



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:49 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

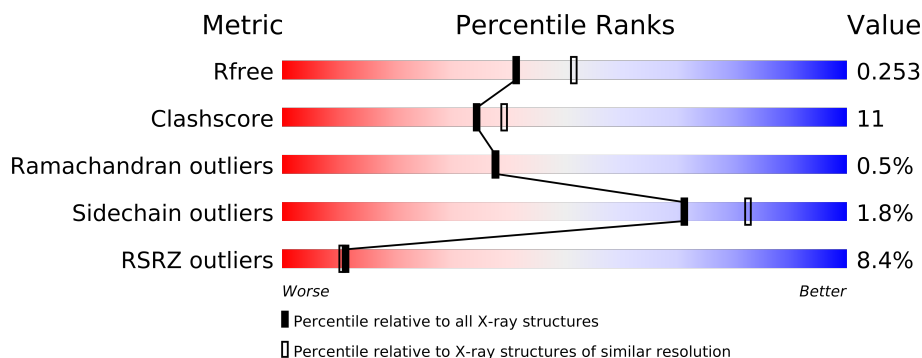
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1001	
2	B	83	
3	C	163	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	EDO	A	1106	-	X
7	EDO	A	1107	-	X
7	EDO	A	1108	-	X
7	EDO	A	1110	-	X
8	SO4	A	1112	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10147 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	977	Total	C	N	O	S	0	0	0
			7673	4907	1254	1473	39			

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
2	B	80	Total	C	N	O	S	0	0	0
			648	396	129	122	1			

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			

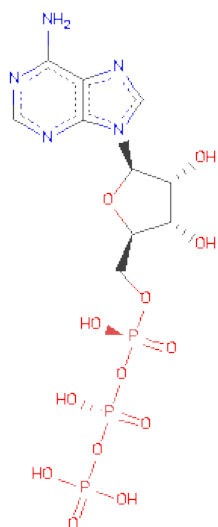
There are 18 discrepancies between the modelled and reference sequences:

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).

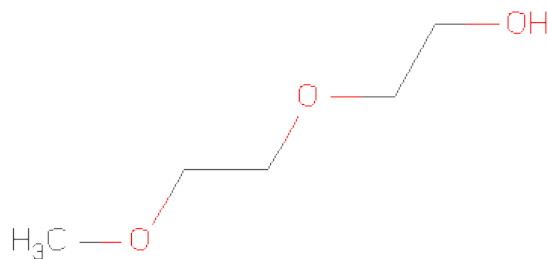
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



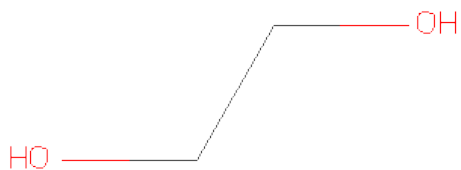
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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



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: $C_2H_6O_2$).



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: O₄S).



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		

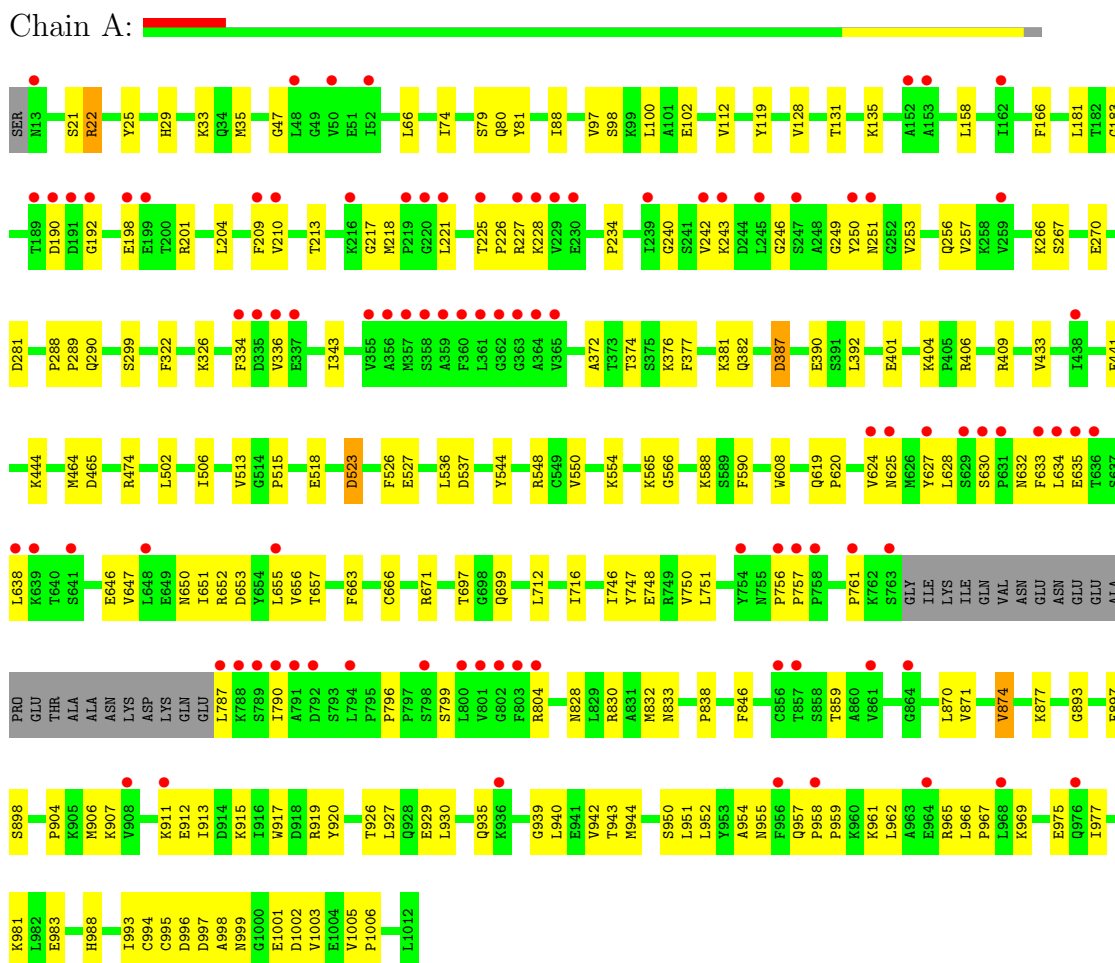
- Molecule 9 is water.

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		

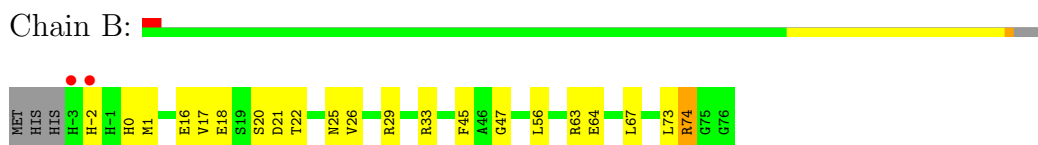
3 Residue-property plots

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

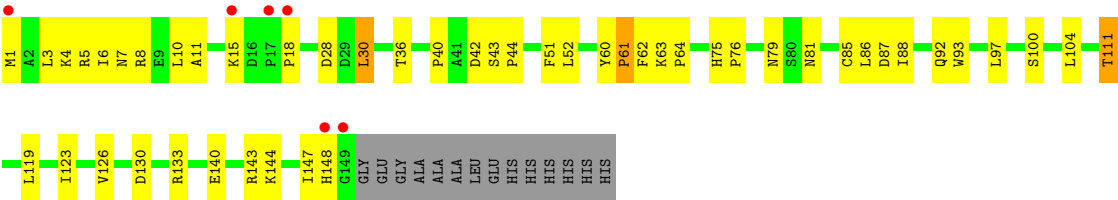


• Molecule 2: Ubiquitin-60S ribosomal protein L40



• 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, 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
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.254 0.214 , 0.253	Depositor DCC
R_{free} test set	4253 reflections (5.05%)	DCC
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 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	5	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (205) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
3:C:140:GLU:CD	3:C:143:ARG:HH21	2.04	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	973/1001 (97%)	918 (94%)	51 (5%)	4 (0%)	43	45
2	B	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
3	C	147/163 (90%)	142 (97%)	3 (2%)	2 (1%)	16	12
All	All	1198/1247 (96%)	1137 (95%)	55 (5%)	6 (0%)	38	38

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%)	75	85
2	B	70/74 (95%)	69 (99%)	1 (1%)	78	88
3	C	130/140 (93%)	126 (97%)	4 (3%)	52	63
All	All	1057/1091 (97%)	1038 (98%)	19 (2%)	71	82

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
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 chains 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	33,33,33	1.24	4 (12%)	52,52,52	1.93	9 (17%)
6	PG0	A	1104	-	6,6,7	0.75	0	5,5,6	1.00	0
7	EDO	A	1105	-	3,3,3	1.16	0	2,2,2	0.19	0
7	EDO	A	1106	-	3,3,3	1.10	0	2,2,2	0.20	0
7	EDO	A	1107	-	3,3,3	1.11	0	2,2,2	0.22	0
7	EDO	A	1108	-	3,3,3	1.09	0	2,2,2	0.21	0
7	EDO	A	1109	-	3,3,3	1.06	0	2,2,2	0.26	0
7	EDO	A	1110	-	3,3,3	1.08	0	2,2,2	0.23	0
8	SO4	A	1111	-	4,4,4	0.26	0	6,6,6	0.08	0
8	SO4	A	1112	-	4,4,4	0.25	0	6,6,6	0.07	0
8	SO4	A	1113	-	4,4,4	0.26	0	6,6,6	0.07	0
7	EDO	B	101	-	3,3,3	1.10	0	2,2,2	0.20	0
8	SO4	B	102	-	4,4,4	0.26	0	6,6,6	0.07	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	-	0/22/38/38	0/1/3/3
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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1103	ATP	C5-C4	2.83	1.46	1.40
5	A	1103	ATP	C4-N9	-2.74	1.33	1.37
5	A	1103	ATP	C2-N3	2.41	1.36	1.32
5	A	1103	ATP	PG-O3B	2.36	1.64	1.60

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	ATP	N3-C2-N1	-8.54	121.57	128.71
5	A	1103	ATP	N3-C4-N9	5.18	134.78	125.43
5	A	1103	ATP	C8-N9-C4	3.34	109.45	106.90
5	A	1103	ATP	C5-C4-N3	-2.70	119.83	125.70
5	A	1103	ATP	C4-C5-N7	-2.60	107.29	109.52
5	A	1103	ATP	C2-N3-C4	2.59	121.37	114.01
5	A	1103	ATP	C1'-N9-C4	-2.52	122.27	126.64
5	A	1103	ATP	O4'-C1'-N9	2.36	110.63	108.44
5	A	1103	ATP	C2-N1-C6	2.13	122.61	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	977/1001 (97%)	0.35	94 (9%) 8 8	28, 46, 100, 120	0
2	B	80/83 (96%)	-0.12	2 (2%) 54 55	32, 52, 67, 91	0
3	C	149/163 (91%)	0.12	6 (4%) 36 37	43, 55, 78, 90	2 (1%)
All	All	1206/1247 (96%)	0.29	102 (8%) 11 10	28, 49, 97, 120	2 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	801	VAL	7.4
1	A	803	PHE	6.7
1	A	756	PRO	6.4
1	A	800	LEU	6.3
3	C	149	GLY	5.7
3	C	18	PRO	5.7
1	A	191	ASP	5.6
1	A	787	LEU	5.4
1	A	229	VAL	5.4
1	A	335	ASP	5.1
1	A	220	GLY	5.1
1	A	209	PHE	4.9
1	A	798	SER	4.9
1	A	243	LYS	4.9
1	A	334	PHE	4.6
3	C	17	PRO	4.6
1	A	199	GLU	4.5
1	A	802	GLY	4.5
1	A	633	PHE	4.3
1	A	790	ILE	4.2
1	A	758	PRO	4.1
1	A	247	SER	4.1
1	A	198	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	655	LEU	3.9
1	A	192	GLY	3.8
1	A	804	ARG	3.7
1	A	788	LYS	3.7
1	A	216	LYS	3.6
1	A	228	LYS	3.6
1	A	190	ASP	3.5
1	A	242	VAL	3.5
1	A	789	SER	3.5
2	B	-2	HIS	3.4
1	A	794	LEU	3.4
1	A	792	ASP	3.4
1	A	365	VAL	3.4
1	A	227	ARG	3.4
1	A	631	PRO	3.4
1	A	757	PRO	3.3
1	A	189	THR	3.3
1	A	259	VAL	3.3
1	A	936	LYS	3.3
1	A	359	ALA	3.2
1	A	791	ALA	3.2
1	A	13	ASN	3.2
3	C	148	HIS	3.1
1	A	908	VAL	3.1
1	A	364	ALA	3.1
1	A	763	SER	3.0
1	A	250	TYR	3.0
1	A	210	VAL	3.0
1	A	634	LEU	3.0
1	A	239	ILE	2.9
1	A	230	GLU	2.9
1	A	624	VAL	2.9
1	A	635	GLU	2.8
1	A	648	LEU	2.8
1	A	162	ILE	2.8
1	A	856	CYS	2.7
1	A	361	LEU	2.7
1	A	357	MET	2.7
1	A	958	PRO	2.7
1	A	48	LEU	2.6
1	A	639	LYS	2.6
1	A	52	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	153	ALA	2.6
1	A	629	SER	2.6
3	C	1	MET	2.6
1	A	225	THR	2.6
1	A	638	LEU	2.6
1	A	356	ALA	2.6
1	A	221	LEU	2.6
1	A	911	LYS	2.5
1	A	861	VAL	2.5
1	A	761	PRO	2.5
1	A	857	THR	2.5
1	A	219	PRO	2.5
1	A	636	THR	2.4
2	B	-3	HIS	2.4
1	A	363	GLY	2.4
1	A	337	GLU	2.3
1	A	956	PHE	2.3
1	A	754	TYR	2.3
3	C	15	LYS	2.3
1	A	438	ILE	2.3
1	A	362	GLY	2.2
1	A	964	GLU	2.2
1	A	630	SER	2.2
1	A	251	ASN	2.2
1	A	245	LEU	2.2
1	A	968	LEU	2.2
1	A	864	GLY	2.2
1	A	625	ASN	2.2
1	A	360	PHE	2.1
1	A	336	VAL	2.1
1	A	355	VAL	2.1
1	A	152	ALA	2.1
1	A	627	TYR	2.1
1	A	358	SER	2.1
1	A	641	SER	2.0
1	A	50	VAL	2.0
1	A	976	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	EDO	A	1110	4/4	0.22	5.96	79,79,80,80	0
7	EDO	A	1106	4/4	0.26	4.53	52,57,58,62	0
8	SO4	A	1112	5/5	0.19	3.09	127,127,127,128	0
7	EDO	A	1107	4/4	0.21	2.65	79,80,81,81	0
7	EDO	A	1108	4/4	0.20	2.41	74,74,74,74	0
7	EDO	A	1109	4/4	0.25	1.15	53,54,55,56	0
7	EDO	B	101	4/4	0.15	1.08	57,59,61,63	0
7	EDO	A	1105	4/4	0.14	0.77	75,75,75,78	0
8	SO4	B	102	5/5	0.14	0.51	135,135,135,135	0
8	SO4	A	1111	5/5	0.14	0.50	122,122,122,122	0
6	PG0	A	1104	7/8	0.17	0.25	47,53,55,56	0
4	MG	A	1102	1/1	0.09	-0.40	47,47,47,47	0
5	ATP	A	1103	31/31	0.11	-0.60	34,38,41,45	0
8	SO4	A	1113	5/5	0.14	-0.82	148,148,148,148	0
4	MG	A	1101	1/1	0.17	-	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.