Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 09:48 PM EDT

PDB ID	:	4II2
Title	:	Crystal structure of Ubiquitin activating enzyme 1 (Uba1) in complex with the Ub E2 Ubc4, ubiquitin, and ATP/Mg
Authors	:	Olsen, S.K.; Lima, C.D.
Deposited on	:	2012-12-19
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 (i) 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 (i)) were used in the production of this report:

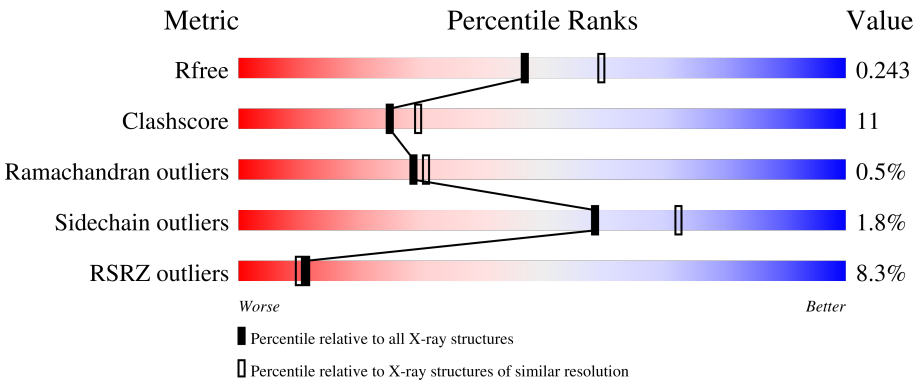
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	1001	9% 77% 20% •
2	B	83	2% 71% 24% • •
3	C	163	3% 61% 28% • 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10147 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	977	7673	4907	1254	1473	39	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	expression tag	UNP O94609

- Molecule 2 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	80	648	396	129	122	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	expression tag	UNP P0CH07
B	-5	HIS	-	expression tag	UNP P0CH07
B	-4	HIS	-	expression tag	UNP P0CH07
B	-3	HIS	-	expression tag	UNP P0CH07
B	-2	HIS	-	expression tag	UNP P0CH07
B	-1	HIS	-	expression tag	UNP P0CH07
B	0	HIS	-	expression tag	UNP P0CH07
B	6	ARG	LYS	engineered mutation	UNP P0CH07
B	11	ARG	LYS	engineered mutation	UNP P0CH07
B	27	ARG	LYS	engineered mutation	UNP P0CH07
B	28	ALA	SER	engineered mutation	UNP P0CH07
B	29	ARG	LYS	engineered mutation	UNP P0CH07
B	33	ARG	LYS	engineered mutation	UNP P0CH07
B	48	ARG	LYS	engineered mutation	UNP P0CH07
B	57	ALA	SER	engineered mutation	UNP P0CH07

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Chain	Residue	Modelled	Actual	Comment	Reference
B	63	ARG	LYS	engineered mutation	UNP P0CH07

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	149	1170	750	199	218	3	2	0	0

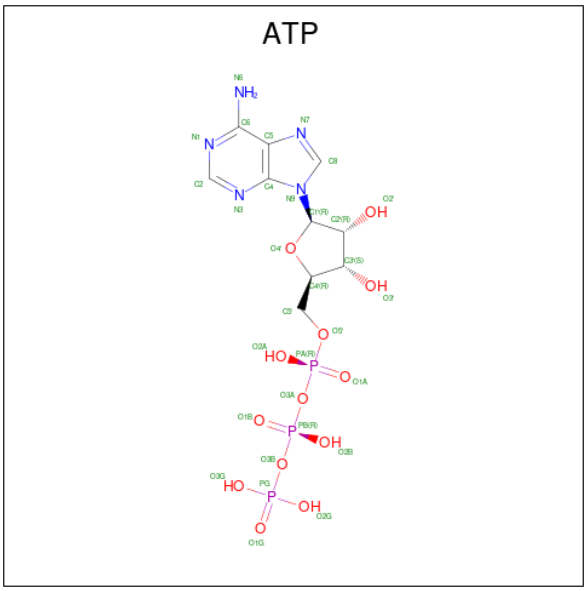
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	SER	CYS	engineered mutation	UNP P46595
C	107	SER	CYS	engineered mutation	UNP P46595
C	148	HIS	-	expression tag	UNP P46595
C	149	GLY	-	expression tag	UNP P46595
C	150	GLY	-	expression tag	UNP P46595
C	151	GLU	-	expression tag	UNP P46595
C	152	GLY	-	expression tag	UNP P46595
C	153	ALA	-	expression tag	UNP P46595
C	154	ALA	-	expression tag	UNP P46595
C	155	ALA	-	expression tag	UNP P46595
C	156	LEU	-	expression tag	UNP P46595
C	157	GLU	-	expression tag	UNP P46595
C	158	HIS	-	expression tag	UNP P46595
C	159	HIS	-	expression tag	UNP P46595
C	160	HIS	-	expression tag	UNP P46595
C	161	HIS	-	expression tag	UNP P46595
C	162	HIS	-	expression tag	UNP P46595
C	163	HIS	-	expression tag	UNP P46595

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

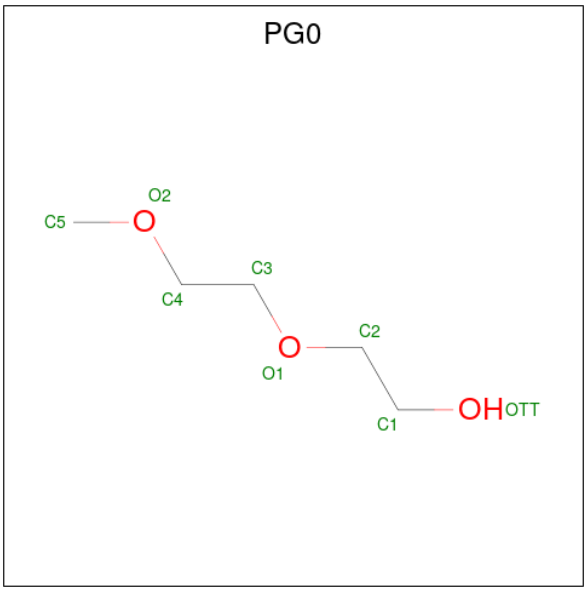
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



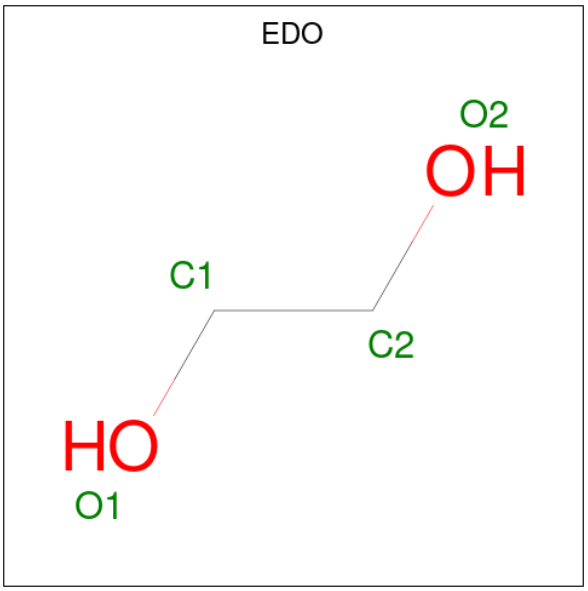
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

- Molecule 6 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



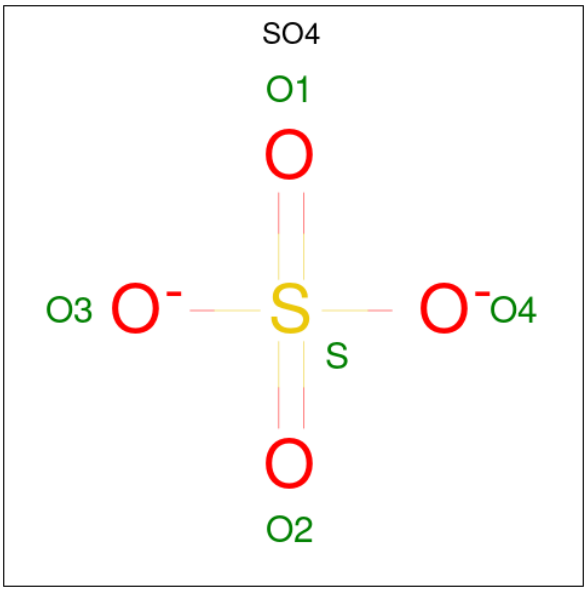
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	4	2	2	0	0
7	A	1	4	2	2	0	0
7	A	1	4	2	2	0	0
7	A	1	4	2	2	0	0
7	A	1	4	2	2	0	0
7	A	1	4	2	2	0	0
7	B	1	4	2	2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
8	A	1	5	4	1	0	0
			Total	O	S		
8	A	1	5	4	1	0	0
			Total	O	S		
8	A	1	5	4	1	0	0
			Total	O	S		
8	B	1	5	4	1	0	0

- Molecule 9 is water.

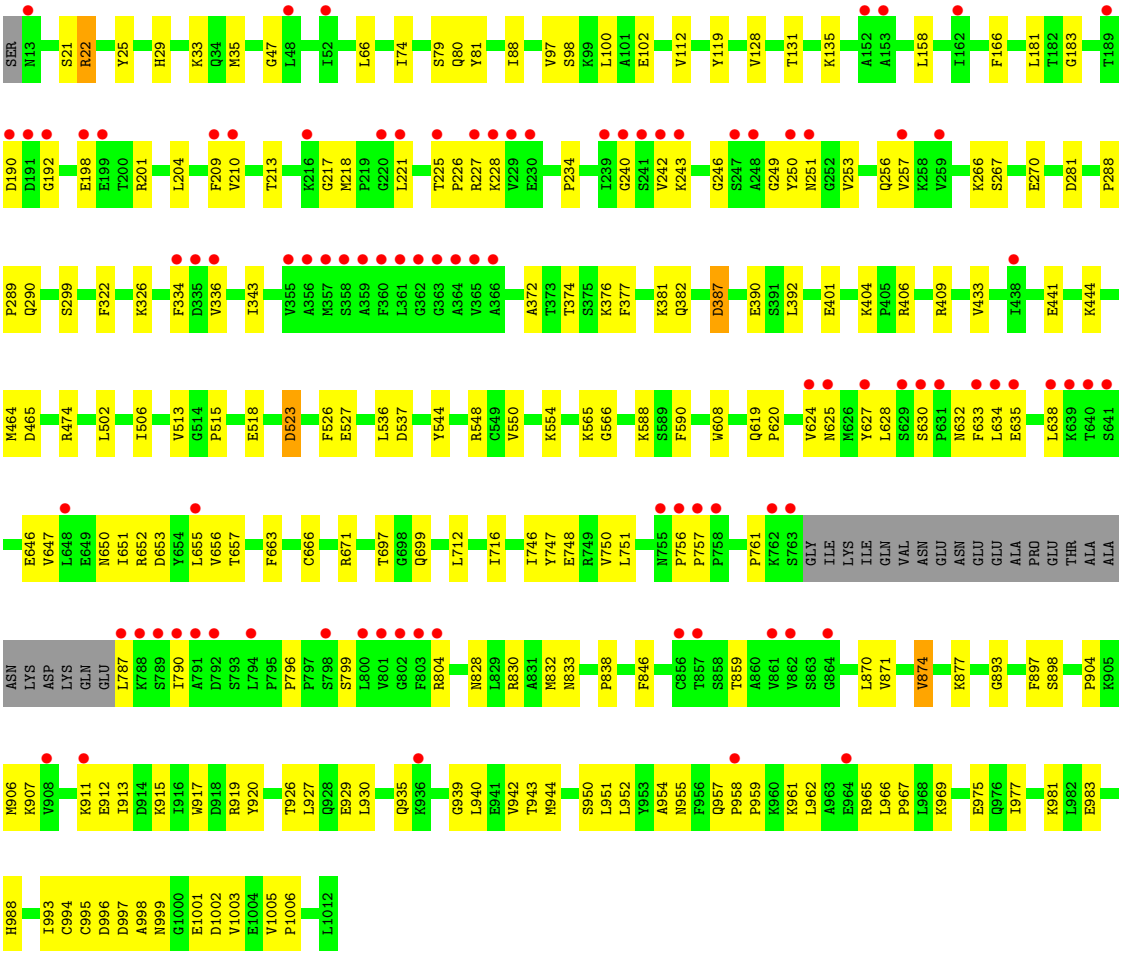
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	471	471	471	0	0
			Total	O		
9	B	41	41	41	0	0
			Total	O		
9	C	56	56	56	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

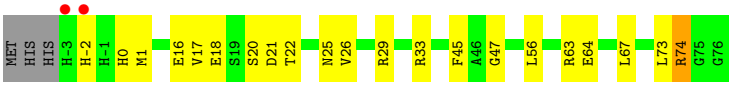
• Molecule 1: Ubiquitin-activating enzyme E1 1

Chain A:



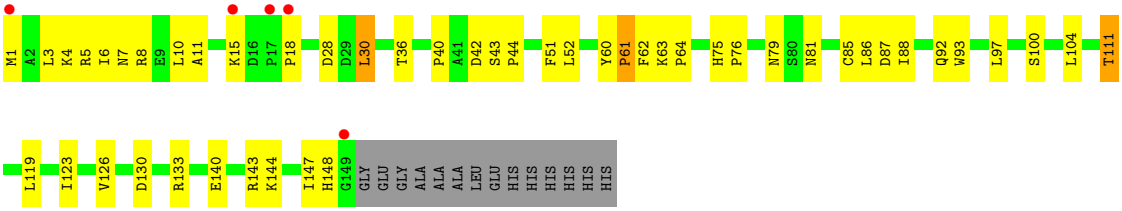
• Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B:



• Molecule 3: Ubiquitin-conjugating enzyme E2 4

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.60Å 111.20Å 181.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 39.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.20) 99.8 (39.80-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.53 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.254 0.206 , 0.243	Depositor DCC
R_{free} test set	4256 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10147	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, EDO, SO4, PG0

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	0.35	0/7844	0.56	0/10618
2	B	0.33	0/656	0.61	0/883
3	C	0.31	0/1206	0.56	0/1647
All	All	0.35	0/9706	0.56	0/13148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7673	0	7607	153	0
2	B	648	0	648	22	0
3	C	1170	0	1149	41	0
4	A	2	0	0	0	0
5	A	31	0	12	2	0
6	A	7	0	8	1	0
7	A	24	0	25	0	0
7	B	4	0	4	0	0
8	A	15	0	0	0	0
8	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	471	0	0	6	0
9	B	41	0	0	2	0
9	C	56	0	0	0	0
All	All	10147	0	9453	205	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 11.

All (205) 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:290:GLN:HB3	1:A:343:ILE:HD11	1.57	0.86
1:A:926:THR:HA	1:A:969:LYS:HA	1.59	0.85
1:A:653:ASP:HA	1:A:657:THR:HB	1.59	0.84
1:A:218:MET:HG3	1:A:246:GLY:HA3	1.61	0.82
2:B:1:MET:HB3	2:B:63:ARG:HG2	1.61	0.82
1:A:697:THR:HG22	1:A:699:GLN:HE21	1.45	0.79
1:A:634:LEU:HD12	1:A:634:LEU:H	1.49	0.78
1:A:656:VAL:HG23	1:A:657:THR:H	1.50	0.76
3:C:87:ASP:HB3	3:C:92:GLN:HG3	1.71	0.72
1:A:209:PHE:HE1	1:A:228:LYS:HG2	1.54	0.72
1:A:904:PRO:HG2	1:A:915:LYS:HB3	1.71	0.72
2:B:22:THR:H	2:B:25:ASN:HD22	1.38	0.68
1:A:81:TYR:CD2	1:A:444:LYS:HD2	2.29	0.68
1:A:210:VAL:HG12	1:A:256:GLN:HA	1.75	0.67
1:A:81:TYR:CE2	1:A:444:LYS:HD2	2.29	0.67
1:A:943:THR:HG21	1:A:996:ASP:OD2	1.94	0.67
1:A:632:ASN:HB3	1:A:635:GLU:HB2	1.76	0.66
3:C:126:VAL:HG11	3:C:133:ARG:HH21	1.61	0.65
1:A:954:ALA:HB3	1:A:957:GLN:HG3	1.79	0.64
3:C:100:SER:O	3:C:104:LEU:HD13	1.96	0.64
1:A:716:ILE:HD13	1:A:748:GLU:HG2	1.79	0.64
1:A:25:TYR:CE1	1:A:846:PHE:HB2	2.33	0.63
1:A:281:ASP:OD2	6:A:1104:PG0:H11	1.98	0.63
3:C:40:PRO:HG2	3:C:111:THR:HG22	1.81	0.63
1:A:871:VAL:HA	1:A:874:VAL:CG1	2.28	0.63
1:A:209:PHE:CE1	1:A:228:LYS:HG2	2.33	0.63
1:A:218:MET:HB2	1:A:221:LEU:HD13	1.81	0.63
1:A:656:VAL:HG23	1:A:657:THR:N	2.15	0.62
3:C:86:LEU:HG	3:C:88:ILE:HG22	1.81	0.62
1:A:625:ASN:OD1	1:A:804:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:GLU:CD	3:C:143:ARG:HH21	2.04	0.61
1:A:638:LEU:HD23	1:A:638:LEU:O	1.99	0.61
1:A:870:LEU:O	1:A:874:VAL:HG12	2.01	0.61
1:A:747:TYR:O	1:A:751:LEU:HD23	2.01	0.60
1:A:334:PHE:CZ	1:A:336:VAL:HB	2.37	0.60
2:B:22:THR:H	2:B:25:ASN:ND2	1.99	0.60
1:A:515:PRO:O	1:A:518:GLU:HG3	2.02	0.60
3:C:6:ILE:HG21	3:C:30:LEU:O	2.00	0.60
1:A:22:ARG:HD2	5:A:1103:ATP:O2G	2.01	0.59
1:A:74:ILE:HD13	1:A:88:ILE:HD11	1.84	0.59
1:A:217:GLY:HA3	1:A:249:GLY:HA2	1.85	0.58
3:C:5:ARG:NH2	3:C:61:PRO:HG3	2.18	0.58
2:B:74:ARG:HD2	9:B:207:HOH:O	2.02	0.58
1:A:112:VAL:HG11	1:A:119:TYR:OH	2.03	0.58
1:A:957:GLN:HE22	1:A:965:ARG:HH12	1.51	0.58
3:C:130:ASP:OD2	3:C:133:ARG:HB2	2.04	0.57
1:A:288:PRO:HB2	1:A:289:PRO:HD3	1.87	0.57
1:A:796:PRO:HG2	1:A:799:SER:HB3	1.87	0.57
1:A:975:GLU:OE1	1:A:981:LYS:HG3	2.05	0.56
3:C:126:VAL:HG11	3:C:133:ARG:NH2	2.19	0.56
1:A:523:ASP:OD2	1:A:988:HIS:HD2	1.88	0.56
1:A:951:LEU:HB2	3:C:30:LEU:HD11	1.87	0.56
1:A:944:MET:HB3	1:A:994:CYS:HB2	1.88	0.56
1:A:913:ILE:HD12	1:A:913:ILE:N	2.20	0.56
1:A:912:GLU:C	1:A:913:ILE:HD12	2.26	0.56
1:A:935:GLN:O	1:A:939:GLY:HA2	2.06	0.55
1:A:940:LEU:HD22	1:A:1003:VAL:HG21	1.87	0.55
2:B:63:ARG:HG3	9:B:226:HOH:O	2.07	0.55
3:C:1:MET:HB2	3:C:4:LYS:HB2	1.88	0.55
1:A:213:THR:HG22	9:A:1302:HOH:O	2.06	0.55
1:A:647:VAL:O	1:A:651:ILE:HG12	2.07	0.55
2:B:17:VAL:HG12	2:B:29:ARG:NH1	2.21	0.55
1:A:201:ARG:HD3	2:B:33:ARG:O	2.07	0.55
1:A:548:ARG:HD3	9:A:1452:HOH:O	2.05	0.55
1:A:997:ASP:HB2	1:A:1003:VAL:HG13	1.88	0.54
2:B:45:PHE:HB2	2:B:67:LEU:HD22	1.89	0.53
1:A:1005:VAL:CG2	1:A:1006:PRO:HD2	2.39	0.53
1:A:441:GLU:HG3	1:A:859:THR:HG22	1.91	0.53
1:A:401:GLU:O	1:A:404:LYS:HG2	2.09	0.53
1:A:619:GLN:HB2	1:A:620:PRO:HD3	1.90	0.53
1:A:433:VAL:HG13	1:A:513:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:HA3	1:A:79:SER:OG	2.08	0.52
1:A:942:VAL:HG22	1:A:993:ILE:HD11	1.91	0.52
3:C:140:GLU:HG3	3:C:144:LYS:HE3	1.92	0.52
1:A:181:LEU:HD12	1:A:204:LEU:HD23	1.92	0.52
1:A:944:MET:HG3	3:C:7:ASN:CG	2.30	0.52
3:C:1:MET:CG	3:C:4:LYS:HD2	2.40	0.51
1:A:966:LEU:N	1:A:967:PRO:HD2	2.24	0.51
1:A:502:LEU:HD13	1:A:506:ILE:HD11	1.93	0.51
1:A:906:MET:HE3	1:A:915:LYS:HB2	1.93	0.51
1:A:35:MET:HG3	1:A:374:THR:HG22	1.93	0.51
3:C:76:PRO:HG3	3:C:123:ILE:HG22	1.93	0.51
1:A:190:ASP:OD2	1:A:243:LYS:HG2	2.11	0.50
1:A:566:GLY:HA2	2:B:73:LEU:HD12	1.93	0.50
1:A:870:LEU:HD23	1:A:870:LEU:C	2.31	0.50
1:A:926:THR:OG1	1:A:929:GLU:HG3	2.11	0.50
1:A:957:GLN:HE22	1:A:965:ARG:NH1	2.07	0.50
3:C:126:VAL:HG13	3:C:133:ARG:HD3	1.92	0.50
1:A:226:PRO:HB3	1:A:257:VAL:HG21	1.93	0.50
1:A:25:TYR:CZ	1:A:846:PHE:HB2	2.47	0.50
1:A:927:LEU:HD23	1:A:966:LEU:HD23	1.94	0.50
1:A:266:LYS:HB3	1:A:270:GLU:HG3	1.94	0.49
1:A:566:GLY:CA	2:B:73:LEU:HD12	2.41	0.49
1:A:951:LEU:HB2	3:C:30:LEU:CD1	2.42	0.49
3:C:43:SER:HB2	3:C:44:PRO:HD2	1.95	0.49
1:A:250:TYR:HD1	1:A:251:ASN:ND2	2.10	0.49
3:C:40:PRO:CG	3:C:111:THR:HG22	2.43	0.49
1:A:930:LEU:O	1:A:930:LEU:HD23	2.13	0.48
1:A:29:HIS:O	1:A:33:LYS:HG3	2.13	0.48
1:A:190:ASP:HA	1:A:242:VAL:HG23	1.96	0.48
1:A:926:THR:HG22	1:A:969:LYS:HG2	1.96	0.48
1:A:97:VAL:HG13	1:A:98:SER:N	2.29	0.48
1:A:630:SER:OG	1:A:633:PHE:HB2	2.13	0.48
1:A:920:TYR:HE2	1:A:1005:VAL:HG22	1.79	0.48
1:A:35:MET:HG3	1:A:374:THR:CG2	2.44	0.48
1:A:166:PHE:CZ	1:A:372:ALA:HB2	2.50	0.47
1:A:433:VAL:HG12	1:A:536:LEU:HD21	1.95	0.47
1:A:390:GLU:O	1:A:877:LYS:HE3	2.14	0.47
2:B:16:GLU:O	2:B:29:ARG:NH1	2.43	0.47
1:A:787:LEU:C	1:A:787:LEU:HD23	2.34	0.47
1:A:209:PHE:HA	1:A:227:ARG:O	2.14	0.47
1:A:712:LEU:HD13	1:A:833:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:PRO:CB	3:C:111:THR:HG22	2.45	0.46
1:A:950:SER:HA	3:C:28:ASP:O	2.15	0.46
3:C:133:ARG:HH21	3:C:133:ARG:HG2	1.80	0.46
3:C:11:ALA:O	3:C:15:LYS:HG3	2.15	0.46
1:A:381:LYS:HA	1:A:382:GLN:HA	1.71	0.46
1:A:537:ASP:HA	2:B:74:ARG:O	2.16	0.46
1:A:1001:GLU:HG3	1:A:1002:ASP:H	1.81	0.46
2:B:18:GLU:HB2	2:B:21:ASP:OD1	2.15	0.46
1:A:201:ARG:HA	1:A:234:PRO:O	2.16	0.46
1:A:952:LEU:HD23	1:A:977:ILE:HD12	1.97	0.46
1:A:993:ILE:HG23	1:A:1005:VAL:CG1	2.46	0.46
3:C:85:CYS:SG	3:C:119:LEU:HB2	2.56	0.46
3:C:87:ASP:HB3	3:C:92:GLN:CG	2.43	0.46
1:A:66:LEU:HD11	1:A:100:LEU:HD12	1.97	0.46
3:C:1:MET:HG2	3:C:4:LYS:HD2	1.96	0.45
3:C:42:ASP:OD1	3:C:111:THR:HB	2.15	0.45
1:A:608:TRP:CD2	1:A:830:ARG:HD2	2.51	0.45
1:A:565:LYS:HB3	2:B:73:LEU:HD11	1.98	0.45
1:A:663:PHE:O	1:A:666:CYS:HB2	2.16	0.45
1:A:1001:GLU:HG3	1:A:1002:ASP:N	2.31	0.45
2:B:-2:HIS:CG	2:B:20:SER:HB3	2.52	0.45
1:A:940:LEU:HB3	1:A:995:CYS:HB3	1.99	0.45
1:A:474:ARG:HG2	1:A:474:ARG:HH11	1.82	0.44
1:A:787:LEU:HD23	1:A:787:LEU:O	2.16	0.44
2:B:26:VAL:HG21	2:B:56:LEU:HD21	1.99	0.44
1:A:98:SER:O	1:A:102:GLU:HG3	2.18	0.44
1:A:544:TYR:OH	1:A:548:ARG:HD2	2.17	0.44
3:C:88:ILE:HG13	3:C:97:LEU:HD13	1.98	0.44
1:A:958:PRO:HA	1:A:959:PRO:HD3	1.91	0.44
1:A:183:GLY:O	1:A:253:VAL:HG13	2.18	0.44
1:A:635:GLU:OE1	1:A:635:GLU:HA	2.18	0.44
1:A:907:LYS:HA	1:A:911:LYS:O	2.17	0.44
3:C:64:PRO:HB3	3:C:93:TRP:CG	2.52	0.43
1:A:627:TYR:CE1	1:A:634:LEU:HD11	2.52	0.43
1:A:29:HIS:HD2	9:A:1498:HOH:O	2.00	0.43
1:A:158:LEU:O	1:A:387:ASP:HA	2.19	0.43
1:A:465:ASP:HB2	5:A:1103:ATP:O2'	2.18	0.43
1:A:250:TYR:CD1	1:A:251:ASN:ND2	2.87	0.43
1:A:267:SER:OG	1:A:270:GLU:HG2	2.18	0.43
1:A:871:VAL:HA	1:A:874:VAL:HG13	2.01	0.43
1:A:656:VAL:CG2	1:A:657:THR:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ILE:O	1:A:750:VAL:HG23	2.19	0.43
1:A:433:VAL:HG13	1:A:513:VAL:CG2	2.48	0.43
3:C:3:LEU:C	3:C:3:LEU:HD23	2.39	0.43
1:A:983:GLU:N	1:A:983:GLU:CD	2.72	0.43
3:C:147:ILE:HG22	3:C:147:ILE:O	2.19	0.43
1:A:550:VAL:HA	1:A:917:TRP:CZ3	2.54	0.43
3:C:133:ARG:NH2	3:C:133:ARG:HG2	2.34	0.43
1:A:131:THR:CG2	1:A:135:LYS:HB2	2.49	0.42
1:A:526:PHE:O	1:A:554:LYS:HE3	2.18	0.42
1:A:376:LYS:O	1:A:377:PHE:HB2	2.18	0.42
1:A:225:THR:O	1:A:227:ARG:HD2	2.19	0.42
1:A:957:GLN:HB3	1:A:961:LYS:HD2	2.00	0.42
1:A:624:VAL:O	1:A:628:LEU:HG	2.19	0.42
1:A:893:GLY:HA2	9:A:1490:HOH:O	2.19	0.42
1:A:22:ARG:HG3	1:A:474:ARG:NH1	2.35	0.42
1:A:404:LYS:NZ	1:A:406:ARG:NH1	2.67	0.42
2:B:1:MET:HB2	2:B:63:ARG:HA	2.02	0.42
1:A:209:PHE:HB3	1:A:226:PRO:HB2	2.02	0.42
1:A:588:LYS:HE3	1:A:590:PHE:CE1	2.55	0.42
3:C:36:THR:HG22	3:C:51:PHE:CD1	2.54	0.42
3:C:79:ASN:OD1	3:C:81:ASN:HB2	2.19	0.42
2:B:1:MET:CB	2:B:63:ARG:HG2	2.41	0.41
1:A:1005:VAL:HG23	1:A:1006:PRO:HD2	2.02	0.41
1:A:181:LEU:CD1	1:A:204:LEU:HD23	2.50	0.41
1:A:957:GLN:HB2	1:A:962:LEU:HD21	2.02	0.41
1:A:952:LEU:HA	1:A:977:ILE:CD1	2.50	0.41
3:C:60:TYR:CD1	3:C:61:PRO:HA	2.55	0.41
1:A:930:LEU:HD23	1:A:930:LEU:C	2.41	0.41
1:A:646:GLU:O	1:A:650:ASN:ND2	2.53	0.41
1:A:651:ILE:O	1:A:655:LEU:HB2	2.20	0.41
1:A:757:PRO:HD2	9:A:1486:HOH:O	2.20	0.41
1:A:898:SER:HA	2:B:47:GLY:O	2.20	0.41
1:A:652:ARG:HH11	1:A:790:ILE:HD12	1.86	0.41
1:A:897:PHE:O	2:B:47:GLY:HA2	2.21	0.41
2:B:0:HIS:ND1	2:B:18:GLU:OE2	2.54	0.41
3:C:51:PHE:C	3:C:52:LEU:HD12	2.40	0.41
1:A:920:TYR:HE2	1:A:1005:VAL:CG2	2.33	0.41
1:A:943:THR:HA	1:A:955:ASN:HB3	2.02	0.41
1:A:993:ILE:HG23	1:A:1005:VAL:HG11	2.03	0.41
3:C:75:HIS:HA	3:C:76:PRO:HD3	1.81	0.41
1:A:671:ARG:HD3	1:A:751:LEU:HD12	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ARG:O	2:B:64:GLU:HB2	2.21	0.41
1:A:322:PHE:CD2	1:A:326:LYS:HE3	2.56	0.40
1:A:627:TYR:HE1	1:A:634:LEU:HD11	1.86	0.40
1:A:838:PRO:HB3	9:A:1466:HOH:O	2.21	0.40
1:A:997:ASP:N	1:A:1001:GLU:O	2.49	0.40
1:A:401:GLU:OE2	1:A:404:LYS:HE2	2.20	0.40
1:A:828:ASN:O	1:A:832:MET:HG3	2.22	0.40
3:C:62:PHE:C	3:C:63:LYS:HD2	2.42	0.40
3:C:93:TRP:HA	3:C:97:LEU:HD12	2.03	0.40
1:A:192:GLY:HA3	1:A:240:GLY:O	2.21	0.40
3:C:4:LYS:O	3:C:8:ARG:HG3	2.21	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	973/1001 (97%)	918 (94%)	51 (5%)	4 (0%)	34 37
2	B	78/83 (94%)	77 (99%)	1 (1%)	0	100 100
3	C	147/163 (90%)	142 (97%)	3 (2%)	2 (1%)	11 8
All	All	1198/1247 (96%)	1137 (95%)	55 (5%)	6 (0%)	29 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
3	C	148	HIS
1	A	998	ALA
1	A	756	PRO
3	C	18	PRO
1	A	761	PRO

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	857/877 (98%)	843 (98%)	14 (2%)	62	76
2	B	70/74 (95%)	69 (99%)	1 (1%)	67	80
3	C	130/140 (93%)	126 (97%)	4 (3%)	40	51
All	All	1057/1091 (97%)	1038 (98%)	19 (2%)	59	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	80	GLN
1	A	128	VAL
1	A	198	GLU
1	A	299	SER
1	A	387	ASP
1	A	392	LEU
1	A	409	ARG
1	A	464	MET
1	A	523	ASP
1	A	527	GLU
1	A	874	VAL
1	A	919	ARG
1	A	999	ASN
2	B	74	ARG
3	C	10	LEU
3	C	30	LEU
3	C	61	PRO
3	C	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	251	ASN

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Mol	Chain	Res	Type
1	A	650	ASN
1	A	688	ASN
1	A	699	GLN
1	A	957	GLN
1	A	988	HIS
1	A	999	ASN
2	B	25	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
6	PG0	A	1104	-	6,6,7	0.84	0	5,5,6	1.06	0
7	EDO	A	1107	-	3,3,3	1.17	0	2,2,2	0.23	0
7	EDO	A	1105	-	3,3,3	1.22	0	2,2,2	0.21	0
7	EDO	A	1106	-	3,3,3	1.16	0	2,2,2	0.21	0
7	EDO	A	1108	-	3,3,3	1.15	0	2,2,2	0.23	0
8	SO4	A	1112	-	4,4,4	0.27	0	6,6,6	0.04	0
7	EDO	A	1110	-	3,3,3	1.14	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SO4	A	1111	-	4,4,4	0.28	0	6,6,6	0.05	0
5	ATP	A	1103	4	26,33,33	1.17	2 (7%)	31,52,52	1.46	5 (16%)
7	EDO	B	101	-	3,3,3	1.16	0	2,2,2	0.22	0
8	SO4	A	1113	-	4,4,4	0.26	0	6,6,6	0.05	0
8	SO4	B	102	-	4,4,4	0.26	0	6,6,6	0.05	0
7	EDO	A	1109	-	3,3,3	1.11	0	2,2,2	0.27	0

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
6	PG0	A	1104	-	-	1/4/4/5	-
7	EDO	A	1107	-	-	0/1/1/1	-
7	EDO	A	1105	-	-	1/1/1/1	-
7	EDO	A	1106	-	-	0/1/1/1	-
7	EDO	A	1108	-	-	1/1/1/1	-
7	EDO	A	1110	-	-	0/1/1/1	-
5	ATP	A	1103	4	-	5/18/38/38	0/3/3/3
7	EDO	B	101	-	-	0/1/1/1	-
7	EDO	A	1109	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1103	ATP	C2-N3	3.01	1.36	1.32
5	A	1103	ATP	C5-C4	2.25	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1103	ATP	N3-C2-N1	-4.55	121.57	128.68
5	A	1103	ATP	C1'-N9-C4	-2.49	122.27	126.64
5	A	1103	ATP	C2-N1-C6	2.26	122.61	118.75
5	A	1103	ATP	O2B-PB-O1B	2.06	122.44	112.24
5	A	1103	ATP	C4-C5-N7	-2.02	107.29	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1103	ATP	O4'-C4'-C5'-O5'
5	A	1103	ATP	C3'-C4'-C5'-O5'
7	A	1105	EDO	O1-C1-C2-O2
7	A	1108	EDO	O1-C1-C2-O2
5	A	1103	ATP	PB-O3A-PA-O2A
6	A	1104	PG0	C1-C2-O1-C3
5	A	1103	ATP	PG-O3B-PB-O1B
5	A	1103	ATP	PB-O3A-PA-O1A

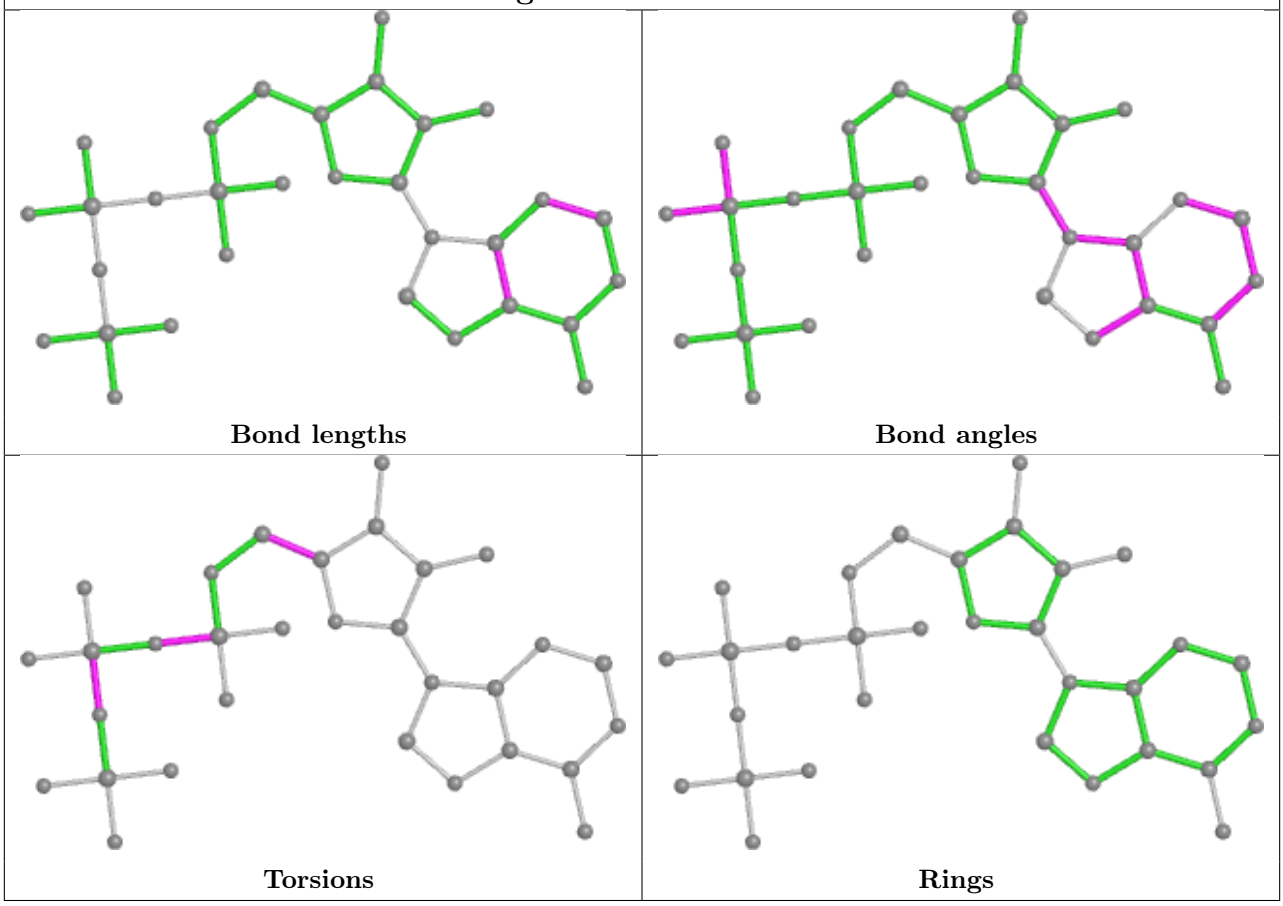
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1104	PG0	1	0
5	A	1103	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 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 A 1103



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	977/1001 (97%)	0.27	93 (9%)	8	7	28, 46, 100, 120	0
2	B	80/83 (96%)	-0.18	2 (2%)	57	55	32, 52, 67, 91	0
3	C	149/163 (91%)	-0.05	5 (3%)	45	43	43, 55, 78, 90	2 (1%)
All	All	1206/1247 (96%)	0.20	100 (8%)	11	10	28, 49, 97, 120	2 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	6.4
1	A	800	LEU	6.3
1	A	801	VAL	6.3
1	A	803	PHE	5.5
1	A	243	LYS	5.4
1	A	334	PHE	5.1
1	A	192	GLY	5.0
1	A	242	VAL	4.8
1	A	335	ASP	4.8
1	A	756	PRO	4.7
1	A	790	ILE	4.5
1	A	787	LEU	4.4
1	A	798	SER	4.3
1	A	190	ASP	4.2
1	A	247	SER	4.2
1	A	199	GLU	4.2
3	C	18	PRO	4.2
1	A	802	GLY	4.1
1	A	229	VAL	4.1
3	C	149	GLY	4.1
1	A	220	GLY	4.0
1	A	633	PHE	4.0
3	C	17	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLU	3.9
1	A	209	PHE	3.9
1	A	908	VAL	3.7
1	A	792	ASP	3.7
1	A	631	PRO	3.5
1	A	250	TYR	3.4
1	A	365	VAL	3.4
1	A	189	THR	3.4
2	B	-2	HIS	3.3
1	A	758	PRO	3.3
1	A	794	LEU	3.2
1	A	364	ALA	3.2
1	A	216	LYS	3.2
1	A	359	ALA	3.2
1	A	239	ILE	3.1
1	A	789	SER	3.1
1	A	228	LYS	3.1
1	A	241	SER	3.0
1	A	361	LEU	3.0
1	A	958	PRO	2.9
1	A	227	ARG	2.9
1	A	162	ILE	2.9
1	A	259	VAL	2.9
1	A	804	ARG	2.9
1	A	791	ALA	2.8
1	A	357	MET	2.8
3	C	1	MET	2.8
1	A	788	LYS	2.8
1	A	635	GLU	2.8
1	A	861	VAL	2.7
1	A	52	ILE	2.7
1	A	230	GLU	2.7
1	A	153	ALA	2.7
1	A	629	SER	2.6
1	A	356	ALA	2.6
1	A	634	LEU	2.5
1	A	639	LYS	2.5
1	A	655	LEU	2.5
1	A	936	LYS	2.5
1	A	13	ASN	2.5
1	A	360	PHE	2.4
1	A	964	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	251	ASN	2.4
1	A	240	GLY	2.4
1	A	911	LYS	2.4
1	A	762	LYS	2.4
1	A	225	THR	2.4
1	A	638	LEU	2.4
1	A	640	THR	2.4
1	A	856	CYS	2.4
1	A	48	LEU	2.3
1	A	630	SER	2.3
1	A	363	GLY	2.3
1	A	152	ALA	2.3
1	A	221	LEU	2.3
1	A	358	SER	2.3
1	A	438	ILE	2.2
1	A	362	GLY	2.2
1	A	210	VAL	2.2
1	A	641	SER	2.2
1	A	336	VAL	2.1
1	A	624	VAL	2.1
1	A	757	PRO	2.1
1	A	355	VAL	2.1
1	A	248	ALA	2.1
1	A	627	TYR	2.1
1	A	763	SER	2.1
1	A	648	LEU	2.1
2	B	-3	HIS	2.1
1	A	625	ASN	2.1
1	A	857	THR	2.1
1	A	366	ALA	2.1
1	A	257	VAL	2.1
1	A	864	GLY	2.0
1	A	862	VAL	2.0
1	A	755	ASN	2.0
3	C	15	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 monosaccharides in this entry.

6.4 Ligands (i)

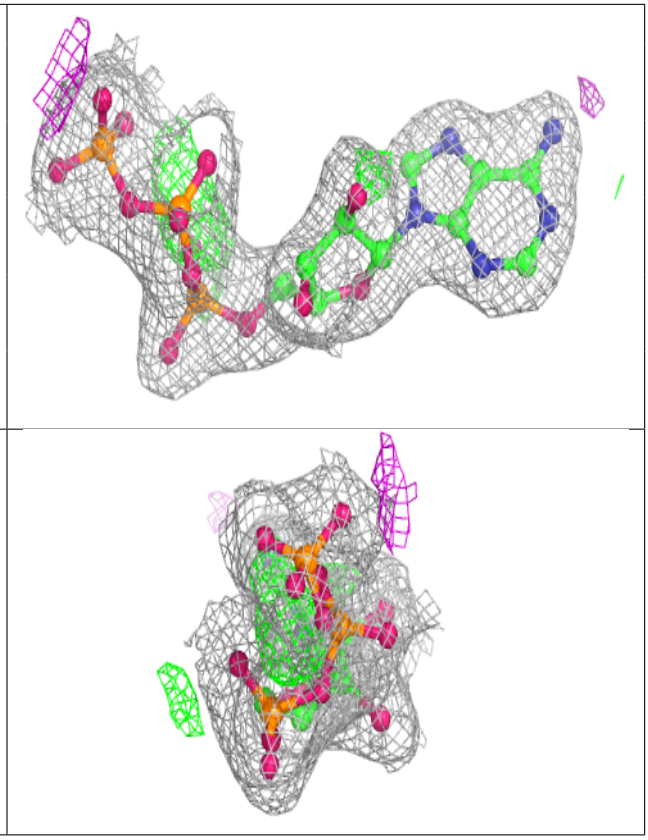
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SO4	A	1113	5/5	0.80	0.14	148,148,148,148	0
8	SO4	A	1112	5/5	0.82	0.23	127,127,127,128	0
4	MG	A	1101	1/1	0.82	0.16	52,52,52,52	0
8	SO4	B	102	5/5	0.84	0.14	135,135,135,135	0
7	EDO	A	1107	4/4	0.87	0.22	79,80,81,81	0
7	EDO	A	1109	4/4	0.88	0.26	53,54,55,56	0
7	EDO	A	1106	4/4	0.89	0.19	52,57,58,62	0
7	EDO	A	1108	4/4	0.89	0.15	74,74,74,74	0
7	EDO	A	1110	4/4	0.90	0.19	79,79,80,80	0
7	EDO	A	1105	4/4	0.91	0.12	75,75,75,78	0
6	PG0	A	1104	7/8	0.92	0.16	47,53,55,56	0
7	EDO	B	101	4/4	0.92	0.16	57,59,61,63	0
8	SO4	A	1111	5/5	0.92	0.18	122,122,122,122	0
4	MG	A	1102	1/1	0.96	0.09	47,47,47,47	0
5	ATP	A	1103	31/31	0.98	0.11	34,38,41,45	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 1103:

$2mF_o$-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.