



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 10:06 pm BST

PDB ID : 8BB0 / pdb_00008bb0
Title : The surface-exposed lipo-protein of BtuG2 in complex with hydroxycobalamin.
Authors : Whittaker, J.; Felices Martinez, J.M.; Guskov, A.; Slotboom, D.J.
Deposited on : 2022-10-12
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
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

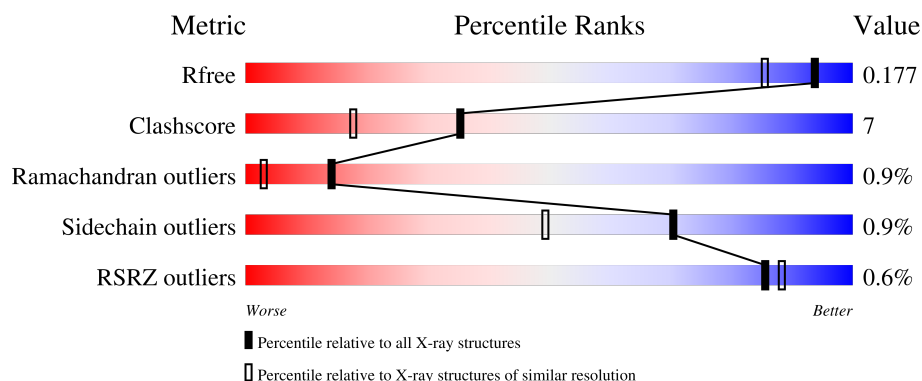
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	327	% 86% 11% .
1	B	327	87% 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
3	SCN	A	413	-	-	X	-
5	ACT	A	424	-	X	X	-
5	ACT	B	417	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6137 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 Surface layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	4	0
			2643	1711	417	504	11			
1	B	321	Total	C	N	O	S	0	0	0
			2626	1696	418	501	11			

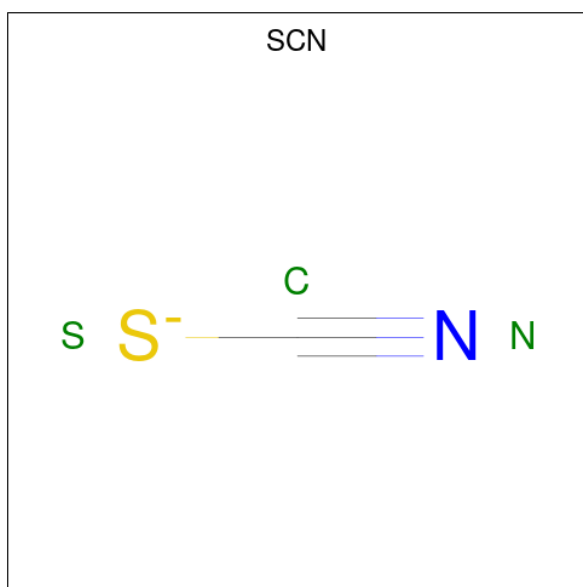
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8A6D0
A	322	LEU	-	expression tag	UNP Q8A6D0
A	323	GLU	-	expression tag	UNP Q8A6D0
A	324	VAL	-	expression tag	UNP Q8A6D0
A	325	LEU	-	expression tag	UNP Q8A6D0
A	326	PHE	-	expression tag	UNP Q8A6D0
A	327	GLN	-	expression tag	UNP Q8A6D0
B	1	MET	-	initiating methionine	UNP Q8A6D0
B	322	LEU	-	expression tag	UNP Q8A6D0
B	323	GLU	-	expression tag	UNP Q8A6D0
B	324	VAL	-	expression tag	UNP Q8A6D0
B	325	LEU	-	expression tag	UNP Q8A6D0
B	326	PHE	-	expression tag	UNP Q8A6D0
B	327	GLN	-	expression tag	UNP Q8A6D0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

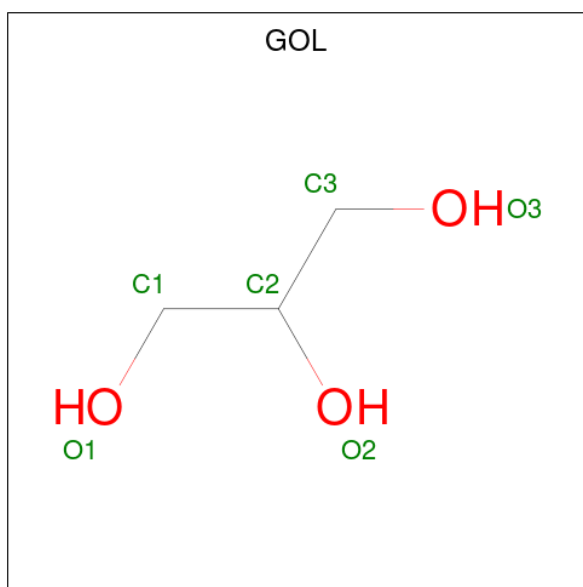
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Na	0	0
			9	9		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



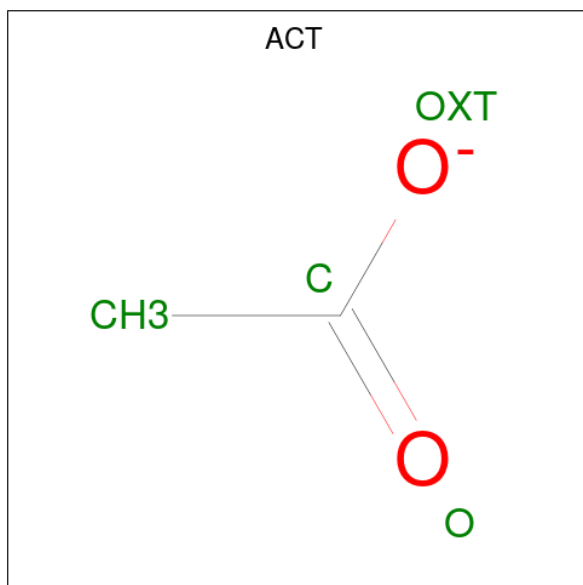
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

Continued on next page...

Continued from previous page...

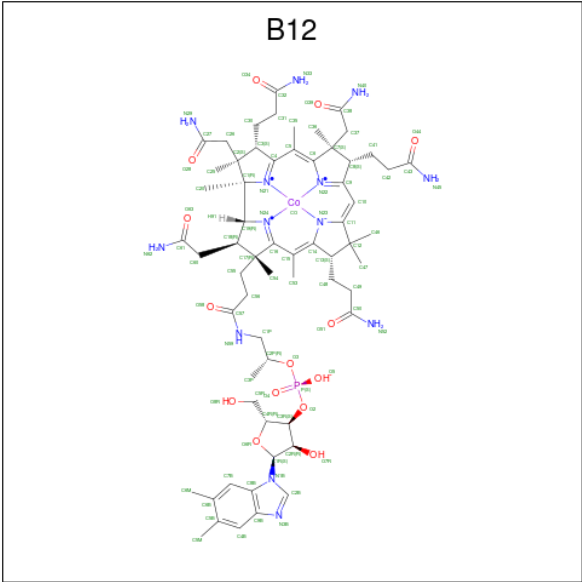
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



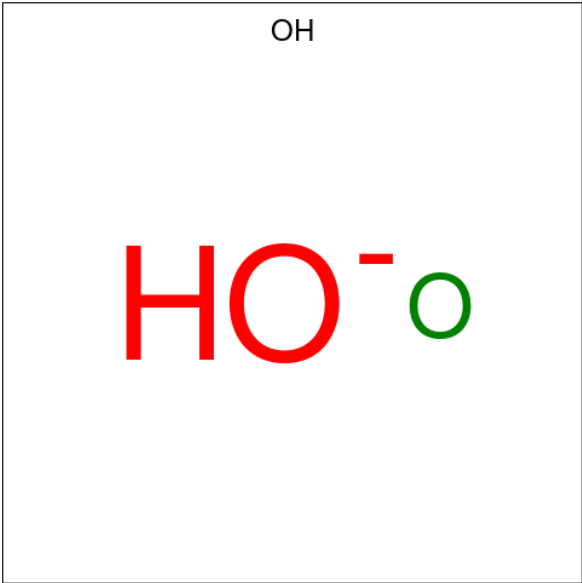
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



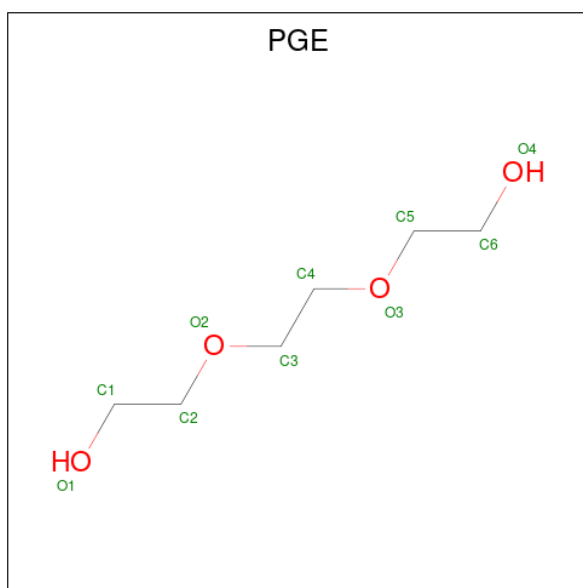
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 7 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



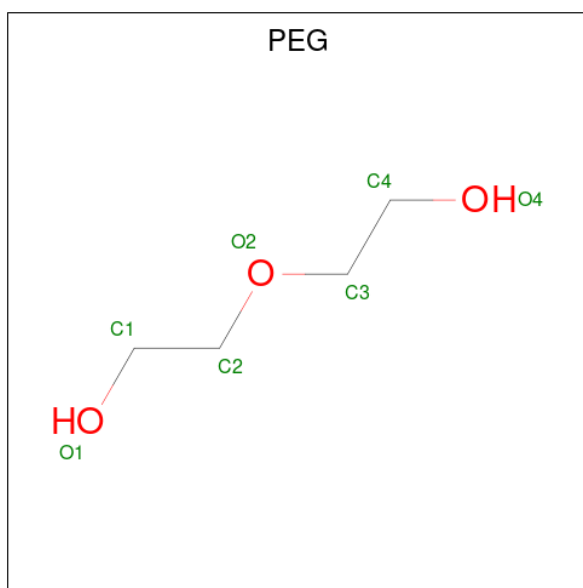
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	1	Total	O	0	0
			1	1		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

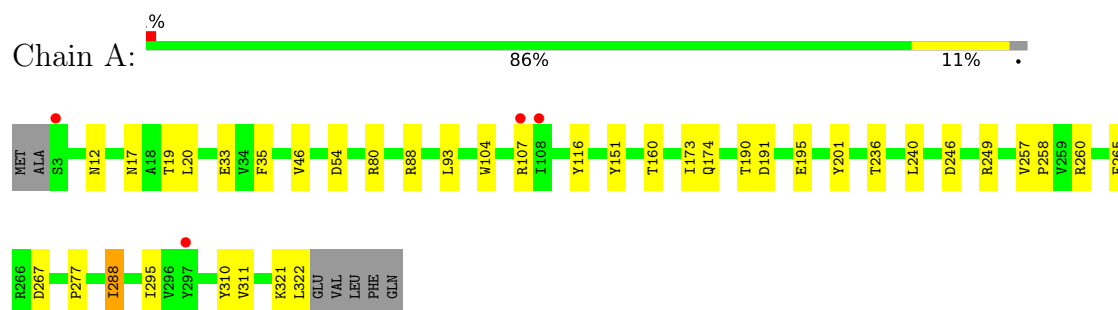
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	263	Total 263	O 263	0	0
10	B	245	Total 245	O 245	0	0

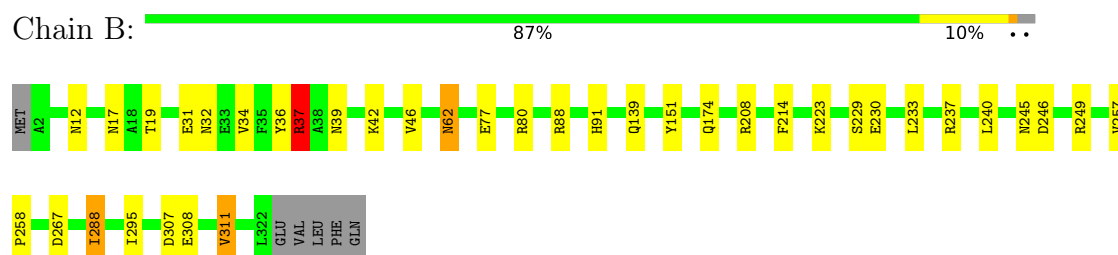
3 Residue-property plots [i](#)

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: Surface layer protein



- Molecule 1: Surface layer protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.11Å 101.10Å 79.89Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	62.40 – 1.50 62.40 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (62.40-1.50) 96.1 (62.40-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.143 , 0.174 0.146 , 0.177	Depositor DCC
R_{free} test set	5900 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6137	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: B12, NA, PGE, PEG, GOL, ACT, OH, SCN

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	0.62	0/2728	0.95	1/3713 (0.0%)
1	B	0.66	0/2699	0.98	3/3674 (0.1%)
All	All	0.64	0/5427	0.97	4/7387 (0.1%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	229	SER	O-C-N	5.87	129.14	123.04
1	B	230	GLU	N-CA-C	5.84	119.31	111.24
1	A	191	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	62	ASN	OD1-CG-ND2	5.12	127.72	122.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	B	208	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	37	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	2643	0	2535	27	0
1	B	2626	0	2506	38	0
2	A	9	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	0	2	0
3	B	3	0	0	0	0
4	A	42	0	56	2	0
4	B	60	0	80	4	0
5	A	8	0	6	9	0
5	B	8	0	6	7	0
6	A	91	0	87	10	0
6	B	91	0	87	11	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	10	0	14	3	0
9	B	14	0	20	5	0
10	A	263	0	0	1	0
10	B	245	0	0	2	0
All	All	6137	0	5397	81	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 7.

All (81) 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)
5:A:424:ACT:C	5:A:424:ACT:CH3	1.74	1.65
5:A:424:ACT:C	5:A:424:ACT:O	1.68	1.42
1:B:42:LYS:CD	5:B:417:ACT:H1	1.85	1.04
1:B:42:LYS:HD2	5:B:417:ACT:CH3	1.89	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:HD2	5:B:417:ACT:H1	1.00	0.97
1:A:20:LEU:H	5:A:424:ACT:H3	1.31	0.95
1:B:307:ASP:OD1	9:B:405:PEG:H12	1.68	0.94
6:A:426:B12:H362	6:A:426:B12:H351	1.48	0.93
1:B:62:ASN:HD21	6:B:418:B12:H331	1.23	0.87
6:B:418:B12:H362	6:B:418:B12:H351	1.57	0.86
1:B:19:THR:HG22	5:B:417:ACT:H3	1.58	0.85
1:B:39:ASN:HD21	1:B:77:GLU:H	1.30	0.80
1:A:88:ARG:HH22	6:A:426:B12:H292	1.30	0.79
1:B:307:ASP:OD1	9:B:405:PEG:C1	2.31	0.78
1:A:33:GLU:HA	5:A:424:ACT:H1	1.66	0.76
6:B:418:B12:H552	6:B:418:B12:H531	1.71	0.73
6:A:426:B12:H531	6:A:426:B12:H552	1.71	0.72
1:B:88:ARG:HH22	6:B:418:B12:H292	1.40	0.70
1:A:19:THR:HG22	5:A:424:ACT:OXT	1.96	0.66
1:A:260:ARG:HH12	1:B:80:ARG:HH22	1.45	0.63
6:A:426:B12:H351	6:A:426:B12:C36	2.27	0.63
1:A:19:THR:HA	5:A:424:ACT:C	2.29	0.63
1:B:42:LYS:CD	5:B:417:ACT:CH3	2.64	0.63
1:B:91:HIS:HE1	1:B:139:GLN:OE1	1.83	0.61
4:B:412:GOL:H12	10:B:676:HOH:O	2.01	0.60
1:B:288:ILE:HD11	1:B:295:ILE:HG22	1.85	0.59
6:A:426:B12:H531	6:A:426:B12:C55	2.31	0.59
1:A:260:ARG:NH1	1:B:80:ARG:HH22	2.01	0.58
1:B:249:ARG:HG3	8:B:401:PGE:H42	1.86	0.58
6:B:418:B12:H291	6:B:418:B12:H3	1.69	0.57
1:B:37:ARG:HH11	1:B:37:ARG:HB2	1.68	0.57
1:B:12:ASN:HD22	1:B:17:ASN:HD21	1.52	0.57
1:B:42:LYS:HE3	10:B:548:HOH:O	2.05	0.57
6:B:418:B12:H531	6:B:418:B12:C55	2.35	0.56
1:A:288:ILE:HD11	1:A:295[B]:ILE:HG22	1.89	0.55
6:A:426:B12:H3	6:A:426:B12:H291	1.71	0.54
6:B:418:B12:H351	6:B:418:B12:C36	2.34	0.54
1:A:12:ASN:HD22	1:A:17:ASN:HD21	1.55	0.53
1:A:321:LYS:NZ	10:A:504:HOH:O	2.43	0.52
1:A:20:LEU:N	5:A:424:ACT:H3	2.14	0.52
1:A:88:ARG:NH2	6:A:426:B12:H292	2.04	0.50
6:B:418:B12:H482	6:B:418:B12:H533	1.95	0.49
1:A:295[A]:ILE:HG12	1:A:310:TYR:CD1	2.48	0.49
1:B:249:ARG:O	8:B:401:PGE:H4	2.12	0.48
1:B:91:HIS:HD2	4:B:406:GOL:O2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:418:B12:H3	6:B:418:B12:N29	2.28	0.48
1:A:93[B]:LEU:CD2	1:A:160:THR:HB	2.43	0.48
1:B:214:PHE:O	5:B:416:ACT:H2	2.13	0.48
1:B:31:GLU:HG2	1:B:34:VAL:HG12	1.95	0.48
1:A:236:THR:HG23	4:A:421:GOL:H32	1.96	0.47
6:A:426:B12:H3	6:A:426:B12:N29	2.26	0.47
1:A:240:LEU:O	1:A:249:ARG:HA	2.15	0.46
1:B:245:ASN:HD22	4:B:411:GOL:C1	2.28	0.46
1:A:80:ARG:O	3:A:413:SCN:S	2.73	0.46
1:A:35:PHE:HB3	5:A:424:ACT:H2	1.97	0.46
1:A:151:TYR:H	1:A:174:GLN:NE2	2.13	0.46
1:B:36:TYR:HB2	5:B:417:ACT:H2	1.99	0.45
1:A:277:PRO:O	4:A:421:GOL:H12	2.17	0.44
6:A:426:B12:H362	6:A:426:B12:C35	2.34	0.44
1:A:116:TYR:O	3:A:413:SCN:N	2.51	0.44
1:B:237:ARG:HG2	9:B:404:PEG:H22	1.99	0.44
5:A:424:ACT:CH3	5:A:424:ACT:OXT	2.54	0.44
1:B:223:LYS:HD3	4:B:411:GOL:C3	2.47	0.44
1:A:265:PHE:CZ	1:A:267:ASP:HA	2.53	0.43
1:A:195:GLU:HG2	1:A:201:TYR:CE2	2.53	0.43
1:B:249:ARG:O	8:B:401:PGE:C4	2.67	0.43
1:B:151:TYR:H	1:B:174:GLN:NE2	2.15	0.43
1:B:31:GLU:CG	1:B:34:VAL:HG12	2.49	0.43
1:B:39:ASN:ND2	1:B:77:GLU:H	2.07	0.42
1:B:37:ARG:HB2	1:B:37:ARG:NH1	2.31	0.42
1:A:104:TRP:HE1	6:A:426:B12:H332	1.68	0.42
1:B:62:ASN:ND2	6:B:418:B12:H331	2.04	0.42
1:B:240:LEU:O	1:B:249:ARG:HA	2.19	0.42
1:B:32:ASN:HD21	1:B:311:VAL:HA	1.85	0.41
1:B:233:LEU:HB2	9:B:404:PEG:H41	2.01	0.41
1:B:257:VAL:HB	1:B:258:PRO:HD2	2.02	0.41
1:B:88:ARG:NH2	6:B:418:B12:H292	2.13	0.41
1:A:257:VAL:HB	1:A:258:PRO:HD2	2.02	0.41
1:A:277:PRO:HG2	1:A:322:LEU:HD11	2.02	0.40
1:A:173:ILE:O	1:A:190:THR:HB	2.22	0.40
1:B:308:GLU:HG3	9:B:405:PEG:H42	2.04	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	322/327 (98%)	301 (94%)	18 (6%)	3 (1%)	14	3
1	B	319/327 (98%)	301 (94%)	15 (5%)	3 (1%)	14	3
All	All	641/654 (98%)	602 (94%)	33 (5%)	6 (1%)	14	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	VAL
1	B	311	VAL
1	B	288	ILE
1	A	46	VAL
1	A	288	ILE
1	B	46	VAL

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	288/290 (99%)	286 (99%)	2 (1%)	76	57
1	B	284/290 (98%)	281 (99%)	3 (1%)	65	41
All	All	572/580 (99%)	567 (99%)	5 (1%)	70	49

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	246	ASP
1	B	37	ARG
1	B	246	ASP
1	B	267	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	32	ASN
1	A	48	GLN
1	A	174	GLN
1	A	184	ASN
1	A	245	ASN
1	B	12	ASN
1	B	32	ASN
1	B	39	ASN
1	B	62	ASN
1	B	73	ASN
1	B	91	HIS
1	B	174	GLN
1	B	232	GLN
1	B	245	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 46 ligands modelled in this entry, 10 are monoatomic and 2 are modelled with single atom - leaving 34 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	$\# Z > 2$
3	SCN	A	415	-	1,2,2	1.30	0	0,1,1	-	-
4	GOL	A	423	-	5,5,5	0.12	0	5,5,5	0.33	0
5	ACT	A	424	-	3,3,3	7.06	3 (100%)	3,3,3	2.32	2 (66%)
3	SCN	A	412	-	1,2,2	0.89	0	0,1,1	-	-
4	GOL	B	406	-	5,5,5	0.18	0	5,5,5	0.39	0
9	PEG	B	404	-	6,6,6	0.19	0	5,5,5	0.22	0
4	GOL	A	418	-	5,5,5	0.12	0	5,5,5	0.24	0
4	GOL	B	410	-	5,5,5	0.14	0	5,5,5	0.35	0
5	ACT	B	417	-	3,3,3	0.71	0	3,3,3	1.19	0
4	GOL	B	415	-	5,5,5	0.17	0	5,5,5	0.35	0
4	GOL	B	411	-	5,5,5	0.12	0	5,5,5	0.37	0
4	GOL	B	412	-	5,5,5	0.14	0	5,5,5	0.53	0
3	SCN	A	413	-	1,2,2	1.63	0	0,1,1	-	-
4	GOL	A	420	-	5,5,5	0.15	0	5,5,5	0.42	0
5	ACT	B	416	-	3,3,3	0.98	0	3,3,3	0.91	0
4	GOL	B	408	-	5,5,5	0.14	0	5,5,5	0.78	0
4	GOL	A	417	-	5,5,5	0.21	0	5,5,5	0.46	0
3	SCN	A	411	-	1,2,2	0.85	0	0,1,1	-	-
5	ACT	A	425	-	3,3,3	1.16	0	3,3,3	0.64	0
4	GOL	A	422	-	5,5,5	0.16	0	5,5,5	0.35	0
3	SCN	A	414	-	1,2,2	0.08	0	0,1,1	-	-
6	B12	B	418	7	93,101,101	1.43	11 (11%)	146,166,166	1.74	29 (19%)
3	SCN	A	416	-	1,2,2	0.63	0	0,1,1	-	-
3	SCN	B	403	-	1,2,2	2.07	1 (100%)	0,1,1	-	-
4	GOL	B	413	-	5,5,5	0.12	0	5,5,5	0.24	0
6	B12	A	426	7,2	93,101,101	1.50	15 (16%)	146,166,166	2.04	31 (21%)
4	GOL	A	419	-	5,5,5	0.16	0	5,5,5	0.70	0
4	GOL	A	421	-	5,5,5	0.15	0	5,5,5	0.60	0
9	PEG	B	405	-	6,6,6	0.38	0	5,5,5	0.30	0
8	PGE	B	401	-	9,9,9	0.49	0	8,8,8	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SCN	A	410	-	1,2,2	2.37	1 (100%)	0,1,1	-	-
4	GOL	B	409	-	5,5,5	0.12	0	5,5,5	0.53	0
4	GOL	B	407	-	5,5,5	0.53	0	5,5,5	1.01	0
4	GOL	B	414	-	5,5,5	0.14	0	5,5,5	0.52	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
4	GOL	A	423	-	-	4/4/4/4	-
9	PEG	B	404	-	-	2/4/4/4	-
4	GOL	B	406	-	-	1/4/4/4	-
4	GOL	A	418	-	-	1/4/4/4	-
4	GOL	B	410	-	-	0/4/4/4	-
4	GOL	B	415	-	-	2/4/4/4	-
4	GOL	B	411	-	-	4/4/4/4	-
4	GOL	B	412	-	-	4/4/4/4	-
4	GOL	A	420	-	-	2/4/4/4	-
4	GOL	B	408	-	-	3/4/4/4	-
4	GOL	A	417	-	-	1/4/4/4	-
4	GOL	A	422	-	-	4/4/4/4	-
6	B12	B	418	7	-	7/56/223/223	0/3/11/11
4	GOL	B	413	-	-	2/4/4/4	-
6	B12	A	426	7,2	-	9/56/223/223	0/3/11/11
4	GOL	A	419	-	-	2/4/4/4	-
4	GOL	A	421	-	-	4/4/4/4	-
9	PEG	B	405	-	-	3/4/4/4	-
8	PGE	B	401	-	-	4/7/7/7	-
4	GOL	B	409	-	-	2/4/4/4	-
4	GOL	B	407	-	-	0/4/4/4	-
4	GOL	B	414	-	-	2/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	424	ACT	O-C	10.12	1.68	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	424	ACT	CH3-C	6.08	1.74	1.49
6	A	426	B12	C12-C11	-4.89	1.43	1.52
6	B	418	B12	C12-C11	-4.77	1.44	1.52
6	A	426	B12	C14-N23	-4.50	1.29	1.35
6	A	426	B12	C9-N22	4.33	1.42	1.30
6	B	418	B12	C14-N23	-4.04	1.29	1.35
6	B	418	B12	C8B-C9B	4.02	1.47	1.40
6	B	418	B12	C9-N22	3.85	1.40	1.30
6	A	426	B12	C6B-C5B	3.81	1.50	1.40
6	A	426	B12	C8B-N1B	-3.25	1.32	1.39
5	A	424	ACT	OXT-C	3.19	1.46	1.30
6	B	418	B12	C8B-N1B	-3.08	1.33	1.39
6	A	426	B12	C8B-C9B	3.07	1.45	1.40
6	A	426	B12	C19-N24	-2.98	1.43	1.48
6	B	418	B12	C46-C12	-2.89	1.47	1.54
6	B	418	B12	C11-N23	-2.89	1.31	1.37
6	B	418	B12	C1-C2	-2.87	1.52	1.58
6	A	426	B12	C11-N23	-2.86	1.31	1.37
6	B	418	B12	C18-C19	-2.84	1.47	1.53
6	A	426	B12	C14-C15	2.52	1.49	1.38
6	A	426	B12	O6R-C4R	-2.46	1.39	1.45
6	A	426	B12	O28-C27	2.38	1.31	1.24
3	A	410	SCN	C-N	2.37	1.23	1.15
6	A	426	B12	C1-C2	-2.37	1.53	1.58
6	B	418	B12	C8-C9	-2.36	1.46	1.51
6	A	426	B12	C18-C19	-2.34	1.48	1.53
6	A	426	B12	C47-C12	-2.27	1.49	1.54
6	B	418	B12	O28-C27	2.23	1.30	1.24
6	A	426	B12	C9B-N3B	-2.19	1.35	1.39
3	B	403	SCN	C-N	-2.07	1.08	1.15

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	418	B12	C1-C19-N24	8.08	115.33	106.24
6	A	426	B12	C9B-N3B-C2B	7.55	113.44	104.44
6	A	426	B12	C12-C11-C10	-7.53	113.57	123.37
6	A	426	B12	C20-C1-C19	-7.24	102.38	109.36
6	A	426	B12	C1-C19-N24	7.11	114.23	106.24
6	A	426	B12	C8B-C9B-N3B	-5.88	103.48	109.97
6	B	418	B12	C12-C11-C10	-5.78	115.85	123.37
6	A	426	B12	N1B-C2B-N3B	-5.74	106.06	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	418	B12	C1-C19-C18	5.63	131.12	121.88
6	B	418	B12	C20-C1-C19	-5.03	104.51	109.36
6	A	426	B12	C1-C19-C18	4.93	129.97	121.88
6	B	418	B12	C12-C11-N23	4.53	118.14	111.83
6	A	426	B12	C8B-N1B-C2B	4.28	110.36	106.37
6	B	418	B12	C2-C1-C19	4.20	125.23	118.60
6	A	426	B12	C12-C11-N23	3.89	117.25	111.83
6	A	426	B12	C2-C1-C19	3.68	124.41	118.60
6	B	418	B12	C7B-C8B-C9B	-3.44	118.44	122.52
6	A	426	B12	O63-C61-C60	3.26	127.72	120.87
6	A	426	B12	C7B-C8B-C9B	-3.24	118.68	122.52
6	B	418	B12	C17-C16-N24	-3.21	106.21	111.15
5	A	424	ACT	OXT-C-O	3.18	133.77	122.05
6	A	426	B12	C18-C19-N24	3.11	107.05	102.31
6	A	426	B12	C9B-C8B-N1B	3.03	106.63	105.35
6	B	418	B12	C18-C19-N24	2.97	106.83	102.31
6	B	418	B12	C3-C4-C5	-2.91	118.91	123.81
6	A	426	B12	C46-C12-C11	2.85	120.32	110.08
6	A	426	B12	C48-C49-C50	-2.82	103.01	112.59
6	B	418	B12	C8B-C9B-N3B	-2.75	106.93	109.97
6	B	418	B12	C13-C14-N23	2.69	112.76	109.10
6	B	418	B12	C13-C12-C11	-2.67	97.94	100.97
6	A	426	B12	C18-C17-C16	-2.63	97.47	100.67
6	B	418	B12	C5-C4-N21	2.63	128.45	124.19
6	A	426	B12	C36-C7-C37	2.58	115.06	110.80
6	A	426	B12	C10-C11-N23	2.58	128.84	124.43
6	B	418	B12	C9B-C8B-N1B	2.57	106.44	105.35
6	A	426	B12	C10-C9-N22	-2.57	122.78	125.73
6	B	418	B12	C10-C9-N22	-2.56	122.79	125.73
6	A	426	B12	C17-C18-C19	2.55	106.26	102.36
6	B	418	B12	C54-C17-C18	-2.50	109.29	112.98
5	A	424	ACT	OXT-C-CH3	-2.45	105.07	115.18
6	B	418	B12	C13-C14-C15	-2.45	120.58	124.32
6	B	418	B12	C46-C12-C11	2.44	118.85	110.08
6	A	426	B12	C13-C12-C11	-2.38	98.27	100.97
6	A	426	B12	C4B-C9B-N3B	2.38	134.59	130.51
6	A	426	B12	C8-C9-C10	2.38	128.46	123.32
6	B	418	B12	C8-C9-C10	2.29	128.26	123.32
6	B	418	B12	C4B-C9B-N3B	2.28	134.42	130.51
6	A	426	B12	C19-C1-N21	2.27	104.49	102.16
6	B	418	B12	C8B-N1B-C2B	2.18	108.40	106.37
6	B	418	B12	C53-C15-C16	-2.17	116.64	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	426	B12	C15-C16-N24	-2.16	119.31	122.42
6	B	418	B12	O39-C38-C37	-2.16	115.17	121.99
6	B	418	B12	C1-C2-C3	2.15	104.34	101.60
6	A	426	B12	C4R-O6R-C1R	2.12	114.15	109.47
6	A	426	B12	O39-C38-N40	2.10	128.23	122.50
6	B	418	B12	C17-C16-C15	2.09	129.56	126.26
6	B	418	B12	O58-C57-N59	2.09	126.97	123.01
6	B	418	B12	O63-C61-C60	2.09	125.27	120.87
6	A	426	B12	C53-C15-C16	-2.06	116.84	120.38
6	A	426	B12	O44-C43-N45	-2.06	116.88	122.50
6	B	418	B12	C36-C7-C37	2.06	114.19	110.80
6	A	426	B12	C13-C14-N23	2.00	111.83	109.10

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	420	GOL	O1-C1-C2-C3
4	A	421	GOL	O1-C1-C2-C3
4	A	422	GOL	O1-C1-C2-C3
4	A	423	GOL	O1-C1-C2-O2
4	A	423	GOL	O1-C1-C2-C3
4	B	408	GOL	O1-C1-C2-C3
4	B	411	GOL	O1-C1-C2-C3
4	B	411	GOL	C1-C2-C3-O3
4	B	412	GOL	O1-C1-C2-O2
4	B	412	GOL	O1-C1-C2-C3
4	B	412	GOL	C1-C2-C3-O3
4	B	412	GOL	O2-C2-C3-O3
4	B	413	GOL	O1-C1-C2-C3
4	B	414	GOL	O1-C1-C2-C3
4	B	415	GOL	O1-C1-C2-C3
6	B	418	B12	C13-C48-C49-C50
4	A	421	GOL	O2-C2-C3-O3
4	B	411	GOL	O1-C1-C2-O2
4	B	413	GOL	O1-C1-C2-O2
8	B	401	PGE	O2-C3-C4-O3
8	B	401	PGE	O3-C5-C6-O4
9	B	404	PEG	O1-C1-C2-O2
9	B	404	PEG	O2-C3-C4-O4
9	B	405	PEG	O2-C3-C4-O4
4	A	418	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	419	GOL	O1-C1-C2-C3
4	A	421	GOL	C1-C2-C3-O3
4	A	422	GOL	C1-C2-C3-O3
4	A	423	GOL	C1-C2-C3-O3
4	B	406	GOL	C1-C2-C3-O3
4	B	409	GOL	C1-C2-C3-O3
4	A	420	GOL	O1-C1-C2-O2
4	A	421	GOL	O1-C1-C2-O2
4	A	423	GOL	O2-C2-C3-O3
4	B	408	GOL	O1-C1-C2-O2
4	B	411	GOL	O2-C2-C3-O3
4	B	414	GOL	O1-C1-C2-O2
6	A	426	B12	C13-C48-C49-C50
9	B	405	PEG	O1-C1-C2-O2
4	A	422	GOL	O1-C1-C2-O2
6	A	426	B12	C2-C26-C27-O28
6	A	426	B12	C2-C26-C27-N29
6	B	418	B12	C2-C26-C27-N29
6	A	426	B12	C41-C42-C43-N45
6	A	426	B12	C41-C42-C43-O44
6	A	426	B12	C30-C31-C32-O34
6	A	426	B12	C7-C37-C38-O39
6	B	418	B12	C41-C42-C43-O44
4	B	409	GOL	O2-C2-C3-O3
4	B	415	GOL	O1-C1-C2-O2
4	A	417	GOL	O1-C1-C2-C3
9	B	405	PEG	C4-C3-O2-C2
6	A	426	B12	C30-C31-C32-N33
6	B	418	B12	C41-C42-C43-N45
6	B	418	B12	C7-C37-C38-N40
8	B	401	PGE	C6-C5-O3-C4
8	B	401	PGE	O1-C1-C2-O2
6	B	418	B12	C2-C26-C27-O28
6	B	418	B12	C7-C37-C38-O39
6	A	426	B12	C7-C37-C38-N40
4	A	419	GOL	O1-C1-C2-O2
4	A	422	GOL	O2-C2-C3-O3
4	B	408	GOL	O2-C2-C3-O3

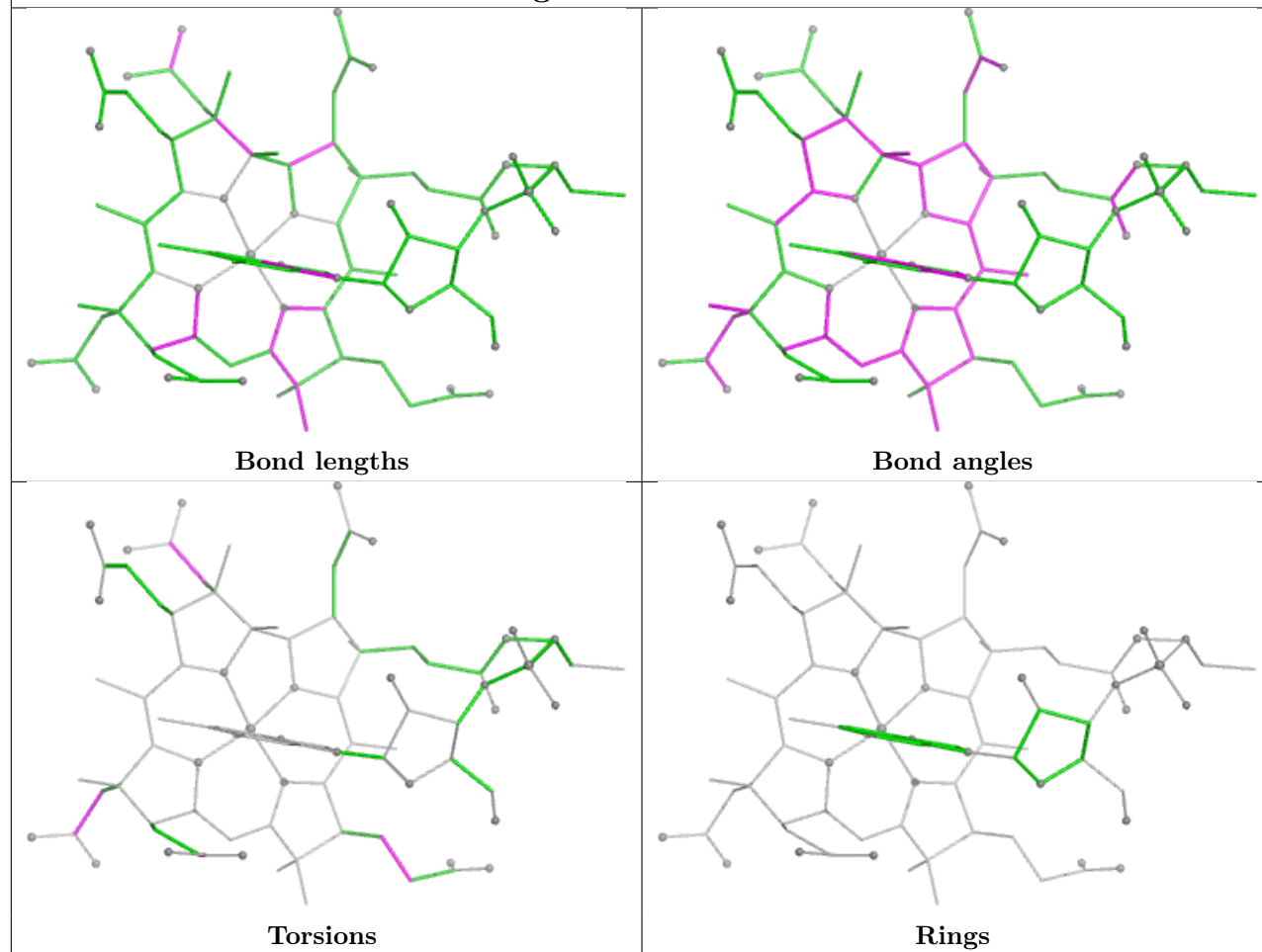
There are no ring outliers.

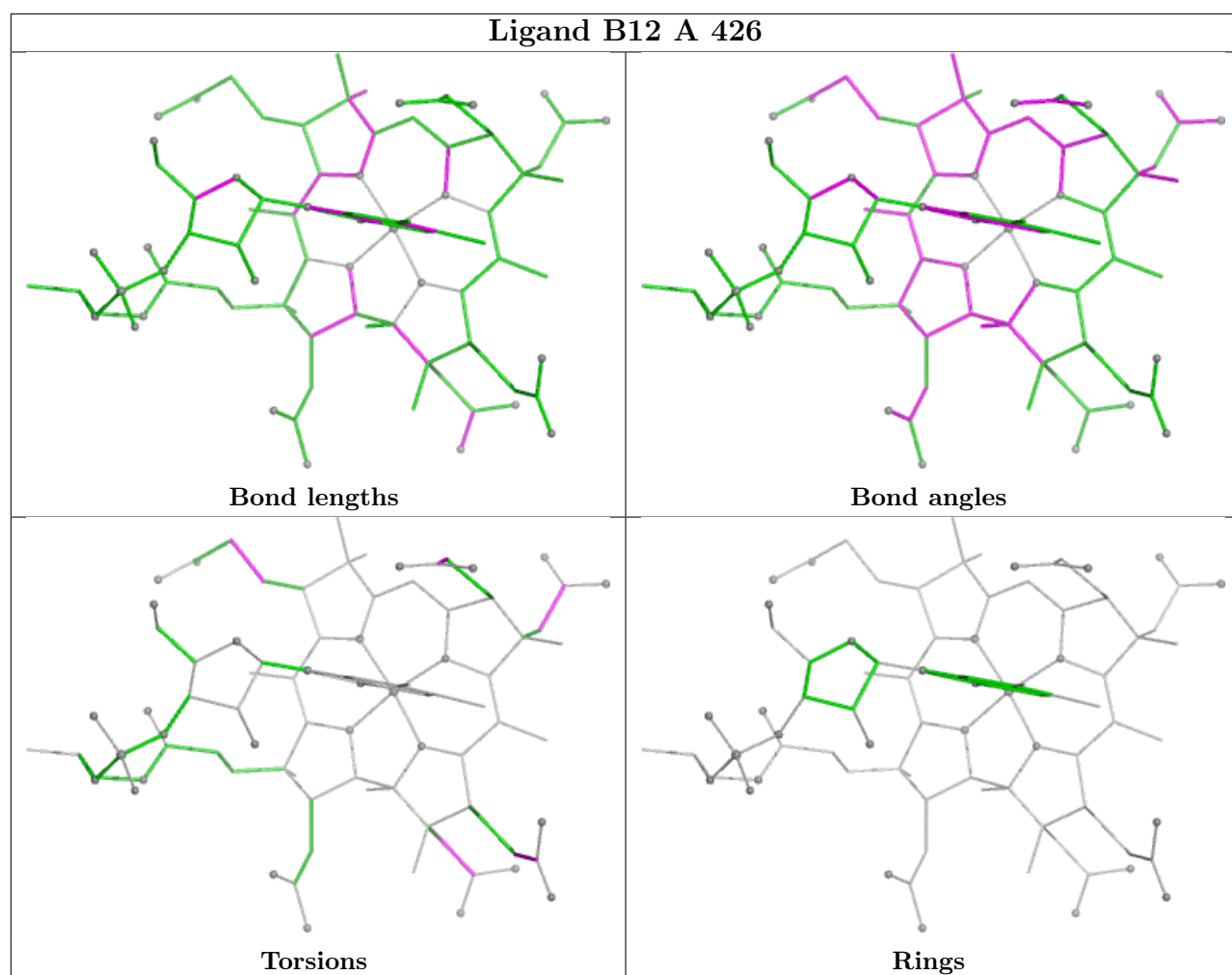
13 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	424	ACT	9	0
4	B	406	GOL	1	0
9	B	404	PEG	2	0
5	B	417	ACT	6	0
4	B	411	GOL	2	0
4	B	412	GOL	1	0
3	A	413	SCN	2	0
5	B	416	ACT	1	0
6	B	418	B12	11	0
6	A	426	B12	10	0
4	A	421	GOL	2	0
9	B	405	PEG	3	0
8	B	401	PGE	3	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.

Ligand B12 B 418





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	320/327 (97%)	-0.40	4 (1%) 75 78	8, 15, 24, 38	4 (1%)
1	B	321/327 (98%)	-0.42	0 100 100	12, 15, 23, 31	0
All	All	641/654 (98%)	-0.41	4 (0%) 85 88	8, 15, 24, 38	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	SER	2.8
1	A	107	ARG	2.7
1	A	108	ILE	2.6
1	A	297	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	OH	A	427	1/1	0.72	0.18	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SCN	A	414	3/3	0.78	0.18	48,48,50,52	0
7	OH	B	419	1/1	0.79	0.16	15,15,15,15	0
5	ACT	A	424	4/4	0.81	0.34	69,125,147,685	0
5	ACT	A	425	4/4	0.82	0.20	45,53,55,55	0
4	GOL	A	423	6/6	0.84	0.20	23,39,43,51	0
4	GOL	B	412	6/6	0.85	0.14	27,33,39,42	0
4	GOL	B	413	6/6	0.85	0.17	33,42,45,52	0
4	GOL	A	418	6/6	0.85	0.18	46,57,62,64	0
4	GOL	B	411	6/6	0.88	0.15	39,41,43,48	0
9	PEG	B	405	7/7	0.88	0.15	23,29,39,41	0
5	ACT	B	416	4/4	0.89	0.15	48,49,49,50	0
8	PGE	B	401	10/10	0.90	0.13	24,30,34,41	0
4	GOL	B	409	6/6	0.90	0.14	27,34,38,39	0
4	GOL	B	415	6/6	0.91	0.12	35,42,44,44	0
4	GOL	A	422	6/6	0.91	0.12	34,40,43,47	0
3	SCN	A	416	3/3	0.91	0.15	48,48,57,66	0
9	PEG	B	404	7/7	0.91	0.15	20,34,44,45	0
4	GOL	A	419	6/6	0.91	0.14	25,34,38,38	0
5	ACT	B	417	4/4	0.92	0.15	18,26,27,30	0
3	SCN	B	403	3/3	0.93	0.10	20,20,23,41	0
3	SCN	A	415	3/3	0.93	0.13	29,29,40,60	0
3	SCN	A	410	3/3	0.93	0.18	17,17,35,48	0
4	GOL	A	421	6/6	0.93	0.13	18,28,39,49	0
3	SCN	A	413	3/3	0.94	0.17	25,25,28,32	0
2	NA	A	409	1/1	0.94	0.09	16,16,16,16	0
4	GOL	B	410	6/6	0.94	0.11	19,32,41,43	0
3	SCN	A	412	3/3	0.94	0.10	42,42,53,68	0
4	GOL	B	408	6/6	0.95	0.08	26,28,29,30	0
4	GOL	B	414	6/6	0.95	0.09	17,23,28,36	0
4	GOL	B	407	6/6	0.96	0.07	15,16,20,20	0
4	GOL	A	420	6/6	0.96	0.09	21,30,34,40	0
3	SCN	A	411	3/3	0.96	0.09	23,23,28,29	0
4	GOL	A	417	6/6	0.97	0.08	17,20,24,26	0
2	NA	B	402	1/1	0.98	0.04	17,17,17,17	0
6	B12	A	426	91/91	0.98	0.06	10,13,21,36	0
6	B12	B	418	91/91	0.98	0.06	12,14,21,36	0
4	GOL	B	406	6/6	0.98	0.06	16,18,21,25	0
2	NA	A	405	1/1	0.99	0.06	20,20,20,20	0
2	NA	A	406	1/1	0.99	0.05	20,20,20,20	0
2	NA	A	407	1/1	0.99	0.07	24,24,24,24	0
2	NA	A	408	1/1	0.99	0.07	23,23,23,23	0
2	NA	A	402	1/1	0.99	0.06	20,20,20,20	0

Continued on next page...

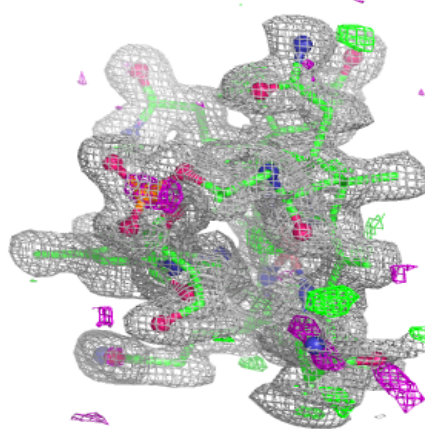
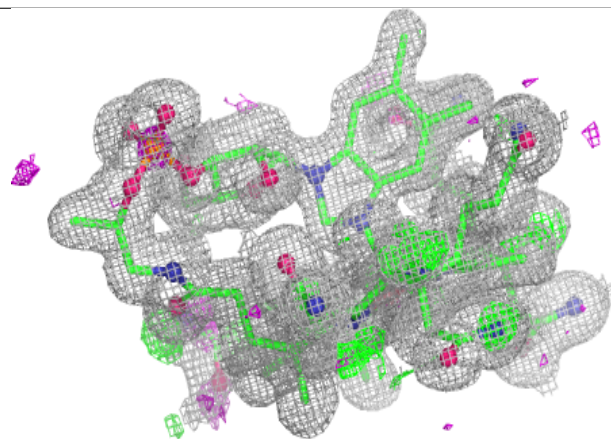
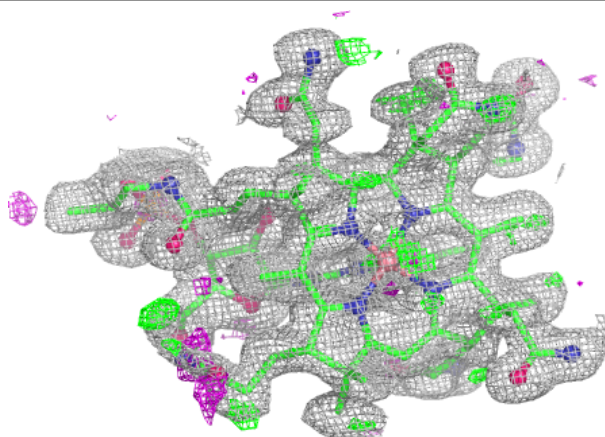
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	403	1/1	0.99	0.07	17,17,17,17	0
2	NA	A	401	1/1	1.00	0.08	12,12,12,12	0
2	NA	A	404	1/1	1.00	0.06	19,19,19,19	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.

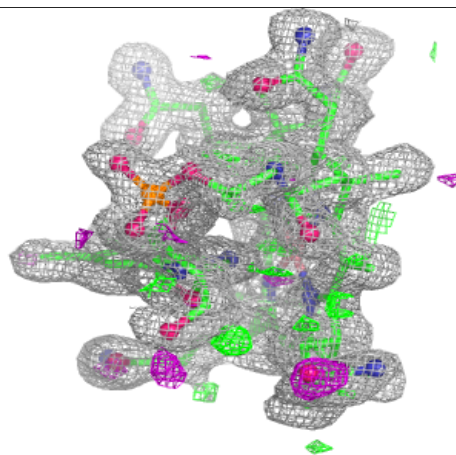
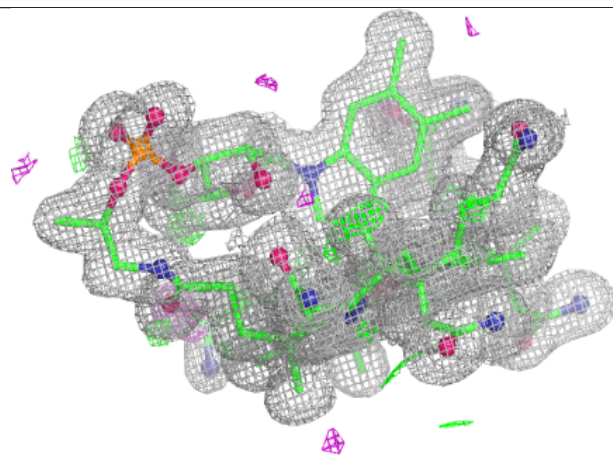
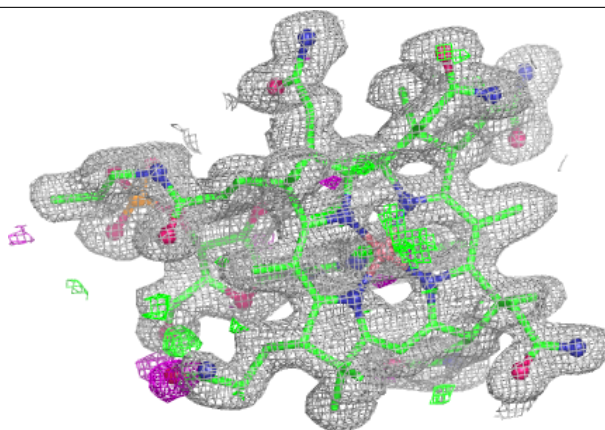
Electron density around B12 A 426:

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 418:

$2mF_o-DF_c$ (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.