



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:37 PM UTC

PDB ID : 6NYA / pdb_00006nya
Title : Crystal Structure of ubiquitin E1 (Uba1) in complex with Ubc3 (Cdc34) and ubiquitin
Authors : Olsen, S.K.; Williams, K.M.; Atkison, J.H.
Deposited on : 2019-02-11
Resolution : 2.06 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

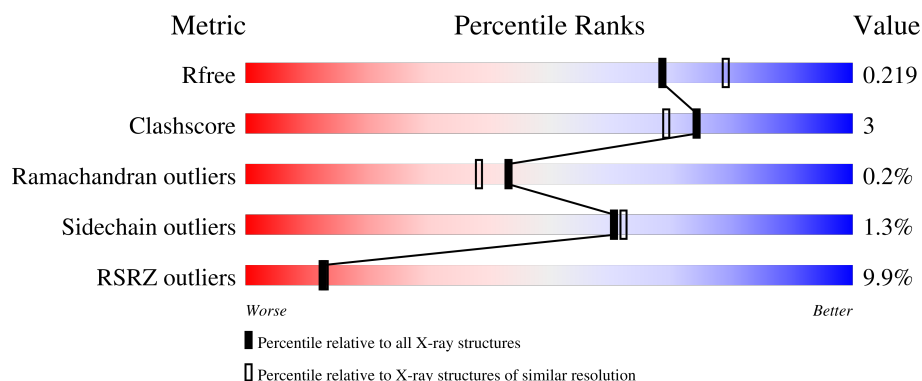
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	1017	4% 89% 8% .
1	D	1017	10% 89% 8% .
2	B	85	5% 84% 7% . 8%
2	E	85	15% 79% 12% 9%
3	C	197	20% 76% 11% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	197	

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
6	SO4	D	1204	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20705 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	987	Total	C	N	O	S	0	0	0
			7800	4979	1288	1510	23			
1	D	987	Total	C	N	O	S	0	0	0
			7796	4977	1288	1508	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP P22515
A	9	ALA	-	expression tag	UNP P22515
A	10	MET	-	expression tag	UNP P22515
D	8	GLY	-	expression tag	UNP P22515
D	9	ALA	-	expression tag	UNP P22515
D	10	MET	-	expression tag	UNP P22515

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			622	380	121	120	1			
2	E	77	Total	C	N	O	S	0	0	0
			618	378	120	119	1			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	initiating methionine	UNP A0A1D6RLC6
B	-7	HIS	-	expression tag	UNP A0A1D6RLC6
B	-6	HIS	-	expression tag	UNP A0A1D6RLC6
B	-5	HIS	-	expression tag	UNP A0A1D6RLC6
B	-4	HIS	-	expression tag	UNP A0A1D6RLC6
B	-3	HIS	-	expression tag	UNP A0A1D6RLC6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A1D6RLC6
B	-1	GLY	-	expression tag	UNP A0A1D6RLC6
B	0	ALA	-	expression tag	UNP A0A1D6RLC6
B	6	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
B	11	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
B	27	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
B	29	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
B	33	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
B	48	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
B	63	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	-8	MET	-	initiating methionine	UNP A0A1D6RLC6
E	-7	HIS	-	expression tag	UNP A0A1D6RLC6
E	-6	HIS	-	expression tag	UNP A0A1D6RLC6
E	-5	HIS	-	expression tag	UNP A0A1D6RLC6
E	-4	HIS	-	expression tag	UNP A0A1D6RLC6
E	-3	HIS	-	expression tag	UNP A0A1D6RLC6
E	-2	HIS	-	expression tag	UNP A0A1D6RLC6
E	-1	GLY	-	expression tag	UNP A0A1D6RLC6
E	0	ALA	-	expression tag	UNP A0A1D6RLC6
E	6	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	11	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	27	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	29	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	33	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	48	ARG	LYS	engineered mutation	UNP A0A1D6RLC6
E	63	ARG	LYS	engineered mutation	UNP A0A1D6RLC6

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2-34 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	170	Total	C	N	O	S	0	0	0
			1381	881	235	260	5			
3	F	167	Total	C	N	O	S	0	0	0
			1356	868	229	254	5			

There are 8 discrepancies between the modelled and reference sequences:

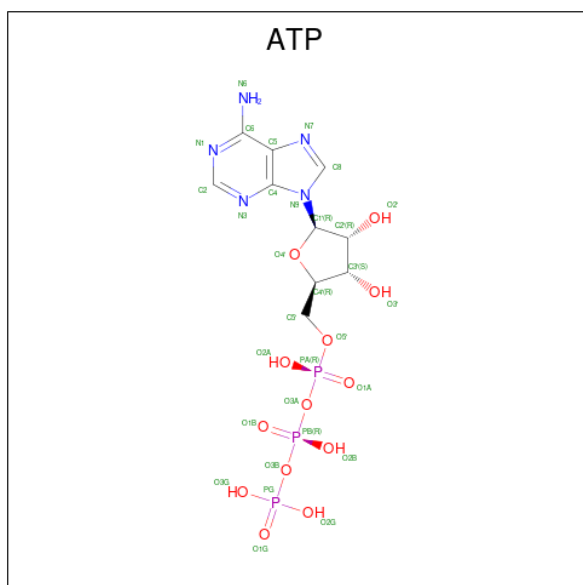
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P14682
C	0	ALA	-	expression tag	UNP P14682
C	1	MET	-	expression tag	UNP P14682
C	2	ALA	-	expression tag	UNP P14682

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P14682
F	0	ALA	-	expression tag	UNP P14682
F	1	MET	-	expression tag	UNP P14682
F	2	ALA	-	expression tag	UNP P14682

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

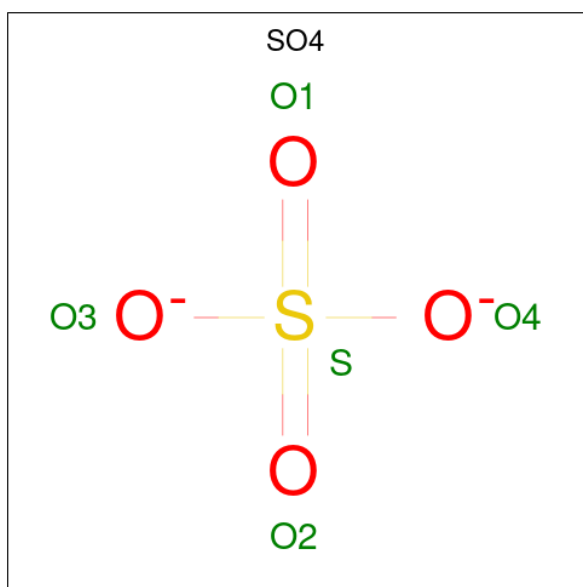


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



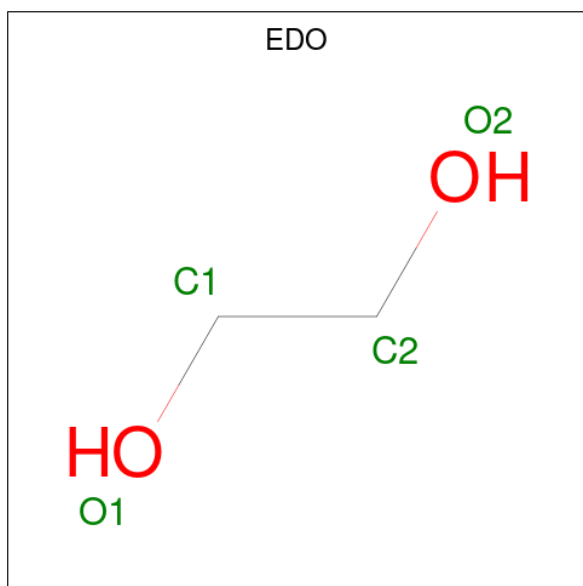
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: 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	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		

Continued on next page...

Continued from previous page...

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

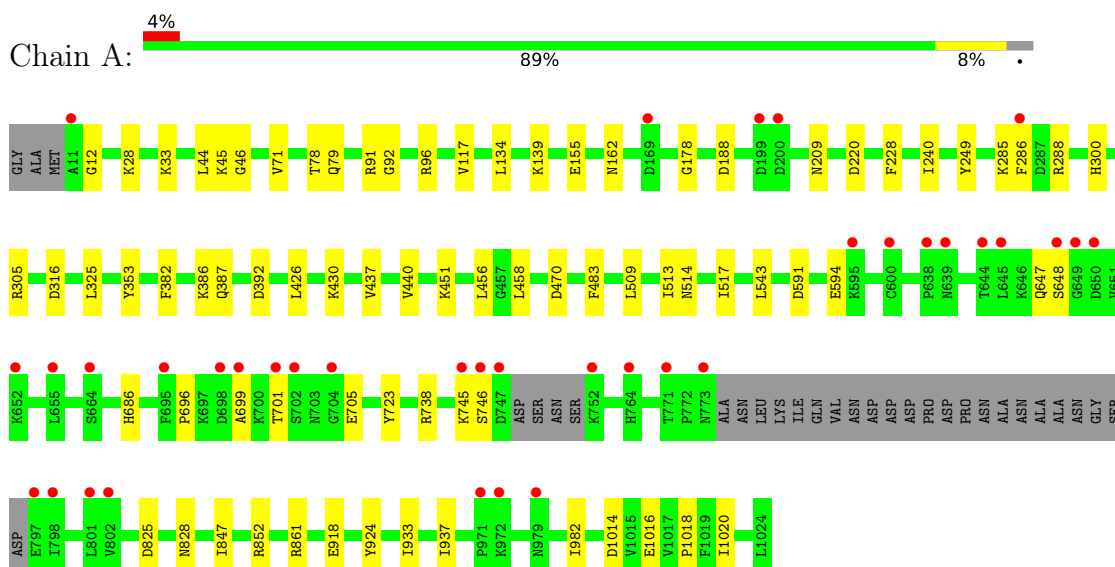
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	471	Total O 471 471	0	0
8	B	29	Total O 29 29	0	0
8	C	9	Total O 9 9	0	0
8	D	373	Total O 373 373	0	0
8	E	21	Total O 21 21	0	0
8	F	6	Total O 6 6	0	0

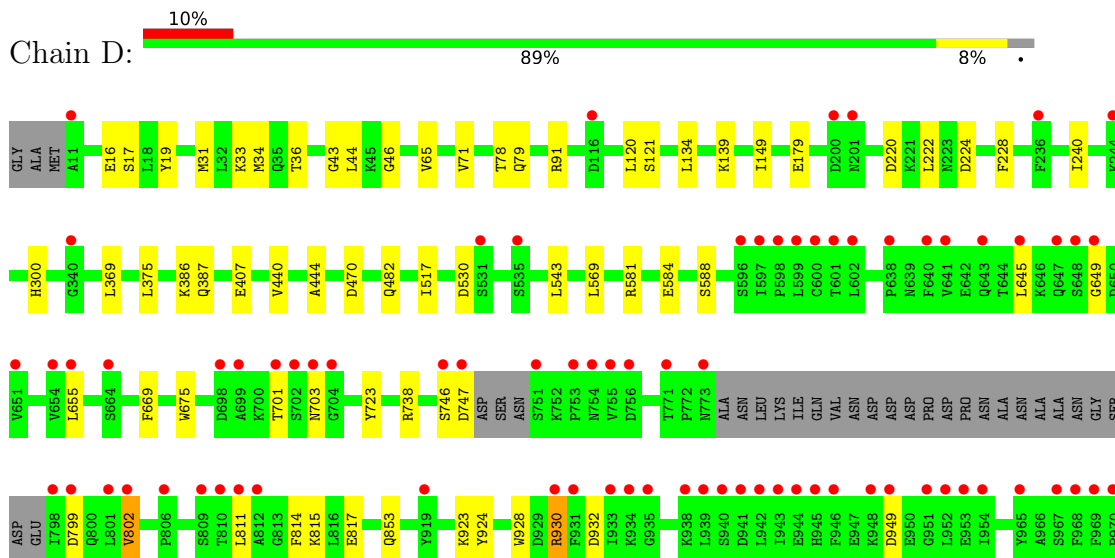
3 Residue-property plots

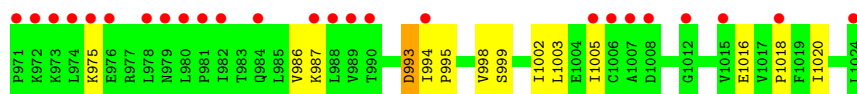
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

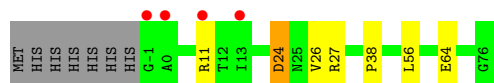
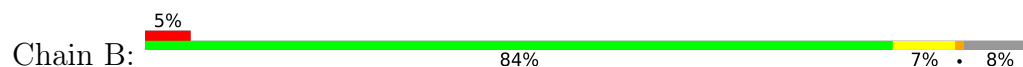


• Molecule 1: Ubiquitin-activating enzyme E1 1

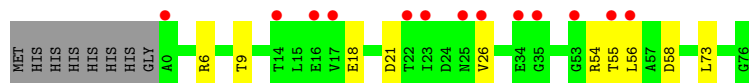
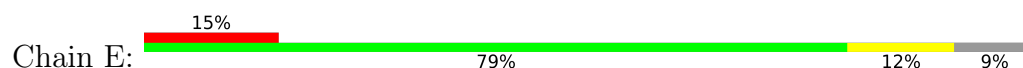




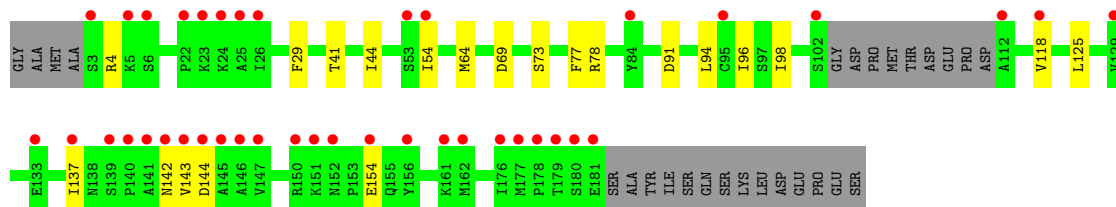
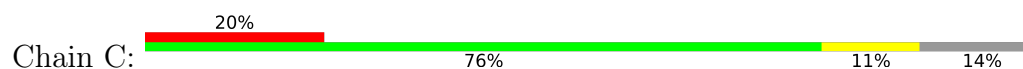
• Molecule 2: Ubiquitin



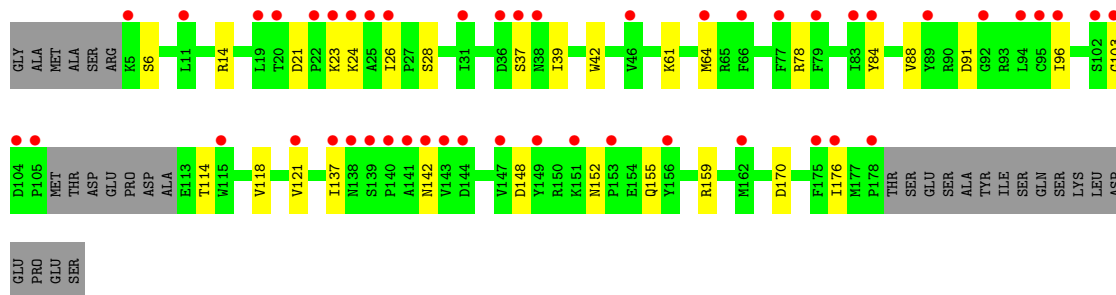
• Molecule 2: Ubiquitin



• Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



• Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.44Å 68.54Å 171.72Å 90.00° 110.72° 90.00°	Depositor
Resolution (Å)	117.03 – 2.06 117.03 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.0 (117.03-2.06) 89.2 (117.03-2.06)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.187 , 0.217 0.188 , 0.219	Depositor DCC
R_{free} test set	2005 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20705	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MG, ATP, 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	0.16	0/7962	0.34	0/10770
1	D	0.16	0/7958	0.32	0/10766
2	B	0.14	0/627	0.36	0/843
2	E	0.14	0/623	0.35	0/838
3	C	0.14	0/1417	0.30	0/1922
3	F	0.15	0/1393	0.31	0/1891
All	All	0.16	0/19980	0.33	0/27030

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7800	0	7721	46	0
1	D	7796	0	7721	50	0
2	B	622	0	633	4	0
2	E	618	0	630	7	0
3	C	1381	0	1351	10	0
3	F	1356	0	1325	14	0
4	A	31	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	31	0	12	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	40	0	0	1	0
6	D	35	0	0	2	0
7	A	44	0	66	2	0
7	C	4	0	6	1	0
7	D	36	0	54	3	0
8	A	471	0	0	7	0
8	B	29	0	0	0	0
8	C	9	0	0	0	0
8	D	373	0	0	3	0
8	E	21	0	0	2	0
8	F	6	0	0	0	0
All	All	20705	0	19531	120	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 3.

All (120) 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:D:930:ARG:NH1	1:D:932:ASP:OD2	2.07	0.88
1:D:1016:GLU:OE2	3:F:14:ARG:NH2	2.21	0.73
3:F:84:TYR:OH	3:F:148:ASP:OD2	2.05	0.73
3:C:143:VAL:HB	3:C:144:ASP:HA	1.72	0.71
1:D:44:LEU:HD21	1:D:65:VAL:HB	1.76	0.66
1:D:811:LEU:HB3	1:D:814:PHE:HB3	1.80	0.61
1:A:71:VAL:HG22	1:A:91:ARG:HG2	1.84	0.60
1:D:655:LEU:HD13	1:D:802:VAL:HG12	1.85	0.58
1:D:71:VAL:HG22	1:D:91:ARG:HG2	1.86	0.58
1:D:1005:ILE:HD13	1:D:1020:ILE:HD11	1.86	0.57
1:A:96:ARG:HH21	7:A:1112:EDO:H11	1.70	0.57
3:F:78:ARG:NH1	3:F:91:ASP:O	2.38	0.57
1:D:17:SER:H	7:D:1212:EDO:H11	1.70	0.57
2:E:26:VAL:HG21	2:E:56:LEU:HD21	1.85	0.56
1:D:440:VAL:HG12	1:D:543:LEU:HD21	1.88	0.55
3:C:142:ASN:ND2	3:C:143:VAL:O	2.39	0.54
1:A:117:VAL:HG21	1:D:723:TYR:HE2	1.72	0.53
1:A:44:LEU:HD12	1:A:92:GLY:HA2	1.90	0.53
1:A:1016:GLU:HG2	3:C:4:ARG:HE	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:987:LYS:HG2	1:D:993:ASP:HA	1.91	0.51
3:F:61:LYS:HE3	3:F:170:ASP:HB3	1.91	0.51
1:A:852:ARG:NH1	8:A:1213:HOH:O	2.43	0.51
1:A:745:LYS:HG2	1:A:746:SER:H	1.76	0.50
1:A:451:LYS:HG3	1:A:483:PHE:HZ	1.76	0.50
3:C:69:ASP:OD2	3:C:73:SER:OG	2.29	0.50
3:C:96:ILE:HG12	3:C:98:ILE:HG22	1.94	0.49
1:A:591:ASP:OD1	8:A:1201:HOH:O	2.19	0.49
1:A:440:VAL:HG12	1:A:543:LEU:HD21	1.94	0.49
1:A:209:ASN:OD1	2:B:11:ARG:NH2	2.45	0.49
1:A:738:ARG:NH2	8:A:1217:HOH:O	2.45	0.48
2:B:26:VAL:HG21	2:B:56:LEU:HD21	1.94	0.48
1:D:34:MET:HE3	1:D:375:LEU:HD22	1.95	0.48
1:D:930:ARG:HG2	6:D:1204:SO4:S	2.54	0.48
2:E:18:GLU:N	2:E:21:ASP:OD2	2.42	0.48
1:A:46:GLY:HA3	1:A:78:THR:OG1	2.12	0.48
1:D:930:ARG:HD2	1:D:932:ASP:OD2	2.14	0.48
1:D:799:ASP:HA	1:D:802:VAL:HG22	1.95	0.48
1:A:155:GLU:HG2	1:A:162:ASN:OD1	2.13	0.48
1:D:930:ARG:HD2	1:D:932:ASP:CG	2.39	0.48
1:A:305:ARG:HH11	1:A:325:LEU:HD21	1.79	0.47
1:D:569:LEU:HB3	2:E:73:LEU:HD22	1.94	0.47
3:F:103:GLY:HA2	3:F:114:THR:HG21	1.96	0.47
1:A:594:GLU:OE1	1:A:861:ARG:NH1	2.41	0.47
1:A:696:PRO:HD2	1:A:699:ALA:HB2	1.97	0.47
3:C:29:PHE:CE1	3:C:125:LEU:HB3	2.50	0.47
3:F:64:MET:HE1	3:F:121:VAL:HG13	1.97	0.47
1:A:228:PHE:HB3	1:A:240:ILE:HB	1.96	0.47
1:A:514:ASN:ND2	6:A:1107:SO4:O1	2.48	0.47
1:D:179:GLU:HG3	2:E:9:THR:HB	1.96	0.47
2:E:54:ARG:NH1	8:E:101:HOH:O	2.47	0.47
3:F:152:ASN:HB3	3:F:155:GLN:HB2	1.96	0.47
3:F:155:GLN:O	3:F:159:ARG:HG2	2.15	0.47
1:D:19:TYR:CG	1:D:31:MET:HE1	2.50	0.47
1:D:407:GLU:OE2	8:D:1301:HOH:O	2.21	0.47
2:B:27:ARG:HB3	2:B:38:PRO:HB3	1.97	0.46
3:C:78:ARG:NH1	3:C:91:ASP:O	2.49	0.46
3:F:21:ASP:HB3	3:F:23:LYS:N	2.31	0.46
1:A:924:TYR:CD1	1:A:1018:PRO:HG3	2.50	0.46
2:B:24:ASP:OD1	2:B:24:ASP:N	2.48	0.46
1:D:121:SER:HA	1:D:149:ILE:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:THR:HG22	1:A:705:GLU:O	2.15	0.45
1:A:117:VAL:HG21	1:D:723:TYR:CE2	2.51	0.45
1:A:723:TYR:CZ	1:D:139:LYS:HD3	2.51	0.45
1:D:581:ARG:H	1:D:928:TRP:CG	2.35	0.45
1:D:815:LYS:HE3	1:D:817:GLU:OE2	2.17	0.45
3:C:77:PHE:H	7:C:201:EDO:H12	1.81	0.44
1:A:933:ILE:HD13	1:A:1020:ILE:HG23	1.99	0.44
1:D:444:ALA:HA	1:D:482:GLN:HG2	2.00	0.44
1:D:16:GLU:HG3	1:D:853:GLN:CD	2.43	0.44
1:D:134:LEU:HB2	1:D:300:HIS:CG	2.53	0.44
1:D:386:LYS:HA	1:D:387:GLN:HA	1.79	0.44
1:D:530:ASP:OD1	1:D:999:SER:OG	2.36	0.44
1:D:1003:LEU:HB2	1:D:1020:ILE:HB	2.00	0.43
3:F:21:ASP:HB3	3:F:24:LYS:H	1.83	0.43
1:A:509:LEU:HD13	1:A:513:ILE:HD11	2.00	0.43
1:D:584:GLU:HB2	1:D:588:SER:CB	2.49	0.43
2:E:55:THR:OG1	2:E:58:ASP:OD1	2.32	0.43
3:F:39:ILE:O	3:F:42:TRP:NE1	2.49	0.43
1:A:386:LYS:HA	1:A:387:GLN:HA	1.69	0.43
1:D:930:ARG:HG2	6:D:1204:SO4:O2	2.19	0.43
1:A:139:LYS:HD3	1:D:723:TYR:CZ	2.54	0.43
3:F:26:ILE:HG22	3:F:28:SER:H	1.84	0.43
1:A:33:LYS:HE2	8:A:1411:HOH:O	2.18	0.43
1:A:178:GLY:HA3	1:A:382:PHE:HE2	1.84	0.42
1:D:701:THR:C	1:D:703:ASN:H	2.27	0.42
1:D:986:VAL:HG11	1:D:994:ILE:HD11	2.01	0.42
1:A:437:VAL:HG11	1:A:458:LEU:HD21	2.00	0.42
2:E:6:ARG:NH1	8:E:104:HOH:O	2.51	0.42
1:A:12:GLY:HA3	1:D:36:THR:HB	2.02	0.42
1:D:43:GLY:C	1:D:44:LEU:HD22	2.45	0.42
1:A:1014:ASP:OD2	3:C:4:ARG:NH2	2.40	0.42
1:D:924:TYR:CD2	1:D:1018:PRO:HG3	2.55	0.42
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.91	0.42
1:A:45:LYS:NZ	8:A:1218:HOH:O	2.45	0.42
1:A:738:ARG:NH1	8:A:1234:HOH:O	2.52	0.42
1:D:1016:GLU:OE2	3:F:6:SER:HB3	2.20	0.42
1:D:46:GLY:HA3	1:D:78:THR:OG1	2.19	0.42
1:D:470:ASP:O	1:D:517:ILE:HA	2.19	0.42
1:D:33:LYS:HE2	8:D:1421:HOH:O	2.20	0.42
1:A:647:GLN:HB3	1:A:648:SER:HA	2.01	0.41
1:A:847:ILE:HA	7:A:1114:EDO:H11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:PHE:HB3	1:D:240:ILE:HB	2.02	0.41
1:A:316:ASP:OD1	1:A:353:TYR:OH	2.27	0.41
1:A:285:LYS:HB3	1:A:288:ARG:HD2	2.02	0.41
1:A:134:LEU:HB2	1:A:300:HIS:CG	2.55	0.41
3:C:44:ILE:HD12	3:C:64:MET:HE3	2.02	0.41
1:D:995:PRO:HG2	1:D:998:VAL:HG23	2.03	0.41
7:D:1213:EDO:H11	8:D:1376:HOH:O	2.20	0.41
1:D:669:PHE:CD2	1:D:746:SER:HB2	2.55	0.41
1:D:923:LYS:HE3	1:D:923:LYS:HB2	1.83	0.41
1:D:224:ASP:OD2	1:D:224:ASP:C	2.63	0.41
1:D:675:TRP:CD2	1:D:738:ARG:HD2	2.56	0.41
1:D:1002:ILE:HD13	7:D:1214:EDO:H11	2.03	0.41
1:A:937:ILE:O	1:A:982:ILE:HG12	2.21	0.40
1:A:188:ASP:HA	1:A:249:TYR:CE2	2.56	0.40
3:F:88:VAL:O	3:F:142:ASN:HB2	2.22	0.40
1:A:426:LEU:HG	1:A:430:LYS:HE2	2.03	0.40
1:A:470:ASP:O	1:A:517:ILE:HA	2.22	0.40
1:A:686:HIS:HE1	8:A:1227:HOH:O	2.04	0.40
1:A:825:ASP:HB3	1:A:828:ASN:ND2	2.36	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	981/1017 (96%)	951 (97%)	29 (3%)	1 (0%)	48	44
1	D	981/1017 (96%)	948 (97%)	31 (3%)	2 (0%)	43	38
2	B	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
2	E	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
3	C	166/197 (84%)	161 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	163/197 (83%)	155 (95%)	7 (4%)	1 (1%)	21	13
All	All	2442/2598 (94%)	2363 (97%)	75 (3%)	4 (0%)	43	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	D	220	ASP
3	F	37	SER
1	D	649	GLY

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	870/893 (97%)	864 (99%)	6 (1%)	76	79
1	D	870/893 (97%)	859 (99%)	11 (1%)	61	62
2	B	67/74 (90%)	65 (97%)	2 (3%)	36	32
2	E	67/74 (90%)	67 (100%)	0	100	100
3	C	157/179 (88%)	151 (96%)	6 (4%)	29	23
3	F	154/179 (86%)	150 (97%)	4 (3%)	40	37
All	All	2185/2292 (95%)	2156 (99%)	29 (1%)	61	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	79	GLN
1	A	286	PHE
1	A	392	ASP
1	A	456	LEU
1	A	918	GLU
2	B	24	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	64	GLU
3	C	41	THR
3	C	54	ILE
3	C	94	LEU
3	C	118	VAL
3	C	137	ILE
3	C	154	GLU
1	D	79	GLN
1	D	120	LEU
1	D	222	LEU
1	D	369	LEU
1	D	645	LEU
1	D	747	ASP
1	D	802	VAL
1	D	930	ARG
1	D	949	ASP
1	D	975	LYS
1	D	993	ASP
3	F	96	ILE
3	F	118	VAL
3	F	137	ILE
3	F	176	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	725	ASN
1	A	844	ASN
1	A	997	HIS
2	B	25	ASN
2	B	68	HIS
1	D	201	ASN
1	D	300	HIS
1	D	725	ASN
1	D	844	ASN
1	D	997	HIS
3	F	30	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	D	1203	-	4,4,4	0.24	0	6,6,6	0.08	0
7	EDO	D	1215	-	3,3,3	0.44	0	2,2,2	0.29	0
7	EDO	A	1119	-	3,3,3	0.42	0	2,2,2	0.47	0
7	EDO	D	1216	-	3,3,3	0.45	0	2,2,2	0.40	0
7	EDO	C	201	-	3,3,3	0.45	0	2,2,2	0.22	0
7	EDO	A	1112	-	3,3,3	0.38	0	2,2,2	0.44	0
6	SO4	A	1106	-	4,4,4	0.24	0	6,6,6	0.10	0
7	EDO	A	1111	-	3,3,3	0.37	0	2,2,2	0.51	0
7	EDO	D	1210	-	3,3,3	0.41	0	2,2,2	0.49	0
6	SO4	A	1110	-	4,4,4	0.24	0	6,6,6	0.06	0
7	EDO	D	1211	-	3,3,3	0.38	0	2,2,2	0.51	0
7	EDO	D	1213	-	3,3,3	0.35	0	2,2,2	0.42	0
7	EDO	D	1217	-	3,3,3	0.46	0	2,2,2	0.28	0
6	SO4	A	1105	-	4,4,4	0.23	0	6,6,6	0.07	0
7	EDO	A	1121	-	3,3,3	0.44	0	2,2,2	0.37	0
6	SO4	A	1107	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	D	1205	-	4,4,4	0.23	0	6,6,6	0.08	0
7	EDO	D	1212	-	3,3,3	0.42	0	2,2,2	0.39	0
4	ATP	D	1202	5	32,33,33	1.47	7 (21%)	48,52,52	1.76	9 (18%)
7	EDO	A	1115	-	3,3,3	0.39	0	2,2,2	0.60	0
6	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.06	0
7	EDO	D	1214	-	3,3,3	0.39	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	D	1206	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	D	1207	-	4,4,4	0.24	0	6,6,6	0.08	0
7	EDO	A	1120	-	3,3,3	0.49	0	2,2,2	0.24	0
7	EDO	D	1218	-	3,3,3	0.43	0	2,2,2	0.40	0
6	SO4	A	1108	-	4,4,4	0.25	0	6,6,6	0.08	0
6	SO4	A	1103	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	D	1209	-	4,4,4	0.24	0	6,6,6	0.07	0
7	EDO	A	1117	-	3,3,3	0.44	0	2,2,2	0.24	0
7	EDO	A	1113	-	3,3,3	0.40	0	2,2,2	0.36	0
6	SO4	A	1109	-	4,4,4	0.24	0	6,6,6	0.12	0
7	EDO	A	1118	-	3,3,3	0.43	0	2,2,2	0.43	0
4	ATP	A	1101	5	32,33,33	1.47	7 (21%)	48,52,52	1.74	9 (18%)
7	EDO	A	1114	-	3,3,3	0.41	0	2,2,2	0.42	0
6	SO4	D	1204	-	4,4,4	0.25	0	6,6,6	0.06	0
6	SO4	D	1208	-	4,4,4	0.25	0	6,6,6	0.06	0
7	EDO	A	1116	-	3,3,3	0.38	0	2,2,2	0.39	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	D	1215	-	-	0/1/1/1	-
7	EDO	A	1119	-	-	0/1/1/1	-
7	EDO	D	1216	-	-	0/1/1/1	-
7	EDO	C	201	-	-	0/1/1/1	-
7	EDO	A	1112	-	-	0/1/1/1	-
7	EDO	A	1111	-	-	0/1/1/1	-
7	EDO	D	1210	-	-	0/1/1/1	-
7	EDO	D	1211	-	-	0/1/1/1	-
7	EDO	D	1213	-	-	0/1/1/1	-
7	EDO	D	1217	-	-	0/1/1/1	-
7	EDO	A	1121	-	-	0/1/1/1	-
7	EDO	D	1212	-	-	0/1/1/1	-
4	ATP	D	1202	5	-	4/22/38/38	0/3/3/3
7	EDO	A	1115	-	-	0/1/1/1	-
7	EDO	D	1214	-	-	0/1/1/1	-
7	EDO	A	1120	-	-	0/1/1/1	-
7	EDO	D	1218	-	-	0/1/1/1	-
7	EDO	A	1117	-	-	0/1/1/1	-
7	EDO	A	1113	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1118	-	-	0/1/1/1	-
4	ATP	A	1101	5	-	5/22/38/38	0/3/3/3
7	EDO	A	1114	-	-	0/1/1/1	-
7	EDO	A	1116	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1202	ATP	C5-C4	4.69	1.47	1.39
4	A	1101	ATP	C5-C4	4.46	1.47	1.39
4	A	1101	ATP	PA-O3A	2.83	1.62	1.59
4	D	1202	ATP	C5-C6	2.81	1.48	1.41
4	A	1101	ATP	C5-C6	2.70	1.48	1.41
4	A	1101	ATP	PB-O3A	2.49	1.62	1.59
4	D	1202	ATP	C8-N7	2.41	1.36	1.31
4	D	1202	ATP	PB-O3A	2.38	1.62	1.59
4	A	1101	ATP	C8-N7	2.30	1.36	1.31
4	D	1202	ATP	C5-N7	-2.26	1.35	1.39
4	D	1202	ATP	PB-O3B	2.25	1.61	1.59
4	A	1101	ATP	PB-O3B	2.19	1.61	1.59
4	A	1101	ATP	C5-N7	-2.18	1.35	1.39
4	D	1202	ATP	PA-O3A	2.10	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1202	ATP	C5-C4-N3	-5.75	118.80	126.72
4	A	1101	ATP	C5-C4-N3	-5.63	118.97	126.72
4	D	1202	ATP	N3-C4-N9	4.62	135.02	127.17
4	A	1101	ATP	N3-C4-N9	4.58	134.96	127.17
4	A	1101	ATP	C2-N3-C4	3.69	120.85	111.83
4	D	1202	ATP	C2-N3-C4	3.65	120.74	111.83
4	D	1202	ATP	C4-C5-N7	-3.45	106.64	110.58
4	A	1101	ATP	N3-C2-N1	-3.43	123.39	128.58
4	D	1202	ATP	N3-C2-N1	-3.19	123.75	128.58
4	A	1101	ATP	C4-C5-N7	-3.18	106.95	110.58
4	A	1101	ATP	C4-N9-C8	2.90	108.78	105.74
4	D	1202	ATP	C4-N9-C8	2.85	108.73	105.74
4	D	1202	ATP	C5-N7-C8	2.62	107.57	103.45
4	A	1101	ATP	C5-N7-C8	2.45	107.31	103.45
4	D	1202	ATP	N9-C8-N7	-2.15	110.88	113.94
4	A	1101	ATP	N9-C8-N7	-2.14	110.90	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1202	ATP	C6-C5-N7	2.07	136.08	132.09
4	A	1101	ATP	C6-C5-N7	2.07	136.07	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

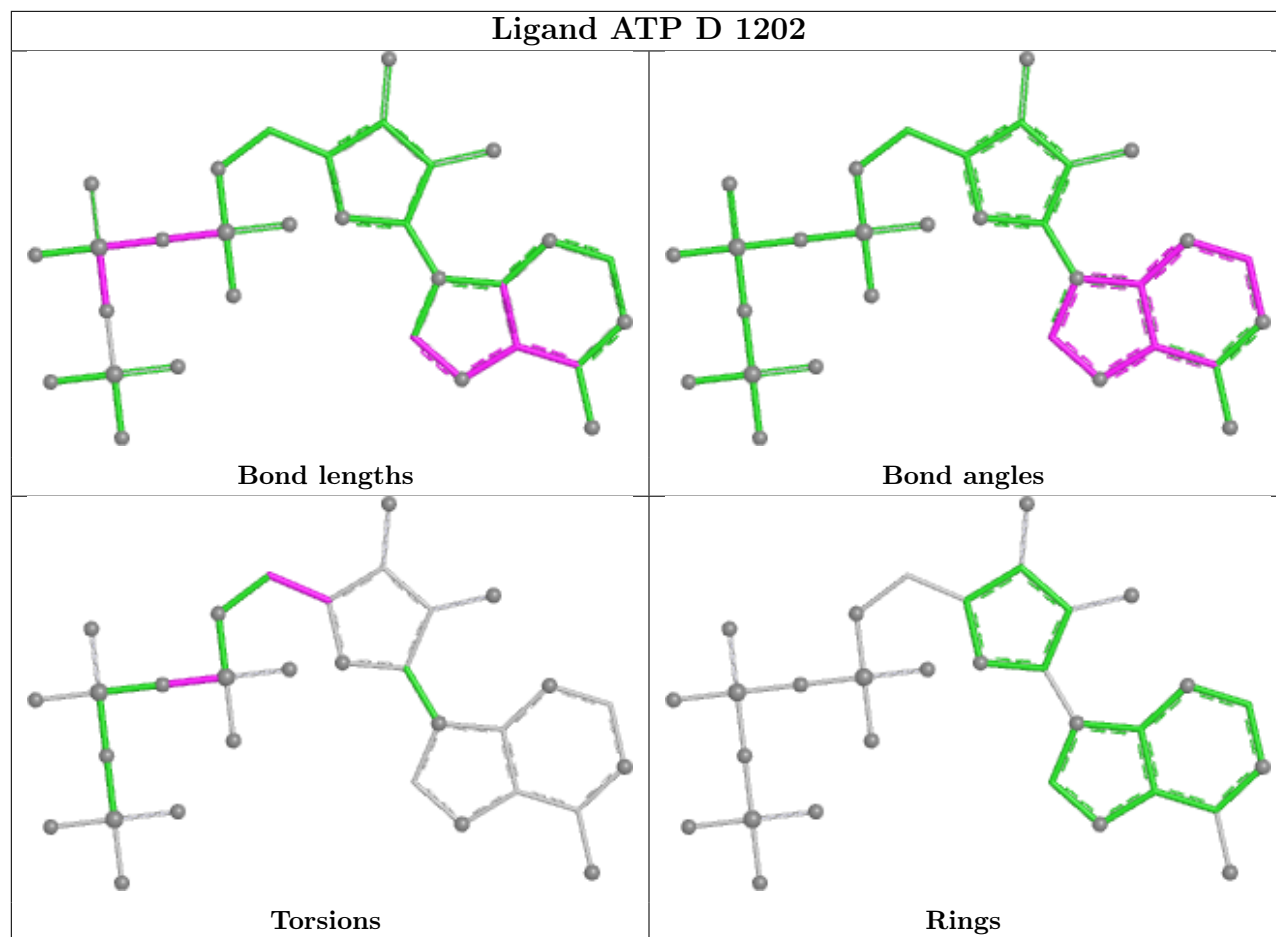
Mol	Chain	Res	Type	Atoms
4	D	1202	ATP	O4'-C4'-C5'-O5'
4	D	1202	ATP	C3'-C4'-C5'-O5'
4	A	1101	ATP	O4'-C4'-C5'-O5'
4	A	1101	ATP	C3'-C4'-C5'-O5'
4	D	1202	ATP	PB-O3A-PA-O2A
4	A	1101	ATP	PB-O3A-PA-O2A
4	A	1101	ATP	PG-O3B-PB-O1B
4	D	1202	ATP	PB-O3A-PA-O1A
4	A	1101	ATP	PG-O3B-PB-O2B

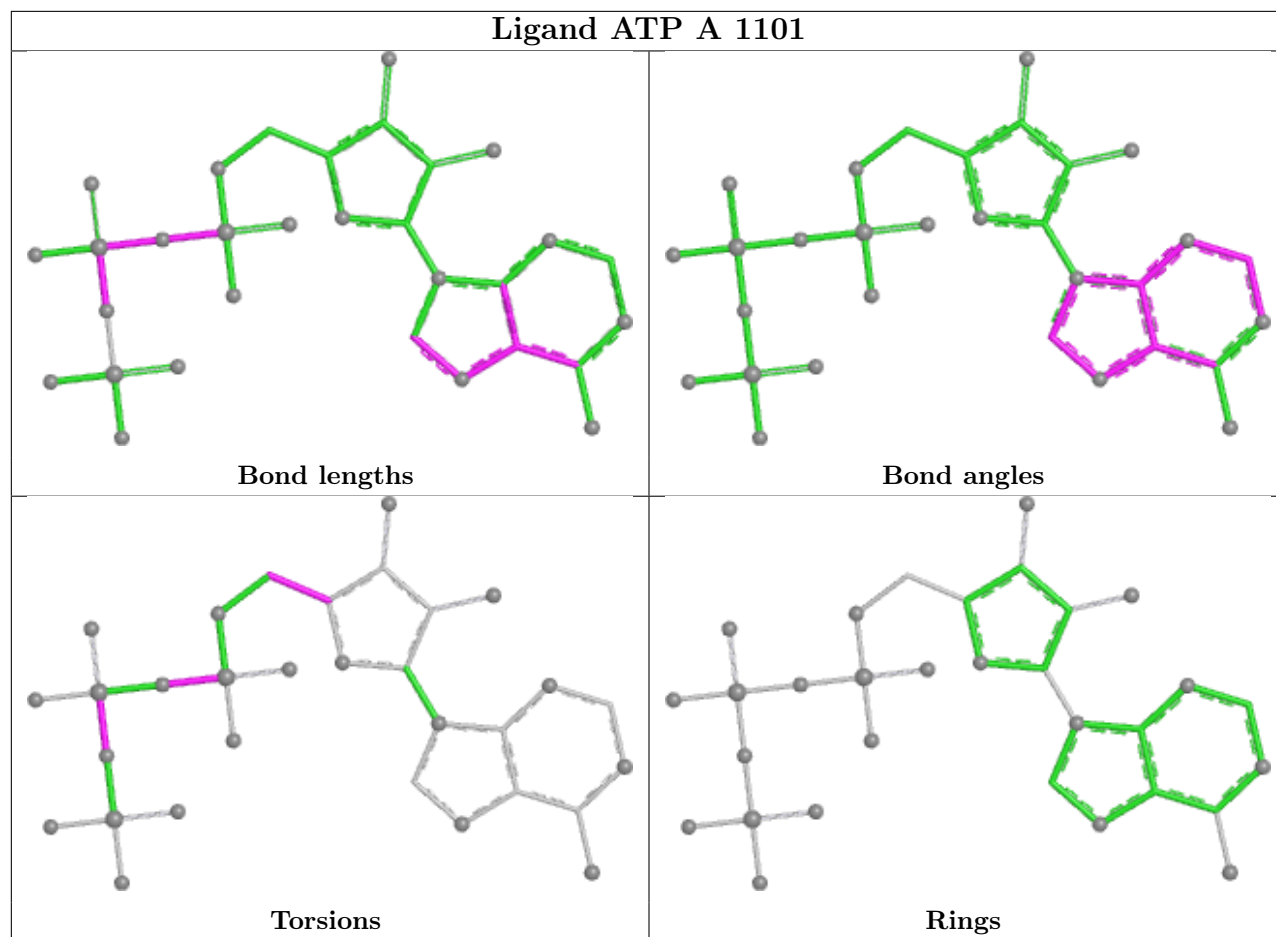
There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	201	EDO	1	0
7	A	1112	EDO	1	0
7	D	1213	EDO	1	0
6	A	1107	SO4	1	0
7	D	1212	EDO	1	0
7	D	1214	EDO	1	0
7	A	1114	EDO	1	0
6	D	1204	SO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	987/1017 (97%)	-0.03	37 (3%)	45 46	19, 33, 77, 152	0
1	D	987/1017 (97%)	0.32	103 (10%)	11 11	19, 39, 100, 137	0
2	B	78/85 (91%)	0.63	4 (5%)	33 33	23, 53, 81, 95	0
2	E	77/85 (90%)	1.03	13 (16%)	4 4	24, 59, 95, 106	0
3	C	170/197 (86%)	1.45	40 (23%)	2 1	43, 66, 104, 139	0
3	F	167/197 (84%)	1.69	48 (28%)	1 1	52, 79, 111, 156	0
All	All	2466/2598 (94%)	0.38	245 (9%)	13 13	19, 40, 98, 156	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	141	ALA	6.4
3	F	105	PRO	6.1
3	C	143	VAL	5.7
1	A	798	ILE	5.4
1	D	978	LEU	5.0
2	E	0	ALA	4.8
1	D	798	ILE	4.7
1	D	602	LEU	4.7
1	D	801	LEU	4.6
1	D	755	VAL	4.5
1	D	11	ALA	4.5
1	D	746	SER	4.4
3	C	147	VAL	4.2
1	D	980	LEU	4.2
1	D	701	THR	4.1
1	A	664	SER	4.1
3	F	89	TYR	4.1
3	F	95	CYS	3.9
1	A	648	SER	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	754	ASN	3.9
2	B	0	ALA	3.9
3	F	94	LEU	3.8
3	F	137	ILE	3.7
1	D	987	LYS	3.7
1	A	11	ALA	3.7
3	C	102	SER	3.7
1	A	801	LEU	3.6
3	C	142	ASN	3.6
1	D	704	GLY	3.5
3	C	24	LYS	3.5
1	D	698	ASP	3.5
3	C	112	ALA	3.5
1	A	655	LEU	3.5
1	D	200	ASP	3.5
1	D	930	ARG	3.5
3	F	5	LYS	3.5
1	A	746	SER	3.4
1	D	810	THR	3.3
1	D	935	GLY	3.3
3	F	102	SER	3.3
3	F	22	PRO	3.3
3	F	96	ILE	3.3
1	D	982	ILE	3.3
3	F	143	VAL	3.2
1	A	773	ASN	3.2
1	A	649	GLY	3.2
3	C	22	PRO	3.2
1	D	699	ALA	3.2
1	D	952	LEU	3.2
1	D	802	VAL	3.1
2	E	34	GLU	3.1
2	B	-1	GLY	3.1
1	A	699	ALA	3.1
1	D	702	SER	3.1
1	D	811	LEU	3.1
3	F	176	ILE	3.1
1	D	648	SER	3.1
1	A	638	PRO	3.1
3	C	23	LYS	3.1
3	C	137	ILE	3.1
3	F	26	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	25	ASN	3.0
1	D	649	GLY	3.0
1	D	979	ASN	3.0
1	D	1012	GLY	3.0
2	E	16	GLU	3.0
1	A	701	THR	3.0
1	D	933	ILE	3.0
2	E	14	THR	3.0
3	F	64	MET	3.0
3	C	6	SER	2.9
3	C	54	ILE	2.9
3	F	84	TYR	2.9
1	A	600	CYS	2.9
1	D	645	LEU	2.9
3	F	11	LEU	2.9
3	F	147	VAL	2.9
1	A	797	GLU	2.9
1	D	969	PHE	2.9
3	F	175	PHE	2.9
1	D	940	SER	2.9
3	F	19	LEU	2.9
1	D	941	ASP	2.9
3	C	176	ILE	2.9
1	A	972	LYS	2.9
2	E	23	ILE	2.8
1	A	745	LYS	2.8
3	C	152	ASN	2.8
2	E	56	LEU	2.8
1	D	944	GLU	2.8
1	D	943	ILE	2.8
3	F	142	ASN	2.8
1	A	286	PHE	2.8
3	F	24	LYS	2.8
3	F	151	LYS	2.8
1	D	664	SER	2.8
1	D	116	ASP	2.8
3	C	146	ALA	2.8
3	F	156	TYR	2.8
1	A	644	THR	2.8
1	D	971	PRO	2.8
1	D	596	SER	2.7
1	D	975	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	599	LEU	2.7
1	D	919	TYR	2.7
1	A	802	VAL	2.7
3	F	37	SER	2.7
3	C	25	ALA	2.7
1	D	965	TYR	2.7
1	D	703	ASN	2.7
1	D	773	ASN	2.7
1	D	989	VAL	2.7
1	D	751	SER	2.7
3	F	104	ASP	2.7
2	E	22	THR	2.7
1	A	639	ASN	2.7
1	D	946	PHE	2.6
3	F	66	PHE	2.6
3	C	140	PRO	2.6
1	A	747	ASP	2.6
3	C	162	MET	2.6
3	F	153	PRO	2.6
1	A	698	ASP	2.6
2	B	13	ILE	2.6
3	F	103	GLY	2.6
3	C	3	SER	2.6
2	E	17	VAL	2.6
1	D	951	GLY	2.6
3	C	145	ALA	2.6
1	A	200	ASP	2.6
1	D	981	PRO	2.6
3	F	77	PHE	2.5
3	F	25	ALA	2.5
1	D	236	PHE	2.5
1	D	1015	VAL	2.5
1	A	764	HIS	2.5
3	F	149	TYR	2.5
1	D	939	LEU	2.5
1	D	638	PRO	2.5
3	F	178	PRO	2.5
1	D	942	LEU	2.5
1	D	988	LEU	2.5
1	A	652	LYS	2.5
1	D	949	ASP	2.4
1	A	702	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	771	THR	2.4
1	D	598	PRO	2.4
1	D	968	PHE	2.4
1	D	643	GLN	2.4
3	C	53	SER	2.4
1	D	970	PRO	2.4
1	D	934	LYS	2.4
1	D	640	PHE	2.4
3	C	181	GLU	2.4
3	F	144	ASP	2.4
1	D	601	THR	2.4
1	D	990	THR	2.4
1	D	756	ASP	2.4
3	F	36	ASP	2.4
1	A	695	PHE	2.4
3	F	20	THR	2.4
1	D	953	GLU	2.3
1	D	974	LEU	2.3
1	D	1024	LEU	2.3
1	D	340	GLY	2.3
3	F	46	VAL	2.3
3	C	179	THR	2.3
1	D	1006	CYS	2.3
3	C	133	GLU	2.3
1	A	199	ASP	2.3
3	C	150	ARG	2.3
1	D	948	LYS	2.3
1	D	972	LYS	2.3
3	F	79	PHE	2.3
1	D	597	ILE	2.3
1	D	641	VAL	2.3
3	C	118	VAL	2.3
3	C	161	LYS	2.3
1	D	954	ILE	2.3
1	D	1005	ILE	2.3
1	D	771	THR	2.3
3	F	138	ASN	2.3
1	D	600	CYS	2.3
1	D	945	HIS	2.2
3	C	154	GLU	2.2
3	C	139	SER	2.2
3	F	139	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	31	ILE	2.2
1	A	971	PRO	2.2
1	A	169	ASP	2.2
1	D	655	LEU	2.2
1	D	976	GLU	2.2
1	D	984	GLN	2.2
1	D	1018	PRO	2.2
3	C	178	PRO	2.2
3	F	23	LYS	2.2
3	F	83	ILE	2.2
1	D	747	ASP	2.2
3	F	162	MET	2.2
1	A	595	LYS	2.2
1	D	244	LYS	2.2
1	D	799	ASP	2.2
1	D	994	ILE	2.2
3	F	121	VAL	2.2
2	E	53	GLY	2.2
1	A	645	LEU	2.2
3	C	95	CYS	2.2
1	D	535	SER	2.2
3	C	156	TYR	2.2
3	C	151	LYS	2.2
3	C	177	MET	2.2
3	F	115	TRP	2.2
1	D	753	PRO	2.1
1	D	1008	ASP	2.2
1	D	651	VAL	2.1
3	C	129	VAL	2.1
1	D	812	ALA	2.1
1	D	1007	ALA	2.1
3	F	141	ALA	2.1
1	D	531	SER	2.1
1	D	809	SER	2.1
3	C	144	ASP	2.1
2	E	55	THR	2.1
1	A	704	GLY	2.1
2	E	26	VAL	2.1
3	F	92	GLY	2.1
1	D	967	SER	2.1
3	F	38	ASN	2.1
1	D	806	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	140	PRO	2.1
2	E	35	GLY	2.1
3	C	26	ILE	2.1
1	D	931	PHE	2.1
1	D	973	LYS	2.1
1	A	979	ASN	2.1
1	D	201	ASN	2.1
1	D	647	GLN	2.1
1	D	938	LYS	2.1
3	C	180	SER	2.1
1	A	650	ASP	2.0
2	B	11	ARG	2.0
1	D	654	VAL	2.0
1	A	752	LYS	2.0
3	C	5	LYS	2.0
3	C	84	TYR	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
6	SO4	A	1105	5/5	0.63	0.19	138,140,140,140	0
6	SO4	A	1103	5/5	0.66	0.17	105,106,107,108	0
6	SO4	D	1209	5/5	0.69	0.13	99,101,102,103	0
6	SO4	A	1107	5/5	0.71	0.21	122,124,125,127	0
6	SO4	A	1104	5/5	0.74	0.20	137,138,139,140	0
6	SO4	D	1208	5/5	0.75	0.16	68,72,76,76	0
6	SO4	D	1207	5/5	0.75	0.13	82,85,86,87	0

Continued on next page...

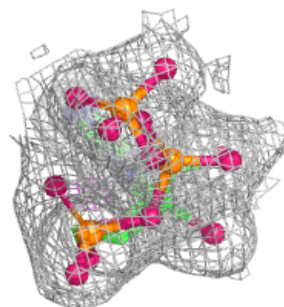
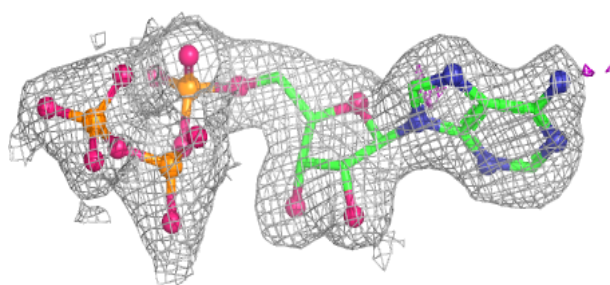
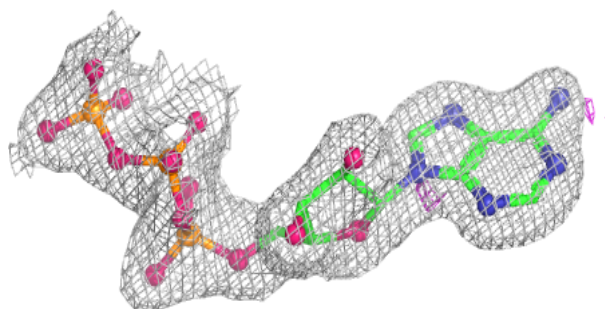
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	1206	5/5	0.77	0.13	91,93,96,98	0
7	EDO	A	1112	4/4	0.80	0.18	42,47,49,57	0
7	EDO	A	1121	4/4	0.80	0.16	64,66,68,69	0
7	EDO	D	1218	4/4	0.80	0.21	57,59,60,60	0
6	SO4	D	1203	5/5	0.81	0.24	126,127,129,130	0
6	SO4	A	1110	5/5	0.81	0.13	82,85,86,89	0
7	EDO	A	1119	4/4	0.82	0.17	51,51,56,60	0
6	SO4	D	1205	5/5	0.82	0.14	105,105,106,107	0
6	SO4	A	1108	5/5	0.82	0.14	61,72,78,78	0
7	EDO	A	1116	4/4	0.83	0.18	47,48,49,55	0
6	SO4	A	1109	5/5	0.83	0.14	86,88,92,93	0
7	EDO	A	1117	4/4	0.84	0.18	53,56,56,60	0
7	EDO	A	1115	4/4	0.84	0.18	46,51,51,52	0
7	EDO	D	1211	4/4	0.85	0.18	49,49,52,57	0
7	EDO	D	1213	4/4	0.86	0.16	42,45,51,51	0
7	EDO	D	1214	4/4	0.86	0.17	58,58,61,65	0
6	SO4	A	1106	5/5	0.86	0.22	110,111,111,113	0
6	SO4	D	1204	5/5	0.87	0.18	120,121,121,122	0
7	EDO	D	1217	4/4	0.87	0.15	47,51,52,52	0
7	EDO	D	1210	4/4	0.87	0.14	36,37,40,43	0
7	EDO	A	1118	4/4	0.88	0.15	33,38,49,60	0
7	EDO	D	1212	4/4	0.88	0.15	51,54,57,61	0
7	EDO	A	1111	4/4	0.91	0.10	27,28,34,36	0
7	EDO	D	1215	4/4	0.91	0.13	52,56,63,68	0
7	EDO	A	1113	4/4	0.92	0.13	32,38,42,45	0
7	EDO	A	1114	4/4	0.92	0.14	46,47,48,55	0
7	EDO	A	1120	4/4	0.93	0.10	34,42,43,45	0
7	EDO	D	1216	4/4	0.93	0.11	30,39,42,43	0
7	EDO	C	201	4/4	0.96	0.07	44,44,44,45	0
4	ATP	A	1101	31/31	0.98	0.04	18,24,28,31	0
4	ATP	D	1202	31/31	0.99	0.05	18,28,36,38	0
5	MG	A	1102	1/1	0.99	0.04	24,24,24,24	0
5	MG	D	1201	1/1	0.99	0.02	31,31,31,31	0

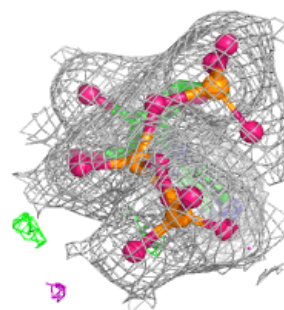
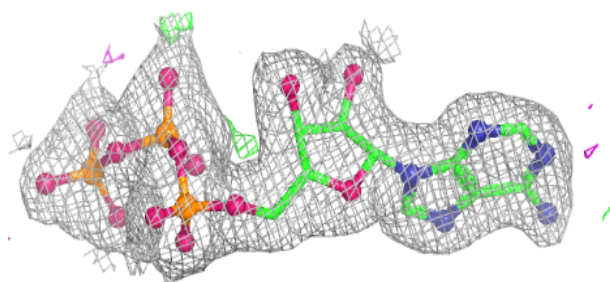
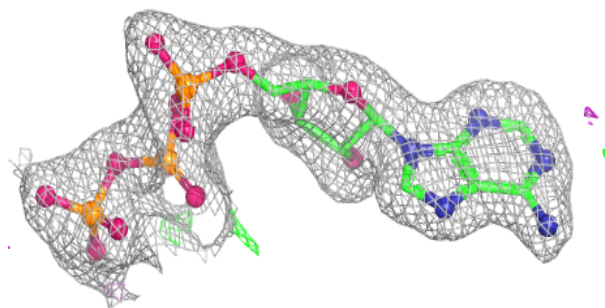
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP D 1202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.