



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:29 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

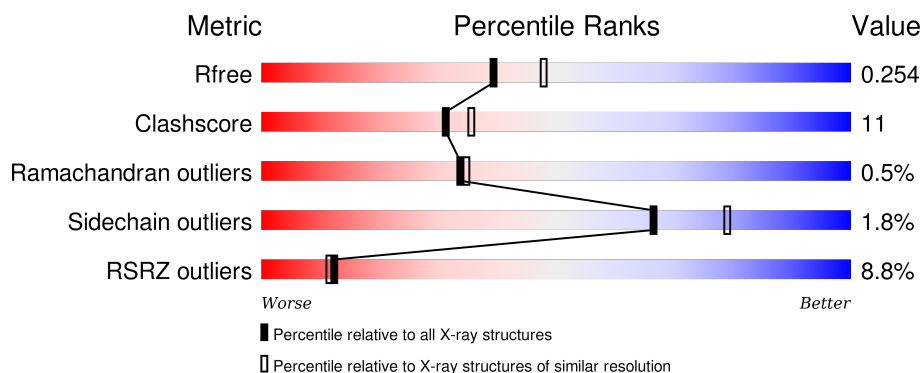
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1001	
2	B	83	
3	C	163	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	A	1107	-	-	-	X
7	EDO	A	1110	-	-	-	X

## 2 Entry composition

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
3	C	149	Total	C	N	O	S	2	0	0
			1170	750	199	218	3			

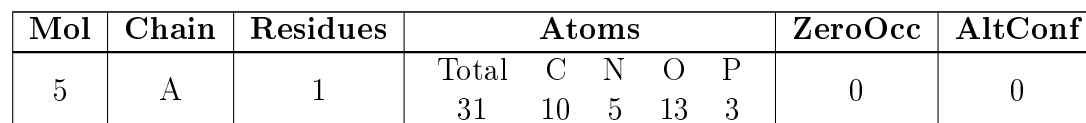
There are 18 discrepancies between the modelled and reference sequences:

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
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



- PGO
- 
- Chemical structure of PGO (pentagynol) is shown, consisting of a five-carbon chain with a carboxylic acid group at C1 and a hydroxyl group at C5. The atoms are labeled C1, C2, C3, C4, C5 for carbons, O1, O2 for oxygens, and H for hydrogen. The structure is shown in a zig-zag conformation.

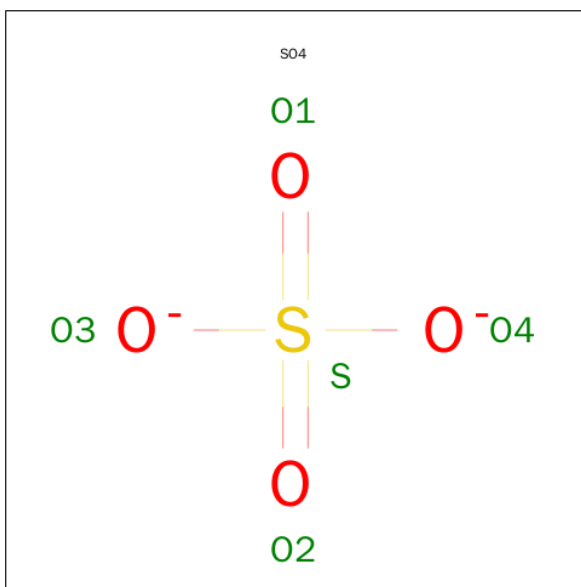
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is water.

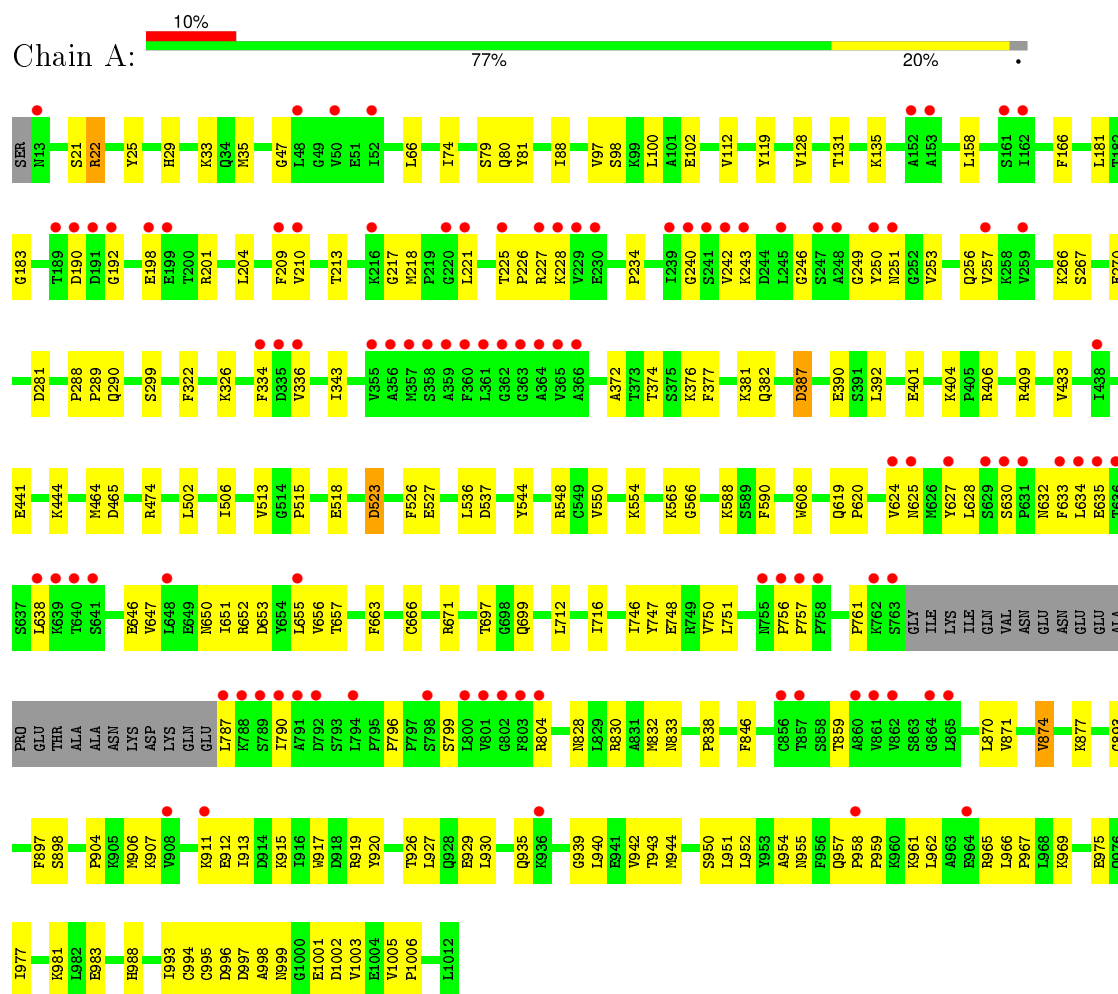
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	471	Total	O	0	0
			471	471		
9	B	41	Total	O	0	0
			41	41		
9	C	56	Total	O	0	0
			56	56		



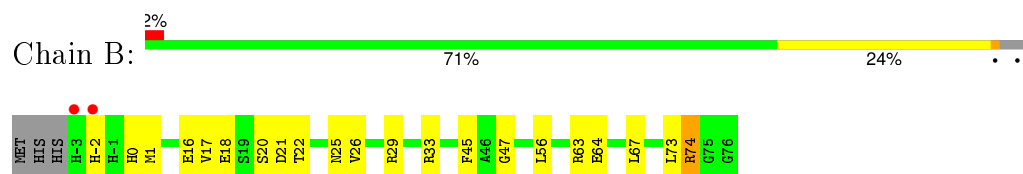
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

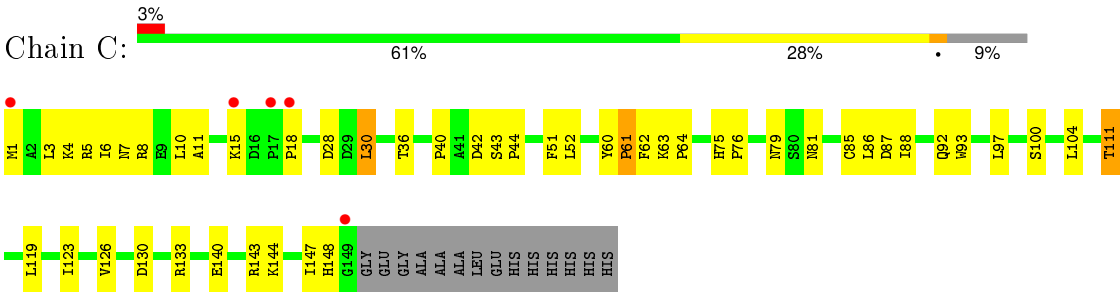
- Molecule 1: Ubiquitin-activating enzyme E1 1



- Molecule 2: Ubiquitin-60S ribosomal protein L40



- Molecule 3: Ubiquitin-conjugating enzyme E2 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.53 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.254 0.213 , 0.254	Depositor DCC
$R_{free}$ test set	4253 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 84338 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

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
3:C:40:PRO:HG2	3:C:111:THR:HG22	1.81	0.63
1:A:281:ASP:OD2	6:A:1104:PG0:H11	1.98	0.63
1:A:871:VAL:HA	1:A:874:VAL:CG1	2.28	0.63
1:A:218:MET:HB2	1:A:221:LEU:HD13	1.81	0.63
1:A:209:PHE:CE1	1:A:228:LYS:HG2	2.33	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:O	1:A:638:LEU:HD23	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
2:B:22:THR:H	2:B:25:ASN:ND2	1.99	0.60
1:A:334:PHE:CZ	1:A:336:VAL:HB	2.37	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:796:PRO:HG2	1:A:799:SER:HB3	1.87	0.57
1:A:288:PRO:HB2	1:A:289:PRO:HD3	1.87	0.57
3:C:126:VAL:HG11	3:C:133:ARG:NH2	2.19	0.56
1:A:975:GLU:OE1	1:A:981:LYS:HG3	2.05	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:N	1:A:913:ILE:HD12	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
2:B:17:VAL:HG12	2:B:29:ARG:NH1	2.21	0.55
1:A:647:VAL:O	1:A:651:ILE:HG12	2.07	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:942:VAL:HG22	1:A:993:ILE:HD11	1.91	0.52
1:A:47:GLY:HA3	1:A:79:SER:OG	2.08	0.52
3:C:140:GLU:HG3	3:C:144:LYS:HE3	1.92	0.52
1:A:944:MET:HG3	3:C:7:ASN:CG	2.30	0.52
1:A:181:LEU:HD12	1:A:204:LEU:HD23	1.92	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
3:C:76:PRO:HG3	3:C:123:ILE:HG22	1.93	0.51
1:A:35:MET:HG3	1:A:374:THR:HG22	1.93	0.51
1:A:566:GLY:HA2	2:B:73:LEU:HD12	1.93	0.50
1:A:190:ASP:OD2	1:A:243:LYS:HG2	2.11	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
1:A:870:LEU:C	1:A:870:LEU:HD23	2.31	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:HD23	1:A:930:LEU:O	2.13	0.48
1:A:190:ASP:HA	1:A:242:VAL:HG23	1.96	0.48
1:A:29:HIS:O	1:A:33:LYS:HG3	2.13	0.48
1:A:926:THR:HG22	1:A:969:LYS:HG2	1.96	0.48
1:A:920:TYR:HE2	1:A:1005:VAL:HG22	1.79	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:35:MET:HG3	1:A:374:THR:CG2	2.44	0.48
1:A:433:VAL:HG12	1:A:536:LEU:HD21	1.95	0.47
1:A:166:PHE:CZ	1:A:372:ALA:HB2	2.50	0.47
2:B:16:GLU:O	2:B:29:ARG:NH1	2.43	0.47
1:A:390:GLU:O	1:A:877:LYS:HE3	2.14	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
3:C:133:ARG:HG2	3:C:133:ARG:HH21	1.80	0.46
1:A:950:SER:HA	3:C:28:ASP:O	2.15	0.46
3:C:11:ALA:O	3:C:15:LYS:HG3	2.15	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:381:LYS:HA	1:A:382:GLN:HA	1.71	0.46
1:A:201:ARG:HA	1:A:234:PRO:O	2.16	0.46
1:A:993:ILE:HG23	1:A:1005:VAL:CG1	2.46	0.46
1:A:952:LEU:HD23	1:A:977:ILE:HD12	1.97	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:42:ASP:OD1	3:C:111:THR:HB	2.15	0.45
3:C:1:MET:HG2	3:C:4:LYS:HD2	1.96	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:HH11	1:A:474:ARG:HG2	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
3:C:88:ILE:HG13	3:C:97:LEU:HD13	1.98	0.44
1:A:544:TYR:OH	1:A:548:ARG:HD2	2.17	0.44
1:A:98:SER:O	1:A:102:GLU:HG3	2.18	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:HA	1:A:635:GLU:OE1	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:465:ASP:HB2	5:A:1103:ATP:O2'	2.18	0.43
1:A:158:LEU:O	1:A:387:ASP:HA	2.19	0.43
1:A:871:VAL:HA	1:A:874:VAL:HG13	2.01	0.43
1:A:267:SER:OG	1:A:270:GLU:HG2	2.18	0.43
1:A:250:TYR:CD1	1:A:251:ASN:ND2	2.87	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:O	3:C:147:ILE:HG22	2.19	0.43
3:C:133:ARG:NH2	3:C:133:ARG:HG2	2.34	0.43
1:A:550:VAL:HA	1:A:917:TRP:CZ3	2.54	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
2:B:1:MET:HB2	2:B:63:ARG:HA	2.02	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
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:957:GLN:HB2	1:A:962:LEU:HD21	2.02	0.41
1:A:181:LEU:CD1	1:A:204:LEU:HD23	2.50	0.41
3:C:60:TYR:CD1	3:C:61:PRO:HA	2.55	0.41
1:A:952:LEU:HA	1:A:977:ILE:CD1	2.50	0.41
1:A:930:LEU:HD23	1:A:930:LEU:C	2.41	0.41
1:A:651:ILE:O	1:A:655:LEU:HB2	2.20	0.41
1:A:646:GLU:O	1:A:650:ASN:ND2	2.53	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
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:897:PHE:O	2:B:47:GLY:HA2	2.21	0.41
1:A:652:ARG:HH11	1:A:790:ILE:HD12	1.86	0.41
1:A:943:THR:HA	1:A:955:ASN:HB3	2.02	0.41
1:A:920:TYR:HE2	1:A:1005:VAL:CG2	2.33	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
2:B:63:ARG:O	2:B:64:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ARG:HD3	1:A:751:LEU:HD12	2.04	0.41
1:A:627:TYR:HE1	1:A:634:LEU:HD11	1.86	0.40
1:A:322:PHE:CD2	1:A:326:LYS:HE3	2.56	0.40
1:A:997:ASP:N	1:A:1001:GLU:O	2.49	0.40
1:A:838:PRO:HB3	9:A:1466:HOH:O	2.21	0.40
3:C:93:TRP:HA	3:C:97:LEU:HD12	2.03	0.40
1:A:401:GLU:OE2	1:A:404:LYS:HE2	2.20	0.40
3:C:62:PHE:C	3:C:63:LYS:HD2	2.42	0.40
1:A:828:ASN:O	1:A:832:MET:HG3	2.22	0.40
3:C:4:LYS:O	3:C:8:ARG:HG3	2.21	0.40
1:A:192:GLY:HA3	1:A:240:GLY:O	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%)	39	42
2	B	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
3	C	147/163 (90%)	142 (97%)	3 (2%)	2 (1%)	14	10
All	All	1198/1247 (96%)	1137 (95%)	55 (5%)	6 (0%)	34	35

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 ⓘ

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%)	70	82
2	B	70/74 (95%)	69 (99%)	1 (1%)	74	85
3	C	130/140 (93%)	126 (97%)	4 (3%)	47	59
All	All	1057/1091 (97%)	1038 (98%)	19 (2%)	66	79

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

Some 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 ⓘ

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 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	$\# Z  > 2$
5	ATP	A	1103	4	24,33,33	1.12	2 (8%)	31,52,52	2.18	5 (16%)
6	PG0	A	1104	-	6,6,7	0.82	0	5,5,6	0.99	0
7	EDO	A	1105	-	3,3,3	1.15	0	2,2,2	0.17	0
7	EDO	A	1106	-	3,3,3	1.10	0	2,2,2	0.17	0
7	EDO	A	1107	-	3,3,3	1.11	0	2,2,2	0.18	0
7	EDO	A	1108	-	3,3,3	1.09	0	2,2,2	0.17	0
7	EDO	A	1109	-	3,3,3	1.05	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	1110	-	3,3,3	1.08	0	2,2,2	0.19	0
8	SO4	A	1111	-	4,4,4	0.22	0	6,6,6	0.09	0
8	SO4	A	1112	-	4,4,4	0.21	0	6,6,6	0.08	0
8	SO4	A	1113	-	4,4,4	0.21	0	6,6,6	0.08	0
7	EDO	B	101	-	3,3,3	1.10	0	2,2,2	0.15	0
8	SO4	B	102	-	4,4,4	0.22	0	6,6,6	0.08	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
5	ATP	A	1103	4	-	0/18/38/38	0/3/3/3
6	PG0	A	1104	-	-	0/4/4/5	0/0/0/0
7	EDO	A	1105	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1106	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1107	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1108	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1109	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1110	-	-	0/1/1/1	0/0/0/0
8	SO4	A	1111	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1112	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1113	-	-	0/0/0/0	0/0/0/0
7	EDO	B	101	-	-	0/1/1/1	0/0/0/0
8	SO4	B	102	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1103	ATP	C2-N3	2.68	1.36	1.32
5	A	1103	ATP	C5-C4	2.83	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	ATP	N3-C2-N1	-9.57	121.57	128.89
5	A	1103	ATP	C1'-N9-C4	-3.09	122.27	126.94
5	A	1103	ATP	C4-C5-N7	-2.38	107.29	109.48
5	A	1103	ATP	O2A-PA-O3A	2.06	114.45	105.09
5	A	1103	ATP	C2-N1-C6	2.15	122.61	118.77

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
5	A	1103	ATP	2	0
6	A	1104	PG0	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	977/1001 (97%)	0.33	99 (10%) 9 8	28, 46, 100, 120	0
2	B	80/83 (96%)	-0.13	2 (2%) 61 60	32, 52, 67, 91	0
3	C	149/163 (91%)	-0.00	5 (3%) 49 47	43, 55, 78, 90	2 (1%)
All	All	1206/1247 (96%)	0.26	106 (8%) 12 11	28, 49, 97, 120	2 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	6.6
1	A	801	VAL	6.6
1	A	800	LEU	6.6
1	A	803	PHE	5.6
1	A	243	LYS	5.5
1	A	192	GLY	5.3
1	A	334	PHE	5.2
1	A	242	VAL	5.1
1	A	335	ASP	4.9
1	A	756	PRO	4.8
1	A	787	LEU	4.7
1	A	790	ILE	4.6
1	A	190	ASP	4.5
1	A	247	SER	4.4
1	A	229	VAL	4.4
1	A	802	GLY	4.3
1	A	798	SER	4.3
3	C	18	PRO	4.2
1	A	199	GLU	4.2
1	A	220	GLY	4.2
1	A	633	PHE	4.2
3	C	149	GLY	4.2
3	C	17	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLU	4.1
1	A	209	PHE	4.0
1	A	908	VAL	3.9
1	A	792	ASP	3.8
1	A	631	PRO	3.8
1	A	250	TYR	3.5
1	A	189	THR	3.5
1	A	365	VAL	3.5
1	A	794	LEU	3.5
2	B	-2	HIS	3.5
1	A	758	PRO	3.4
1	A	359	ALA	3.4
1	A	364	ALA	3.3
1	A	239	ILE	3.3
1	A	789	SER	3.3
1	A	216	LYS	3.2
1	A	228	LYS	3.2
1	A	241	SER	3.1
1	A	361	LEU	3.1
1	A	259	VAL	3.1
1	A	162	ILE	3.0
1	A	958	PRO	3.0
1	A	227	ARG	3.0
1	A	791	ALA	3.0
3	C	1	MET	3.0
1	A	357	MET	2.9
1	A	861	VAL	2.9
1	A	804	ARG	2.9
1	A	153	ALA	2.9
1	A	52	ILE	2.9
1	A	635	GLU	2.8
1	A	788	LYS	2.8
1	A	230	GLU	2.8
1	A	356	ALA	2.7
1	A	629	SER	2.7
1	A	639	LYS	2.7
1	A	634	LEU	2.6
1	A	240	GLY	2.6
1	A	360	PHE	2.6
1	A	251	ASN	2.6
1	A	640	THR	2.6
1	A	762	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	964	GLU	2.5
1	A	655	LEU	2.5
1	A	856	CYS	2.5
1	A	13	ASN	2.5
1	A	638	LEU	2.5
1	A	936	LYS	2.5
1	A	911	LYS	2.5
1	A	48	LEU	2.4
1	A	210	VAL	2.4
1	A	363	GLY	2.4
1	A	152	ALA	2.4
1	A	225	THR	2.4
1	A	630	SER	2.4
1	A	438	ILE	2.4
1	A	221	LEU	2.4
1	A	358	SER	2.4
1	A	362	GLY	2.3
1	A	641	SER	2.3
1	A	624	VAL	2.3
1	A	757	PRO	2.3
1	A	336	VAL	2.3
1	A	355	VAL	2.2
2	B	-3	HIS	2.2
1	A	625	ASN	2.2
1	A	648	LEU	2.2
1	A	366	ALA	2.2
1	A	257	VAL	2.2
1	A	627	TYR	2.2
1	A	862	VAL	2.1
1	A	864	GLY	2.1
1	A	857	THR	2.1
1	A	248	ALA	2.1
1	A	763	SER	2.1
1	A	50	VAL	2.1
1	A	755	ASN	2.1
1	A	161	SER	2.1
1	A	245	LEU	2.1
1	A	865	LEU	2.1
3	C	15	LYS	2.1
1	A	636	THR	2.0
1	A	860	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	A	1110	4/4	0.90	0.18	3.65	79,79,80,80	0
7	EDO	A	1107	4/4	0.86	0.23	3.18	79,80,81,81	0
7	EDO	A	1109	4/4	0.88	0.26	1.40	53,54,55,56	0
7	EDO	B	101	4/4	0.93	0.16	1.40	57,59,61,63	0
7	EDO	A	1105	4/4	0.91	0.12	0.34	75,75,75,78	0
6	PG0	A	1104	7/8	0.92	0.16	-0.12	47,53,55,56	0
5	ATP	A	1103	31/31	0.98	0.11	-0.62	34,38,41,45	0
8	SO4	B	102	5/5	0.84	0.14	-	135,135,135,135	0
7	EDO	A	1106	4/4	0.89	0.18	-	52,57,58,62	0
4	MG	A	1102	1/1	0.96	0.08	-	47,47,47,47	0
8	SO4	A	1111	5/5	0.92	0.18	-	122,122,122,122	0
8	SO4	A	1113	5/5	0.80	0.14	-	148,148,148,148	0
4	MG	A	1101	1/1	0.81	0.16	-	52,52,52,52	0
8	SO4	A	1112	5/5	0.81	0.23	-	127,127,127,128	0
7	EDO	A	1108	4/4	0.88	0.15	-	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.