



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:38 AM UTC

PDB ID : 4II2 / pdb_00004ii2
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

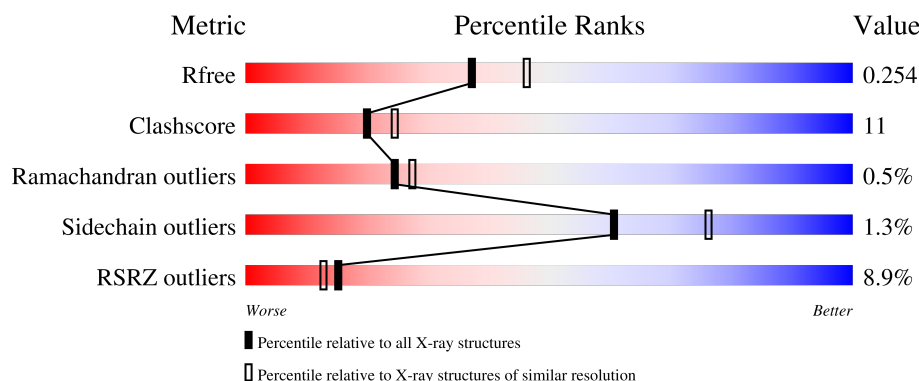
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1001	9% 75% 22% ..
2	B	83	4% 70% 27% .
3	C	163	6% 61% 28% . 9%

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
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			

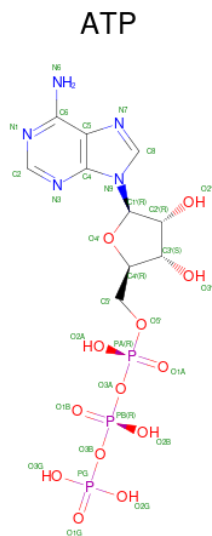
There are 18 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

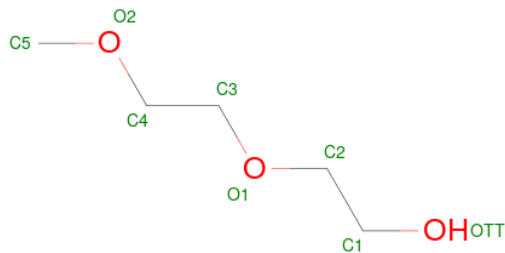
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 6 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: 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 (CCD ID: 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 (CCD ID: 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		

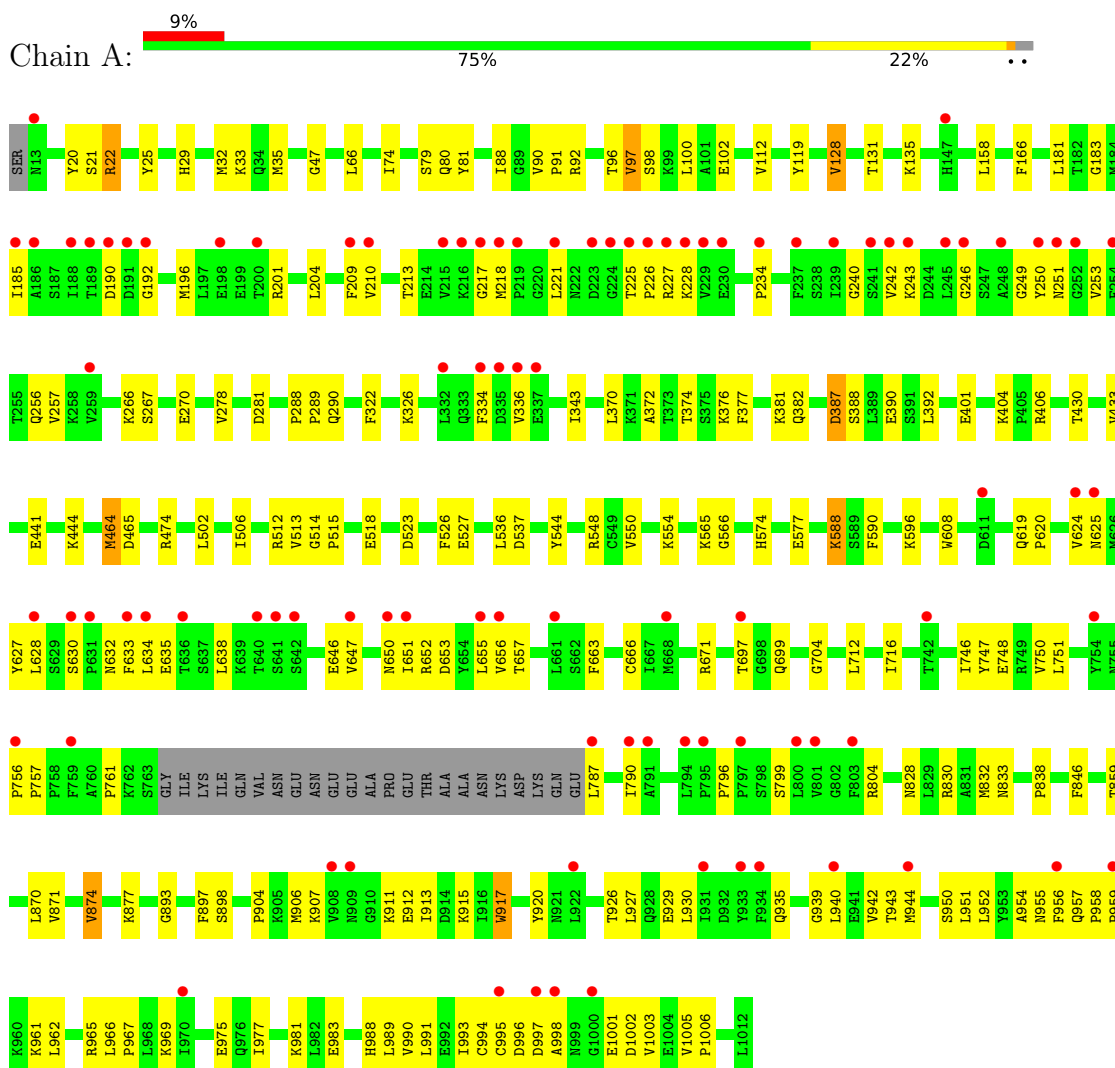
- Molecule 9 is water.

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 [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

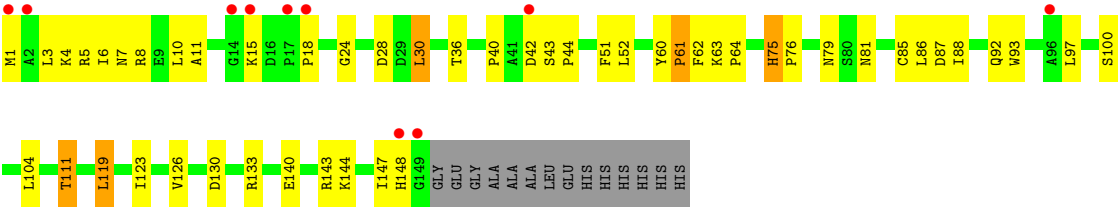


• Molecule 2: Ubiquitin-60S ribosomal protein L40





● 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 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.20) 99.8 (40.00-2.20)	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 0.213 , 0.254	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 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.

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

5 Model quality

5.1 Standard geometry

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

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	0.41	0/7844	0.86	14/10618 (0.1%)
2	B	0.40	0/656	0.86	1/883 (0.1%)
3	C	0.40	0/1206	0.95	5/1647 (0.3%)
All	All	0.40	0/9706	0.87	20/13148 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	119	LEU	N-CA-C	-7.91	103.84	113.97
1	A	97	VAL	N-CA-C	7.36	118.09	110.36
1	A	388	SER	N-CA-C	-7.10	99.90	110.06
3	C	75	HIS	CA-C-N	6.60	126.54	119.28
3	C	75	HIS	C-N-CA	6.60	126.54	119.28
1	A	577	GLU	N-CA-C	-6.49	102.16	110.53
1	A	596	LYS	N-CA-C	6.47	117.99	111.07
3	C	24	GLY	CA-C-N	5.87	125.88	119.89
3	C	24	GLY	C-N-CA	5.87	125.88	119.89
1	A	430	THR	N-CA-C	5.37	118.34	109.85
1	A	278	VAL	N-CA-C	-5.36	99.93	107.75
1	A	917	TRP	N-CA-C	5.29	119.83	112.90
1	A	704	GLY	CA-C-N	5.25	124.87	119.56
1	A	704	GLY	C-N-CA	5.25	124.87	119.56
1	A	128	VAL	N-CA-C	5.24	115.52	107.77
1	A	514	GLY	CA-C-N	5.19	124.64	119.24
1	A	514	GLY	C-N-CA	5.19	124.64	119.24
1	A	96	THR	N-CA-C	5.12	118.68	112.23
2	B	70	VAL	N-CA-C	5.11	116.54	109.29
1	A	92	ARG	N-CA-C	5.02	117.41	111.33

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	163	0
2	B	648	0	648	22	0
3	C	1170	0	1149	43	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
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	217	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 (217) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:906:MET:HE3	1:A:915:LYS:HB2	1.76	0.66
1:A:632:ASN:HB3	1:A:635:GLU:HB2	1.76	0.66
3:C:140:GLU:CD	3:C:143:ARG:HH21	2.04	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:PGO: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
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
1:A:334:PHE:CZ	1:A:336:VAL:HB	2.37	0.60
1:A:912:GLU:C	1:A:913:ILE:HD12	2.26	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
1:A:944:MET:HG3	3:C:7:ASN:CG	2.30	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:870:LEU:C	1:A:870:LEU:HD23	2.31	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
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:787:LEU:C	1:A:787:LEU:HD23	2.34	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:ILE:CD1	1:A:196:MET:HE1	2.43	0.48
1:A:930:LEU:HD23	1:A:930:LEU:O	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
3:C:3:LEU:C	3:C:3:LEU:HD23	2.39	0.47
1:A:983:GLU:CD	1:A:983:GLU:N	2.72	0.47
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: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
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:930:LEU:HD23	1:A:930:LEU:C	2.41	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
3:C:51:PHE:C	3:C:52:LEU:HD12	2.40	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
1:A:464:MET:HE3	1:A:512:ARG:CZ	2.45	0.45
3:C:1:MET:HG2	3:C:4:LYS:HD2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:62:PHE:C	3:C:63:LYS:HD2	2.42	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
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:20:TYR:CG	1:A:32:MET:HE1	2.52	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:954:ALA:C	1:A:956:PHE:H	2.26	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
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
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:464:MET:HE3	1:A:512:ARG:NH2	2.35	0.42
1:A:990:VAL:C	1:A:991:LEU:HD12	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ILE:O	3:C:147:ILE:HG22	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
3:C:1:MET:HE2	3:C:1:MET:N	2.34	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
3:C:87:ASP:C	3:C:92:GLN:HB2	2.45	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: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:944:MET:HE3	1:A:994:CYS:SG	2.61	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
1:A:90:VAL:O	1:A:91:PRO:C	2.63	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
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:35:MET:HE3	1:A:370:LEU:HD22	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:HIS:H	1:A:917:TRP:CG	2.38	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%)	30	34
2	B	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
3	C	147/163 (90%)	142 (97%)	3 (2%)	2 (1%)	9	7
All	All	1198/1247 (96%)	1137 (95%)	55 (5%)	6 (0%)	24	27

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%)	847 (99%)	10 (1%)	63	78
2	B	70/74 (95%)	70 (100%)	0	100	100
3	C	130/140 (93%)	126 (97%)	4 (3%)	35	48
All	All	1057/1091 (97%)	1043 (99%)	14 (1%)	61	76

All (14) 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	387	ASP
1	A	392	LEU
1	A	464	MET
1	A	527	GLU
1	A	588	LYS
1	A	874	VAL
1	A	989	LEU
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	146	ASN
1	A	251	ASN
1	A	623	ASN
1	A	650	ASN
1	A	688	ASN
1	A	699	GLN
1	A	833	ASN
1	A	921	ASN
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 oligosaccharides 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	$\# Z > 2$
7	EDO	A	1107	-	3,3,3	1.19	0	2,2,2	0.18	0
7	EDO	A	1110	-	3,3,3	1.15	0	2,2,2	0.19	0
7	EDO	A	1106	-	3,3,3	1.17	0	2,2,2	0.16	0
8	SO4	A	1113	-	4,4,4	0.37	0	6,6,6	0.07	0
8	SO4	B	102	-	4,4,4	0.37	0	6,6,6	0.07	0
7	EDO	A	1108	-	3,3,3	1.16	0	2,2,2	0.17	0
7	EDO	A	1109	-	3,3,3	1.12	0	2,2,2	0.21	0
7	EDO	B	101	-	3,3,3	1.18	0	2,2,2	0.16	0
8	SO4	A	1112	-	4,4,4	0.38	0	6,6,6	0.07	0
5	ATP	A	1103	4	32,33,33	1.52	5 (15%)	48,52,52	1.97	14 (29%)
7	EDO	A	1105	-	3,3,3	1.23	0	2,2,2	0.16	0
6	PG0	A	1104	-	6,6,7	0.85	0	5,5,6	1.05	0
8	SO4	A	1111	-	4,4,4	0.38	0	6,6,6	0.09	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
7	EDO	A	1107	-	-	0/1/1/1	-
7	EDO	A	1110	-	-	0/1/1/1	-
7	EDO	A	1106	-	-	0/1/1/1	-
7	EDO	A	1108	-	-	1/1/1/1	-
7	EDO	A	1109	-	-	0/1/1/1	-
7	EDO	B	101	-	-	0/1/1/1	-
5	ATP	A	1103	4	-	5/22/38/38	0/3/3/3
7	EDO	A	1105	-	-	1/1/1/1	-
6	PG0	A	1104	-	-	1/4/4/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1103	ATP	C5-C4	4.37	1.46	1.39
5	A	1103	ATP	PB-O3B	3.59	1.63	1.59
5	A	1103	ATP	C5-C6	3.09	1.49	1.41
5	A	1103	ATP	C5-N7	-2.05	1.35	1.39
5	A	1103	ATP	C8-N7	2.04	1.35	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	ATP	C5-C4-N3	-5.00	119.83	126.72
5	A	1103	ATP	N3-C2-N1	-4.63	121.57	128.58
5	A	1103	ATP	N3-C4-N9	4.48	134.78	127.17
5	A	1103	ATP	C2-N3-C4	3.91	121.37	111.83
5	A	1103	ATP	C4-N9-C8	3.54	109.45	105.74
5	A	1103	ATP	C4-C5-N7	-2.88	107.29	110.58
5	A	1103	ATP	O3A-PA-O1A	-2.69	102.62	110.70
5	A	1103	ATP	O2A-PA-O3A	2.65	114.45	107.27
5	A	1103	ATP	O3A-PB-O1B	-2.55	103.03	110.70
5	A	1103	ATP	C5-N7-C8	2.45	107.30	103.45
5	A	1103	ATP	N9-C8-N7	-2.38	110.56	113.94
5	A	1103	ATP	C2-N1-C6	2.36	122.61	118.73
5	A	1103	ATP	C6-C5-N7	2.20	136.33	132.09
5	A	1103	ATP	O2B-PB-O1B	2.15	122.44	112.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

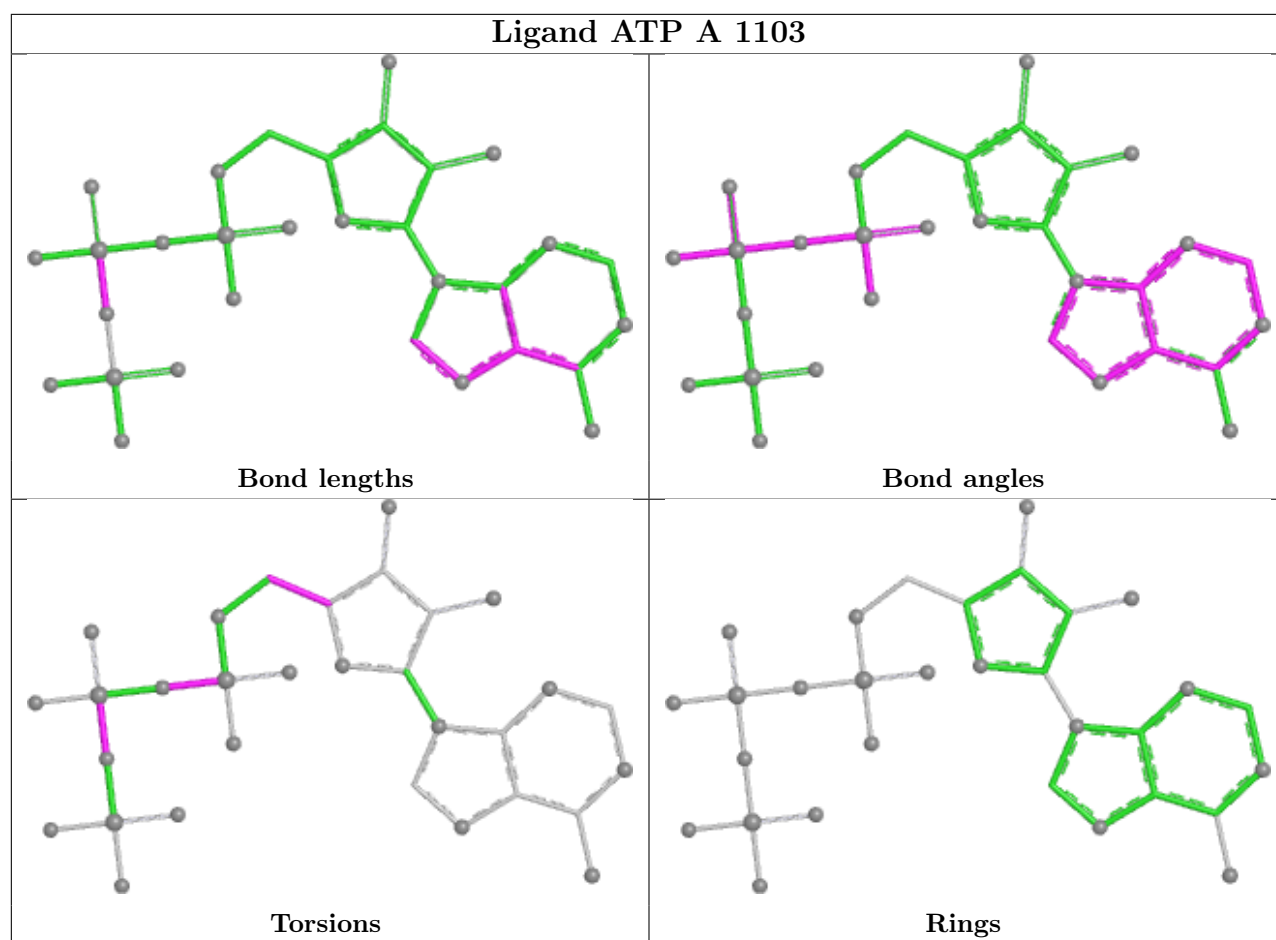
Mol	Chain	Res	Type	Atoms
7	A	1105	EDO	O1-C1-C2-O2
5	A	1103	ATP	O4'-C4'-C5'-O5'
5	A	1103	ATP	C3'-C4'-C5'-O5'
7	A	1108	EDO	O1-C1-C2-O2
5	A	1103	ATP	PB-O3A-PA-O2A
6	A	1104	PG0	C1-C2-O1-C3
5	A	1103	ATP	PG-O3B-PB-O1B
5	A	1103	ATP	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1103	ATP	2	0
6	A	1104	PG0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	977/1001 (97%)	0.37	94 (9%) 13 11	28, 46, 100, 120	0
2	B	80/83 (96%)	0.38	3 (3%) 44 41	32, 52, 67, 91	0
3	C	149/163 (91%)	0.57	10 (6%) 24 21	43, 55, 78, 90	2 (1%)
All	All	1206/1247 (96%)	0.40	107 (8%) 15 13	28, 49, 97, 120	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	790	ILE	5.1
1	A	245	LEU	4.9
1	A	801	VAL	4.6
1	A	226	PRO	4.6
1	A	787	LEU	4.3
1	A	803	PHE	4.3
1	A	191	ASP	4.2
1	A	229	VAL	4.1
1	A	242	VAL	4.1
1	A	800	LEU	4.1
2	B	-3	HIS	4.0
3	C	18	PRO	3.7
1	A	334	PHE	3.6
1	A	221	LEU	3.6
1	A	624	VAL	3.6
1	A	634	LEU	3.5
1	A	219	PRO	3.5
1	A	1000	GLY	3.4
1	A	239	ILE	3.3
3	C	2	ALA	3.3
1	A	217	GLY	3.3
3	C	149	GLY	3.3
1	A	631	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	GLY	3.1
1	A	227	ARG	3.1
1	A	756	PRO	3.0
1	A	243	LYS	3.0
1	A	791	ALA	2.9
3	C	148	HIS	2.9
1	A	754	TYR	2.9
1	A	209	PHE	2.9
1	A	998	ALA	2.9
3	C	17	PRO	2.8
1	A	630	SER	2.8
3	C	1	MET	2.8
1	A	633	PHE	2.8
1	A	188	ILE	2.7
1	A	944	MET	2.7
1	A	147	HIS	2.7
1	A	225	THR	2.7
1	A	628	LEU	2.7
1	A	13	ASN	2.7
1	A	218	MET	2.7
1	A	210	VAL	2.7
1	A	636	THR	2.7
1	A	742	THR	2.7
1	A	655	LEU	2.7
1	A	336	VAL	2.6
1	A	650	ASN	2.6
1	A	246	GLY	2.6
1	A	335	ASP	2.6
1	A	216	LYS	2.6
1	A	223	ASP	2.6
1	A	625	ASN	2.6
1	A	252	GLY	2.6
1	A	697	THR	2.6
1	A	224	GLY	2.5
1	A	234	PRO	2.5
1	A	651	ILE	2.5
1	A	908	VAL	2.4
1	A	933	TYR	2.4
1	A	248	ALA	2.4
1	A	230	GLU	2.4
1	A	251	ASN	2.4
1	A	259	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	970	ILE	2.4
1	A	794	LEU	2.4
1	A	198	GLU	2.4
1	A	250	TYR	2.3
1	A	640	THR	2.3
1	A	641	SER	2.3
1	A	647	VAL	2.3
3	C	14	GLY	2.3
1	A	200	THR	2.3
2	B	74	ARG	2.3
1	A	185	ILE	2.3
1	A	934	PHE	2.3
1	A	190	ASP	2.3
1	A	959	PRO	2.3
1	A	332	LEU	2.2
3	C	42	ASP	2.2
1	A	797	PRO	2.2
1	A	189	THR	2.2
1	A	241	SER	2.2
1	A	642	SER	2.2
1	A	956	PHE	2.2
1	A	995	CYS	2.2
1	A	215	VAL	2.2
1	A	228	LYS	2.2
1	A	337	GLU	2.2
2	B	36	ILE	2.1
1	A	909	ASN	2.1
1	A	668	MET	2.1
1	A	656	VAL	2.1
3	C	96	ALA	2.1
1	A	661	LEU	2.1
1	A	922	LEU	2.1
1	A	931	ILE	2.1
1	A	940	LEU	2.1
1	A	997	ASP	2.1
1	A	237	PHE	2.1
1	A	611	ASP	2.1
1	A	254	PHE	2.1
1	A	759	PHE	2.1
3	C	15	LYS	2.0
1	A	186	ALA	2.0
1	A	795	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

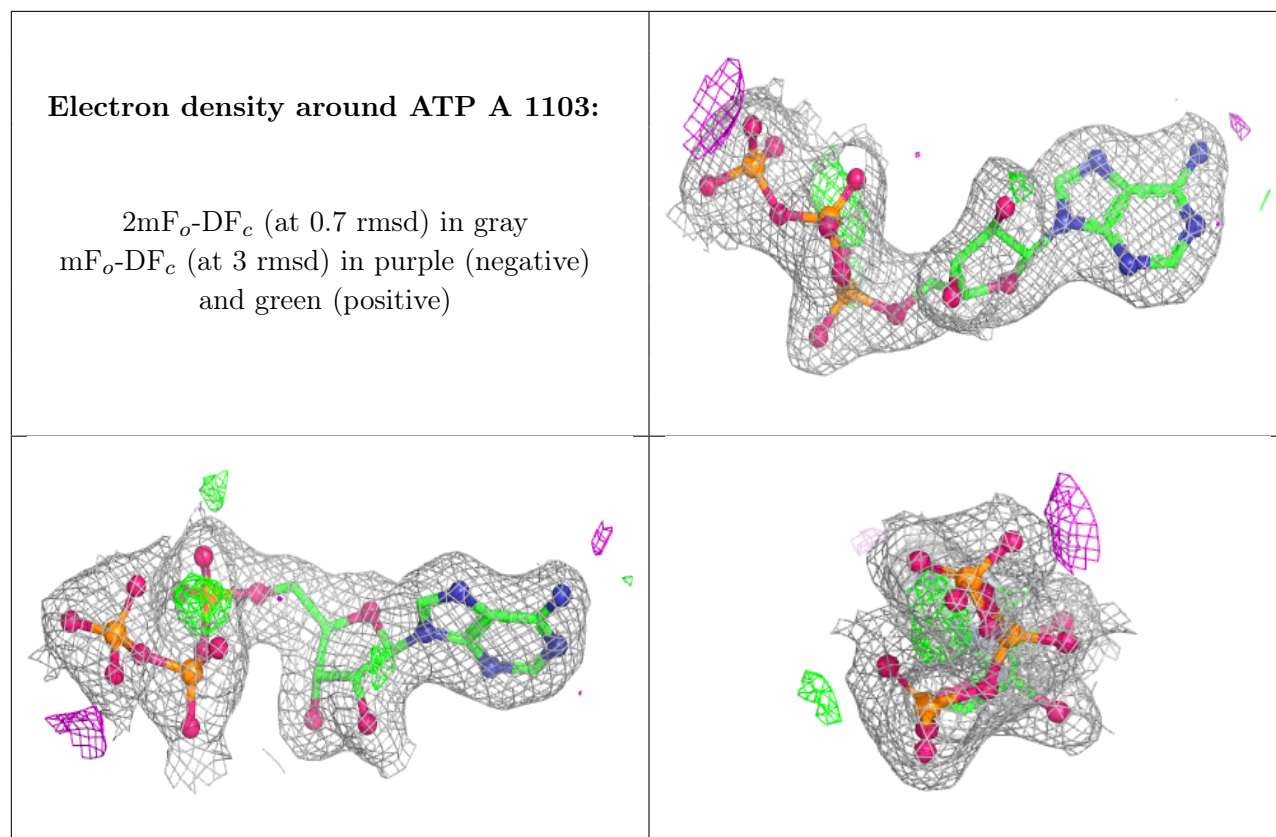
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	A	1113	5/5	0.60	0.12	148,148,148,148	0
8	SO4	B	102	5/5	0.69	0.16	135,135,135,135	0
8	SO4	A	1111	5/5	0.71	0.13	122,122,122,122	0
8	SO4	A	1112	5/5	0.71	0.17	127,127,127,128	0
7	EDO	A	1110	4/4	0.81	0.25	79,79,80,80	0
7	EDO	A	1108	4/4	0.86	0.14	74,74,74,74	0
7	EDO	A	1105	4/4	0.87	0.16	75,75,75,78	0
7	EDO	A	1107	4/4	0.87	0.17	79,80,81,81	0
7	EDO	A	1106	4/4	0.88	0.17	52,57,58,62	0
4	MG	A	1101	1/1	0.89	0.10	52,52,52,52	0
6	PG0	A	1104	7/8	0.90	0.13	47,53,55,56	0
7	EDO	A	1109	4/4	0.91	0.13	53,54,55,56	0
7	EDO	B	101	4/4	0.91	0.16	57,59,61,63	0
4	MG	A	1102	1/1	0.97	0.08	47,47,47,47	0
5	ATP	A	1103	31/31	0.98	0.06	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.