MET:HG3	1:A:2070:LEU:CD2	2.49	0.43
1:A:2052:ILE:HB	1:A:2092:PHE:CE1	2.53	0.43
1:A:3185:ARG:O	1:A:3189:GLN:NE2	2.51	0.43
1:A:3673:GLN:HA	1:A:3676:LEU:HD12	2.01	0.43
1:A:4030:LYS:O	1:A:4034:GLU:HB2	2.18	0.43
1:A:4100:VAL:HB	1:A:4105:THR:HG23	1.99	0.43
1:A:4124:PRO:HD2	1:A:4127:TRP:CE3	2.53	0.43
1:A:4147:ARG:HG2	1:A:4172:GLU:O	2.19	0.43
1:A:1558:HIS:HB3	1:A:1560:LEU:HG	1.99	0.43
1:A:1603:ILE:O	1:A:1606:ASN:HB2	2.19	0.43
1:A:2004:LYS:HB3	1:A:2050:SER:HA	2.00	0.43
1:A:2284:LYS:CE	1:A:2401:GLN:CB	2.77	0.43
1:A:2601:LYS:C	1:A:2602:LEU:HD12	2.44	0.43
1:A:3654:ASN:O	1:A:3657:CYS:HB3	2.19	0.43
1:A:4201:VAL:HG23	1:A:4253:ILE:CD1	2.48	0.43
1:A:1294:ASP:O	1:A:1297:ASP:HB3	2.19	0.43
1:A:1518:CYS:HB2	1:A:1534:PHE:CE1	2.53	0.43
1:A:2699:GLN:C	1:A:2699:GLN:CD	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3200:LEU:HD23	1:A:3200:LEU:C	2.44	0.43
1:A:3281:ILE:HD12	1:A:3391:ASN:HB3	1.99	0.43
1:A:3300:LEU:HD12	1:A:3300:LEU:C	2.44	0.43
1:A:3374:ASN:ND2	1:A:3377:PRO:CD	2.78	0.43
1:A:3686:LEU:HD22	1:A:3690:MET:SD	2.59	0.43
1:A:4100:VAL:N	1:A:4105:THR:HG21	2.34	0.43
1:A:1281:TYR:O	1:A:1288:THR:HA	2.19	0.43
1:A:2201:ASN:OD1	1:A:2201:ASN:N	2.51	0.43
1:A:3808:TRP:C	1:A:3809:LEU:HG	2.43	0.43
1:A:1475:ALA:HB1	1:A:1484:VAL:O	2.19	0.43
1:A:2590:GLN:HG3	1:A:2591:PRO:HD3	2.01	0.43
1:A:2288:ILE:HD12	1:A:2426:ARG:O	2.19	0.43
1:A:2296:GLY:CA	5:A:4405:ADP:O1A	2.67	0.43
1:A:2312:GLN:HB2	1:A:2351:CYS:SG	2.59	0.43
1:A:2357:TYR:O	1:A:2358:LEU:HD23	2.19	0.43
1:A:2745:GLU:N	1:A:2746:PRO:HD2	2.34	0.43
1:A:3510:SER:HA	1:A:3516:TYR:HB2	2.00	0.43
1:A:4171:SER:O	1:A:4308:VAL:C	2.61	0.43
1:A:1584:PRO:C	1:A:1587:THR:HG22	2.44	0.42
1:A:2667:LEU:O	1:A:2668:VAL:C	2.62	0.42
1:A:3230:THR:HG23	1:A:3235:LEU:O	2.19	0.42
1:A:3493:LEU:N	1:A:3494:PRO:CD	2.82	0.42
1:A:3502:MET:HE1	1:A:3551:LEU:CD1	2.44	0.42
1:A:3577:ARG:HD2	1:A:3589:TRP:CZ3	2.54	0.42
1:A:3822:LEU:O	1:A:3823:GLN:C	2.61	0.42
1:A:4304:LEU:HD12	1:A:4304:LEU:C	2.44	0.42
1:A:2652:LEU:HD22	1:A:2805:VAL:HG13	2.01	0.42
1:A:2851:PHE:CE2	1:A:3201:PRO:HB2	2.54	0.42
1:A:3238:PHE:CZ	1:A:3243:PHE:CB	3.01	0.42
1:A:3336:LEU:CD2	1:A:3336:LEU:N	2.82	0.42
1:A:3512:ILE:HG23	1:A:4021:LEU:HD21	1.95	0.42
1:A:4057:ILE:HD12	1:A:4149:LEU:HD22	1.98	0.42
1:A:1741:ASP:C	1:A:1742:GLU:HG2	2.44	0.42
1:A:1879:LEU:C	1:A:1883:LEU:HD23	2.44	0.42
1:A:1918:PHE:CD1	1:A:1918:PHE:C	2.97	0.42
1:A:2167:SER:O	1:A:2170:GLY:N	2.52	0.42
1:A:2200:LEU:HD12	1:A:2205:ARG:HA	2.01	0.42
1:A:2301:LEU:HD13	1:A:2357:TYR:CE1	2.55	0.42
1:A:2503:VAL:HG13	1:A:2504:LEU:HD13	2.01	0.42
1:A:2606:ASP:O	1:A:2610:VAL:HG23	2.19	0.42
1:A:2664:ILE:HD12	1:A:2664:ILE:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:LYS:HD3	1:A:1461:ILE:C	2.44	0.42
1:A:1515:LEU:HD13	1:A:1538:ILE:HG23	2.01	0.42
1:A:2029:TRP:HE1	1:A:2031:ASP:HA	1.84	0.42
1:A:2163:VAL:HG23	1:A:2164:VAL:HG23	1.99	0.42
1:A:2212:VAL:HA	1:A:2215:TRP:CE3	2.48	0.42
1:A:3403:LEU:O	1:A:3404:LEU:C	2.61	0.42
1:A:4072:ILE:HB	1:A:4186:GLU:HG3	2.00	0.42
1:A:4075:PHE:O	1:A:4078:LEU:HB2	2.20	0.42
1:A:4130:LYS:HD3	1:A:4130:LYS:C	2.45	0.42
1:A:4227:PHE:CD2	1:A:4232:LEU:HD21	2.54	0.42
1:A:1593:GLU:OE1	1:A:1593:GLU:N	2.47	0.42
1:A:3321:GLY:HA2	1:A:3366:PHE:HB2	2.02	0.42
1:A:3374:ASN:HB2	1:A:3820:ILE:CD1	2.47	0.42
1:A:3545:GLN:HA	1:A:3548:ILE:HG22	2.01	0.42
1:A:1684:GLY:O	1:A:1812:PHE:HA	2.19	0.42
1:A:1731:LEU:HD23	1:A:1731:LEU:HA	1.91	0.42
1:A:1862:TYR:HB3	1:A:1864:TRP:CH2	2.54	0.42
1:A:2193:ILE:HG21	1:A:2209:THR:HG22	2.02	0.42
1:A:4147:ARG:NH2	1:A:4308:VAL:C	2.78	0.42
1:A:1514:LEU:HD11	1:A:1534:PHE:CD1	2.54	0.42
1:A:2041:VAL:HG21	1:A:2050:SER:HB2	2.01	0.42
1:A:2276:LYS:N	1:A:2277:PRO:HD2	2.35	0.42
1:A:3239:ASP:OD1	1:A:3239:ASP:N	2.52	0.42
1:A:3277:CYS:SG	1:A:3368:LEU:CD2	3.07	0.42
1:A:4134:PRO:HG2	1:A:4140:TYR:CA	2.50	0.42
1:A:2662:ARG:NH1	1:A:2662:ARG:HG2	2.35	0.42
1:A:3248:SER:O	1:A:3252:ILE:HG13	2.20	0.42
1:A:3299:ARG:HE	1:A:3322:LYS:HD2	1.84	0.42
1:A:3518:PHE:CD1	1:A:3518:PHE:N	2.87	0.42
1:A:3583:LEU:H	1:A:3583:LEU:HG	1.68	0.42
1:A:3788:TRP:O	1:A:3788:TRP:HD1	2.03	0.42
1:A:3860:ARG:HB3	1:A:3907:PHE:CD2	2.55	0.42
1:A:4271:VAL:HA	1:A:4302:LEU:O	2.19	0.42
1:A:1581:SER:C	1:A:1584:PRO:HD2	2.45	0.42
1:A:1866:LEU:HD12	2:A:4401:AOV:O4'	2.20	0.42
1:A:2296:GLY:HA2	5:A:4405:ADP:O1A	2.20	0.42
1:A:2517:ASN:HB2	1:A:2519:PRO:HB3	1.99	0.42
1:A:4281:VAL:CG2	1:A:4304:LEU:HD23	2.48	0.42
1:A:1289:MET:HE2	1:A:1289:MET:HB3	1.82	0.42
1:A:1481:GLY:O	1:A:1591:ILE:HD13	2.20	0.42
1:A:1693:THR:HG21	1:A:1817:MET:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2076:LEU:HD12	1:A:2077:THR:H	1.85	0.42
1:A:3512:ILE:HD12	1:A:3513:ASN:CB	2.46	0.42
1:A:1906:THR:HG22	1:A:1910:PHE:CE1	2.55	0.41
1:A:3847:TRP:CH2	1:A:3900:TYR:CG	3.08	0.41
1:A:3919:HIS:HB2	1:A:3944:LEU:HB3	2.03	0.41
1:A:3965:PHE:HB3	1:A:3966:PRO:HD3	2.02	0.41
1:A:4030:LYS:O	1:A:4034:GLU:N	2.44	0.41
1:A:1624:TRP:HZ2	1:A:3906:LEU:HD13	1.85	0.41
1:A:1962:ALA:O	1:A:1965:LEU:HB3	2.19	0.41
1:A:1986:SER:HB3	1:A:2095:GLU:OE2	2.19	0.41
1:A:2710:LEU:C	1:A:2710:LEU:HD13	2.45	0.41
1:A:3309:ASN:OD1	1:A:3309:ASN:N	2.53	0.41
1:A:3567:ASP:O	1:A:3570:MET:HB2	2.19	0.41
1:A:3836:LEU:O	1:A:3840:LEU:HD13	2.19	0.41
1:A:2153:LEU:HD22	1:A:2157:LEU:HD11	2.03	0.41
1:A:2230:TYR:O	1:A:2239:ALA:HA	2.20	0.41
1:A:2276:LYS:N	1:A:2277:PRO:CD	2.83	0.41
1:A:2460:TRP:CH2	1:A:2523:VAL:HG11	2.55	0.41
1:A:3836:LEU:HD23	1:A:3991:ASP:HB3	2.00	0.41
1:A:3915:TRP:O	1:A:3918:VAL:HB	2.20	0.41
1:A:4086:LEU:O	1:A:4087:VAL:C	2.60	0.41
1:A:1496:VAL:HA	1:A:1499:TRP:HE1	1.84	0.41
1:A:1691:ALA:HA	2:A:4401:AOV:O1G	2.20	0.41
1:A:1982:GLY:HA2	4:A:4403:ATP:C5'	2.50	0.41
1:A:2186:ASP:HB3	1:A:2238:LEU:HD21	2.01	0.41
1:A:3214:LEU:HD12	1:A:3214:LEU:N	2.35	0.41
1:A:1289:MET:CE	1:A:1379:MET:HG2	2.51	0.41
1:A:1514:LEU:HD23	1:A:1538:ILE:CD1	2.50	0.41
1:A:2171:THR:O	1:A:2172:VAL:C	2.64	0.41
1:A:2296:GLY:HA2	5:A:4405:ADP:H5'1	2.03	0.41
1:A:3271:ILE:HD12	1:A:3271:ILE:C	2.45	0.41
1:A:3551:LEU:HD13	1:A:3555:VAL:HG23	2.02	0.41
1:A:3790:PRO:O	1:A:3794:LYS:HB2	2.20	0.41
1:A:1440:ILE:HD11	1:A:1453:HIS:CB	2.51	0.41
1:A:1563:ILE:O	1:A:1566:GLN:HB3	2.20	0.41
1:A:2402:ILE:C	1:A:2403:VAL:HG23	2.46	0.41
1:A:3270:VAL:O	1:A:3273:GLN:HB3	2.19	0.41
1:A:1849:PHE:CE2	1:A:1869:LEU:HB2	2.56	0.41
1:A:3238:PHE:CG	1:A:3238:PHE:O	2.72	0.41
1:A:3249:GLU:HA	1:A:3252:ILE:HD12	2.03	0.41
1:A:3648:TRP:CZ3	1:A:3662:PRO:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1690:PRO:CD	1:A:1818:SER:HA	2.48	0.41
1:A:1908:SER:HA	1:A:1964:GLU:CD	2.45	0.41
1:A:2099:LEU:O	1:A:2100:SER:C	2.63	0.41
1:A:2223:PHE:CD2	1:A:2224:HIS:HB2	2.55	0.41
1:A:2335:CYS:SG	1:A:2348:PRO:HA	2.60	0.41
1:A:2534:LEU:HD12	1:A:2534:LEU:N	2.36	0.41
1:A:4153:ASN:O	1:A:4157:LYS:HG2	2.21	0.41
1:A:4166:GLU:HG2	1:A:4167:THR:N	2.36	0.41
1:A:1352:LEU:O	1:A:1356:PHE:N	2.47	0.41
1:A:1388:VAL:CG1	1:A:1389:THR:N	2.84	0.41
1:A:1486:PHE:CD1	1:A:1506:GLU:OE1	2.74	0.41
1:A:1591:ILE:O	1:A:1592:LEU:HB2	2.21	0.41
1:A:1640:CYS:SG	1:A:1641:CYS:N	2.94	0.41
1:A:1718:GLY:HA2	1:A:1746:LEU:HD12	2.03	0.41
1:A:1729:VAL:O	1:A:1732:VAL:HG22	2.21	0.41
1:A:1925:VAL:HG23	1:A:1926:PHE:CD1	2.53	0.41
1:A:2067:ASN:O	1:A:2071:ASP:HB2	2.20	0.41
1:A:2152:ALA:O	1:A:2156:VAL:HG23	2.21	0.41
1:A:2229:THR:C	1:A:2239:ALA:HB1	2.46	0.41
1:A:2421:PHE:HA	1:A:2424:ILE:HD12	2.02	0.41
1:A:2524:LEU:HD12	1:A:2564:ILE:HG21	2.03	0.41
1:A:2573:TYR:CZ	1:A:2601:LYS:HG3	2.56	0.41
1:A:3244:LEU:C	1:A:3244:LEU:HD13	2.46	0.41
1:A:3505:ILE:HD11	1:A:3578:GLY:HA3	2.03	0.41
1:A:3570:MET:HE2	1:A:3570:MET:HB3	2.00	0.41
1:A:3759:GLN:O	1:A:3762:LEU:HG	2.21	0.41
1:A:4072:ILE:O	1:A:4075:PHE:HB3	2.21	0.41
1:A:4238:ASP:OD1	1:A:4239:SER:N	2.54	0.41
1:A:4291:ASN:OD1	1:A:4294:GLN:HB2	2.21	0.41
1:A:1906:THR:CG2	1:A:1910:PHE:CE1	3.04	0.41
1:A:2230:TYR:OH	1:A:2270:ARG:N	2.53	0.41
1:A:2338:ILE:HD11	1:A:2345:VAL:HG13	2.03	0.41
1:A:2689:GLN:CG	1:A:2690:PHE:N	2.83	0.41
1:A:3552:GLN:O	1:A:3555:VAL:HB	2.21	0.41
1:A:1591:ILE:HG22	1:A:1592:LEU:N	2.36	0.40
1:A:1624:TRP:CD1	1:A:3914:GLN:HB2	2.56	0.40
1:A:1673:LEU:HD12	1:A:1673:LEU:C	2.46	0.40
1:A:1693:THR:HG21	1:A:1817:MET:CB	2.51	0.40
1:A:1710:VAL:HA	1:A:1737:TRP:O	2.20	0.40
1:A:1789:ILE:O	1:A:1789:ILE:HG13	2.21	0.40
1:A:1980:PRO:O	1:A:1983:ALA:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2156:VAL:HG13	1:A:2200:LEU:HD21	2.04	0.40
1:A:2266:PRO:O	1:A:2267:ASP:C	2.62	0.40
1:A:2476:VAL:O	1:A:2477:TYR:C	2.64	0.40
1:A:2523:VAL:O	1:A:2527:VAL:HG23	2.21	0.40
1:A:2739:TYR:CB	1:A:2744:LEU:HD21	2.51	0.40
1:A:2873:MET:HE2	5:A:4406:ADP:N3	2.36	0.40
1:A:3202:LYS:O	1:A:3206:LEU:HG	2.21	0.40
1:A:3230:THR:CG2	1:A:3235:LEU:O	2.70	0.40
1:A:3387:VAL:HG12	1:A:3388:THR:N	2.36	0.40
1:A:3512:ILE:CG2	1:A:4021:LEU:HD23	2.52	0.40
1:A:3640:LEU:CD1	1:A:3642:PHE:CZ	3.04	0.40
1:A:3686:LEU:O	1:A:3689:ALA:HB3	2.21	0.40
1:A:1539:LEU:O	1:A:1543:GLU:HG2	2.21	0.40
1:A:2553:THR:HG22	1:A:2557:GLN:NE2	2.36	0.40
1:A:3670:SER:OG	1:A:3673:GLN:HG3	2.22	0.40
1:A:3675:ILE:HD11	1:A:3693:PHE:CB	2.49	0.40
1:A:3687:GLN:HB3	1:A:4007:GLN:OE1	2.22	0.40
1:A:4220:LEU:C	1:A:4221:LEU:HG	2.46	0.40
1:A:1437:LEU:HD23	1:A:1437:LEU:C	2.46	0.40
1:A:1741:ASP:O	1:A:1742:GLU:HB2	2.21	0.40
1:A:1982:GLY:HA2	4:A:4403:ATP:H5'1	2.04	0.40
1:A:2174:ASN:HA	1:A:2426:ARG:HD2	2.03	0.40
1:A:2766:ASN:O	1:A:2769:THR:HB	2.21	0.40
1:A:1986:SER:HA	1:A:1989:TRP:NE1	2.37	0.40
1:A:2453:ASN:ND2	1:A:2512:GLU:HA	2.36	0.40
1:A:2664:ILE:CD1	1:A:2664:ILE:H	2.34	0.40
1:A:3858:THR:HG23	1:A:3859:HIS:N	2.36	0.40
1:A:4200:PHE:HB2	1:A:4252:TRP:CZ3	2.57	0.40
1:A:1567:LEU:HB3	1:A:1607:ILE:HD11	2.04	0.40
1:A:2175:GLY:HA3	1:A:2196:LEU:CD2	2.51	0.40
1:A:2659:VAL:O	1:A:2659:VAL:HG13	2.21	0.40
1:A:3277:CYS:SG	1:A:3368:LEU:HD23	2.61	0.40
1:A:3486:ASP:O	1:A:3490:ASP:N	2.42	0.40
1:A:3493:LEU:C	1:A:3493:LEU:HD12	2.47	0.40
1:A:3588:GLU:HA	1:A:3633:LEU:HD11	2.03	0.40
1:A:3755:MET:HB2	1:A:3780:LYS:O	2.21	0.40
1:A:3939:VAL:HG22	1:A:4296:ILE:HG22	2.04	0.40
1:A:4073:LEU:O	1:A:4077:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2995/3450 (87%)	2834 (95%)	153 (5%)	8 (0%)	36 65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1820	PRO
1	A	3965	PHE
1	A	1589	SER
1	A	1645	VAL
1	A	3375	PRO
1	A	4027	ALA
1	A	1529	VAL
1	A	3952	VAL

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	2286/3065 (75%)	2169 (95%)	117 (5%)	21 47

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1307	CYS
1	A	1361	LEU
1	A	1378	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1390	THR
1	A	1392	THR
1	A	1397	ILE
1	A	1402	LEU
1	A	1437	LEU
1	A	1465	CYS
1	A	1509	LYS
1	A	1513	GLN
1	A	1536	SER
1	A	1539	LEU
1	A	1570	LYS
1	A	1680	LYS
1	A	1705	LEU
1	A	1787	ILE
1	A	1796	LYS
1	A	1879	LEU
1	A	1944	LYS
1	A	1977	ILE
1	A	1978	VAL
1	A	1997	CYS
1	A	1999	THR
1	A	2008	MET
1	A	2050	SER
1	A	2052	ILE
1	A	2064	GLU
1	A	2116	SER
1	A	2164	VAL
1	A	2178	HIS
1	A	2248	ASP
1	A	2258	LEU
1	A	2260	LEU
1	A	2322	THR
1	A	2345	VAL
1	A	2374	LEU
1	A	2379	GLN
1	A	2401	GLN
1	A	2402	ILE
1	A	2417	LEU
1	A	2435	ARG
1	A	2533	ARG
1	A	2570	ASP
1	A	2574	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2615	LEU
1	A	2625	LEU
1	A	2627	ILE
1	A	2635	GLU
1	A	2659	VAL
1	A	2664	ILE
1	A	2668	VAL
1	A	2687	LEU
1	A	2707	GLN
1	A	2716	GLN
1	A	2774	GLN
1	A	2782	MET
1	A	2804	GLN
1	A	2852	LEU
1	A	2890	LEU
1	A	3189	GLN
1	A	3211	ILE
1	A	3236	GLU
1	A	3244	LEU
1	A	3309	ASN
1	A	3333	GLU
1	A	3336	LEU
1	A	3345	VAL
1	A	3357	ASP
1	A	3391	ASN
1	A	3397	SER
1	A	3493	LEU
1	A	3495	LEU
1	A	3532	GLN
1	A	3582	GLU
1	A	3583	LEU
1	A	3590	ASP
1	A	3640	LEU
1	A	3641	CYS
1	A	3667	LYS
1	A	3671	LEU
1	A	3688	SER
1	A	3690	MET
1	A	3700	LEU
1	A	3706	LEU
1	A	3718	LEU
1	A	3755	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3761	ASP
1	A	3762	LEU
1	A	3792	LEU
1	A	3816	ASN
1	A	3821	LEU
1	A	3828	ILE
1	A	3842	ARG
1	A	3847	TRP
1	A	3877	ARG
1	A	3903	ILE
1	A	3904	ASP
1	A	3921	LEU
1	A	3976	SER
1	A	4023	ARG
1	A	4026	THR
1	A	4030	LYS
1	A	4051	ASN
1	A	4073	LEU
1	A	4100	VAL
1	A	4118	LEU
1	A	4164	LEU
1	A	4180	LEU
1	A	4201	VAL
1	A	4215	ILE
1	A	4228	ASP
1	A	4246	LEU
1	A	4253	ILE
1	A	4268	SER
1	A	4298	CYS
1	A	4302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1686	ASN
1	A	1744	ASN
1	A	1810	GLN
1	A	1893	ASN
1	A	2133	GLN
1	A	2140	ASN
1	A	2178	HIS
1	A	2362	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2518	HIS
1	A	2595	HIS
1	A	2623	GLN
1	A	2696	HIS
1	A	2773	GLN
1	A	2786	ASN
1	A	2894	GLN
1	A	3742	ASN
1	A	3883	GLN
1	A	4214	GLN

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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
5	ADP	A	4405	-	28,29,29	1.44	6 (21%)	43,45,45	2.08	13 (30%)
5	ADP	A	4406	-	28,29,29	1.54	6 (21%)	43,45,45	1.95	13 (30%)
4	ATP	A	4403	3	32,33,33	1.27	5 (15%)	48,52,52	1.98	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AOV	A	4401	3	32,34,34	5.10	7 (21%)	42,56,56	2.27	12 (28%)

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
5	ADP	A	4405	-	-	2/16/32/32	0/3/3/3
5	ADP	A	4406	-	-	0/16/32/32	0/3/3/3
4	ATP	A	4403	3	-	0/22/38/38	0/3/3/3
2	AOV	A	4401	3	-	0/16/39/39	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4401	AOV	O1G-VG	27.68	2.10	1.61
2	A	4401	AOV	C5-C4	4.74	1.47	1.39
5	A	4406	ADP	C5-C4	3.80	1.45	1.39
5	A	4405	ADP	C5-C4	3.78	1.45	1.39
4	A	4403	ATP	C5-C4	3.75	1.45	1.39
5	A	4405	ADP	C5-N7	-3.39	1.32	1.39
5	A	4406	ADP	PB-O1B	3.30	1.60	1.50
5	A	4406	ADP	C5-N7	-2.84	1.33	1.39
2	A	4401	AOV	C5-C6	2.84	1.48	1.41
5	A	4406	ADP	C5-C6	2.76	1.48	1.41
5	A	4405	ADP	C4-N9	-2.71	1.32	1.37
5	A	4406	ADP	C4-N9	-2.66	1.32	1.37
2	A	4401	AOV	C8-N9	-2.59	1.33	1.37
2	A	4401	AOV	C5-N7	-2.53	1.34	1.39
4	A	4403	ATP	C5-N7	-2.52	1.34	1.39
2	A	4401	AOV	PA-O3A	-2.50	1.56	1.59
4	A	4403	ATP	C5-C6	2.49	1.47	1.41
4	A	4403	ATP	C4-N9	-2.42	1.32	1.37
4	A	4403	ATP	C8-N9	-2.37	1.33	1.37
5	A	4405	ADP	C8-N9	-2.35	1.33	1.37
2	A	4401	AOV	C8-N7	2.35	1.36	1.31
5	A	4405	ADP	C5-C6	2.22	1.47	1.41
5	A	4405	ADP	C8-N7	2.20	1.35	1.31
5	A	4406	ADP	C8-N9	-2.13	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4401	AOV	C5-C4-N3	-7.25	116.74	126.72
5	A	4405	ADP	C5-C4-N3	-6.87	117.25	126.72
4	A	4403	ATP	C5-C4-N3	-6.30	118.04	126.72
2	A	4401	AOV	N3-C4-N9	5.68	136.83	127.17
5	A	4406	ADP	C5-C4-N3	-5.41	119.27	126.72
4	A	4403	ATP	N3-C4-N9	5.38	136.31	127.17
5	A	4405	ADP	C4-C5-N7	-4.83	105.06	110.58
2	A	4401	AOV	C4-C5-N7	-4.56	105.36	110.58
5	A	4405	ADP	N3-C4-N9	4.45	134.74	127.17
2	A	4401	AOV	C2-N3-C4	4.28	122.29	111.83
4	A	4403	ATP	C2-N3-C4	4.25	122.20	111.83
5	A	4406	ADP	N3-C4-N9	4.20	134.30	127.17
5	A	4406	ADP	C2-N3-C4	3.99	121.57	111.83
4	A	4403	ATP	C4-N9-C8	3.96	109.90	105.74
5	A	4406	ADP	N3-C2-N1	-3.83	122.78	128.58
4	A	4403	ATP	N3-C2-N1	-3.80	122.83	128.58
2	A	4401	AOV	O2B-PB-O3A	3.77	117.47	107.27
2	A	4401	AOV	N3-C2-N1	-3.50	123.28	128.58
5	A	4405	ADP	C2-N3-C4	3.50	120.37	111.83
2	A	4401	AOV	C5-N7-C8	3.45	108.87	103.45
4	A	4403	ATP	C4-C5-N7	-3.39	106.71	110.58
5	A	4406	ADP	C4-C5-N7	-3.35	106.75	110.58
5	A	4405	ADP	C5-N7-C8	3.32	108.67	103.45
2	A	4401	AOV	C4-N9-C8	2.86	108.74	105.74
5	A	4406	ADP	O3B-PB-O2B	2.86	118.52	107.80
4	A	4403	ATP	N9-C8-N7	-2.77	110.01	113.94
4	A	4403	ATP	C5-N7-C8	2.72	107.73	103.45
5	A	4406	ADP	C4-N9-C8	2.66	108.53	105.74
5	A	4405	ADP	C3'-C2'-C1'	2.61	106.40	101.46
5	A	4406	ADP	O2A-PA-O1A	2.57	124.41	112.44
2	A	4401	AOV	O3A-PA-O1A	-2.53	103.09	110.70
5	A	4405	ADP	N9-C8-N7	-2.51	110.38	113.94
5	A	4406	ADP	C6-C5-N7	2.45	136.81	132.09
2	A	4401	AOV	N9-C8-N7	-2.36	110.59	113.94
5	A	4406	ADP	C5-N7-C8	2.34	107.12	103.45
4	A	4403	ATP	C6-C5-N7	2.31	136.53	132.09
5	A	4405	ADP	O2A-PA-O1A	2.29	123.10	112.44
5	A	4405	ADP	C2'-C1'-N9	-2.28	107.64	113.30
2	A	4401	AOV	C6-C5-N7	2.25	136.42	132.09
5	A	4406	ADP	O4'-C4'-C3'	2.24	109.60	105.15
5	A	4405	ADP	N3-C2-N1	-2.24	125.19	128.58
2	A	4401	AOV	C2'-C1'-N9	-2.21	107.82	113.30
4	A	4403	ATP	O3A-PA-O1A	-2.20	104.09	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4405	ADP	O2B-PB-O3A	2.13	111.76	104.64
4	A	4403	ATP	O4'-C1'-N9	-2.09	104.08	108.09
5	A	4406	ADP	C5'-C4'-C3'	-2.08	107.71	115.21
4	A	4403	ATP	O4'-C4'-C3'	2.02	109.17	105.15
5	A	4405	ADP	C4-N9-C8	2.02	107.86	105.74
5	A	4405	ADP	C5-C4-N9	2.01	108.00	105.81
5	A	4406	ADP	C2'-C1'-N9	-2.01	108.31	113.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4405	ADP	C5'-O5'-PA-O2A
5	A	4405	ADP	C5'-O5'-PA-O3A

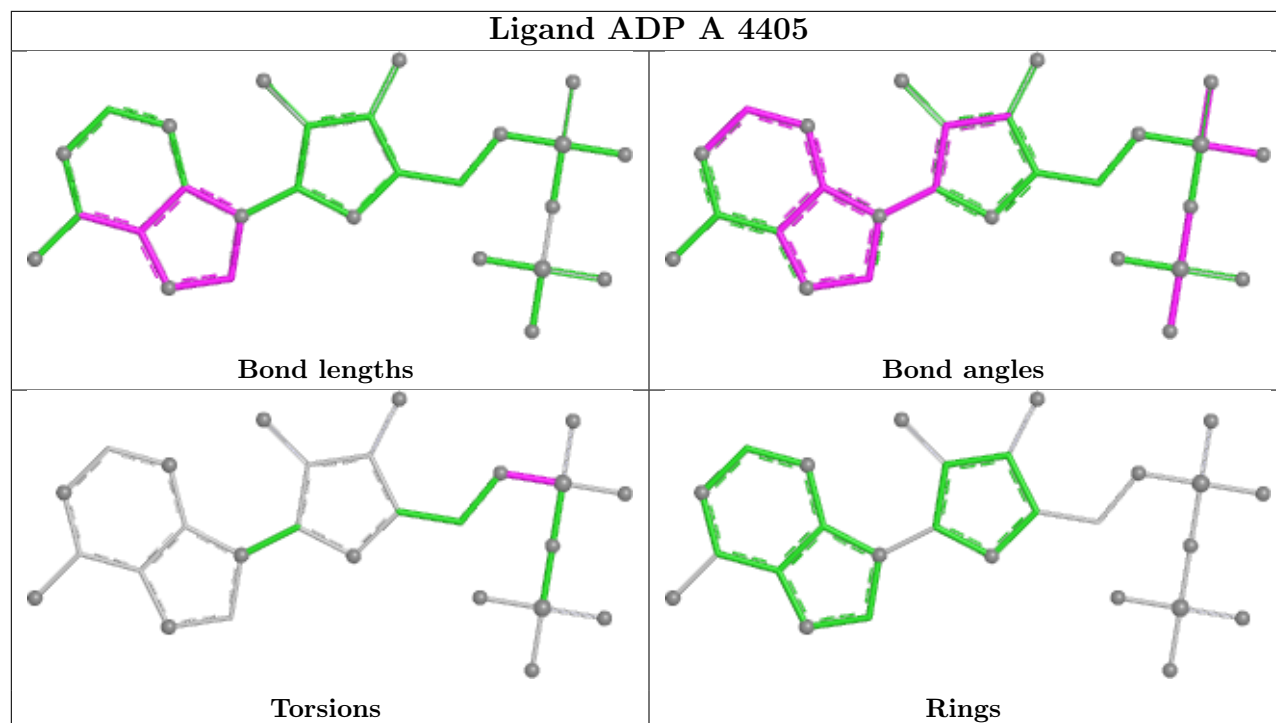
There are no ring outliers.

4 monomers are involved in 26 short contacts:

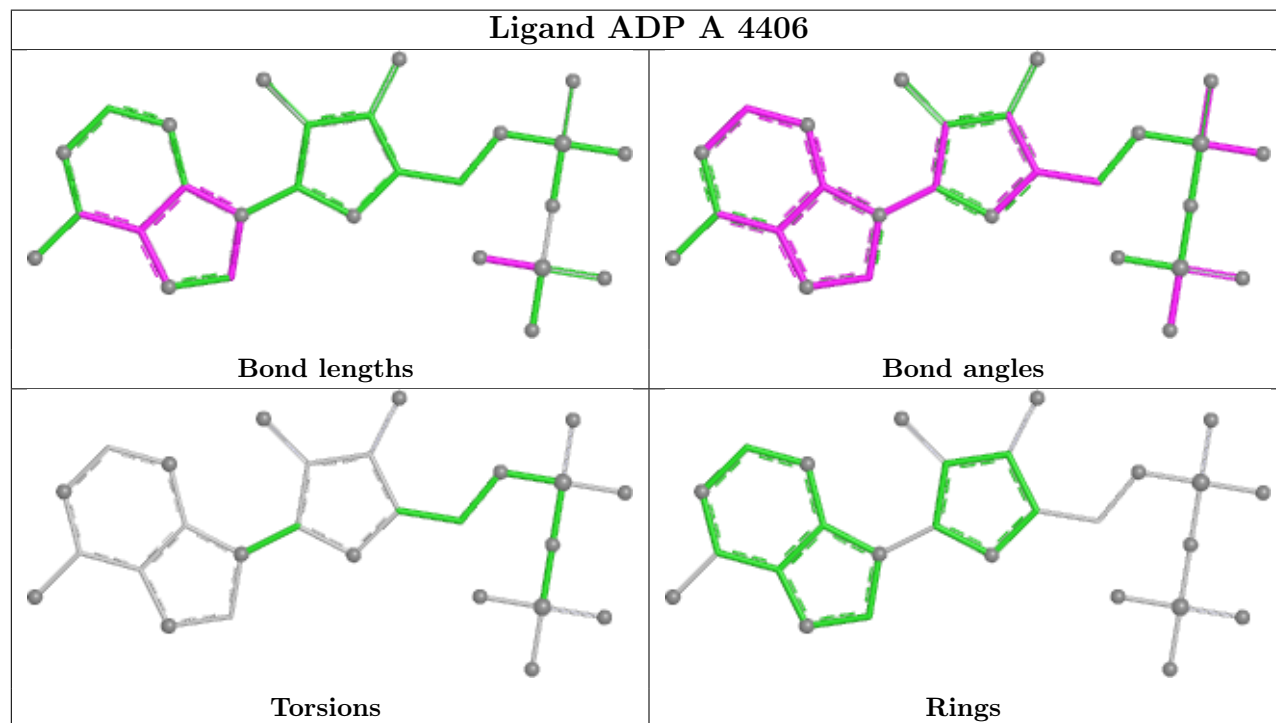
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4405	ADP	4	0
5	A	4406	ADP	6	0
4	A	4403	ATP	4	0
2	A	4401	AOV	12	0

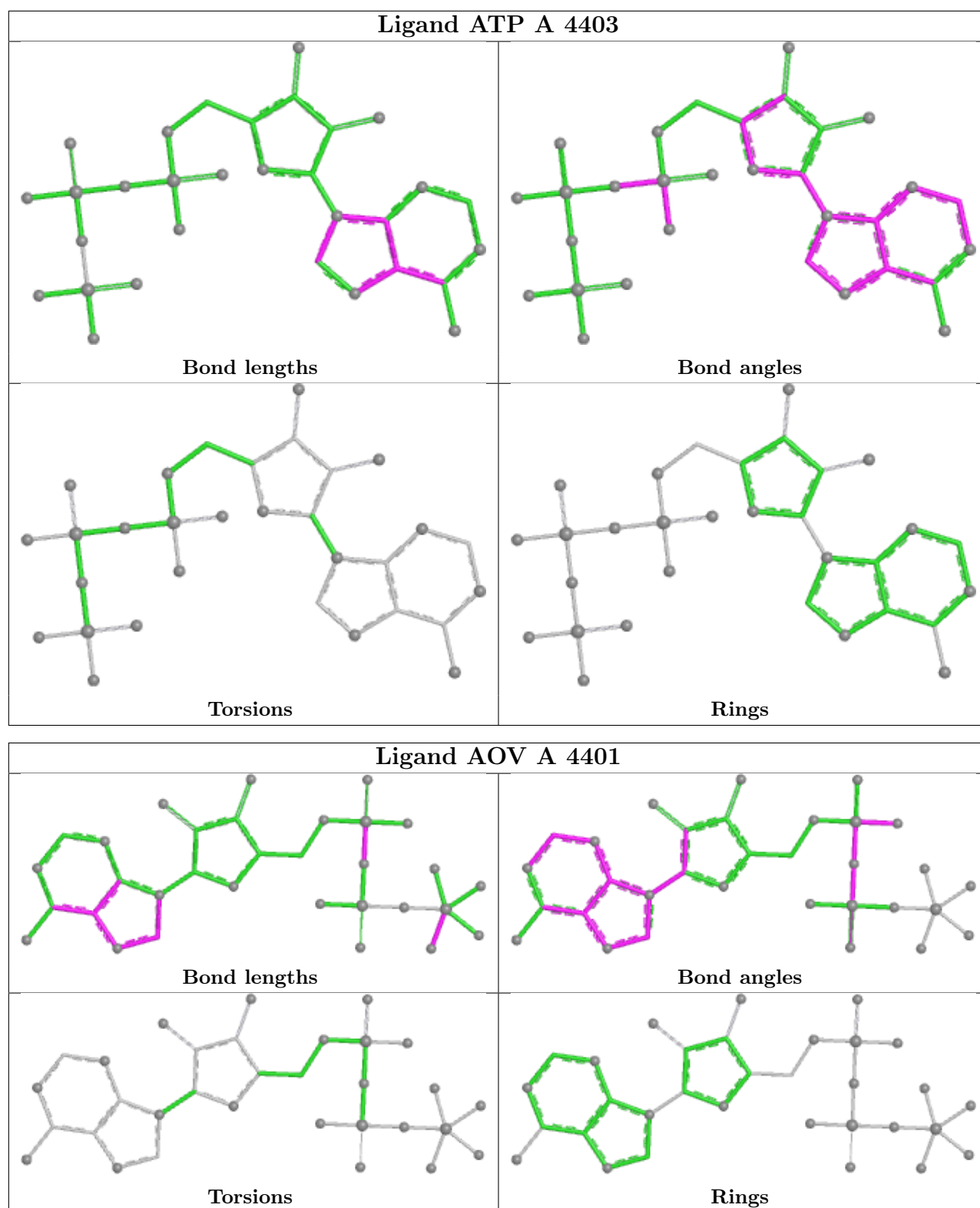
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP A 4405



Ligand ADP A 4406





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	3005/3450 (87%)	0.32	166 (5%)	30 23	39, 110, 274, 477	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1578	ASP	5.9
1	A	3015	ASP	4.6
1	A	4026	THR	4.6
1	A	3964	ILE	4.5
1	A	3018	GLU	4.4
1	A	3642	PHE	4.4
1	A	3073	SER	4.3
1	A	3037	PHE	4.2
1	A	4031	PHE	4.2
1	A	2999	SER	4.0
1	A	3377	PRO	3.9
1	A	2811	TRP	3.9
1	A	1821	ASP	3.8
1	A	3182	GLU	3.8
1	A	3562	CYS	3.7
1	A	2824	PHE	3.6
1	A	3019	GLY	3.6
1	A	4056	LEU	3.5
1	A	3932	ASP	3.5
1	A	1818	SER	3.5
1	A	2137	TYR	3.4
1	A	2217	ARG	3.4
1	A	2336	MET	3.4
1	A	3274	SER	3.4
1	A	1529	VAL	3.4
1	A	3969	VAL	3.4
1	A	2587	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1378	ILE	3.4
1	A	3990	ASP	3.4
1	A	3031	TRP	3.3
1	A	3489	ARG	3.3
1	A	3085	ALA	3.3
1	A	2826	GLU	3.3
1	A	3267	ASN	3.2
1	A	4030	LYS	3.2
1	A	1798	TYR	3.2
1	A	3033	SER	3.2
1	A	2865	TYR	3.2
1	A	2228	ASP	3.1
1	A	3070	ASN	3.1
1	A	3178	GLN	3.1
1	A	3966	PRO	3.1
1	A	1344	HIS	3.1
1	A	3968	SER	3.1
1	A	1362	PRO	3.1
1	A	3075	ASP	3.1
1	A	4025	ILE	3.1
1	A	1532	SER	3.0
1	A	1579	THR	3.0
1	A	4035	ILE	3.0
1	A	3028	ASP	3.0
1	A	3916	GLU	2.9
1	A	3155	ALA	2.9
1	A	2566	ASP	2.9
1	A	1739	CYS	2.9
1	A	3054	ASN	2.9
1	A	3134	LEU	2.9
1	A	3011	ASP	2.8
1	A	3099	TYR	2.8
1	A	3451	ILE	2.8
1	A	3392	PHE	2.8
1	A	1594	LEU	2.8
1	A	3029	THR	2.8
1	A	4125	LEU	2.8
1	A	3952	VAL	2.7
1	A	3614	LEU	2.7
1	A	1717	GLU	2.7
1	A	3965	PHE	2.7
1	A	2907	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	4294	GLN	2.7
1	A	3294	HIS	2.7
1	A	1591	ILE	2.6
1	A	2223	PHE	2.6
1	A	3478	SER	2.6
1	A	3063	VAL	2.6
1	A	3034	MET	2.6
1	A	1612	GLN	2.6
1	A	1741	ASP	2.6
1	A	2982	GLN	2.6
1	A	3647	LEU	2.6
1	A	1892	ALA	2.6
1	A	3275	ARG	2.6
1	A	2588	PRO	2.5
1	A	1296	LYS	2.5
1	A	4055	ASN	2.5
1	A	3488	GLU	2.5
1	A	2237	ARG	2.5
1	A	2436	GLU	2.5
1	A	2218	GLU	2.5
1	A	3030	SER	2.4
1	A	4057	ILE	2.4
1	A	3564	PHE	2.4
1	A	3130	LEU	2.4
1	A	3076	PRO	2.4
1	A	3088	PRO	2.4
1	A	3424	GLN	2.4
1	A	2161	ASP	2.4
1	A	4289	GLY	2.4
1	A	2932	ALA	2.4
1	A	3414	ASP	2.4
1	A	1967	GLU	2.4
1	A	2519	PRO	2.4
1	A	1653	TYR	2.3
1	A	3020	VAL	2.3
1	A	2564	ILE	2.3
1	A	3107	HIS	2.3
1	A	3919	HIS	2.3
1	A	2072	ASP	2.3
1	A	2933	ASP	2.3
1	A	3456	ASP	2.3
1	A	2954	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	4022	GLY	2.3
1	A	3052	ALA	2.3
1	A	3074	PHE	2.3
1	A	4102	ARG	2.3
1	A	3481	LEU	2.3
1	A	2214	HIS	2.3
1	A	3859	HIS	2.3
1	A	4129	SER	2.3
1	A	2274	TYR	2.3
1	A	2893	ARG	2.3
1	A	3154	GLU	2.2
1	A	1360	ALA	2.2
1	A	2899	ALA	2.2
1	A	3025	GLY	2.2
1	A	3206	LEU	2.2
1	A	3920	GLY	2.2
1	A	3056	SER	2.2
1	A	1822	ASN	2.2
1	A	3640	LEU	2.2
1	A	2929	GLN	2.2
1	A	2019	LEU	2.2
1	A	2015	ARG	2.2
1	A	3277	CYS	2.2
1	A	3047	ILE	2.1
1	A	1562	GLN	2.1
1	A	2473	MET	2.1
1	A	3477	GLU	2.1
1	A	2810	GLY	2.1
1	A	3413	PRO	2.1
1	A	3584	PHE	2.1
1	A	2685	TYR	2.1
1	A	1361	LEU	2.1
1	A	3520	LEU	2.1
1	A	3692	LEU	2.1
1	A	4027	ALA	2.1
1	A	3036	SER	2.1
1	A	3950	SER	2.1
1	A	1640	CYS	2.1
1	A	3016	ILE	2.1
1	A	4019	ARG	2.1
1	A	3148	PHE	2.1
1	A	3238	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1934	VAL	2.1
1	A	4278	ASP	2.1
1	A	4224	GLY	2.1
1	A	3012	VAL	2.0
1	A	3239	ASP	2.0
1	A	3757	GLN	2.0
1	A	4061	VAL	2.0
1	A	1624	TRP	2.0
1	A	3092	TRP	2.0
1	A	4229	GLY	2.0
1	A	3002	GLU	2.0
1	A	3023	LEU	2.0
1	A	2939	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

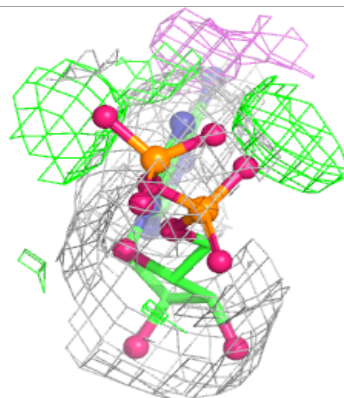
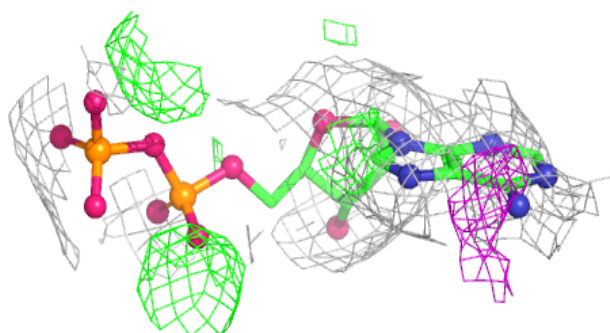
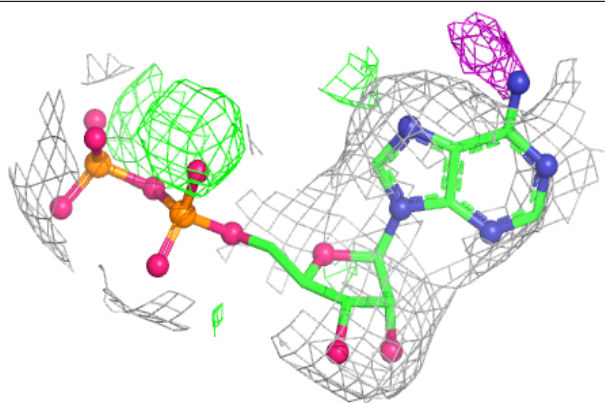
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ADP	A	4406	27/27	0.95	0.10	66,85,103,111	0
4	ATP	A	4403	31/31	0.98	0.06	49,80,97,108	0
5	ADP	A	4405	27/27	0.98	0.05	42,46,57,61	0
2	AOV	A	4401	32/32	0.98	0.07	41,69,88,93	0
3	MG	A	4404	1/1	0.99	0.09	22,22,22,22	0
3	MG	A	4402	1/1	1.00	0.01	31,31,31,31	0

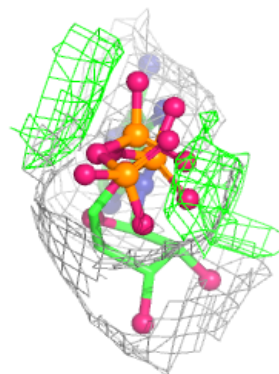
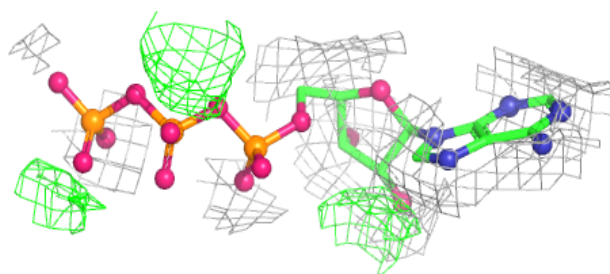
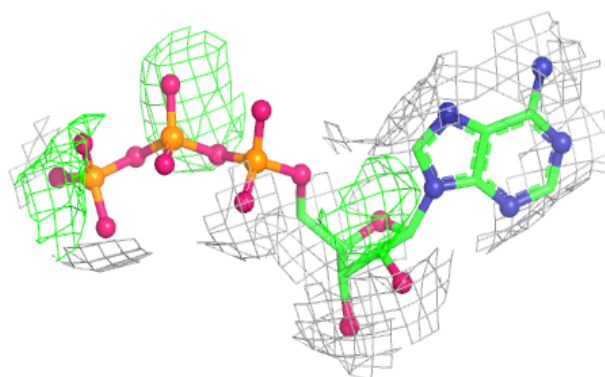
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 4406:

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

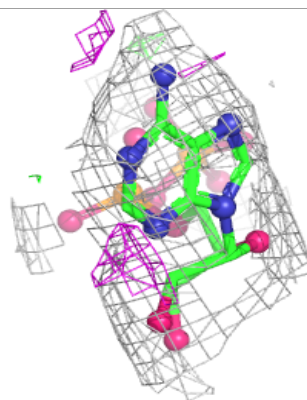
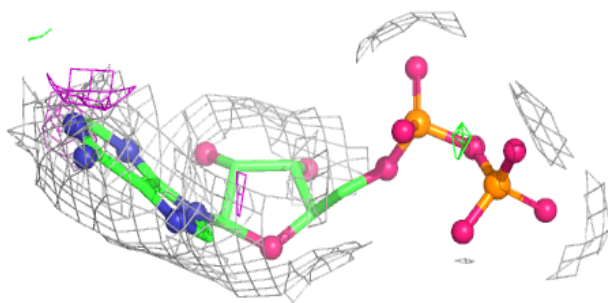
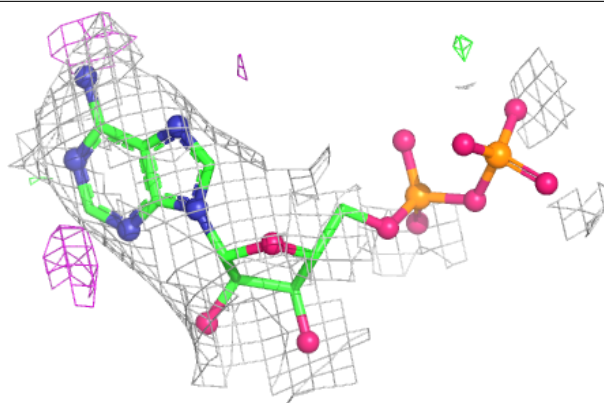
**Electron density around ATP A 4403:**

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

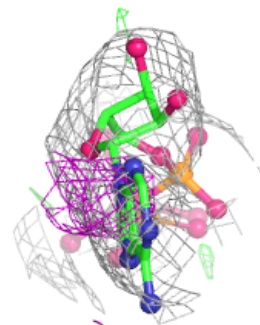
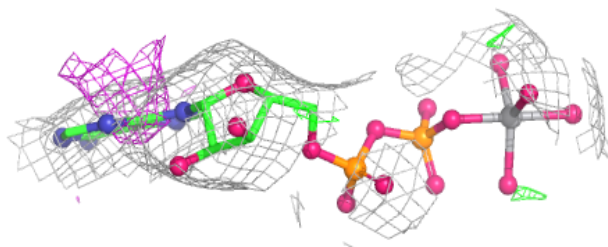
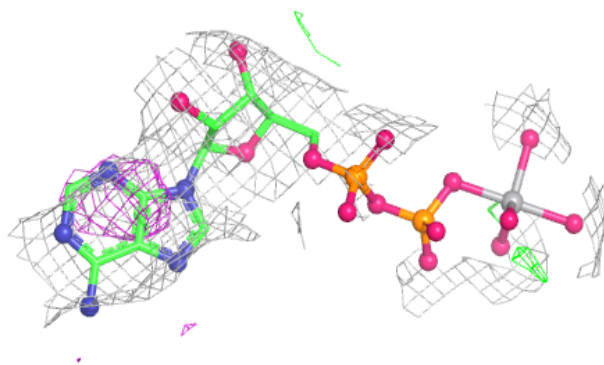


Electron density around ADP A 4405:

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

**Electron density around AOV A 4401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.