



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 02:03 am BST

PDB ID : 3K5H
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

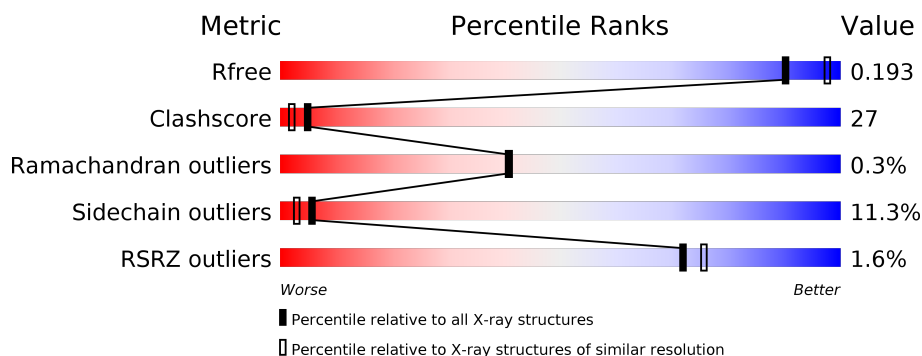
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	
1	B	403	
1	C	403	
1	D	403	

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...

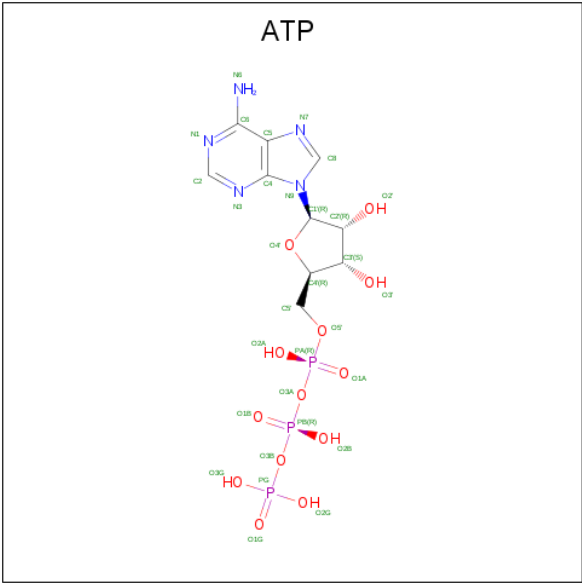
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP A1CII2
B	-17	SER	-	EXPRESSION TAG	UNP A1CII2
B	-16	SER	-	EXPRESSION TAG	UNP A1CII2
B	-15	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-14	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-13	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-12	HIS	-	EXPRESSION TAG	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 (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Continued from previous page...

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

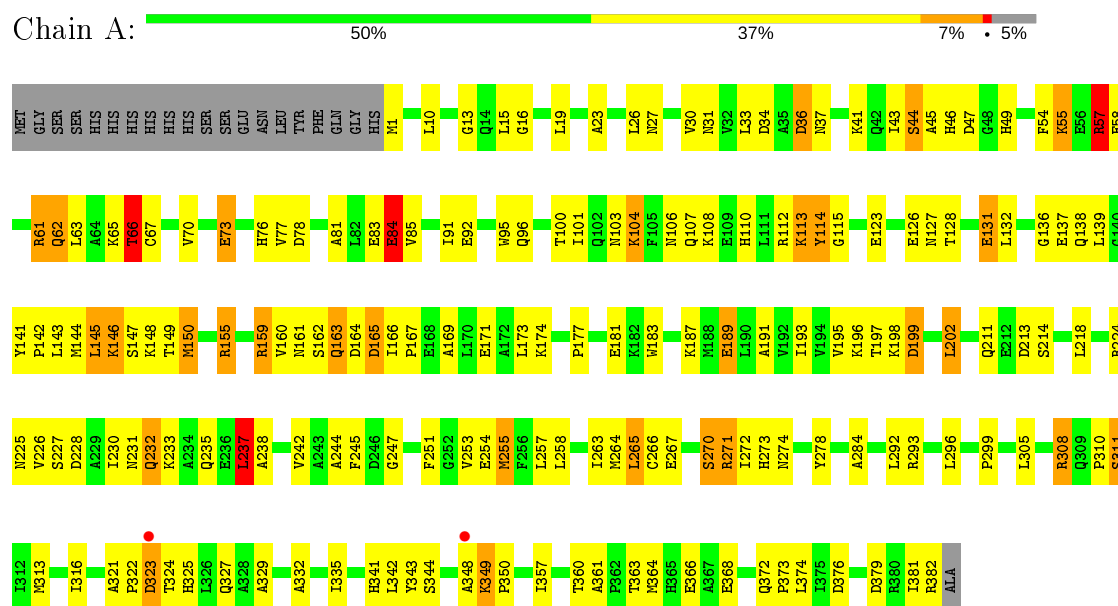
- Molecule 4 is water.

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		

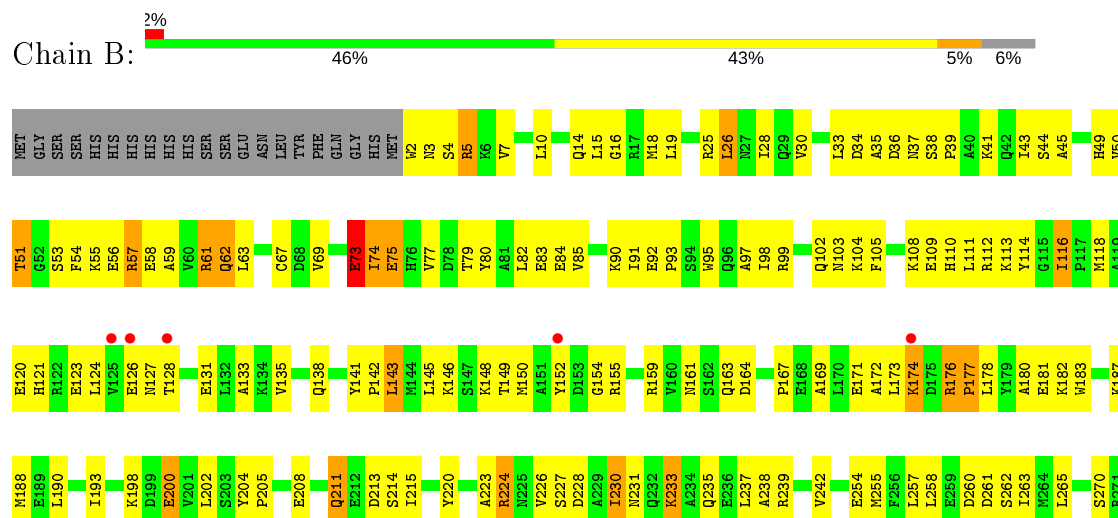
3 Residue-property plots

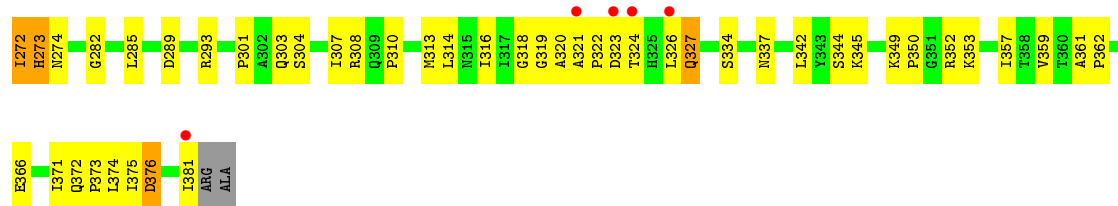
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

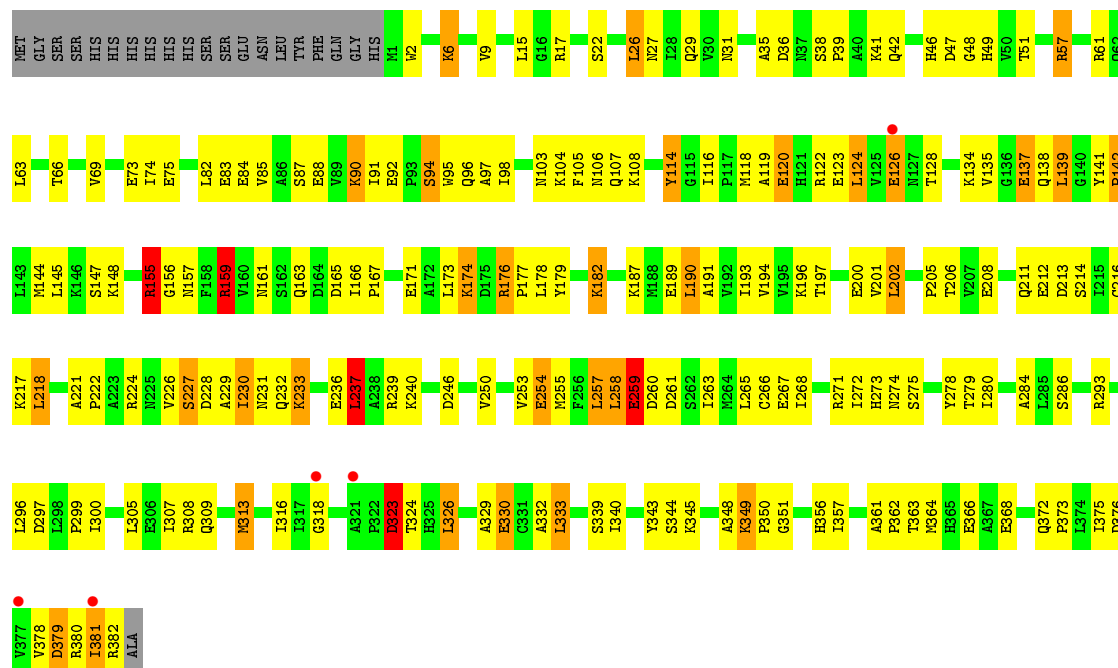


• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

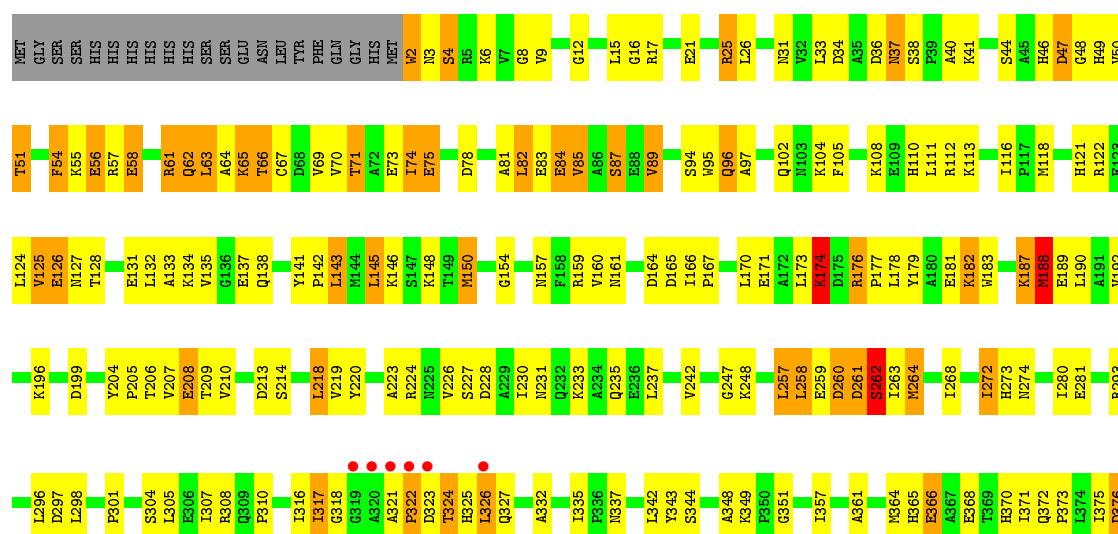
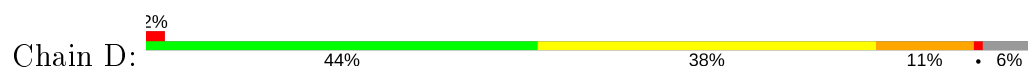


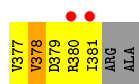


• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase



• 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	75.90 Å 134.40 Å 99.60 Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 40.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.10) 93.5 (40.62-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.63 (at 2.10 Å)	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)	0.32 , 104.3	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	0.94	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: MG, ATP

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	0.79	1/3046 (0.0%)	1.49	29/4124 (0.7%)
1	B	0.79	1/3042 (0.0%)	1.53	31/4120 (0.8%)
1	C	0.77	1/3036 (0.0%)	1.46	20/4110 (0.5%)
1	D	0.73	1/3005 (0.0%)	1.55	42/4071 (1.0%)
All	All	0.77	4/12129 (0.0%)	1.51	122/16425 (0.7%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	CYS	CB-SG	-6.34	1.71	1.82
1	A	189	GLU	CD-OE1	-5.96	1.19	1.25
1	C	137	GLU	CB-CG	-5.77	1.41	1.52
1	D	188	MET	SD-CE	-5.67	1.46	1.77

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	LEU	CB-CG-CD1	-11.52	91.42	111.00
1	C	144	MET	CG-SD-CE	-10.85	82.85	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	127	ASN	N-CA-CB	-10.72	91.30	110.60
1	A	376	ASP	CB-CG-OD1	-9.95	109.34	118.30
1	B	289	ASP	CB-CG-OD2	9.28	126.66	118.30
1	B	257	LEU	CB-CG-CD1	9.11	126.48	111.00
1	A	376	ASP	CB-CG-OD2	8.89	126.30	118.30
1	C	323	ASP	CB-CA-C	-8.18	94.03	110.40
1	C	381	ILE	CB-CA-C	-8.16	95.27	111.60
1	B	224	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	57	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	36	ASP	CB-CG-OD1	-7.53	111.52	118.30
1	B	224	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	239	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	D	228	ASP	CB-CG-OD1	7.41	124.97	118.30
1	D	376	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	D	261	ASP	CB-CG-OD2	7.25	124.82	118.30
1	D	273	HIS	N-CA-CB	-7.24	97.58	110.60
1	B	273	HIS	N-CA-CB	-7.22	97.60	110.60
1	D	305	LEU	CB-CG-CD1	-7.22	98.72	111.00
1	A	374	LEU	CB-CG-CD1	7.21	123.25	111.00
1	C	349	LYS	N-CA-C	-7.16	91.68	111.00
1	B	376	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	D	308	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	C	379	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	B	202	LEU	CB-CG-CD2	-6.95	99.19	111.00
1	C	155	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	84	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	B	5	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	66	THR	N-CA-CB	-6.84	97.30	110.30
1	B	374	LEU	CB-CG-CD1	-6.83	99.39	111.00
1	D	67	CYS	CA-CB-SG	-6.83	101.71	114.00
1	D	85	VAL	CB-CA-C	-6.82	98.44	111.40
1	A	379	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	C	124	LEU	CB-CG-CD2	-6.76	99.50	111.00
1	C	94	SER	CB-CA-C	-6.70	97.37	110.10
1	C	271	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	A	278	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	D	224	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	25	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	D	317	ILE	CB-CA-C	-6.42	98.77	111.60
1	D	69	VAL	CB-CA-C	-6.41	99.22	111.40
1	B	159	ARG	NE-CZ-NH2	6.34	123.47	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	LEU	CA-CB-CG	-6.33	100.74	115.30
1	B	164	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	D	143	LEU	CB-CA-C	-6.29	98.24	110.20
1	B	69	VAL	CB-CA-C	-6.26	99.51	111.40
1	C	190	LEU	CB-CG-CD2	-6.25	100.38	111.00
1	C	176	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	143	LEU	CA-CB-CG	6.19	129.53	115.30
1	C	333	LEU	CB-CG-CD1	-6.07	100.67	111.00
1	D	376	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	319	GLY	N-CA-C	-6.03	98.01	113.10
1	A	237	LEU	CB-CG-CD2	6.03	121.25	111.00
1	D	89	VAL	CG1-CB-CG2	5.95	120.43	110.90
1	D	260	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	323	ASP	CB-CA-C	-5.92	98.55	110.40
1	A	273	HIS	N-CA-CB	-5.90	99.97	110.60
1	B	51	THR	CB-CA-C	-5.90	95.68	111.60
1	B	99	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	99	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	255	MET	CA-CB-CG	-5.83	103.39	113.30
1	D	143	LEU	CB-CG-CD2	-5.82	101.10	111.00
1	D	261	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	78	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	335	ILE	CG1-CB-CG2	5.79	124.15	111.40
1	A	36	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	197	THR	CA-CB-CG2	-5.79	104.30	112.40
1	D	257	LEU	CB-CG-CD1	5.78	120.82	111.00
1	D	199	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	155	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	308	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	254	GLU	OE1-CD-OE2	-5.72	116.43	123.30
1	D	21	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	D	371	ILE	N-CA-C	5.64	126.22	111.00
1	D	262	SER	N-CA-C	-5.62	95.83	111.00
1	B	116	ILE	CG1-CB-CG2	5.59	123.69	111.40
1	A	278	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	220	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	D	308	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	145	LEU	CB-CG-CD1	5.56	120.46	111.00
1	D	174	LYS	CB-CA-C	-5.56	99.28	110.40
1	B	120	GLU	N-CA-CB	-5.55	100.61	110.60
1	B	349	LYS	N-CA-C	-5.53	96.07	111.00
1	B	18	MET	CA-CB-CG	-5.53	103.90	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	GLU	CB-CA-C	-5.53	99.34	110.40
1	B	143	LEU	CB-CA-C	-5.52	99.71	110.20
1	D	281	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	D	82	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	D	165	ASP	N-CA-C	-5.48	96.22	111.00
1	B	345	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	D	51	THR	CB-CA-C	-5.47	96.83	111.60
1	C	9	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	D	164	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	A	349	LYS	N-CA-C	-5.38	96.47	111.00
1	C	237	LEU	CB-CG-CD2	5.37	120.13	111.00
1	D	218	LEU	CB-CA-C	-5.36	100.02	110.20
1	A	195	VAL	CB-CA-C	-5.32	101.30	111.40
1	B	177	PRO	N-CA-C	-5.30	98.31	112.10
1	A	165	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	B	61	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	146	LYS	CD-CE-NZ	5.25	123.77	111.70
1	C	165	ASP	CB-CA-C	-5.22	99.96	110.40
1	D	322	PRO	N-CA-C	5.22	125.66	112.10
1	C	159	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	181	GLU	CB-CA-C	-5.21	99.97	110.40
1	B	73	GLU	CA-CB-CG	5.18	124.79	113.40
1	D	44	SER	N-CA-CB	-5.17	102.75	110.50
1	C	116	ILE	CG1-CB-CG2	5.15	122.73	111.40
1	D	179	TYR	N-CA-C	-5.13	97.16	111.00
1	D	208	GLU	N-CA-CB	-5.13	101.37	110.60
1	C	230	ILE	CG1-CB-CG2	-5.12	100.14	111.40
1	C	200	GLU	CB-CA-C	-5.11	100.19	110.40
1	D	258	LEU	CA-CB-CG	-5.09	103.59	115.30
1	A	202	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	D	2	TRP	N-CA-CB	5.08	119.74	110.60
1	D	280	ILE	CA-CB-CG1	5.05	120.61	111.00
1	B	176	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	228	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	343	TYR	N-CA-C	5.03	124.58	111.00
1	D	26	LEU	CB-CG-CD1	-5.01	102.49	111.00

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
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	135	0
1	B	2969	0	2965	161	0
1	C	2975	0	2991	162	0
1	D	2948	0	2960	205	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	9	0
4	D	196	0	0	12	0
All	All	12850	0	11952	659	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 27.

All (659) 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:174:LYS:HD2	1:B:174:LYS:H	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:HG3	1:C:61[B]:ARG:HH11	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:HH11	1:C:155:ARG:HG2	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: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:201:VAL:C	1:C:202:LEU:HD23	1.95	0.86
1:C:233:LYS:HB3	1:C:263:ILE:HD12	1.58	0.84
1:B:59:ALA:HA	1:B:62[B]:GLN:HG3	1.58	0.84
1:D:54:PHE:H	1:D:54:PHE:HD1	1.24	0.84
1:A:66:THR:HG22	1:A:67[B]:CYS:SG	2.18	0.82
1:B:174:LYS:CD	1:B:174:LYS:H	1.92	0.82
1:B:174:LYS:N	1:B:174:LYS:HD2	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:D:112:ARG:HG3	1:D:118:MET:CE	2.12	0.80
1:B:108:LYS:O	1:B:118:MET:HE1	1.82	0.80
1:C:6:LYS:HE2	1:C:29:GLN:CD	2.02	0.79
1:B:188:MET:HE1	1:B:226:VAL:HG21	1.63	0.79
1:B:112:ARG:HG2	1:B:118:MET:HE3	1.65	0.78
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:D:112:ARG:HG3	1:D:118:MET:HE3	1.66	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:188:MET:CE	1:B:226:VAL:HG21	2.17	0.74
1:B:36:ASP:O	1:B:37:ASN:HB3	1.87	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:126:GLU:HB3	1:C:128:THR:HG23	1.70	0.73
1:C:6:LYS:HE2	1:C:29:GLN:NE2	2.03	0.73
1:B:188:MET:HE2	1:B:190:LEU:HD21	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: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: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: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:HA	1:D:62:GLN:HE21	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:15:LEU:HB2	1:D:73:GLU:HG2	1.74	0.69
1:B:112:ARG:HG2	1:B:118:MET:CE	2.21	0.69
1:D:33:LEU:HB2	1:D:63:LEU:HG	1.73	0.69
1:C:318:GLY:HA3	1:C:349:LYS:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:148:LYS:HD2	1:B:177:PRO:HB2	1.76	0.68
1:B:146:LYS:HE3	1:B:181:GLU:OE1	1.92	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:141:TYR:HB3	1:D:142:PRO:HA	1.75	0.68
1:D:54:PHE:N	1:D:54:PHE:CD1	2.51	0.68
1:A:361:ALA:HB1	1:A:366:GLU:HG2	1.75	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: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: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:B:57:ARG:HG3	1:B:58:GLU:N	2.11	0.65
1:A:143:LEU:CD1	1:A:160:VAL:HB	2.27	0.65
1:D:2:TRP:C	1:D:4:SER:H	2.00	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:258:LEU:O	1:C:261:ASP:N	2.26	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:A:110:HIS:O	1:A:113:LYS:HD3	1.97	0.63
1:D:108:LYS:O	1:D:118:MET:HE3	1.99	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:D:188:MET:HE3	1:D:190:LEU:HD21	1.80	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:D:323:ASP:O	1:D:324:THR:C	2.36	0.63
1:A:166:ILE:CB	1:A:167:PRO:HD3	2.28	0.63
1:D:141:TYR:HA	1:D:142:PRO:C	2.19	0.63
1:D:323:ASP:O	1:D:326:LEU:N	2.31	0.63
1:D:188:MET:HE3	1:D:190:LEU:CD2	2.29	0.62
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: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:364:MET:O	1:C:368:GLU:HG3	1.99	0.62
1:C:94:SER:OG	1:C:246:ASP:HB2	1.98	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:B:74:ILE:HD12	1:B:77:VAL:HG13	1.82	0.62
1:D:126:GLU:HB2	1:D:131:GLU:CD	2.20	0.62
1:C:85:VAL:O	1:C:85:VAL:HG22	1.99	0.61
1:B:353:LYS:HE3	4:B:431:HOH:O	2.00	0.61
1:B:53:SER:HB3	1:B:56:GLU:HG3	1.81	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:A:381:ILE:O	1:A:382:ARG:C	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:381:ILE:HG22	1:C:382:ARG:N	2.16	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:HB3	1:D:61:ARG:HH11	1.66	0.60
1:A:143:LEU:HD12	1:A:143:LEU:O	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: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: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:B:150:MET:HA	1:B:150:MET:HE3	1.85	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:N	1:B:174:LYS:CD	2.60	0.57
1:C:258:LEU:C	1:C:260:ASP:H	2.08	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:188:MET:HE1	1:B:226:VAL:CG2	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:120:GLU:HB2	1:C:182:LYS:HD2	1.87	0.57
1:D:110:HIS:HA	1:D:113:LYS:CE	2.31	0.57
1:D:46:HIS:ND1	1:D:48:GLY:N	2.52	0.57
1:B:238:ALA:O	1:B:242:VAL:HG23	2.05	0.57
1:D:112:ARG:HG3	1:D:118:MET:HE2	1.85	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:308:ARG:NH1	4:B:472:HOH:O	2.31	0.56
1:A:137:GLU:O	1:A:137:GLU:HG3	2.05	0.56
1:B:226:VAL:HG13	1:B:230:ILE:CG2	2.35	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:B:188:MET:HE3	1:B:190:LEU:CD2	2.35	0.56
1:D:173:LEU:HD13	1:D:178:LEU:CD2	2.36	0.56
1:A:112:ARG:HB3	1:A:112:ARG:HH11	1.71	0.56
1:A:213:ASP:O	1:A:214:SER:HB2	2.05	0.56
1:C:372:GLN:NE2	1:C:376:ASP:OD1	2.38	0.56
1:B:85:VAL:HG23	1:B:91:ILE:HD11	1.87	0.56
1:C:202:LEU:N	1:C:202:LEU:HD23	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:30:VAL:O	1:A:46:HIS:NE2	2.39	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: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:HA	1:A:232:GLN:OE1	2.06	0.55
1:A:143:LEU:HD12	1:A:160:VAL:HB	1.89	0.55
1:A:31:ASN:HD22	1:A:66:THR:HG23	1.72	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:C:155:ARG:HG2	1:C:155:ARG:NH1	2.03	0.55
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:N	1:B:124:LEU:HD12	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:273:HIS:CE1	1:C:275:SER:HB3	2.43	0.54
1:D:73:GLU:C	1:D:74:ILE:HG13	2.26	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: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:A:237:LEU:HD12	1:A:237:LEU:C	2.28	0.54
1:B:198:LYS:HG3	4:B:529:HOH:O	2.08	0.53
1:D:127:ASN:ND2	1:D:178:LEU:HD12	2.20	0.53
1:A:163:GLN:HA	1:A:166:ILE:HG13	1.90	0.53
1:A:101:ILE:HD12	1:A:270:SER:HB3	1.90	0.53
1:A:293:ARG:HD3	1:A:299:PRO:O	2.09	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:194:VAL:HG13	1:C:202:LEU:O	2.09	0.53
1:C:61[B]:ARG:HG3	1:C:61[B]:ARG:NH1	2.08	0.53
1:A:36:ASP:HA	4:A:507:HOH:O	2.09	0.53
1:C:201:VAL:O	1:C:202:LEU:HD23	2.07	0.53
1:C:31:ASN:HD22	1:C:66:THR:CG2	2.21	0.53
1:A:54:PHE:HB2	1:A:77:VAL:HG12	1.91	0.53
1:C:258:LEU:C	1:C:260:ASP:N	2.63	0.53
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:92:GLU:HA	1:B:93:PRO:C	2.29	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:34:ASP:O	1:D:41:LYS:NZ	2.26	0.52
1:D:188:MET:HE1	1:D:226:VAL:CG2	2.40	0.52
1:A:76:HIS:HB3	1:A:150:MET:HE3	1.92	0.52
1:C:187:LYS:HD3	1:C:259:GLU:HA	1.91	0.52
1:D:148:LYS:HD2	1:D:177:PRO:HB2	1.91	0.52
1:D:33:LEU:HD12	1:D:34:ASP:N	2.25	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:173:LEU:HD12	1:D:178:LEU:HD22	1.91	0.51
1:D:96:GLN:HG2	4:D:404:HOH:O	2.09	0.51
1:A:113:LYS:C	1:A:115:GLY:H	2.14	0.51
1:A:91:ILE:C	1:A:92:GLU:HG2	2.29	0.51
1:C:61[A]:ARG:NH2	1:C:84:GLU:OE2	2.43	0.51
1:D:173:LEU:CD1	1:D:178:LEU:HD22	2.41	0.51
1:D:61:ARG:CB	1:D:61:ARG:HH11	2.23	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:308:ARG:NH1	4:C:691:HOH:O	2.27	0.51
1:C:95:TRP:CH2	1:C:96:GLN:HG3	2.44	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:D:375:ILE:O	1:D:376:ASP:C	2.48	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:116:ILE:O	1:D:118:MET:HG2	2.10	0.51
1:C:356:HIS:C	1:C:356:HIS:CD2	2.85	0.50
1:D:204:TYR:HB3	1:D:205:PRO:CD	2.41	0.50
1:D:188:MET:HE1	1:D:226:VAL:HG21	1.92	0.50
1:A:83:GLU:HG3	1:A:95:TRP:CZ2	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:HIS:HB2	4:B:426:HOH:O	2.12	0.50
1:C:104:LYS:O	1:C:108:LYS:HG3	2.12	0.50
1:D:316:ILE:HG21	1:D:325:HIS:HB2	1.94	0.50
1:A:143:LEU:C	1:A:143:LEU:HD12	2.32	0.50
1:A:55:LYS:HE3	1:A:150:MET:HE2	1.94	0.50
1:B:114:TYR:CD2	1:B:114:TYR:N	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:B:375:ILE:O	1:B:376:ASP:C	2.50	0.49
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:D:85:VAL:C	1:D:87:SER:N	2.66	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:N	1:D:260:ASP:OD1	2.45	0.49
1:D:317:ILE:O	1:D:318:GLY:C	2.50	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:D:85:VAL:C	1:D:87:SER:H	2.15	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:B:126:GLU:CB	1:B:128:THR:HG23	2.43	0.49
1:A:284:ALA:CB	1:B:337:ASN:HA	2.42	0.49
1:A:104:LYS:O	1:A:108:LYS:HG3	2.13	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:135:VAL:O	1:D:138:GLN:N	2.44	0.48
1:D:192:VAL:HG22	1:D:206:THR:HA	1.94	0.48
1:D:15:LEU:CB	1:D:73:GLU:HG2	2.42	0.48
1:B:110:HIS:O	1:B:113:LYS:HG3	2.12	0.48
1:B:57:ARG:CG	1:B:58:GLU:N	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:188:MET:HE2	1:B:226:VAL:HG21	1.96	0.48
1:B:169:ALA:O	1:B:172:ALA:HB3	2.14	0.48
1:C:224:ARG:NH2	1:C:368:GLU:OE1	2.45	0.48
1:C:94:SER:CB	1:C:97:ALA:H	2.27	0.48
1:D:260:ASP:OD1	1:D:262:SER:HB3	2.13	0.48
1:D:33:LEU:O	1:D:34:ASP:HB2	2.14	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: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:142:PRO:HB3	1:B:161:ASN:HA	1.96	0.47
1:D:188:MET:SD	1:D:208:GLU:HG3	2.54	0.47
1:B:258:LEU:HB2	1:B:262:SER:OG	2.14	0.47
1:B:237:LEU:HD23	1:B:263:ILE:HG22	1.95	0.47
1:D:173:LEU:CD1	1:D:178:LEU:CD2	2.93	0.47
1:D:34:ASP:O	1:D:51:THR:HA	2.14	0.47
1:D:62:GLN:CA	1:D:62:GLN:NE2	2.77	0.47
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:141:TYR:HB3	1:A:161:ASN:O	2.15	0.47
1:A:381:ILE:CG2	1:A:381:ILE:O	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:378:VAL:O	1:C:381:ILE:HB	2.15	0.47
1:B:301:PRO:O	1:B:304:SER:HB2	2.15	0.47
1:C:221:ALA:HA	1:C:222:PRO:C	2.34	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:D:230:ILE:O	1:D:231:ASN:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ILE:HG12	1:B:272:ILE:O	2.14	0.47
1:B:79:THR:CG2	1:B:98:ILE:HG22	2.44	0.47
1:C:299:PRO:C	1:C:300:ILE:HD12	2.34	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:A:55:LYS:CE	1:A:150:MET:HE2	2.44	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:166:ILE:CB	1:A:167:PRO:CD	2.94	0.46
1:A:67[A]:CYS:SG	1:A:70:VAL:HG22	2.54	0.46
1:A:16:GLY:H	1:A:73:GLU:HG3	1.73	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: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: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:16:GLY:CA	1:A:73:GLU:HG3	2.46	0.46
1:C:124:LEU:N	1:C:124:LEU:HD12	2.31	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: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
1:B:188:MET:HE1	1:B:223:ALA:HB1	1.96	0.46
1:C:379:ASP:O	1:C:382:ARG:HD2	2.16	0.46
1:B:123:GLU:C	1:B:124:LEU:HD12	2.36	0.46
1:C:135:VAL:HA	1:C:138:GLN:HE21	1.79	0.46
1:D:33:LEU:C	1:D:33:LEU:HD12	2.36	0.46
1:D:54:PHE:CD2	1:D:74:ILE:CD1	2.98	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:B:318:GLY:N	1:B:352:ARG:O	2.43	0.46
1:C:166:ILE:HB	1:C:167:PRO:HD3	1.98	0.46
1:D:324:THR:O	1:D:325:HIS:C	2.54	0.46
1:D:65:LYS:HE3	1:D:65:LYS:HB3	1.75	0.46
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:332:ALA:HA	1:D:335:ILE:HG13	1.98	0.45
1:D:104:LYS:NZ	2:D:400:ATP:O2B	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:228:ASP:O	1:C:229:ALA:C	2.53	0.45
1:D:372:GLN:N	1:D:373:PRO:CD	2.79	0.45
1:D:70:VAL:HG21	1:D:89:VAL:HG11	1.97	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:112:ARG:N	1:D:118:MET:HE1	2.32	0.45
1:D:85:VAL:O	1:D:87:SER:N	2.50	0.45
1:B:133:ALA:HB1	1:B:163:GLN:NE2	2.31	0.45
1:C:375:ILE:O	1:C:376:ASP:C	2.55	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
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:C:349:LYS:HA	1:C:349:LYS:HD2	1.79	0.44
1:C:92:GLU:HA	1:C:92:GLU:OE1	2.17	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:258:LEU:O	1:D:261:ASP:N	2.48	0.44
1:D:16:GLY:H	1:D:73:GLU:HG3	1.76	0.44
1:B:116:ILE:O	1:B:118:MET:HG2	2.18	0.44
1:B:313:MET:HG2	1:B:314:LEU:N	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ALA:HA	1:C:362:PRO:HD3	1.69	0.44
1:D:264:MET:HE2	1:D:264:MET:HB2	1.45	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: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:342:LEU:HD23	1:A:342:LEU:HA	1.65	0.44
1:A:45:ALA:HB2	1:B:45:ALA:HB2	1.99	0.44
1:B:141:TYR:HA	1:B:142:PRO:C	2.36	0.44
1:C:107:GLN:OE1	1:C:268:ILE:HG22	2.18	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: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
1:D:150:MET:HE2	1:D:150:MET:HB3	1.89	0.43
1:D:379:ASP:O	1:D:380:ARG:C	2.54	0.43
1:D:380:ARG:HD3	4:D:411:HOH:O	2.17	0.43
1:B:254:GLU:C	1:B:255:MET:HG3	2.38	0.43
1:C:22:SER:HB3	4:C:464:HOH:O	2.17	0.43
1:C:57:ARG:HB2	1:C:57:ARG:HE	1.16	0.43
1:D:75:GLU:H	1:D:75:GLU:HG3	1.59	0.43
1:A:163:GLN:HG3	1:A:164:ASP:N	2.34	0.43
1:A:171:GLU:O	1:A:174:LYS:HB3	2.19	0.43
1:C:236:GLU:O	1:C:237:LEU:C	2.57	0.43
1:D:343:TYR:CD2	1:D:343:TYR:N	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:227:SER:O	1:B:228:ASP:C	2.55	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: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:64:ALA:C	1:D:66:THR:N	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:97:ALA:O	1:B:98:ILE:C	2.55	0.43
1:C:166:ILE:O	1:C:167:PRO:C	2.57	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:146:LYS:HE2	2:B:400:ATP:N7	2.34	0.42
1:B:14:GLN:HG2	1:B:15:LEU:N	2.34	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:348:ALA:O	1:A:349:LYS:HD3	2.19	0.42
1:A:58:GLU:HA	1:A:61:ARG:HB2	2.01	0.42
1:C:94:SER:HB3	1:C:97:ALA:H	1.84	0.42
1:D:188:MET:CE	1:D:226:VAL:CG2	2.98	0.42
1:D:8:GLY:HA2	1:D:31:ASN:O	2.19	0.42
1:D:342:LEU:HA	1:D:342:LEU:HD23	1.78	0.42
1:A:226:VAL:HG12	1:A:227:SER:O	2.18	0.42
1:A:321:ALA:HA	1:A:322:PRO:HD3	1.95	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:237:LEU:HD12	1:D:237:LEU:O	2.19	0.42
1:D:187:LYS:HE3	1:D:259:GLU:HA	2.01	0.42
1:A:321:ALA:HB1	1:A:323:ASP:OD1	2.18	0.42
1:C:171:GLU:CD	1:C:174:LYS:HE3	2.40	0.42
1:C:296:LEU:O	1:C:297:ASP:HB2	2.19	0.42
1:D:170:LEU:HA	1:D:170:LEU:HD23	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:D:37:ASN:C	1:D:37:ASN:ND2	2.73	0.42
1:C:122:ARG:HG2	1:C:139:LEU:HD21	2.02	0.42
1:C:69:VAL:HG23	1:C:90:LYS:HB3	2.01	0.42
1:D:188:MET:HG3	1:D:189:GLU:N	2.34	0.42
1:A:321:ALA:O	1:A:324:THR:HG23	2.20	0.42
1:D:325:HIS:CE1	1:D:348:ALA:HB2	2.55	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:26:LEU:O	1:A:27:ASN:HB2	2.20	0.41
1:B:293:ARG:HD3	1:B:293:ARG:HH11	1.73	0.41
1:A:292:LEU:O	1:A:296:LEU:HD12	2.19	0.41
1:A:372:GLN:O	1:A:373:PRO:C	2.58	0.41
1:A:62:GLN:O	1:A:63:LEU:C	2.57	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:D:226:VAL:HG13	1:D:230:ILE:HB	2.03	0.41
1:D:375:ILE:O	1:D:378:VAL:N	2.53	0.41
1:A:198:LYS:HG3	1:A:199:ASP:CG	2.41	0.41
1:A:36:ASP:O	1:A:37[B]:ASN:HB3	2.20	0.41
1:C:103:ASN:CB	1:C:106:ASN:ND2	2.83	0.41
1:C:141:TYR:HA	1:C:142:PRO:C	2.39	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: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:113:LYS:C	1:A:115:GLY:N	2.74	0.41
1:A:341:HIS:CE1	1:B:25:ARG:NH1	2.88	0.41
1:B:112:ARG:HG2	1:B:118:MET:HE1	2.02	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:126:GLU:H	1:D:131:GLU:CD	2.23	0.41
1:D:146:LYS:HB3	1:D:157:ASN:OD1	2.20	0.41
1:A:55:LYS:NZ	1:A:150:MET:HE2	2.36	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: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:70:VAL:CG2	1:D:89:VAL:HG11	2.50	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:110:HIS:CA	1:D:113:LYS:HE3	2.34	0.41
1:D:25:ARG:NH1	4:D:849:HOH:O	2.50	0.41
1:A:324:THR:O	1:A:327:GLN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:MET:HE3	1:B:190:LEU:HD21	1.93	0.41
1:C:213:ASP:O	1:C:214:SER:HB2	2.21	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:D:41:LYS:HE2	1:D:49:HIS:HB3	2.02	0.41
1:A:196:LYS:HD3	1:A:247:GLY:O	2.21	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:82:LEU:O	1:C:83:GLU:C	2.59	0.41
1:D:293:ARG:HA	1:D:298:LEU:HB2	2.01	0.41
1:A:224:ARG:O	1:A:225:ASN:HB2	2.20	0.41
1:C:330:GLU:HB2	1:D:2:TRP:NE1	2.36	0.41
1:D:3:ASN:OD1	1:D:3:ASN:N	2.54	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:A:33:LEU:HD12	1:A:34:ASP:N	2.36	0.41
1:B:193:ILE:HA	1:B:193:ILE:HD13	1.93	0.41
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:B:55:LYS:HE2	4:B:760:HOH:O	2.21	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:196:LYS:NZ	1:D:247:GLY:O	2.38	0.40
1:D:46:HIS:CE1	1:D:48:GLY:HA3	2.56	0.40
1:A:316:ILE:CG2	1:A:325:HIS:HA	2.51	0.40
1:B:19:LEU:HA	1:B:19:LEU:HD12	1.62	0.40
1:B:285:LEU:HG	1:B:304:SER:HB3	2.03	0.40
1:C:233:LYS:HB3	1:C:263:ILE:CD1	2.39	0.40
1:A:254:GLU:OE2	1:A:267:GLU:HG2	2.21	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

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%)	41	41
1	B	383/403 (95%)	368 (96%)	15 (4%)	0	100	100
1	C	382/403 (95%)	361 (94%)	19 (5%)	2 (0%)	29	26
1	D	379/403 (94%)	351 (93%)	27 (7%)	1 (0%)	41	41
All	All	1528/1612 (95%)	1443 (94%)	81 (5%)	4 (0%)	41	41

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%)	282 (88%)	40 (12%)	4	2
1	B	321/336 (96%)	293 (91%)	28 (9%)	10	7
1	C	320/336 (95%)	280 (88%)	40 (12%)	4	2
1	D	317/336 (94%)	281 (89%)	36 (11%)	5	3
All	All	1280/1344 (95%)	1136 (89%)	144 (11%)	6	3

All (144) 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	57	ARG
1	A	61	ARG
1	A	62	GLN
1	A	65	LYS
1	A	66	THR
1	A	73	GLU
1	A	84	GLU
1	A	104	LYS
1	A	113	LYS
1	A	131	GLU
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	193	ILE
1	A	199	ASP
1	A	202	LEU
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	274	ASN
1	A	305	LEU
1	A	311	SER
1	A	344	SER
1	A	350	PRO
1	B	4	SER
1	B	5	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	LEU
1	B	39	PRO
1	B	44	SER
1	B	57	ARG
1	B	62[A]	GLN
1	B	62[B]	GLN
1	B	73	GLU
1	B	74	ILE
1	B	75	GLU
1	B	102	GLN
1	B	143	LEU
1	B	167	PRO
1	B	174	LYS
1	B	178	LEU
1	B	200	GLU
1	B	211	GLN
1	B	230	ILE
1	B	233	LYS
1	B	265	LEU
1	B	272	ILE
1	B	274	ASN
1	B	327	GLN
1	B	334	SER
1	B	344	SER
1	B	362	PRO
1	B	381	ILE
1	C	6	LYS
1	C	26	LEU
1	C	47	ASP
1	C	57	ARG
1	C	73	GLU
1	C	87	SER
1	C	88	GLU
1	C	90	LYS
1	C	114	TYR
1	C	118	MET
1	C	120	GLU
1	C	126	GLU
1	C	139	LEU
1	C	142	PRO
1	C	155	ARG
1	C	159	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	GLN
1	C	174	LYS
1	C	182	LYS
1	C	196	LYS
1	C	197	THR
1	C	202	LEU
1	C	208	GLU
1	C	218	LEU
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	274	ASN
1	C	313	MET
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	D	4	SER
1	D	6	LYS
1	D	37	ASN
1	D	47	ASP
1	D	54	PHE
1	D	55	LYS
1	D	56	GLU
1	D	58	GLU
1	D	61	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	96	GLN
1	D	125	VAL
1	D	126	GLU
1	D	150	MET
1	D	174	LYS
1	D	176	ARG
1	D	182	LYS
1	D	187	LYS
1	D	188	MET
1	D	248	LYS
1	D	262	SER
1	D	264	MET
1	D	272	ILE
1	D	274	ASN
1	D	326	LEU
1	D	344	SER
1	D	366	GLU
1	D	378	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	138	GLN
1	A	225	ASN
1	B	106	ASN
1	B	163	GLN
1	B	232	GLN
1	C	102	GLN
1	C	106	ASN
1	C	232	GLN
1	D	62	GLN
1	D	106	ASN
1	D	127	ASN
1	D	138	GLN
1	D	325	HIS

5.3.3 RNA ⓘ

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 carbohydrates 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	26,33,33	1.04	2 (7%)	31,52,52	2.27	10 (32%)
2	ATP	D	400	3	26,33,33	0.94	1 (3%)	31,52,52	2.95	7 (22%)
2	ATP	A	400	3	26,33,33	0.89	1 (3%)	31,52,52	2.75	11 (35%)
2	ATP	C	400	3	26,33,33	0.78	0	31,52,52	1.79	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	400	3	-	3/18/38/38	0/3/3/3
2	ATP	D	400	3	-	5/18/38/38	0/3/3/3
2	ATP	A	400	3	-	6/18/38/38	0/3/3/3
2	ATP	C	400	3	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	ATP	C2-N1	2.62	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ATP	C6-N6	-2.50	1.24	1.34
2	B	400	ATP	C2-N1	2.18	1.38	1.33
2	A	400	ATP	C2-N1	2.11	1.37	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	ATP	C2-N1-C6	9.33	134.72	118.75
2	A	400	ATP	C5-C6-N6	8.77	133.69	120.35
2	B	400	ATP	C5-C6-N6	8.51	133.28	120.35
2	D	400	ATP	C5-C6-N1	-8.12	101.94	120.35
2	D	400	ATP	C5-C6-N6	6.58	130.35	120.35
2	A	400	ATP	C2-N1-C6	6.32	129.56	118.75
2	A	400	ATP	C5-C6-N1	-6.30	106.07	120.35
2	C	400	ATP	C5-C6-N6	4.91	127.82	120.35
2	D	400	ATP	N6-C6-N1	4.37	127.64	118.57
2	D	400	ATP	N3-C2-N1	-3.98	122.46	128.68
2	C	400	ATP	N3-C2-N1	-3.33	123.47	128.68
2	A	400	ATP	O3G-PG-O3B	3.32	115.76	104.64
2	C	400	ATP	C3'-C2'-C1'	3.29	105.92	100.98
2	C	400	ATP	O4'-C1'-C2'	-3.19	102.27	106.93
2	B	400	ATP	N6-C6-N1	-3.10	112.13	118.57
2	B	400	ATP	O3'-C3'-C2'	3.10	121.86	111.82
2	A	400	ATP	O3'-C3'-C4'	-2.94	102.56	111.05
2	C	400	ATP	O3G-PG-O3B	2.93	114.45	104.64
2	B	400	ATP	O2A-PA-O5'	-2.93	94.15	107.75
2	B	400	ATP	O2B-PB-O1B	2.85	126.31	112.24
2	B	400	ATP	O3G-PG-O2G	2.74	118.09	107.64
2	A	400	ATP	N3-C2-N1	-2.72	124.43	128.68
2	B	400	ATP	C5-C6-N1	-2.55	114.58	120.35
2	A	400	ATP	O5'-PA-O1A	2.53	118.94	109.07
2	A	400	ATP	O2G-PG-O3B	-2.47	96.34	104.64
2	C	400	ATP	PA-O5'-C5'	-2.43	107.45	121.68
2	A	400	ATP	C2'-C3'-C4'	-2.38	98.02	102.64
2	B	400	ATP	O2'-C2'-C1'	-2.29	102.41	110.85
2	B	400	ATP	O4'-C4'-C3'	-2.27	100.62	105.11
2	A	400	ATP	O4'-C4'-C3'	-2.24	100.69	105.11
2	D	400	ATP	PB-O3B-PG	-2.20	125.29	132.83
2	D	400	ATP	O3'-C3'-C2'	2.19	118.91	111.82
2	B	400	ATP	C3'-C2'-C1'	2.07	104.10	100.98
2	A	400	ATP	O2G-PG-O1G	2.02	118.58	110.68
2	C	400	ATP	O4'-C4'-C3'	-2.01	101.14	105.11

There are no chirality outliers.

All (17) torsion outliers are listed below:

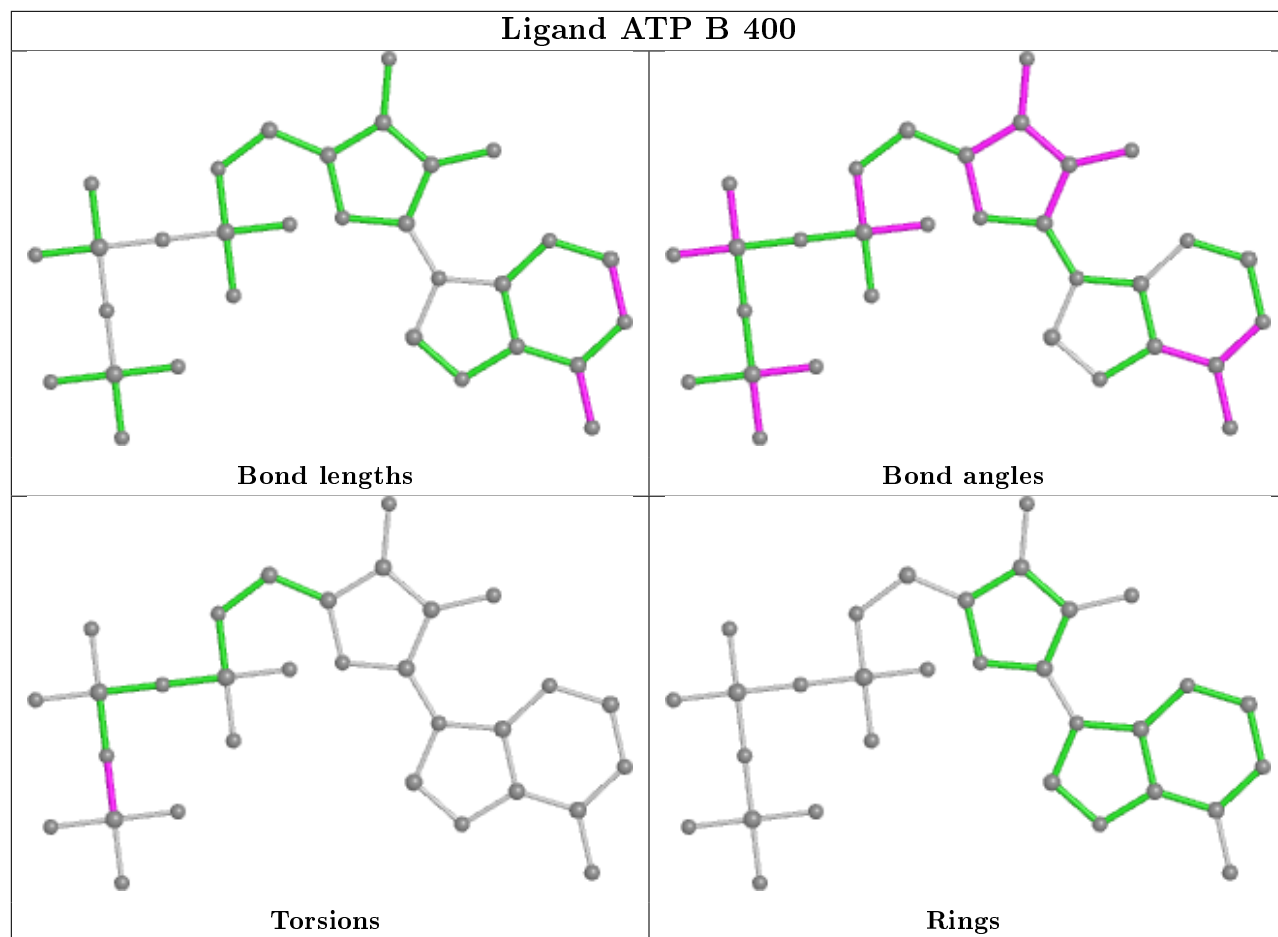
Mol	Chain	Res	Type	Atoms
2	C	400	ATP	PB-O3B-PG-O3G
2	B	400	ATP	PB-O3B-PG-O3G
2	D	400	ATP	PB-O3B-PG-O2G
2	D	400	ATP	PB-O3B-PG-O3G
2	A	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	PB-O3B-PG-O3G
2	A	400	ATP	C5'-O5'-PA-O1A
2	C	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	O4'-C4'-C5'-O5'
2	D	400	ATP	PG-O3B-PB-O2B
2	C	400	ATP	PB-O3B-PG-O1G
2	B	400	ATP	PB-O3B-PG-O1G
2	B	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	C5'-O5'-PA-O3A
2	D	400	ATP	PG-O3B-PB-O1B
2	A	400	ATP	PG-O3B-PB-O1B
2	D	400	ATP	PB-O3B-PG-O1G

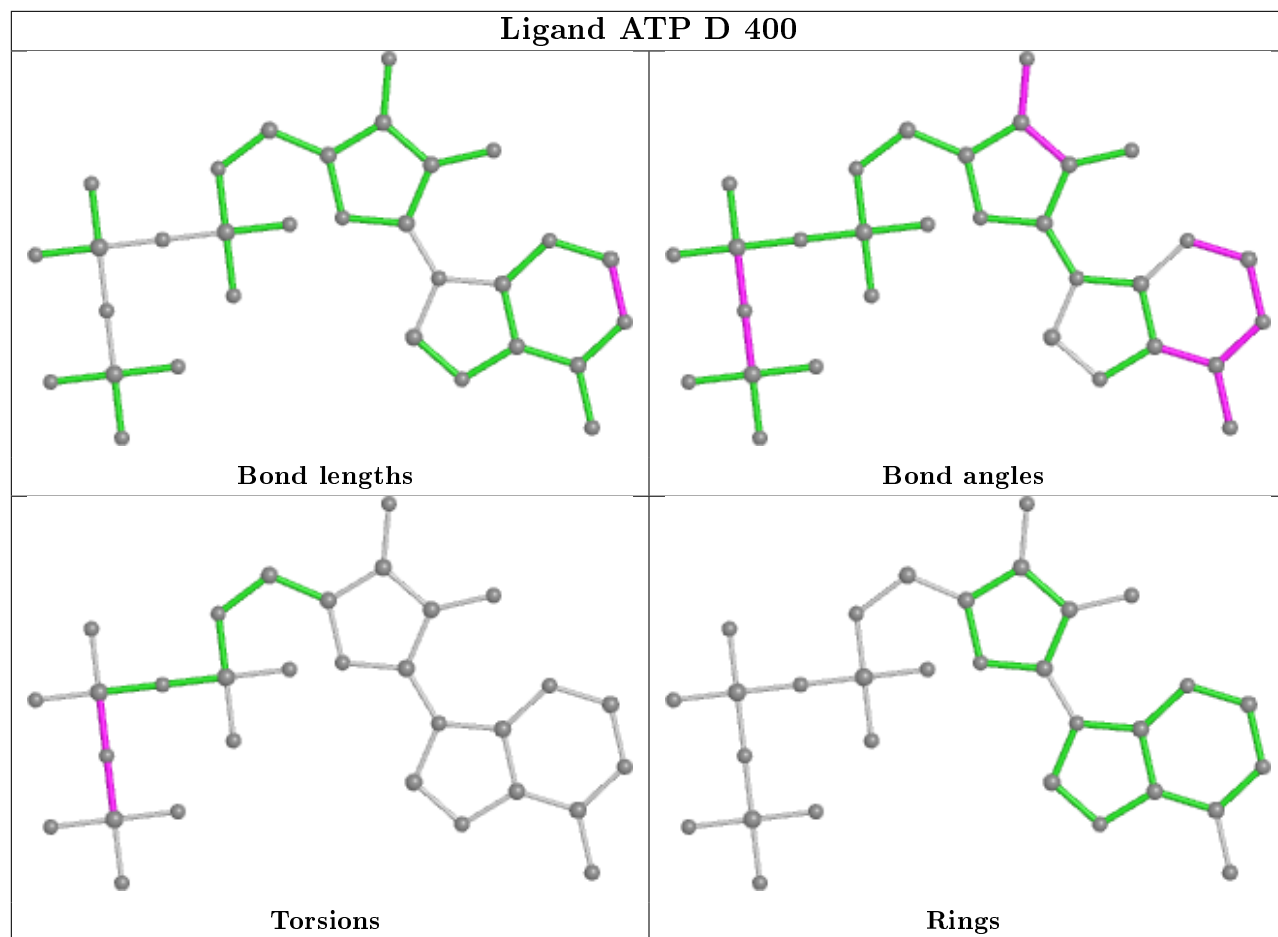
There are no ring outliers.

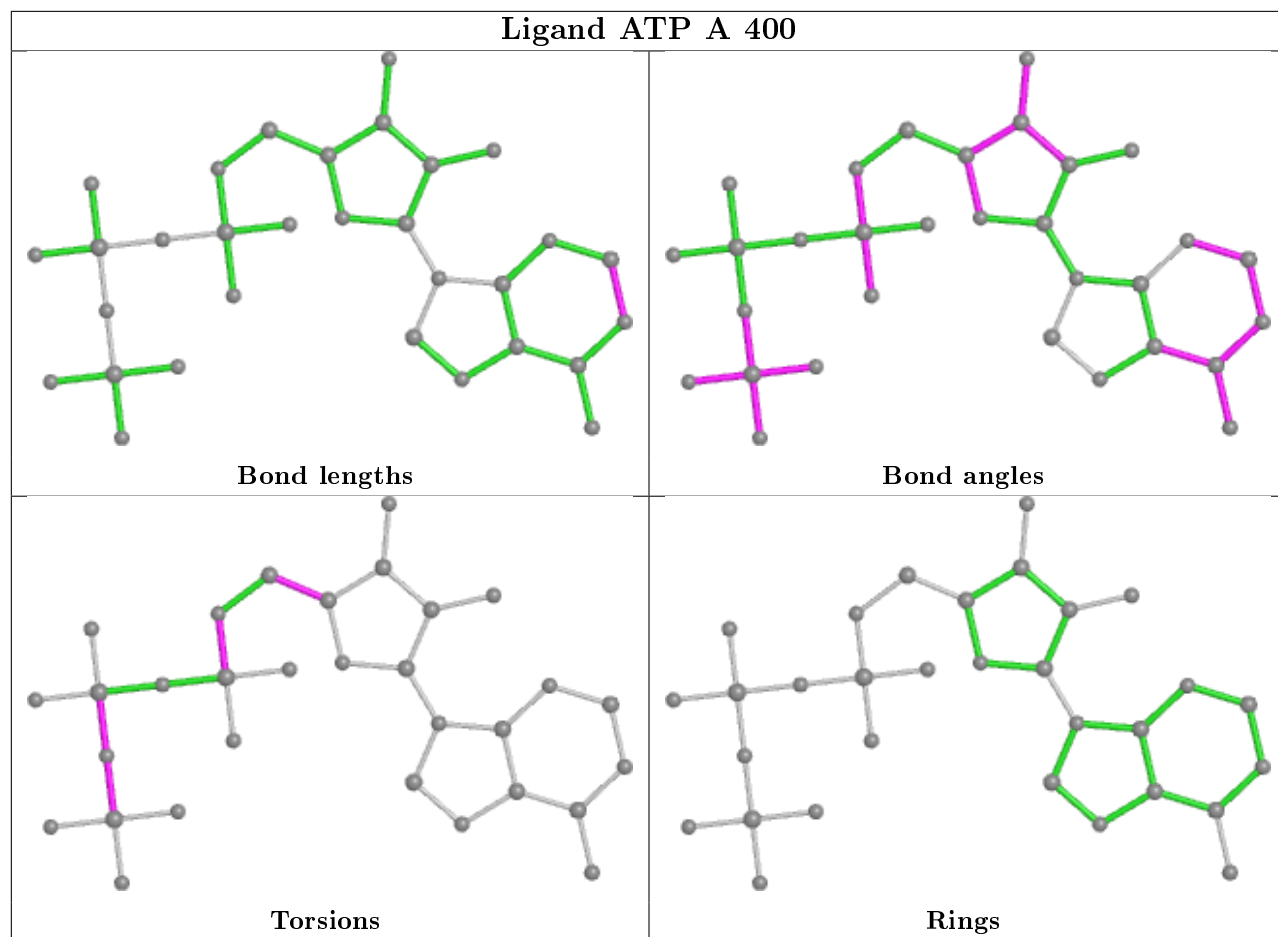
4 monomers are involved in 6 short contacts:

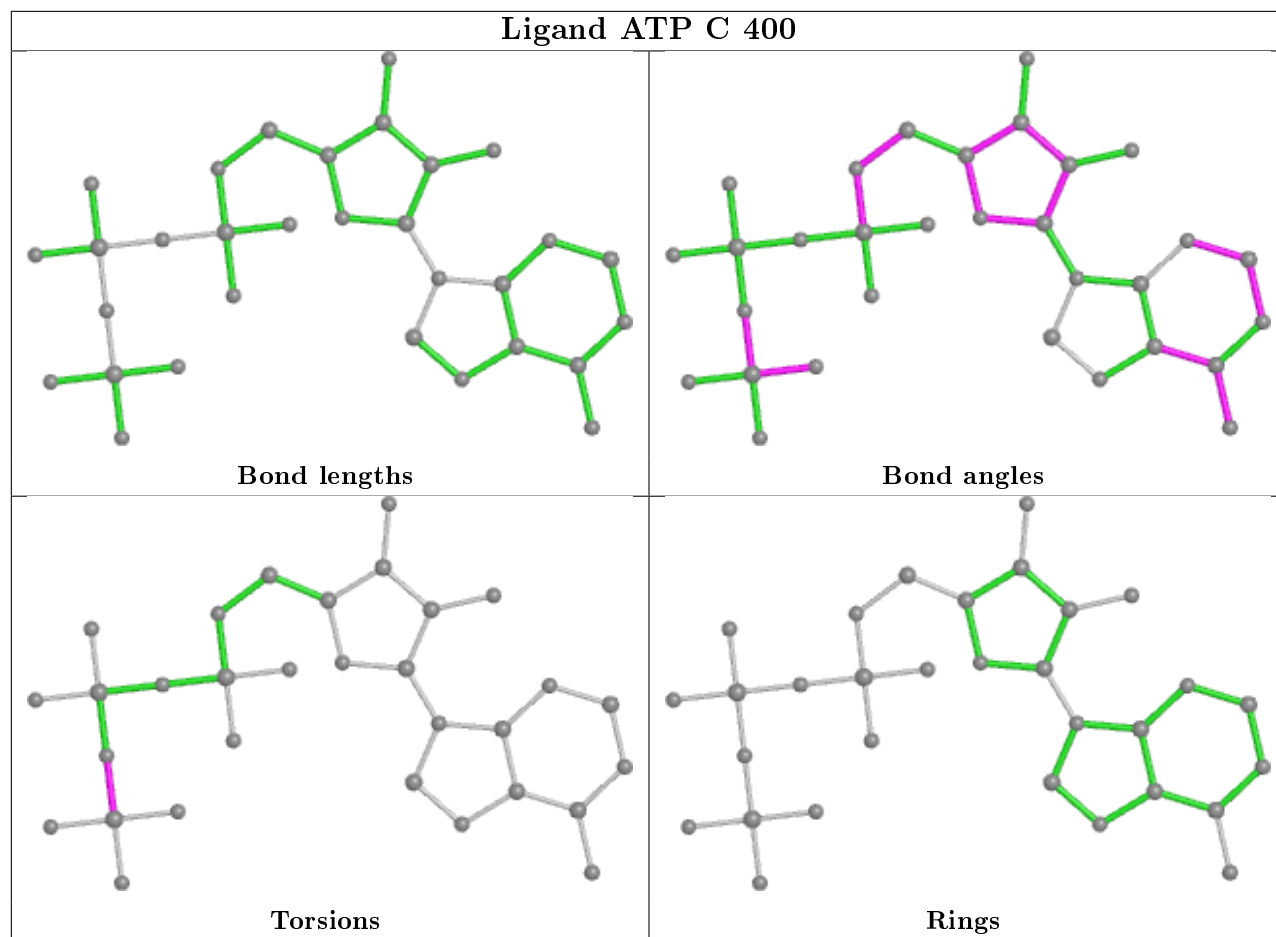
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ATP	2	0
2	D	400	ATP	2	0
2	A	400	ATP	1	0
2	C	400	ATP	1	0

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%)	-0.14	2 (0%) 91 92	7, 25, 62, 81	0
1	B	380/403 (94%)	-0.10	10 (2%) 56 61	6, 24, 64, 86	0
1	C	382/403 (94%)	-0.04	5 (1%) 77 80	12, 31, 69, 93	0
1	D	380/403 (94%)	0.03	8 (2%) 63 68	11, 29, 70, 93	0
All	All	1524/1612 (94%)	-0.06	25 (1%) 72 75	6, 28, 67, 93	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	381	ILE	6.1
1	D	381	ILE	5.7
1	B	323	ASP	3.9
1	B	321	ALA	3.1
1	D	326	LEU	3.1
1	C	318	GLY	3.0
1	B	125	VAL	2.7
1	C	321	ALA	2.6
1	D	380	ARG	2.6
1	D	321	ALA	2.5
1	D	322	PRO	2.5
1	C	126	GLU	2.5
1	B	174	LYS	2.5
1	D	319	GLY	2.5
1	A	323	ASP	2.5
1	D	323	ASP	2.5
1	B	326	LEU	2.4
1	D	320	ALA	2.4
1	B	128	THR	2.3
1	B	126	GLU	2.3
1	A	348	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	377	VAL	2.1
1	B	152	TYR	2.1
1	C	381	ILE	2.1
1	B	324	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

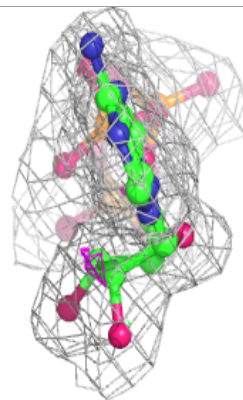
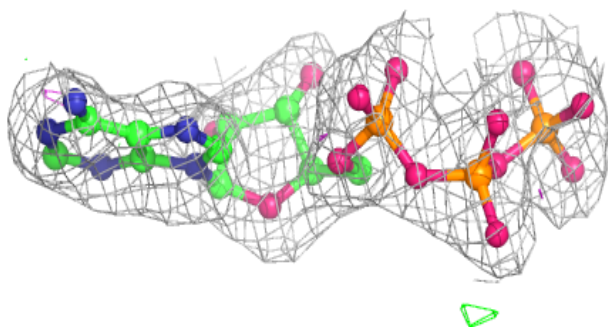
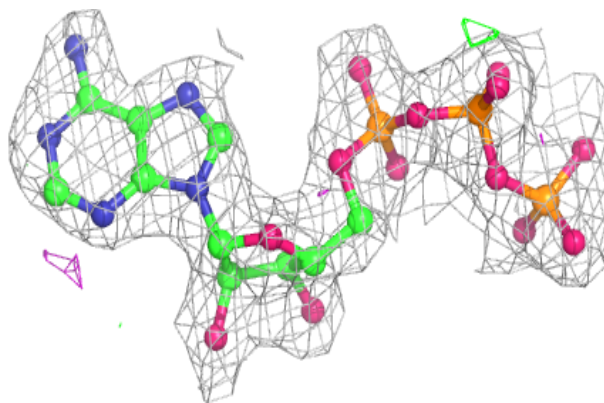
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	401	1/1	0.84	0.09	22,22,22,22	0
3	MG	C	401	1/1	0.85	0.07	40,40,40,40	0
3	MG	D	401	1/1	0.87	0.08	33,33,33,33	0
3	MG	B	402	1/1	0.92	0.08	25,25,25,25	0
2	ATP	C	400	31/31	0.96	0.10	12,30,82,100	0
3	MG	D	402	1/1	0.96	0.05	24,24,24,24	0
2	ATP	B	400	31/31	0.96	0.10	7,28,44,63	0
3	MG	C	402	1/1	0.96	0.09	22,22,22,22	0
2	ATP	D	400	31/31	0.97	0.09	12,26,56,100	0
2	ATP	A	400	31/31	0.97	0.08	9,23,33,75	0
3	MG	A	401	1/1	0.97	0.04	14,14,14,14	0
3	MG	A	402	1/1	0.97	0.06	24,24,24,24	0

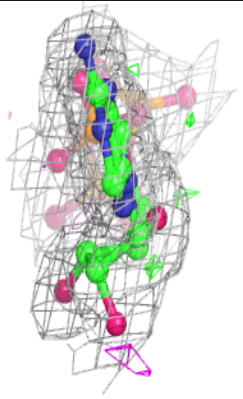
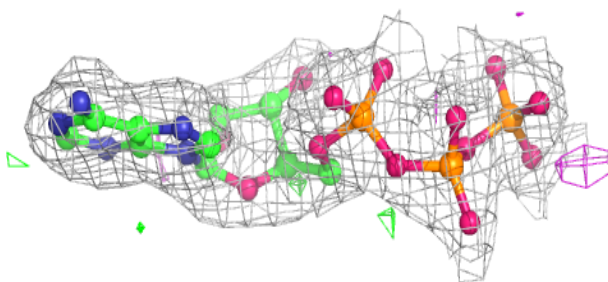
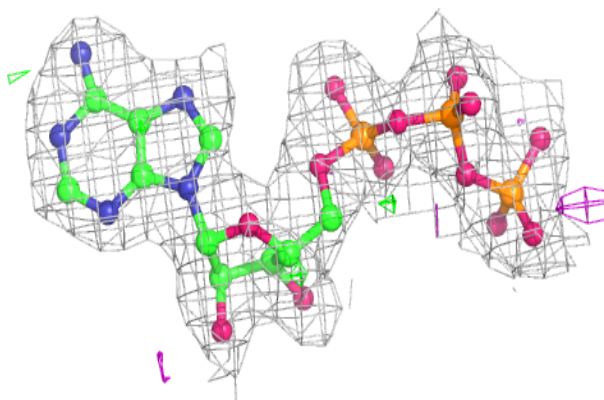
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP 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)

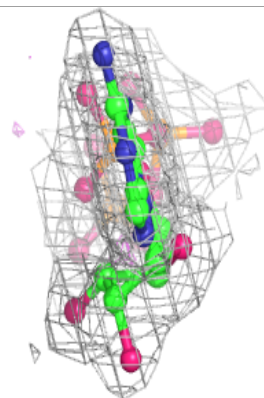
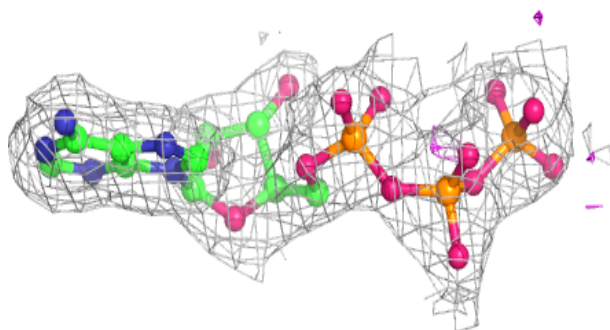
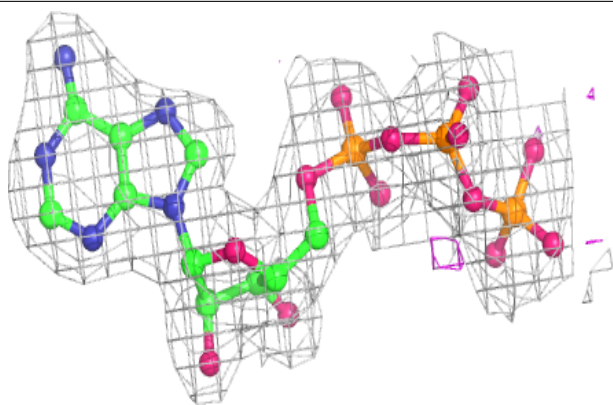
**Electron density around ATP B 400:**

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

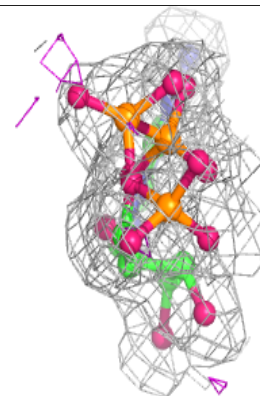
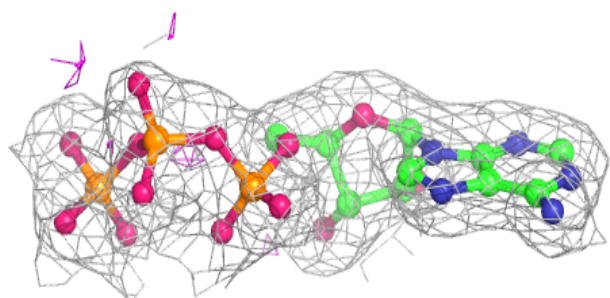
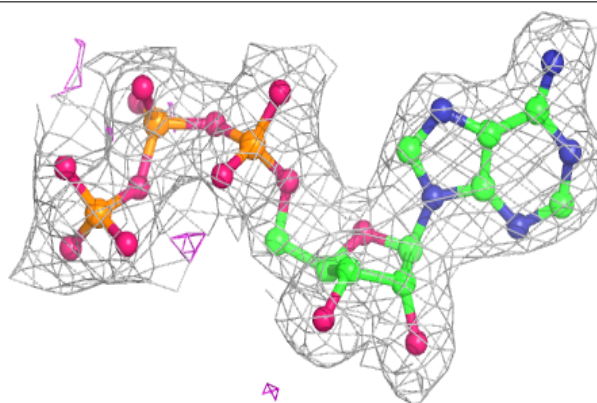


Electron density around ATP D 400:

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

**Electron density around ATP 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

There are no such residues in this entry.