



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:19 AM BST

PDB ID : 6DT1
Title : Crystal structure of the ligase from bacteriophage T4 complexed with DNA intermediate
Authors : Shi, K.; Aihara, H.
Deposited on : 2018-06-14
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

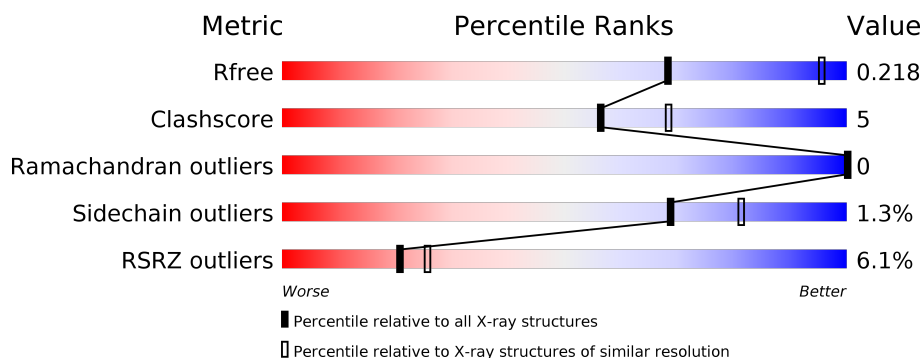
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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	507	<div> <div>80%</div> <div>11%</div> <div>8%</div> </div>
1	E	507	<div> <div>12%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>
2	B	11	<div> <div>45%</div> <div>55%</div> </div>
2	F	11	<div> <div>36%</div> <div>55%</div> <div>9%</div> </div>
3	C	10	<div> <div>70%</div> <div>30%</div> </div>
3	G	10	<div> <div>70%</div> <div>30%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	21	 <div>62%38%</div>
4	H	21	 <div>62%38%</div>

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
8	CL	A	516	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9524 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 DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	1	0
			3711	2365	631	699	16			
1	E	459	Total	C	N	O	S	0	0	0
			3660	2335	621	688	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P00970
A	-18	GLY	-	expression tag	UNP P00970
A	-17	SER	-	expression tag	UNP P00970
A	-16	SER	-	expression tag	UNP P00970
A	-15	HIS	-	expression tag	UNP P00970
A	-14	HIS	-	expression tag	UNP P00970
A	-13	HIS	-	expression tag	UNP P00970
A	-12	HIS	-	expression tag	UNP P00970
A	-11	HIS	-	expression tag	UNP P00970
A	-10	HIS	-	expression tag	UNP P00970
A	-9	SER	-	expression tag	UNP P00970
A	-8	SER	-	expression tag	UNP P00970
A	-7	GLY	-	expression tag	UNP P00970
A	-6	LEU	-	expression tag	UNP P00970
A	-5	VAL	-	expression tag	UNP P00970
A	-4	PRO	-	expression tag	UNP P00970
A	-3	ARG	-	expression tag	UNP P00970
A	-2	GLY	-	expression tag	UNP P00970
A	-1	SER	-	expression tag	UNP P00970
A	0	HIS	-	expression tag	UNP P00970
E	-19	MET	-	initiating methionine	UNP P00970
E	-18	GLY	-	expression tag	UNP P00970
E	-17	SER	-	expression tag	UNP P00970
E	-16	SER	-	expression tag	UNP P00970
E	-15	HIS	-	expression tag	UNP P00970

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP P00970
E	-13	HIS	-	expression tag	UNP P00970
E	-12	HIS	-	expression tag	UNP P00970
E	-11	HIS	-	expression tag	UNP P00970
E	-10	HIS	-	expression tag	UNP P00970
E	-9	SER	-	expression tag	UNP P00970
E	-8	SER	-	expression tag	UNP P00970
E	-7	GLY	-	expression tag	UNP P00970
E	-6	LEU	-	expression tag	UNP P00970
E	-5	VAL	-	expression tag	UNP P00970
E	-4	PRO	-	expression tag	UNP P00970
E	-3	ARG	-	expression tag	UNP P00970
E	-2	GLY	-	expression tag	UNP P00970
E	-1	SER	-	expression tag	UNP P00970
E	0	HIS	-	expression tag	UNP P00970

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*TP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total 222	C 107	N 40	O 65	P 10	0	0	0
2	F	11	Total 222	C 107	N 40	O 65	P 10	0	0	0

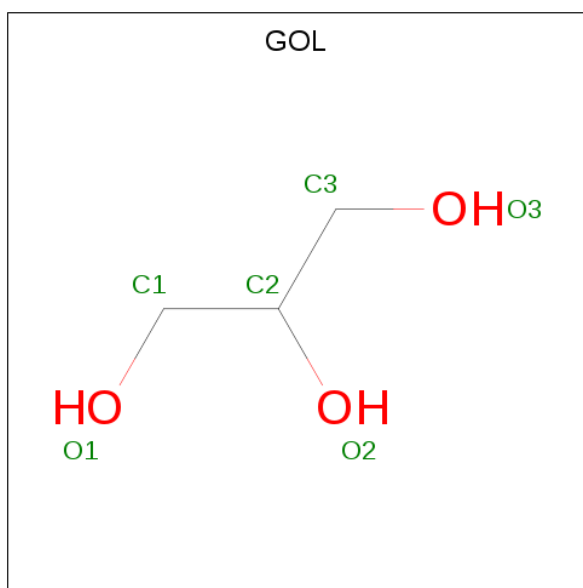
- Molecule 3 is a DNA chain called DNA (5'-D((AMP)*GP*TP*CP*GP*GP*AP*CP*TP*GP*AP*)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total 208	C 98	N 40	O 60	P 10	0	0	0
3	G	10	Total 208	C 98	N 40	O 60	P 10	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*CP*AP*GP*TP*CP*CP*GP*AP*CP*GP*AP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3').

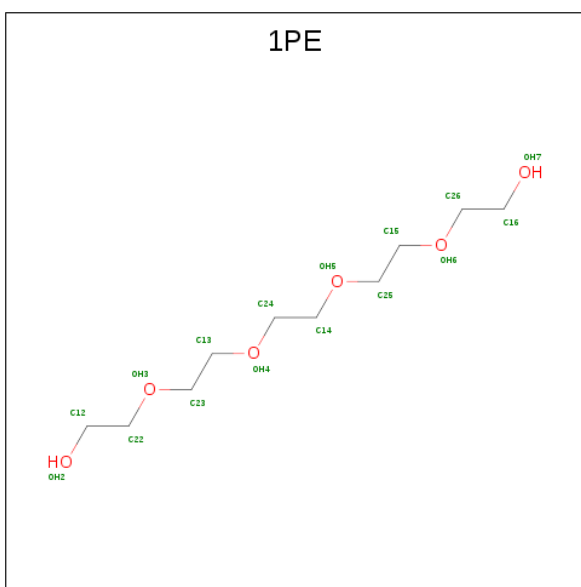
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	21	Total 424	C 202	N 80	O 122	P 20	0	0	0
4	H	21	Total 424	C 202	N 80	O 122	P 20	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



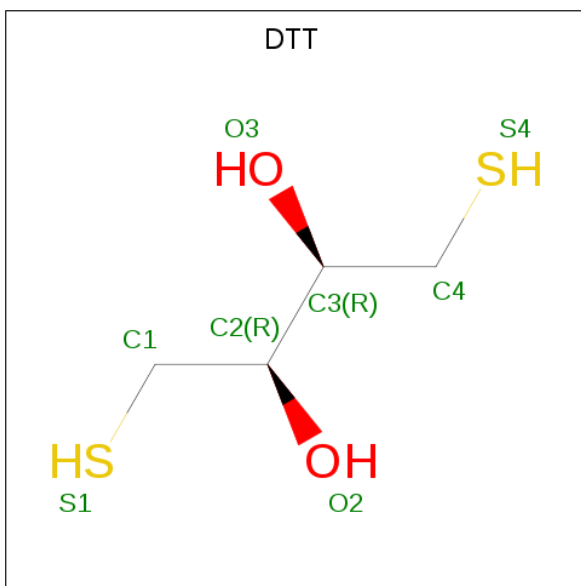
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			8	4	2	2		
7	A	1	Total	C	O	S	0	0
			8	4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			8	4	2	2		
7	D	1	Total	C	O	S	0	0
			8	4	2	2		
7	D	1	Total	C	O	S	0	0
			8	4	2	2		

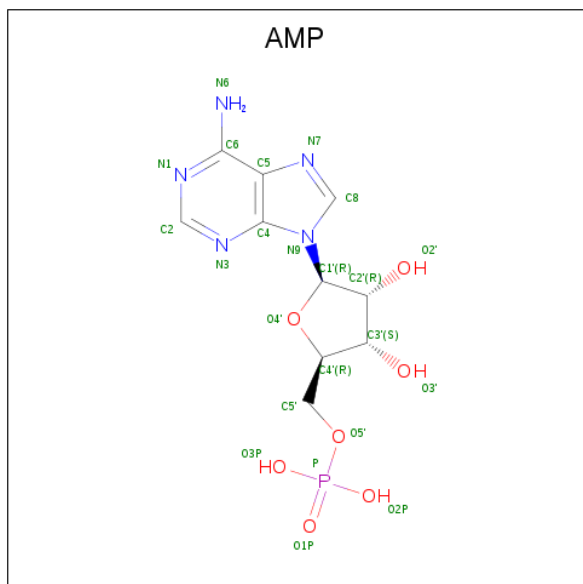
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	E	1	Total	Cl	0	0
			1	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

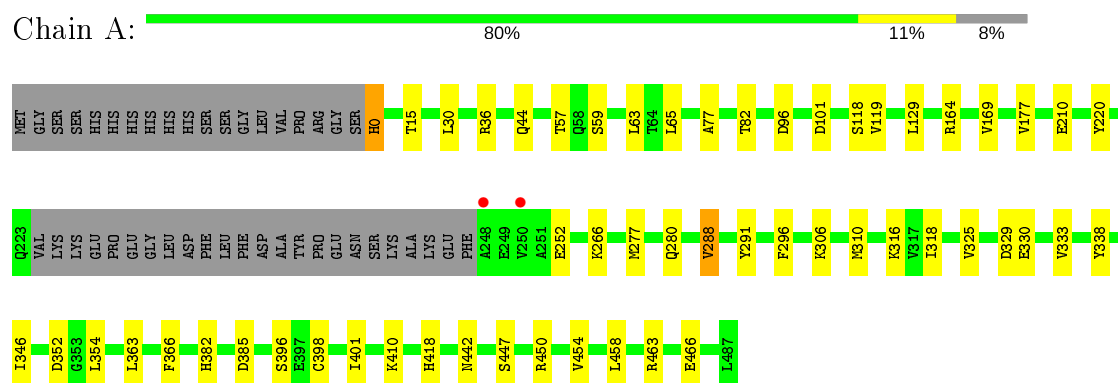
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	170	Total	O	0	1
			171	171		
11	E	13	Total	O	0	0
			13	13		
11	B	23	Total	O	0	0
			23	23		
11	C	22	Total	O	0	0
			22	22		
11	D	29	Total	O	0	0
			29	29		
11	F	2	Total	O	0	0
			2	2		
11	H	8	Total	O	0	0
			8	8		

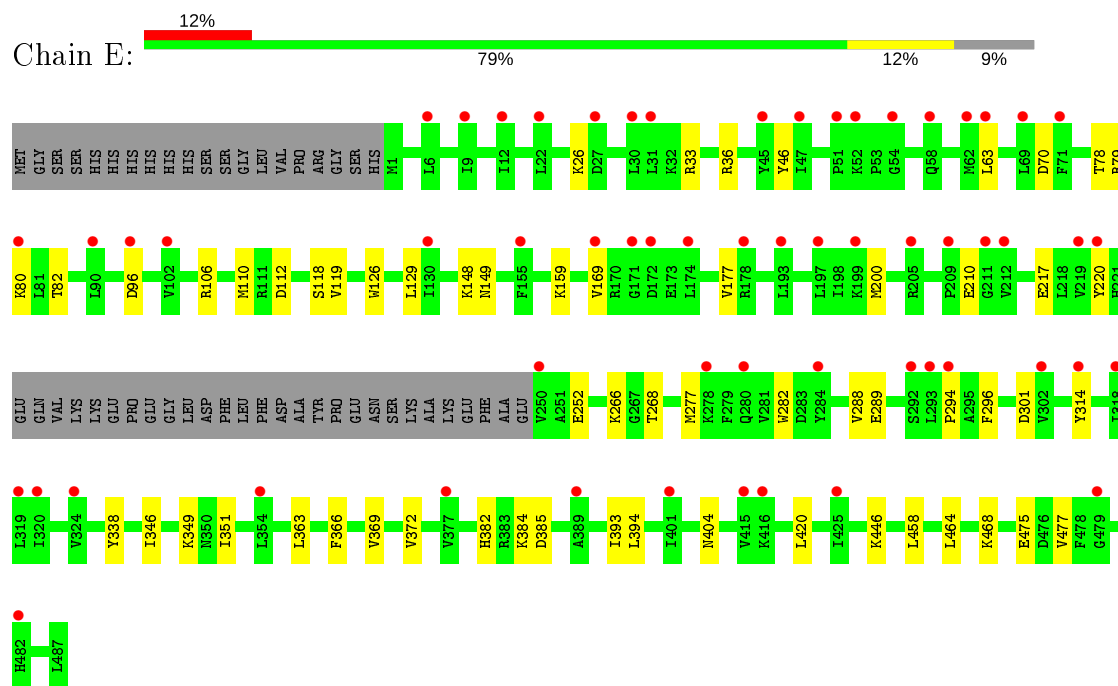
3 Residue-property plots

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: DNA ligase

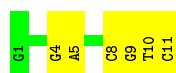


- Molecule 1: DNA ligase

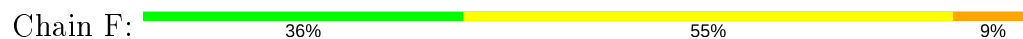


- Molecule 2: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*TP*(DOC))-3')





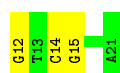
- Molecule 2: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*TP*(DOC))-3')



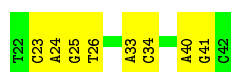
- Molecule 3: DNA (5'-D((AMP)*GP*TP*CP*GP*GP*AP*CP*TP*GP*AP*))-3')



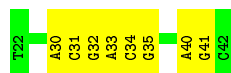
- Molecule 3: DNA (5'-D((AMP)*GP*TP*CP*GP*GP*AP*CP*TP*GP*AP*))-3')



- Molecule 4: DNA (5'-D(*TP*CP*AP*GP*TP*CP*CP*GP*AP*CP*GP*AP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3')



- Molecule 4: DNA (5'-D(*TP*CP*AP*GP*TP*CP*CP*GP*AP*CP*GP*AP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.53Å 67.43Å 114.64Å 88.78° 80.94° 62.97°	Depositor
Resolution (Å)	113.02 – 2.75 113.02 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (113.02-2.75) 98.6 (113.02-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.14rc1_3177: ???)	Depositor
R, R_{free}	0.170 , 0.219 0.170 , 0.218	Depositor DCC
R_{free} test set	2155 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9524	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: GOL, MG, CL, DOC, 1PE, AMP, DTT

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	0.36	0/3771	0.54	0/5071
1	E	0.27	0/3719	0.45	0/5002
2	B	0.82	0/228	0.97	0/351
2	F	0.79	0/228	1.04	0/351
3	C	0.80	0/233	0.91	0/358
3	G	0.70	0/233	0.88	0/358
4	D	0.81	0/475	0.92	0/730
4	H	0.70	0/475	0.89	0/730
All	All	0.44	0/9362	0.62	0/12951

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3711	0	3785	34	0
1	E	3660	0	3739	34	0
2	B	222	0	126	4	0
2	F	222	0	126	7	0
3	C	208	0	113	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	208	0	113	2	0
4	D	424	0	236	5	0
4	H	424	0	236	6	0
5	A	72	0	96	3	0
6	A	16	0	22	3	0
7	A	16	0	20	1	0
7	B	8	0	10	0	0
7	D	16	0	20	1	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
9	A	1	0	0	0	0
10	C	23	0	12	1	0
10	E	23	0	11	1	0
11	A	171	0	0	3	0
11	B	23	0	0	1	0
11	C	22	0	0	1	0
11	D	29	0	0	1	0
11	E	13	0	0	0	0
11	F	2	0	0	0	0
11	H	8	0	0	0	0
All	All	9524	0	8665	89	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 5.

All (89) 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:E:112:ASP:OD2	1:E:384:LYS:NZ	2.17	0.77
1:A:57:THR:HG23	1:A:59:SER:H	1.51	0.73
1:A:398:CYS:SG	11:A:768:HOH:O	2.46	0.72
3:C:12:DG:OP1	11:C:201:HOH:O	2.08	0.72
4:H:33:DA:H2'	4:H:34:DC:C6	2.28	0.69
4:D:41:DG:N7	11:D:501:HOH:O	2.26	0.68
1:E:220:TYR:HD2	1:E:252:GLU:HG3	1.59	0.68
1:A:82:THR:HA	6:A:506:1PE:H121	1.77	0.67
1:A:325:VAL:HG23	1:A:330:GLU:HB2	1.77	0.67
7:A:513:DTT:H41	7:A:513:DTT:S1	2.35	0.66
1:A:210:GLU:HG3	1:A:288:VAL:HG13	1.79	0.63
2:B:9:DG:H2'	2:B:10:DT:C6	2.32	0.63
1:E:63:LEU:HD22	1:E:96:ASP:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TYR:HD2	1:A:252:GLU:HG3	1.66	0.61
2:F:9:DG:H2'	2:F:10:DT:C6	2.38	0.58
2:B:4:DG:N3	11:B:501:HOH:O	2.33	0.55
1:E:346:ILE:HG12	1:E:366:PHE:HB2	1.89	0.55
4:D:33:DA:H2'	4:D:34:DC:C6	2.42	0.54
2:F:4:DG:H2''	2:F:5:DA:H8	1.73	0.54
1:E:382:HIS:HE2	4:H:30:DA:H4'	1.72	0.53
1:A:354:LEU:HB2	5:A:509:GOL:H32	1.90	0.53
1:E:266:LYS:HB2	1:E:268:THR:HG22	1.90	0.52
4:D:40:DA:H2''	4:D:41:DG:H5''	1.90	0.52
1:A:410:LYS:HG3	1:A:418:HIS:CG	2.45	0.52
1:A:266:LYS:NZ	6:A:506:1PE:H161	2.25	0.51
4:H:40:DA:H2''	4:H:41:DG:H5''	1.93	0.51
2:F:11:DOC:C2	4:H:32:DG:H22	2.23	0.51
1:A:442:ASN:HB2	1:A:458:LEU:HD12	1.92	0.50
1:E:393:ILE:HA	1:E:404:ASN:HD22	1.76	0.50
1:E:169:VAL:HG13	1:E:177:VAL:HG22	1.94	0.50
1:E:79:ARG:HE	1:E:82:THR:HG22	1.76	0.50
1:A:291:TYR:HB2	5:A:504:GOL:H32	1.94	0.49
1:A:169:VAL:HG13	1:A:177:VAL:HG22	1.95	0.48
1:A:0:HIS:N	1:A:101:ASP:OD1	2.47	0.48
1:E:289:GLU:HA	1:E:294:PRO:HG3	1.96	0.48
1:E:118:SER:OG	1:E:119:VAL:N	2.46	0.47
1:A:36:ARG:HB2	1:A:129:LEU:HD11	1.97	0.47
3:G:14:DC:H2''	3:G:15:DG:C8	2.50	0.47
2:F:6:DT:H4'	2:F:7:DG:OP1	2.14	0.47
1:A:63:LEU:HD22	1:A:96:ASP:HB2	1.96	0.47
1:E:210:GLU:HG3	1:E:288:VAL:HG13	1.97	0.46
1:E:46:TYR:CE2	1:E:79:ARG:HD3	2.51	0.46
1:A:316:LYS:HD3	11:A:606:HOH:O	2.14	0.46
1:A:396:SER:HB3	1:A:401:ILE:HB	1.96	0.46
2:F:4:DG:H4'	2:F:5:DA:OP1	2.15	0.46
1:E:220:TYR:HD1	1:E:277:MET:HE2	1.81	0.46
1:E:301:ASP:HB2	1:E:351:ILE:HG22	1.97	0.45
2:F:4:DG:H2''	2:F:5:DA:C8	2.50	0.45
1:A:44:GLN:O	1:A:77:ALA:HA	2.17	0.45
1:E:36:ARG:HB2	1:E:129:LEU:HD11	1.98	0.45
1:E:33:ARG:NH2	1:E:70:ASP:OD1	2.39	0.44
1:E:458:LEU:HD22	3:G:12:DG:H2''	1.99	0.44
1:A:164:ARG:HD3	10:C:100:AMP:O2'	2.18	0.44
1:E:338:TYR:HD2	1:E:346:ILE:HG22	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:HE1	1:E:369:VAL:HB	1.82	0.44
1:E:106:ARG:O	1:E:110:MET:HG2	2.18	0.43
1:A:306:LYS:O	1:A:310:MET:HB2	2.19	0.43
1:E:78:THR:OG1	1:E:80:LYS:HG2	2.18	0.43
2:B:4:DG:H2''	2:B:5:DA:O5'	2.19	0.43
1:A:410:LYS:HE2	11:A:655:HOH:O	2.19	0.42
1:E:420:LEU:HD21	1:E:464:LEU:HG	2.01	0.42
4:H:30:DA:H2'	4:H:31:DC:C6	2.54	0.42
1:A:63:LEU:HD21	5:A:507:GOL:H2	2.01	0.42
1:E:46:TYR:HA	2:F:7:DG:O3'	2.19	0.42
1:E:26:LYS:HA	1:E:126:TRP:CZ2	2.54	0.42
4:D:25:DG:C8	4:D:26:DT:H72	2.54	0.42
1:E:220:TYR:CD2	1:E:252:GLU:HG3	2.47	0.42
1:E:159:LYS:HA	10:E:501:AMP:N7	2.34	0.42
1:E:349:LYS:HG2	1:E:363:LEU:HD22	2.02	0.42
1:A:447:SER:HB3	1:A:450:ARG:CZ	2.50	0.42
1:E:382:HIS:HB3	1:E:385:ASP:O	2.20	0.41
3:C:19:DT:H2''	3:C:20:DG:C8	2.56	0.41
4:H:34:DC:H2''	4:H:35:DG:C8	2.55	0.41
1:E:217:GLU:HB2	1:E:282:TRP:HZ3	1.85	0.41
1:E:372:VAL:HG23	1:E:477:VAL:HG21	2.02	0.41
1:A:15:THR:HG21	7:D:401:DTT:S1	2.60	0.41
1:A:30:LEU:HD21	1:A:65:LEU:HD23	2.03	0.41
1:A:346:ILE:HG12	1:A:366:PHE:HB2	2.03	0.41
1:E:148:LYS:HD2	1:E:149:ASN:OD1	2.21	0.41
1:E:200:MET:HB3	1:E:314:TYR:CZ	2.55	0.41
1:A:338:TYR:HD2	1:A:346:ILE:HG22	1.85	0.41
1:A:329:ASP:O	1:A:333:VAL:HG23	2.21	0.41
1:A:382:HIS:HB3	1:A:385:ASP:O	2.21	0.41
1:A:118:SER:OG	1:A:119:VAL:N	2.53	0.41
1:A:220:TYR:HD1	1:A:277:MET:HE2	1.86	0.41
1:A:352:ASP:OD2	1:E:468:LYS:NZ	2.33	0.40
6:A:506:1PE:H152	2:B:8:DC:H4'	2.02	0.40
1:A:280:GLN:HA	1:A:318:ILE:O	2.22	0.40
4:D:23:DC:H2''	4:D:24:DA:C8	2.56	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	461/507 (91%)	448 (97%)	13 (3%)	0	100	100
1	E	455/507 (90%)	443 (97%)	12 (3%)	0	100	100
All	All	916/1014 (90%)	891 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	401/437 (92%)	395 (98%)	6 (2%)	65	78
1	E	396/437 (91%)	392 (99%)	4 (1%)	76	85
All	All	797/874 (91%)	787 (99%)	10 (1%)	69	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	288	VAL
1	A	363	LEU
1	A	454	VAL
1	A	463	ARG
1	A	466	GLU
1	E	296	PHE
1	E	394	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	446	LYS
1	E	475	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	GLN
1	E	404	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	DOC	B	11	2,4	14,19,20	3.00	1 (7%)	13,26,29	2.19	5 (38%)
2	DOC	F	11	2,4	14,19,20	3.13	2 (14%)	13,26,29	2.15	6 (46%)

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
2	DOC	B	11	2,4	-	1/4/18/19	0/2/2/2
2	DOC	F	11	2,4	-	1/4/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	11	DOC	C6-N1	10.99	1.49	1.35
2	B	11	DOC	C6-N1	10.70	1.49	1.35
2	F	11	DOC	C4-N3	2.72	1.40	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	11	DOC	C4'-O4'-C1'	-4.26	105.79	109.81
2	F	11	DOC	C4'-O4'-C1'	-3.98	106.05	109.81
2	B	11	DOC	C2-N3-C4	3.45	119.84	116.34
2	B	11	DOC	C2'-C3'-C4'	-3.10	96.92	102.72
2	F	11	DOC	C2-N3-C4	2.92	119.30	116.34
2	B	11	DOC	C5-C6-N1	-2.83	114.37	120.68
2	F	11	DOC	C5-C6-N1	-2.82	114.38	120.68
2	F	11	DOC	O4'-C4'-C3'	-2.80	100.16	104.80
2	F	11	DOC	C2'-C3'-C4'	-2.57	97.91	102.72
2	B	11	DOC	O4'-C4'-C3'	-2.43	100.77	104.80
2	F	11	DOC	N4-C4-N3	2.25	120.04	116.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	11	DOC	O4'-C4'-C5'-O5'
2	B	11	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	11	DOC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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
10	AMP	C	100	3	22,25,25	0.89	1 (4%)	25,38,38	1.38	6 (24%)
5	GOL	A	505	-	5,5,5	0.99	0	5,5,5	0.90	0
5	GOL	A	504	-	5,5,5	0.85	0	5,5,5	0.97	0
7	DTT	B	401	-	7,7,7	0.74	0	4,8,8	0.79	0
5	GOL	A	503	-	5,5,5	1.16	0	5,5,5	0.81	0
5	GOL	A	511	-	5,5,5	0.90	0	5,5,5	1.05	0
10	AMP	E	501	3	22,25,25	0.87	1 (4%)	25,38,38	1.43	4 (16%)
5	GOL	A	502	-	5,5,5	1.24	0	5,5,5	0.76	0
7	DTT	D	401	-	7,7,7	0.58	0	4,8,8	0.57	0
5	GOL	A	515	-	5,5,5	1.04	0	5,5,5	0.92	0
7	DTT	D	402	-	7,7,7	0.67	0	4,8,8	0.74	0
5	GOL	A	508	-	5,5,5	0.98	0	5,5,5	0.97	0
5	GOL	A	510	-	5,5,5	1.04	0	5,5,5	0.89	0
7	DTT	A	513	-	7,7,7	0.78	0	4,8,8	0.73	0
5	GOL	A	507	-	5,5,5	0.87	0	5,5,5	1.06	0
6	1PE	A	506	-	15,15,15	0.56	0	14,14,14	0.39	0
5	GOL	A	514	-	5,5,5	0.99	0	5,5,5	0.96	0
7	DTT	A	512	-	7,7,7	0.74	0	4,8,8	0.22	0
5	GOL	A	509	-	5,5,5	1.03	0	5,5,5	0.87	0
5	GOL	A	501	-	5,5,5	1.04	0	5,5,5	0.97	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
10	AMP	C	100	3	-	1/6/26/26	0/3/3/3
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	A	504	-	-	2/4/4/4	-
7	DTT	B	401	-	-	0/8/8/8	-
5	GOL	A	503	-	-	0/4/4/4	-
5	GOL	A	511	-	-	0/4/4/4	-
10	AMP	E	501	3	-	1/6/26/26	0/3/3/3
5	GOL	A	502	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DTT	D	401	-	-	0/8/8/8	-
5	GOL	A	515	-	-	0/4/4/4	-
7	DTT	D	402	-	-	0/8/8/8	-
5	GOL	A	508	-	-	2/4/4/4	-
5	GOL	A	510	-	-	2/4/4/4	-
7	DTT	A	513	-	-	0/8/8/8	-
5	GOL	A	507	-	-	0/4/4/4	-
6	1PE	A	506	-	-	9/13/13/13	-
5	GOL	A	514	-	-	2/4/4/4	-
7	DTT	A	512	-	-	0/8/8/8	-
5	GOL	A	509	-	-	3/4/4/4	-
5	GOL	A	501	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	501	AMP	C5-C4	2.55	1.47	1.40
10	C	100	AMP	C5-C4	2.30	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	501	AMP	O3P-P-O2P	3.42	120.72	107.64
10	C	100	AMP	N3-C2-N1	-3.18	123.71	128.68
10	E	501	AMP	N3-C2-N1	-3.07	123.87	128.68
10	E	501	AMP	O3P-P-O5'	-2.76	99.38	106.73
10	C	100	AMP	N6-C6-N1	2.59	123.94	118.57
10	E	501	AMP	C4-C5-N7	-2.43	106.87	109.40
10	C	100	AMP	O2P-P-O1P	2.17	119.17	110.68
10	C	100	AMP	O2P-P-O5'	-2.04	101.30	106.73
10	C	100	AMP	O3P-P-O2P	2.03	115.41	107.64
10	C	100	AMP	C3'-C2'-C1'	2.03	104.03	100.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	509	GOL	O1-C1-C2-O2
5	A	509	GOL	O1-C1-C2-C3
5	A	508	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	510	GOL	C1-C2-C3-O3
5	A	514	GOL	O2-C2-C3-O3
5	A	505	GOL	O2-C2-C3-O3
5	A	505	GOL	C1-C2-C3-O3
5	A	514	GOL	C1-C2-C3-O3
5	A	508	GOL	O2-C2-C3-O3
10	E	501	AMP	C4'-C5'-O5'-P
5	A	510	GOL	O2-C2-C3-O3
6	A	506	1PE	OH6-C15-C25-OH5
6	A	506	1PE	C13-C23-OH3-C22
5	A	504	GOL	O1-C1-C2-O2
10	C	100	AMP	C4'-C5'-O5'-P
6	A	506	1PE	C12-C22-OH3-C23
5	A	509	GOL	C1-C2-C3-O3
6	A	506	1PE	C24-C14-OH5-C25
6	A	506	1PE	C15-C25-OH5-C14
6	A	506	1PE	C14-C24-OH4-C13
5	A	504	GOL	O1-C1-C2-C3
6	A	506	1PE	C25-C15-OH6-C26
6	A	506	1PE	OH5-C14-C24-OH4
6	A	506	1PE	OH4-C13-C23-OH3

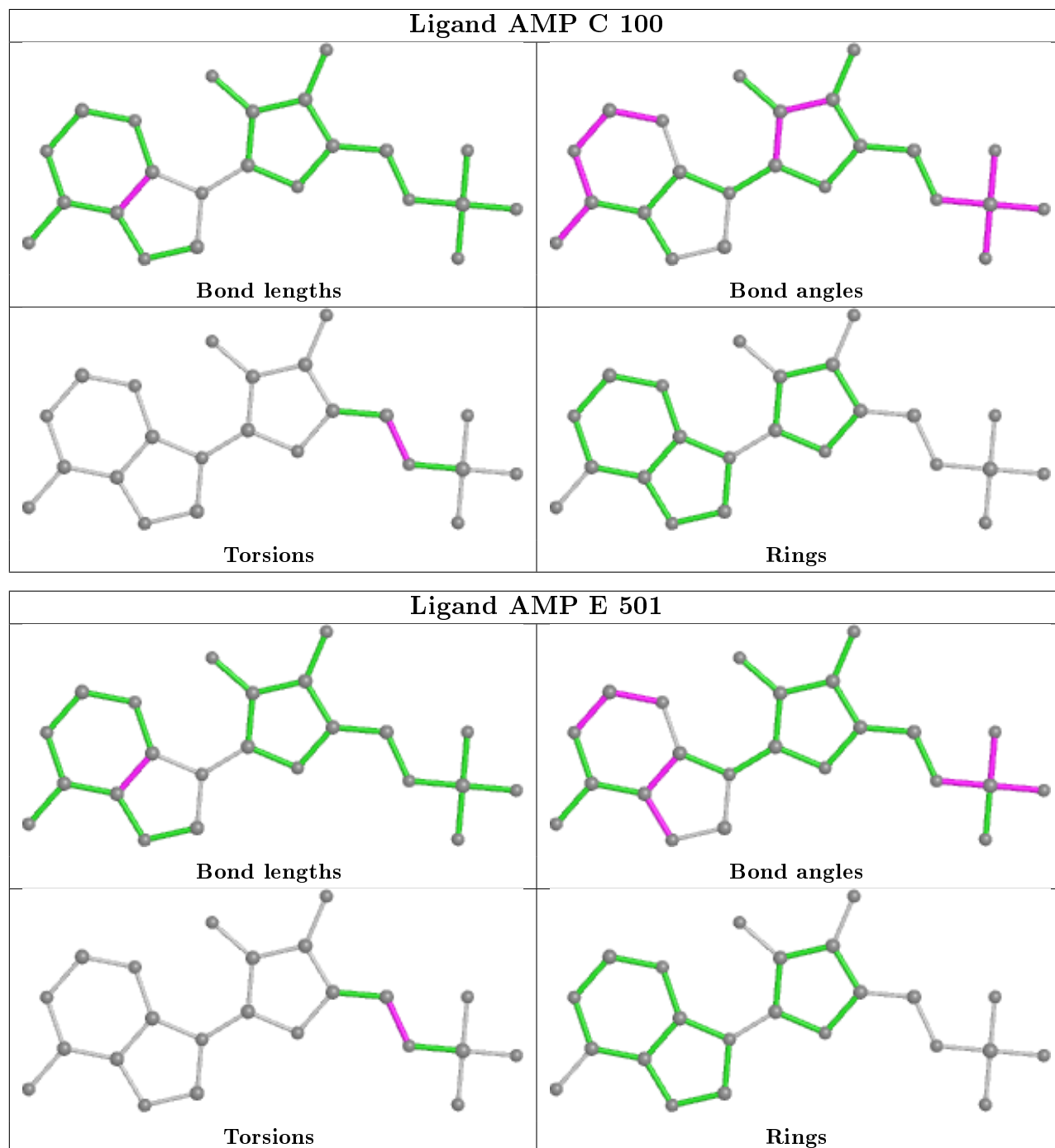
There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	100	AMP	1	0
5	A	504	GOL	1	0
10	E	501	AMP	1	0
7	D	401	DTT	1	0
7	A	513	DTT	1	0
5	A	507	GOL	1	0
6	A	506	1PE	3	0
5	A	509	GOL	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 ⓘ

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	464/507 (91%)	0.25	2 (0%) 92 95	28, 47, 80, 130	0
1	E	459/507 (90%)	0.89	59 (12%) 3 4	58, 106, 155, 178	0
2	B	10/11 (90%)	0.06	0 100 100	36, 41, 64, 68	0
2	F	10/11 (90%)	-0.25	0 100 100	70, 77, 88, 89	0
3	C	10/10 (100%)	0.17	0 100 100	32, 40, 78, 89	0
3	G	10/10 (100%)	-0.10	0 100 100	60, 76, 91, 101	0
4	D	21/21 (100%)	0.15	0 100 100	34, 40, 77, 98	0
4	H	21/21 (100%)	-0.22	0 100 100	58, 78, 94, 116	0
All	All	1005/1098 (91%)	0.52	61 (6%) 21 26	28, 74, 143, 178	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	51	PRO	5.0
1	E	102	VAL	4.9
1	E	284	TYR	4.9
1	E	63	LEU	4.6
1	E	22	LEU	4.4
1	E	209	PRO	4.3
1	E	293	LEU	4.2
1	E	12	ILE	4.0
1	E	58	GLN	3.7
1	E	479	GLY	3.5
1	E	389	ALA	3.5
1	E	52	LYS	3.5
1	E	171	GLY	3.4
1	E	193	LEU	3.4
1	E	250	VAL	3.4
1	E	69	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	278	LYS	3.3
1	E	320	ILE	3.3
1	E	416	LYS	3.2
1	E	96	ASP	3.2
1	E	174	LEU	3.2
1	E	62	MET	3.1
1	E	54	GLY	3.1
1	E	199	LYS	3.1
1	E	130	ILE	3.0
1	E	324	VAL	2.9
1	A	248	ALA	2.8
1	E	90	LEU	2.8
1	E	377	VAL	2.8
1	E	178	ARG	2.8
1	E	169	VAL	2.7
1	E	212	VAL	2.7
1	E	425	ILE	2.7
1	A	250	VAL	2.6
1	E	211	GLY	2.4
1	E	292	SER	2.4
1	E	220	TYR	2.3
1	E	314	TYR	2.3
1	E	415	VAL	2.3
1	E	319	LEU	2.3
1	E	27	ASP	2.3
1	E	6	LEU	2.3
1	E	30	LEU	2.3
1	E	302	VAL	2.2
1	E	294	PRO	2.2
1	E	45	TYR	2.2
1	E	31	LEU	2.2
1	E	280	GLN	2.2
1	E	197	LEU	2.1
1	E	482	HIS	2.1
1	E	172	ASP	2.1
1	E	205	ARG	2.1
1	E	9	ILE	2.1
1	E	401	ILE	2.0
1	E	80	LYS	2.0
1	E	155	PHE	2.0
1	E	354	LEU	2.0
1	E	219	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	47	ILE	2.0
1	E	318	ILE	2.0
1	E	71	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOC	F	11	18/19	0.97	0.20	44,59,77,78	0
2	DOC	B	11	18/19	0.99	0.21	22,33,41,47	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

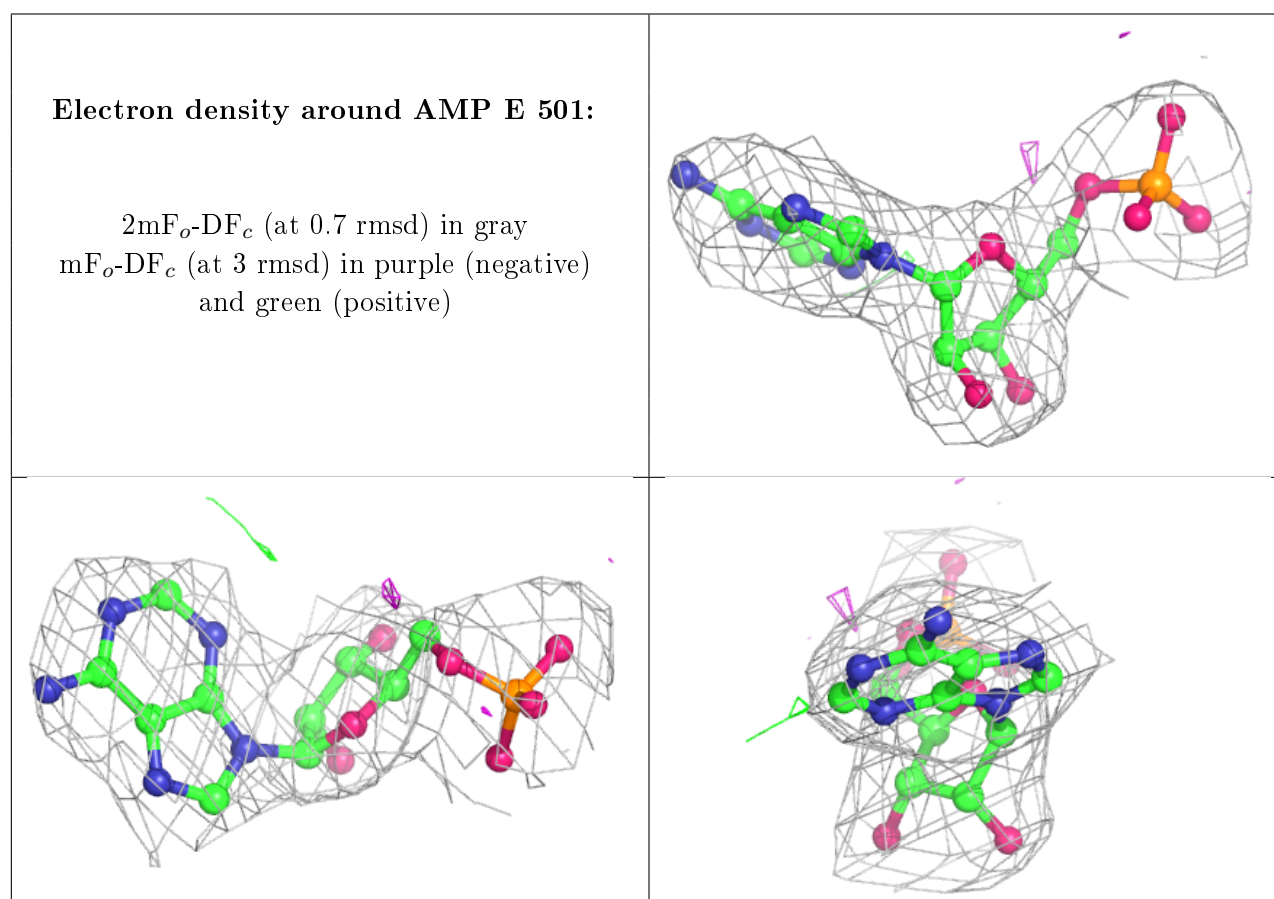
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CL	A	516	1/1	0.62	0.55	189,189,189,189	0
7	DTT	D	401	8/8	0.81	0.34	104,123,125,127	0
6	1PE	A	506	16/16	0.81	0.35	68,85,96,99	0
5	GOL	A	510	6/6	0.82	0.25	72,75,76,76	0
5	GOL	A	509	6/6	0.83	0.25	63,70,73,74	0
5	GOL	A	505	6/6	0.83	0.36	59,81,88,90	0
7	DTT	A	512	8/8	0.85	0.35	95,101,109,119	0
7	DTT	A	513	8/8	0.86	0.21	65,84,103,117	0
5	GOL	A	514	6/6	0.86	0.32	69,80,87,91	0
8	CL	E	502	1/1	0.86	0.22	88,88,88,88	0
7	DTT	B	401	8/8	0.86	0.26	69,84,101,110	0
5	GOL	A	502	6/6	0.88	0.18	59,68,69,73	0
7	DTT	D	402	8/8	0.89	0.28	81,87,106,116	0

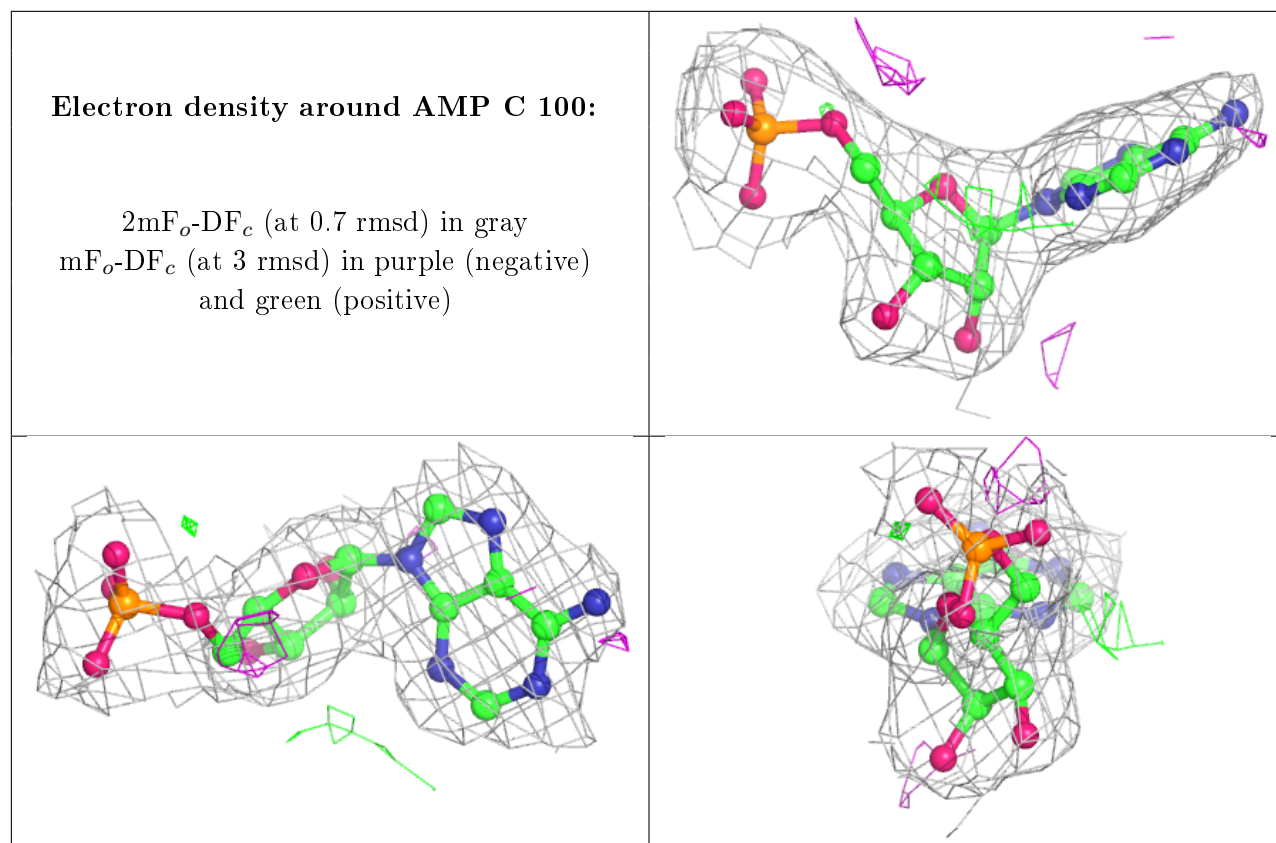
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	515	6/6	0.89	0.24	75,79,81,81	0
5	GOL	A	508	6/6	0.92	0.26	46,57,64,73	0
5	GOL	A	501	6/6	0.92	0.20	57,63,71,75	0
5	GOL	A	504	6/6	0.93	0.29	63,67,73,79	0
5	GOL	A	507	6/6	0.93	0.16	73,82,84,86	0
5	GOL	A	503	6/6	0.93	0.21	49,67,81,85	0
5	GOL	A	511	6/6	0.93	0.26	60,67,87,93	0
10	AMP	E	501	23/23	0.96	0.16	63,75,79,85	0
9	MG	A	517	1/1	0.99	0.31	51,51,51,51	0
10	AMP	C	100	23/23	0.99	0.20	30,36,40,42	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.