



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:19 PM UTC

PDB ID : 2FSG / pdb_00002fsg
Title : Complex SecA:ATP from Escherichia coli
Authors : Papanikolaou, Y.; Petratos, K.; Economou, A.
Deposited on : 2006-01-23
Resolution : 2.20 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

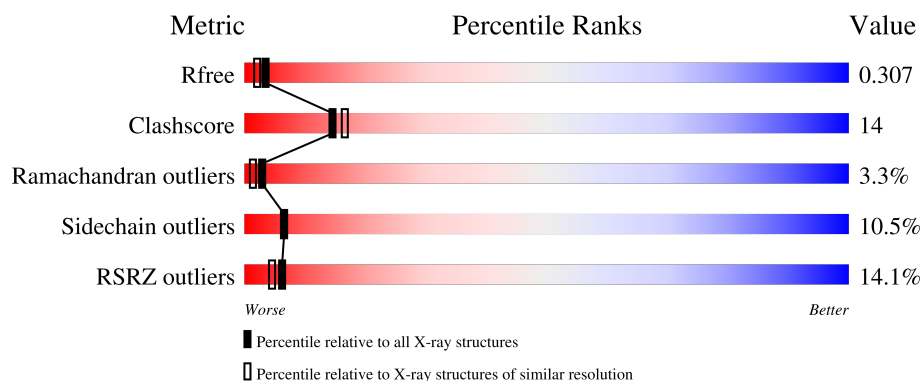
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	853	 4% 50% 23% 5% 20%
1	B	853	 18% 44% 30% 11% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11809 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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	Se	0	0	0
			5401	3392	953	1030	1	25			
1	B	743	Total	C	N	O	S	Se	0	0	0
			5915	3712	1045	1128	1	29			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	modified residue	UNP P10408
A	31	MSE	MET	modified residue	UNP P10408
A	35	MSE	MET	modified residue	UNP P10408
A	81	MSE	MET	modified residue	UNP P10408
A	92	MSE	MET	modified residue	UNP P10408
A	102	MSE	MET	modified residue	UNP P10408
A	161	MSE	MET	modified residue	UNP P10408
A	191	MSE	MET	modified residue	UNP P10408
A	235	MSE	MET	modified residue	UNP P10408
A	292	MSE	MET	modified residue	UNP P10408
A	305	MSE	MET	modified residue	UNP P10408
A	307	MSE	MET	modified residue	UNP P10408
A	344	MSE	MET	modified residue	UNP P10408
A	390	MSE	MET	modified residue	UNP P10408
A	418	MSE	MET	modified residue	UNP P10408
A	429	MSE	MET	modified residue	UNP P10408
A	506	MSE	MET	modified residue	UNP P10408
A	590	MSE	MET	modified residue	UNP P10408
A	595	MSE	MET	modified residue	UNP P10408
A	606	MSE	MET	modified residue	UNP P10408
A	607	MSE	MET	modified residue	UNP P10408
A	612	MSE	MET	modified residue	UNP P10408
A	700	MSE	MET	modified residue	UNP P10408
A	758	MSE	MET	modified residue	UNP P10408
A	759	MSE	MET	modified residue	UNP P10408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	767	MSE	MET	modified residue	UNP P10408
A	782	MSE	MET	modified residue	UNP P10408
A	810	MSE	MET	modified residue	UNP P10408
A	814	MSE	MET	modified residue	UNP P10408
A	833	MSE	MET	modified residue	UNP P10408
A	846	MSE	MET	modified residue	UNP P10408
A	854	MSE	MET	modified residue	UNP P10408
B	21	MSE	MET	modified residue	UNP P10408
B	31	MSE	MET	modified residue	UNP P10408
B	35	MSE	MET	modified residue	UNP P10408
B	81	MSE	MET	modified residue	UNP P10408
B	92	MSE	MET	modified residue	UNP P10408
B	102	MSE	MET	modified residue	UNP P10408
B	161	MSE	MET	modified residue	UNP P10408
B	191	MSE	MET	modified residue	UNP P10408
B	235	MSE	MET	modified residue	UNP P10408
B	292	MSE	MET	modified residue	UNP P10408
B	305	MSE	MET	modified residue	UNP P10408
B	307	MSE	MET	modified residue	UNP P10408
B	344	MSE	MET	modified residue	UNP P10408
B	390	MSE	MET	modified residue	UNP P10408
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B	429	MSE	MET	modified residue	UNP P10408
B	506	MSE	MET	modified residue	UNP P10408
B	590	MSE	MET	modified residue	UNP P10408
B	595	MSE	MET	modified residue	UNP P10408
B	606	MSE	MET	modified residue	UNP P10408
B	607	MSE	MET	modified residue	UNP P10408
B	612	MSE	MET	modified residue	UNP P10408
B	700	MSE	MET	modified residue	UNP P10408
B	758	MSE	MET	modified residue	UNP P10408
B	759	MSE	MET	modified residue	UNP P10408
B	767	MSE	MET	modified residue	UNP P10408
B	782	MSE	MET	modified residue	UNP P10408
B	810	MSE	MET	modified residue	UNP P10408
B	814	MSE	MET	modified residue	UNP P10408
B	833	MSE	MET	modified residue	UNP P10408
B	846	MSE	MET	modified residue	UNP P10408
B	854	MSE	MET	modified residue	UNP P10408

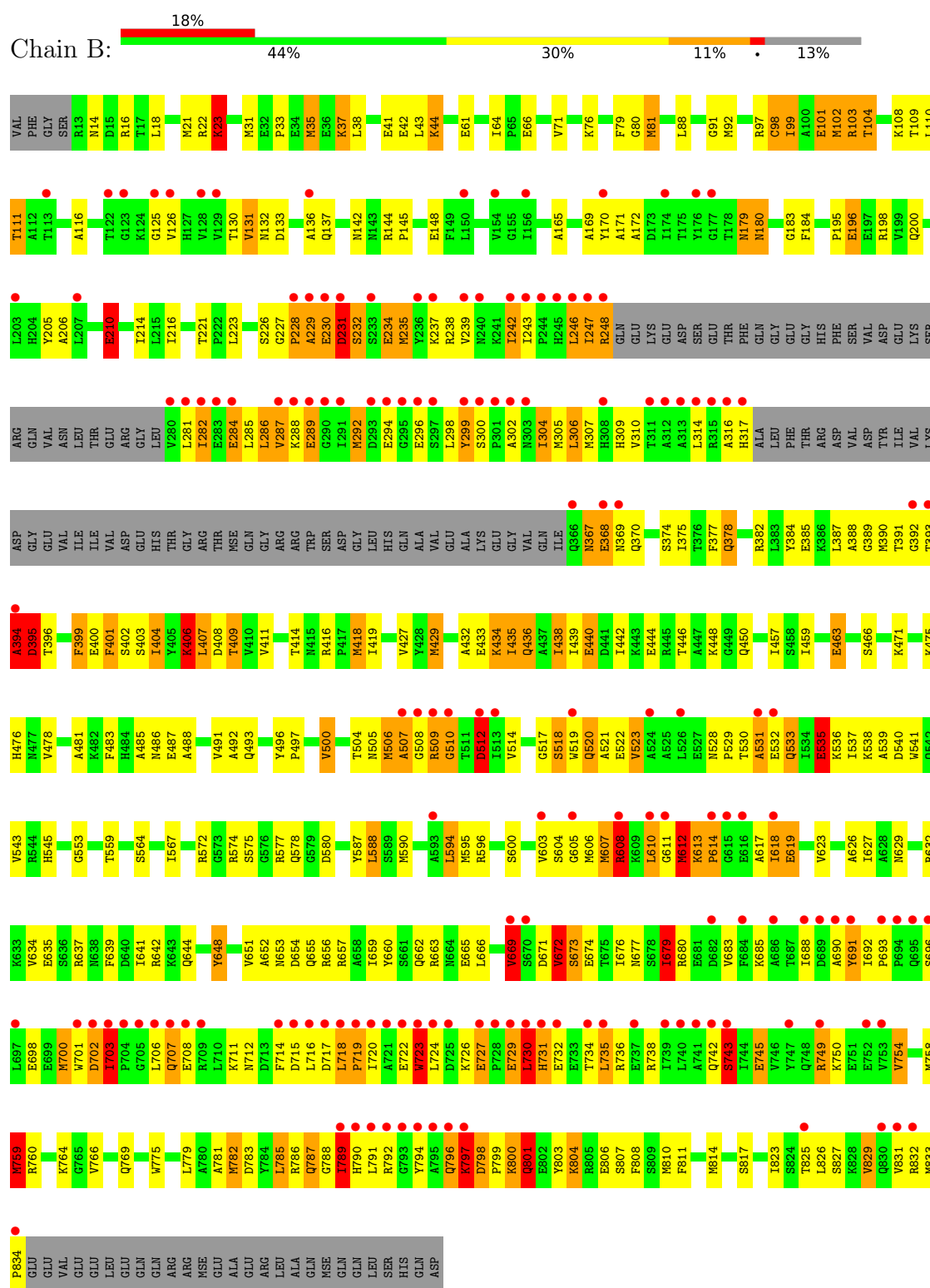
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	233	Total	O	0	0
			233	233		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.38Å 89.48Å 163.35Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	19.61 – 2.20 19.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.61-2.20) 96.8 (19.61-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.270 0.262 , 0.307	Depositor DCC
R_{free} test set	5245 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

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	1.85	95/5466 (1.7%)	1.50	53/7334 (0.7%)
1	B	1.91	135/5983 (2.3%)	1.50	60/8023 (0.7%)
All	All	1.88	230/11449 (2.0%)	1.50	113/15357 (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	3
1	B	0	7
All	All	0	10

All (230) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ILE	CA-CB	-11.97	1.47	1.54
1	B	626	ALA	CA-CB	-10.66	1.36	1.53
1	B	806	GLU	C-O	-10.18	1.12	1.24
1	A	172	ALA	CA-CB	-9.48	1.38	1.53
1	A	782	MSE	SE-CE	9.34	2.23	1.95
1	A	833	MSE	SE-CE	9.31	2.23	1.95
1	B	23	LYS	CE-NZ	9.11	1.76	1.49
1	A	740	LEU	C-O	9.08	1.34	1.24
1	A	700	MSE	SE-CE	9.05	2.22	1.95
1	B	64	ILE	CA-CB	8.91	1.59	1.54
1	A	438	ILE	CA-CB	-8.88	1.44	1.54
1	B	700	MSE	SE-CE	8.84	2.21	1.95
1	B	660	TYR	C-O	-8.66	1.12	1.24
1	A	620	HIS	N-CA	-8.41	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	MSE	SE-CE	8.22	2.20	1.95
1	B	109	THR	CA-CB	8.16	1.66	1.53
1	B	126	VAL	C-O	-8.04	1.15	1.24
1	B	184	PHE	C-O	-8.01	1.14	1.24
1	A	590	MSE	SE-CE	7.68	2.18	1.95
1	B	580	ASP	C-O	7.64	1.32	1.23
1	B	393	THR	CA-CB	7.60	1.67	1.53
1	A	79	PHE	CA-C	-7.58	1.42	1.52
1	B	506	MSE	SE-CE	7.56	2.18	1.95
1	B	612	MSE	SE-CE	7.56	2.18	1.95
1	B	572	ARG	CZ-NH2	-7.54	1.23	1.33
1	A	136	ALA	CA-CB	7.54	1.65	1.53
1	B	672	VAL	CA-CB	7.49	1.64	1.54
1	A	506	MSE	SE-CE	7.42	2.17	1.95
1	A	825	THR	C-O	-7.29	1.15	1.24
1	B	394	ALA	CA-C	7.23	1.62	1.52
1	B	607	MSE	SE-CE	7.22	2.17	1.95
1	A	466	SER	C-O	7.15	1.32	1.24
1	A	395	ASP	CA-C	7.15	1.62	1.52
1	B	35	MSE	SE-CE	7.15	2.16	1.95
1	B	811	PHE	CA-C	7.06	1.61	1.52
1	A	799	PRO	C-O	-7.05	1.16	1.23
1	A	21	MSE	SE-CE	7.03	2.16	1.95
1	B	42	GLU	CA-C	-7.02	1.44	1.52
1	B	492	ALA	CA-CB	6.97	1.64	1.53
1	B	401	PHE	C-O	-6.95	1.15	1.24
1	B	642	ARG	N-CA	-6.95	1.37	1.46
1	B	418	MSE	SE-CE	6.95	2.16	1.95
1	A	404	ILE	CA-CB	-6.93	1.45	1.54
1	B	403	SER	C-O	-6.90	1.15	1.24
1	A	776	LYS	N-CA	-6.88	1.38	1.46
1	B	789	ILE	CA-CB	6.87	1.63	1.54
1	B	766	VAL	C-O	-6.84	1.16	1.24
1	A	651	VAL	CA-CB	6.79	1.61	1.54
1	B	196	GLU	N-CA	6.79	1.55	1.46
1	B	406	LYS	CE-NZ	6.76	1.69	1.49
1	A	817	SER	CA-C	6.75	1.61	1.52
1	A	559	THR	N-CA	6.73	1.54	1.46
1	A	640	ASP	C-O	-6.73	1.16	1.24
1	B	210	GLU	CG-CD	6.72	1.68	1.52
1	B	703	ILE	CA-C	6.71	1.59	1.52
1	B	476	HIS	C-O	-6.71	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	MSE	SE-CE	6.71	2.15	1.95
1	B	653	ASN	C-O	-6.66	1.16	1.24
1	B	639	PHE	N-CA	-6.63	1.38	1.46
1	B	485	ALA	CA-CB	-6.61	1.42	1.53
1	B	404	ILE	C-O	6.58	1.32	1.24
1	B	829	VAL	CA-CB	6.57	1.61	1.54
1	B	98	CYS	C-O	-6.52	1.15	1.23
1	B	76	LYS	C-O	-6.51	1.16	1.24
1	B	198	ARG	CA-C	-6.49	1.44	1.52
1	B	669	VAL	CA-C	6.48	1.60	1.52
1	B	408	ASP	C-O	6.46	1.32	1.23
1	B	80	GLY	C-O	-6.45	1.15	1.23
1	B	88	LEU	C-O	-6.42	1.16	1.24
1	B	775	TRP	N-CA	-6.42	1.38	1.46
1	A	429	MSE	SE-CE	6.42	2.14	1.95
1	B	803	TYR	N-CA	-6.41	1.38	1.46
1	A	488	ALA	CA-C	6.41	1.61	1.52
1	B	759	MSE	SE-CE	6.39	2.14	1.95
1	A	634	VAL	C-O	-6.34	1.17	1.24
1	B	512	ASP	CA-C	6.33	1.60	1.52
1	B	572	ARG	CB-CG	-6.32	1.33	1.52
1	A	62	ASN	C-O	-6.31	1.16	1.24
1	A	131	VAL	C-O	-6.30	1.15	1.24
1	B	758	MSE	SE-CE	-6.29	1.76	1.95
1	B	377	PHE	CA-C	-6.28	1.44	1.52
1	A	564	SER	CA-C	6.27	1.60	1.52
1	B	205	TYR	C-O	-6.23	1.17	1.23
1	A	657	ARG	CZ-NH2	6.22	1.41	1.33
1	A	759	MSE	SE-CE	6.22	2.14	1.95
1	B	785	LEU	C-O	-6.21	1.16	1.24
1	A	156	ILE	CA-CB	6.18	1.62	1.54
1	B	206	ALA	CA-CB	6.18	1.62	1.53
1	A	582	GLY	C-O	-6.16	1.17	1.24
1	B	399	PHE	C-O	-6.15	1.17	1.24
1	A	180	ASN	CB-CG	-6.13	1.36	1.52
1	B	42	GLU	C-O	6.13	1.31	1.24
1	A	723	TRP	CA-C	-6.13	1.45	1.52
1	A	439	ILE	CA-CB	6.12	1.61	1.54
1	B	37	LYS	CG-CD	6.12	1.70	1.52
1	B	130	THR	C-O	-6.09	1.16	1.23
1	A	383	LEU	C-O	-6.08	1.16	1.24
1	B	769	GLN	CA-C	6.08	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	GLU	CB-CG	-6.08	1.34	1.52
1	A	662	GLN	N-CA	-6.06	1.39	1.46
1	B	44	LYS	CE-NZ	6.04	1.67	1.49
1	A	31	MSE	SE-CE	6.02	2.13	1.95
1	A	180	ASN	N-CA	-6.00	1.39	1.46
1	B	804	LYS	C-O	-5.99	1.17	1.24
1	A	492	ALA	N-CA	-5.95	1.38	1.46
1	B	385	GLU	CD-OE1	5.94	1.36	1.25
1	B	31	MSE	SE-CE	5.94	2.13	1.95
1	B	475	LYS	CA-C	-5.93	1.45	1.52
1	A	800	LYS	N-CA	5.92	1.53	1.46
1	A	214	ILE	CA-CB	-5.91	1.46	1.54
1	B	574	ARG	C-O	-5.91	1.16	1.24
1	B	22	ARG	CA-C	5.91	1.60	1.52
1	A	462	SER	C-O	5.88	1.30	1.24
1	B	111	THR	C-O	-5.87	1.17	1.24
1	A	97	ARG	C-O	5.87	1.30	1.23
1	A	161	MSE	SE-CE	5.87	2.13	1.95
1	B	307	MSE	SE-CE	5.85	2.12	1.95
1	A	555	HIS	CA-C	-5.84	1.45	1.52
1	A	122	THR	C-O	-5.84	1.15	1.24
1	A	129	VAL	CA-CB	5.84	1.60	1.54
1	A	800	LYS	CA-C	-5.84	1.45	1.52
1	A	437	ALA	C-O	-5.83	1.17	1.24
1	A	454	VAL	C-N	-5.83	1.28	1.33
1	A	501	THR	C-O	-5.82	1.17	1.24
1	A	499	ALA	N-CA	-5.81	1.38	1.45
1	A	566	ARG	C-O	-5.80	1.17	1.24
1	A	683	VAL	CA-CB	5.80	1.61	1.54
1	B	512	ASP	CB-CG	5.80	1.66	1.52
1	B	375	ILE	CA-CB	5.80	1.63	1.55
1	B	81	MSE	SE-CE	-5.79	1.78	1.95
1	A	548	VAL	CA-CB	-5.78	1.46	1.54
1	B	679	ILE	CA-C	-5.78	1.45	1.52
1	B	814	MSE	SE-CE	5.75	2.12	1.95
1	B	66	GLU	CD-OE2	5.75	1.36	1.25
1	A	394	ALA	CA-C	5.74	1.60	1.52
1	B	387	LEU	C-O	-5.73	1.17	1.23
1	A	216	ILE	N-CA	-5.72	1.39	1.46
1	A	174	ILE	CA-CB	5.72	1.62	1.54
1	A	791	LEU	CA-C	5.72	1.60	1.52
1	B	463	GLU	N-CA	-5.71	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	GLN	N-CA	-5.69	1.39	1.46
1	B	442	ILE	CA-CB	-5.69	1.47	1.54
1	B	665	GLU	CG-CD	5.69	1.66	1.52
1	B	434	LYS	CA-C	5.68	1.60	1.52
1	B	44	LYS	N-CA	5.67	1.53	1.46
1	B	116	ALA	CA-CB	5.67	1.62	1.53
1	B	662	GLN	N-CA	-5.67	1.39	1.46
1	A	156	ILE	CA-C	5.63	1.59	1.52
1	B	76	LYS	CE-NZ	5.62	1.66	1.49
1	B	172	ALA	CA-CB	-5.62	1.44	1.53
1	B	214	ILE	CA-CB	-5.59	1.47	1.54
1	B	540	ASP	C-O	-5.58	1.17	1.24
1	B	488	ALA	CA-C	5.58	1.59	1.52
1	B	402	SER	N-CA	-5.58	1.39	1.46
1	A	572	ARG	CB-CG	-5.57	1.35	1.52
1	B	414	THR	CA-C	5.56	1.60	1.52
1	B	578	GLN	CA-C	-5.55	1.45	1.53
1	A	614	PRO	N-CA	5.55	1.53	1.47
1	B	61	GLU	CG-CD	5.50	1.65	1.52
1	B	391	THR	C-O	-5.49	1.17	1.23
1	A	777	GLU	CD-OE1	5.49	1.35	1.25
1	A	514	VAL	N-CA	-5.46	1.40	1.46
1	B	282	ILE	CA-CB	5.45	1.60	1.54
1	B	432	ALA	CA-CB	5.41	1.62	1.53
1	B	825	THR	C-O	-5.41	1.17	1.24
1	B	500	VAL	C-O	-5.41	1.18	1.24
1	B	131	VAL	CA-CB	5.41	1.61	1.54
1	A	561	ARG	CZ-NH2	-5.39	1.26	1.33
1	A	208	VAL	C-O	-5.39	1.18	1.24
1	B	384	TYR	N-CA	5.38	1.52	1.46
1	B	102	MSE	N-CA	-5.36	1.39	1.46
1	B	634	VAL	CA-C	5.36	1.59	1.52
1	A	661	SER	C-O	-5.35	1.18	1.24
1	A	583	SER	N-CA	5.34	1.52	1.45
1	B	184	PHE	N-CA	-5.33	1.40	1.46
1	B	419	ILE	CA-CB	5.32	1.61	1.54
1	B	179	ASN	CG-ND2	5.29	1.44	1.33
1	B	808	PHE	N-CA	5.29	1.52	1.46
1	B	663	ARG	C-O	-5.28	1.17	1.24
1	A	632	ARG	CG-CD	5.28	1.68	1.52
1	B	137	GLN	N-CA	-5.28	1.40	1.46
1	A	111	THR	CA-C	5.27	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	782	MSE	SE-CE	5.27	2.11	1.95
1	B	92	MSE	CG-SE	5.26	2.11	1.95
1	B	388	ALA	CA-CB	5.26	1.63	1.53
1	B	514	VAL	CA-CB	5.26	1.60	1.54
1	B	393	THR	N-CA	5.25	1.53	1.46
1	A	618	ILE	CA-CB	5.25	1.59	1.55
1	A	547	ALA	C-O	-5.24	1.17	1.24
1	B	23	LYS	CG-CD	5.23	1.68	1.52
1	B	71	VAL	CA-CB	5.23	1.61	1.54
1	B	131	VAL	C-O	-5.22	1.17	1.24
1	B	429	MSE	SE-CE	5.22	2.11	1.95
1	B	171	ALA	CA-CB	5.21	1.62	1.53
1	A	567	ILE	N-CA	-5.21	1.40	1.46
1	A	643	LYS	CA-C	5.19	1.59	1.52
1	A	410	VAL	N-CA	5.19	1.52	1.46
1	B	659	ILE	CA-C	5.19	1.60	1.52
1	A	591	GLU	N-CA	5.18	1.53	1.46
1	A	161	MSE	C-O	-5.18	1.17	1.24
1	B	133	ASP	CA-C	-5.18	1.45	1.52
1	B	438	ILE	CA-C	5.17	1.59	1.52
1	B	652	ALA	CA-CB	5.16	1.61	1.53
1	B	169	ALA	C-O	5.16	1.30	1.24
1	A	630	ALA	CA-C	5.15	1.59	1.52
1	A	655	GLN	N-CA	-5.15	1.40	1.46
1	B	148	GLU	N-CA	5.14	1.52	1.46
1	B	478	VAL	C-O	-5.14	1.17	1.24
1	A	517	GLY	C-O	-5.13	1.19	1.23
1	A	502	ILE	CG1-CD1	-5.12	1.31	1.51
1	A	443	LYS	CD-CE	5.10	1.67	1.52
1	B	692	ILE	CA-C	5.09	1.57	1.53
1	B	136	ALA	N-CA	-5.09	1.40	1.46
1	A	612	MSE	SE-CE	5.08	2.10	1.95
1	B	657	ARG	C-O	-5.08	1.18	1.24
1	B	806	GLU	C-N	-5.08	1.27	1.33
1	A	193	PHE	CA-C	-5.07	1.45	1.52
1	A	476	HIS	C-O	-5.07	1.18	1.24
1	B	195	PRO	C-O	5.06	1.30	1.24
1	A	472	ALA	C-O	-5.05	1.17	1.24
1	A	636	SER	N-CA	-5.05	1.40	1.46
1	B	287	VAL	CA-CB	5.05	1.61	1.54
1	A	35	MSE	SE-CE	5.04	2.10	1.95
1	A	734	THR	CA-CB	5.04	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLU	CA-C	-5.04	1.46	1.52
1	A	661	SER	C-N	-5.03	1.27	1.33
1	A	675	THR	CA-CB	-5.03	1.45	1.53
1	A	762	PHE	CA-C	5.03	1.59	1.52
1	B	92	MSE	CA-C	-5.02	1.46	1.52
1	B	97	ARG	CZ-NH2	-5.01	1.26	1.33

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	HIS	CA-C-N	9.88	132.19	119.84
1	A	620	HIS	C-N-CA	9.88	132.19	119.84
1	B	743	SER	N-CA-C	-9.67	100.70	111.14
1	B	669	VAL	N-CA-CB	-8.82	100.95	111.00
1	B	798	ASP	CA-C-N	8.09	129.96	119.84
1	B	798	ASP	C-N-CA	8.09	129.96	119.84
1	A	517	GLY	N-CA-C	-7.91	103.47	111.85
1	B	648	TYR	N-CA-C	-7.84	102.81	111.36
1	B	613	LYS	CA-C-N	7.52	129.24	119.84
1	B	613	LYS	C-N-CA	7.52	129.24	119.84
1	B	669	VAL	CB-CA-C	7.50	120.03	110.96
1	B	91	GLY	N-CA-C	7.48	121.96	112.83
1	B	23	LYS	CD-CE-NZ	7.39	135.56	111.90
1	A	534	ILE	CB-CA-C	-7.37	102.39	112.04
1	B	378	GLN	N-CA-C	-7.36	103.19	111.07
1	B	790	HIS	N-CA-C	-7.28	104.53	113.41
1	A	581	ALA	N-CA-C	-7.22	100.32	110.50
1	B	801	GLN	N-CA-CB	7.14	122.55	110.49
1	B	466	SER	N-CA-C	7.12	119.71	111.02
1	B	677	ASN	N-CA-C	-6.96	103.77	111.36
1	B	37	LYS	CB-CG-CD	6.91	127.20	111.30
1	A	672	VAL	N-CA-CB	-6.89	102.98	111.94
1	A	214	ILE	N-CA-C	6.80	117.59	110.72
1	B	783	ASP	N-CA-C	-6.80	103.95	111.36
1	A	784	TYR	CA-CB-CG	6.61	125.81	113.90
1	A	651	VAL	N-CA-C	-6.61	103.89	110.30
1	B	442	ILE	CB-CA-C	-6.53	103.61	111.97
1	A	385	GLU	N-CA-C	6.51	118.38	111.28
1	A	72	ARG	NE-CZ-NH2	6.48	125.03	119.20
1	B	660	TYR	N-CA-C	-6.45	104.10	112.23
1	A	144	ARG	CA-C-N	-6.31	112.50	119.19
1	A	144	ARG	C-N-CA	-6.31	112.50	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	679	ILE	CB-CA-C	-6.26	103.68	112.14
1	A	568	ASP	N-CA-C	-6.26	104.54	111.36
1	B	533	GLN	N-CA-C	-6.21	105.83	113.41
1	B	817	SER	N-CA-C	-6.21	104.62	111.82
1	A	827	SER	N-CA-C	6.14	117.64	111.07
1	A	723	TRP	N-CA-C	-6.11	104.31	110.97
1	A	51	ARG	N-CA-C	6.10	117.93	111.28
1	B	759	MSE	N-CA-C	6.03	117.65	111.14
1	B	299	TYR	N-CA-C	-5.99	106.32	113.21
1	B	679	ILE	N-CA-C	5.99	116.73	110.62
1	B	607	MSE	CG-SE-CE	5.98	112.08	98.92
1	B	673	SER	N-CA-C	5.97	117.79	111.28
1	B	827	SER	N-CA-C	5.97	118.28	111.11
1	B	43	LEU	N-CA-C	5.97	118.27	111.11
1	B	679	ILE	N-CA-CB	5.89	118.55	110.54
1	A	597	ILE	CB-CA-C	-5.87	100.57	111.79
1	B	165	ALA	N-CA-C	5.86	117.34	111.07
1	B	116	ALA	N-CA-C	-5.83	105.00	111.36
1	A	156	ILE	CB-CA-C	5.83	118.83	110.33
1	A	168	GLU	N-CA-C	5.81	117.61	111.28
1	B	517	GLY	N-CA-C	-5.79	105.80	112.29
1	A	398	ALA	N-CA-C	5.79	117.59	111.28
1	A	522	GLU	N-CA-C	-5.75	105.03	112.68
1	A	647	GLU	N-CA-C	-5.73	105.03	111.28
1	B	688	ILE	CB-CA-C	-5.70	104.61	112.24
1	B	80	GLY	N-CA-C	-5.67	106.34	115.08
1	A	72	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	A	672	VAL	CB-CA-C	5.60	120.03	112.36
1	A	218	GLU	N-CA-C	5.59	120.21	113.17
1	A	454	VAL	CA-C-N	-5.57	117.55	122.73
1	A	454	VAL	C-N-CA	-5.57	117.55	122.73
1	B	654	ASP	N-CA-C	-5.57	105.29	111.36
1	B	370	GLN	N-CA-C	5.56	117.71	110.43
1	B	785	LEU	CB-CA-C	-5.54	101.55	110.74
1	B	786	ARG	NE-CZ-NH1	-5.54	115.97	121.50
1	A	415	ASN	N-CA-C	-5.51	105.18	111.07
1	A	674	GLU	N-CA-C	-5.50	105.18	111.07
1	A	184	PHE	N-CA-C	5.49	120.43	111.37
1	B	656	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	B	442	ILE	N-CA-C	5.47	115.67	110.42
1	A	141	GLU	N-CA-C	5.42	117.27	111.36
1	A	533	GLN	N-CA-C	-5.42	105.38	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	THR	N-CA-C	5.40	117.17	111.28
1	B	400	GLU	N-CA-C	5.39	117.23	111.36
1	A	777	GLU	CB-CA-C	-5.38	101.86	110.79
1	A	627	ILE	N-CA-C	5.35	115.56	110.42
1	B	98	CYS	CA-C-N	5.35	129.74	122.90
1	B	98	CYS	C-N-CA	5.35	129.74	122.90
1	A	64	ILE	N-CA-C	-5.33	105.96	112.35
1	B	703	ILE	N-CA-C	5.32	120.37	108.88
1	A	801	GLN	N-CA-CB	5.29	119.44	110.49
1	A	800	LYS	N-CA-C	-5.29	99.53	110.80
1	A	544	ARG	N-CA-C	-5.28	104.95	111.40
1	B	64	ILE	CA-C-N	-5.27	113.20	119.05
1	B	64	ILE	C-N-CA	-5.27	113.20	119.05
1	A	467	ASN	N-CA-C	5.26	117.02	111.28
1	A	795	ALA	N-CA-C	5.26	117.70	107.71
1	B	125	GLY	N-CA-C	5.26	118.84	112.48
1	B	101	GLU	CB-CA-C	-5.24	102.17	110.81
1	A	760	ARG	N-CA-C	-5.21	105.50	111.07
1	A	370	GLN	N-CA-C	5.18	118.00	109.72
1	A	673	SER	N-CA-C	5.18	117.00	111.36
1	A	565	ARG	N-CA-C	5.17	118.69	112.38
1	B	723	TRP	CA-CB-CG	5.17	123.42	113.60
1	A	18	LEU	N-CA-C	5.15	116.58	111.07
1	B	572	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	612	MSE	N-CA-C	5.15	119.86	111.37
1	B	142	ASN	N-CA-CB	5.14	117.77	110.16
1	A	395	ASP	N-CA-C	5.12	121.71	110.80
1	A	799	PRO	O-C-N	-5.09	117.27	123.03
1	B	518	SER	N-CA-C	5.09	117.04	109.25
1	B	676	ILE	CB-CA-C	-5.06	105.41	112.04
1	B	221	THR	CA-C-N	-5.06	114.58	119.90
1	B	221	THR	C-N-CA	-5.06	114.58	119.90
1	B	37	LYS	CA-C-N	5.04	127.93	120.82
1	B	37	LYS	C-N-CA	5.04	127.93	120.82
1	A	664	ASN	N-CA-C	5.04	116.77	111.28
1	A	573	GLY	N-CA-C	-5.04	109.13	114.67
1	B	486	ASN	N-CA-C	-5.03	105.87	111.36
1	A	511	THR	N-CA-C	5.03	117.59	110.10
1	B	407	LEU	N-CA-C	-5.01	100.56	108.73

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	ALA	Peptide
1	A	796	GLN	Peptide
1	A	800	LYS	Peptide
1	B	228	PRO	Peptide
1	B	246	LEU	Peptide
1	B	394	ALA	Peptide
1	B	530	THR	Peptide
1	B	719	PRO	Peptide
1	B	730	LEU	Peptide
1	B	789	ILE	Peptide

5.2 Too-close contacts [i](#)

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	5401	0	5406	126	0
1	B	5915	0	5921	193	0
2	A	31	0	12	0	0
2	B	31	0	12	2	0
3	A	198	0	0	15	0
3	B	233	0	0	17	0
All	All	11809	0	11351	318	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 14.

All (318) 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:B:44:LYS:CE	1:B:44:LYS:NZ	1.67	1.55
1:B:406:LYS:CE	1:B:406:LYS:NZ	1.69	1.52
1:B:759:MSE:SE	1:B:759:MSE:CE	2.14	1.45
1:A:429:MSE:SE	1:A:429:MSE:CE	2.14	1.45
1:B:23:LYS:CE	1:B:23:LYS:NZ	1.76	1.45
1:B:235:MSE:SE	1:B:235:MSE:CE	2.15	1.45
1:B:607:MSE:SE	1:B:607:MSE:CE	2.17	1.43
1:A:21:MSE:CE	1:A:21:MSE:SE	2.16	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:MSE:SE	1:A:506:MSE:CE	2.17	1.42
1:B:35:MSE:SE	1:B:35:MSE:CE	2.16	1.42
1:A:590:MSE:CE	1:A:590:MSE:SE	2.18	1.42
1:B:418:MSE:CE	1:B:418:MSE:SE	2.16	1.42
1:B:506:MSE:CE	1:B:506:MSE:SE	2.18	1.41
1:B:612:MSE:SE	1:B:612:MSE:CE	2.18	1.41
1:A:418:MSE:SE	1:A:418:MSE:CE	2.20	1.39
1:B:700:MSE:SE	1:B:700:MSE:CE	2.22	1.38
1:A:833:MSE:CE	1:A:833:MSE:SE	2.23	1.37
1:A:700:MSE:SE	1:A:700:MSE:CE	2.22	1.36
1:A:782:MSE:SE	1:A:782:MSE:CE	2.23	1.35
1:B:305:MSE:HE3	3:B:1070:HOH:O	1.46	1.16
2:B:901:ATP:O3A	2:B:901:ATP:O2G	1.73	1.03
1:B:788:GLY:HA3	3:B:1023:HOH:O	1.66	0.95
1:B:782:MSE:HE1	1:B:810:MSE:SE	2.21	0.90
1:B:101:GLU:OE2	1:B:395:ASP:HB3	1.72	0.90
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.72	0.88
1:A:612:MSE:HB3	3:A:1047:HOH:O	1.74	0.87
1:A:618:ILE:O	1:A:619:GLU:HB2	1.75	0.86
1:A:731:HIS:NE2	1:A:734:THR:OG1	2.10	0.85
1:B:14:ASN:HD21	1:B:411:VAL:H	1.25	0.84
1:B:782:MSE:HG3	3:B:949:HOH:O	1.79	0.82
1:B:102:MSE:HE3	1:B:108:LYS:HG2	1.60	0.82
1:B:679:ILE:O	1:B:683:VAL:HG23	1.81	0.80
1:B:759:MSE:CE	1:B:759:MSE:HA	2.11	0.80
1:B:610:LEU:O	1:B:612:MSE:N	2.17	0.77
1:B:754:VAL:HG11	1:B:759:MSE:HE3	1.66	0.77
1:B:796:GLN:O	1:B:797:LYS:O	2.02	0.77
1:B:587:TYR:C	1:B:588:LEU:HG	2.07	0.77
1:B:18:LEU:HD23	1:B:21:MSE:CE	2.15	0.76
1:A:789:ILE:O	1:A:790:HIS:CG	2.40	0.75
1:B:228:PRO:C	1:B:230:GLU:H	1.95	0.74
1:A:531:ALA:HB1	1:A:532:GLU:OE1	1.87	0.74
1:B:707:GLN:NE2	1:B:708:GLU:OE2	2.21	0.74
1:B:807:SER:HA	1:B:810:MSE:HE3	1.70	0.74
1:B:395:ASP:HA	3:B:946:HOH:O	1.88	0.74
1:B:367:ASN:O	1:B:368:GLU:O	2.06	0.73
1:A:594:LEU:HG	1:A:597:ILE:HD13	1.69	0.73
1:A:786:ARG:O	1:A:789:ILE:HB	1.89	0.72
1:A:612:MSE:CB	3:A:1047:HOH:O	2.36	0.72
1:A:799:PRO:O	1:A:800:LYS:CB	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:THR:HG23	3:B:939:HOH:O	1.90	0.71
1:B:718:LEU:O	1:B:720:ILE:N	2.24	0.70
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.21	0.70
1:A:799:PRO:O	1:A:800:LYS:HG3	1.93	0.69
1:B:693:PRO:O	1:B:696:SER:HB3	1.93	0.69
1:B:732:GLU:O	1:B:736:ARG:HG3	1.93	0.69
1:B:595:MSE:HE3	1:B:604:SER:OG	1.93	0.68
1:A:530:THR:O	1:A:532:GLU:N	2.26	0.68
1:A:17:THR:O	1:A:21:MSE:HG3	1.93	0.68
1:A:620:HIS:HD2	3:A:992:HOH:O	1.75	0.68
1:A:458:SER:HB2	1:A:460:GLU:OE1	1.94	0.67
1:A:618:ILE:O	1:A:619:GLU:CB	2.42	0.67
1:A:223:LEU:HD21	1:A:377:PHE:CZ	2.30	0.67
1:A:731:HIS:CE1	1:A:734:THR:HG1	2.12	0.67
1:B:247:ILE:O	1:B:247:ILE:HG23	1.94	0.67
1:B:759:MSE:HA	1:B:759:MSE:HE2	1.76	0.66
1:B:637:ARG:HH11	1:B:641:ILE:HD11	1.59	0.66
1:B:239:VAL:O	1:B:242:ILE:HG22	1.96	0.65
1:B:789:ILE:HG22	1:B:789:ILE:O	1.96	0.65
1:B:703:ILE:HA	1:B:706:LEU:HB3	1.78	0.65
1:B:595:MSE:CE	1:B:604:SER:OG	2.45	0.65
1:A:102:MSE:HE1	1:A:390:MSE:SE	2.48	0.64
1:A:529:PRO:HA	1:A:533:GLN:HE21	1.63	0.64
1:B:316:ALA:O	1:B:317:HIS:CG	2.51	0.64
1:B:800:LYS:O	1:B:801:GLN:HB2	1.97	0.64
1:B:605:GLY:O	1:B:608:ARG:HB2	1.97	0.64
1:A:799:PRO:O	1:A:800:LYS:CG	2.46	0.64
1:B:600:SER:HB3	1:B:603:VAL:HB	1.81	0.63
1:B:519:TRP:CH2	1:B:538:LYS:HE3	2.34	0.63
1:A:435:ILE:HG21	1:A:468:GLU:HG3	1.80	0.62
1:B:629:ASN:HD22	1:B:632:ARG:HH22	1.47	0.62
1:B:102:MSE:HE1	1:B:390:MSE:SE	2.49	0.62
1:A:429:MSE:HB2	1:A:433:GLU:OE2	1.99	0.61
1:A:566:ARG:HD2	3:A:1093:HOH:O	2.00	0.61
1:B:618:ILE:O	1:B:619:GLU:HB2	2.01	0.60
1:B:693:PRO:O	1:B:696:SER:CB	2.48	0.60
1:B:787:GLN:C	1:B:789:ILE:H	2.08	0.60
1:B:730:LEU:HG	1:B:731:HIS:H	1.67	0.59
1:A:405:TYR:O	1:A:406:LYS:HB2	2.01	0.59
1:B:833:MSE:HG3	1:B:834:PRO:HD2	1.83	0.59
1:A:730:LEU:HD12	1:A:734:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HB2	3:B:1094:HOH:O	2.03	0.59
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.84	0.59
1:B:722:GLU:O	1:B:723:TRP:C	2.46	0.59
1:A:395:ASP:HA	3:A:1028:HOH:O	2.03	0.58
1:B:14:ASN:ND2	1:B:411:VAL:H	2.00	0.58
1:B:180:ASN:HD22	1:B:180:ASN:H	1.51	0.58
1:B:564:SER:HB3	1:B:567:ILE:HD12	1.85	0.58
1:B:429:MSE:HB2	1:B:433:GLU:OE2	2.02	0.58
1:A:102:MSE:HE3	1:A:108:LYS:HG2	1.86	0.58
1:B:723:TRP:O	1:B:727:GLU:HG2	2.02	0.58
1:A:507:ALA:HB3	3:A:1094:HOH:O	2.02	0.58
1:A:800:LYS:HA	1:A:803:TYR:HB3	1.86	0.57
1:B:216:ILE:HD11	1:B:401:PHE:CE1	2.39	0.57
1:B:523:VAL:HG22	3:B:1121:HOH:O	2.05	0.57
1:A:529:PRO:HA	1:A:533:GLN:NE2	2.20	0.57
1:B:79:PHE:HB3	1:B:81:MSE:HE2	1.85	0.57
1:B:671:ASP:OD1	1:B:673:SER:HB2	2.04	0.57
1:B:238:ARG:NE	1:B:238:ARG:HA	2.19	0.57
1:B:782:MSE:HE1	1:B:810:MSE:CE	2.35	0.57
1:B:18:LEU:HD23	1:B:21:MSE:HE3	1.86	0.56
1:B:826:LEU:O	1:B:829:VAL:HG12	2.05	0.56
1:B:679:ILE:HG13	1:B:823:ILE:HD11	1.87	0.56
1:B:512:ASP:OD1	1:B:577:ARG:HD3	2.06	0.56
1:B:785:LEU:O	1:B:789:ILE:HB	2.06	0.55
1:B:435:ILE:O	1:B:436:GLN:C	2.47	0.55
1:A:441:ASP:O	1:A:445:ARG:HG3	2.06	0.55
1:B:104:THR:HG21	1:B:577:ARG:NH2	2.22	0.55
1:B:294:GLU:O	1:B:294:GLU:HG3	2.06	0.55
1:B:457:ILE:HA	1:B:505:ASN:OD1	2.06	0.55
1:A:461:LYS:O	1:A:465:VAL:HG12	2.07	0.55
1:B:648:TYR:OH	1:B:800:LYS:HB3	2.06	0.54
1:B:789:ILE:O	1:B:789:ILE:CG2	2.55	0.54
1:A:731:HIS:CD2	1:A:734:THR:HG1	2.25	0.54
1:B:607:MSE:HE2	1:B:623:VAL:HG13	1.90	0.54
1:B:247:ILE:O	1:B:247:ILE:CG2	2.56	0.54
1:A:519:TRP:CZ3	1:A:538:LYS:HD3	2.43	0.53
1:B:170:TYR:CZ	1:B:200:GLN:HG2	2.43	0.53
1:B:292:MSE:HG2	1:B:296:GLU:HB2	1.90	0.53
1:A:711:LYS:HG2	1:A:717:ASP:HB2	1.90	0.53
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.07	0.53
1:B:507:ALA:HB3	3:B:1043:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:LEU:HD11	1:B:810:MSE:HE1	1.89	0.53
1:B:760:ARG:CB	3:B:1124:HOH:O	2.56	0.53
1:B:637:ARG:NH1	1:B:641:ILE:HD11	2.24	0.52
1:B:228:PRO:O	1:B:230:GLU:N	2.40	0.52
1:B:531:ALA:O	1:B:535:GLU:HB2	2.10	0.52
1:A:531:ALA:CB	1:A:532:GLU:OE1	2.58	0.52
1:B:18:LEU:HA	1:B:21:MSE:HE2	1.92	0.52
1:B:651:VAL:O	1:B:655:GLN:HG3	2.10	0.52
1:B:504:THR:O	1:B:505:ASN:C	2.53	0.52
1:A:460:GLU:OE1	1:A:460:GLU:N	2.30	0.51
1:B:716:LEU:HG	1:B:718:LEU:CD1	2.40	0.51
1:A:427:VAL:HB	1:A:612:MSE:HE2	1.92	0.51
1:A:590:MSE:HG3	1:A:608:ARG:HG2	1.93	0.51
1:A:763:GLU:O	1:A:767:MSE:HG3	2.10	0.51
1:B:520:GLN:C	1:B:522:GLU:N	2.69	0.50
1:B:438:ILE:HD13	1:B:559:THR:HG22	1.93	0.50
1:B:508:GLY:O	1:B:510:GLY:N	2.43	0.50
1:B:590:MSE:HE1	1:B:604:SER:O	2.11	0.50
1:A:16:ARG:NH1	3:A:1005:HOH:O	2.44	0.50
1:A:742:GLN:O	1:A:746:VAL:HG23	2.11	0.50
1:B:16:ARG:CB	3:B:1094:HOH:O	2.58	0.50
1:B:520:GLN:C	1:B:522:GLU:H	2.19	0.50
1:A:727:GLU:HB2	1:A:729:GLU:HB2	1.93	0.50
2:B:901:ATP:O2G	2:B:901:ATP:PA	2.70	0.50
1:B:79:PHE:HB3	1:B:81:MSE:CE	2.41	0.50
1:B:587:TYR:O	1:B:588:LEU:HG	2.11	0.50
1:B:539:ALA:O	1:B:543:VAL:HG23	2.12	0.49
1:B:801:GLN:HA	1:B:801:GLN:OE1	2.10	0.49
1:B:782:MSE:CE	1:B:810:MSE:SE	3.05	0.49
1:B:102:MSE:CE	1:B:390:MSE:SE	3.10	0.49
1:A:727:GLU:HG3	1:A:730:LEU:HB3	1.93	0.49
1:B:691:TYR:HD1	1:B:702:ASP:OD2	1.96	0.49
1:B:800:LYS:HD2	1:B:804:LYS:HE3	1.93	0.49
1:B:648:TYR:CZ	1:B:800:LYS:HB3	2.47	0.49
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.53	0.49
1:B:680:ARG:HD2	1:B:743:SER:OG	2.13	0.49
1:B:787:GLN:C	1:B:789:ILE:N	2.71	0.49
1:B:227:GLY:C	1:B:229:ALA:N	2.71	0.48
1:A:742:GLN:HA	1:A:745:GLU:HG2	1.94	0.48
1:A:731:HIS:CE1	1:A:733:GLU:HB3	2.48	0.48
1:A:731:HIS:HE1	1:A:733:GLU:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ILE:O	1:A:789:ILE:CG2	2.61	0.48
1:B:246:LEU:HD13	1:B:314:LEU:HD21	1.94	0.48
1:B:434:LYS:NZ	1:B:559:THR:O	2.41	0.48
1:A:503:ALA:HB1	1:A:506:MSE:HG2	1.95	0.48
1:A:538:LYS:NZ	1:B:528:ASN:ND2	2.61	0.48
1:B:99:ILE:HD11	1:B:407:LEU:HD13	1.95	0.48
1:B:179:ASN:OD1	3:B:1055:HOH:O	2.20	0.48
1:B:228:PRO:C	1:B:230:GLU:N	2.63	0.48
1:B:730:LEU:HG	1:B:731:HIS:N	2.28	0.48
1:B:708:GLU:O	1:B:712:ASN:N	2.37	0.48
1:A:789:ILE:O	1:A:790:HIS:ND1	2.46	0.48
1:A:571:LEU:O	1:A:574:ARG:HB2	2.14	0.48
1:A:747:TYR:OH	1:A:763:GLU:OE2	2.24	0.48
1:A:799:PRO:O	1:A:800:LYS:HB3	2.11	0.48
1:A:32:GLU:HB3	1:A:33:PRO:HD3	1.96	0.47
1:A:642:ARG:NH1	3:A:1000:HOH:O	2.46	0.47
1:B:459:ILE:O	1:B:463:GLU:HG3	2.14	0.47
1:A:594:LEU:O	1:A:597:ILE:HG12	2.15	0.47
1:A:731:HIS:HB3	3:A:1026:HOH:O	2.14	0.47
1:A:487:GLU:O	1:A:491:VAL:HG23	2.14	0.47
1:A:531:ALA:O	1:A:534:ILE:HB	2.14	0.47
1:A:727:GLU:HG3	1:A:730:LEU:CB	2.44	0.47
1:A:64:ILE:N	1:A:65:PRO:CD	2.78	0.47
1:B:367:ASN:O	1:B:368:GLU:HG3	2.15	0.47
1:B:520:GLN:O	1:B:522:GLU:N	2.48	0.47
1:A:66:GLU:HG3	3:A:957:HOH:O	2.13	0.47
1:A:535:GLU:OE1	1:A:535:GLU:HA	2.15	0.47
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.95	0.47
1:B:446:THR:HG21	1:B:500:VAL:CG2	2.45	0.47
1:B:144:ARG:HB3	1:B:145:PRO:HD3	1.97	0.47
1:A:785:LEU:HD22	1:A:810:MSE:HE1	1.97	0.47
1:B:239:VAL:O	1:B:242:ILE:CG2	2.61	0.47
1:B:493:GLN:HG2	3:B:1047:HOH:O	2.14	0.47
1:B:131:VAL:HG11	1:B:210:GLU:HG2	1.97	0.46
1:B:440:GLU:O	1:B:444:GLU:HG3	2.15	0.46
1:B:131:VAL:CG1	1:B:210:GLU:HG2	2.45	0.46
1:B:404:ILE:HG22	1:B:404:ILE:O	2.16	0.46
1:A:731:HIS:CD2	1:A:734:THR:OG1	2.67	0.46
1:B:394:ALA:HB3	3:B:1054:HOH:O	2.15	0.46
1:A:589:SER:H	1:A:592:ASP:CG	2.24	0.46
1:B:228:PRO:HG3	1:B:369:ASN:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:THR:N	3:B:1016:HOH:O	2.48	0.46
1:B:613:LYS:HA	1:B:614:PRO:HD2	1.71	0.46
1:B:749:ARG:HD3	1:B:833:MSE:HE3	1.97	0.46
1:B:760:ARG:HB3	3:B:1124:HOH:O	2.16	0.46
1:A:103:ARG:NE	3:A:1082:HOH:O	2.35	0.46
1:A:563:GLU:HA	1:A:594:LEU:HD11	1.96	0.46
1:A:133:ASP:O	1:A:137:GLN:HG3	2.15	0.46
1:A:395:ASP:OD2	1:A:396:THR:N	2.49	0.46
1:B:110:LEU:O	1:B:111:THR:C	2.58	0.45
1:A:428:TYR:O	1:A:589:SER:HA	2.15	0.45
1:A:47:THR:O	1:A:51:ARG:HG3	2.15	0.45
1:A:434:LYS:NZ	1:A:560:GLU:HG3	2.31	0.45
1:A:590:MSE:HG3	1:A:608:ARG:CG	2.46	0.45
1:B:99:ILE:HA	1:B:389:GLY:O	2.16	0.45
1:B:588:LEU:HD13	1:B:627:ILE:HD13	1.98	0.45
1:A:650:ASP:OD2	3:A:1068:HOH:O	2.20	0.45
1:B:457:ILE:O	1:B:505:ASN:ND2	2.49	0.45
1:B:144:ARG:N	1:B:145:PRO:HD2	2.32	0.45
1:B:496:TYR:O	1:B:497:PRO:C	2.60	0.45
1:A:409:THR:HG23	3:A:1007:HOH:O	2.17	0.45
1:B:716:LEU:HG	1:B:718:LEU:HD11	1.99	0.45
1:B:281:LEU:HA	1:B:284:GLU:HG2	1.98	0.45
1:B:727:GLU:O	1:B:730:LEU:HD22	2.16	0.45
1:B:520:GLN:HA	3:B:1121:HOH:O	2.17	0.44
1:A:38:LEU:HG	1:A:42:GLU:HB3	1.97	0.44
1:A:74:ALA:O	1:A:78:VAL:HG23	2.17	0.44
1:B:644:GLN:NE2	1:B:800:LYS:HE3	2.31	0.44
1:B:282:ILE:HD11	1:B:286:LEU:HD21	1.99	0.44
1:A:486:ASN:HD21	1:B:132:ASN:HD21	1.65	0.44
1:B:483:PHE:O	1:B:487:GLU:HG3	2.18	0.44
1:A:32:GLU:N	1:A:33:PRO:CD	2.81	0.44
1:B:735:LEU:HA	1:B:738:ARG:HB2	1.99	0.44
1:B:796:GLN:HB3	1:B:797:LYS:H	1.73	0.44
1:A:101:GLU:HB2	1:A:411:VAL:HA	2.00	0.44
1:A:800:LYS:O	1:A:801:GLN:HB2	2.18	0.44
1:B:33:PRO:O	1:B:37:LYS:HD3	2.16	0.44
1:B:742:GLN:O	1:B:745:GLU:HG2	2.18	0.44
1:B:243:ILE:HG21	1:B:317:HIS:NE2	2.33	0.44
1:A:25:VAL:HG23	1:A:92:MSE:HE1	2.00	0.44
1:A:457:ILE:HG22	1:A:562:HIS:CE1	2.53	0.44
1:A:507:ALA:O	1:A:508:GLY:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:GLU:O	1:B:491:VAL:HG23	2.18	0.44
1:A:27:ILE:O	1:A:31:MSE:HG3	2.19	0.43
1:A:101:GLU:OE1	1:A:411:VAL:HG22	2.18	0.43
1:B:789:ILE:HG13	1:B:792:ARG:HB2	1.99	0.43
1:A:496:TYR:O	1:A:497:PRO:C	2.61	0.43
1:A:532:GLU:N	1:A:532:GLU:CD	2.77	0.43
1:B:223:LEU:O	1:B:374:SER:HA	2.19	0.43
1:B:711:LYS:HE2	1:B:717:ASP:HA	2.00	0.43
1:A:594:LEU:C	1:A:596:ARG:N	2.70	0.43
1:B:183:GLY:HA3	1:B:223:LEU:CD1	2.48	0.43
1:B:299:TYR:CD1	1:B:299:TYR:O	2.71	0.43
1:B:304:ILE:HG21	1:B:781:ALA:HB1	2.00	0.43
1:A:18:LEU:O	1:A:22:ARG:HG3	2.18	0.43
1:A:594:LEU:O	1:A:595:MSE:C	2.61	0.43
1:A:629:ASN:HD22	1:A:632:ARG:HE	1.65	0.43
1:B:103:ARG:NH2	1:B:575:SER:O	2.52	0.43
1:B:298:LEU:HD13	1:B:306:LEU:HD13	2.00	0.43
1:B:669:VAL:HG12	1:B:672:VAL:HG23	2.01	0.43
1:B:306:LEU:O	1:B:309:HIS:HB2	2.19	0.43
1:B:230:GLU:HB3	1:B:367:ASN:ND2	2.33	0.42
1:B:595:MSE:HE3	1:B:604:SER:HG	1.80	0.42
1:B:735:LEU:O	1:B:736:ARG:C	2.60	0.42
1:A:378:GLN:O	1:A:382:ARG:HG3	2.19	0.42
1:A:721:ALA:O	1:A:725:ASP:HB3	2.19	0.42
1:A:792:ARG:O	1:A:794:TYR:CD1	2.73	0.42
1:B:298:LEU:C	1:B:300:SER:H	2.27	0.41
1:B:798:ASP:HA	1:B:799:PRO:HD2	1.52	0.41
1:B:399:PHE:HZ	1:B:635:GLU:HG3	1.84	0.41
1:B:792:ARG:NH2	3:B:1023:HOH:O	2.52	0.41
1:A:453:LEU:HD21	1:A:506:MSE:SE	2.70	0.41
1:A:63:LEU:O	1:A:64:ILE:C	2.64	0.41
1:B:714:PHE:O	1:B:715:ASP:C	2.63	0.41
1:A:81:MSE:HE3	1:A:110:LEU:HD13	2.03	0.41
1:B:170:TYR:CE2	1:B:200:GLN:HG2	2.55	0.41
1:B:231:ASP:OD1	1:B:232:SER:HB2	2.20	0.41
1:A:486:ASN:ND2	1:B:132:ASN:HD21	2.19	0.41
1:A:566:ARG:CD	3:A:1093:HOH:O	2.65	0.41
1:A:701:TRP:CD1	1:A:701:TRP:N	2.86	0.41
1:A:719:PRO:HB2	1:A:722:GLU:CD	2.45	0.41
1:A:731:HIS:O	1:A:735:LEU:HB2	2.21	0.41
1:B:406:LYS:NZ	1:B:406:LYS:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:VAL:O	1:B:612:MSE:HG2	2.20	0.41
1:A:16:ARG:HH21	1:A:19:ARG:HD2	1.86	0.41
1:A:797:LYS:NZ	3:A:1079:HOH:O	2.50	0.41
1:B:316:ALA:O	1:B:317:HIS:CD2	2.74	0.41
1:B:378:GLN:O	1:B:382:ARG:HG3	2.21	0.41
1:B:666:LEU:O	1:B:764:LYS:HE3	2.21	0.41
1:A:519:TRP:CE3	1:A:538:LYS:HD3	2.57	0.40
1:A:679:ILE:HD13	1:A:679:ILE:HG21	1.92	0.40
1:A:800:LYS:H	1:A:803:TYR:H	1.68	0.40
1:B:693:PRO:HG2	1:B:696:SER:OG	2.21	0.40
1:A:785:LEU:HD11	1:A:806:GLU:OE2	2.21	0.40
1:B:519:TRP:CZ2	1:B:538:LYS:HE3	2.57	0.40
1:B:698:GLU:HA	1:B:701:TRP:CD2	2.56	0.40
1:A:32:GLU:OE2	1:A:82:ARG:HD2	2.20	0.40
1:B:102:MSE:O	1:B:392:GLY:HA2	2.20	0.40
1:B:644:GLN:HE22	1:B:800:LYS:CE	2.34	0.40
1:A:457:ILE:HD13	1:A:457:ILE:HG21	1.81	0.40
1:A:632:ARG:HB2	1:A:632:ARG:NH1	2.36	0.40
1:A:740:LEU:O	1:A:741:ALA:C	2.65	0.40
1:A:745:GLU:HG3	1:A:746:VAL:N	2.36	0.40
1:B:247:ILE:O	1:B:248:ARG:HG2	2.22	0.40
1:B:450:GLN:HG3	1:B:553:GLY:O	2.22	0.40
1:B:541:TRP:CZ2	1:B:545:HIS:CD2	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	675/853 (79%)	635 (94%)	31 (5%)	9 (1%)	9 8
1	B	737/853 (86%)	651 (88%)	49 (7%)	37 (5%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1412/1706 (83%)	1286 (91%)	80 (6%)	46 (3%)	3 1

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	A	395	ASP
1	A	508	GLY
1	A	509	ARG
1	A	531	ALA
1	B	229	ALA
1	B	230	GLU
1	B	289	GLU
1	B	368	GLU
1	B	395	ASP
1	B	507	ALA
1	B	509	ARG
1	B	521	ALA
1	B	531	ALA
1	B	611	GLY
1	B	612	MSE
1	B	729	GLU
1	B	730	LEU
1	B	731	HIS
1	B	796	GLN
1	B	797	LYS
1	A	510	GLY
1	A	619	GLU
1	A	790	HIS
1	B	231	ASP
1	B	302	ALA
1	B	394	ALA
1	B	594	LEU
1	B	801	GLN
1	B	234	GLU
1	B	608	ARG
1	B	614	PRO
1	B	617	ALA
1	B	707	GLN
1	B	794	TYR
1	A	613	LYS
1	B	286	LEU

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Mol	Chain	Res	Type
1	B	690	ALA
1	B	691	TYR
1	B	481	ALA
1	B	535	GLU
1	B	619	GLU
1	B	719	PRO
1	B	703	ILE
1	B	510	GLY
1	B	287	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	575/696 (83%)	532 (92%)	43 (8%)	12	14
1	B	632/696 (91%)	548 (87%)	84 (13%)	4	3
All	All	1207/1392 (87%)	1080 (90%)	127 (10%)	6	6

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	ARG
1	A	22	ARG
1	A	37	LYS
1	A	38	LEU
1	A	41	GLU
1	A	72	ARG
1	A	156	ILE
1	A	194	SER
1	A	225	ILE
1	A	369	ASN
1	A	396	THR
1	A	409	THR
1	A	427	VAL

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Mol	Chain	Res	Type
1	A	461	LYS
1	A	506	MSE
1	A	527	GLU
1	A	532	GLU
1	A	533	GLN
1	A	535	GLU
1	A	538	LYS
1	A	566	ARG
1	A	596	ARG
1	A	597	ILE
1	A	604	SER
1	A	610	LEU
1	A	618	ILE
1	A	632	ARG
1	A	637	ARG
1	A	661	SER
1	A	669	VAL
1	A	672	VAL
1	A	674	GLU
1	A	725	ASP
1	A	727	GLU
1	A	735	LEU
1	A	742	GLN
1	A	749	ARG
1	A	789	ILE
1	A	791	LEU
1	A	794	TYR
1	A	800	LYS
1	A	816	GLU
1	B	23	LYS
1	B	38	LEU
1	B	41	GLU
1	B	98	CYS
1	B	99	ILE
1	B	103	ARG
1	B	104	THR
1	B	180	ASN
1	B	196	GLU
1	B	210	GLU
1	B	226	SER
1	B	231	ASP
1	B	232	SER

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	237	LYS
1	B	242	ILE
1	B	247	ILE
1	B	248	ARG
1	B	284	GLU
1	B	285	LEU
1	B	288	LYS
1	B	289	GLU
1	B	292	MSE
1	B	304	ILE
1	B	306	LEU
1	B	310	VAL
1	B	367	ASN
1	B	395	ASP
1	B	406	LYS
1	B	409	THR
1	B	416	ARG
1	B	435	ILE
1	B	436	GLN
1	B	439	ILE
1	B	440	GLU
1	B	448	LYS
1	B	471	LYS
1	B	509	ARG
1	B	512	ASP
1	B	518	SER
1	B	520	GLN
1	B	523	VAL
1	B	529	PRO
1	B	532	GLU
1	B	533	GLN
1	B	535	GLU
1	B	536	LYS
1	B	537	ILE
1	B	588	LEU
1	B	594	LEU
1	B	596	ARG
1	B	606	MSE
1	B	608	ARG
1	B	610	LEU
1	B	618	ILE

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Mol	Chain	Res	Type
1	B	669	VAL
1	B	672	VAL
1	B	674	GLU
1	B	679	ILE
1	B	685	LYS
1	B	702	ASP
1	B	703	ILE
1	B	718	LEU
1	B	723	TRP
1	B	724	LEU
1	B	726	LYS
1	B	727	GLU
1	B	729	GLU
1	B	734	THR
1	B	735	LEU
1	B	743	SER
1	B	745	GLU
1	B	749	ARG
1	B	750	LYS
1	B	754	VAL
1	B	759	MSE
1	B	779	LEU
1	B	787	GLN
1	B	791	LEU
1	B	797	LYS
1	B	800	LYS
1	B	801	GLN
1	B	831	VAL
1	B	832	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	A	370	GLN
1	A	486	ASN
1	A	520	GLN
1	A	528	ASN
1	A	620	HIS
1	A	629	ASN
1	A	638	ASN
1	A	662	GLN

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Mol	Chain	Res	Type
1	A	742	GLN
1	A	761	HIS
1	B	14	ASN
1	B	180	ASN
1	B	309	HIS
1	B	367	ASN
1	B	486	ASN
1	B	520	GLN
1	B	528	ASN
1	B	542	GLN
1	B	545	HIS
1	B	629	ASN
1	B	638	ASN
1	B	644	GLN
1	B	664	ASN
1	B	707	GLN
1	B	731	HIS
1	B	748	GLN
1	B	787	GLN
1	B	830	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	900	-	32,33,33	1.71	7 (21%)	48,52,52	2.29	19 (39%)
2	ATP	B	901	-	32,33,33	2.63	13 (40%)	48,52,52	2.48	20 (41%)

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	A	900	-	-	3/22/38/38	0/3/3/3
2	ATP	B	901	-	-	7/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	PB-O3A	8.78	1.69	1.59
2	A	900	ATP	C5-C4	5.11	1.48	1.39
2	B	901	ATP	C5-C4	4.39	1.46	1.39
2	B	901	ATP	PA-O5'	3.78	1.74	1.59
2	B	901	ATP	PA-O3A	3.76	1.63	1.59
2	A	900	ATP	PB-O3B	3.62	1.63	1.59
2	B	901	ATP	C5-N7	-3.57	1.32	1.39
2	B	901	ATP	PA-O1A	3.14	1.61	1.50
2	B	901	ATP	C8-N9	-3.07	1.32	1.37
2	A	900	ATP	C5-N7	-2.98	1.33	1.39
2	A	900	ATP	PB-O3A	2.98	1.62	1.59
2	B	901	ATP	O4'-C1'	2.95	1.48	1.42
2	B	901	ATP	C5'-C4'	2.92	1.60	1.51
2	B	901	ATP	C5-C6	2.90	1.49	1.41
2	A	900	ATP	C8-N7	2.82	1.37	1.31
2	B	901	ATP	PB-O3B	2.64	1.62	1.59
2	A	900	ATP	C5-C6	2.50	1.48	1.41
2	A	900	ATP	PB-O2B	-2.17	1.45	1.55
2	B	901	ATP	C4-N3	2.12	1.38	1.34
2	B	901	ATP	C6-N1	-2.00	1.30	1.35

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	O2B-PB-O3A	6.54	124.94	107.27
2	A	900	ATP	C5-C4-N3	-6.28	118.07	126.72
2	B	901	ATP	N3-C4-N9	5.71	136.87	127.17
2	A	900	ATP	N3-C4-N9	5.65	136.78	127.17
2	B	901	ATP	C5-C4-N3	-5.53	119.11	126.72
2	A	900	ATP	N3-C2-N1	-4.60	121.62	128.58
2	B	901	ATP	C2'-C3'-C4'	4.51	111.32	102.61
2	A	900	ATP	C2-N3-C4	4.39	122.54	111.83
2	B	901	ATP	O5'-C5'-C4'	4.18	123.22	108.99
2	B	901	ATP	O3'-C3'-C2'	-3.60	100.27	111.82
2	A	900	ATP	C5-N7-C8	3.30	108.64	103.45
2	B	901	ATP	N3-C2-N1	-3.24	123.68	128.58
2	B	901	ATP	PA-O5'-C5'	3.14	139.32	121.35
2	B	901	ATP	O4'-C4'-C3'	-3.09	99.03	105.15
2	A	900	ATP	O2A-PA-O3A	3.04	115.50	107.27
2	A	900	ATP	C4-N9-C8	2.98	108.86	105.74
2	B	901	ATP	O5'-PA-O1A	2.96	120.67	108.94
2	B	901	ATP	C2-N1-C6	2.91	123.52	118.73
2	A	900	ATP	C4-C5-N7	-2.87	107.30	110.58
2	B	901	ATP	O2G-PG-O3B	-2.80	95.25	104.64
2	A	900	ATP	O5'-PA-O1A	2.80	120.02	108.94
2	A	900	ATP	N9-C8-N7	-2.75	110.03	113.94
2	A	900	ATP	C5-C6-N6	-2.75	116.47	123.29
2	B	901	ATP	C2-N3-C4	2.75	118.55	111.83
2	A	900	ATP	N6-C6-N1	2.72	124.44	118.38
2	B	901	ATP	O4'-C4'-C5'	2.66	117.87	109.33
2	B	901	ATP	O3G-PG-O3B	2.57	113.24	104.64
2	B	901	ATP	O3B-PB-O1B	-2.55	103.02	110.70
2	A	900	ATP	O2B-PB-O3B	2.42	113.82	107.27
2	B	901	ATP	C4-N9-C8	2.38	108.24	105.74
2	B	901	ATP	C5'-C4'-C3'	2.32	123.58	115.21
2	A	900	ATP	PA-O5'-C5'	2.28	134.39	121.35
2	A	900	ATP	O2'-C2'-C3'	2.26	119.07	111.82
2	A	900	ATP	O3A-PB-O1B	-2.21	104.04	110.70
2	B	901	ATP	O4'-C1'-N9	-2.14	103.97	108.09
2	A	900	ATP	O3A-PA-O1A	-2.10	104.39	110.70
2	B	901	ATP	O2A-PA-O3A	-2.09	101.63	107.27
2	A	900	ATP	C6-C5-N7	2.04	136.02	132.09
2	A	900	ATP	O3B-PG-O1G	-2.01	100.45	111.04

There are no chirality outliers.

All (10) torsion outliers are listed below:

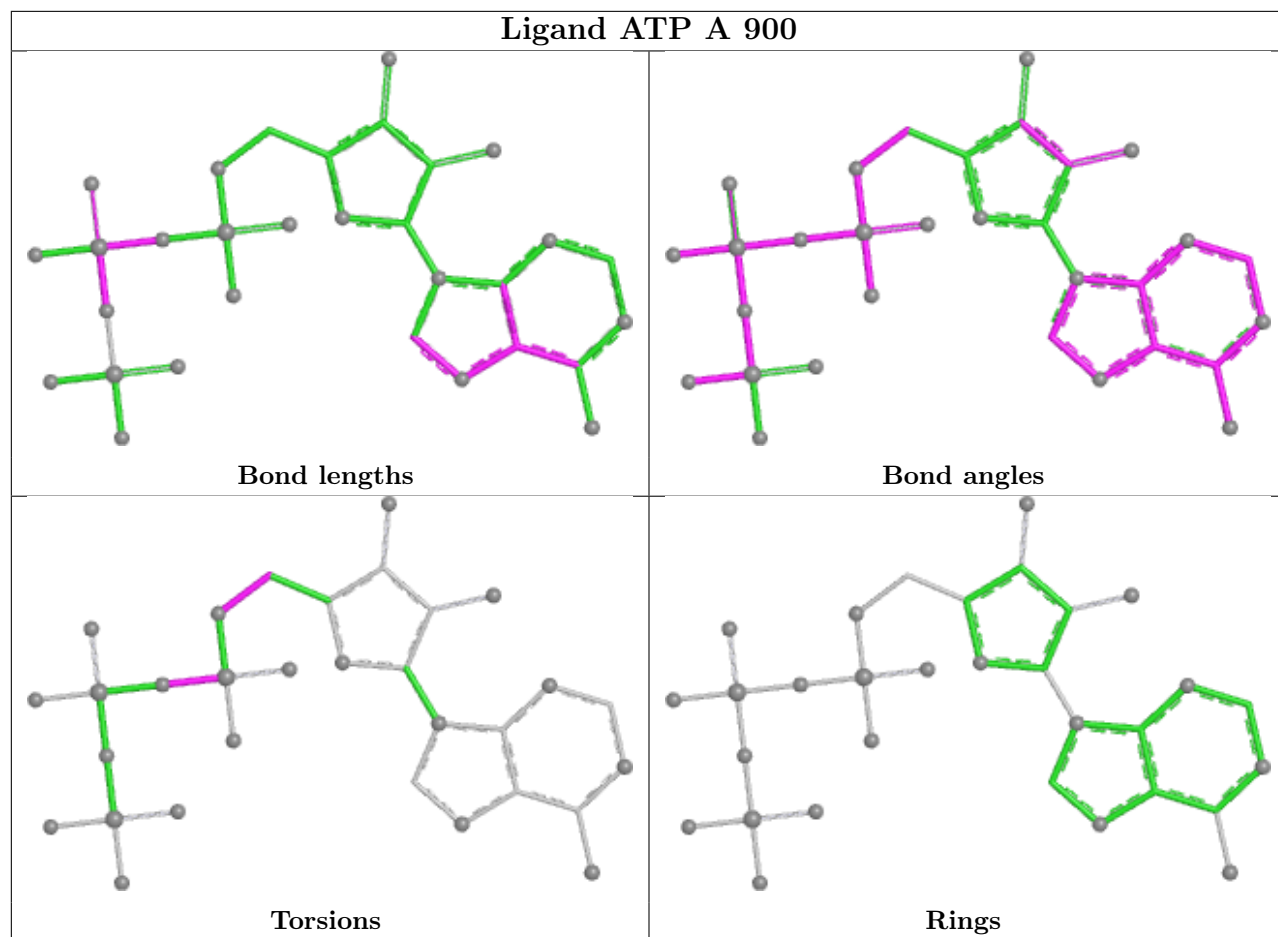
Mol	Chain	Res	Type	Atoms
2	B	901	ATP	C5'-O5'-PA-O3A
2	B	901	ATP	C4'-C5'-O5'-PA
2	B	901	ATP	C3'-C4'-C5'-O5'
2	B	901	ATP	O4'-C4'-C5'-O5'
2	B	901	ATP	PB-O3A-PA-O5'
2	A	900	ATP	PB-O3A-PA-O2A
2	B	901	ATP	C5'-O5'-PA-O1A
2	A	900	ATP	PB-O3A-PA-O1A
2	A	900	ATP	C4'-C5'-O5'-PA
2	B	901	ATP	PG-O3B-PB-O2B

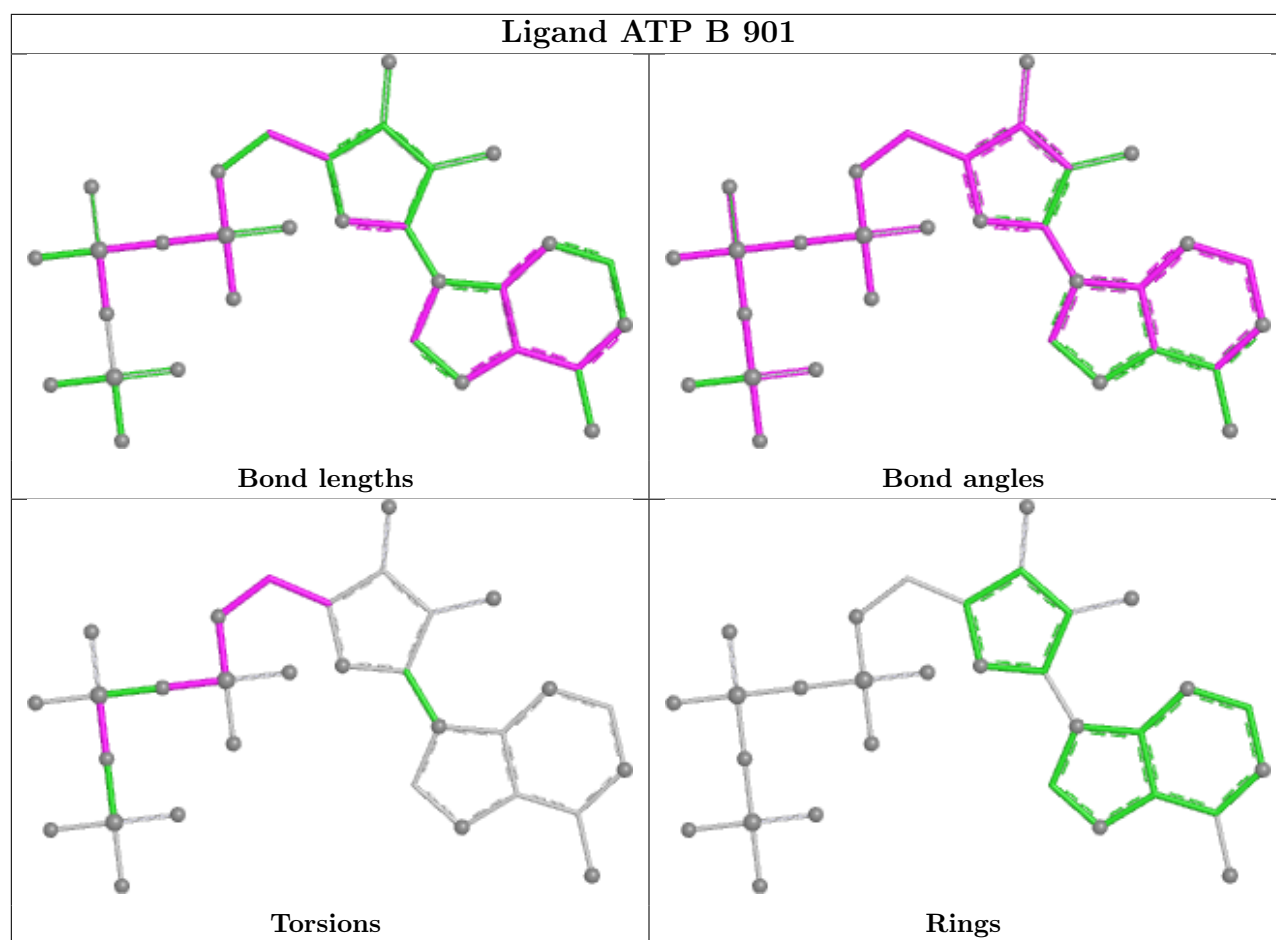
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ATP	2	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	654/853 (76%)	0.38	38 (5%) 29 25	5, 19, 43, 62	0
1	B	714/853 (83%)	1.06	155 (21%) 2 1	3, 21, 46, 64	0
All	All	1368/1706 (80%)	0.73	193 (14%) 6 4	3, 20, 44, 64	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	LEU	8.2
1	B	287	VAL	7.3
1	A	793	GLY	6.8
1	A	791	LEU	6.4
1	B	299	TYR	6.3
1	B	315	ARG	6.2
1	B	294	GLU	6.1
1	B	793	GLY	6.0
1	B	789	ILE	6.0
1	B	707	GLN	5.7
1	B	702	ASP	5.7
1	B	794	TYR	5.6
1	B	706	LEU	5.5
1	A	597	ILE	5.4
1	B	728	PRO	5.4
1	B	791	LEU	5.4
1	B	301	PRO	5.3
1	B	696	SER	5.2
1	B	684	PHE	5.2
1	A	615	GLY	5.1
1	B	233	SER	5.0
1	A	794	TYR	4.9
1	B	704	PRO	4.9
1	B	316	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	697	LEU	4.8
1	B	317	HIS	4.8
1	B	283	GLU	4.8
1	A	604	SER	4.8
1	B	228	PRO	4.8
1	B	290	GLY	4.7
1	B	703	ILE	4.6
1	B	795	ALA	4.6
1	B	236	TYR	4.6
1	B	244	PRO	4.5
1	B	727	GLU	4.4
1	B	792	ARG	4.4
1	B	247	ILE	4.4
1	B	614	PRO	4.3
1	B	705	GLY	4.3
1	A	611	GLY	4.3
1	B	719	PRO	4.2
1	B	753	VAL	4.1
1	B	289	GLU	3.9
1	A	790	HIS	3.9
1	B	246	LEU	3.9
1	B	714	PHE	3.8
1	A	792	ARG	3.8
1	B	281	LEU	3.7
1	B	366	GLN	3.7
1	B	730	LEU	3.7
1	B	295	GLY	3.6
1	B	743	SER	3.6
1	A	610	LEU	3.6
1	B	735	LEU	3.6
1	B	239	VAL	3.6
1	B	694	PRO	3.6
1	B	691	TYR	3.5
1	B	731	HIS	3.5
1	B	312	ALA	3.5
1	B	701	TRP	3.5
1	B	291	ILE	3.5
1	B	243	ILE	3.5
1	B	280	VAL	3.5
1	B	603	VAL	3.5
1	B	297	SER	3.4
1	B	834	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	795	ALA	3.4
1	B	724	LEU	3.4
1	B	230	GLU	3.4
1	B	296	GLU	3.4
1	B	709	ARG	3.4
1	B	741	ALA	3.4
1	B	245	HIS	3.3
1	B	242	ILE	3.3
1	A	614	PRO	3.3
1	B	721	ALA	3.3
1	B	303	ASN	3.3
1	B	723	TRP	3.3
1	B	689	ASP	3.2
1	B	790	HIS	3.2
1	B	593	ALA	3.2
1	A	723	TRP	3.2
1	B	128	VAL	3.2
1	B	725	ASP	3.1
1	B	519	TRP	3.1
1	B	293	ASP	3.1
1	B	240	ASN	3.1
1	B	203	LEU	3.1
1	A	789	ILE	3.1
1	B	729	GLU	3.1
1	A	834	PRO	3.1
1	B	248	ARG	3.1
1	B	797	LYS	3.0
1	A	745	GLU	3.0
1	B	796	GLN	3.0
1	B	830	GLN	3.0
1	B	136	ALA	2.9
1	B	718	LEU	2.9
1	B	508	GLY	2.9
1	B	670	SER	2.8
1	A	799	PRO	2.8
1	B	392	GLY	2.8
1	B	693	PRO	2.8
1	B	229	ALA	2.8
1	B	302	ALA	2.8
1	B	509	ARG	2.8
1	B	615	GLY	2.8
1	B	610	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	521	ALA	2.8
1	A	798	ASP	2.7
1	B	688	ILE	2.7
1	B	237	LYS	2.7
1	B	313	ALA	2.7
1	B	510	GLY	2.7
1	A	784	TYR	2.7
1	B	282	ILE	2.7
1	B	507	ALA	2.7
1	B	695	GLN	2.7
1	A	725	ASP	2.7
1	A	831	VAL	2.7
1	B	284	GLU	2.7
1	B	300	SER	2.7
1	B	526	LEU	2.7
1	B	531	ALA	2.6
1	B	752	GLU	2.6
1	B	618	ILE	2.6
1	B	747	TYR	2.6
1	B	177	GLY	2.6
1	B	734	THR	2.6
1	A	602	ARG	2.6
1	B	832	ARG	2.6
1	B	611	GLY	2.6
1	B	686	ALA	2.6
1	B	715	ASP	2.6
1	B	605	GLY	2.5
1	A	616	GLU	2.5
1	B	532	GLU	2.5
1	A	16	ARG	2.5
1	A	730	LEU	2.5
1	B	123	GLY	2.5
1	B	608	ARG	2.5
1	B	831	VAL	2.5
1	B	722	GLU	2.4
1	B	716	LEU	2.4
1	A	797	LYS	2.4
1	B	207	LEU	2.4
1	A	691	TYR	2.4
1	B	176	TYR	2.4
1	B	669	VAL	2.4
1	B	717	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	742	GLN	2.4
1	B	524	ALA	2.3
1	B	113	THR	2.3
1	B	150	LEU	2.3
1	B	740	LEU	2.3
1	A	507	ALA	2.3
1	B	394	ALA	2.3
1	B	749	ARG	2.3
1	B	231	ASP	2.3
1	B	512	ASP	2.3
1	B	125	GLY	2.3
1	A	609	LYS	2.3
1	B	129	VAL	2.3
1	B	732	GLU	2.2
1	B	690	ALA	2.2
1	B	739	ILE	2.2
1	B	393	THR	2.2
1	B	825	THR	2.2
1	B	170	TYR	2.2
1	A	17	THR	2.2
1	A	832	ARG	2.1
1	B	368	GLU	2.1
1	B	369	ASN	2.1
1	B	126	VAL	2.1
1	B	308	HIS	2.1
1	B	156	ILE	2.1
1	B	513	ILE	2.1
1	B	122	THR	2.1
1	A	532	GLU	2.1
1	B	737	GLU	2.1
1	B	174	ILE	2.1
1	B	682	ASP	2.1
1	B	720	ILE	2.1
1	B	154	VAL	2.1
1	B	311	THR	2.0
1	B	616	GLU	2.0
1	A	724	LEU	2.0
1	A	728	PRO	2.0
1	A	527	GLU	2.0
1	B	708	GLU	2.0
1	A	731	HIS	2.0
1	A	203	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	288	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](#)

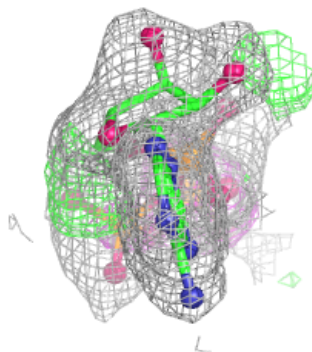
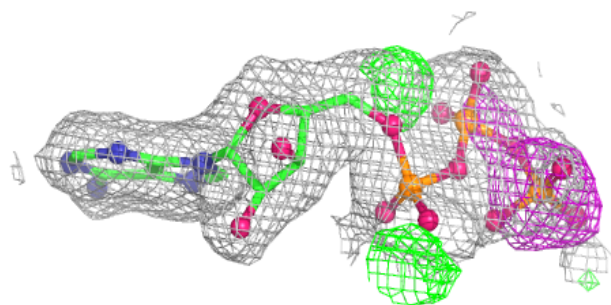
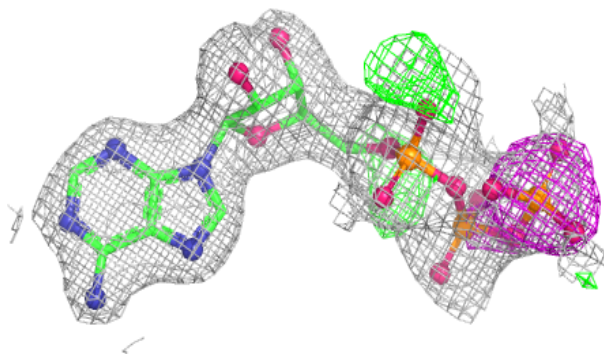
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	B	901	31/31	0.87	0.11	9,19,24,26	0
2	ATP	A	900	31/31	0.90	0.09	11,24,29,30	0

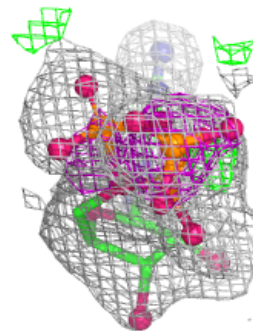
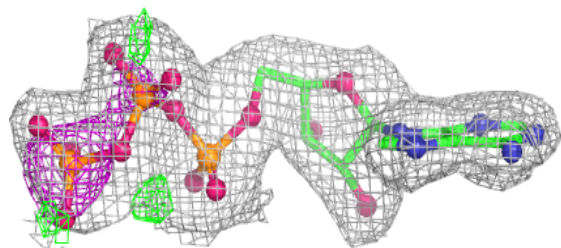
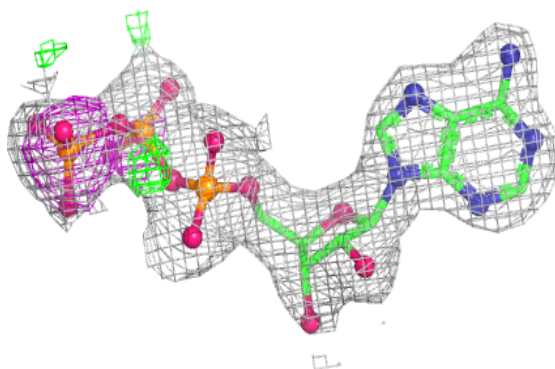
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 901:

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

**Electron density around ATP A 900:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.