Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:45 pm BST

PDB ID	:	2W00
Title	:	Crystal structure of the HsdR subunit of the EcoR124I restriction enzyme in complex with ATP
Authors	:	Lapkouski, M.; Panjikar, S.; Kuta Smatanova, I.; Ettrich, R.; Csefalvay, E.
Deposited on	:	2008-08-08
Resolution	:	2.60 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:

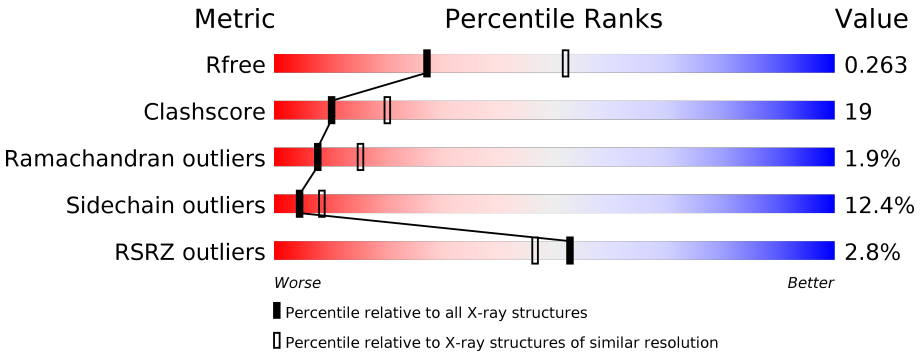
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	1038	2% 54% 20% 6% 19%
1	B	1038	2% 55% 20% 6% 18%

2 Entry composition

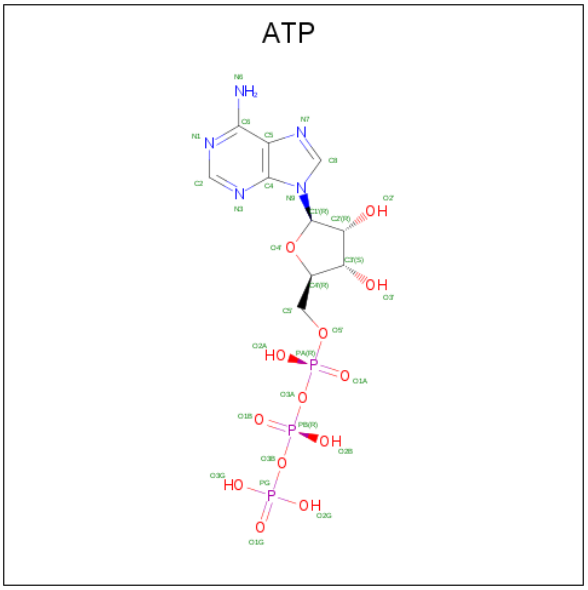
There are 4 unique types of molecules in this entry. The entry contains 14386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HSDR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	Se	0	0	0
			6825	4341	1154	1314	3	13			
1	B	852	Total	C	N	O	S	Se	0	0	0
			6915	4393	1172	1334	3	13			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

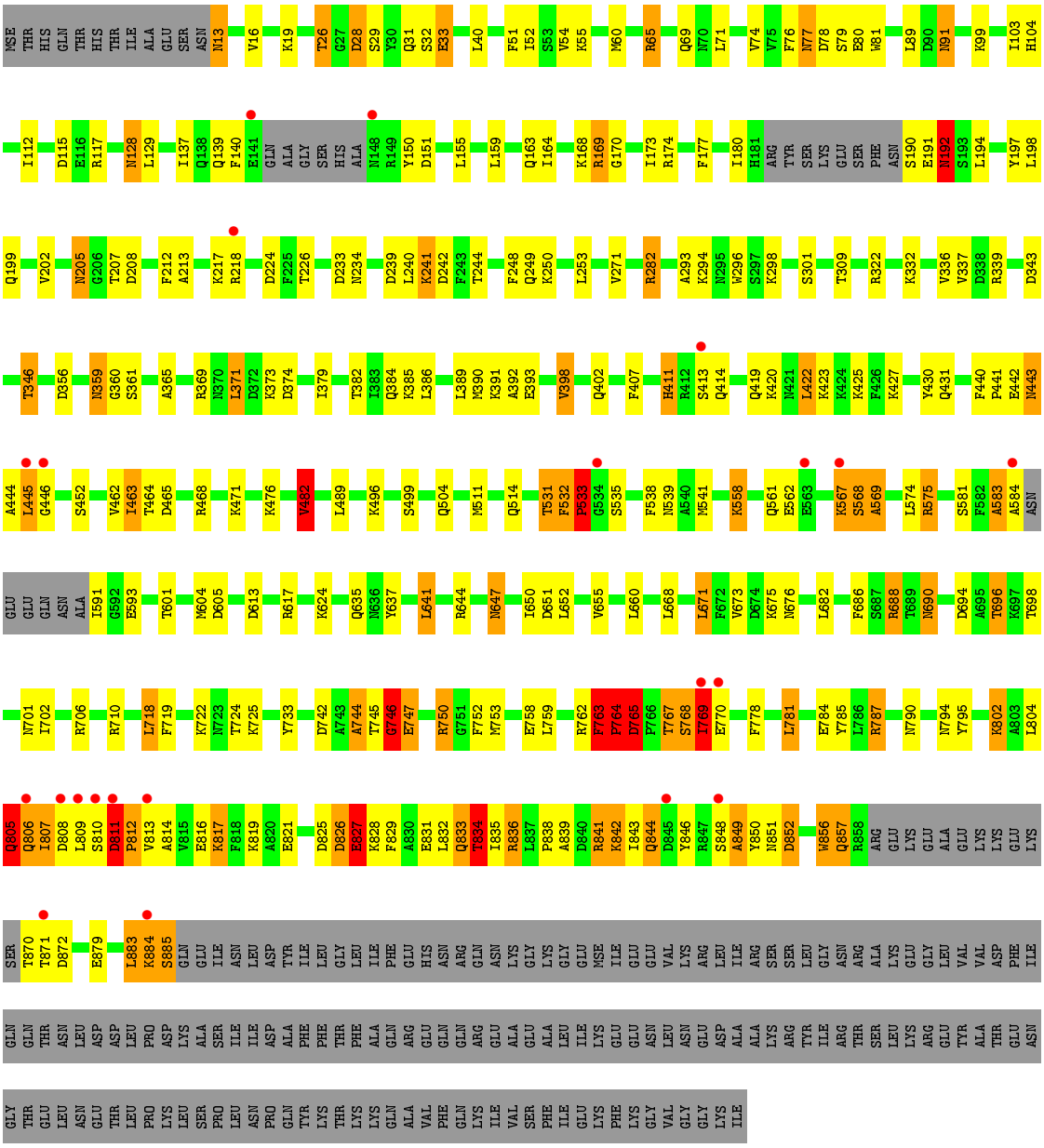
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	286	Total O 286 286	0	0
4	B	296	Total O 296 296	0	0

3 Residue-property plots (i)

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.

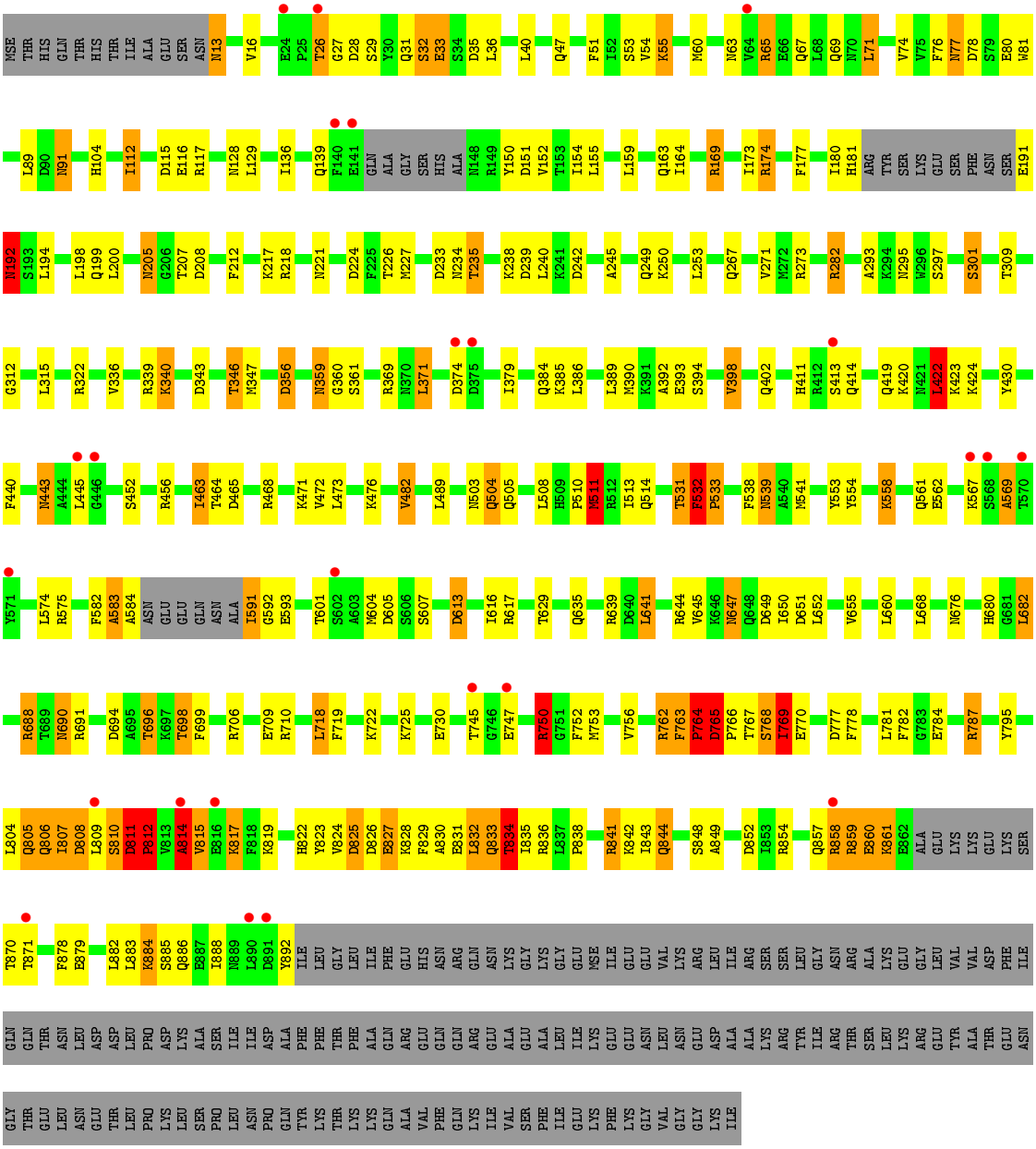
- Molecule 1: HSDR

Chain A: 2% 54% 20% 6% 19%



• Molecule 1: HSDR

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.91Å 129.92Å 161.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.60) 100.0 (19.97-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.265 0.220 , 0.263	Depositor DCC
R_{free} test set	977 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14386	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.62	3/6942 (0.0%)	0.72	2/9341 (0.0%)
1	B	0.65	8/7034 (0.1%)	0.70	5/9464 (0.1%)
All	All	0.64	11/13976 (0.1%)	0.71	7/18805 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	40
1	B	2	37
All	All	3	77

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	827	GLU	CD-OE2	13.17	1.40	1.25
1	A	827	GLU	CD-OE2	8.36	1.34	1.25
1	B	892	TYR	CG-CD2	6.75	1.48	1.39
1	B	825	ASP	CG-OD1	6.38	1.40	1.25
1	B	892	TYR	CE1-CZ	6.15	1.46	1.38
1	B	825	ASP	CG-OD2	5.75	1.38	1.25
1	A	115	ASP	N-CA	5.72	1.57	1.46
1	A	19	LYS	CD-CE	5.68	1.65	1.51
1	B	819	LYS	CE-NZ	5.50	1.62	1.49
1	B	834	THR	CB-OG1	5.08	1.53	1.43
1	B	293	ALA	C-O	5.05	1.32	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	811	ASP	C-N-CD	-18.35	80.23	120.60
1	A	533	PRO	N-CA-CB	6.11	110.63	103.30
1	B	511	MSE	N-CA-C	6.09	127.44	111.00
1	B	511	MSE	CB-CG-SE	-5.99	94.74	112.70
1	B	422	LEU	CA-CB-CG	5.89	128.85	115.30
1	B	765	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	765	ASP	N-CA-CB	5.32	120.17	110.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	207	THR	CB
1	B	207	THR	CB
1	B	511	MSE	CA

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	PHE	Peptide
1	A	170	GLY	Peptide
1	A	190	SER	Peptide
1	A	192	ASN	Peptide
1	A	26	THR	Peptide
1	A	28	ASP	Peptide
1	A	392	ALA	Peptide
1	A	411	HIS	Peptide
1	A	444	ALA	Peptide
1	A	445	LEU	Peptide
1	A	533	PRO	Peptide
1	A	567	LYS	Peptide
1	A	569	ALA	Peptide
1	A	583	ALA	Peptide
1	A	744	ALA	Peptide
1	A	745	THR	Peptide
1	A	746	GLY	Peptide
1	A	750	ARG	Peptide
1	A	762	ARG	Peptide
1	A	763	PHE	Peptide
1	A	764	PRO	Peptide
1	A	765	ASP	Peptide
1	A	768	SER	Peptide
1	A	769	ILE	Peptide
1	A	805	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	806	GLN	Peptide
1	A	807	ILE	Peptide
1	A	808	ASP	Peptide
1	A	811	ASP	Peptide
1	A	812	PRO	Peptide
1	A	826	ASP	Mainchain
1	A	833	GLN	Peptide
1	A	834	THR	Peptide
1	A	848	SER	Peptide
1	A	850	TYR	Peptide
1	A	851	ASN	Peptide
1	A	856	TRP	Peptide
1	A	857	GLN	Peptide
1	A	870	THR	Peptide
1	A	872	ASP	Peptide
1	B	192	ASN	Peptide
1	B	26	THR	Peptide
1	B	392	ALA	Peptide
1	B	411	HIS	Peptide
1	B	445	LEU	Peptide
1	B	510	PRO	Peptide
1	B	532	PHE	Peptide
1	B	567	LYS	Peptide
1	B	569	ALA	Peptide
1	B	583	ALA	Peptide
1	B	591	ILE	Peptide
1	B	592	GLY	Peptide
1	B	750	ARG	Peptide
1	B	762	ARG	Peptide
1	B	763	PHE	Peptide
1	B	764	PRO	Peptide
1	B	765	ASP	Peptide
1	B	768	SER	Peptide
1	B	769	ILE	Peptide
1	B	805	GLN	Peptide
1	B	806	GLN	Peptide
1	B	807	ILE	Peptide
1	B	808	ASP	Peptide
1	B	809	LEU	Peptide
1	B	810	SER	Peptide
1	B	811	ASP	Peptide
1	B	812	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	814	ALA	Peptide
1	B	826	ASP	Peptide
1	B	830	ALA	Peptide
1	B	832	LEU	Peptide
1	B	833	GLN	Peptide
1	B	834	THR	Peptide
1	B	859	ARG	Peptide
1	B	860	GLU	Peptide
1	B	870	THR	Peptide
1	B	885	SER	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	6825	0	6665	257	0
1	B	6915	0	6741	258	0
2	A	31	0	12	1	0
2	B	31	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	286	0	0	11	0
4	B	296	0	0	14	0
All	All	14386	0	13430	512	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 19.

All (512) 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:810:SER:CA	1:A:812:PRO:CD	1.90	1.46
1:B:769:ILE:HG22	1:B:770:GLU:HA	1.20	1.17
1:A:533:PRO:HA	1:A:535:SER:H	1.12	1.14
1:A:769:ILE:HD13	1:A:769:ILE:H	1.06	1.12
1:A:769:ILE:CD1	1:A:769:ILE:H	1.60	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:SER:CA	1:A:812:PRO:HD3	1.67	1.11
1:B:769:ILE:HD13	1:B:769:ILE:H	1.09	1.09
1:A:810:SER:CA	1:A:812:PRO:CG	2.33	1.06
1:A:810:SER:CA	1:A:812:PRO:HD2	1.79	1.05
1:B:767:THR:C	1:B:769:ILE:O	1.95	1.04
1:B:752:PHE:HD2	1:B:753:MSE:HE3	1.24	1.03
1:B:752:PHE:CD2	1:B:753:MSE:HE3	1.94	1.03
1:B:456:ARG:NH2	4:B:2150:HOH:O	1.92	1.02
1:A:169:ARG:HG3	1:A:169:ARG:HH11	0.86	1.02
1:B:696:THR:HG21	4:B:2245:HOH:O	1.59	1.02
1:B:169:ARG:CG	1:B:169:ARG:HH11	1.73	1.02
1:B:768:SER:N	1:B:769:ILE:O	1.93	1.00
1:B:698:THR:HG22	1:B:699:PHE:CD1	1.98	0.99
1:A:768:SER:N	1:A:769:ILE:O	1.93	0.99
1:B:769:ILE:H	1:B:769:ILE:CD1	1.75	0.98
1:B:169:ARG:HG3	1:B:169:ARG:HH11	0.83	0.98
1:A:440:PHE:H	1:A:443:ASN:HD21	1.03	0.97
1:A:752:PHE:CD2	1:A:753:MSE:CE	2.48	0.97
1:B:532:PHE:CD2	1:B:533:PRO:HD2	1.99	0.96
1:A:752:PHE:HD2	1:A:753:MSE:CE	1.78	0.95
1:B:765:ASP:HB2	1:B:766:PRO:HA	1.44	0.95
1:B:169:ARG:HG3	1:B:169:ARG:NH1	1.63	0.94
1:A:169:ARG:CG	1:A:169:ARG:HH11	1.80	0.94
1:A:91:ASN:HD22	1:A:91:ASN:H	1.07	0.94
1:B:810:SER:O	1:B:812:PRO:HB3	1.68	0.93
1:A:787:ARG:HB3	1:A:787:ARG:HH11	1.33	0.93
1:A:787:ARG:CB	1:A:787:ARG:HH11	1.80	0.93
1:B:752:PHE:CD2	1:B:753:MSE:CE	2.53	0.92
1:B:440:PHE:H	1:B:443:ASN:HD21	1.07	0.91
1:A:769:ILE:N	1:A:769:ILE:HD13	1.86	0.91
1:B:91:ASN:H	1:B:91:ASN:HD22	0.91	0.90
1:A:169:ARG:HG3	1:A:169:ARG:NH1	1.65	0.90
1:B:765:ASP:CB	1:B:766:PRO:HA	2.02	0.89
1:B:54:VAL:HG11	1:B:60:MSE:HG3	1.54	0.89
1:B:531:THR:O	1:B:532:PHE:O	1.92	0.88
1:A:386:LEU:HG	1:A:390:MSE:HE2	1.56	0.87
1:A:810:SER:C	1:A:812:PRO:HD3	1.95	0.87
1:A:359:ASN:HD22	1:A:361:SER:H	1.22	0.87
1:A:443:ASN:H	1:A:443:ASN:HD22	1.18	0.87
1:B:91:ASN:N	1:B:91:ASN:HD22	1.70	0.87
1:B:218:ARG:HH22	1:B:884:LYS:NZ	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ASN:H	1:B:443:ASN:HD22	1.21	0.86
1:B:91:ASN:ND2	1:B:91:ASN:H	1.73	0.86
1:B:860:GLU:H	1:B:861:LYS:CA	1.87	0.86
1:A:752:PHE:CD2	1:A:753:MSE:HE2	2.10	0.86
1:B:538:PHE:HZ	1:B:696:THR:HG22	1.41	0.86
1:A:769:ILE:HG22	1:A:770:GLU:HA	1.57	0.85
1:A:767:THR:C	1:A:769:ILE:O	2.15	0.84
1:A:825:ASP:HB3	1:A:828:LYS:H	1.43	0.84
1:B:787:ARG:CB	1:B:787:ARG:HH11	1.90	0.83
1:B:769:ILE:CG2	1:B:770:GLU:HA	2.06	0.83
1:A:511:MSE:HA	1:A:511:MSE:HE3	1.61	0.83
1:A:533:PRO:CB	4:A:2189:HOH:O	2.26	0.82
1:A:769:ILE:N	1:A:769:ILE:CD1	2.33	0.82
1:B:359:ASN:HD22	1:B:361:SER:H	1.27	0.82
1:B:769:ILE:HD13	1:B:769:ILE:N	1.93	0.82
1:A:752:PHE:HD2	1:A:753:MSE:HE2	1.45	0.82
1:B:174:ARG:NH1	4:B:2049:HOH:O	2.07	0.82
1:B:765:ASP:HB2	1:B:766:PRO:CA	2.07	0.81
1:A:694:ASP:OD1	1:A:696:THR:HB	1.81	0.81
1:B:419:GLN:HE21	1:B:423:LYS:HE2	1.46	0.81
1:A:538:PHE:CZ	1:A:696:THR:HG22	2.16	0.79
1:A:538:PHE:HZ	1:A:696:THR:HG22	1.47	0.79
1:A:809:LEU:HD23	1:A:810:SER:N	1.98	0.79
1:A:371:LEU:HD13	1:A:379:ILE:HD13	1.64	0.78
1:B:150:TYR:O	1:B:151:ASP:OD1	2.01	0.77
1:A:533:PRO:HA	1:A:535:SER:N	1.94	0.77
1:A:440:PHE:N	1:A:443:ASN:HD21	1.81	0.77
1:B:511:MSE:HE1	1:B:514:GLN:NE2	2.00	0.77
1:B:767:THR:O	1:B:769:ILE:O	2.03	0.77
1:A:65:ARG:HD3	1:A:69:GLN:NE2	2.00	0.76
1:A:371:LEU:HD13	1:A:379:ILE:CD1	2.15	0.76
1:A:139:GLN:O	1:A:139:GLN:HG2	1.85	0.76
1:A:91:ASN:ND2	1:A:91:ASN:H	1.84	0.75
1:B:694:ASP:OD1	1:B:696:THR:HB	1.86	0.75
1:B:583:ALA:HB1	1:B:584:ALA:CA	2.16	0.75
1:A:651:ASP:OD2	4:A:2218:HOH:O	2.04	0.75
1:A:809:LEU:HA	1:A:810:SER:C	2.05	0.75
1:B:340:LYS:HD3	4:B:2205:HOH:O	1.87	0.75
1:B:77:ASN:ND2	1:B:80:GLU:H	1.84	0.75
1:A:561:GLN:HE22	1:A:574:LEU:H	1.33	0.74
1:A:838:PRO:HG2	1:A:843:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:PRO:CA	1:A:535:SER:H	1.97	0.74
1:A:856:TRP:CG	1:A:856:TRP:O	2.40	0.74
1:B:787:ARG:HH11	1:B:787:ARG:HB3	1.52	0.74
1:A:742:ASP:O	1:A:746:GLY:HA2	1.87	0.74
1:B:386:LEU:HG	1:B:390:MSE:HE2	1.70	0.74
1:B:343:ASP:OD2	1:B:346:THR:HB	1.86	0.73
1:A:343:ASP:OD2	1:A:346:THR:HB	1.88	0.73
1:A:763:PHE:H	1:A:764:PRO:HD3	1.52	0.73
1:A:825:ASP:CB	1:A:828:LYS:H	2.00	0.73
1:B:752:PHE:CE2	1:B:753:MSE:CE	2.71	0.73
1:B:402:GLN:NE2	1:B:430:TYR:OH	2.21	0.73
1:A:150:TYR:O	1:A:151:ASP:OD1	2.05	0.73
1:A:617:ARG:HD3	4:A:2204:HOH:O	1.89	0.73
1:B:769:ILE:HG22	1:B:770:GLU:CA	2.11	0.73
1:A:752:PHE:HD2	1:A:753:MSE:HE3	1.53	0.72
1:A:77:ASN:C	1:A:77:ASN:HD22	1.92	0.72
1:B:752:PHE:HD2	1:B:753:MSE:CE	1.93	0.72
1:B:538:PHE:CZ	1:B:696:THR:HG22	2.24	0.72
1:A:339:ARG:HD3	1:A:384:GLN:CD	2.10	0.72
1:B:65:ARG:HD3	1:B:69:GLN:NE2	2.05	0.72
1:A:360:GLY:H	1:A:635:GLN:HE22	1.36	0.72
1:A:810:SER:CA	1:A:812:PRO:HG3	2.20	0.72
1:B:104:HIS:HE1	1:B:199:GLN:OE1	1.72	0.72
1:B:561:GLN:HE22	1:B:574:LEU:H	1.36	0.72
1:B:660:LEU:O	1:B:688:ARG:HD3	1.90	0.71
1:B:360:GLY:H	1:B:635:GLN:HE22	1.39	0.70
1:A:128:ASN:ND2	4:A:2055:HOH:O	2.24	0.70
1:B:806:GLN:H	1:B:807:ILE:HG12	1.57	0.70
1:B:371:LEU:HD13	1:B:379:ILE:HD13	1.72	0.70
1:B:440:PHE:H	1:B:443:ASN:ND2	1.87	0.69
1:A:750:ARG:NH1	1:A:784:GLU:OE1	2.25	0.69
1:B:745:THR:OG1	1:B:747:GLU:HG2	1.92	0.69
1:A:752:PHE:CD2	1:A:753:MSE:HE3	2.28	0.69
1:B:849:ALA:O	1:B:852:ASP:HB2	1.93	0.69
1:B:218:ARG:HH22	1:B:884:LYS:HZ1	1.40	0.68
1:A:809:LEU:HD23	1:A:809:LEU:C	2.13	0.68
1:B:414:GLN:NE2	1:B:414:GLN:HA	2.09	0.68
1:B:139:GLN:O	1:B:139:GLN:HG2	1.94	0.67
1:A:787:ARG:CG	1:A:787:ARG:HH11	2.06	0.67
1:B:218:ARG:NH2	1:B:884:LYS:NZ	2.41	0.67
1:A:191:GLU:CB	1:A:192:ASN:HA	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:NH2	4:B:2104:HOH:O	2.28	0.67
1:B:402:GLN:HE21	1:B:430:TYR:HE1	1.43	0.67
1:B:768:SER:CA	1:B:769:ILE:O	2.41	0.67
1:B:829:PHE:O	1:B:833:GLN:HB2	1.95	0.67
1:A:660:LEU:O	1:A:688:ARG:HD3	1.95	0.67
1:B:233:ASP:OD1	1:B:235:THR:HB	1.95	0.66
1:B:825:ASP:HB3	1:B:827:GLU:HB2	1.76	0.66
1:A:856:TRP:CD2	1:A:856:TRP:O	2.48	0.66
1:A:805:GLN:O	1:A:806:GLN:CD	2.34	0.66
1:B:765:ASP:CB	1:B:766:PRO:CA	2.71	0.66
1:A:139:GLN:NE2	1:A:150:TYR:HA	2.10	0.65
1:A:769:ILE:CG2	1:A:770:GLU:HA	2.27	0.65
1:A:752:PHE:CE2	1:A:753:MSE:CE	2.79	0.65
1:A:360:GLY:H	1:A:635:GLN:NE2	1.93	0.65
1:A:65:ARG:HG3	1:A:81:TRP:CD2	2.32	0.65
1:B:371:LEU:HD13	1:B:379:ILE:CD1	2.27	0.65
1:A:205:ASN:HD22	1:A:205:ASN:C	2.00	0.64
1:A:322:ARG:NH2	4:A:2116:HOH:O	2.30	0.64
1:A:443:ASN:N	1:A:443:ASN:HD22	1.91	0.64
1:B:787:ARG:HD3	1:B:879:GLU:CD	2.18	0.64
1:A:825:ASP:HB2	1:A:828:LYS:HB2	1.80	0.64
1:B:463:ILE:HG13	4:B:2155:HOH:O	1.96	0.64
1:A:91:ASN:N	1:A:91:ASN:HD22	1.88	0.63
1:B:339:ARG:HD3	1:B:384:GLN:CD	2.18	0.63
1:A:65:ARG:HG3	1:A:81:TRP:CE2	2.34	0.63
1:A:763:PHE:H	1:A:764:PRO:CD	2.10	0.63
1:B:218:ARG:HH22	1:B:884:LYS:HZ3	1.45	0.63
1:B:440:PHE:N	1:B:443:ASN:HD21	1.89	0.63
1:A:389:LEU:O	1:A:393:GLU:HB2	1.99	0.63
1:B:834:THR:O	1:B:834:THR:CG2	2.46	0.63
1:B:359:ASN:ND2	1:B:361:SER:H	1.97	0.62
1:A:359:ASN:ND2	1:A:361:SER:H	1.93	0.62
1:B:295:ASN:O	1:B:301:SER:HB3	1.98	0.62
1:A:561:GLN:HE22	1:A:574:LEU:N	1.97	0.62
1:A:768:SER:CA	1:A:769:ILE:O	2.46	0.62
1:A:759:LEU:O	1:A:763:PHE:HB2	1.99	0.62
1:B:834:THR:O	1:B:834:THR:HG22	2.00	0.62
1:A:809:LEU:CA	1:A:810:SER:C	2.68	0.62
1:B:205:ASN:HD22	1:B:205:ASN:C	2.01	0.62
1:A:765:ASP:H	1:A:768:SER:HB2	1.64	0.62
1:A:371:LEU:CD1	1:A:379:ILE:CD1	2.77	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ASN:HD22	1:B:443:ASN:N	1.95	0.61
1:B:139:GLN:NE2	1:B:150:TYR:HA	2.15	0.61
1:A:531:THR:HG22	1:A:532:PHE:N	2.15	0.61
1:A:567:LYS:N	1:A:568:SER:O	2.33	0.61
1:A:810:SER:C	1:A:812:PRO:CD	2.61	0.61
1:B:698:THR:HG22	1:B:699:PHE:CE1	2.36	0.60
1:A:841:ARG:HG3	1:A:842:LYS:N	2.16	0.60
1:A:54:VAL:HG11	1:A:60:MSE:HG3	1.83	0.60
1:B:690:ASN:C	1:B:690:ASN:HD22	2.05	0.60
1:A:825:ASP:HB2	1:A:828:LYS:CB	2.29	0.60
1:A:60:MSE:HE2	1:A:194:LEU:CD1	2.32	0.60
1:B:688:ARG:H	1:B:688:ARG:HD2	1.67	0.60
1:B:825:ASP:CB	1:B:828:LYS:H	2.15	0.60
1:B:805:GLN:O	1:B:806:GLN:CD	2.40	0.60
1:A:531:THR:HG22	1:A:532:PHE:H	1.67	0.59
1:A:104:HIS:HE1	1:A:199:GLN:OE1	1.85	0.59
1:B:558:LYS:O	1:B:562:GLU:HG2	2.02	0.59
1:B:688:ARG:N	1:B:688:ARG:HD2	2.18	0.59
1:A:601:THR:O	1:A:604:MSE:HG3	2.02	0.59
1:B:838:PRO:HG2	1:B:843:ILE:HD11	1.85	0.59
1:A:593:GLU:HA	1:A:593:GLU:OE2	2.03	0.59
1:A:769:ILE:HD12	1:A:769:ILE:H	1.62	0.59
1:B:191:GLU:CB	1:B:192:ASN:HA	2.31	0.59
1:B:787:ARG:HD3	1:B:879:GLU:OE2	2.03	0.59
1:B:769:ILE:N	1:B:769:ILE:CD1	2.48	0.59
1:B:371:LEU:CD1	1:B:379:ILE:CD1	2.81	0.59
1:B:825:ASP:HB3	1:B:828:LYS:H	1.68	0.58
1:A:16:VAL:O	1:A:282:ARG:NH2	2.36	0.58
1:B:688:ARG:NH2	2:B:1893:ATP:O2G	2.26	0.58
1:A:205:ASN:ND2	1:A:208:ASP:H	2.01	0.58
1:B:77:ASN:C	1:B:77:ASN:HD22	2.07	0.58
1:B:77:ASN:HD21	1:B:80:GLU:H	1.51	0.58
1:B:65:ARG:HG3	1:B:81:TRP:CD2	2.39	0.58
1:A:60:MSE:HE2	1:A:194:LEU:HD13	1.85	0.58
1:A:849:ALA:O	1:A:852:ASP:HB2	2.03	0.58
1:A:511:MSE:HE1	1:A:514:GLN:HE21	1.68	0.58
1:A:831:GLU:C	1:A:833:GLN:H	2.06	0.58
1:A:77:ASN:HD22	1:A:78:ASP:N	2.02	0.57
1:A:402:GLN:HE21	1:A:430:TYR:HE1	1.52	0.57
1:A:558:LYS:O	1:A:562:GLU:HG2	2.03	0.57
1:A:77:ASN:C	1:A:77:ASN:ND2	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:PHE:CD2	1:B:533:PRO:CD	2.81	0.57
1:B:104:HIS:CE1	1:B:199:GLN:OE1	2.57	0.57
1:B:753:MSE:HE2	1:B:753:MSE:HA	1.87	0.57
1:B:778:PHE:CE1	1:B:782:PHE:HB2	2.40	0.57
1:A:169:ARG:CG	1:A:169:ARG:NH1	2.49	0.57
1:B:343:ASP:H	1:B:346:THR:HG22	1.70	0.57
1:B:360:GLY:H	1:B:635:GLN:NE2	2.03	0.57
1:B:814:ALA:HA	1:B:817:LYS:HB2	1.87	0.57
1:B:538:PHE:CZ	1:B:696:THR:CG2	2.88	0.56
1:B:787:ARG:CB	1:B:787:ARG:NH1	2.67	0.56
1:B:860:GLU:HA	1:B:860:GLU:OE1	2.05	0.56
1:B:511:MSE:CE	1:B:514:GLN:NE2	2.68	0.56
1:A:531:THR:CG2	1:A:532:PHE:N	2.69	0.56
1:A:402:GLN:NE2	1:A:430:TYR:OH	2.38	0.56
1:A:787:ARG:HB3	1:A:787:ARG:NH1	2.13	0.56
1:B:833:GLN:O	1:B:833:GLN:HG2	2.06	0.56
1:B:616:ILE:HD12	1:B:629:THR:HG22	1.88	0.55
1:A:838:PRO:CG	1:A:843:ILE:HD11	2.36	0.55
1:B:647:ASN:C	1:B:647:ASN:HD22	2.11	0.55
1:A:13:ASN:OD1	1:A:13:ASN:N	2.38	0.55
1:A:688:ARG:NH2	2:A:1886:ATP:O2G	2.24	0.55
1:A:205:ASN:HD21	1:A:208:ASP:H	1.53	0.55
1:A:832:LEU:HA	1:A:835:ILE:HD12	1.88	0.55
1:A:213:ALA:HB2	1:A:271:VAL:HG23	1.88	0.55
1:A:389:LEU:O	1:A:393:GLU:CB	2.55	0.54
1:A:52:ILE:HG13	1:A:137:ILE:HG22	1.89	0.54
1:A:769:ILE:HG22	1:A:770:GLU:CA	2.35	0.54
1:A:839:ALA:O	1:A:843:ILE:HG12	2.06	0.54
1:A:218:ARG:HH22	1:A:884:LYS:NZ	2.05	0.54
1:B:698:THR:CG2	1:B:699:PHE:CD1	2.82	0.54
1:B:65:ARG:HG3	1:B:81:TRP:CE2	2.43	0.54
1:B:511:MSE:HE1	1:B:514:GLN:HE22	1.69	0.54
1:A:511:MSE:CE	1:A:511:MSE:HA	2.35	0.54
1:A:809:LEU:CD2	1:A:809:LEU:C	2.76	0.54
1:A:826:ASP:O	1:A:829:PHE:HB3	2.08	0.54
1:B:359:ASN:HD21	1:B:385:LYS:NZ	2.05	0.54
1:A:575:ARG:NH1	4:A:2199:HOH:O	2.41	0.54
1:A:462:VAL:O	1:A:465:ASP:HB2	2.08	0.53
1:A:180:ILE:HG22	1:A:180:ILE:O	2.09	0.53
1:B:882:LEU:O	1:B:886:GLN:HB2	2.07	0.53
1:A:414:GLN:NE2	1:A:414:GLN:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:MSE:HE1	1:A:514:GLN:NE2	2.24	0.53
1:B:69:GLN:HE21	1:B:76:PHE:HD1	1.56	0.53
1:B:831:GLU:C	1:B:833:GLN:H	2.11	0.53
1:A:249:GLN:HE21	1:A:249:GLN:HA	1.73	0.53
1:B:503:ASN:OD1	1:B:505:GLN:HB2	2.09	0.53
1:B:65:ARG:NH1	1:B:78:ASP:OD1	2.34	0.53
1:B:541:MSE:HG3	1:B:668:LEU:HD11	1.90	0.53
1:A:422:LEU:C	1:A:422:LEU:HD12	2.30	0.53
1:B:152:VAL:O	1:B:164:ILE:HD12	2.09	0.53
1:B:532:PHE:CZ	1:B:886:GLN:HG2	2.44	0.52
1:A:778:PHE:C	1:A:778:PHE:CD1	2.82	0.52
1:B:422:LEU:HD12	1:B:422:LEU:C	2.28	0.52
1:B:593:GLU:HA	1:B:593:GLU:OE2	2.09	0.52
1:A:769:ILE:HD12	1:A:769:ILE:N	2.21	0.52
1:B:31:GLN:HE21	1:B:169:ARG:HB2	1.75	0.52
1:B:690:ASN:C	1:B:690:ASN:ND2	2.60	0.52
1:B:16:VAL:O	1:B:282:ARG:NH2	2.42	0.52
1:A:445:LEU:HD12	1:A:446:GLY:H	1.75	0.52
1:B:539:ASN:HB2	1:B:651:ASP:O	2.10	0.52
1:A:538:PHE:CZ	1:A:696:THR:CG2	2.90	0.52
1:A:814:ALA:HA	1:A:817:LYS:HB2	1.92	0.52
1:B:698:THR:CG2	1:B:699:PHE:CE1	2.93	0.52
1:B:752:PHE:CE2	1:B:753:MSE:HE3	2.38	0.52
1:A:688:ARG:N	1:A:688:ARG:HD2	2.25	0.51
1:A:752:PHE:CE2	1:A:753:MSE:HE1	2.45	0.51
1:A:51:PHE:C	1:A:51:PHE:CD2	2.83	0.51
1:B:60:MSE:HE2	1:B:194:LEU:CD1	2.40	0.51
1:A:583:ALA:HB1	1:A:584:ALA:HA	1.91	0.51
1:B:32:SER:O	1:B:35:ASP:HB2	2.10	0.51
1:A:233:ASP:O	1:A:234:ASN:HB2	2.10	0.51
1:B:267:GLN:NE2	4:B:2092:HOH:O	2.43	0.51
1:A:805:GLN:H	1:A:805:GLN:HE21	1.58	0.51
1:B:69:GLN:NE2	1:B:76:PHE:H	2.09	0.51
1:A:511:MSE:HE3	1:A:511:MSE:CA	2.36	0.50
1:B:860:GLU:N	1:B:861:LYS:CA	2.61	0.50
1:A:541:MSE:HG3	1:A:668:LEU:HD11	1.94	0.50
1:A:69:GLN:HE21	1:A:76:PHE:HD1	1.59	0.50
1:A:77:ASN:ND2	1:A:80:GLU:H	2.09	0.50
1:B:53:SER:OG	1:B:55:LYS:HE2	2.11	0.50
1:B:752:PHE:CE2	1:B:753:MSE:HE1	2.47	0.50
1:A:647:ASN:HD22	1:A:647:ASN:C	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:THR:HG22	1:A:724:THR:HG23	1.94	0.50
1:A:476:LYS:HE3	1:A:794:ASN:O	2.11	0.50
1:B:218:ARG:O	1:B:221:ASN:HB2	2.12	0.50
1:A:425:LYS:O	1:A:427:LYS:HE2	2.12	0.49
1:B:51:PHE:C	1:B:51:PHE:CD2	2.86	0.49
1:B:810:SER:C	1:B:812:PRO:HB3	2.29	0.49
1:A:337:VAL:O	1:A:382:THR:HA	2.12	0.49
1:B:112:ILE:O	1:B:112:ILE:HG22	2.12	0.49
1:A:671:LEU:HD13	1:A:673:VAL:CG2	2.42	0.49
1:B:27:GLY:HA2	1:B:28:ASP:O	2.13	0.49
1:A:581:SER:HA	1:A:604:MSE:HE3	1.94	0.49
1:A:77:ASN:ND2	1:A:79:SER:H	2.10	0.49
1:B:532:PHE:CG	1:B:533:PRO:CD	2.95	0.49
1:B:419:GLN:HE21	1:B:423:LYS:CE	2.21	0.49
1:B:155:LEU:HA	1:B:159:LEU:O	2.13	0.49
1:B:180:ILE:HB	1:B:181:HIS:CD2	2.48	0.49
1:B:647:ASN:HD22	1:B:649:ASP:H	1.61	0.49
1:A:205:ASN:C	1:A:205:ASN:ND2	2.66	0.48
1:B:832:LEU:HA	1:B:835:ILE:HD12	1.95	0.48
1:A:239:ASP:OD1	1:A:242:ASP:OD2	2.30	0.48
1:A:644:ARG:HA	1:A:647:ASN:ND2	2.27	0.48
1:A:476:LYS:HE2	1:A:795:TYR:CZ	2.48	0.48
1:B:249:GLN:O	1:B:250:LYS:C	2.52	0.48
1:B:465:ASP:HA	1:B:468:ARG:NH1	2.27	0.48
1:B:709:GLU:HG3	4:B:2053:HOH:O	2.13	0.48
1:A:742:ASP:OD1	1:A:744:ALA:HB3	2.13	0.48
1:A:77:ASN:HD22	1:A:79:SER:H	1.62	0.48
1:B:414:GLN:NE2	1:B:414:GLN:CA	2.74	0.48
1:B:63:ASN:O	1:B:67:GLN:HG2	2.13	0.48
1:B:593:GLU:OE2	1:B:680:HIS:NE2	2.38	0.48
1:A:644:ARG:CB	1:A:650:ILE:HD12	2.44	0.48
1:A:690:ASN:C	1:A:690:ASN:HD22	2.16	0.48
1:A:883:LEU:O	1:A:885:SER:N	2.47	0.48
1:B:181:HIS:C	4:B:2055:HOH:O	2.51	0.48
1:A:197:TYR:O	1:A:198:LEU:C	2.52	0.48
1:A:440:PHE:H	1:A:443:ASN:ND2	1.88	0.48
1:A:443:ASN:ND2	1:A:443:ASN:H	1.97	0.48
1:B:443:ASN:ND2	1:B:443:ASN:H	2.01	0.48
1:B:838:PRO:CG	1:B:843:ILE:HD11	2.43	0.48
1:A:365:ALA:HB3	1:B:116:GLU:HB3	1.96	0.47
1:A:471:LYS:HE3	4:A:2078:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:GLU:OE1	1:A:770:GLU:N	2.47	0.47
1:A:759:LEU:HG	1:A:781:LEU:HD13	1.96	0.47
1:B:227:MSE:HE1	1:B:271:VAL:HB	1.96	0.47
1:B:471:LYS:HE3	4:B:2072:HOH:O	2.12	0.47
1:A:676:ASN:ND2	1:A:706:ARG:NH1	2.62	0.47
1:B:660:LEU:C	1:B:688:ARG:HD3	2.34	0.47
1:A:163:GLN:HG3	1:A:198:LEU:HD11	1.96	0.47
1:A:644:ARG:HB3	1:A:650:ILE:HD12	1.96	0.47
1:A:660:LEU:C	1:A:688:ARG:HD3	2.35	0.47
1:A:802:LYS:O	1:A:805:GLN:HB2	2.14	0.47
1:B:47:GLN:HE22	1:B:245:ALA:HA	1.80	0.47
1:B:831:GLU:O	1:B:833:GLN:N	2.48	0.47
1:A:65:ARG:NH1	1:A:78:ASP:OD1	2.38	0.47
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.44	0.47
1:A:112:ILE:HD13	1:B:356:ASP:HB2	1.95	0.47
1:A:249:GLN:HA	1:A:249:GLN:NE2	2.29	0.47
1:A:33:GLU:HG2	1:A:33:GLU:H	1.33	0.46
1:B:369:ARG:NH1	4:B:2126:HOH:O	2.47	0.46
1:B:768:SER:C	1:B:769:ILE:O	2.53	0.46
1:B:13:ASN:N	1:B:13:ASN:OD1	2.47	0.46
1:A:177:PHE:CD2	1:A:177:PHE:C	2.88	0.46
1:A:163:GLN:HG3	1:A:198:LEU:CD1	2.45	0.46
1:A:104:HIS:CE1	1:A:199:GLN:OE1	2.68	0.46
1:A:212:PHE:CD2	1:A:226:THR:HG22	2.51	0.46
1:A:787:ARG:CG	1:A:787:ARG:NH1	2.70	0.46
1:B:205:ASN:C	1:B:205:ASN:ND2	2.68	0.46
1:B:532:PHE:CE2	1:B:533:PRO:HD2	2.49	0.46
1:B:644:ARG:HA	1:B:647:ASN:ND2	2.30	0.46
1:B:482:VAL:HG21	1:B:823:TYR:CG	2.50	0.46
1:B:858:ARG:HB3	1:B:858:ARG:CZ	2.42	0.46
1:B:641:LEU:CD2	1:B:650:ILE:HD13	2.45	0.46
1:A:77:ASN:HD22	1:A:79:SER:N	2.13	0.46
1:B:613:ASP:O	1:B:617:ARG:HG3	2.15	0.46
1:A:765:ASP:H	1:A:768:SER:CB	2.29	0.46
1:B:371:LEU:HG	1:B:398:VAL:HG21	1.96	0.46
1:B:810:SER:N	1:B:811:ASP:HA	2.30	0.46
1:A:686:PHE:CZ	1:A:702:ILE:HG21	2.51	0.46
1:B:676:ASN:ND2	1:B:706:ARG:NH1	2.64	0.46
1:B:752:PHE:HE2	1:B:753:MSE:HE1	1.79	0.46
1:B:822:HIS:O	1:B:824:VAL:HG23	2.16	0.46
1:A:790:ASN:OD1	4:A:2264:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:GLN:H	1:A:807:ILE:HG12	1.80	0.46
1:B:690:ASN:ND2	1:B:691:ARG:HD2	2.31	0.46
1:A:155:LEU:HA	1:A:159:LEU:O	2.15	0.45
1:A:787:ARG:HD2	1:A:879:GLU:OE2	2.17	0.45
1:B:765:ASP:H	1:B:768:SER:HB2	1.81	0.45
1:A:168:LYS:HE2	1:A:168:LYS:HB3	1.80	0.45
1:B:787:ARG:HB2	1:B:787:ARG:HH11	1.75	0.45
1:B:476:LYS:HE2	1:B:795:TYR:CZ	2.51	0.45
1:B:389:LEU:O	1:B:393:GLU:HB2	2.16	0.45
1:A:831:GLU:O	1:A:833:GLN:N	2.50	0.45
1:B:752:PHE:CD2	1:B:753:MSE:HE2	2.47	0.45
1:A:768:SER:C	1:A:769:ILE:O	2.55	0.45
1:A:419:GLN:HE21	1:A:423:LYS:HE2	1.81	0.45
1:A:244:THR:O	1:A:248:PHE:HB2	2.17	0.45
1:A:690:ASN:C	1:A:690:ASN:ND2	2.69	0.45
1:B:233:ASP:O	1:B:234:ASN:HB2	2.17	0.45
1:B:343:ASP:H	1:B:346:THR:CG2	2.28	0.45
1:B:465:ASP:OD1	1:B:468:ARG:NH1	2.28	0.45
1:A:778:PHE:HE2	1:A:846:TYR:CD1	2.35	0.45
1:B:807:ILE:H	1:B:808:ASP:HB2	1.81	0.45
1:B:402:GLN:NE2	1:B:430:TYR:CZ	2.85	0.45
1:B:641:LEU:HD23	1:B:650:ILE:HD13	1.98	0.45
1:B:67:GLN:HA	1:B:67:GLN:NE2	2.32	0.45
1:B:762:ARG:HH22	1:B:777:ASP:HB3	1.82	0.45
1:B:218:ARG:NH2	1:B:884:LYS:HZ3	2.11	0.45
1:A:369:ARG:NH2	1:B:116:GLU:O	2.45	0.44
1:B:718:LEU:HD13	1:B:719:PHE:CZ	2.52	0.44
1:A:675:LYS:NZ	4:A:2225:HOH:O	2.42	0.44
1:A:834:THR:CG2	1:A:834:THR:O	2.65	0.44
1:B:561:GLN:HE22	1:B:574:LEU:N	2.09	0.44
1:A:644:ARG:HA	1:A:647:ASN:HD21	1.82	0.44
1:B:340:LYS:CD	4:B:2205:HOH:O	2.58	0.44
1:A:218:ARG:NH2	1:A:884:LYS:NZ	2.65	0.44
1:B:857:GLN:C	1:B:859:ARG:N	2.70	0.44
1:A:671:LEU:HD13	1:A:673:VAL:HG22	1.99	0.44
1:A:77:ASN:ND2	1:A:79:SER:N	2.65	0.44
1:B:339:ARG:HD3	1:B:384:GLN:CG	2.48	0.44
1:B:647:ASN:ND2	1:B:649:ASP:H	2.15	0.44
1:B:812:PRO:O	1:B:815:VAL:HB	2.17	0.44
1:B:218:ARG:NH2	1:B:884:LYS:HZ1	2.10	0.44
1:B:763:PHE:H	1:B:764:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:NE2	1:A:76:PHE:H	2.15	0.44
1:A:249:GLN:O	1:A:250:LYS:C	2.57	0.44
1:A:688:ARG:H	1:A:688:ARG:HD2	1.83	0.44
1:A:841:ARG:O	1:A:844:GLN:HG3	2.18	0.44
1:B:420:LYS:HE3	1:B:420:LYS:HB3	1.76	0.44
1:B:504:GLN:HG2	1:B:504:GLN:H	1.39	0.44
1:A:293:ALA:O	1:A:294:LYS:HB2	2.18	0.43
1:A:322:ARG:NH1	4:A:2117:HOH:O	2.50	0.43
1:B:163:GLN:HG3	1:B:198:LEU:CD1	2.49	0.43
1:B:91:ASN:N	1:B:91:ASN:ND2	2.42	0.43
1:A:825:ASP:HB3	1:A:827:GLU:HB3	1.99	0.43
1:B:831:GLU:C	1:B:833:GLN:N	2.71	0.43
1:A:31:GLN:HE21	1:A:169:ARG:HB2	1.84	0.43
1:A:624:LYS:HD3	1:A:624:LYS:HA	1.90	0.43
1:A:825:ASP:O	1:A:829:PHE:HB2	2.18	0.43
1:A:443:ASN:ND2	1:A:443:ASN:N	2.63	0.43
1:B:32:SER:O	1:B:36:LEU:HD13	2.18	0.43
1:B:690:ASN:HD22	1:B:691:ARG:N	2.17	0.43
1:A:414:GLN:CA	1:A:414:GLN:NE2	2.81	0.43
1:A:465:ASP:HA	1:A:468:ARG:NH1	2.34	0.43
1:A:65:ARG:HD3	1:A:69:GLN:HE22	1.80	0.43
1:A:831:GLU:C	1:A:833:GLN:N	2.69	0.43
1:A:164:ILE:HA	1:A:202:VAL:O	2.19	0.43
1:A:359:ASN:HD21	1:A:385:LYS:NZ	2.16	0.43
1:A:103:ILE:HD13	1:A:103:ILE:HA	1.83	0.43
1:A:99:LYS:HD2	1:A:197:TYR:CZ	2.53	0.43
1:A:836:ARG:HE	1:A:836:ARG:HB3	1.60	0.43
1:B:463:ILE:H	1:B:463:ILE:HG13	1.40	0.43
1:A:676:ASN:ND2	1:A:706:ARG:HH11	2.16	0.43
1:A:765:ASP:C	1:A:767:THR:H	2.22	0.43
1:B:699:PHE:CD1	1:B:730:GLU:HG3	2.54	0.43
1:B:508:LEU:HA	1:B:513:ILE:HD11	2.01	0.43
1:A:463:ILE:H	1:A:463:ILE:HG13	1.44	0.42
1:A:758:GLU:HB3	1:A:781:LEU:HD11	2.00	0.42
1:B:841:ARG:HA	1:B:844:GLN:NE2	2.35	0.42
1:A:641:LEU:HD23	1:A:650:ILE:HD13	2.00	0.42
1:A:476:LYS:HE2	1:A:795:TYR:CE1	2.54	0.42
1:B:676:ASN:ND2	1:B:706:ARG:HH11	2.18	0.42
1:B:419:GLN:NE2	1:B:423:LYS:HE2	2.25	0.42
1:B:787:ARG:NH1	1:B:787:ARG:HB2	2.34	0.42
1:B:583:ALA:CB	1:B:584:ALA:CA	2.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:HE22	1:A:150:TYR:HA	1.84	0.42
1:A:763:PHE:N	1:A:764:PRO:CD	2.81	0.42
1:B:163:GLN:HG3	1:B:198:LEU:HD11	2.01	0.42
1:B:212:PHE:HB3	1:B:226:THR:HA	2.02	0.42
1:B:841:ARG:O	1:B:844:GLN:HG3	2.19	0.42
1:A:441:PRO:HD2	1:A:442:GLU:OE2	2.19	0.42
1:B:71:LEU:HA	1:B:71:LEU:HD23	1.89	0.42
1:B:115:ASP:O	1:B:116:GLU:CB	2.68	0.42
1:A:282:ARG:NH1	4:A:2110:HOH:O	2.50	0.42
1:B:177:PHE:CD2	1:B:177:PHE:C	2.93	0.42
1:B:192:ASN:HA	1:B:192:ASN:HD22	1.63	0.42
1:B:205:ASN:ND2	1:B:208:ASP:H	2.18	0.42
1:B:806:GLN:N	1:B:807:ILE:HG12	2.30	0.42
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.75	0.41
1:A:371:LEU:HG	1:A:398:VAL:HG21	2.02	0.41
1:A:541:MSE:HE1	1:A:660:LEU:HD23	2.02	0.41
1:B:473:LEU:HB3	1:B:699:PHE:HA	2.02	0.41
1:A:733:TYR:HB2	1:A:795:TYR:CD2	2.55	0.41
1:B:239:ASP:OD1	1:B:242:ASP:OD2	2.38	0.41
1:B:33:GLU:HG2	1:B:33:GLU:H	1.35	0.41
1:B:77:ASN:C	1:B:77:ASN:ND2	2.73	0.41
1:A:482:VAL:O	1:A:482:VAL:HG13	2.19	0.41
1:A:752:PHE:HE2	1:A:753:MSE:HE1	1.82	0.41
1:B:601:THR:O	1:B:604:MSE:HG3	2.20	0.41
1:A:765:ASP:C	1:A:767:THR:N	2.73	0.41
1:B:60:MSE:HE2	1:B:194:LEU:HD12	2.01	0.41
1:B:347:MSE:HE2	1:B:639:ARG:NH1	2.36	0.41
1:B:750:ARG:NH1	1:B:784:GLU:OE1	2.54	0.41
1:B:641:LEU:O	1:B:645:VAL:HG23	2.20	0.41
1:B:854:ARG:HB2	1:B:878:PHE:CE2	2.56	0.41
1:A:817:LYS:HE3	1:A:821:GLU:OE2	2.20	0.41
1:A:841:ARG:HA	1:A:844:GLN:HG3	2.02	0.41
1:B:136:ILE:HG22	1:B:154:ILE:HG12	2.03	0.41
1:B:817:LYS:NZ	4:B:2278:HOH:O	2.49	0.41
1:B:884:LYS:C	1:B:886:GLN:H	2.23	0.41
1:A:339:ARG:HD3	1:A:384:GLN:OE1	2.21	0.41
1:B:312:GLY:HA2	2:B:1893:ATP:PA	2.61	0.41
1:B:227:MSE:SE	1:B:273:ARG:HG2	2.71	0.41
1:B:752:PHE:O	1:B:756:VAL:HG23	2.20	0.41
1:A:407:PHE:HE1	1:A:431:GLN:HE21	1.68	0.41
1:A:52:ILE:HG13	1:A:137:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:NH1	1:B:384:GLN:HG2	2.35	0.41
1:B:582:PHE:CE2	1:B:583:ALA:O	2.74	0.41
1:B:682:LEU:HD13	1:B:682:LEU:C	2.40	0.41
1:A:420:LYS:HB3	1:A:420:LYS:HE3	1.84	0.40
1:B:200:LEU:HD13	1:B:271:VAL:HG21	2.03	0.40
1:B:750:ARG:O	4:B:2265:HOH:O	2.22	0.40
1:B:539:ASN:H	1:B:539:ASN:HD22	1.69	0.40
1:A:701:ASN:O	1:A:702:ILE:HD13	2.21	0.40
1:A:637:TYR:O	1:A:641:LEU:HB2	2.21	0.40
1:A:718:LEU:HD13	1:A:719:PHE:CZ	2.57	0.40
1:A:785:TYR:CD1	1:A:785:TYR:C	2.95	0.40
1:A:816:GLU:OE2	1:A:819:LYS:HE3	2.22	0.40
1:B:339:ARG:HD3	1:B:384:GLN:HG2	2.03	0.40
1:B:553:TYR:O	1:B:554:TYR:C	2.58	0.40
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.96	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	832/1038 (80%)	754 (91%)	60 (7%)	18 (2%)	6 12
1	B	842/1038 (81%)	768 (91%)	61 (7%)	13 (2%)	10 21
All	All	1674/2076 (81%)	1522 (91%)	121 (7%)	31 (2%)	8 15

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	411	HIS
1	A	532	PHE

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Mol	Chain	Res	Type
1	A	568	SER
1	A	763	PHE
1	A	769	ILE
1	A	811	ASP
1	A	852	ASP
1	B	532	PHE
1	B	769	ILE
1	B	815	VAL
1	A	569	ALA
1	A	764	PRO
1	A	805	GLN
1	B	511	MSE
1	B	569	ALA
1	B	765	ASP
1	B	861	LYS
1	A	746	GLY
1	A	827	GLU
1	A	849	ALA
1	A	883	LEU
1	B	812	PRO
1	B	814	ALA
1	A	482	VAL
1	A	747	GLU
1	A	765	ASP
1	B	811	ASP
1	B	764	PRO
1	B	533	PRO
1	B	888	ILE

5.3.2 Protein sidechains (i)

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	740/912 (81%)	648 (88%)	92 (12%)	4 8
1	B	750/912 (82%)	657 (88%)	93 (12%)	4 8
All	All	1490/1824 (82%)	1305 (88%)	185 (12%)	4 8

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	26	THR
1	A	29	SER
1	A	32	SER
1	A	33	GLU
1	A	40	LEU
1	A	55	LYS
1	A	65	ARG
1	A	71	LEU
1	A	74	VAL
1	A	77	ASN
1	A	89	LEU
1	A	91	ASN
1	A	117	ARG
1	A	128	ASN
1	A	129	LEU
1	A	169	ARG
1	A	173	ILE
1	A	174	ARG
1	A	192	ASN
1	A	205	ASN
1	A	207	THR
1	A	217	LYS
1	A	224	ASP
1	A	240	LEU
1	A	241	LYS
1	A	253	LEU
1	A	282	ARG
1	A	296	TRP
1	A	298	LYS
1	A	301	SER
1	A	309	THR
1	A	332	LYS
1	A	336	VAL
1	A	346	THR
1	A	356	ASP
1	A	359	ASN
1	A	371	LEU
1	A	373	LYS
1	A	374	ASP
1	A	391	LYS
1	A	398	VAL

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Mol	Chain	Res	Type
1	A	413	SER
1	A	422	LEU
1	A	443	ASN
1	A	452	SER
1	A	463	ILE
1	A	482	VAL
1	A	489	LEU
1	A	496	LYS
1	A	499	SER
1	A	504	GLN
1	A	531	THR
1	A	539	ASN
1	A	558	LYS
1	A	575	ARG
1	A	591	ILE
1	A	605	ASP
1	A	613	ASP
1	A	641	LEU
1	A	647	ASN
1	A	652	LEU
1	A	655	VAL
1	A	671	LEU
1	A	682	LEU
1	A	688	ARG
1	A	690	ASN
1	A	696	THR
1	A	698	THR
1	A	710	ARG
1	A	718	LEU
1	A	722	LYS
1	A	725	LYS
1	A	747	GLU
1	A	767	THR
1	A	769	ILE
1	A	781	LEU
1	A	787	ARG
1	A	802	LYS
1	A	804	LEU
1	A	805	GLN
1	A	813	VAL
1	A	817	LYS
1	A	834	THR

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Mol	Chain	Res	Type
1	A	836	ARG
1	A	841	ARG
1	A	842	LYS
1	A	844	GLN
1	A	857	GLN
1	A	871	THR
1	A	884	LYS
1	A	885	SER
1	B	13	ASN
1	B	26	THR
1	B	29	SER
1	B	32	SER
1	B	33	GLU
1	B	40	LEU
1	B	55	LYS
1	B	65	ARG
1	B	71	LEU
1	B	74	VAL
1	B	77	ASN
1	B	89	LEU
1	B	91	ASN
1	B	112	ILE
1	B	117	ARG
1	B	128	ASN
1	B	129	LEU
1	B	169	ARG
1	B	173	ILE
1	B	174	ARG
1	B	192	ASN
1	B	205	ASN
1	B	207	THR
1	B	217	LYS
1	B	224	ASP
1	B	235	THR
1	B	238	LYS
1	B	240	LEU
1	B	253	LEU
1	B	282	ARG
1	B	297	SER
1	B	301	SER
1	B	309	THR
1	B	315	LEU

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Mol	Chain	Res	Type
1	B	336	VAL
1	B	340	LYS
1	B	346	THR
1	B	356	ASP
1	B	359	ASN
1	B	371	LEU
1	B	374	ASP
1	B	394	SER
1	B	398	VAL
1	B	413	SER
1	B	422	LEU
1	B	424	LYS
1	B	443	ASN
1	B	452	SER
1	B	463	ILE
1	B	464	THR
1	B	472	VAL
1	B	482	VAL
1	B	489	LEU
1	B	504	GLN
1	B	511	MSE
1	B	531	THR
1	B	539	ASN
1	B	558	LYS
1	B	575	ARG
1	B	591	ILE
1	B	605	ASP
1	B	607	SER
1	B	613	ASP
1	B	641	LEU
1	B	647	ASN
1	B	652	LEU
1	B	655	VAL
1	B	682	LEU
1	B	688	ARG
1	B	690	ASN
1	B	696	THR
1	B	698	THR
1	B	710	ARG
1	B	718	LEU
1	B	722	LYS
1	B	725	LYS

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Mol	Chain	Res	Type
1	B	750	ARG
1	B	765	ASP
1	B	769	ILE
1	B	781	LEU
1	B	787	ARG
1	B	804	LEU
1	B	817	LYS
1	B	834	THR
1	B	836	ARG
1	B	841	ARG
1	B	842	LYS
1	B	844	GLN
1	B	848	SER
1	B	858	ARG
1	B	871	THR
1	B	883	LEU
1	B	884	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	31	GLN
1	A	47	GLN
1	A	67	GLN
1	A	69	GLN
1	A	77	ASN
1	A	91	ASN
1	A	104	HIS
1	A	128	ASN
1	A	192	ASN
1	A	205	ASN
1	A	214	ASN
1	A	249	GLN
1	A	295	ASN
1	A	359	ASN
1	A	376	ASN
1	A	402	GLN
1	A	414	GLN
1	A	419	GLN
1	A	431	GLN
1	A	443	ASN

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Mol	Chain	Res	Type
1	A	504	GLN
1	A	505	GLN
1	A	526	GLN
1	A	539	ASN
1	A	561	GLN
1	A	635	GLN
1	A	643	GLN
1	A	647	ASN
1	A	676	ASN
1	A	690	ASN
1	A	805	GLN
1	A	833	GLN
1	B	13	ASN
1	B	31	GLN
1	B	47	GLN
1	B	67	GLN
1	B	69	GLN
1	B	77	ASN
1	B	91	ASN
1	B	104	HIS
1	B	128	ASN
1	B	181	HIS
1	B	192	ASN
1	B	205	ASN
1	B	214	ASN
1	B	249	GLN
1	B	295	ASN
1	B	359	ASN
1	B	376	ASN
1	B	402	GLN
1	B	414	GLN
1	B	419	GLN
1	B	431	GLN
1	B	443	ASN
1	B	504	GLN
1	B	526	GLN
1	B	539	ASN
1	B	561	GLN
1	B	635	GLN
1	B	647	ASN
1	B	676	ASN
1	B	690	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1893	3	26,33,33	0.87	0	31,52,52	1.43	5 (16%)
2	ATP	A	1886	3	26,33,33	0.82	1 (3%)	31,52,52	1.51	5 (16%)

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	1893	3	-	0/18/38/38	0/3/3/3
2	ATP	A	1886	3	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1886	ATP	C5-C4	2.12	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1886	ATP	N3-C2-N1	-3.72	122.86	128.68
2	B	1893	ATP	PB-O3B-PG	-3.63	120.37	132.83
2	A	1886	ATP	PB-O3B-PG	-2.84	123.09	132.83
2	B	1893	ATP	C4-C5-N7	-2.78	106.51	109.40
2	A	1886	ATP	C2-N1-C6	2.60	123.20	118.75
2	B	1893	ATP	N3-C2-N1	-2.59	124.62	128.68
2	A	1886	ATP	C4-C5-N7	-2.56	106.73	109.40
2	A	1886	ATP	O3B-PG-O1G	-2.23	98.80	111.19
2	B	1893	ATP	O4'-C1'-C2'	-2.19	103.72	106.93
2	B	1893	ATP	PA-O3A-PB	-2.16	125.43	132.83

There are no chirality outliers.

There are no torsion outliers.

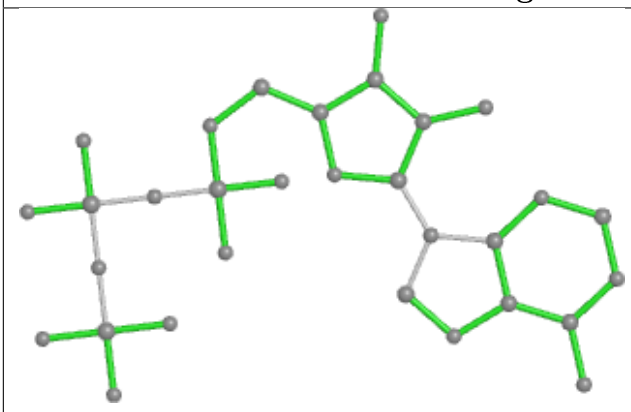
There are no ring outliers.

2 monomers are involved in 3 short contacts:

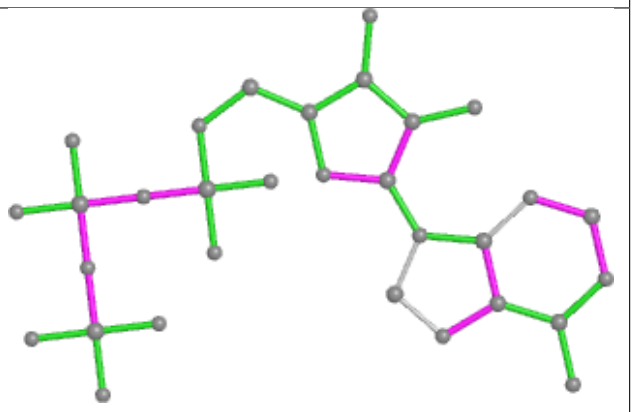
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1893	ATP	2	0
2	A	1886	ATP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

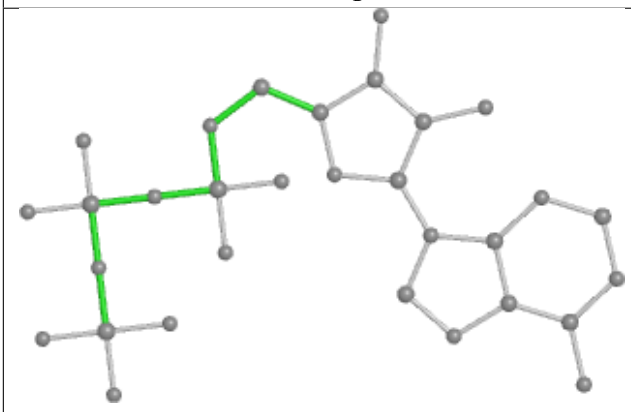
Ligand ATP B 1893



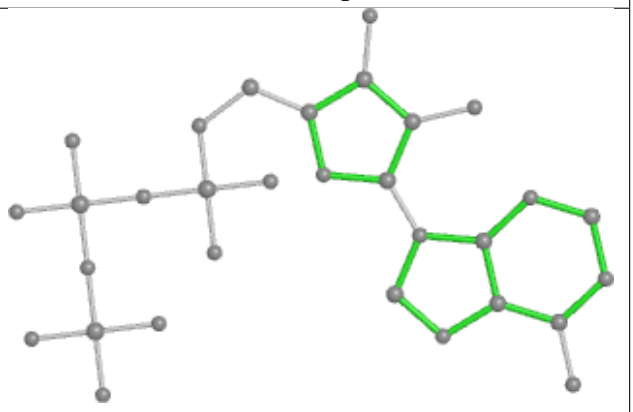
Bond lengths



Bond angles

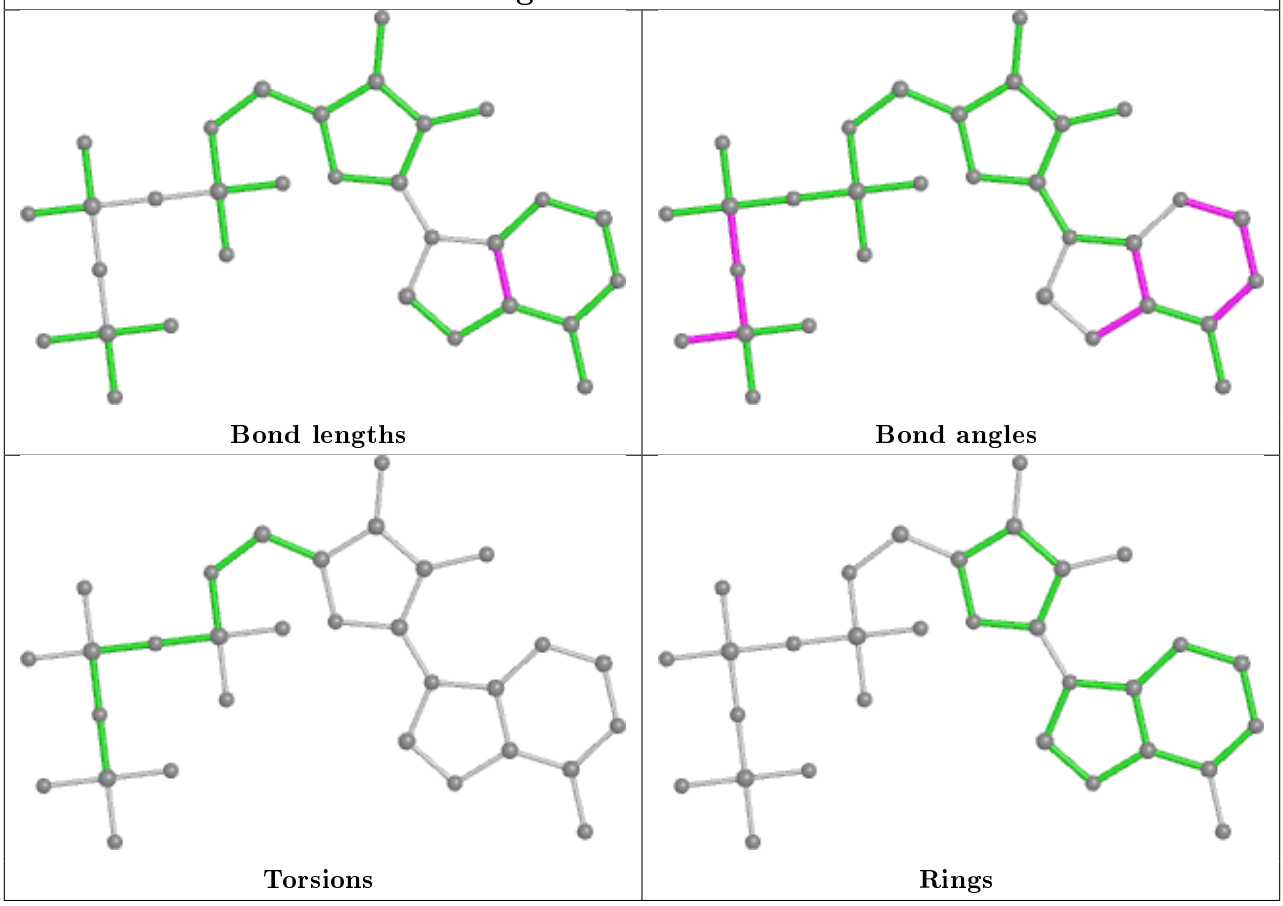


Torsions



Rings

Ligand ATP A 1886



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, 95^{th} 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	829/1038 (79%)	-0.12	22 (2%) 54 48	24, 40, 53, 66	0
1	B	839/1038 (80%)	-0.08	24 (2%) 51 45	25, 40, 53, 66	0
All	All	1668/2076 (80%)	-0.10	46 (2%) 53 46	24, 40, 53, 66	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	LEU	4.7
1	B	375	ASP	4.5
1	B	26	THR	4.4
1	B	446	GLY	4.1
1	B	141	GLU	4.1
1	A	810	SER	4.0
1	B	871	THR	3.6
1	B	891	ASP	3.4
1	B	567	LYS	3.3
1	B	814	ALA	3.1
1	A	218	ARG	3.1
1	A	769	ILE	3.0
1	A	871	THR	3.0
1	A	413	SER	3.0
1	B	140	PHE	3.0
1	A	809	LEU	2.9
1	A	584	ALA	2.9
1	A	770	GLU	2.9
1	A	148	ASN	2.8
1	B	24	GLU	2.8
1	B	445	LEU	2.8
1	A	813	VAL	2.8
1	B	374	ASP	2.8
1	A	845	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	808	ASP	2.5
1	A	446	GLY	2.5
1	A	884	LYS	2.5
1	A	811	ASP	2.5
1	B	858	ARG	2.4
1	A	567	LYS	2.4
1	B	568	SER	2.4
1	A	563	GLU	2.4
1	B	809	LEU	2.3
1	B	745	THR	2.3
1	A	848	SER	2.2
1	A	534	GLY	2.2
1	B	747	GLU	2.1
1	A	806	GLN	2.1
1	B	816	GLU	2.1
1	A	141	GLU	2.1
1	B	890	LEU	2.1
1	B	602	SER	2.1
1	B	570	THR	2.0
1	B	571	TYR	2.0
1	B	413	SER	2.0
1	B	64	VAL	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, 95^{th} 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
3	MG	A	1887	1/1	0.97	0.04	11,11,11,11	0

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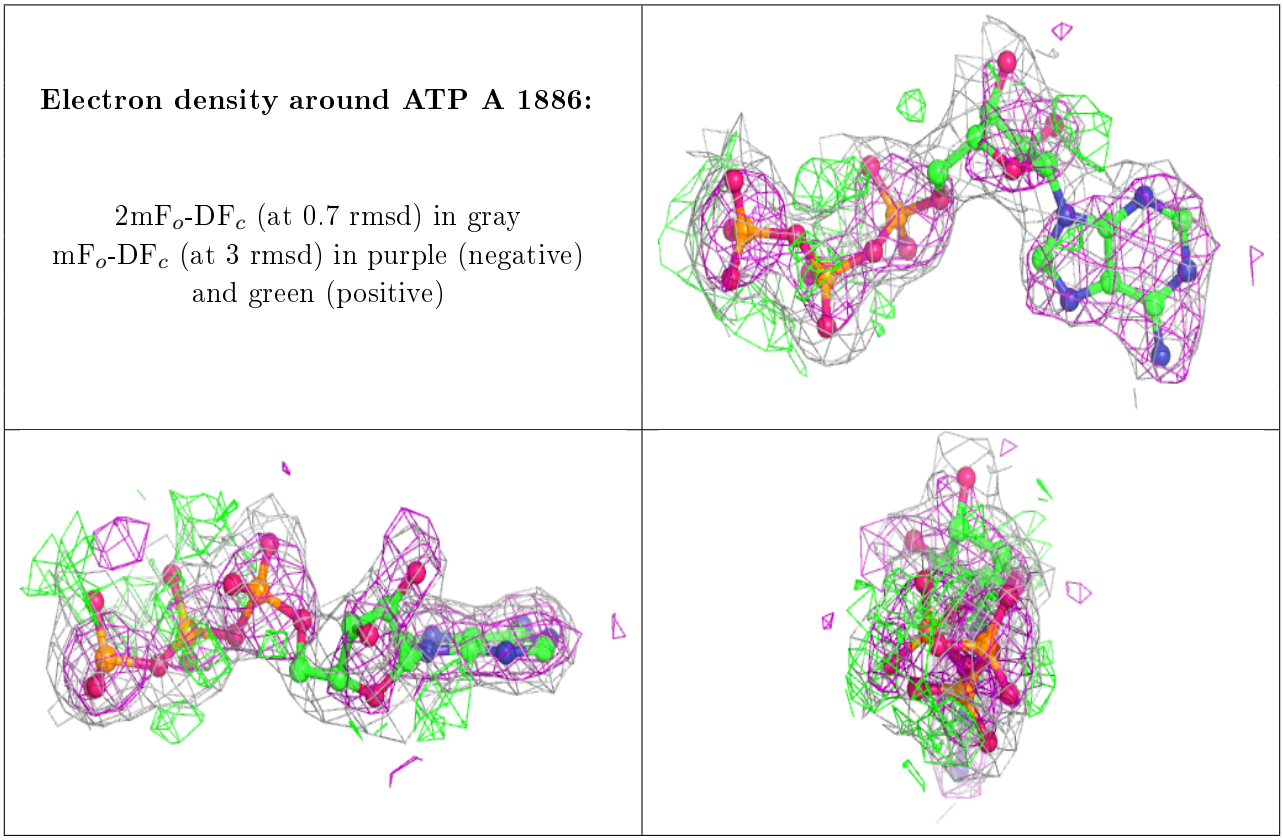
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	1894	1/1	0.98	0.09	13,13,13,13	0
2	ATP	A	1886	31/31	0.98	0.12	17,26,31,33	0
2	ATP	B	1893	31/31	0.99	0.10	20,26,30,33	0

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.

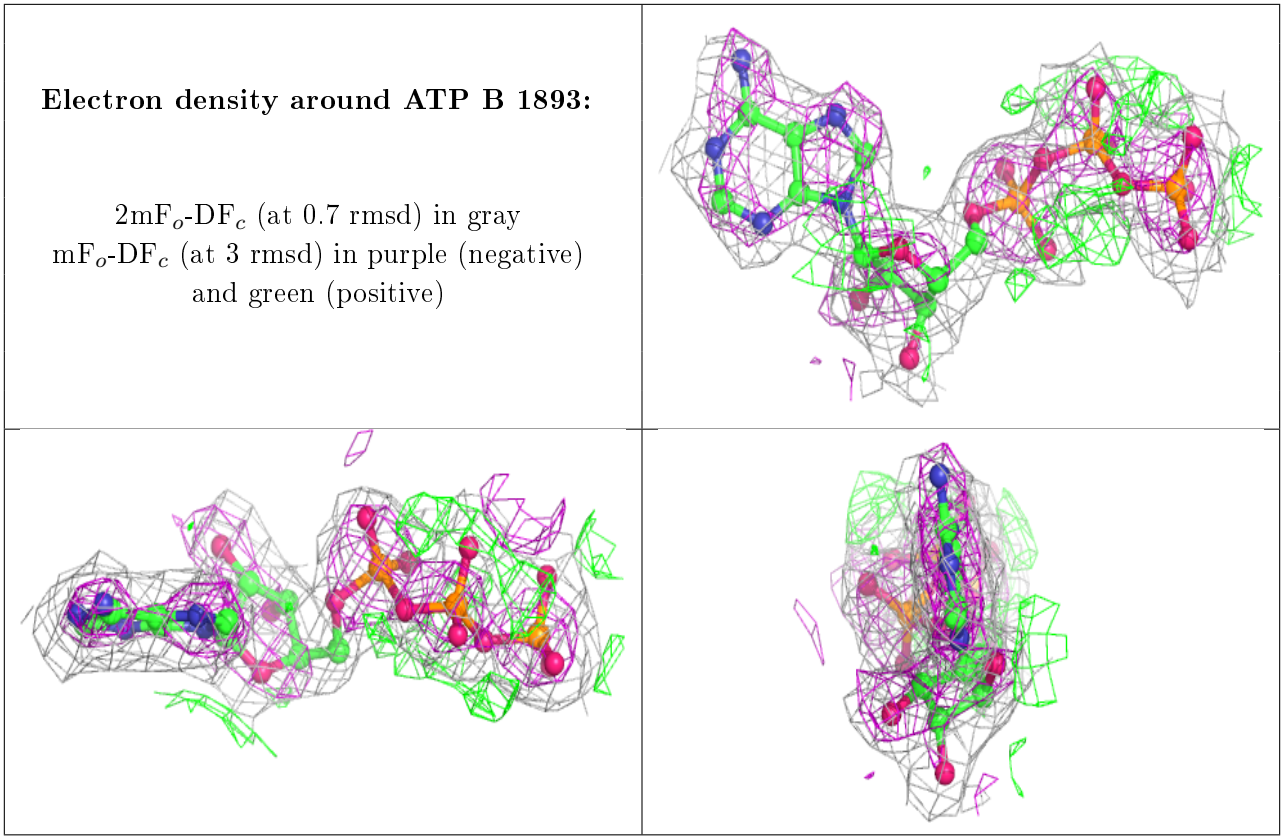
Electron density around ATP A 1886:

$2mF_o$-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 1893:

$2mF_o$-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.