Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 05:16 AM EDT

PDB ID	:	5D0B / pdb_00005d0b
Title	:	Crystal structure of epoxyqueuosine reductase with a tRNA-TYR epoxyqueu osine-modified tRNA stem loop
Authors	:	Dowling, D.P.; Miles, Z.D.; Kohrer, C.; Bandarian, V.; Drennan, C.L.
Deposited on	:	2015-08-03
Resolution	:	2.65 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 (i) 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 (i)) were used in the production of this report:

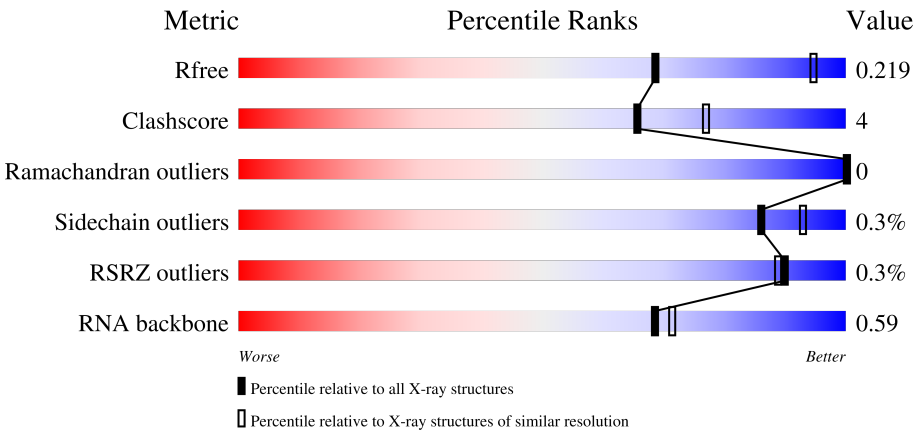
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)
RNA backbone	3983	1043 (2.88-2.40)

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 <=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	437	75% 11% 14%
1	B	437	80% 6% 14%
2	F	17	65% 24% 6% 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6586 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 Epoxyqueuosine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	2962	1880	504	561	17	0	1	0
1	B	375	2956	1877	503	559	17	0	2	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P97030
A	-26	ALA	-	expression tag	UNP P97030
A	-25	SER	-	expression tag	UNP P97030
A	-24	ARG	-	expression tag	UNP P97030
A	-23	GLY	-	expression tag	UNP P97030
A	-22	SER	-	expression tag	UNP P97030
A	-21	HIS	-	expression tag	UNP P97030
A	-20	HIS	-	expression tag	UNP P97030
A	-19	HIS	-	expression tag	UNP P97030
A	-18	HIS	-	expression tag	UNP P97030
A	-17	HIS	-	expression tag	UNP P97030
A	-16	HIS	-	expression tag	UNP P97030
A	-15	GLY	-	expression tag	UNP P97030
A	-14	ALA	-	expression tag	UNP P97030
A	-13	GLY	-	expression tag	UNP P97030
A	-12	ASP	-	expression tag	UNP P97030
A	-11	ARG	-	expression tag	UNP P97030
A	-10	GLY	-	expression tag	UNP P97030
A	-9	PRO	-	expression tag	UNP P97030
A	-8	GLU	-	expression tag	UNP P97030
A	-7	PHE	-	expression tag	UNP P97030
A	-6	GLU	-	expression tag	UNP P97030
A	-5	LEU	-	expression tag	UNP P97030
A	-4	GLY	-	expression tag	UNP P97030
A	-3	THR	-	expression tag	UNP P97030

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ARG	-	expression tag	UNP P97030
A	-1	GLY	-	expression tag	UNP P97030
A	0	SER	-	expression tag	UNP P97030
A	387	GLY	-	expression tag	UNP P97030
A	388	SER	-	expression tag	UNP P97030
A	389	LEU	-	expression tag	UNP P97030
A	390	GLU	-	expression tag	UNP P97030
A	391	VAL	-	expression tag	UNP P97030
A	392	ASP	-	expression tag	UNP P97030
A	393	LEU	-	expression tag	UNP P97030
A	394	GLN	-	expression tag	UNP P97030
A	395	GLY	-	expression tag	UNP P97030
A	396	ASP	-	expression tag	UNP P97030
A	397	HIS	-	expression tag	UNP P97030
A	398	GLY	-	expression tag	UNP P97030
A	399	LEU	-	expression tag	UNP P97030
A	400	SER	-	expression tag	UNP P97030
A	401	ALA	-	expression tag	UNP P97030
A	402	TRP	-	expression tag	UNP P97030
A	403	SER	-	expression tag	UNP P97030
A	404	HIS	-	expression tag	UNP P97030
A	405	PRO	-	expression tag	UNP P97030
A	406	GLN	-	expression tag	UNP P97030
A	407	PHE	-	expression tag	UNP P97030
A	408	GLU	-	expression tag	UNP P97030
A	409	LYS	-	expression tag	UNP P97030
B	-27	MET	-	initiating methionine	UNP P97030
B	-26	ALA	-	expression tag	UNP P97030
B	-25	SER	-	expression tag	UNP P97030
B	-24	ARG	-	expression tag	UNP P97030
B	-23	GLY	-	expression tag	UNP P97030
B	-22	SER	-	expression tag	UNP P97030
B	-21	HIS	-	expression tag	UNP P97030
B	-20	HIS	-	expression tag	UNP P97030
B	-19	HIS	-	expression tag	UNP P97030
B	-18	HIS	-	expression tag	UNP P97030
B	-17	HIS	-	expression tag	UNP P97030
B	-16	HIS	-	expression tag	UNP P97030
B	-15	GLY	-	expression tag	UNP P97030
B	-14	ALA	-	expression tag	UNP P97030
B	-13	GLY	-	expression tag	UNP P97030
B	-12	ASP	-	expression tag	UNP P97030

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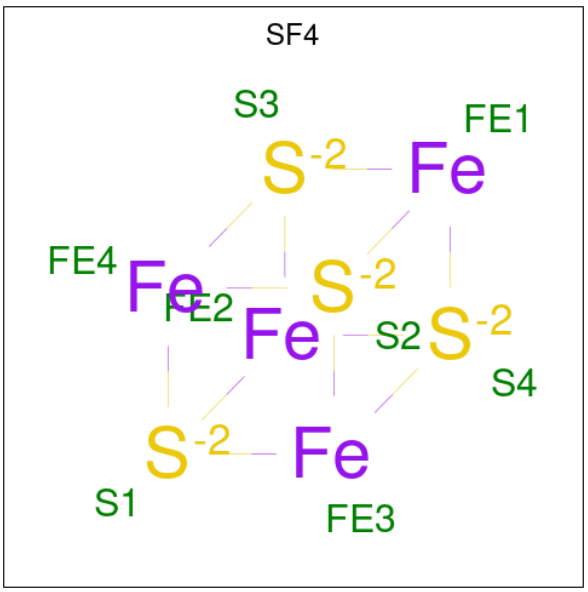
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	ARG	-	expression tag	UNP P97030
B	-10	GLY	-	expression tag	UNP P97030
B	-9	PRO	-	expression tag	UNP P97030
B	-8	GLU	-	expression tag	UNP P97030
B	-7	PHE	-	expression tag	UNP P97030
B	-6	GLU	-	expression tag	UNP P97030
B	-5	LEU	-	expression tag	UNP P97030
B	-4	GLY	-	expression tag	UNP P97030
B	-3	THR	-	expression tag	UNP P97030
B	-2	ARG	-	expression tag	UNP P97030
B	-1	GLY	-	expression tag	UNP P97030
B	0	SER	-	expression tag	UNP P97030
B	387	GLY	-	expression tag	UNP P97030
B	388	SER	-	expression tag	UNP P97030
B	389	LEU	-	expression tag	UNP P97030
B	390	GLU	-	expression tag	UNP P97030
B	391	VAL	-	expression tag	UNP P97030
B	392	ASP	-	expression tag	UNP P97030
B	393	LEU	-	expression tag	UNP P97030
B	394	GLN	-	expression tag	UNP P97030
B	395	GLY	-	expression tag	UNP P97030
B	396	ASP	-	expression tag	UNP P97030
B	397	HIS	-	expression tag	UNP P97030
B	398	GLY	-	expression tag	UNP P97030
B	399	LEU	-	expression tag	UNP P97030
B	400	SER	-	expression tag	UNP P97030
B	401	ALA	-	expression tag	UNP P97030
B	402	TRP	-	expression tag	UNP P97030
B	403	SER	-	expression tag	UNP P97030
B	404	HIS	-	expression tag	UNP P97030
B	405	PRO	-	expression tag	UNP P97030
B	406	GLN	-	expression tag	UNP P97030
B	407	PHE	-	expression tag	UNP P97030
B	408	GLU	-	expression tag	UNP P97030
B	409	LYS	-	expression tag	UNP P97030

- Molecule 2 is a RNA chain called RNA (5'-D(*GP*CP*AP*GP*AP*CP*UP*(56B)P*UP*AP*AP*AP*UP*CP*UP*GP*C)-3').

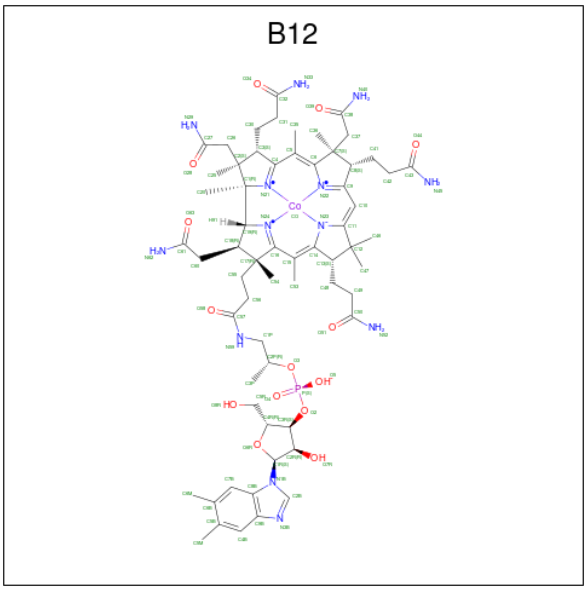
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	17	368	169	65	118	16	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



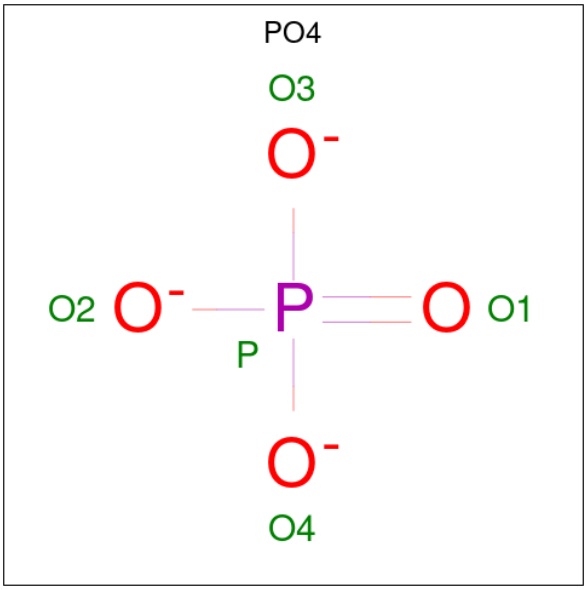
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0

- Molecule 4 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



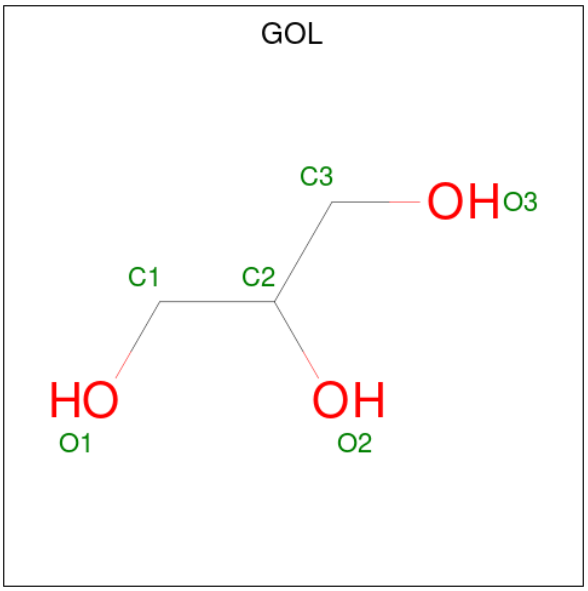
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
4	A	1	91	62	1	13	14	1	0	0
4	B	1	91	62	1	13	14	1	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

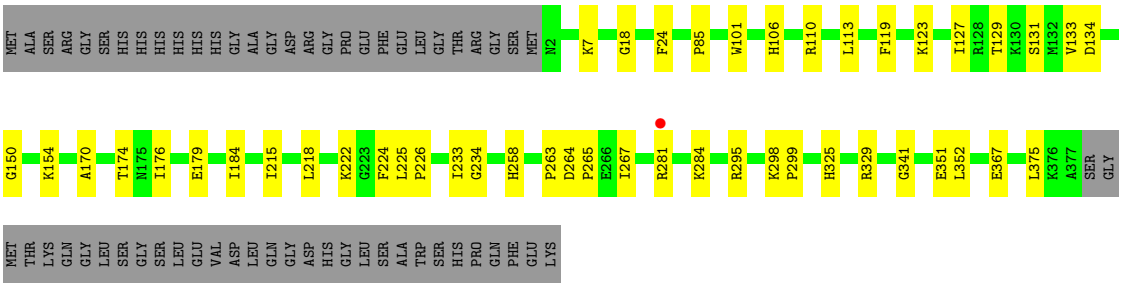
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	35	35	35	0	0
			Total	O		
7	B	27	27	27	0	0
			Total	O		
7	F	8	8	8	0	0

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.

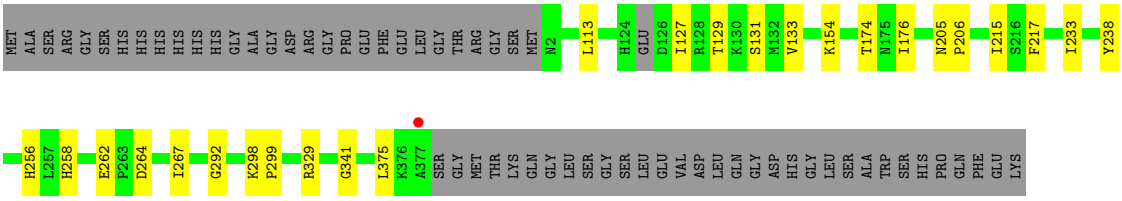
• Molecule 1: Epoxyqueuosine reductase

Chain A:



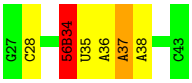
• Molecule 1: Epoxyqueuosine reductase

Chain B:



• Molecule 2: RNA (5'-D(*GP*CP*AP*GP*AP*CP*UP*(56B)P*UP*AP*AP*AP*UP*CP*UP*GP*C)-3')

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.64Å 110.75Å 99.22Å 90.00° 95.16° 90.00°	Depositor
Resolution (Å)	32.05 – 2.65 32.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.5 (32.05-2.65) 87.3 (32.05-2.65)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.221 0.193 , 0.219	Depositor DCC
R_{free} test set	1318 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 25.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6586	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 56B, PO4, SF4, GOL, B12

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	0.34	0/3024	0.73	2/4079 (0.0%)
1	B	0.32	0/3020	0.73	4/4072 (0.1%)
2	F	0.14	0/374	0.22	0/578
All	All	0.32	0/6418	0.70	6/8729 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ARG	CA-C-N	5.86	126.00	119.32
1	B	329	ARG	C-N-CA	5.86	126.00	119.32
1	B	258	HIS	CA-C-N	5.41	125.48	119.32
1	B	258	HIS	C-N-CA	5.41	125.48	119.32
1	A	329	ARG	CA-C-N	5.07	125.10	119.32
1	A	329	ARG	C-N-CA	5.07	125.10	119.32

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	2962	0	2991	28	0
1	B	2956	0	2989	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	368	0	174	5	0
3	A	16	0	0	1	0
3	B	16	0	0	1	0
4	A	91	0	88	1	0
4	B	91	0	88	4	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	6	0	8	2	0
7	A	35	0	0	1	0
7	B	27	0	0	1	0
7	F	8	0	0	0	0
All	All	6586	0	6338	49	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 4.

All (49) 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)
6:A:505:GOL:H31	2:F:36:A:H61	1.61	0.65
1:B:341:GLY:HA2	1:B:375:LEU:HG	1.80	0.64
1:A:341:GLY:HA2	1:A:375:LEU:HG	1.81	0.62
1:B:264:ASP:HB3	1:B:267:ILE:HG12	1.84	0.58
1:A:113:LEU:HD13	1:A:131:SER:HB3	1.87	0.57
1:A:106:HIS:NE2	1:A:134:ASP:OD2	2.37	0.56
1:B:113:LEU:HD13	1:B:131:SER:HB3	1.89	0.54
1:B:127:ILE:HD13	1:B:176:ILE:HD11	1.90	0.54
6:A:505:GOL:H12	2:F:36:A:N1	2.23	0.54
1:A:325:HIS:NE2	1:A:351:GLU:HG3	2.22	0.54
1:A:352:LEU:HD12	1:A:375:LEU:HD12	1.92	0.51
2:F:34:56B:O6	2:F:34:56B:N10	2.42	0.51
1:B:205:ASN:OD1	7:B:601:HOH:O	2.20	0.50
1:B:256:HIS:ND1	1:B:262:GLU:OE2	2.30	0.50
1:A:215:ILE:HD12	1:A:233:ILE:HD13	1.94	0.50
1:B:154:LYS:HD2	3:B:501:SF4:S3	2.51	0.50
1:A:154:LYS:HD2	3:A:501:SF4:S3	2.52	0.49
1:A:281:ARG:NH1	2:F:28:C:OP1	2.46	0.48
1:A:7:LYS:NZ	1:A:179:GLU:O	2.45	0.48
1:A:234:GLY:O	7:A:601:HOH:O	2.20	0.48
1:B:217:PHE:HB2	4:B:503:B12:H471	1.95	0.47
1:A:222:LYS:HE3	1:A:295:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:HD12	1:B:233:ILE:HD13	1.96	0.47
1:A:129:THR:HG22	1:A:174:THR:HG22	1.96	0.47
1:A:119:PHE:CZ	1:A:123:LYS:HE3	2.50	0.47
1:A:85:PRO:HD3	1:A:265:PRO:HB2	1.97	0.47
1:A:264:ASP:HB3	1:A:267:ILE:HG12	1.97	0.46
1:A:7:LYS:HE3	1:A:24:PHE:CD2	2.51	0.45
4:A:503:B12:H351	4:A:503:B12:H362	1.99	0.45
1:A:284:LYS:HE3	1:A:284:LYS:HB2	1.83	0.45
4:B:503:B12:H262	4:B:503:B12:H91	1.86	0.44
1:B:238:TYR:CZ	1:B:292:GLY:HA2	2.53	0.43
1:A:150:GLY:HA2	1:A:184:ILE:HD11	1.99	0.43
1:A:101:TRP:HB3	1:A:263:PRO:HB3	2.01	0.43
1:A:224:PHE:CE2	1:A:367:GLU:HG3	2.53	0.43
1:B:154:LYS:HG2	1:B:206:PRO:HB3	2.01	0.42
1:A:225:LEU:HD12	1:A:226:PRO:HD2	2.01	0.42
1:B:129:THR:HG22	1:B:174:THR:HG22	2.01	0.42
1:A:298:LYS:HB3	1:A:299:PRO:HD3	2.02	0.42
1:A:127:ILE:HD13	1:A:176:ILE:HD11	2.02	0.41
1:A:218:LEU:HB3	1:A:225:LEU:HD11	2.01	0.41
4:B:503:B12:H253	4:B:503:B12:H301	1.87	0.41
4:B:503:B12:H362	4:B:503:B12:H351	2.01	0.41
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.84	0.41
1:A:110:ARG:HA	1:A:110:ARG:HD2	1.89	0.41
1:A:18:GLY:O	1:A:258:HIS:HE1	2.04	0.41
1:B:298:LYS:HB3	1:B:299:PRO:HD3	2.02	0.40
1:A:113:LEU:HD11	1:A:170:ALA:HB1	2.03	0.40
2:F:37:A:O2'	2:F:38:A:H5"	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	375/437 (86%)	367 (98%)	8 (2%)	0	100	100
1	B	373/437 (85%)	367 (98%)	6 (2%)	0	100	100
All	All	748/874 (86%)	734 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	322/368 (88%)	321 (100%)	1 (0%)	86	93
1	B	322/368 (88%)	321 (100%)	1 (0%)	86	93
All	All	644/736 (88%)	642 (100%)	2 (0%)	86	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	VAL
1	B	133	VAL

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

Mol	Chain	Res	Type
1	A	220	GLN
1	B	220	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	16/17 (94%)	3 (18%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	34	56B
2	F	35	U
2	F	37	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	56B	F	34	2	29,35,36	0.69	1 (3%)	34,52,55	1.06	1 (2%)

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	56B	F	34	2	-	4/12/43/44	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	34	56B	C9-N10	2.27	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	34	56B	C7-C5-C4	-4.48	107.54	112.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	34	56B	C5-C7-C9-N10
2	F	34	56B	O4'-C4'-C5'-O5'
2	F	34	56B	C3'-C4'-C5'-O5'
2	F	34	56B	C8-C7-C9-N10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	34	56B	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands 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	$\#\|Z\| > 2$
4	B12	B	503	-	94,101,101	0.68	3 (3%)	149,166,166	1.04	13 (8%)
6	GOL	A	505	-	5,5,5	0.38	0	5,5,5	0.26	0
5	PO4	B	504	-	4,4,4	1.05	0	6,6,6	0.40	0
5	PO4	A	504	-	4,4,4	1.08	0	6,6,6	0.50	0
3	SF4	B	501	1	0,12,12	-	-	-		
3	SF4	A	501	1	0,12,12	-	-	-		
3	SF4	B	502	1	0,12,12	-	-	-		
3	SF4	A	502	1	0,12,12	-	-	-		
4	B12	A	503	-	94,101,101	0.69	3 (3%)	149,166,166	1.04	12 (8%)

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
4	B12	B	503	-	-	12/56/223/223	0/3/11/11
6	GOL	A	505	-	-	2/4/4/4	-
3	SF4	B	501	1	-	-	0/6/5/5
3	SF4	A	501	1	-	-	0/6/5/5
3	SF4	B	502	1	-	-	0/6/5/5
3	SF4	A	502	1	-	-	0/6/5/5
4	B12	A	503	-	-	14/56/223/223	0/3/11/11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	B12	C14-N23	3.86	1.40	1.35
4	B	503	B12	C14-N23	3.85	1.40	1.35
4	A	503	B12	C16-C15	2.72	1.52	1.44
4	B	503	B12	C16-C15	2.60	1.52	1.44
4	A	503	B12	C1P-C2P	2.29	1.57	1.51
4	B	503	B12	C1P-C2P	2.28	1.57	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	B12	C20-C1-C19	-3.97	105.53	109.35
4	A	503	B12	C9-N22-C6	3.52	109.51	105.28
4	B	503	B12	C9-N22-C6	3.45	109.43	105.28
4	B	503	B12	C20-C1-C19	-3.20	106.27	109.35
4	B	503	B12	C55-C17-C18	-3.03	105.34	111.12
4	A	503	B12	C19-N24-C16	2.90	110.47	107.29
4	B	503	B12	C35-C5-C6	2.86	127.02	122.41
4	A	503	B12	C55-C17-C18	-2.84	105.70	111.12
4	A	503	B12	C1-C19-C18	-2.82	117.33	121.90
4	B	503	B12	C1-C19-C18	-2.78	117.40	121.90
4	A	503	B12	C35-C5-C6	2.76	126.86	122.41
4	B	503	B12	C19-N24-C16	2.72	110.27	107.29
4	B	503	B12	C15-C16-N24	-2.61	118.70	122.42
4	A	503	B12	C15-C16-N24	-2.54	118.80	122.42
4	A	503	B12	C10-C9-N22	2.47	128.56	125.74
4	B	503	B12	C10-C9-N22	2.43	128.52	125.74
4	B	503	B12	C30-C3-C2	-2.36	113.80	119.00
4	A	503	B12	C17-C18-C19	2.32	105.88	102.36
4	B	503	B12	C17-C18-C19	2.24	105.75	102.36
4	A	503	B12	C35-C5-C4	-2.24	112.26	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	503	B12	C35-C5-C4	-2.18	112.36	116.79
4	B	503	B12	P-O3-C2P	2.17	128.52	121.10
4	A	503	B12	C30-C3-C2	-2.17	114.22	119.00
4	B	503	B12	C17-C16-N24	2.05	114.29	111.17
4	A	503	B12	P-O3-C2P	2.05	128.10	121.10

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	B12	C14-C13-C48-C49
4	A	503	B12	C1P-C2P-O3-P
4	A	503	B12	C3P-C2P-O3-P
4	A	503	B12	C2P-O3-P-O2
4	B	503	B12	C14-C13-C48-C49
4	B	503	B12	C1P-C2P-O3-P
4	B	503	B12	C3P-C2P-O3-P
4	B	503	B12	C2P-O3-P-O2
6	A	505	GOL	O1-C1-C2-C3
4	A	503	B12	C2R-C3R-O2-P
4	B	503	B12	C2R-C3R-O2-P
4	A	503	B12	O6R-C1R-N1B-C8B
4	B	503	B12	O6R-C1R-N1B-C8B
6	A	505	GOL	O1-C1-C2-O2
4	B	503	B12	C4R-C3R-O2-P
4	A	503	B12	C4R-C3R-O2-P
4	A	503	B12	C2R-C1R-N1B-C8B
4	B	503	B12	C2R-C1R-N1B-C8B
4	A	503	B12	C2-C3-C30-C31
4	A	503	B12	C2P-O3-P-O4
4	B	503	B12	C2P-O3-P-O4
4	B	503	B12	C2-C3-C30-C31
4	A	503	B12	C8-C41-C42-C43
4	A	503	B12	C3R-O2-P-O4
4	A	503	B12	C3R-O2-P-O5
4	B	503	B12	C3R-O2-P-O4
4	A	503	B12	C25-C2-C26-C27
4	B	503	B12	C25-C2-C26-C27

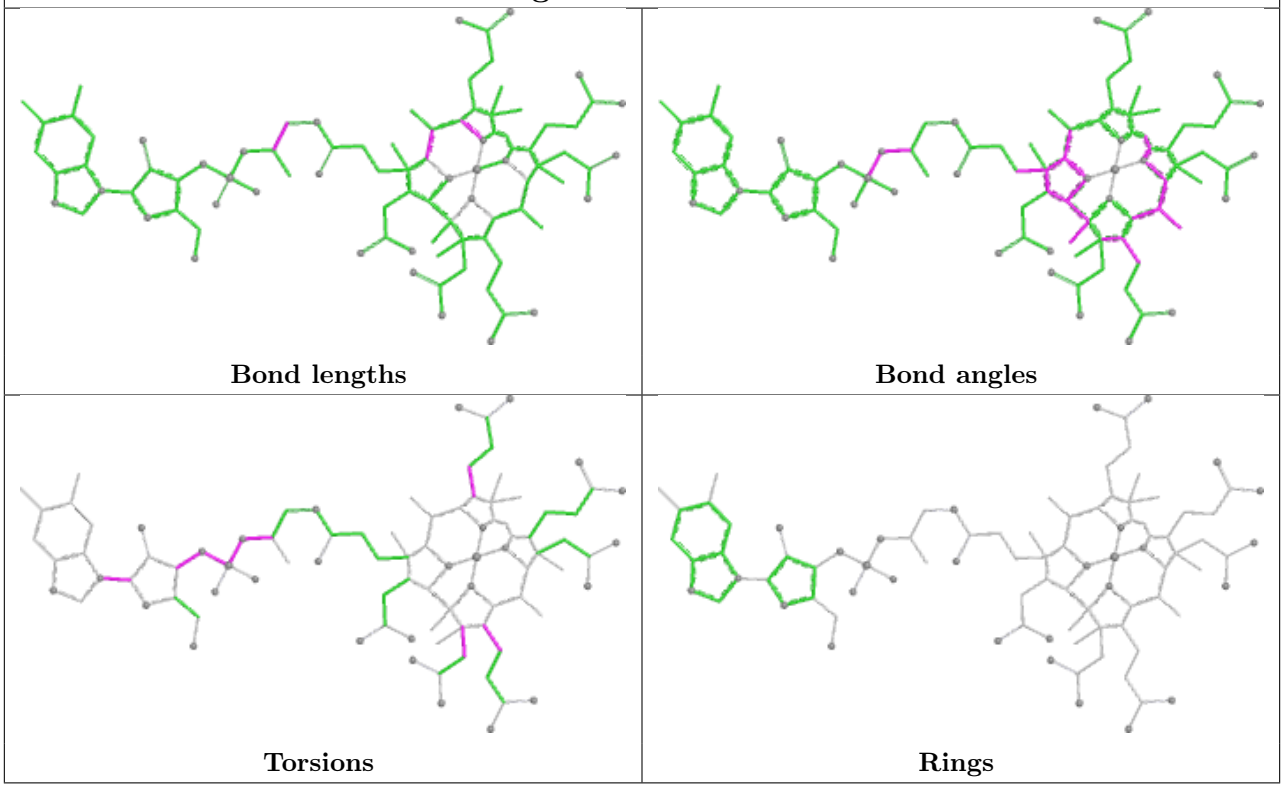
There are no ring outliers.

5 monomers are involved in 9 short contacts:

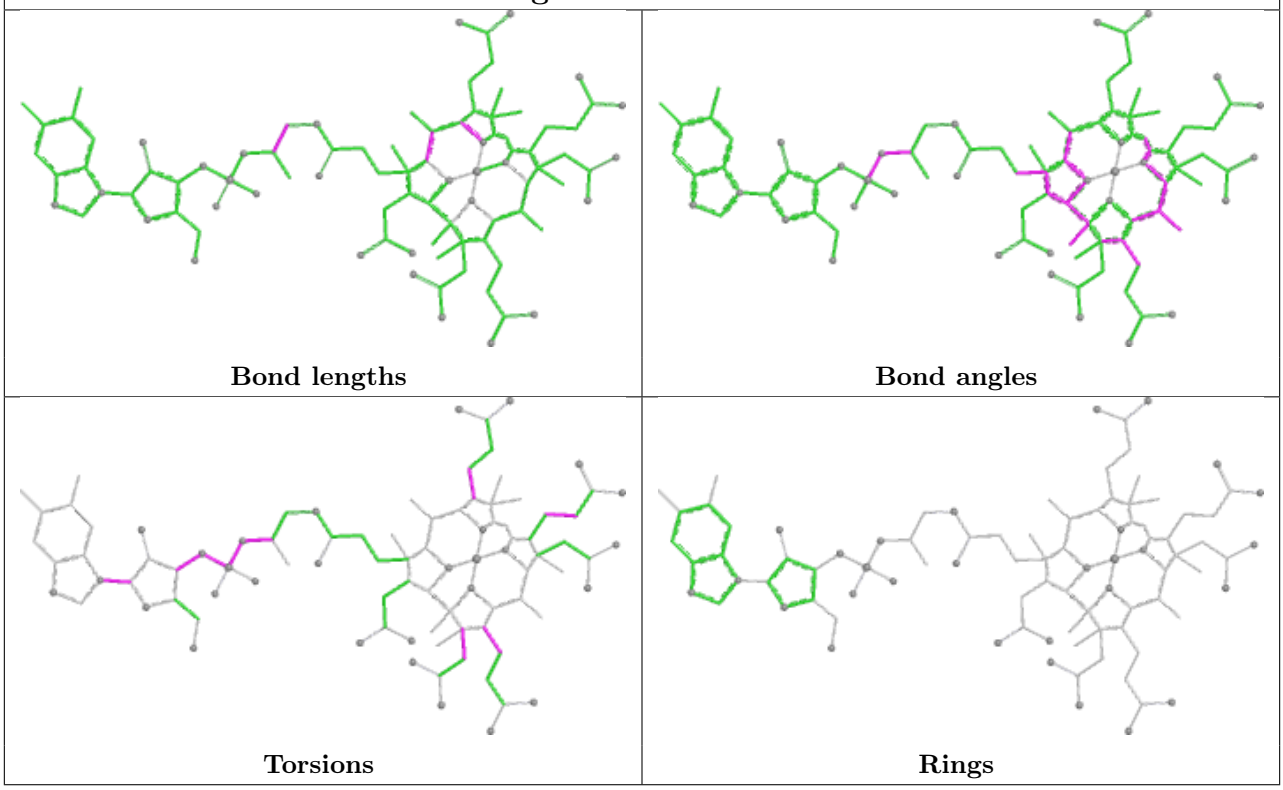
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	B12	4	0
6	A	505	GOL	2	0
3	B	501	SF4	1	0
3	A	501	SF4	1	0
4	A	503	B12	1	0

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 then 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.

Ligand B12 B 503



Ligand B12 A 503



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	376/437 (86%)	-0.03	1 (0%)	90	89	20, 29, 45, 65	1 (0%)
1	B	375/437 (85%)	-0.15	1 (0%)	90	89	19, 29, 45, 62	2 (0%)
2	F	16/17 (94%)	0.02	0	100	100	29, 38, 52, 55	0
All	All	767/891 (86%)	-0.09	2 (0%)	90	89	19, 29, 45, 65	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ARG	3.9
1	B	377	ALA	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	56B	F	34	32/33	0.86	0.13	29,32,48,50	0

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,

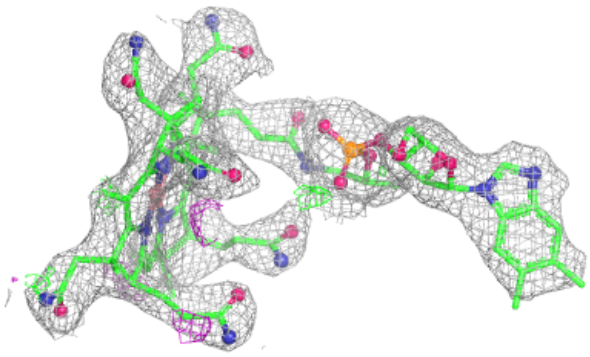
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

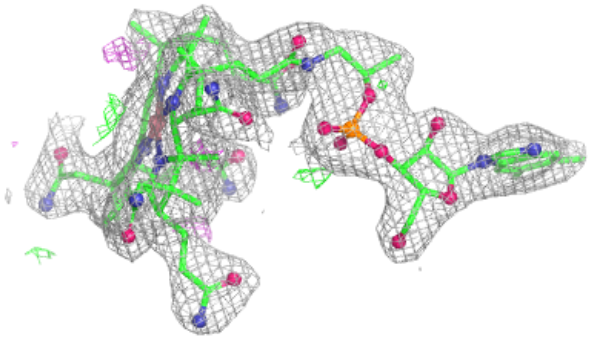
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	505	6/6	0.82	0.15	34,34,38,40	0
5	PO4	A	504	5/5	0.94	0.08	28,30,31,32	0
4	B12	A	503	91/91	0.96	0.08	16,22,33,36	0
5	PO4	B	504	5/5	0.96	0.06	29,31,32,33	0
4	B12	B	503	91/91	0.96	0.08	18,22,35,38	0
3	SF4	A	502	8/8	0.99	0.04	19,21,24,26	0
3	SF4	B	501	8/8	0.99	0.03	21,27,29,35	0
3	SF4	B	502	8/8	0.99	0.03	23,25,26,27	0
3	SF4	A	501	8/8	0.99	0.04	20,24,26,30	0

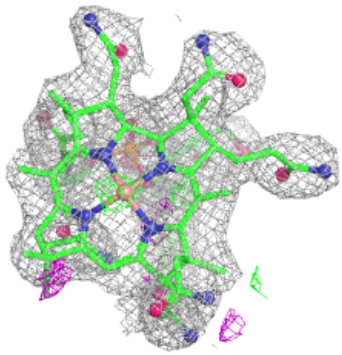
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

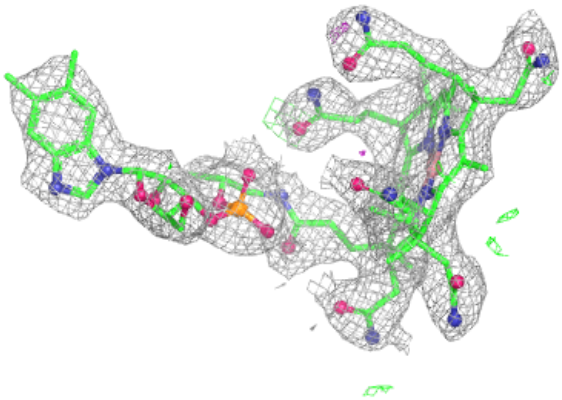
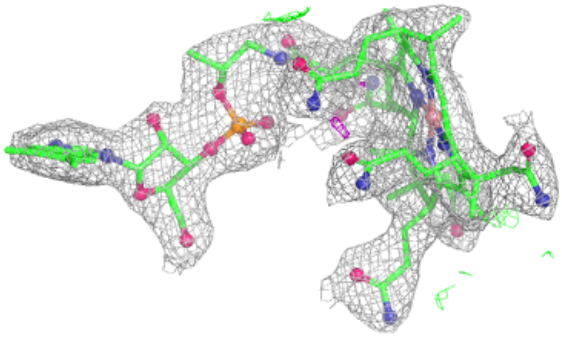
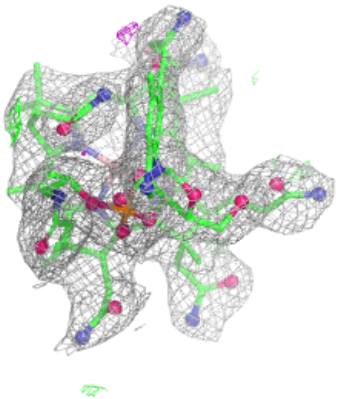
Electron density around B12 A 503:

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







Electron density around B12 B 503: $2mF_o$-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.