



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:34 PM UTC

PDB ID : 3K5H / pdb_00003k5h
Title : Crystal structure of carboxyaminoimidazole ribonucleotide synthase from asperigillus clavatus complexed with ATP
Authors : Thoden, J.B.; Holden, H.M.; Paritala, H.; Firestine, S.M.
Deposited on : 2009-10-07
Resolution : 2.10 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

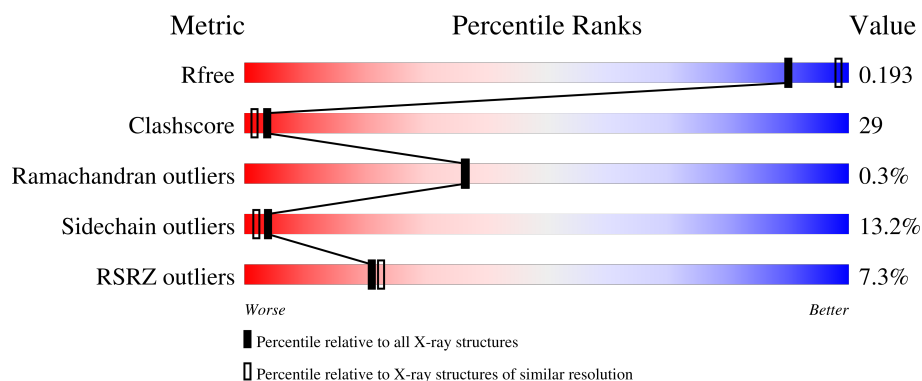
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	403	5% 41% 40% 12% 5%
1	B	403	6% 37% 44% 12% 6%
1	C	403	8% 38% 41% 14% 5%
1	D	403	8% 37% 39% 14% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12850 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 Phosphoribosyl-aminoimidazole carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	4	0
			2977	1869	525	566	17			
1	B	380	Total	C	N	O	S	0	5	0
			2969	1865	519	570	15			
1	C	382	Total	C	N	O	S	0	2	0
			2975	1868	527	564	16			
1	D	380	Total	C	N	O	S	0	1	0
			2948	1854	518	561	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A1CII2
A	-18	GLY	-	expression tag	UNP A1CII2
A	-17	SER	-	expression tag	UNP A1CII2
A	-16	SER	-	expression tag	UNP A1CII2
A	-15	HIS	-	expression tag	UNP A1CII2
A	-14	HIS	-	expression tag	UNP A1CII2
A	-13	HIS	-	expression tag	UNP A1CII2
A	-12	HIS	-	expression tag	UNP A1CII2
A	-11	HIS	-	expression tag	UNP A1CII2
A	-10	HIS	-	expression tag	UNP A1CII2
A	-9	SER	-	expression tag	UNP A1CII2
A	-8	SER	-	expression tag	UNP A1CII2
A	-7	GLU	-	expression tag	UNP A1CII2
A	-6	ASN	-	expression tag	UNP A1CII2
A	-5	LEU	-	expression tag	UNP A1CII2
A	-4	TYR	-	expression tag	UNP A1CII2
A	-3	PHE	-	expression tag	UNP A1CII2
A	-2	GLN	-	expression tag	UNP A1CII2
A	-1	GLY	-	expression tag	UNP A1CII2
A	0	HIS	-	expression tag	UNP A1CII2
B	-19	MET	-	expression tag	UNP A1CII2

Continued on next page...

Continued from previous page...

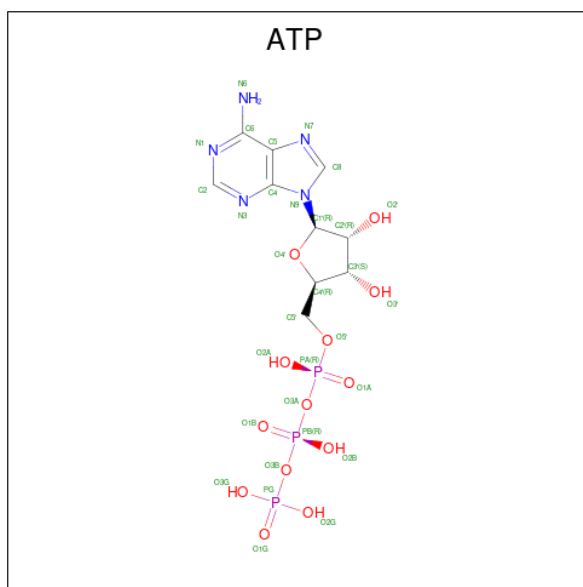
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A1CII2
B	-17	SER	-	expression tag	UNP A1CII2
B	-16	SER	-	expression tag	UNP A1CII2
B	-15	HIS	-	expression tag	UNP A1CII2
B	-14	HIS	-	expression tag	UNP A1CII2
B	-13	HIS	-	expression tag	UNP A1CII2
B	-12	HIS	-	expression tag	UNP A1CII2
B	-11	HIS	-	expression tag	UNP A1CII2
B	-10	HIS	-	expression tag	UNP A1CII2
B	-9	SER	-	expression tag	UNP A1CII2
B	-8	SER	-	expression tag	UNP A1CII2
B	-7	GLU	-	expression tag	UNP A1CII2
B	-6	ASN	-	expression tag	UNP A1CII2
B	-5	LEU	-	expression tag	UNP A1CII2
B	-4	TYR	-	expression tag	UNP A1CII2
B	-3	PHE	-	expression tag	UNP A1CII2
B	-2	GLN	-	expression tag	UNP A1CII2
B	-1	GLY	-	expression tag	UNP A1CII2
B	0	HIS	-	expression tag	UNP A1CII2
C	-19	MET	-	expression tag	UNP A1CII2
C	-18	GLY	-	expression tag	UNP A1CII2
C	-17	SER	-	expression tag	UNP A1CII2
C	-16	SER	-	expression tag	UNP A1CII2
C	-15	HIS	-	expression tag	UNP A1CII2
C	-14	HIS	-	expression tag	UNP A1CII2
C	-13	HIS	-	expression tag	UNP A1CII2
C	-12	HIS	-	expression tag	UNP A1CII2
C	-11	HIS	-	expression tag	UNP A1CII2
C	-10	HIS	-	expression tag	UNP A1CII2
C	-9	SER	-	expression tag	UNP A1CII2
C	-8	SER	-	expression tag	UNP A1CII2
C	-7	GLU	-	expression tag	UNP A1CII2
C	-6	ASN	-	expression tag	UNP A1CII2
C	-5	LEU	-	expression tag	UNP A1CII2
C	-4	TYR	-	expression tag	UNP A1CII2
C	-3	PHE	-	expression tag	UNP A1CII2
C	-2	GLN	-	expression tag	UNP A1CII2
C	-1	GLY	-	expression tag	UNP A1CII2
C	0	HIS	-	expression tag	UNP A1CII2
D	-19	MET	-	expression tag	UNP A1CII2
D	-18	GLY	-	expression tag	UNP A1CII2
D	-17	SER	-	expression tag	UNP A1CII2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A1CII2
D	-15	HIS	-	expression tag	UNP A1CII2
D	-14	HIS	-	expression tag	UNP A1CII2
D	-13	HIS	-	expression tag	UNP A1CII2
D	-12	HIS	-	expression tag	UNP A1CII2
D	-11	HIS	-	expression tag	UNP A1CII2
D	-10	HIS	-	expression tag	UNP A1CII2
D	-9	SER	-	expression tag	UNP A1CII2
D	-8	SER	-	expression tag	UNP A1CII2
D	-7	GLU	-	expression tag	UNP A1CII2
D	-6	ASN	-	expression tag	UNP A1CII2
D	-5	LEU	-	expression tag	UNP A1CII2
D	-4	TYR	-	expression tag	UNP A1CII2
D	-3	PHE	-	expression tag	UNP A1CII2
D	-2	GLN	-	expression tag	UNP A1CII2
D	-1	GLY	-	expression tag	UNP A1CII2
D	0	HIS	-	expression tag	UNP A1CII2

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

Continued on next page...

Continued from previous page...

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

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

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

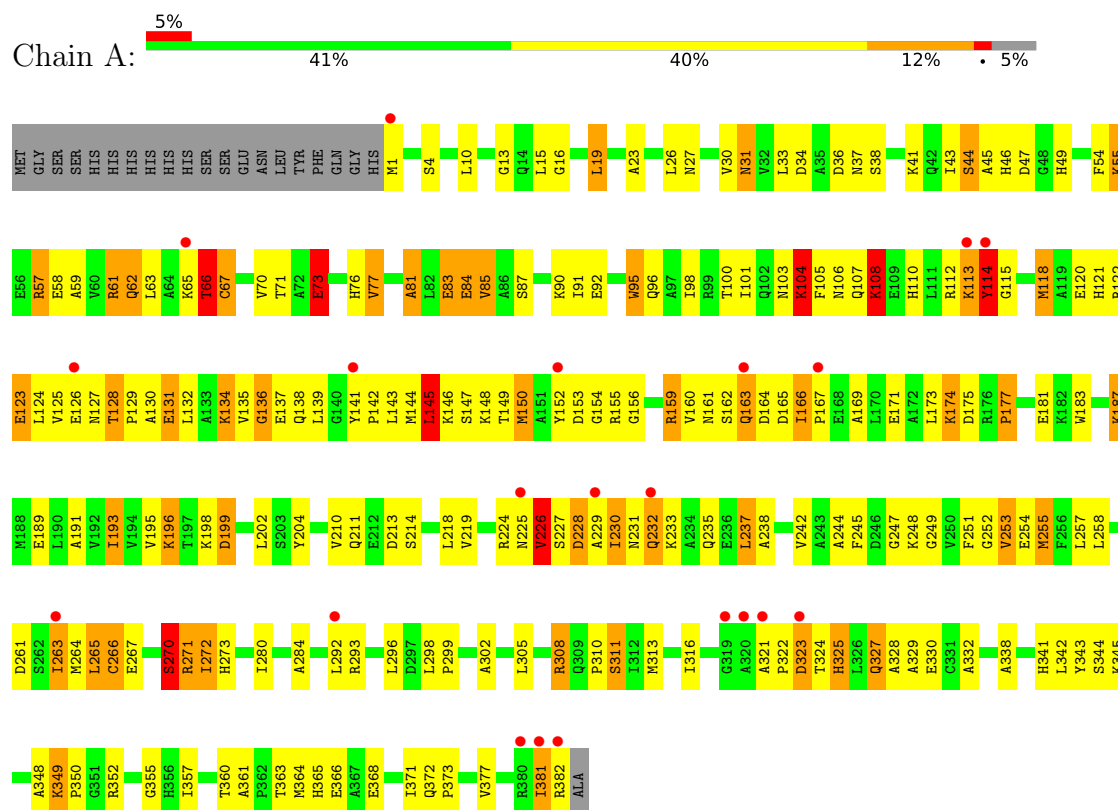
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	247	Total	O	0	0
			247	247		
4	C	179	Total	O	0	0
			179	179		
4	D	196	Total	O	0	0
			196	196		

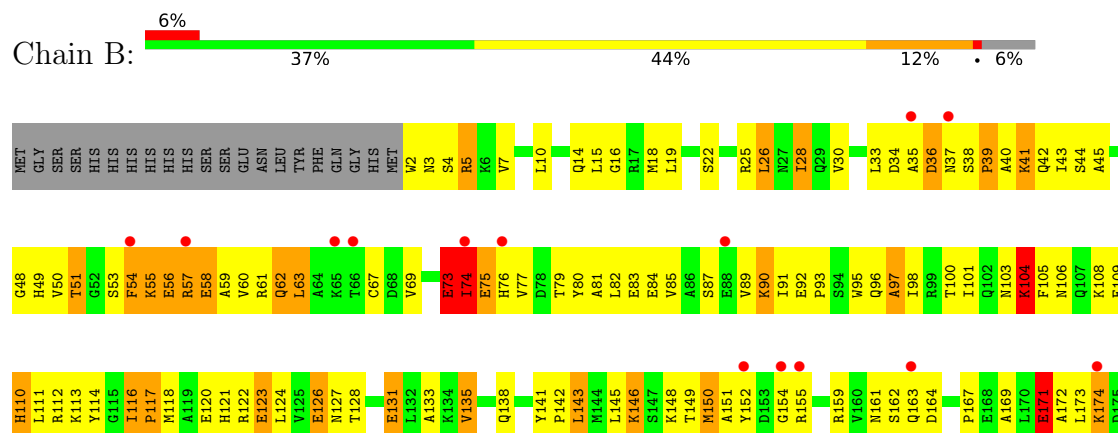
3 Residue-property plots [i](#)

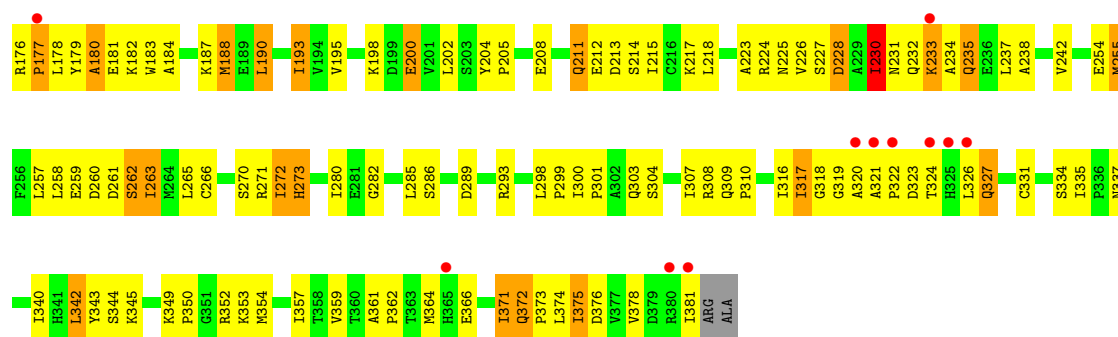
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoribosyl-aminoimidazole carboxylase

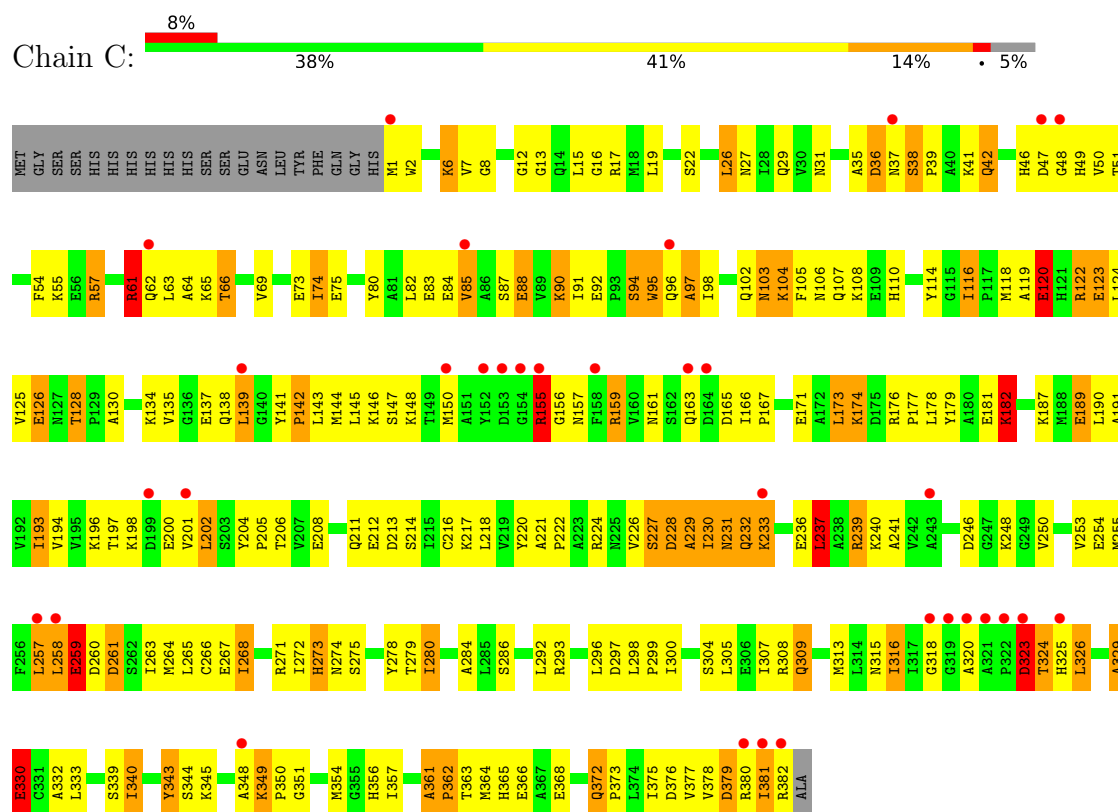


• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

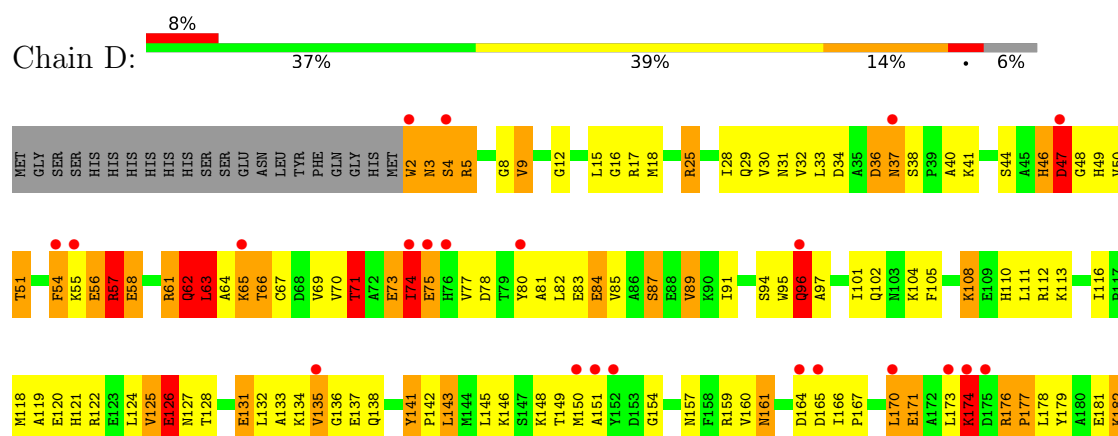


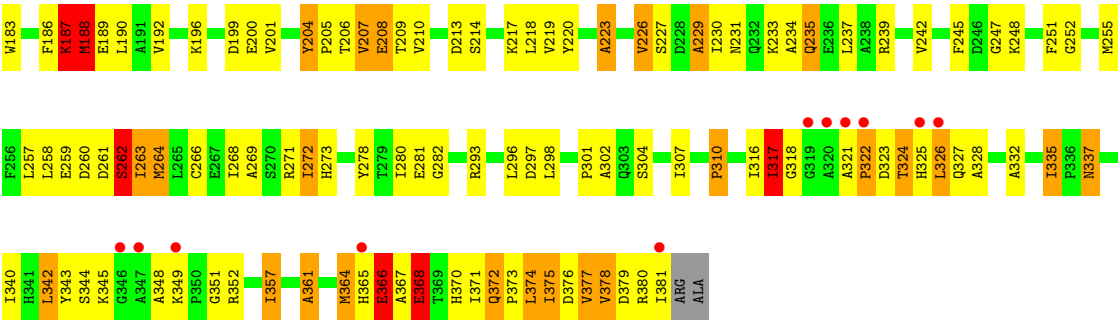


• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase



• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.90Å 134.40Å 99.60Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.10) 93.7 (30.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.63 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.196 , 0.261 0.195 , 0.193	Depositor DCC
R_{free} test set	10356 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 105.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12850	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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: ATP, MG

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	0.97	2/3046 (0.1%)	1.90	84/4124 (2.0%)
1	B	1.02	8/3042 (0.3%)	1.97	103/4120 (2.5%)
1	C	0.96	5/3036 (0.2%)	1.95	95/4110 (2.3%)
1	D	0.97	4/3005 (0.1%)	2.01	116/4071 (2.8%)
All	All	0.98	19/12129 (0.2%)	1.96	398/16425 (2.4%)

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	1
1	C	0	1
1	D	1	0
All	All	1	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	188	MET	SD-CE	-13.38	1.46	1.79
1	B	63	LEU	C-O	-7.98	1.14	1.24
1	B	255	MET	SD-CE	7.41	1.98	1.79
1	D	364	MET	SD-CE	7.30	1.97	1.79
1	A	252	GLY	CA-C	7.03	1.57	1.52
1	D	63	LEU	C-O	-7.03	1.15	1.24
1	C	1	MET	SD-CE	6.96	1.97	1.79
1	D	255	MET	SD-CE	6.90	1.96	1.79
1	A	352	ARG	C-O	-6.61	1.15	1.23
1	B	159	ARG	C-O	-6.61	1.16	1.24
1	C	55	LYS	C-O	-6.43	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	ALA	CA-CB	5.90	1.60	1.53
1	B	67	CYS	C-O	-5.69	1.16	1.23
1	B	110	HIS	C-O	-5.55	1.17	1.24
1	C	329	ALA	CA-CB	-5.54	1.44	1.53
1	C	50	VAL	CA-CB	-5.47	1.47	1.54
1	B	354	MET	SD-CE	5.42	1.93	1.79
1	B	188	MET	SD-CE	-5.27	1.66	1.79
1	C	47	ASP	C-O	-5.08	1.16	1.23

All (398) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	ASP	N-CA-C	-13.47	96.22	113.72
1	C	381	ILE	CB-CA-C	-12.80	95.27	112.04
1	C	349	LYS	N-CA-C	-12.35	91.68	110.32
1	A	127	ASN	N-CA-CB	-11.98	91.30	110.11
1	B	60	VAL	N-CA-C	-11.66	98.72	110.62
1	B	55	LYS	N-CA-C	-11.52	98.74	113.72
1	B	349	LYS	N-CA-C	-10.02	96.07	110.40
1	D	262	SER	N-CA-C	-9.90	95.83	110.48
1	D	371	ILE	N-CA-C	9.87	126.22	112.50
1	A	343	TYR	N-CA-C	9.42	124.58	113.18
1	C	95	TRP	N-CA-C	-9.23	100.60	112.23
1	C	230	ILE	N-CA-C	9.18	119.21	110.30
1	B	101	ILE	N-CA-C	9.11	121.00	110.62
1	C	231[A]	ASN	N-CA-C	-8.97	100.34	111.11
1	C	231[B]	ASN	N-CA-C	-8.97	100.34	111.11
1	D	187	LYS	N-CA-C	-8.97	102.11	113.23
1	C	7	VAL	CA-C-N	-8.92	113.73	122.20
1	C	7	VAL	C-N-CA	-8.92	113.73	122.20
1	A	66	THR	N-CA-CB	-8.92	97.30	110.49
1	A	371	ILE	N-CA-C	8.91	123.38	111.44
1	D	375	ILE	N-CA-C	-8.91	101.66	110.30
1	B	262	SER	N-CA-C	-8.74	99.26	110.53
1	B	375	ILE	N-CA-C	-8.69	102.08	110.42
1	B	51	THR	CB-CA-C	-8.69	95.68	109.84
1	D	281	GLU	N-CA-C	-8.66	102.85	113.50
1	C	323	ASP	CB-CA-C	-8.51	94.03	110.11
1	A	302	ALA	N-CA-C	8.47	121.46	111.71
1	B	54	PHE	N-CA-C	-8.34	103.59	112.93
1	B	230	ILE	N-CA-C	-8.29	102.17	110.62
1	D	317	ILE	N-CA-C	8.27	119.74	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171[A]	GLU	N-CA-C	-8.21	102.41	111.36
1	B	171[B]	GLU	N-CA-C	-8.21	102.41	111.36
1	C	144	MET	CG-SD-CE	-8.21	82.85	100.90
1	D	372	GLN	CA-C-O	8.18	125.85	118.33
1	C	150	MET	N-CA-C	-8.12	103.32	113.23
1	D	317	ILE	CB-CA-C	-8.10	98.77	110.83
1	C	309	GLN	N-CA-C	-8.03	100.99	108.22
1	A	187	LYS	N-CA-C	-8.03	103.50	113.38
1	D	51	THR	CB-CA-C	-8.02	96.83	110.22
1	D	57	ARG	N-CA-C	7.96	124.43	111.37
1	A	349	LYS	N-CA-C	-7.95	96.47	109.82
1	D	73	GLU	N-CA-C	-7.95	103.66	112.72
1	B	89	VAL	N-CA-C	7.91	121.75	108.86
1	B	36	ASP	N-CA-C	-7.88	100.13	110.53
1	D	5	ARG	N-CA-C	7.88	121.06	110.35
1	A	73	GLU	N-CA-C	-7.85	103.51	113.72
1	C	120	GLU	N-CA-C	-7.80	98.93	110.48
1	D	179	TYR	N-CA-C	-7.79	97.16	109.23
1	D	149	THR	N-CA-C	7.78	121.58	110.14
1	D	80	TYR	N-CA-C	-7.75	101.67	112.45
1	A	175	ASP	CB-CA-C	-7.74	101.10	111.63
1	D	161	ASN	N-CA-C	7.72	120.77	111.82
1	A	66	THR	N-CA-C	7.70	122.87	113.17
1	D	229	ALA	CA-C-N	-7.67	110.89	120.56
1	D	229	ALA	C-N-CA	-7.67	110.89	120.56
1	D	204	TYR	CA-C-N	7.67	127.59	119.85
1	D	204	TYR	C-N-CA	7.67	127.59	119.85
1	B	177	PRO	N-CA-C	-7.61	98.31	111.32
1	D	273	HIS	N-CA-CB	-7.58	97.58	111.37
1	A	130	ALA	N-CA-C	-7.58	102.96	111.07
1	B	135	VAL	N-CA-C	-7.56	103.17	110.42
1	B	73	GLU	CA-C-N	7.54	130.56	122.11
1	B	73	GLU	C-N-CA	7.54	130.56	122.11
1	D	164	ASP	N-CA-C	7.52	121.07	112.57
1	C	146	LYS	N-CA-C	7.52	121.66	109.40
1	B	104	LYS	N-CA-C	7.52	120.35	111.71
1	D	62	GLN	N-CA-C	-7.51	102.79	110.97
1	C	193	ILE	N-CA-C	-7.50	97.63	108.36
1	B	273	HIS	N-CA-CB	-7.49	97.60	111.53
1	C	204	TYR	N-CA-C	-7.48	101.34	110.31
1	C	62	GLN	N-CA-C	-7.46	102.75	111.03
1	D	252	GLY	CA-C-N	-7.42	113.23	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	GLY	C-N-CA	-7.42	113.23	123.10
1	C	232	GLN	N-CA-C	7.40	118.99	111.07
1	D	101	ILE	N-CA-C	7.32	118.09	110.62
1	C	241	ALA	N-CA-C	7.32	118.90	111.07
1	D	345	LYS	N-CA-C	-7.31	103.33	112.90
1	C	343	TYR	N-CA-C	7.31	122.22	113.16
1	C	237	LEU	N-CA-C	-7.30	102.35	111.11
1	B	309	GLN	N-CA-C	-7.25	99.83	108.25
1	D	69	VAL	CB-CA-C	-7.17	99.22	110.69
1	B	69	VAL	CB-CA-C	-7.14	99.51	110.50
1	D	96	GLN	CA-C-N	7.13	129.71	120.44
1	D	96	GLN	C-N-CA	7.13	129.71	120.44
1	A	355	GLY	O-C-N	-7.12	117.08	123.92
1	D	141	TYR	O-C-N	7.11	127.60	121.20
1	A	280	ILE	N-CA-C	-7.09	103.87	110.53
1	C	361	ALA	CA-C-N	7.08	126.70	119.19
1	C	361	ALA	C-N-CA	7.08	126.70	119.19
1	B	179	TYR	N-CA-C	-7.07	98.56	109.24
1	A	105	PHE	N-CA-C	-7.06	103.52	111.14
1	C	340	ILE	N-CA-C	7.05	119.02	108.23
1	B	345	LYS	N-CA-C	-7.04	104.50	113.23
1	A	228	ASP	CA-C-N	7.04	129.59	120.44
1	A	228	ASP	C-N-CA	7.04	129.59	120.44
1	D	266	CYS	N-CA-C	-7.02	102.06	111.96
1	A	90	LYS	N-CA-C	-6.99	100.14	110.48
1	A	323	ASP	CB-CA-C	-6.99	98.55	109.80
1	D	89	VAL	N-CA-C	6.89	119.46	108.85
1	A	166	ILE	N-CA-C	6.89	123.75	108.88
1	A	123	GLU	N-CA-C	-6.84	100.86	110.50
1	D	251	PHE	CA-C-N	-6.82	115.72	122.20
1	D	251	PHE	C-N-CA	-6.82	115.72	122.20
1	C	229	ALA	N-CA-C	-6.80	102.95	111.11
1	C	123	GLU	N-CA-C	-6.74	100.55	110.52
1	B	42	GLN	N-CA-C	6.74	120.95	112.87
1	C	372	GLN	N-CA-C	6.73	122.65	113.77
1	D	18	MET	N-CA-C	-6.71	104.03	111.82
1	B	48	GLY	N-CA-C	6.71	122.05	114.67
1	C	104	LYS	N-CA-C	6.70	119.42	111.71
1	C	66	THR	N-CA-C	6.70	121.05	113.01
1	D	199	ASP	CA-C-N	-6.69	110.36	121.80
1	D	199	ASP	C-N-CA	-6.69	110.36	121.80
1	A	230	ILE	N-CA-C	6.68	117.44	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	VAL	CB-CA-C	-6.67	101.30	110.77
1	C	80	TYR	N-CA-C	-6.64	103.22	112.45
1	D	71	THR	N-CA-C	6.62	119.46	109.41
1	A	87	SER	N-CA-C	-6.60	105.23	113.28
1	D	136	GLY	N-CA-C	-6.60	104.78	112.83
1	C	130	ALA	N-CA-C	-6.60	104.17	111.36
1	B	146	LYS	N-CA-C	6.59	120.14	109.40
1	A	248	LYS	N-CA-C	-6.57	100.48	110.14
1	C	94	SER	CB-CA-C	-6.56	97.37	110.42
1	C	64	ALA	N-CA-C	6.55	118.42	111.28
1	A	381	ILE	CB-CA-C	-6.51	102.47	111.65
1	B	81	ALA	N-CA-C	-6.43	104.27	111.28
1	D	143	LEU	CB-CG-CD1	-6.43	91.42	110.70
1	B	340	ILE	N-CA-C	6.42	117.55	108.36
1	C	198	LYS	CA-C-N	-6.42	112.16	122.24
1	C	198	LYS	C-N-CA	-6.42	112.16	122.24
1	B	120	GLU	N-CA-CB	-6.42	100.61	110.04
1	D	322	PRO	N-CA-C	6.41	125.66	112.47
1	B	319	GLY	N-CA-C	-6.40	98.01	113.18
1	A	135	VAL	N-CA-C	-6.40	104.52	110.53
1	B	143	LEU	N-CA-CB	-6.40	100.42	111.55
1	A	85	VAL	N-CA-C	6.39	121.82	113.07
1	D	141	TYR	C-N-CD	6.37	134.61	120.60
1	C	173	LEU	N-CA-C	-6.34	102.04	111.81
1	C	365	HIS	CA-C-N	-6.33	111.30	120.29
1	C	365	HIS	C-N-CA	-6.33	111.30	120.29
1	D	282	GLY	N-CA-C	6.33	123.35	113.86
1	C	228	ASP	N-CA-C	-6.32	104.62	112.90
1	C	324	THR	N-CA-C	6.31	124.23	110.80
1	C	85	VAL	N-CA-C	6.30	122.44	109.34
1	C	110	HIS	N-CA-C	-6.28	103.97	111.69
1	A	104	LYS	N-CA-C	6.27	118.92	111.71
1	C	182	LYS	N-CA-C	-6.25	102.24	110.43
1	C	54	PHE	N-CA-C	-6.25	105.62	113.18
1	D	46	HIS	CA-C-N	-6.25	112.69	123.25
1	D	46	HIS	C-N-CA	-6.25	112.69	123.25
1	A	59	ALA	N-CA-C	-6.25	104.39	111.14
1	C	354	MET	N-CA-C	6.23	120.08	112.23
1	D	377	VAL	CB-CA-C	-6.22	104.01	111.97
1	A	273	HIS	N-CA-CB	-6.21	99.97	111.53
1	B	96	GLN	N-CA-C	-6.21	104.43	111.14
1	B	90	LYS	N-CA-CB	6.19	119.14	110.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	TYR	N-CA-C	-6.17	102.91	110.31
1	D	302	ALA	N-CA-C	6.15	117.99	111.28
1	C	42	GLN	N-CA-C	6.15	120.25	112.87
1	B	190	LEU	N-CA-CB	-6.12	101.29	111.20
1	B	117	PRO	CB-CA-C	-6.11	101.47	111.56
1	A	31	ASN	N-CA-C	-6.11	98.56	108.52
1	B	126	GLU	N-CA-C	6.11	119.93	112.23
1	B	280	ILE	N-CA-C	-6.11	104.79	110.53
1	D	235	GLN	CA-C-O	6.10	127.23	120.82
1	C	36	ASP	CA-C-N	-6.09	113.49	123.05
1	C	36	ASP	C-N-CA	-6.09	113.49	123.05
1	A	95	TRP	CA-C-N	-6.07	112.15	120.28
1	A	95	TRP	C-N-CA	-6.07	112.15	120.28
1	D	174	LYS	CB-CA-C	-6.07	99.28	109.65
1	B	122	ARG	CB-CA-C	-6.06	100.80	110.14
1	B	343	TYR	N-CA-C	6.04	120.50	113.20
1	D	135	VAL	CA-C-N	6.03	126.79	120.03
1	D	135	VAL	C-N-CA	6.03	126.79	120.03
1	A	120	GLU	N-CA-C	-6.03	101.55	110.48
1	B	36	ASP	CA-C-N	-6.03	114.41	125.02
1	B	36	ASP	C-N-CA	-6.03	114.41	125.02
1	C	12	GLY	CA-C-N	6.02	128.23	122.27
1	C	12	GLY	C-N-CA	6.02	128.23	122.27
1	A	330	GLU	N-CA-C	6.02	118.62	111.33
1	B	212	GLU	N-CA-C	-6.02	98.59	108.76
1	C	122	ARG	N-CA-C	-6.01	98.83	109.06
1	B	317	ILE	CB-CA-C	-6.01	101.87	110.83
1	D	280	ILE	CA-CB-CG1	6.00	120.61	110.40
1	A	270	SER	CB-CA-C	-5.99	103.80	111.22
1	B	164	ASP	N-CA-C	5.98	119.84	112.54
1	D	25	ARG	N-CA-C	-5.98	104.84	111.36
1	B	151	ALA	N-CA-C	5.97	119.12	110.28
1	B	298	LEU	N-CA-C	-5.96	101.45	110.50
1	C	372	GLN	CA-C-O	5.95	124.03	118.44
1	B	97	ALA	N-CA-C	-5.93	104.72	111.07
1	B	180	ALA	CA-C-N	-5.93	113.50	122.81
1	B	180	ALA	C-N-CA	-5.93	113.50	122.81
1	B	372	GLN	CA-C-O	5.92	123.78	118.33
1	B	54	PHE	N-CA-CB	-5.92	102.40	110.56
1	D	186	PHE	O-C-N	5.91	129.68	123.06
1	C	61[A]	ARG	N-CA-C	5.91	118.67	111.82
1	C	61[B]	ARG	N-CA-C	5.91	118.67	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	VAL	CB-CA-C	-5.89	102.36	110.96
1	D	143	LEU	CB-CA-C	-5.88	98.24	109.66
1	C	13	GLY	CA-C-O	-5.88	116.40	122.28
1	C	261	ASP	N-CA-C	5.88	122.65	113.72
1	D	340	ILE	N-CA-C	5.88	117.05	108.58
1	B	5	ARG	CA-C-N	-5.88	114.89	123.00
1	B	5	ARG	C-N-CA	-5.88	114.89	123.00
1	A	98	ILE	N-CA-C	-5.87	104.64	110.62
1	C	19	LEU	N-CA-C	-5.87	104.97	111.36
1	A	328	ALA	N-CA-C	-5.84	104.83	111.14
1	C	116	ILE	N-CA-C	5.84	114.31	107.77
1	B	195	VAL	CA-C-N	-5.83	115.02	122.77
1	B	195	VAL	C-N-CA	-5.83	115.02	122.77
1	A	325	HIS	N-CA-C	-5.82	104.30	111.75
1	D	366	GLU	N-CA-C	-5.81	104.85	111.07
1	A	67[A]	CYS	N-CA-C	5.81	117.05	108.86
1	A	67[B]	CYS	N-CA-C	5.81	117.05	108.86
1	A	38	SER	CA-C-N	5.80	127.09	119.84
1	A	38	SER	C-N-CA	5.80	127.09	119.84
1	D	29	GLN	N-CA-C	5.79	118.97	109.76
1	D	245	PHE	N-CA-C	5.78	118.98	109.85
1	C	189	GLU	N-CA-C	-5.77	100.30	109.59
1	C	128	THR	N-CA-C	-5.75	101.30	110.10
1	B	289	ASP	N-CA-C	-5.75	104.94	111.14
1	D	234	ALA	N-CA-C	-5.74	105.10	111.36
1	B	271	ARG	CA-CB-CG	-5.74	102.62	114.10
1	B	123	GLU	N-CA-C	-5.72	102.44	110.50
1	D	32	VAL	CB-CA-C	-5.72	103.07	110.84
1	C	103	ASN	N-CA-C	-5.71	98.43	108.20
1	D	239	ARG	N-CA-C	5.71	117.50	111.28
1	D	223	ALA	CA-C-N	-5.70	113.28	121.42
1	D	223	ALA	C-N-CA	-5.70	113.28	121.42
1	C	155	ARG	N-CA-C	-5.69	105.44	112.90
1	C	315	ASN	N-CA-C	-5.69	102.06	110.48
1	B	235	GLN	CA-C-O	5.69	126.80	120.82
1	D	131	GLU	N-CA-C	-5.69	105.00	111.14
1	D	310	PRO	N-CA-C	-5.69	102.16	111.15
1	A	377	VAL	N-CA-C	5.68	115.88	110.42
1	A	229	ALA	N-CA-C	-5.67	105.01	111.07
1	D	263	ILE	CB-CA-C	-5.65	102.27	110.63
1	A	134	LYS	N-CA-C	-5.65	105.27	111.82
1	C	19	LEU	CB-CA-C	-5.64	101.27	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	GLY	O-C-N	-5.63	119.28	123.61
1	B	74	ILE	CB-CA-C	-5.62	103.48	111.40
1	B	40	ALA	N-CA-C	5.61	118.33	111.82
1	A	145	LEU	N-CA-C	-5.60	100.85	109.76
1	B	22	SER	N-CA-C	5.60	117.38	111.28
1	D	200	GLU	N-CA-CB	-5.60	102.84	111.46
1	C	316	ILE	CB-CA-C	-5.59	103.42	111.19
1	D	273	HIS	N-CA-C	5.59	118.33	109.50
1	C	165	ASP	CB-CA-C	-5.58	99.96	110.01
1	B	217	LYS	N-CA-C	-5.58	105.51	112.93
1	D	126	GLU	N-CA-C	5.57	120.20	112.45
1	D	36	ASP	N-CA-C	-5.57	103.18	110.53
1	D	342	LEU	N-CA-C	-5.56	100.65	109.76
1	A	128	THR	CA-C-N	5.55	125.91	119.47
1	A	128	THR	C-N-CA	5.55	125.91	119.47
1	D	208	GLU	N-CA-CB	-5.55	101.37	110.42
1	D	368	GLU	CA-C-O	5.55	126.35	119.97
1	D	30	VAL	N-CA-C	5.55	115.88	108.11
1	A	164	ASP	N-CA-C	-5.53	105.64	112.38
1	B	228	ASP	N-CA-C	-5.53	104.68	111.75
1	C	103	ASN	CB-CA-C	-5.52	101.94	110.78
1	D	67	CYS	CA-CB-SG	-5.52	101.71	114.40
1	D	368	GLU	CA-C-N	-5.52	112.93	120.44
1	D	368	GLU	C-N-CA	-5.52	112.93	120.44
1	A	210	VAL	O-C-N	5.51	128.70	123.03
1	C	97	ALA	CA-C-N	-5.51	112.77	120.53
1	C	97	ALA	C-N-CA	-5.51	112.77	120.53
1	B	371	ILE	N-CA-C	5.50	120.61	113.07
1	C	125	VAL	CB-CA-C	-5.50	104.68	110.62
1	C	239	ARG	N-CA-C	5.50	116.95	111.07
1	C	8	GLY	CA-C-N	-5.49	115.95	123.14
1	C	8	GLY	C-N-CA	-5.49	115.95	123.14
1	A	83	GLU	N-CA-C	-5.48	105.33	112.23
1	A	108	LYS	CA-C-N	-5.48	112.39	120.28
1	A	108	LYS	C-N-CA	-5.48	112.39	120.28
1	C	200	GLU	CB-CA-C	-5.46	100.19	111.22
1	C	362	PRO	N-CA-C	-5.46	106.42	113.57
1	B	106	ASN	CA-C-N	-5.46	113.34	120.44
1	B	106	ASN	C-N-CA	-5.46	113.34	120.44
1	D	74	ILE	CB-CA-C	-5.45	103.71	111.40
1	C	116	ILE	CB-CA-C	-5.45	104.51	110.78
1	C	37	ASN	N-CA-C	5.45	119.51	112.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	CYS	N-CA-C	-5.44	104.30	111.96
1	D	2	TRP	N-CA-CB	5.43	119.74	110.50
1	B	58	GLU	N-CA-C	5.42	119.15	112.54
1	B	300	ILE	CA-C-N	-5.42	113.97	119.83
1	B	300	ILE	C-N-CA	-5.42	113.97	119.83
1	D	108	LYS	CA-C-O	5.42	126.28	120.70
1	D	271	ARG	N-CA-C	5.42	115.52	107.88
1	B	232	GLN	CA-C-O	5.41	126.28	120.55
1	B	335	ILE	CA-C-N	-5.41	114.21	119.78
1	B	335	ILE	C-N-CA	-5.41	114.21	119.78
1	A	4	SER	CA-CB-OG	-5.41	100.29	111.10
1	D	352	ARG	CB-CA-C	-5.40	100.42	109.65
1	D	337	ASN	N-CA-CB	-5.40	104.23	112.28
1	D	91	ILE	N-CA-CB	-5.39	104.63	111.64
1	A	196	LYS	CB-CA-C	-5.39	101.45	110.19
1	D	151	ALA	N-CA-C	5.39	117.50	109.25
1	B	266	CYS	N-CA-C	-5.39	103.32	111.56
1	B	286	SER	N-CA-C	-5.39	103.58	110.53
1	B	218	LEU	N-CA-C	5.38	117.86	109.52
1	B	41	LYS	N-CA-C	-5.38	105.97	112.54
1	D	281	GLU	CA-C-N	-5.38	113.56	120.34
1	D	281	GLU	C-N-CA	-5.38	113.56	120.34
1	C	320	ALA	N-CA-C	5.37	116.82	111.07
1	C	102	GLN	N-CA-C	5.37	119.09	112.54
1	A	327	GLN	CA-C-N	-5.37	113.14	120.44
1	A	327	GLN	C-N-CA	-5.37	113.14	120.44
1	A	19	LEU	N-CA-C	-5.37	105.34	111.14
1	B	131	GLU	N-CA-C	-5.36	105.34	111.07
1	A	255	MET	CA-CB-CG	-5.35	103.39	114.10
1	A	129	PRO	N-CA-C	-5.35	106.05	113.81
1	B	345	LYS	CA-C-O	5.34	125.52	119.27
1	C	38	SER	CA-CB-OG	-5.34	100.41	111.10
1	B	73	GLU	CA-CB-CG	5.34	124.79	114.10
1	C	200	GLU	N-CA-C	5.34	117.38	109.69
1	C	325	HIS	N-CA-C	-5.34	105.87	112.38
1	D	47	ASP	N-CA-C	-5.32	103.69	111.30
1	C	271	ARG	CB-CA-C	-5.31	101.27	111.78
1	C	88	GLU	CB-CA-C	-5.31	100.64	109.55
1	B	263	ILE	N-CA-C	5.30	115.76	108.12
1	D	269	ALA	N-CA-C	-5.30	99.77	108.41
1	D	164	ASP	N-CA-CB	5.29	119.27	110.91
1	A	226	VAL	N-CA-C	-5.29	99.94	107.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ILE	CB-CA-C	-5.28	103.75	110.98
1	B	56	GLU	N-CA-C	5.27	117.22	108.20
1	B	273	HIS	N-CA-C	5.27	117.39	109.23
1	A	177	PRO	N-CA-C	-5.26	101.97	110.55
1	D	201	VAL	CB-CA-C	5.26	116.99	110.73
1	D	44	SER	N-CA-CB	-5.26	102.75	111.96
1	B	257	LEU	CB-CG-CD1	5.26	126.48	110.70
1	B	225	ASN	CB-CA-C	-5.26	104.13	111.80
1	D	36	ASP	CA-C-N	-5.26	115.77	125.02
1	D	36	ASP	C-N-CA	-5.26	115.77	125.02
1	A	249	GLY	CA-C-N	-5.25	114.09	122.50
1	A	249	GLY	C-N-CA	-5.25	114.09	122.50
1	A	219	VAL	CA-C-O	-5.25	114.80	120.36
1	A	249	GLY	CA-C-O	5.25	126.46	122.16
1	B	259[A]	GLU	CA-C-N	-5.25	113.94	122.65
1	B	259[A]	GLU	C-N-CA	-5.25	113.94	122.65
1	B	259[B]	GLU	CA-C-N	-5.25	113.94	122.65
1	B	259[B]	GLU	C-N-CA	-5.25	113.94	122.65
1	A	71	THR	N-CA-C	-5.24	101.47	108.86
1	C	66	THR	N-CA-CB	-5.24	101.22	110.39
1	C	273	HIS	N-CA-CB	-5.24	101.83	111.37
1	C	323	ASP	CA-C-O	5.24	126.39	120.00
1	A	136	GLY	N-CA-C	-5.23	106.45	112.83
1	D	217	LYS	N-CA-C	-5.22	105.98	112.93
1	A	81	ALA	N-CA-C	-5.21	105.69	111.36
1	B	299	PRO	CB-CA-C	-5.21	104.56	111.23
1	D	368	GLU	N-CA-C	-5.21	105.78	111.82
1	A	308	ARG	N-CA-C	5.20	117.03	111.36
1	C	330	GLU	CB-CA-C	5.19	119.41	110.79
1	A	77	VAL	CB-CA-C	-5.18	103.44	110.90
1	D	204	TYR	N-CA-C	-5.18	101.49	109.41
1	D	328	ALA	N-CA-C	-5.17	105.72	111.36
1	D	374	LEU	N-CA-C	-5.15	105.74	111.36
1	A	181	GLU	CB-CA-C	-5.13	99.97	109.37
1	D	170	LEU	CB-CA-C	5.13	119.31	110.79
1	A	338	ALA	CA-C-N	5.13	129.51	122.84
1	A	338	ALA	C-N-CA	5.13	129.51	122.84
1	C	36	ASP	N-CA-C	-5.12	102.70	110.28
1	A	131	GLU	N-CA-C	5.12	116.66	111.14
1	D	119	ALA	N-CA-C	5.11	117.64	110.23
1	B	193	ILE	CB-CA-C	-5.10	104.79	110.96
1	C	280	ILE	N-CA-C	-5.10	105.73	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	ILE	CA-C-N	5.10	128.76	120.60
1	D	101	ILE	C-N-CA	5.10	128.76	120.60
1	A	263	ILE	CB-CA-C	-5.10	103.02	110.62
1	B	18	MET	CA-CB-CG	-5.10	103.90	114.10
1	C	298	LEU	N-CA-C	-5.10	102.63	110.58
1	B	375	ILE	CA-C-N	-5.09	113.71	120.79
1	B	375	ILE	C-N-CA	-5.09	113.71	120.79
1	B	73	GLU	N-CA-CB	-5.08	102.79	110.92
1	B	200	GLU	CB-CA-C	-5.08	99.34	110.67
1	D	3	ASN	CA-C-N	5.07	127.34	120.44
1	D	3	ASN	C-N-CA	5.07	127.34	120.44
1	C	16	GLY	N-CA-C	-5.07	106.65	112.73
1	A	298	LEU	N-CA-C	-5.07	103.76	110.40
1	D	77	VAL	N-CA-CB	-5.07	106.06	112.60
1	C	292	LEU	CB-CA-C	-5.07	102.90	110.90
1	C	379	ASP	N-CA-C	-5.06	105.76	111.28
1	D	141	TYR	CA-C-N	-5.06	114.85	127.00
1	D	141	TYR	C-N-CA	-5.06	114.85	127.00
1	D	188	MET	CA-C-N	-5.06	114.72	122.87
1	D	188	MET	C-N-CA	-5.06	114.72	122.87
1	B	116	ILE	CA-C-O	5.06	122.14	119.15
1	C	220	TYR	N-CA-C	-5.04	100.31	108.52
1	B	69	VAL	CA-C-N	-5.03	116.12	123.06
1	B	69	VAL	C-N-CA	-5.03	116.12	123.06
1	D	361	ALA	N-CA-C	-5.03	103.61	108.13
1	B	234	ALA	N-CA-C	-5.02	105.81	111.28
1	B	100	THR	N-CA-C	-5.02	105.50	110.97
1	B	331	CYS	N-CA-C	-5.01	105.70	111.07
1	B	342	LEU	N-CA-C	-5.01	101.06	109.24
1	A	345	LYS	CA-C-O	5.01	124.86	119.15
1	A	114	TYR	N-CA-C	-5.00	107.20	113.15
1	D	177	PRO	N-CA-C	-5.00	103.34	111.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	280	ILE	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	114	TYR	Sidechain

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	2977	0	2988	142	0
1	B	2969	0	2965	171	0
1	C	2975	0	2991	171	0
1	D	2948	0	2960	210	0
2	A	31	0	12	1	0
2	B	31	0	12	2	0
2	C	31	0	12	1	0
2	D	31	0	12	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	227	0	0	3	0
4	B	247	0	0	11	0
4	C	179	0	0	11	0
4	D	196	0	0	12	0
All	All	12850	0	11952	690	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 29.

All (690) 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:145:LEU:HD13	1:A:173:LEU:HD12	1.25	1.15
1:B:112:ARG:HG2	1:B:118:MET:HE3	1.29	1.15
1:D:112:ARG:HG3	1:D:118:MET:HE3	1.22	1.08
1:B:174:LYS:H	1:B:174:LYS:HD2	1.11	1.07
1:C:41:LYS:HE2	1:C:49:HIS:HB3	1.36	1.05
1:D:132:LEU:HD23	1:D:166:ILE:HG23	1.40	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:VAL:HA	1:D:138:GLN:HE21	1.19	1.02
1:D:135:VAL:HA	1:D:138:GLN:NE2	1.78	0.98
1:C:206:THR:HB	1:C:231[A]:ASN:ND2	1.78	0.97
1:C:61[B]:ARG:HH11	1:C:61[B]:ARG:HG3	1.28	0.96
1:B:316:ILE:HD11	1:B:357:ILE:HD11	1.47	0.96
1:D:110:HIS:HA	1:D:113:LYS:HE3	1.48	0.96
1:C:155:ARG:HG2	1:C:155:ARG:HH11	1.26	0.95
1:B:33:LEU:HD13	1:B:50:VAL:HG12	1.50	0.94
1:C:145:LEU:HD23	1:C:173:LEU:HD12	1.48	0.94
1:A:41:LYS:HE2	1:A:49:HIS:HB3	1.49	0.93
1:C:201:VAL:C	1:C:202:LEU:HD23	1.95	0.91
1:D:205:PRO:HG2	1:D:307:ILE:HD12	1.50	0.91
1:C:217:LYS:HG2	1:C:218:LEU:HD12	1.55	0.89
1:A:145:LEU:CD1	1:A:173:LEU:HD12	2.03	0.88
1:A:16:GLY:N	1:A:73:GLU:HG3	1.88	0.88
1:B:57:ARG:O	1:B:61:ARG:HG3	1.72	0.87
1:C:15:LEU:HB3	1:C:272:ILE:CD1	2.04	0.87
1:C:233:LYS:HB3	1:C:263:ILE:HD12	1.58	0.84
1:C:6:LYS:HE2	1:C:29:GLN:CD	2.02	0.84
1:B:59:ALA:HA	1:B:62[B]:GLN:HG3	1.58	0.84
1:D:54:PHE:HD1	1:D:54:PHE:H	1.24	0.84
1:A:66:THR:HG22	1:A:67[B]:CYS:SG	2.18	0.82
1:B:174:LYS:H	1:B:174:LYS:CD	1.92	0.82
1:B:174:LYS:HD2	1:B:174:LYS:N	1.92	0.81
1:D:16:GLY:N	1:D:73:GLU:HG3	1.95	0.81
1:A:63:LEU:O	1:A:66:THR:HB	1.80	0.80
1:D:142:PRO:HB3	1:D:161:ASN:HA	1.64	0.80
1:A:321:ALA:HB3	1:A:324:THR:CG2	2.12	0.80
1:A:166:ILE:HB	1:A:167:PRO:HD3	1.64	0.78
1:D:365:HIS:HA	4:D:474:HOH:O	1.82	0.78
1:C:63:LEU:O	1:C:66:THR:HB	1.84	0.78
1:B:16:GLY:N	1:B:73:GLU:HG3	1.99	0.77
1:C:145:LEU:CD2	1:C:173:LEU:HD12	2.13	0.77
1:B:2:TRP:HZ3	1:B:26:LEU:HD13	1.49	0.77
1:B:205:PRO:HG2	1:B:307:ILE:HG13	1.66	0.77
1:D:127:ASN:HD21	1:D:178:LEU:HD12	1.50	0.77
1:B:188:MET:HE1	1:B:226:VAL:HG21	1.66	0.76
1:D:83:GLU:HG3	1:D:95:TRP:CZ2	2.20	0.76
1:C:15:LEU:HB3	1:C:272:ILE:HD12	1.67	0.76
1:B:233:LYS:HE2	1:B:233:LYS:HA	1.66	0.75
1:A:238:ALA:O	1:A:242:VAL:HG23	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HB3	1:D:166:ILE:HD13	1.69	0.75
1:C:363:THR:OG1	1:C:366:GLU:HB2	1.87	0.75
1:C:120:GLU:H	1:C:182:LYS:HD3	1.50	0.75
1:B:372:GLN:HB3	1:B:373:PRO:HD3	1.67	0.74
1:C:211:GLN:OE1	1:C:216:CYS:HA	1.86	0.74
1:A:166:ILE:O	1:A:169:ALA:HB3	1.88	0.74
1:B:36:ASP:O	1:B:37:ASN:HB3	1.87	0.74
1:B:188:MET:CE	1:B:226:VAL:HG21	2.17	0.74
1:B:188:MET:CE	1:B:190:LEU:HD21	2.17	0.74
1:A:311:SER:HB3	1:A:360:THR:HG22	1.69	0.73
1:C:6:LYS:HE2	1:C:29:GLN:NE2	2.03	0.73
1:C:126:GLU:HB3	1:C:128:THR:HG23	1.70	0.73
1:C:94:SER:O	1:C:98:ILE:HG13	1.88	0.73
1:D:111:LEU:HD11	1:D:268:ILE:HD12	1.70	0.73
1:D:112:ARG:HG3	1:D:118:MET:CE	2.12	0.73
1:B:316:ILE:HD11	1:B:357:ILE:CD1	2.17	0.73
1:D:171:GLU:O	1:D:174:LYS:HG3	1.88	0.73
1:C:15:LEU:HB3	1:C:272:ILE:HD11	1.71	0.72
1:A:162:SER:O	1:A:165:ASP:HB2	1.89	0.72
1:D:176:ARG:HB2	4:D:464:HOH:O	1.89	0.72
1:A:322:PRO:HA	1:A:348:ALA:HB3	1.72	0.72
1:C:147:SER:HA	1:C:178:LEU:HD23	1.70	0.72
1:D:373:PRO:O	1:D:377:VAL:HG23	1.90	0.72
1:D:209:THR:HG22	1:D:219:VAL:HG22	1.70	0.72
1:B:282:GLY:O	1:B:308:ARG:HG3	1.91	0.71
1:D:188:MET:HE3	1:D:190:LEU:HD21	1.73	0.71
1:D:36:ASP:O	1:D:37:ASN:ND2	2.23	0.71
1:A:324:THR:O	1:A:327:GLN:HB2	1.90	0.71
1:B:188:MET:HE2	1:B:190:LEU:HD21	1.73	0.70
1:C:326:LEU:N	1:C:326:LEU:HD23	2.06	0.70
1:C:61[B]:ARG:HH11	1:C:61[B]:ARG:CG	2.01	0.70
1:D:62:GLN:HE21	1:D:62:GLN:HA	1.56	0.70
1:B:359:VAL:CG2	1:B:371:ILE:HD12	2.21	0.70
1:B:2:TRP:CZ3	1:B:26:LEU:HD13	2.27	0.70
1:C:36:ASP:OD1	1:C:51:THR:HG23	1.92	0.69
1:D:2:TRP:C	1:D:4:SER:H	2.00	0.69
1:D:15:LEU:HB2	1:D:73:GLU:HG2	1.74	0.69
1:C:318:GLY:HA3	1:C:349:LYS:O	1.92	0.69
1:D:33:LEU:HB2	1:D:63:LEU:HG	1.73	0.69
1:D:62:GLN:HA	1:D:62:GLN:NE2	2.08	0.69
1:B:34:ASP:OD1	1:B:35:ALA:N	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TYR:O	1:B:84:GLU:HG3	1.93	0.68
1:A:159:ARG:HD3	1:A:161:ASN:OD1	1.94	0.68
1:B:146:LYS:HE3	1:B:181:GLU:OE1	1.92	0.68
1:B:148:LYS:HD2	1:B:177:PRO:HB2	1.76	0.68
1:B:75:GLU:HB3	1:B:270:SER:OG	1.93	0.68
1:B:33:LEU:HB2	1:B:63:LEU:HD22	1.75	0.68
1:D:54:PHE:CD1	1:D:54:PHE:N	2.51	0.68
1:D:141:TYR:HB3	1:D:142:PRO:HA	1.75	0.68
1:D:323:ASP:O	1:D:324:THR:C	2.36	0.68
1:A:361:ALA:HB1	1:A:366:GLU:HG2	1.75	0.67
1:D:141:TYR:HA	1:D:142:PRO:C	2.19	0.67
1:D:188:MET:HE3	1:D:190:LEU:CD2	2.24	0.67
1:C:372:GLN:HB3	1:C:373:PRO:HD3	1.75	0.67
1:C:134:LYS:O	1:C:137:GLU:HB3	1.94	0.67
1:B:204:TYR:HB3	1:B:205:PRO:HD2	1.76	0.67
1:D:141:TYR:CB	1:D:142:PRO:HA	2.25	0.66
1:D:15:LEU:HB2	1:D:73:GLU:CG	2.25	0.66
1:D:126:GLU:HB3	1:D:128:THR:HG23	1.76	0.66
1:D:126:GLU:HB2	1:D:131:GLU:CD	2.20	0.66
1:B:83:GLU:HG3	1:B:95:TRP:CZ2	2.30	0.66
1:C:95:TRP:CZ3	1:C:96:GLN:HG3	2.31	0.66
1:A:381:ILE:O	1:A:382:ARG:C	2.37	0.66
1:A:187:LYS:HE2	1:A:258:LEU:O	1.95	0.65
1:D:83:GLU:HG3	1:D:95:TRP:CE2	2.32	0.65
1:C:212:GLU:OE2	1:C:382:ARG:NH2	2.23	0.65
1:D:208:GLU:HB3	1:D:220:TYR:HB2	1.76	0.65
1:C:96:GLN:HB2	4:C:832:HOH:O	1.95	0.65
1:D:54:PHE:CE2	1:D:74:ILE:HD13	2.30	0.65
1:A:372:GLN:HB3	1:A:373:PRO:HD3	1.79	0.65
1:D:56:GLU:HG3	1:D:58:GLU:OE2	1.96	0.65
1:C:231[A]:ASN:ND2	4:C:481:HOH:O	2.30	0.65
1:A:143:LEU:CD1	1:A:160:VAL:HB	2.27	0.65
1:B:33:LEU:HD13	1:B:50:VAL:CG1	2.26	0.64
1:A:44:SER:HB3	1:A:49:HIS:HE2	1.61	0.64
1:A:95:TRP:CZ3	1:A:96[B]:GLN:HG3	2.32	0.64
1:C:258:LEU:O	1:C:260:ASP:N	2.29	0.64
1:B:16:GLY:O	1:B:19:LEU:HB3	1.98	0.64
1:A:15:LEU:HB2	1:A:73:GLU:HG2	1.80	0.64
1:D:310:PRO:HD2	1:D:361:ALA:O	1.98	0.64
1:A:226:VAL:HG13	1:A:230:ILE:HB	1.79	0.64
1:C:31:ASN:HD22	1:C:66:THR:HG22	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:O	1:C:261:ASP:N	2.26	0.64
1:A:110:HIS:O	1:A:113:LYS:HD3	1.97	0.63
1:D:78:ASP:OD1	1:D:81:ALA:N	2.28	0.63
1:B:15:LEU:HB2	1:B:73:GLU:HG2	1.79	0.63
1:C:318:GLY:O	1:C:350:PRO:HA	1.98	0.63
1:C:376:ASP:O	1:C:380:ARG:HG3	1.99	0.63
1:C:379:ASP:O	1:C:382:ARG:HG2	1.98	0.63
1:A:323:ASP:OD1	1:A:324:THR:N	2.31	0.63
1:A:166:ILE:CB	1:A:167:PRO:HD3	2.28	0.63
1:D:323:ASP:O	1:D:326:LEU:N	2.31	0.63
1:D:33:LEU:HD13	1:D:50:VAL:HG12	1.81	0.62
1:A:265:LEU:HG	1:A:266:CYS:N	2.13	0.62
1:C:187:LYS:NZ	1:C:261:ASP:OD1	2.31	0.62
1:B:150:MET:HE3	1:B:150:MET:HA	1.80	0.62
1:B:204:TYR:HB3	1:B:205:PRO:CD	2.30	0.62
1:D:372:GLN:N	1:D:373:PRO:HD2	2.14	0.62
1:A:61:ARG:HH22	1:A:84:GLU:HG2	1.62	0.62
1:C:94:SER:OG	1:C:246:ASP:HB2	1.98	0.62
1:C:364:MET:O	1:C:368:GLU:HG3	1.99	0.62
1:B:227:SER:OG	1:B:230:ILE:HD12	2.00	0.62
1:C:119:ALA:HA	1:C:182:LYS:HE3	1.81	0.62
1:D:105:PHE:HB2	1:D:148:LYS:HG2	1.80	0.62
1:C:258:LEU:C	1:C:260:ASP:H	2.08	0.62
1:A:76:HIS:HB3	1:A:150:MET:HE3	1.81	0.62
1:B:74:ILE:HD12	1:B:77:VAL:HG13	1.82	0.62
1:C:85:VAL:HG22	1:C:85:VAL:O	1.99	0.61
1:D:34:ASP:O	1:D:41:LYS:NZ	2.26	0.61
1:B:53:SER:HB3	1:B:56:GLU:HG3	1.81	0.61
1:B:353:LYS:HE3	4:B:431:HOH:O	2.00	0.61
1:C:293:ARG:HD3	1:C:299:PRO:O	1.99	0.61
1:C:309:GLN:HB3	1:C:361:ALA:O	2.00	0.61
1:C:27:ASN:HB3	4:C:790:HOH:O	2.00	0.61
1:A:13:GLY:N	1:A:73:GLU:OE2	2.34	0.60
1:B:38:SER:OG	1:B:41:LYS:HG3	2.00	0.60
1:D:227:SER:HB2	4:D:468:HOH:O	2.00	0.60
1:C:217:LYS:HG2	1:C:218:LEU:CD1	2.30	0.60
1:C:230:ILE:HG21	1:C:257:LEU:HD11	1.83	0.60
1:D:205:PRO:CG	1:D:307:ILE:HD12	2.27	0.60
1:D:372:GLN:HB3	1:D:373:PRO:HD3	1.83	0.60
1:B:33:LEU:HA	1:B:50:VAL:O	2.01	0.60
1:A:10:LEU:HD22	1:A:33:LEU:HD23	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HD2	1:A:177:PRO:HB2	1.82	0.60
1:B:105:PHE:CB	1:B:148:LYS:HE2	2.31	0.60
1:D:205:PRO:HG2	1:D:307:ILE:CD1	2.28	0.60
1:D:47:ASP:HA	4:D:389:HOH:O	2.01	0.60
1:D:33:LEU:HA	1:D:50:VAL:O	2.01	0.60
1:A:76:HIS:HB3	1:A:150:MET:CE	2.32	0.60
1:C:318:GLY:O	1:C:351:GLY:N	2.29	0.60
1:A:31:ASN:ND2	1:A:66:THR:HG23	2.16	0.60
1:A:166:ILE:HG22	1:A:167:PRO:N	2.16	0.60
1:D:61:ARG:HH11	1:D:61:ARG:HB3	1.66	0.60
1:A:143:LEU:O	1:A:143:LEU:HD12	2.01	0.59
1:D:57:ARG:HD2	1:D:84:GLU:OE1	2.02	0.59
1:B:127:ASN:N	1:B:131:GLU:OE1	2.32	0.59
1:C:361:ALA:HB1	1:C:362:PRO:HD2	1.82	0.59
1:C:284:ALA:CB	1:D:337:ASN:HA	2.32	0.59
1:D:134:LYS:O	1:D:138:GLN:HG3	2.02	0.59
1:A:226:VAL:HG11	1:A:231:ASN:OD1	2.03	0.59
1:B:188:MET:HE3	1:B:190:LEU:CD2	2.33	0.59
1:D:95:TRP:CZ3	1:D:96:GLN:HG3	2.37	0.59
1:C:141:TYR:HB3	1:C:142:PRO:HA	1.84	0.59
1:C:273:HIS:ND1	1:C:275:SER:HB3	2.17	0.59
1:B:54:PHE:CD1	1:B:54:PHE:N	2.65	0.59
1:B:316:ILE:CD1	1:B:357:ILE:HD11	2.29	0.59
1:C:382:ARG:CZ	1:C:382:ARG:HB2	2.32	0.59
1:A:321:ALA:HB3	1:A:324:THR:HG22	1.83	0.59
1:D:208:GLU:HB2	1:D:223:ALA:HA	1.85	0.58
1:D:73:GLU:C	1:D:74:ILE:HG13	2.26	0.58
1:A:329:ALA:O	1:A:332:ALA:HB3	2.03	0.58
1:D:318:GLY:HA3	1:D:349:LYS:O	2.03	0.58
1:A:237:LEU:C	1:A:237:LEU:HD12	2.28	0.58
1:A:61:ARG:NH2	1:A:84:GLU:HG2	2.19	0.58
1:D:324:THR:O	1:D:327:GLN:N	2.30	0.58
1:B:174:LYS:CD	1:B:174:LYS:N	2.60	0.57
1:D:380:ARG:HG3	4:D:411:HOH:O	2.05	0.57
1:B:323:ASP:O	1:B:326:LEU:N	2.35	0.57
1:C:308:ARG:NH1	4:C:434:HOH:O	2.37	0.57
1:D:231:ASN:OD1	1:D:235:GLN:NE2	2.35	0.57
1:C:206:THR:HB	1:C:231[A]:ASN:HD21	1.66	0.57
1:B:359:VAL:HG23	1:B:371:ILE:HD12	1.86	0.57
1:A:141:TYR:CD1	1:A:162:SER:HA	2.40	0.57
1:B:57:ARG:HG3	1:B:58:GLU:N	2.11	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLU:HB2	1:C:182:LYS:HD2	1.87	0.57
1:D:46:HIS:ND1	1:D:48:GLY:N	2.52	0.57
1:D:110:HIS:HA	1:D:113:LYS:CE	2.31	0.57
1:B:238:ALA:O	1:B:242:VAL:HG23	2.05	0.57
1:D:2:TRP:CZ3	1:D:3:ASN:HB3	2.40	0.57
1:B:26:LEU:HB3	1:B:28:ILE:HD12	1.86	0.56
1:B:226:VAL:HG13	1:B:230:ILE:CG2	2.35	0.56
1:B:308:ARG:NH1	4:B:472:HOH:O	2.31	0.56
1:D:188:MET:CE	1:D:226:VAL:HG21	2.35	0.56
1:B:104:LYS:NZ	2:B:400:ATP:O2B	2.39	0.56
1:D:173:LEU:HD13	1:D:178:LEU:CD2	2.36	0.56
1:A:112:ARG:HH11	1:A:112:ARG:HB3	1.71	0.56
1:A:113:LYS:C	1:A:115:GLY:H	2.14	0.56
1:A:213:ASP:O	1:A:214:SER:HB2	2.05	0.56
1:B:92:GLU:HA	1:B:93:PRO:C	2.29	0.56
1:C:372:GLN:NE2	1:C:376:ASP:OD1	2.38	0.56
1:A:91:ILE:C	1:A:92:GLU:HG2	2.29	0.56
1:B:85:VAL:HG23	1:B:91:ILE:HD11	1.87	0.56
1:C:202:LEU:HD23	1:C:202:LEU:N	2.21	0.56
1:D:142:PRO:CB	1:D:161:ASN:HA	2.34	0.56
1:B:74:ILE:HD12	1:B:77:VAL:CG1	2.36	0.56
1:C:145:LEU:HD23	1:C:173:LEU:CD1	2.30	0.56
1:D:111:LEU:HD11	1:D:268:ILE:CD1	2.34	0.56
1:A:137:GLU:HG3	1:A:137:GLU:O	2.05	0.56
1:A:30:VAL:O	1:A:46:HIS:NE2	2.39	0.55
1:D:375:ILE:O	1:D:376:ASP:C	2.48	0.55
1:A:132:LEU:HD12	1:A:132:LEU:O	2.06	0.55
1:C:278:TYR:CZ	1:C:279:THR:HG22	2.41	0.55
1:B:111:LEU:HB2	1:B:118:MET:HE1	1.88	0.55
1:C:120:GLU:H	1:C:182:LYS:CD	2.19	0.55
1:C:257:LEU:CD2	1:C:261:ASP:HA	2.36	0.55
1:D:159:ARG:NE	1:D:161:ASN:OD1	2.34	0.55
1:A:232:GLN:OE1	1:A:232:GLN:HA	2.06	0.55
1:C:258:LEU:C	1:C:260:ASP:N	2.63	0.55
1:C:356:HIS:CD2	1:C:356:HIS:C	2.85	0.55
1:A:31:ASN:HD22	1:A:66:THR:HG23	1.72	0.55
1:A:143:LEU:HD12	1:A:160:VAL:HB	1.89	0.55
1:B:105:PHE:CZ	1:B:123:GLU:HB2	2.42	0.55
1:A:321:ALA:HB3	1:A:324:THR:HG23	1.85	0.55
1:B:310:PRO:HB3	1:B:364:MET:HE2	1.89	0.55
1:C:155:ARG:HG2	1:C:155:ARG:NH1	2.03	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:HA	1:B:149:THR:HG22	1.89	0.55
1:D:210:VAL:HB	1:D:218:LEU:HB2	1.89	0.55
1:A:136:GLY:HA3	1:A:141:TYR:OH	2.07	0.54
1:B:124:LEU:HD12	1:B:124:LEU:N	2.21	0.54
1:A:143:LEU:HD12	1:A:143:LEU:C	2.32	0.54
1:A:187:LYS:N	1:A:257:LEU:O	2.37	0.54
1:B:359:VAL:HG21	1:B:371:ILE:HD12	1.90	0.54
1:C:323:ASP:O	1:C:326:LEU:HB2	2.07	0.54
1:D:108:LYS:O	1:D:118:MET:HE1	2.07	0.54
1:B:33:LEU:CB	1:B:63:LEU:HD22	2.37	0.54
1:C:82:LEU:HB3	1:C:91:ILE:HD13	1.89	0.54
1:B:188:MET:HE1	1:B:226:VAL:CG2	2.35	0.54
1:B:375:ILE:O	1:B:376:ASP:C	2.50	0.54
1:C:273:HIS:CE1	1:C:275:SER:HB3	2.43	0.54
2:A:400:ATP:H5'2	4:A:432:HOH:O	2.07	0.54
1:D:188:MET:CE	1:D:190:LEU:HD21	2.37	0.54
1:D:317:ILE:O	1:D:318:GLY:C	2.50	0.54
1:A:15:LEU:HB2	1:A:73:GLU:CG	2.38	0.54
1:D:143:LEU:HB2	1:D:160:VAL:HB	1.90	0.54
1:A:143:LEU:HD11	1:A:160:VAL:HB	1.90	0.54
1:D:296:LEU:O	1:D:297:ASP:HB2	2.07	0.54
1:B:198:LYS:HG3	4:B:529:HOH:O	2.08	0.53
1:D:85:VAL:C	1:D:87:SER:H	2.15	0.53
1:D:127:ASN:ND2	1:D:178:LEU:HD12	2.20	0.53
1:A:101:ILE:HD12	1:A:270:SER:HB3	1.90	0.53
1:A:163:GLN:HA	1:A:166:ILE:HG13	1.90	0.53
1:A:293:ARG:HD3	1:A:299:PRO:O	2.09	0.53
1:D:85:VAL:C	1:D:87:SER:N	2.66	0.53
1:B:105:PHE:CE1	1:B:123:GLU:HB2	2.43	0.53
1:D:102:GLN:HG2	4:D:458:HOH:O	2.08	0.53
1:D:301:PRO:O	1:D:304:SER:HB2	2.08	0.53
1:D:317:ILE:CG2	1:D:351:GLY:HA2	2.39	0.53
1:C:191:ALA:HA	1:C:253:VAL:O	2.08	0.53
1:A:174:LYS:O	1:A:174:LYS:HG2	2.08	0.53
1:D:373:PRO:O	1:D:376:ASP:HB2	2.09	0.53
1:C:61[B]:ARG:HG3	1:C:61[B]:ARG:NH1	2.08	0.53
1:C:194:VAL:HG13	1:C:202:LEU:O	2.09	0.53
1:A:36:ASP:HA	4:A:507:HOH:O	2.09	0.53
1:C:31:ASN:HD22	1:C:66:THR:CG2	2.21	0.53
1:C:201:VAL:O	1:C:202:LEU:HD23	2.07	0.53
1:A:54:PHE:HB2	1:A:77:VAL:HG12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLU:O	1:C:190:LEU:HD23	2.10	0.52
1:B:188:MET:CE	1:B:223:ALA:HB1	2.39	0.52
1:C:31:ASN:ND2	1:C:66:THR:CG2	2.72	0.52
1:C:329:ALA:O	1:C:332:ALA:HB3	2.09	0.52
1:D:204:TYR:HB3	1:D:205:PRO:HD2	1.90	0.52
1:D:376:ASP:HB3	1:D:380:ARG:NH1	2.24	0.52
1:B:105:PHE:HB3	1:B:148:LYS:HE2	1.91	0.52
1:B:372:GLN:N	1:B:373:PRO:CD	2.73	0.52
1:B:10:LEU:HD11	1:B:82:LEU:HD21	1.91	0.52
1:C:148:LYS:HG3	1:C:177:PRO:O	2.10	0.52
1:C:187:LYS:HD3	1:C:259:GLU:HA	1.91	0.52
1:D:33:LEU:HD12	1:D:34:ASP:N	2.25	0.52
1:D:148:LYS:HD2	1:D:177:PRO:HB2	1.91	0.52
1:C:123:GLU:HA	1:C:179:TYR:HA	1.93	0.51
1:C:254:GLU:OE2	1:C:267:GLU:HG2	2.10	0.51
1:D:96:GLN:HG2	4:D:404:HOH:O	2.09	0.51
1:D:173:LEU:HD12	1:D:178:LEU:HD22	1.91	0.51
1:C:61[A]:ARG:NH2	1:C:84:GLU:OE2	2.43	0.51
1:C:299:PRO:C	1:C:300:ILE:HD12	2.34	0.51
1:D:61:ARG:HH11	1:D:61:ARG:CB	2.23	0.51
1:D:173:LEU:CD1	1:D:178:LEU:HD22	2.41	0.51
1:D:230:ILE:O	1:D:231:ASN:C	2.53	0.51
1:C:17:ARG:HD2	1:C:39:PRO:O	2.10	0.51
1:D:54:PHE:CE2	1:D:74:ILE:CD1	2.93	0.51
1:C:221:ALA:HA	1:C:222:PRO:C	2.34	0.51
1:C:95:TRP:CH2	1:C:96:GLN:HG3	2.44	0.51
1:C:308:ARG:NH1	4:C:691:HOH:O	2.27	0.51
1:A:196:LYS:HE3	1:A:245:PHE:O	2.10	0.51
1:B:90:LYS:HB3	4:B:432:HOH:O	2.10	0.51
1:D:75:GLU:O	1:D:102:GLN:HG3	2.11	0.51
1:A:308:ARG:NH1	4:A:427:HOH:O	2.43	0.51
1:D:372:GLN:HB3	1:D:373:PRO:CD	2.40	0.51
1:B:123:GLU:C	1:B:124:LEU:HD12	2.36	0.51
1:B:188:MET:HE2	1:B:226:VAL:HG21	1.93	0.51
1:C:381:ILE:HG22	1:C:382:ARG:N	2.16	0.51
1:A:31:ASN:HD22	1:A:66:THR:CG2	2.24	0.51
1:C:226:VAL:HG12	1:C:227:SER:O	2.11	0.51
1:D:33:LEU:HD12	1:D:33:LEU:C	2.36	0.51
1:D:116:ILE:O	1:D:118:MET:HG2	2.10	0.51
1:D:204:TYR:HB3	1:D:205:PRO:CD	2.41	0.50
1:A:83:GLU:HG3	1:A:95:TRP:CZ2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:CB	1:B:118:MET:HE1	2.41	0.50
1:B:233:LYS:HE2	1:B:233:LYS:CA	2.39	0.50
1:A:361:ALA:CB	1:A:366:GLU:HG2	2.41	0.50
1:D:272:ILE:HG12	1:D:272:ILE:O	2.10	0.50
1:A:196:LYS:HD2	1:A:251:PHE:CE1	2.47	0.50
1:B:145:LEU:HD23	1:B:173:LEU:HD12	1.94	0.50
1:D:377:VAL:O	1:D:381:ILE:HG12	2.12	0.50
1:B:49:HIS:HB2	4:B:426:HOH:O	2.12	0.50
1:B:141:TYR:HA	1:B:142:PRO:C	2.36	0.50
1:C:104:LYS:O	1:C:108:LYS:HG3	2.12	0.50
1:C:228:ASP:O	1:C:229:ALA:C	2.53	0.50
1:D:316:ILE:HG21	1:D:325:HIS:HB2	1.94	0.50
1:B:114:TYR:N	1:B:114:TYR:CD2	2.80	0.50
1:B:208:GLU:OE1	1:B:224:ARG:HB2	2.12	0.50
1:C:38:SER:O	1:C:42:GLN:HG3	2.12	0.50
1:D:233:LYS:HD3	1:D:263:ILE:HD12	1.94	0.49
1:C:205:PRO:HG2	1:C:307:ILE:HG13	1.93	0.49
1:D:182:LYS:HG3	1:D:183:TRP:N	2.25	0.49
1:D:361:ALA:HB1	1:D:366:GLU:HB3	1.94	0.49
1:C:375:ILE:O	1:C:376:ASP:C	2.55	0.49
1:B:376:ASP:HA	4:B:493:HOH:O	2.11	0.49
1:C:2:TRP:CZ3	1:C:26:LEU:HD13	2.47	0.49
1:D:260:ASP:OD1	1:D:260:ASP:N	2.45	0.49
1:B:16:GLY:CA	1:B:73:GLU:HG3	2.41	0.49
1:B:260:ASP:N	1:B:260:ASP:OD1	2.41	0.49
1:C:361:ALA:HB1	1:C:362:PRO:CD	2.43	0.49
1:D:207:VAL:HB	1:D:220:TYR:O	2.12	0.49
1:B:142:PRO:O	1:B:183:TRP:HB2	2.12	0.49
1:C:105:PHE:CE1	1:C:123:GLU:HB3	2.47	0.49
1:D:124:LEU:HD21	1:D:145:LEU:HD11	1.95	0.49
1:C:145:LEU:O	1:C:157:ASN:HA	2.13	0.49
1:D:213:ASP:O	1:D:214:SER:HB2	2.11	0.49
1:A:284:ALA:CB	1:B:337:ASN:HA	2.42	0.49
1:B:126:GLU:CB	1:B:128:THR:HG23	2.43	0.49
1:A:104:LYS:O	1:A:108:LYS:HG3	2.13	0.48
1:B:108:LYS:O	1:B:118:MET:HE1	2.12	0.48
1:A:142:PRO:O	1:A:183:TRP:HB2	2.13	0.48
1:C:83:GLU:HG3	1:C:95:TRP:CZ2	2.48	0.48
1:D:15:LEU:CB	1:D:73:GLU:HG2	2.42	0.48
1:D:112:ARG:N	1:D:118:MET:HE1	2.28	0.48
1:D:135:VAL:O	1:D:138:GLN:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:VAL:HG22	1:D:206:THR:HA	1.94	0.48
1:D:324:THR:O	1:D:325:HIS:C	2.54	0.48
1:B:57:ARG:CG	1:B:58:GLU:N	2.75	0.48
1:B:110:HIS:O	1:B:113:LYS:HG3	2.12	0.48
1:C:171:GLU:OE1	1:C:174:LYS:HE3	2.13	0.48
1:A:159:ARG:HG3	1:A:183:TRP:CZ3	2.48	0.48
1:B:58:GLU:O	1:B:62[B]:GLN:HG2	2.14	0.48
1:B:188:MET:HE1	1:B:223:ALA:HB1	1.93	0.48
1:A:126:GLU:HB3	1:A:128:THR:HG23	1.93	0.48
1:D:127:ASN:HD21	1:D:178:LEU:CD1	2.24	0.48
1:B:254:GLU:C	1:B:255:MET:HG3	2.38	0.48
1:D:379:ASP:O	1:D:380:ARG:C	2.54	0.48
1:B:169:ALA:O	1:B:172:ALA:HB3	2.14	0.48
1:B:227:SER:O	1:B:228:ASP:C	2.55	0.48
1:C:94:SER:CB	1:C:97:ALA:H	2.27	0.48
1:C:224:ARG:NH2	1:C:368:GLU:OE1	2.45	0.48
1:C:236:GLU:O	1:C:237:LEU:C	2.57	0.48
1:D:33:LEU:O	1:D:34:ASP:HB2	2.14	0.48
1:D:260:ASP:OD1	1:D:262:SER:HB3	2.13	0.48
1:D:190:LEU:HD11	1:D:257:LEU:HB2	1.95	0.48
1:B:121:HIS:HB3	1:B:181:GLU:HB2	1.95	0.48
1:C:159:ARG:HD3	1:C:161:ASN:OD1	2.13	0.48
1:A:55:LYS:NZ	1:A:150:MET:HE2	2.29	0.48
1:A:128:THR:O	1:A:131:GLU:N	2.47	0.48
1:A:191:ALA:HA	1:A:253:VAL:O	2.14	0.48
1:B:154:GLY:HA2	4:B:409:HOH:O	2.13	0.48
1:C:193:ILE:CG2	1:C:250:VAL:HG13	2.44	0.48
1:B:113:LYS:HB2	1:B:114:TYR:CD2	2.49	0.47
1:D:125:VAL:HG22	1:D:131:GLU:OE2	2.13	0.47
1:D:133:ALA:O	1:D:137:GLU:HG3	2.14	0.47
1:D:159:ARG:HD2	1:D:183:TRP:CH2	2.49	0.47
1:B:112:ARG:HG2	1:B:118:MET:CE	2.21	0.47
1:B:142:PRO:HB3	1:B:161:ASN:HA	1.96	0.47
1:C:166:ILE:O	1:C:167:PRO:C	2.57	0.47
1:D:188:MET:SD	1:D:208:GLU:HG3	2.54	0.47
1:B:237:LEU:HD23	1:B:263:ILE:HG22	1.95	0.47
1:B:258:LEU:HB2	1:B:262:SER:OG	2.14	0.47
1:D:34:ASP:O	1:D:51:THR:HA	2.14	0.47
1:D:62:GLN:NE2	1:D:62:GLN:CA	2.77	0.47
1:D:173:LEU:CD1	1:D:178:LEU:CD2	2.93	0.47
1:B:97:ALA:O	1:B:98:ILE:C	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:TYR:CE2	1:C:279:THR:HG22	2.48	0.47
1:B:109:GLU:HA	1:B:112:ARG:HG3	1.97	0.47
1:C:2:TRP:HZ3	1:C:26:LEU:HD13	1.79	0.47
1:D:154:GLY:N	2:D:400:ATP:O1B	2.44	0.47
1:A:55:LYS:CE	1:A:150:MET:HE2	2.43	0.47
1:A:141:TYR:HB3	1:A:161:ASN:O	2.15	0.47
1:A:381:ILE:O	1:A:381:ILE:CG2	2.54	0.47
1:C:46:HIS:ND1	1:C:48:GLY:N	2.63	0.47
1:B:135:VAL:HG11	1:B:180:ALA:HB3	1.97	0.47
1:C:166:ILE:N	1:C:167:PRO:CD	2.78	0.47
1:C:171:GLU:CD	1:C:174:LYS:HE3	2.40	0.47
1:C:378:VAL:O	1:C:381:ILE:HB	2.15	0.47
1:D:37:ASN:ND2	1:D:37:ASN:C	2.73	0.47
1:D:188:MET:HE1	1:D:226:VAL:HG21	1.95	0.47
1:B:301:PRO:O	1:B:304:SER:HB2	2.15	0.47
1:C:280:ILE:HA	1:C:286:SER:HB3	1.97	0.47
1:C:316:ILE:HD11	1:C:357:ILE:HD11	1.97	0.47
1:B:79:THR:CG2	1:B:98:ILE:HG22	2.44	0.47
1:B:272:ILE:O	1:B:272:ILE:HG12	2.14	0.47
1:D:332:ALA:HB2	1:D:357:ILE:HD12	1.97	0.47
1:A:364:MET:O	1:A:368:GLU:HG3	2.15	0.46
1:B:316:ILE:CD1	1:B:357:ILE:CD1	2.90	0.46
1:D:17:ARG:N	1:D:40:ALA:HB2	2.30	0.46
1:A:16:GLY:H	1:A:73:GLU:HG3	1.73	0.46
1:A:67[A]:CYS:SG	1:A:70:VAL:HG22	2.54	0.46
1:A:166:ILE:CB	1:A:167:PRO:CD	2.94	0.46
1:B:26:LEU:CB	1:B:28:ILE:HD12	2.45	0.46
1:B:59:ALA:CA	1:B:62[B]:GLN:HG3	2.35	0.46
1:D:188:MET:HE1	1:D:226:VAL:CG2	2.46	0.46
1:A:218:LEU:HA	1:A:313:MET:O	2.15	0.46
1:D:57:ARG:O	1:D:61:ARG:HG3	2.15	0.46
1:A:16:GLY:CA	1:A:73:GLU:HG3	2.46	0.46
1:A:114:TYR:CD1	1:A:244:ALA:HB2	2.50	0.46
1:A:363:THR:OG1	1:A:366:GLU:HB3	2.15	0.46
1:A:372:GLN:O	1:A:373:PRO:C	2.58	0.46
1:C:35:ALA:O	1:C:41:LYS:HD2	2.15	0.46
1:C:74:ILE:HG13	1:C:75:GLU:N	2.30	0.46
1:C:124:LEU:N	1:C:124:LEU:HD12	2.31	0.46
1:A:198:LYS:HG3	1:A:199:ASP:CG	2.41	0.46
1:A:271:ARG:HD2	1:A:272:ILE:O	2.16	0.46
1:D:73:GLU:OE2	4:D:427:HOH:O	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HE3	1:A:150:MET:HE2	1.97	0.46
1:C:379:ASP:O	1:C:382:ARG:HD2	2.16	0.46
1:D:126:GLU:H	1:D:131:GLU:CD	2.23	0.46
1:C:135:VAL:HA	1:C:138:GLN:HE21	1.79	0.46
1:D:54:PHE:CD2	1:D:74:ILE:CD1	2.98	0.46
1:A:113:LYS:C	1:A:115:GLY:N	2.74	0.46
1:A:144:MET:HG3	1:A:146:LYS:HG2	1.97	0.46
1:B:372:GLN:N	1:B:373:PRO:HD2	2.31	0.46
1:D:108:LYS:NZ	1:D:181:GLU:OE2	2.41	0.46
1:A:62:GLN:O	1:A:63:LEU:C	2.57	0.46
1:B:318:GLY:N	1:B:352:ARG:O	2.43	0.46
1:C:141:TYR:HA	1:C:142:PRO:C	2.39	0.46
1:C:166:ILE:HB	1:C:167:PRO:HD3	1.98	0.46
1:D:65:LYS:HB3	1:D:65:LYS:HE3	1.75	0.46
1:C:82:LEU:O	1:C:83:GLU:C	2.59	0.45
1:C:103:ASN:HB3	1:C:106:ASN:HB2	1.97	0.45
1:C:265:LEU:HG	1:C:266:CYS:N	2.30	0.45
1:D:31:ASN:OD1	1:D:46:HIS:HE1	1.99	0.45
1:D:104:LYS:NZ	2:D:400:ATP:O2B	2.47	0.45
1:D:332:ALA:HA	1:D:335:ILE:HG13	1.98	0.45
1:B:303:GLN:HB2	4:B:514:HOH:O	2.16	0.45
1:C:333:LEU:HD23	1:C:340:ILE:CD1	2.46	0.45
1:D:124:LEU:CD2	1:D:145:LEU:HD11	2.46	0.45
1:D:364:MET:O	1:D:368:GLU:HG3	2.17	0.45
1:B:57:ARG:CD	1:B:61:ARG:HD3	2.47	0.45
1:B:83:GLU:HG3	1:B:95:TRP:CE2	2.51	0.45
1:D:70:VAL:HG21	1:D:89:VAL:HG11	1.97	0.45
1:D:372:GLN:N	1:D:373:PRO:CD	2.79	0.45
1:A:227:SER:H	1:A:230:ILE:HD12	1.81	0.45
1:B:149:THR:O	1:B:150:MET:HB2	2.16	0.45
1:D:322:PRO:O	1:D:325:HIS:HE1	1.99	0.45
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.46	0.45
1:B:123:GLU:OE1	1:B:148:LYS:NZ	2.49	0.45
1:D:85:VAL:O	1:D:87:SER:N	2.50	0.45
1:D:187:LYS:NZ	1:D:261:ASP:OD1	2.42	0.45
1:B:133:ALA:HB1	1:B:163:GLN:NE2	2.31	0.45
1:B:317:ILE:O	1:B:318:GLY:C	2.58	0.45
1:D:64:ALA:C	1:D:66:THR:N	2.71	0.45
1:A:118:MET:HE2	1:A:118:MET:HB3	1.81	0.45
1:A:57:ARG:HD2	1:A:81:ALA:HB2	1.99	0.45
1:B:126:GLU:HB3	1:B:128:THR:HG23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLU:HA	1:C:179:TYR:CB	2.48	0.45
1:D:70:VAL:HG23	1:D:89:VAL:HG21	1.98	0.45
1:C:326:LEU:HD22	1:C:326:LEU:HA	1.52	0.44
1:B:76:HIS:HB3	1:B:150:MET:HE1	1.98	0.44
1:C:92:GLU:OE1	1:C:92:GLU:HA	2.17	0.44
1:C:349:LYS:HD2	1:C:349:LYS:HA	1.79	0.44
1:D:12:GLY:O	1:D:38:SER:HB2	2.17	0.44
1:D:95:TRP:CH2	1:D:96:GLN:HG3	2.52	0.44
1:B:176:ARG:HH21	1:B:176:ARG:HD3	1.60	0.44
1:B:182:LYS:HE2	4:B:475:HOH:O	2.18	0.44
1:B:316:ILE:CG1	1:B:357:ILE:CD1	2.96	0.44
1:B:361:ALA:HB1	1:B:366:GLU:HB3	1.99	0.44
1:C:293:ARG:O	1:C:297:ASP:N	2.50	0.44
1:D:82:LEU:HA	1:D:82:LEU:HD23	1.43	0.44
1:C:156:GLY:HA2	1:C:173:LEU:HD22	1.98	0.44
1:D:16:GLY:H	1:D:73:GLU:HG3	1.76	0.44
1:D:258:LEU:O	1:D:261:ASP:N	2.48	0.44
1:B:116:ILE:O	1:B:118:MET:HG2	2.18	0.44
1:C:171:GLU:OE2	1:C:174:LYS:HE3	2.17	0.44
1:A:23:ALA:HB2	1:A:292:LEU:HD11	1.99	0.44
1:A:332:ALA:CB	1:A:357:ILE:HD12	2.48	0.44
1:C:361:ALA:HA	1:C:362:PRO:HD3	1.69	0.44
1:A:123:GLU:HG3	1:A:148:LYS:HZ3	1.83	0.44
1:B:34:ASP:O	1:B:51:THR:HA	2.18	0.44
1:C:189:GLU:C	1:C:190:LEU:HD23	2.42	0.44
1:D:321:ALA:HA	1:D:322:PRO:HD3	1.70	0.44
1:D:332:ALA:CB	1:D:357:ILE:CD1	2.95	0.44
1:A:45:ALA:HB2	1:B:45:ALA:HB2	1.99	0.44
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.65	0.44
1:B:374:LEU:O	1:B:375:ILE:C	2.57	0.44
1:C:107:GLN:OE1	1:C:268:ILE:HG22	2.18	0.44
1:C:143:LEU:C	1:C:143:LEU:HD12	2.43	0.44
1:C:226:VAL:O	1:C:227:SER:O	2.36	0.44
1:C:379:ASP:O	1:C:382:ARG:CG	2.65	0.44
1:D:121:HIS:O	1:D:122:ARG:HD3	2.18	0.44
1:D:143:LEU:HA	1:D:143:LEU:HD23	1.55	0.44
1:A:152:TYR:O	1:A:153:ASP:C	2.58	0.44
1:C:193:ILE:HG23	1:C:250:VAL:HG13	1.99	0.44
1:A:95:TRP:CE3	1:A:96[B]:GLN:HG3	2.53	0.43
1:B:310:PRO:HD2	1:B:361:ALA:O	2.18	0.43
1:C:318:GLY:HA2	1:C:348:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ARG:HD3	4:D:411:HOH:O	2.17	0.43
1:C:22:SER:HB3	4:C:464:HOH:O	2.17	0.43
1:C:57:ARG:HE	1:C:57:ARG:HB2	1.16	0.43
1:D:75:GLU:H	1:D:75:GLU:HG3	1.59	0.43
1:A:171:GLU:O	1:A:174:LYS:HB3	2.19	0.43
1:B:188:MET:HE3	1:B:190:LEU:HD21	1.89	0.43
1:D:343:TYR:N	1:D:343:TYR:CD2	2.83	0.43
1:A:15:LEU:HD13	1:A:272:ILE:HG13	2.00	0.43
1:A:310:PRO:HG2	1:A:363:THR:CA	2.49	0.43
1:B:213:ASP:O	1:B:214:SER:HB2	2.18	0.43
1:B:320:ALA:HA	1:B:350:PRO:HG3	2.00	0.43
1:C:361:ALA:CB	1:C:362:PRO:CD	2.96	0.43
1:D:110:HIS:O	1:D:113:LYS:HB2	2.18	0.43
1:D:324:THR:O	1:D:327:GLN:HB3	2.18	0.43
1:B:38:SER:O	1:B:39:PRO:C	2.60	0.43
1:B:324:THR:O	1:B:327:GLN:HB2	2.18	0.43
1:B:124:LEU:N	1:B:124:LEU:CD1	2.81	0.43
1:C:297:ASP:HA	4:C:406:HOH:O	2.17	0.43
1:D:264:MET:HB2	1:D:264:MET:HE2	1.50	0.43
1:A:33:LEU:HD12	1:A:33:LEU:C	2.43	0.43
1:A:364:MET:O	1:A:365:HIS:C	2.60	0.43
1:D:94:SER:O	1:D:97:ALA:HB3	2.19	0.43
1:A:81:ALA:O	1:A:85:VAL:HG22	2.19	0.43
1:B:226:VAL:HG13	1:B:230:ILE:HG21	1.99	0.43
1:D:229:ALA:O	1:D:230:ILE:C	2.55	0.43
1:B:152:TYR:OH	1:B:155:ARG:NH1	2.52	0.42
1:D:38:SER:OG	1:D:41:LYS:HG3	2.19	0.42
1:D:61:ARG:HB3	1:D:61:ARG:NH1	2.34	0.42
1:B:14:GLN:HG2	1:B:15:LEU:N	2.34	0.42
1:B:146:LYS:HE2	2:B:400:ATP:N7	2.34	0.42
1:C:226:VAL:C	1:C:227:SER:O	2.60	0.42
1:C:378:VAL:HG23	1:C:379:ASP:N	2.34	0.42
1:D:141:TYR:HB3	1:D:161:ASN:O	2.19	0.42
1:A:58:GLU:HA	1:A:61:ARG:HB2	2.01	0.42
1:A:348:ALA:O	1:A:349:LYS:HD3	2.19	0.42
1:C:94:SER:HB3	1:C:97:ALA:H	1.84	0.42
1:C:304:SER:OG	4:C:466:HOH:O	2.22	0.42
1:D:8:GLY:HA2	1:D:31:ASN:O	2.19	0.42
1:D:188:MET:CE	1:D:226:VAL:CG2	2.98	0.42
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.78	0.42
1:A:226:VAL:HG12	1:A:227:SER:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ALA:HA	1:A:322:PRO:HD3	1.95	0.42
1:A:323:ASP:OD1	1:A:323:ASP:C	2.60	0.42
1:B:231:ASN:OD1	1:B:235:GLN:NE2	2.49	0.42
1:B:321:ALA:HA	1:B:322:PRO:HD3	1.72	0.42
1:D:166:ILE:N	1:D:167:PRO:CD	2.82	0.42
1:D:187:LYS:HE3	1:D:259:GLU:HA	2.01	0.42
1:D:237:LEU:O	1:D:237:LEU:HD12	2.19	0.42
1:A:321:ALA:HB1	1:A:323:ASP:OD1	2.18	0.42
1:C:296:LEU:O	1:C:297:ASP:HB2	2.19	0.42
1:D:170:LEU:HD23	1:D:170:LEU:HA	1.93	0.42
1:D:196:LYS:HD2	1:D:242:VAL:HG12	2.02	0.42
1:D:332:ALA:HB2	1:D:357:ILE:CD1	2.49	0.42
1:D:368:GLU:HG3	4:D:474:HOH:O	2.18	0.42
1:B:95:TRP:C	1:B:95:TRP:CE3	2.98	0.42
1:C:69:VAL:HG23	1:C:90:LYS:HB3	2.01	0.42
1:C:122:ARG:HG2	1:C:139:LEU:HD21	2.02	0.42
1:D:188:MET:HG3	1:D:189:GLU:N	2.34	0.42
1:D:278:TYR:CD2	1:D:278:TYR:C	2.97	0.42
1:A:321:ALA:O	1:A:324:THR:HG23	2.20	0.42
1:C:206:THR:HB	1:C:231[A]:ASN:CG	2.40	0.42
1:D:325:HIS:CE1	1:D:348:ALA:HB2	2.55	0.42
1:B:371:ILE:C	1:B:373:PRO:HD2	2.45	0.42
1:C:97:ALA:O	1:C:98:ILE:C	2.60	0.42
1:C:104:LYS:HE2	4:C:414:HOH:O	2.20	0.42
1:C:202:LEU:HD12	1:C:305:LEU:HD11	2.01	0.42
1:D:323:ASP:O	1:D:324:THR:O	2.38	0.42
1:A:43:ILE:HA	1:B:43:ILE:O	2.20	0.42
1:B:7:VAL:O	1:B:30:VAL:HA	2.20	0.42
1:B:152:TYR:C	1:B:154:GLY:N	2.76	0.42
1:D:37:ASN:O	1:D:38:SER:C	2.61	0.42
1:A:26:LEU:O	1:A:27:ASN:HB2	2.20	0.41
1:B:293:ARG:HH11	1:B:293:ARG:HD3	1.73	0.41
1:A:292:LEU:O	1:A:296:LEU:HD12	2.19	0.41
1:A:55:LYS:NZ	1:A:150:MET:CE	2.84	0.41
1:A:231:ASN:O	1:A:235:GLN:HG2	2.20	0.41
1:B:3:ASN:OD1	1:B:3:ASN:N	2.53	0.41
1:B:85:VAL:C	1:B:87:SER:N	2.77	0.41
1:D:226:VAL:HG13	1:D:230:ILE:HB	2.03	0.41
1:D:374:LEU:O	1:D:375:ILE:C	2.61	0.41
1:D:375:ILE:O	1:D:378:VAL:N	2.53	0.41
1:A:36:ASP:O	1:A:37[B]:ASN:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASN:CB	1:C:106:ASN:ND2	2.83	0.41
1:C:218:LEU:HA	1:C:313:MET:O	2.21	0.41
1:C:343:TYR:HB2	1:C:345:LYS:HD2	2.02	0.41
1:D:112:ARG:CG	1:D:118:MET:HE3	2.16	0.41
1:D:379:ASP:O	1:D:381:ILE:N	2.53	0.41
1:A:100:THR:HG22	1:A:107:GLN:HA	2.01	0.41
1:A:341:HIS:CE1	1:B:25:ARG:NH1	2.88	0.41
1:B:211:GLN:HA	1:B:215:ILE:O	2.21	0.41
1:B:237:LEU:HD23	1:B:263:ILE:CG2	2.50	0.41
2:C:400:ATP:H5'2	4:C:398:HOH:O	2.19	0.41
1:D:146:LYS:HB3	1:D:157:ASN:OD1	2.20	0.41
1:B:237:LEU:O	1:B:237:LEU:HD12	2.21	0.41
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.86	0.41
1:C:174:LYS:O	1:C:176:ARG:HG3	2.20	0.41
1:C:300:ILE:HD12	1:C:300:ILE:N	2.36	0.41
1:D:70:VAL:CG2	1:D:89:VAL:HG11	2.50	0.41
1:D:74:ILE:HG22	1:D:75:GLU:N	2.36	0.41
1:D:74:ILE:HG22	1:D:75:GLU:H	1.86	0.41
1:D:379:ASP:C	1:D:381:ILE:N	2.78	0.41
1:A:103:ASN:HB3	1:A:106:ASN:HB2	2.02	0.41
1:A:123:GLU:HG3	1:A:148:LYS:NZ	2.36	0.41
1:D:25:ARG:NH1	4:D:849:HOH:O	2.50	0.41
1:D:110:HIS:CA	1:D:113:LYS:HE3	2.34	0.41
1:A:324:THR:O	1:A:327:GLN:N	2.54	0.41
1:C:213:ASP:O	1:C:214:SER:HB2	2.21	0.41
1:D:41:LYS:HE2	1:D:49:HIS:HB3	2.02	0.41
1:D:141:TYR:HB3	1:D:142:PRO:CA	2.49	0.41
1:D:370:HIS:O	4:D:471:HOH:O	2.22	0.41
1:A:154:GLY:C	1:A:156:GLY:H	2.28	0.41
1:A:196:LYS:HD3	1:A:247:GLY:O	2.21	0.41
1:A:224:ARG:O	1:A:225:ASN:HB2	2.20	0.41
1:C:226:VAL:HG13	1:C:230:ILE:HB	2.03	0.41
1:C:237:LEU:HD13	1:C:255:MET:SD	2.61	0.41
1:C:330:GLU:HB2	1:D:2:TRP:NE1	2.36	0.41
1:D:293:ARG:HA	1:D:298:LEU:HB2	2.01	0.41
1:A:33:LEU:HD12	1:A:34:ASP:N	2.36	0.41
1:A:189:GLU:OE1	1:A:211:GLN:NE2	2.44	0.41
1:A:255:MET:HB3	1:A:263:ILE:CG2	2.51	0.41
1:B:193:ILE:HD13	1:B:193:ILE:HA	1.93	0.41
1:C:248:LYS:NZ	4:C:589:HOH:O	2.50	0.41
1:B:55:LYS:HE2	4:B:760:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:O	1:B:138:GLN:N	2.50	0.40
1:B:258:LEU:O	1:B:261:ASP:N	2.50	0.40
1:C:349:LYS:HA	1:C:350:PRO:HD3	1.85	0.40
1:D:2:TRP:CE3	1:D:3:ASN:HB3	2.56	0.40
1:D:366:GLU:O	1:D:367:ALA:C	2.62	0.40
1:D:46:HIS:CE1	1:D:48:GLY:HA3	2.56	0.40
1:D:196:LYS:NZ	1:D:247:GLY:O	2.38	0.40
1:A:316:ILE:CG2	1:A:325:HIS:HA	2.51	0.40
1:B:19:LEU:HD12	1:B:19:LEU:HA	1.62	0.40
1:B:285:LEU:HG	1:B:304:SER:HB3	2.03	0.40
1:C:226:VAL:O	1:C:227:SER:C	2.64	0.40
1:C:233:LYS:HB3	1:C:263:ILE:CD1	2.39	0.40
1:A:121:HIS:C	1:A:122:ARG:HG2	2.47	0.40
1:A:187:LYS:NZ	1:A:261:ASP:OD1	2.48	0.40
1:A:254:GLU:OE2	1:A:267:GLU:HG2	2.21	0.40
1:B:162:SER:O	1:B:163:GLN:C	2.63	0.40
1:C:126:GLU:HB3	1:C:128:THR:CG2	2.45	0.40
1:D:378:VAL:O	1:D:381:ILE:HG12	2.22	0.40
1:A:10:LEU:HD23	1:A:63:LEU:HD22	2.03	0.40
1:B:273:HIS:CD2	4:B:547:HOH:O	2.74	0.40
1:C:381:ILE:O	1:C:382:ARG:C	2.64	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	384/403 (95%)	363 (94%)	20 (5%)	1 (0%)	36	36
1	B	383/403 (95%)	368 (96%)	15 (4%)	0	100	100
1	C	382/403 (95%)	361 (94%)	19 (5%)	2 (0%)	24	22
1	D	379/403 (94%)	351 (93%)	27 (7%)	1 (0%)	36	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1528/1612 (95%)	1443 (94%)	81 (5%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	GLU
1	C	227	SER
1	D	324	THR
1	A	57	ARG

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	322/336 (96%)	277 (86%)	45 (14%)	3	2
1	B	321/336 (96%)	287 (89%)	34 (11%)	6	4
1	C	320/336 (95%)	275 (86%)	45 (14%)	3	2
1	D	317/336 (94%)	270 (85%)	47 (15%)	3	1
All	All	1280/1344 (95%)	1109 (87%)	171 (13%)	4	2

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	LEU
1	A	44	SER
1	A	47	ASP
1	A	55	LYS
1	A	61	ARG
1	A	62	GLN
1	A	65	LYS
1	A	66	THR
1	A	73	GLU
1	A	84	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	104	LYS
1	A	108	LYS
1	A	113	LYS
1	A	118	MET
1	A	124	LEU
1	A	125	VAL
1	A	134	LYS
1	A	138	GLN
1	A	139	LEU
1	A	145	LEU
1	A	147	SER
1	A	149	THR
1	A	150	MET
1	A	155	ARG
1	A	159	ARG
1	A	163	GLN
1	A	174	LYS
1	A	193	ILE
1	A	199	ASP
1	A	202	LEU
1	A	226	VAL
1	A	228	ASP
1	A	232	GLN
1	A	233	LYS
1	A	237	LEU
1	A	264	MET
1	A	265	LEU
1	A	270	SER
1	A	271	ARG
1	A	272	ILE
1	A	305	LEU
1	A	311	SER
1	A	344	SER
1	A	350	PRO
1	B	4	SER
1	B	5	ARG
1	B	26	LEU
1	B	28	ILE
1	B	39	PRO
1	B	44	SER
1	B	57	ARG
1	B	62[A]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62[B]	GLN
1	B	73	GLU
1	B	74	ILE
1	B	75	GLU
1	B	104	LYS
1	B	117	PRO
1	B	143	LEU
1	B	150	MET
1	B	167	PRO
1	B	171[A]	GLU
1	B	171[B]	GLU
1	B	174	LYS
1	B	178	LEU
1	B	200	GLU
1	B	202	LEU
1	B	211	GLN
1	B	230	ILE
1	B	233	LYS
1	B	265	LEU
1	B	272	ILE
1	B	327	GLN
1	B	334	SER
1	B	344	SER
1	B	362	PRO
1	B	378	VAL
1	B	381	ILE
1	C	6	LYS
1	C	26	LEU
1	C	57	ARG
1	C	61[A]	ARG
1	C	61[B]	ARG
1	C	65	LYS
1	C	73	GLU
1	C	74	ILE
1	C	87	SER
1	C	88	GLU
1	C	90	LYS
1	C	116	ILE
1	C	118	MET
1	C	120	GLU
1	C	126	GLU
1	C	139	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	142	PRO
1	C	155	ARG
1	C	159	ARG
1	C	163	GLN
1	C	174	LYS
1	C	181	GLU
1	C	182	LYS
1	C	196	LYS
1	C	197	THR
1	C	202	LEU
1	C	208	GLU
1	C	232	GLN
1	C	233	LYS
1	C	237	LEU
1	C	239	ARG
1	C	240	LYS
1	C	257	LEU
1	C	258	LEU
1	C	259	GLU
1	C	264	MET
1	C	268	ILE
1	C	274	ASN
1	C	323	ASP
1	C	324	THR
1	C	326	LEU
1	C	330	GLU
1	C	339	SER
1	C	344	SER
1	C	377	VAL
1	D	4	SER
1	D	5	ARG
1	D	9[A]	VAL
1	D	9[B]	VAL
1	D	28	ILE
1	D	37	ASN
1	D	47	ASP
1	D	54	PHE
1	D	55	LYS
1	D	56	GLU
1	D	57	ARG
1	D	58	GLU
1	D	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	62	GLN
1	D	63	LEU
1	D	65	LYS
1	D	66	THR
1	D	71	THR
1	D	74	ILE
1	D	75	GLU
1	D	84	GLU
1	D	87	SER
1	D	96	GLN
1	D	120	GLU
1	D	125	VAL
1	D	126	GLU
1	D	150	MET
1	D	171	GLU
1	D	174	LYS
1	D	176	ARG
1	D	182	LYS
1	D	187	LYS
1	D	188	MET
1	D	207	VAL
1	D	226	VAL
1	D	248	LYS
1	D	262	SER
1	D	264	MET
1	D	272	ILE
1	D	317	ILE
1	D	326	LEU
1	D	335	ILE
1	D	344	SER
1	D	357	ILE
1	D	366	GLU
1	D	368	GLU
1	D	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	138	GLN
1	A	225	ASN
1	A	303	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	327	GLN
1	B	106	ASN
1	B	211	GLN
1	B	232	GLN
1	C	29	GLN
1	C	106	ASN
1	C	232	GLN
1	D	62	GLN
1	D	102	GLN
1	D	106	ASN
1	D	127	ASN
1	D	138	GLN
1	D	325	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	$\# Z > 2$
2	ATP	B	400	3	32,33,33	1.09	3 (9%)	48,52,52	1.75	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	D	400	3	32,33,33	1.10	3 (9%)	48,52,52	2.59	14 (29%)
2	ATP	C	400	3	32,33,33	0.89	1 (3%)	48,52,52	1.63	12 (25%)
2	ATP	A	400	3	32,33,33	1.03	2 (6%)	48,52,52	2.16	16 (33%)

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	ATP	B	400	3	-	3/22/38/38	0/3/3/3
2	ATP	D	400	3	-	5/22/38/38	0/3/3/3
2	ATP	C	400	3	-	3/22/38/38	0/3/3/3
2	ATP	A	400	3	-	6/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ATP	C6-N6	-3.70	1.24	1.34
2	D	400	ATP	C2-N1	2.73	1.38	1.33
2	A	400	ATP	C6-N6	-2.72	1.27	1.34
2	D	400	ATP	C2-N3	-2.52	1.29	1.33
2	D	400	ATP	C6-N6	-2.44	1.28	1.34
2	B	400	ATP	C2-N1	2.27	1.38	1.33
2	A	400	ATP	C2-N1	2.20	1.37	1.33
2	B	400	ATP	C2-N3	-2.10	1.30	1.33
2	C	400	ATP	C6-N6	-2.02	1.29	1.34

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	ATP	C2-N1-C6	9.73	134.72	118.73
2	A	400	ATP	C2-N1-C6	6.59	129.56	118.73
2	D	400	ATP	C5-C6-N1	-6.13	101.94	117.51
2	D	400	ATP	O3B-PB-O1B	-5.56	93.97	110.70
2	B	400	ATP	O4'-C1'-N9	-5.02	98.45	108.09
2	A	400	ATP	C2'-C1'-N9	-4.69	101.65	113.30
2	A	400	ATP	C5-C6-N1	-4.51	106.07	117.51
2	A	400	ATP	C5-C6-N6	4.20	133.69	123.29
2	D	400	ATP	N6-C6-N1	4.16	127.64	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	ATP	N3-C2-N1	-4.04	122.46	128.58
2	B	400	ATP	C5-C6-N6	4.04	133.28	123.29
2	C	400	ATP	C2'-C1'-N9	-4.01	103.34	113.30
2	C	400	ATP	C4'-O4'-C1'	3.71	117.65	109.47
2	D	400	ATP	C6-C5-C4	3.68	122.20	117.18
2	C	400	ATP	N3-C2-N1	-3.38	123.47	128.58
2	A	400	ATP	O3G-PG-O3B	3.32	115.76	104.64
2	C	400	ATP	O3A-PA-O1A	3.18	120.27	110.70
2	B	400	ATP	O3'-C3'-C2'	3.13	121.86	111.82
2	D	400	ATP	N3-C4-N9	-3.10	121.89	127.17
2	D	400	ATP	C5-C4-N3	3.09	130.97	126.72
2	B	400	ATP	O2B-PB-O1B	2.98	126.31	112.44
2	A	400	ATP	O3'-C3'-C4'	-2.97	102.56	111.08
2	B	400	ATP	O2A-PA-O5'	-2.96	94.15	107.57
2	B	400	ATP	O2B-PB-O3A	-2.95	99.30	107.27
2	C	400	ATP	O3G-PG-O3B	2.93	114.45	104.64
2	D	400	ATP	O2A-PA-O3A	2.92	115.17	107.27
2	A	400	ATP	C6-C5-C4	2.86	121.08	117.18
2	D	400	ATP	C5-C6-N6	2.86	130.35	123.29
2	B	400	ATP	N6-C6-N1	-2.80	112.13	118.38
2	D	400	ATP	O3A-PA-O1A	-2.77	102.37	110.70
2	B	400	ATP	O3G-PG-O2G	2.74	118.09	107.80
2	A	400	ATP	N3-C2-N1	-2.74	124.43	128.58
2	D	400	ATP	O2B-PB-O3B	2.72	114.63	107.27
2	C	400	ATP	C5-C4-N3	-2.61	123.12	126.72
2	A	400	ATP	O5'-PA-O1A	2.52	118.94	108.94
2	D	400	ATP	O3A-PB-O1B	-2.50	103.17	110.70
2	A	400	ATP	O2G-PG-O3B	-2.47	96.34	104.64
2	C	400	ATP	PA-O5'-C5'	-2.43	107.45	121.35
2	A	400	ATP	C4-C5-N7	-2.41	107.82	110.58
2	A	400	ATP	C2'-C3'-C4'	-2.37	98.02	102.61
2	C	400	ATP	O4'-C1'-N9	2.36	112.62	108.09
2	C	400	ATP	C3'-C2'-C1'	2.36	105.92	101.46
2	A	400	ATP	N3-C4-N9	-2.32	123.23	127.17
2	B	400	ATP	O4'-C4'-C3'	-2.28	100.62	105.15
2	B	400	ATP	O2A-PA-O3A	2.28	113.44	107.27
2	A	400	ATP	O4'-C4'-C3'	-2.25	100.69	105.15
2	B	400	ATP	O2'-C2'-C1'	-2.24	102.41	110.10
2	D	400	ATP	O3'-C3'-C2'	2.21	118.91	111.82
2	A	400	ATP	O4'-C1'-N9	-2.13	104.00	108.09
2	A	400	ATP	N9-C8-N7	-2.08	110.98	113.94
2	C	400	ATP	O4'-C1'-C2'	-2.03	102.27	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	ATP	C2-N3-C4	2.02	116.77	111.83
2	C	400	ATP	O4'-C4'-C3'	-2.02	101.14	105.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	PB-O3B-PG-O3G
2	A	400	ATP	C5'-O5'-PA-O1A
2	B	400	ATP	PB-O3B-PG-O3G
2	C	400	ATP	PB-O3B-PG-O3G
2	D	400	ATP	PB-O3B-PG-O2G
2	D	400	ATP	PB-O3B-PG-O3G
2	C	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	O4'-C4'-C5'-O5'
2	D	400	ATP	PG-O3B-PB-O2B
2	B	400	ATP	PB-O3B-PG-O1G
2	C	400	ATP	PB-O3B-PG-O1G
2	B	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	PG-O3B-PB-O1B
2	D	400	ATP	PG-O3B-PB-O1B
2	D	400	ATP	PB-O3B-PG-O1G
2	A	400	ATP	PG-O3B-PB-O2B

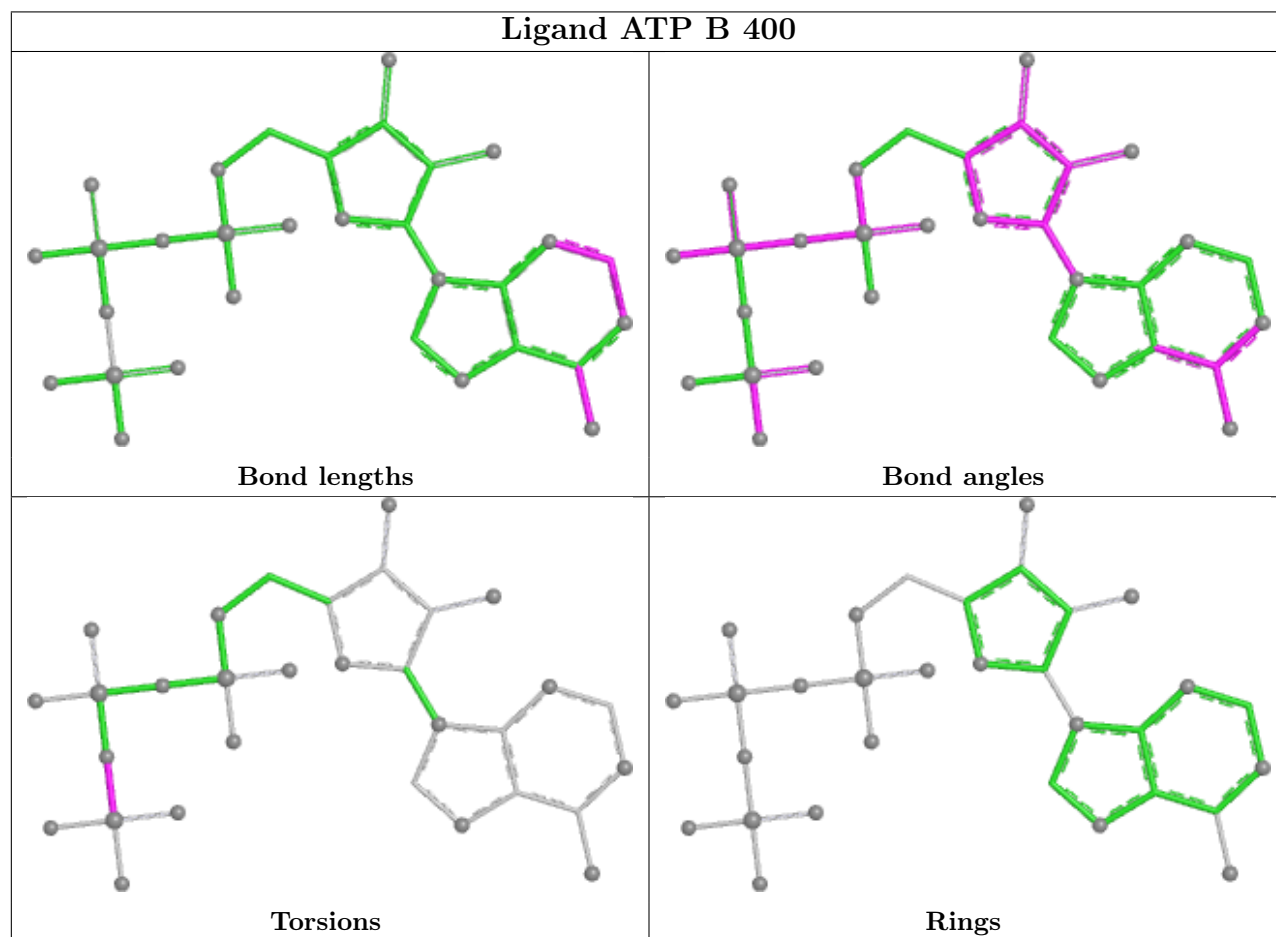
There are no ring outliers.

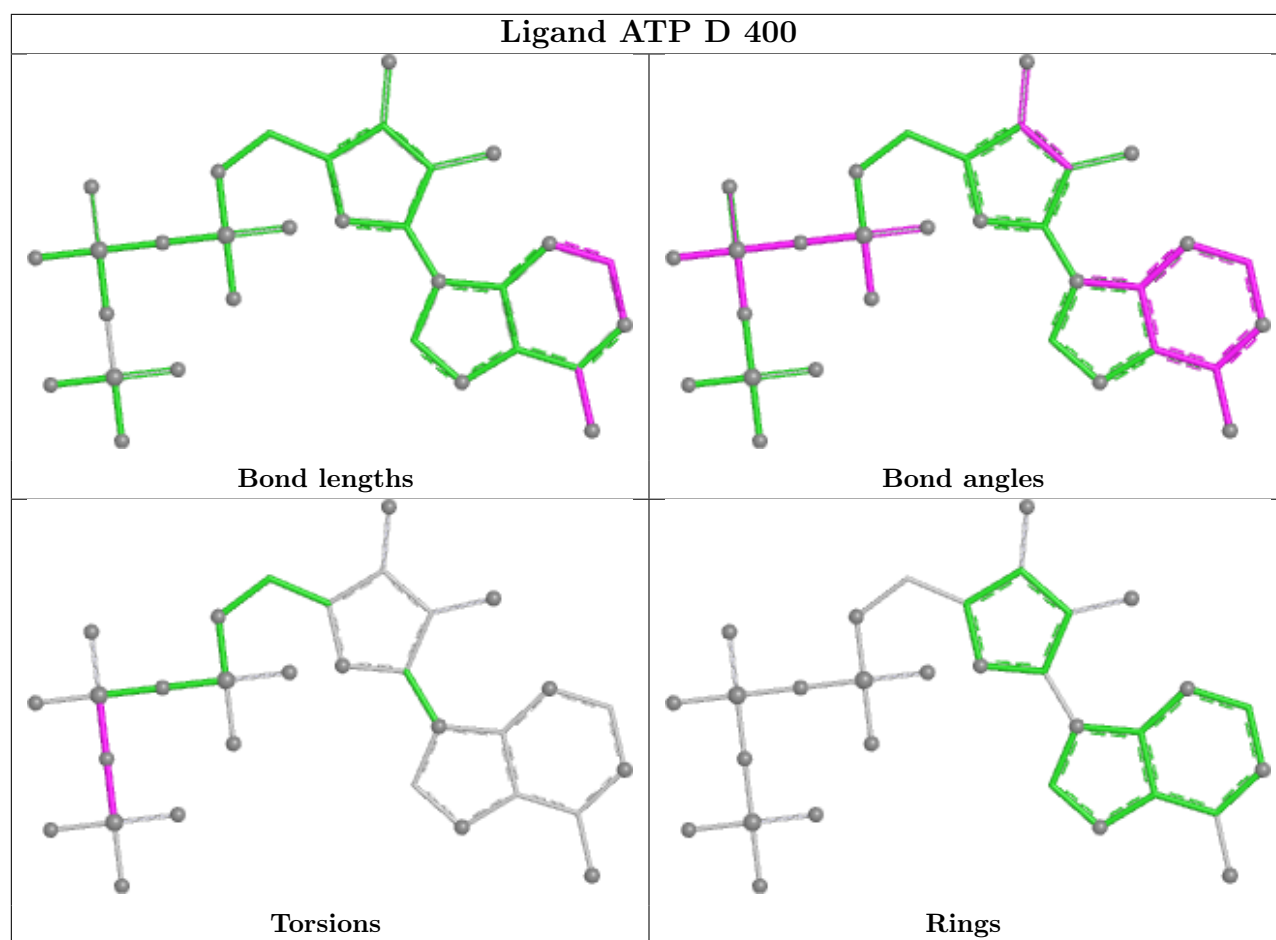
4 monomers are involved in 6 short contacts:

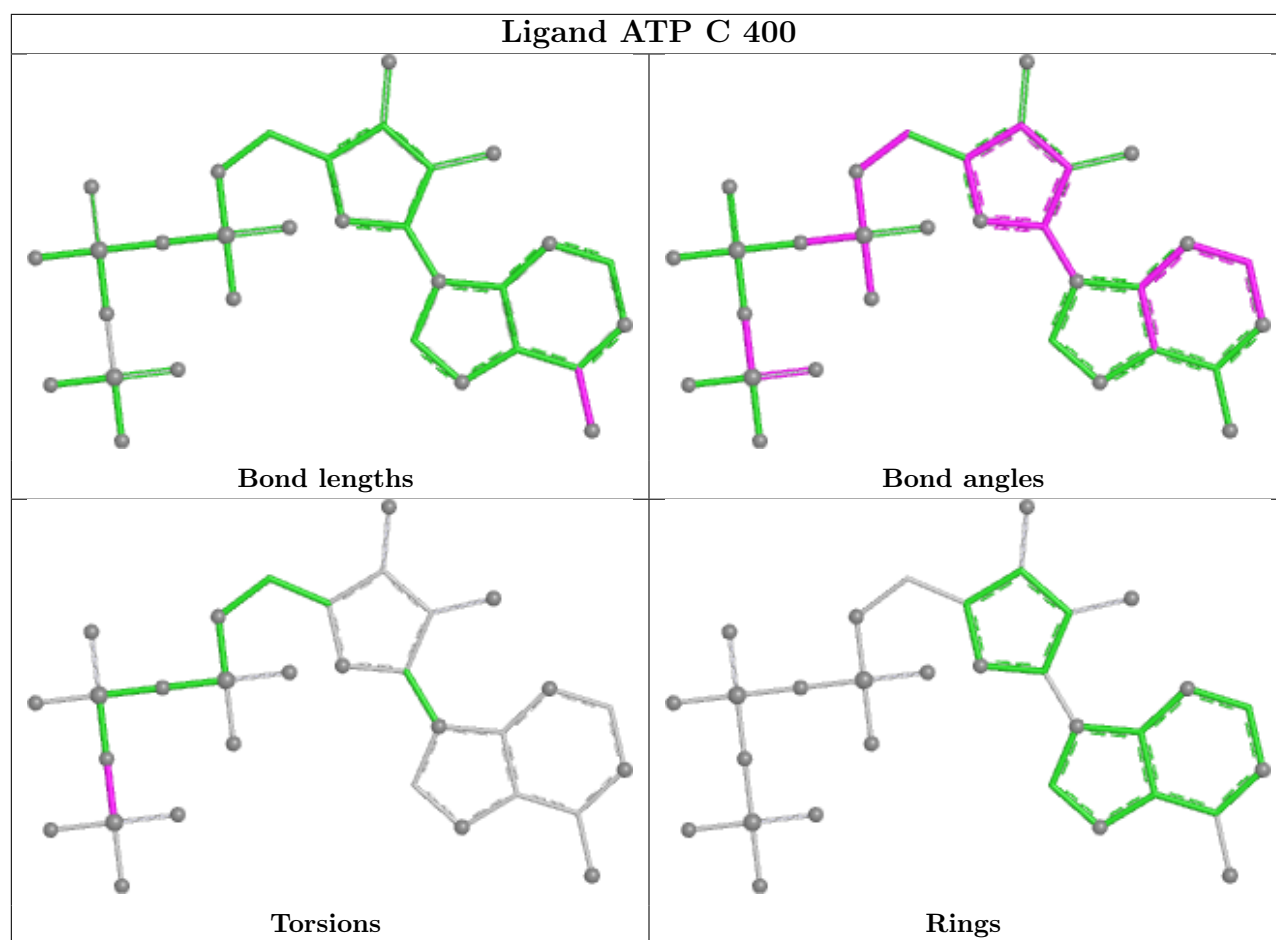
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ATP	2	0
2	D	400	ATP	2	0
2	C	400	ATP	1	0
2	A	400	ATP	1	0

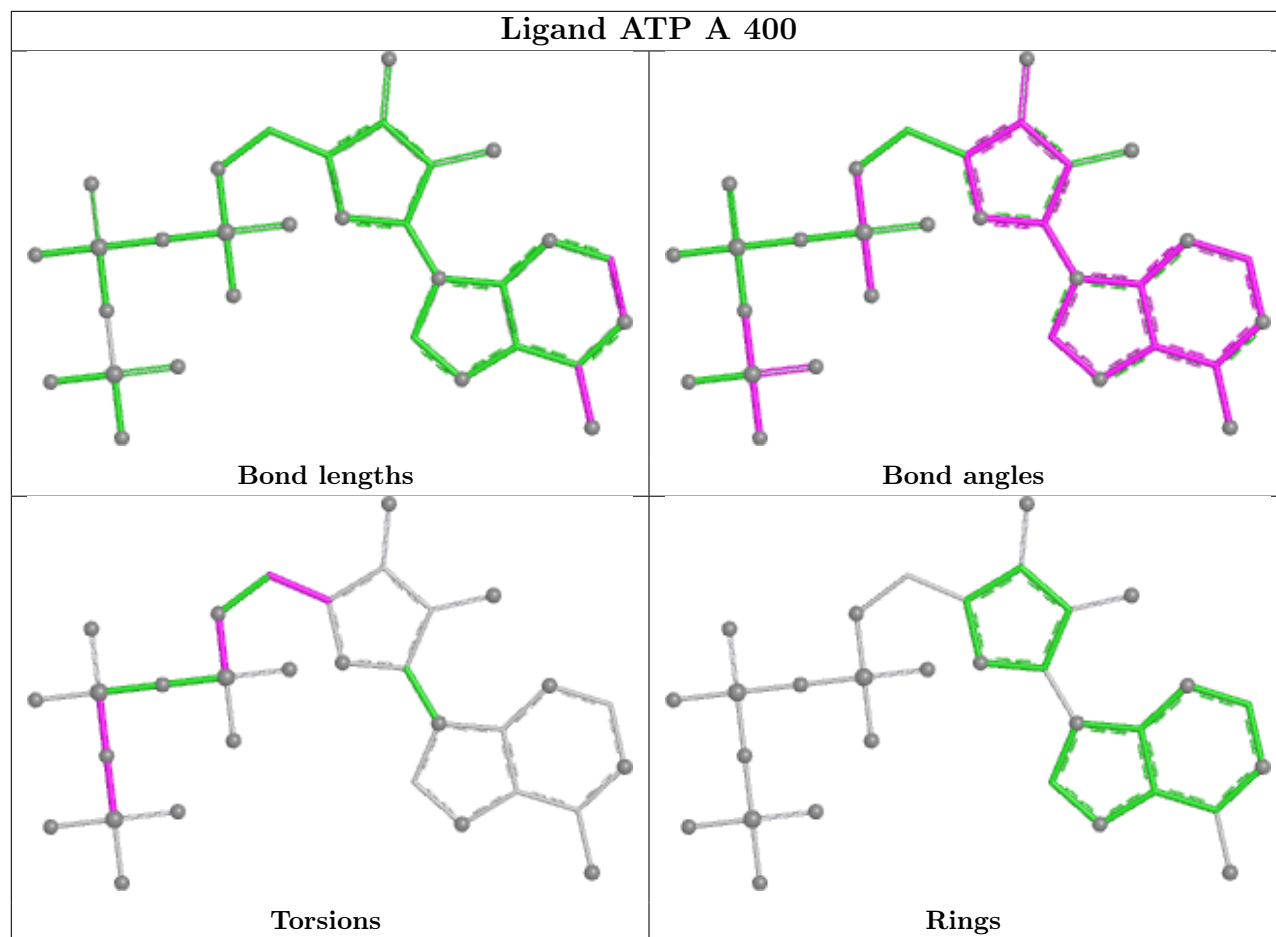
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	382/403 (94%)	0.20	21 (5%)	30	32	6, 25, 62, 81	4 (1%)
1	B	380/403 (94%)	0.18	25 (6%)	24	26	6, 24, 64, 86	5 (1%)
1	C	382/403 (94%)	0.46	33 (8%)	16	17	12, 30, 69, 93	2 (0%)
1	D	380/403 (94%)	0.39	33 (8%)	16	16	11, 29, 70, 93	1 (0%)
All	All	1524/1612 (94%)	0.31	112 (7%)	21	22	6, 27, 67, 93	12 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	381	ILE	5.4
1	C	321	ALA	4.7
1	B	320	ALA	4.6
1	D	381	ILE	4.5
1	D	320	ALA	4.4
1	B	54	PHE	4.2
1	D	54	PHE	4.2
1	A	167	PRO	4.1
1	C	320	ALA	3.9
1	D	346	GLY	3.9
1	B	152	TYR	3.8
1	A	321	ALA	3.7
1	A	1	MET	3.7
1	B	37	ASN	3.7
1	C	322	PRO	3.6
1	A	382	ARG	3.5
1	C	96	GLN	3.4
1	D	326	LEU	3.3
1	A	319	GLY	3.3
1	C	154	GLY	3.3
1	C	47	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	177	PRO	3.2
1	D	175	ASP	3.2
1	D	74	ILE	3.1
1	C	257	LEU	3.1
1	C	1	MET	3.1
1	C	381	ILE	3.1
1	C	152	TYR	3.1
1	D	37	ASN	3.0
1	C	319	GLY	3.0
1	D	347	ALA	3.0
1	B	88	GLU	2.9
1	C	318	GLY	2.8
1	D	55	LYS	2.8
1	C	323	ASP	2.7
1	C	233	LYS	2.7
1	C	158	PHE	2.7
1	A	323	ASP	2.7
1	A	229	ALA	2.7
1	B	322	PRO	2.7
1	B	325	HIS	2.7
1	D	322	PRO	2.6
1	D	174	LYS	2.6
1	C	380	ARG	2.6
1	D	321	ALA	2.6
1	B	324	THR	2.6
1	C	258	LEU	2.6
1	D	325	HIS	2.6
1	A	163	GLN	2.5
1	B	35	ALA	2.5
1	D	2	TRP	2.5
1	D	150	MET	2.5
1	A	114	TYR	2.5
1	D	319	GLY	2.5
1	C	85	VAL	2.5
1	D	135	VAL	2.5
1	D	173	LEU	2.5
1	B	174	LYS	2.5
1	C	37	ASN	2.5
1	C	153	ASP	2.4
1	D	152	TYR	2.4
1	A	381	ILE	2.4
1	C	155	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	382	ARG	2.4
1	B	326	LEU	2.4
1	B	57	ARG	2.4
1	A	152	TYR	2.4
1	B	76	HIS	2.4
1	B	163	GLN	2.4
1	C	199	ASP	2.4
1	D	164	ASP	2.4
1	A	263	ILE	2.4
1	B	321	ALA	2.3
1	A	65	LYS	2.3
1	C	150	MET	2.3
1	A	232	GLN	2.3
1	D	75	GLU	2.3
1	B	66	THR	2.3
1	B	380	ARG	2.3
1	A	126	GLU	2.2
1	D	80	TYR	2.2
1	D	76	HIS	2.2
1	C	62	GLN	2.2
1	D	4	SER	2.2
1	C	164	ASP	2.2
1	D	47	ASP	2.2
1	D	165	ASP	2.2
1	D	170	LEU	2.2
1	A	380	ARG	2.2
1	D	349	LYS	2.2
1	B	154	GLY	2.2
1	B	365	HIS	2.2
1	D	96	GLN	2.1
1	C	325	HIS	2.1
1	B	155	ARG	2.1
1	C	348	ALA	2.1
1	B	233	LYS	2.1
1	D	365	HIS	2.1
1	C	48	GLY	2.1
1	A	225	ASN	2.1
1	C	163	GLN	2.1
1	A	141	TYR	2.1
1	A	113	LYS	2.1
1	A	320	ALA	2.1
1	C	243	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	292	LEU	2.0
1	B	65	LYS	2.0
1	B	74	ILE	2.0
1	C	201	VAL	2.0
1	D	151	ALA	2.0
1	C	139	LEU	2.0
1	D	65	LYS	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](#)

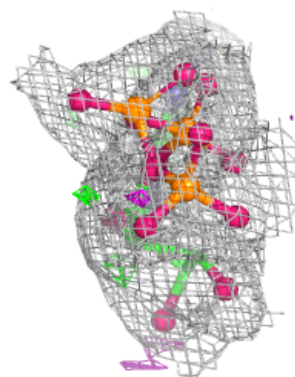
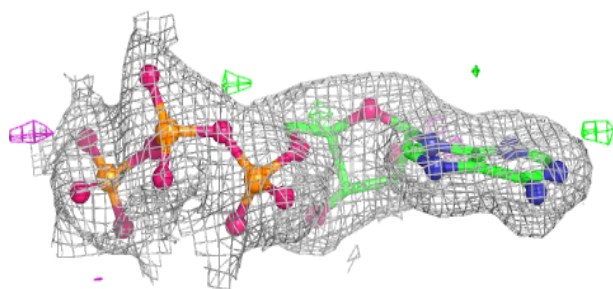
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	MG	A	401	1/1	0.94	0.03	14,14,14,14	0
2	ATP	B	400	31/31	0.96	0.08	7,28,44,63	0
3	MG	B	401	1/1	0.96	0.05	22,22,22,22	0
3	MG	D	401	1/1	0.96	0.04	33,33,33,33	0
2	ATP	D	400	31/31	0.97	0.07	12,26,56,100	0
2	ATP	C	400	31/31	0.97	0.08	12,30,82,100	0
2	ATP	A	400	31/31	0.98	0.06	9,23,33,75	0
3	MG	B	402	1/1	0.98	0.03	25,25,25,25	0
3	MG	C	401	1/1	0.98	0.04	40,40,40,40	0
3	MG	C	402	1/1	0.98	0.05	22,22,22,22	0
3	MG	A	402	1/1	0.98	0.03	24,24,24,24	0
3	MG	D	402	1/1	0.98	0.04	24,24,24,24	0

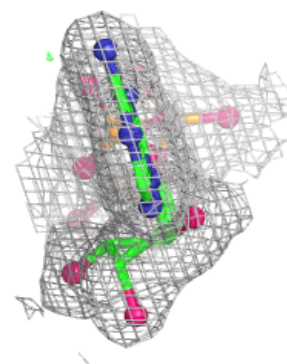
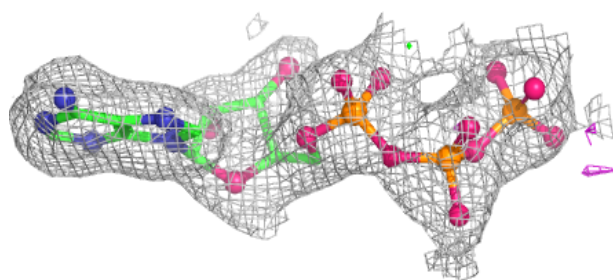
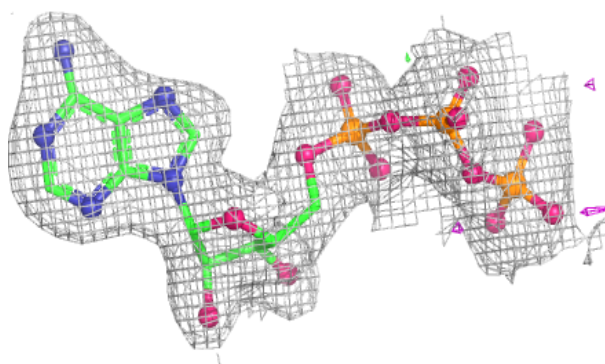
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 400:

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

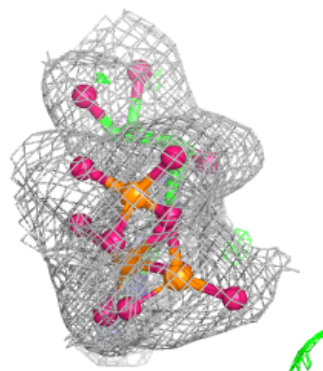
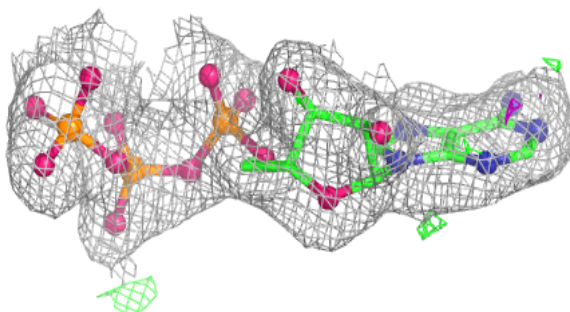
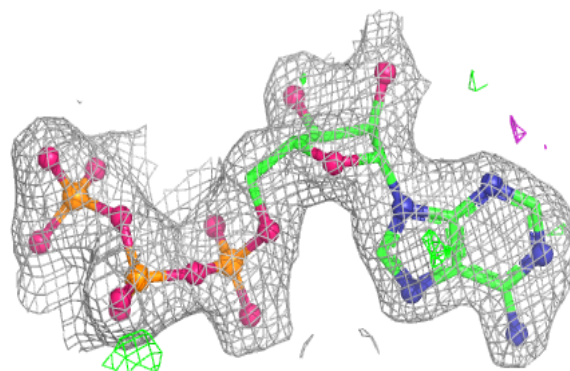
**Electron density around ATP D 400:**

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

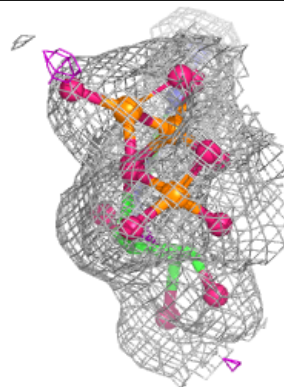
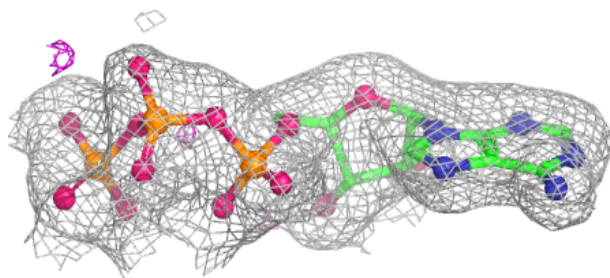
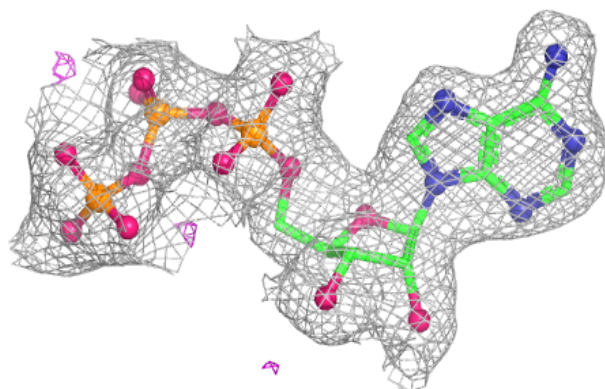


Electron density around ATP C 400:

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

**Electron density around ATP A 400:**

$2mF_o-DF_c$ (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.