Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 10:15 AM EDT

PDB ID	:	9CBP / pdb_00009cbp
Title	:	Methionine synthase from Thermus thermophilus HB8, Homocysteine, Folate, and Cobalamin Domains, Pre-Catalytic State (Pre-Hcy-on)
Authors	:	Yamada, K.; Mendoza, J.; Koutmos, M.
Deposited on	:	2024-06-19
Resolution	:	2.45 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:

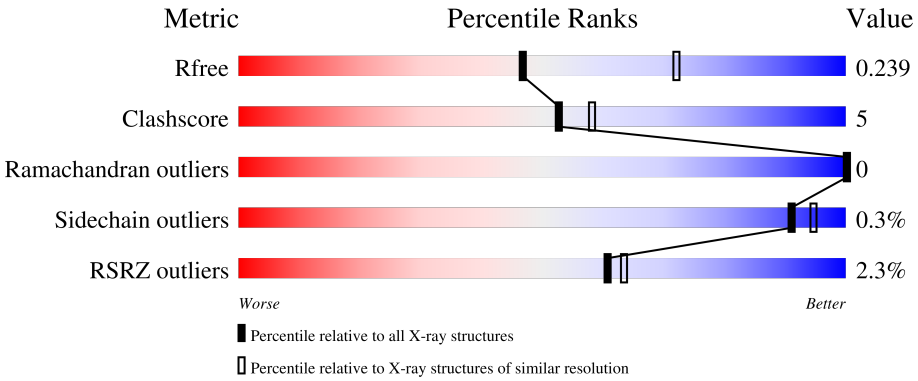
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.45 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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	874	2% 88% 10%

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
2	GOL	A	908	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6977 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.

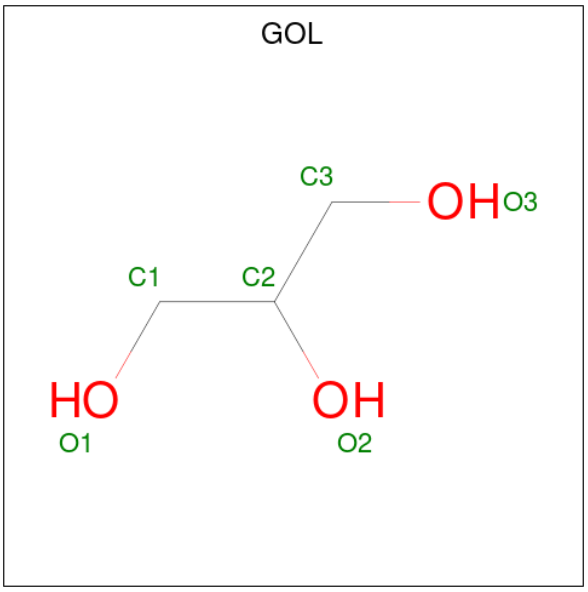
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	862	6623	4213	1159	1222	29	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

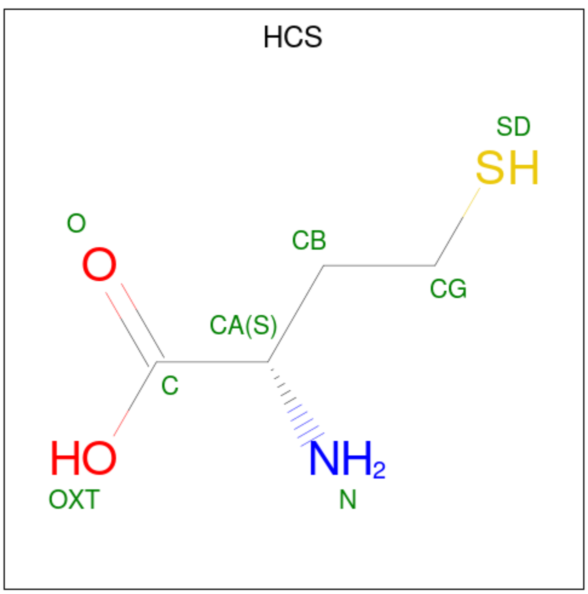
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	PHE	engineered mutation	UNP Q5SKM5
A	123	ALA	GLU	engineered mutation	UNP Q5SKM5
A	124	ALA	GLU	engineered mutation	UNP Q5SKM5
A	296	ALA	TYR	engineered mutation	UNP Q5SKM5
A	651	ALA	ASP	engineered mutation	UNP Q5SKM5
A	652	ALA	PRO	engineered mutation	UNP Q5SKM5
A	653	ALA	GLY	engineered mutation	UNP Q5SKM5

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (CCD ID: HCS) (formula: $C_4H_9NO_2S$).

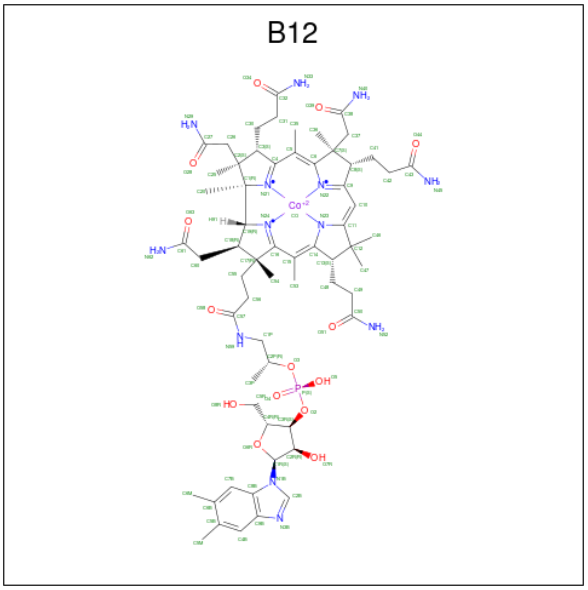


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	8	4	1	2	1	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0

- Molecule 7 is water.

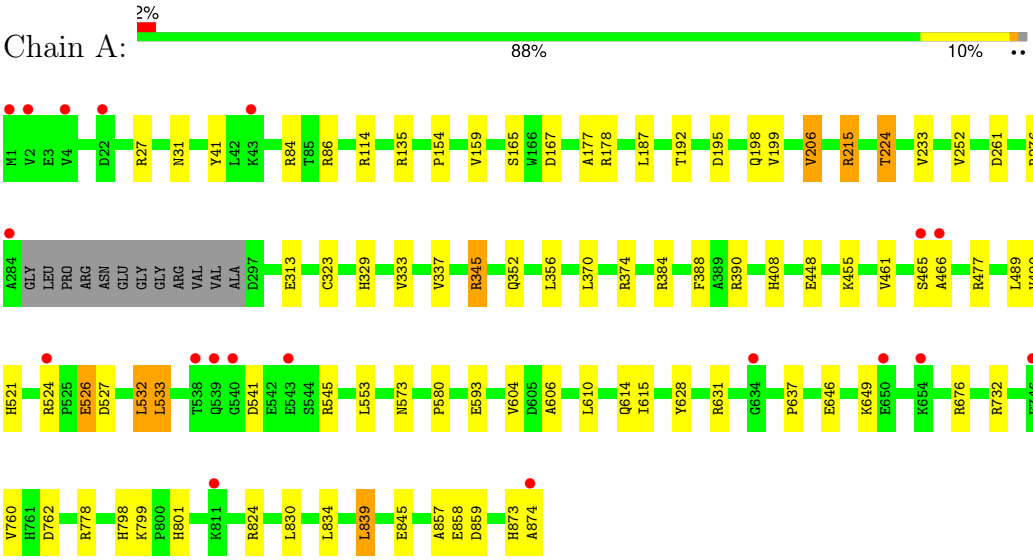
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	198	Total O 198 198	0	0

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: Methionine synthase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.95Å 83.82Å 163.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.99 – 2.45 81.86 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.1 (81.99-2.45) 98.4 (81.86-2.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.161 , 0.237 0.172 , 0.239	Depositor DCC
R_{free} test set	1817 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6977	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B12, ZN, HCS, K, GOL

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	0.93	3/6743 (0.0%)	1.42	24/9124 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	ARG	NE-CZ	8.22	1.42	1.33
1	A	521	HIS	CE1-NE2	5.66	1.38	1.32
1	A	84	ARG	NE-CZ	5.14	1.38	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ARG	NE-CZ-NH1	-9.04	112.47	121.50
1	A	858	GLU	CB-CG-CD	7.72	125.72	112.60
1	A	86	ARG	NH1-CZ-NH2	7.31	128.81	119.30
1	A	533	LEU	N-CA-CB	-6.95	100.42	110.36
1	A	532	LEU	N-CA-C	-6.80	98.54	109.96
1	A	337	VAL	N-CA-CB	-6.42	105.15	112.21
1	A	845	GLU	CB-CG-CD	6.36	123.41	112.60
1	A	859	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	526	GLU	CB-CG-CD	5.93	122.68	112.60
1	A	345	ARG	NE-CZ-NH2	-5.67	114.09	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	839	LEU	N-CA-CB	-5.66	101.18	110.52
1	A	224	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	31	ASN	CA-C-N	5.50	127.91	120.65
1	A	31	ASN	C-N-CA	5.50	127.91	120.65
1	A	313	GLU	CB-CG-CD	-5.36	103.50	112.60
1	A	199	VAL	N-CA-C	-5.35	105.28	110.42
1	A	830	LEU	N-CA-CB	-5.24	102.11	110.03
1	A	461	VAL	N-CA-CB	-5.24	102.08	112.24
1	A	215	ARG	CG-CD-NE	-5.23	100.49	112.00
1	A	801	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	491	VAL	N-CA-CB	-5.21	105.34	111.90
1	A	573	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	448	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	261	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ARG	Sidechain
1	A	178	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	27	ARG	Sidechain
1	A	374	ARG	Sidechain
1	A	390	ARG	Sidechain
1	A	477	ARG	Sidechain
1	A	732	ARG	Sidechain
1	A	778	ARG	Sidechain
1	A	824	ARG	Sidechain

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	6623	0	6743	60	0
2	A	54	0	72	15	0
3	A	8	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	91	0	87	11	0
6	A	1	0	0	0	0
7	A	198	0	0	10	0
All	All	6977	0	6909	67	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 (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:HB3	2:A:909:GOL:O3	1.40	1.19
1:A:533:LEU:N	7:A:1001:HOH:O	1.89	1.04
5:A:912:B12:H362	5:A:912:B12:H351	1.54	0.88
1:A:167:ASP:CG	2:A:908:GOL:O3	2.31	0.74
5:A:912:B12:H552	5:A:912:B12:H531	1.70	0.73
1:A:604:VAL:O	2:A:905:GOL:O3	2.08	0.70
1:A:370:LEU:H	1:A:408:HIS:HD1	1.41	0.69
1:A:532:LEU:C	7:A:1001:HOH:O	2.27	0.68
1:A:167:ASP:CG	2:A:908:GOL:HO3	2.00	0.68
1:A:159:VAL:HG22	2:A:910:GOL:H31	1.77	0.66
1:A:198:GLN:HB3	2:A:902:GOL:O1	1.95	0.66
1:A:649:LYS:HG3	7:A:1002:HOH:O	1.96	0.65
5:A:912:B12:H531	5:A:912:B12:C55	2.28	0.64
1:A:167:ASP:OD2	2:A:908:GOL:O3	2.16	0.63
1:A:465:SER:H	1:A:490:VAL:HB	1.63	0.62
1:A:195:ASP:HB3	1:A:198:GLN:HG3	1.82	0.61
1:A:748:LYS:HD3	1:A:874:ALA:HB2	1.81	0.60
1:A:159:VAL:H	1:A:198:GLN:HE21	1.51	0.58
5:A:912:B12:H351	5:A:912:B12:C36	2.29	0.58
2:A:905:GOL:H12	7:A:1015:HOH:O	2.04	0.57
1:A:532:LEU:CA	7:A:1001:HOH:O	2.51	0.56
1:A:252:VAL:O	1:A:278:VAL:HA	2.05	0.56
1:A:646:GLU:O	1:A:649:LYS:HG3	2.05	0.55
1:A:455:LYS:HE2	2:A:907:GOL:H12	1.88	0.55
1:A:762:ASP:H	5:A:912:B12:H522	1.55	0.55
1:A:233:VAL:HG22	7:A:1056:HOH:O	2.07	0.54
1:A:41:TYR:CE2	1:A:187:LEU:HD22	2.43	0.54
1:A:857:ALA:CB	5:A:912:B12:HM62	2.39	0.53
1:A:233:VAL:CG2	7:A:1056:HOH:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:LEU:HB3	1:A:839:LEU:HD21	1.93	0.51
1:A:524:ARG:HG2	1:A:527:ASP:CG	2.36	0.51
1:A:873:HIS:O	1:A:874:ALA:HB3	2.11	0.51
1:A:610:LEU:HD11	1:A:615:ILE:HG12	1.92	0.50
1:A:352:GLN:NE2	7:A:1010:HOH:O	2.44	0.49
1:A:524:ARG:CD	1:A:526:GLU:HB2	2.43	0.49
5:A:912:B12:H203	5:A:912:B12:H301	1.95	0.49
1:A:541:ASP:O	1:A:545:ARG:HG3	2.12	0.49
1:A:524:ARG:CB	2:A:909:GOL:O3	2.34	0.48
1:A:384:ARG:HG3	1:A:388:PHE:CZ	2.48	0.48
1:A:192:THR:HA	1:A:224:THR:OG1	2.13	0.48
1:A:466:ALA:HB2	1:A:489:LEU:HD11	1.96	0.48
1:A:545:ARG:HD2	1:A:631:ARG:HH21	1.79	0.47
1:A:159:VAL:HG12	1:A:198:GLN:HG2	1.96	0.47
1:A:41:TYR:CZ	1:A:187:LEU:HD22	2.50	0.47
1:A:276:ARG:O	1:A:345:ARG:HD3	2.14	0.47
1:A:545:ARG:HA	2:A:901:GOL:H12	1.97	0.47
1:A:159:VAL:CG1	1:A:198:GLN:HG2	2.45	0.47
1:A:277:PHE:HA	1:A:345:ARG:HD2	1.98	0.46
1:A:614:GLN:NE2	7:A:1007:HOH:O	2.41	0.46
1:A:759:ASP:HA	5:A:912:B12:H452	1.82	0.45
5:A:912:B12:H482	5:A:912:B12:H533	1.97	0.44
1:A:676:ARG:HD3	7:A:1101:HOH:O	2.17	0.44
1:A:760:VAL:HG22	5:A:912:B12:C43	2.48	0.43
1:A:857:ALA:HB3	5:A:912:B12:HM62	2.00	0.43
1:A:283:ASN:HB2	1:A:323:CYS:O	2.19	0.43
1:A:154:PRO:HA	2:A:902:GOL:H2	2.00	0.43
1:A:329:HIS:O	1:A:333:VAL:HG23	2.19	0.43
1:A:187:LEU:C	1:A:187:LEU:HD12	2.44	0.42
1:A:798:HIS:O	1:A:799:LYS:C	2.62	0.42
1:A:637:PRO:HG2	2:A:901:GOL:C3	2.48	0.42
1:A:593:GLU:OE1	1:A:628:TYR:OH	2.35	0.42
1:A:165:SER:HB2	2:A:908:GOL:H32	2.01	0.41
1:A:177:ALA:HB2	1:A:206:VAL:HG22	2.02	0.41
1:A:873:HIS:O	1:A:874:ALA:CB	2.68	0.41
1:A:233:VAL:CG2	1:A:356:LEU:HD11	2.50	0.41
1:A:503:ARG:NH1	1:A:553:LEU:HD13	2.36	0.41
1:A:606:ALA:N	2:A:905:GOL:O1	2.49	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	858/874 (98%)	840 (98%)	18 (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	679/687 (99%)	677 (100%)	2 (0%)	91 95

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

Mol	Chain	Res	Type
1	A	206	VAL
1	A	580	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	273	HIS
1	A	352	GLN
1	A	431	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
2	GOL	A	908	-	5,5,5	0.30	0	5,5,5	0.74	0
2	GOL	A	911	-	5,5,5	0.25	0	5,5,5	0.43	0
2	GOL	A	905	-	5,5,5	0.20	0	5,5,5	0.38	0
2	GOL	A	910	-	5,5,5	0.37	0	5,5,5	0.77	0
2	GOL	A	901	-	5,5,5	0.26	0	5,5,5	0.74	0
2	GOL	A	909	-	5,5,5	0.24	0	5,5,5	0.90	0
2	GOL	A	906	-	5,5,5	0.22	0	5,5,5	0.56	0
2	GOL	A	902	-	5,5,5	0.98	0	5,5,5	1.22	0
3	HCS	A	903	4	6,7,7	0.97	0	5,8,8	1.37	1 (20%)
2	GOL	A	907	-	5,5,5	0.58	0	5,5,5	0.79	0
5	B12	A	912	1	91,101,101	1.56	16 (17%)	140,166,166	1.99	34 (24%)

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	GOL	A	908	-	-	0/4/4/4	-
2	GOL	A	911	-	-	0/4/4/4	-
2	GOL	A	905	-	-	2/4/4/4	-
2	GOL	A	910	-	-	4/4/4/4	-
2	GOL	A	901	-	-	2/4/4/4	-
2	GOL	A	909	-	-	1/4/4/4	-
2	GOL	A	906	-	-	3/4/4/4	-
2	GOL	A	902	-	-	0/4/4/4	-
3	HCS	A	903	4	-	2/7/7/7	-
2	GOL	A	907	-	-	4/4/4/4	-
5	B12	A	912	1	-	7/52/223/223	0/3/11/11

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	912	B12	C19-N24	-7.94	1.39	1.49
5	A	912	B12	O6R-C1R	3.48	1.45	1.40
5	A	912	B12	C16-C15	-3.44	1.34	1.44
5	A	912	B12	C10-C9	2.83	1.47	1.39
5	A	912	B12	C4B-C9B	-2.79	1.37	1.41
5	A	912	B12	C8B-C9B	2.67	1.45	1.40
5	A	912	B12	C1-C2	-2.67	1.52	1.58
5	A	912	B12	C9-N22	2.54	1.36	1.30
5	A	912	B12	C3-C4	-2.52	1.45	1.51
5	A	912	B12	O6R-C4R	-2.39	1.39	1.45
5	A	912	B12	C14-C15	2.33	1.48	1.38
5	A	912	B12	C6B-C5B	2.20	1.46	1.40
5	A	912	B12	C14-N23	-2.17	1.32	1.35
5	A	912	B12	O7R-C2R	2.17	1.48	1.43
5	A	912	B12	P-O4	2.09	1.58	1.50
5	A	912	B12	C36-C7	2.01	1.57	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	912	B12	C18-C19-N24	7.74	113.97	102.33
5	A	912	B12	C1-C19-N24	7.50	114.60	106.25
5	A	912	B12	C20-C1-C19	-6.03	103.55	109.35
5	A	912	B12	O6R-C1R-N1B	-5.73	101.14	108.75
5	A	912	B12	C60-C61-N62	4.82	127.74	116.19
5	A	912	B12	C13-C14-N23	4.66	115.41	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	912	B12	C19-N24-C16	-4.49	102.38	107.29
5	A	912	B12	C13-C14-C15	-4.36	117.69	124.32
5	A	912	B12	C1-C19-C18	4.08	128.52	121.90
5	A	912	B12	C55-C17-C16	3.79	124.00	116.59
5	A	912	B12	C19-C1-N21	3.46	105.71	102.14
5	A	912	B12	C41-C8-C9	3.30	116.94	111.19
5	A	912	B12	C9-N22-C6	-3.24	101.39	105.28
5	A	912	B12	O34-C32-N33	-3.22	113.94	122.53
5	A	912	B12	O28-C27-N29	-3.11	114.22	122.53
5	A	912	B12	C60-C18-C19	2.98	122.33	114.59
5	A	912	B12	O5-P-O4	2.92	126.04	112.44
5	A	912	B12	C5-C6-N22	-2.90	119.50	123.88
5	A	912	B12	C2P-C1P-N59	-2.70	108.96	112.92
5	A	912	B12	C4B-C9B-C8B	-2.65	118.39	121.10
5	A	912	B12	C2-C1-C19	2.61	122.68	118.61
5	A	912	B12	O3-C2P-C1P	2.58	112.06	106.94
5	A	912	B12	O63-C61-C60	-2.55	115.54	120.87
5	A	912	B12	C25-C2-C1	2.48	117.47	113.75
5	A	912	B12	C41-C42-C43	-2.37	104.48	112.55
5	A	912	B12	C26-C27-N29	2.35	123.78	116.49
5	A	912	B12	O63-C61-N62	-2.27	116.47	122.53
5	A	912	B12	C7-C6-N22	2.24	112.01	107.94
5	A	912	B12	C30-C3-C4	2.23	114.88	109.66
5	A	912	B12	C2R-C3R-C4R	2.19	107.06	103.24
3	A	903	HCS	CG-CB-CA	2.17	116.67	113.14
5	A	912	B12	O2-P-O4	-2.16	102.89	109.81
5	A	912	B12	C1-C2-C3	-2.15	98.89	101.60
5	A	912	B12	C4B-C9B-N3B	2.14	136.60	130.88
5	A	912	B12	C7-C37-C38	-2.07	108.16	114.28

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	C1-C2-C3-O3
2	A	906	GOL	C1-C2-C3-O3
2	A	910	GOL	O1-C1-C2-C3
3	A	903	HCS	N-CA-CB-CG
3	A	903	HCS	C-CA-CB-CG
5	A	912	B12	C3-C30-C31-C32
5	A	912	B12	C18-C60-C61-O63
5	A	912	B12	C18-C60-C61-N62

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Mol	Chain	Res	Type	Atoms
2	A	910	GOL	O1-C1-C2-O2
2	A	905	GOL	O1-C1-C2-C3
2	A	907	GOL	O1-C1-C2-C3
2	A	907	GOL	C1-C2-C3-O3
2	A	910	GOL	C1-C2-C3-O3
2	A	901	GOL	O2-C2-C3-O3
2	A	906	GOL	O2-C2-C3-O3
2	A	907	GOL	O2-C2-C3-O3
2	A	910	GOL	O2-C2-C3-O3
2	A	907	GOL	O1-C1-C2-O2
5	A	912	B12	C48-C49-C50-N52
2	A	905	GOL	O1-C1-C2-O2
2	A	909	GOL	O1-C1-C2-O2
5	A	912	B12	C48-C49-C50-O51
5	A	912	B12	C2-C26-C27-N29
5	A	912	B12	O6R-C4R-C5R-O8R
2	A	906	GOL	O1-C1-C2-C3

There are no ring outliers.

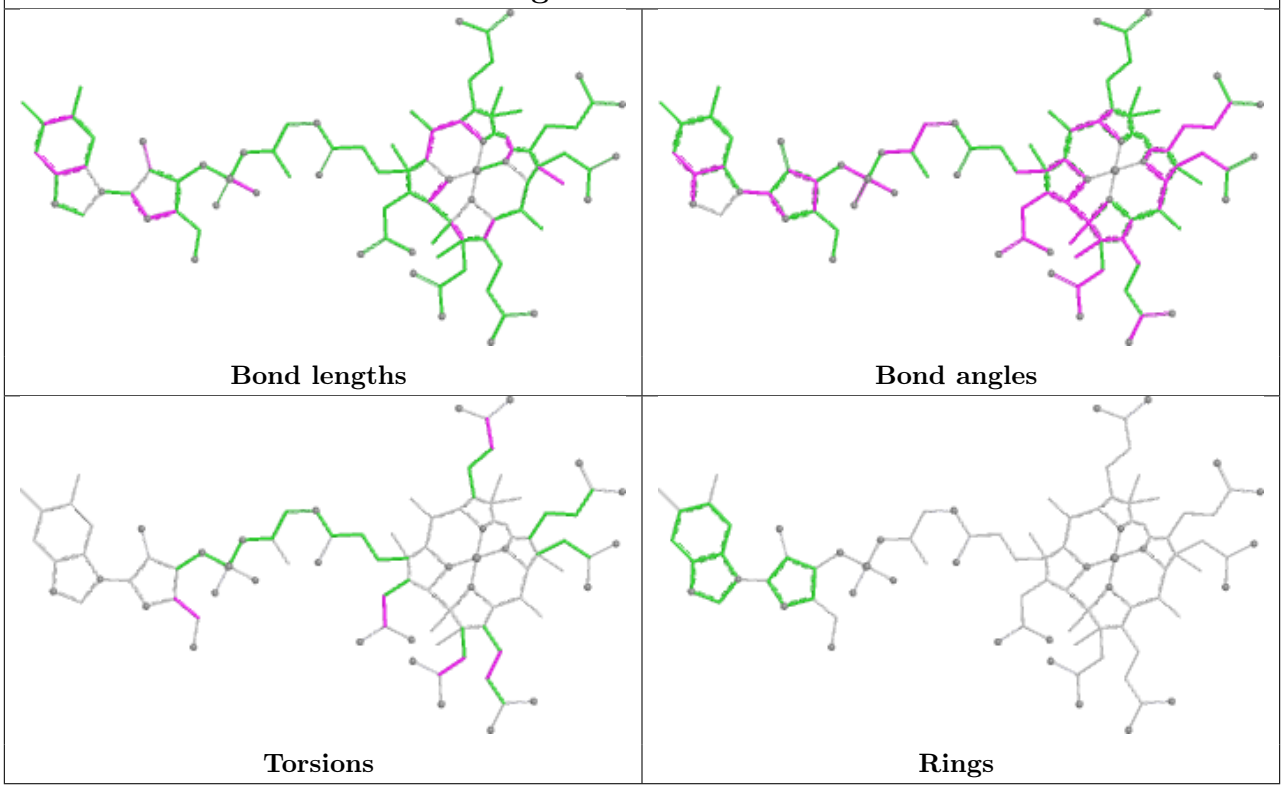
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	908	GOL	4	0
2	A	905	GOL	3	0
2	A	910	GOL	1	0
2	A	901	GOL	2	0
2	A	909	GOL	2	0
2	A	902	GOL	2	0
2	A	907	GOL	1	0
5	A	912	B12	11	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 A 912



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, 95^{th} 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	862/874 (98%)	0.03	20 (2%) 61 63	46, 60, 91, 145	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	ALA	3.7
1	A	874	ALA	3.6
1	A	2	VAL	3.5
1	A	465	SER	3.3
1	A	283	ASN	3.3
1	A	539	GLN	3.1
1	A	540	GLY	2.9
1	A	4	VAL	2.8
1	A	634	GLY	2.8
1	A	654	LYS	2.7
1	A	1	MET	2.6
1	A	524	ARG	2.5
1	A	284	ALA	2.5
1	A	22	ASP	2.5
1	A	746	GLU	2.3
1	A	811	LYS	2.3
1	A	650	GLU	2.3
1	A	43	LYS	2.2
1	A	538	THR	2.2
1	A	543	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

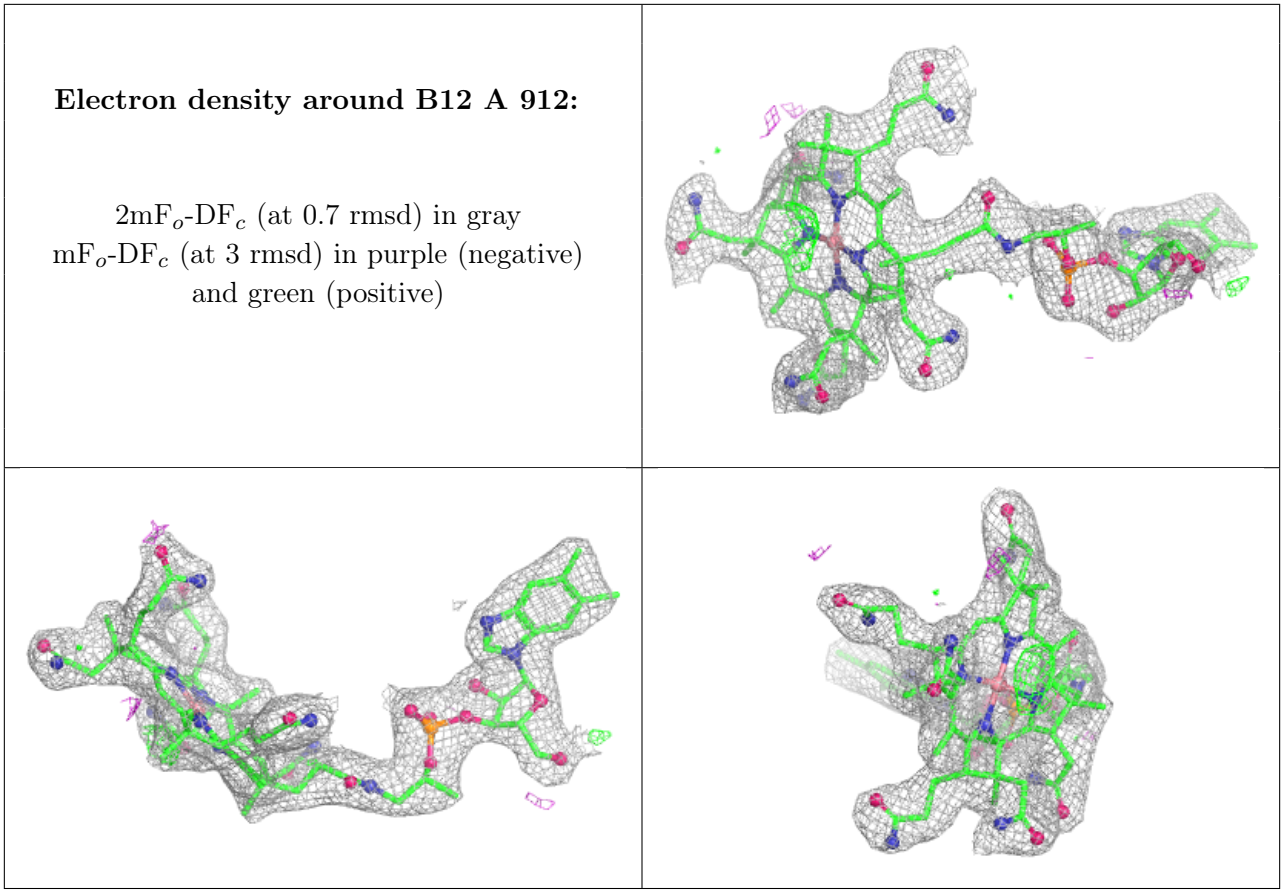
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	K	A	914	1/1	0.65	0.39	30,30,30,30	0
2	GOL	A	902	6/6	0.84	0.23	50,68,79,81	0
2	GOL	A	901	6/6	0.89	0.18	80,101,112,124	0
2	GOL	A	907	6/6	0.90	0.17	71,85,93,95	0
2	GOL	A	911	6/6	0.92	0.15	60,73,81,83	0
2	GOL	A	909	6/6	0.92	0.13	64,67,71,89	0
2	GOL	A	906	6/6	0.94	0.11	50,59,72,89	0
2	GOL	A	910	6/6	0.94	0.13	63,77,84,100	0
3	HCS	A	903	8/8	0.95	0.09	58,69,73,75	0
2	GOL	A	905	6/6	0.95	0.12	57,66,81,127	0
2	GOL	A	908	6/6	0.96	0.10	54,71,88,95	0
5	B12	A	912	91/91	0.97	0.09	39,59,78,82	0
4	ZN	A	904	1/1	0.98	0.07	75,75,75,75	0
4	ZN	A	913	1/1	0.99	0.02	54,54,54,54	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 912:

$2mF_o$-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

There are no such residues in this entry.