



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:26 pm BST

PDB ID : 3ABR
Title : Crystal structure of ethanolamine ammonia-lyase from Escherichia coli complexed with CN-Cbl (substrate-free form)
Authors : Shibata, N.
Deposited on : 2009-12-21
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

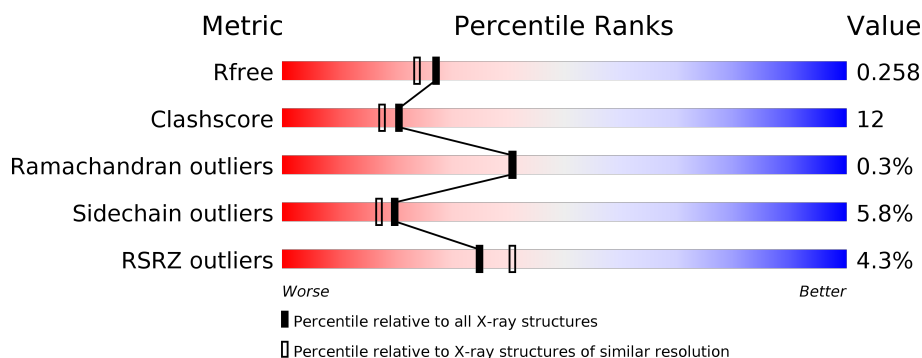
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	453	<div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div>87% 12% .</div>
1	C	453	<div> <div style="width: 85%;"></div> <div style="width: 13%;"></div> <div style="width: 2%;"></div> </div> <div>85% 13% .</div>
2	B	306	<div> <div style="width: 5%;"></div> <div style="width: 58%;"></div> <div style="width: 21%;"></div> <div style="width: 18%;"></div> </div> <div>5% 58% 21% 18%</div>
2	D	306	<div> <div style="width: 14%;"></div> <div style="width: 54%;"></div> <div style="width: 23%;"></div> <div style="width: 6%;"></div> <div style="width: 18%;"></div> </div> <div>14% 54% 23% 6% 18%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	B12	B	601	-	-	X	-
5	B12	D	601	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11985 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 Ethanolamine ammonia-lyase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3464	2170	593	679	22			
1	C	453	Total	C	N	O	S	0	0	0
			3464	2170	593	679	22			

- Molecule 2 is a protein called Ethanolamine ammonia-lyase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1916	1197	347	362	10			
2	D	252	Total	C	N	O	S	0	0	0
			1916	1197	347	362	10			

There are 22 discrepancies between the modelled and reference sequences:

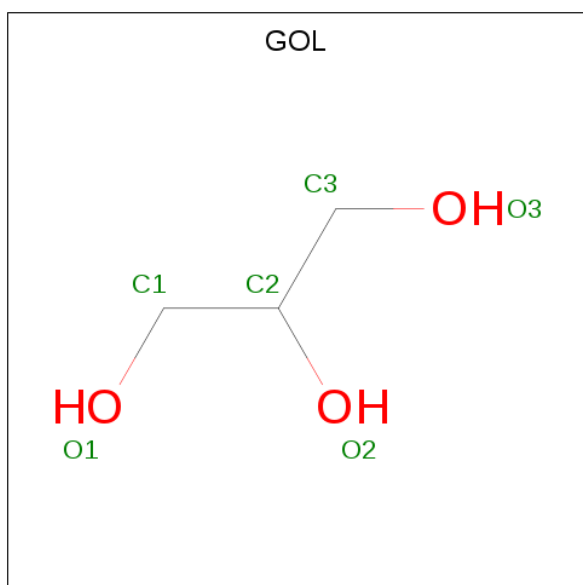
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	EXPRESSION TAG	UNP P19636
B	-9	ASP	-	EXPRESSION TAG	UNP P19636
B	-8	GLN	-	EXPRESSION TAG	UNP P19636
B	-7	SER	-	EXPRESSION TAG	UNP P19636
B	-6	SER	-	EXPRESSION TAG	UNP P19636
B	-5	HIS	-	EXPRESSION TAG	UNP P19636
B	-4	HIS	-	EXPRESSION TAG	UNP P19636
B	-3	HIS	-	EXPRESSION TAG	UNP P19636
B	-2	HIS	-	EXPRESSION TAG	UNP P19636
B	-1	HIS	-	EXPRESSION TAG	UNP P19636
B	0	HIS	-	EXPRESSION TAG	UNP P19636
D	-10	MET	-	EXPRESSION TAG	UNP P19636
D	-9	ASP	-	EXPRESSION TAG	UNP P19636
D	-8	GLN	-	EXPRESSION TAG	UNP P19636
D	-7	SER	-	EXPRESSION TAG	UNP P19636
D	-6	SER	-	EXPRESSION TAG	UNP P19636

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP P19636
D	-4	HIS	-	EXPRESSION TAG	UNP P19636
D	-3	HIS	-	EXPRESSION TAG	UNP P19636
D	-2	HIS	-	EXPRESSION TAG	UNP P19636
D	-1	HIS	-	EXPRESSION TAG	UNP P19636
D	0	HIS	-	EXPRESSION TAG	UNP P19636

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

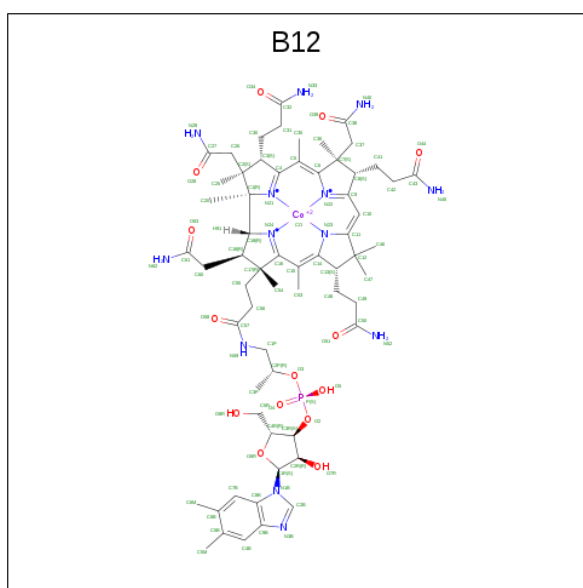


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	3	Total Na 3 3	0	0
4	D	2	Total Na 2 2	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

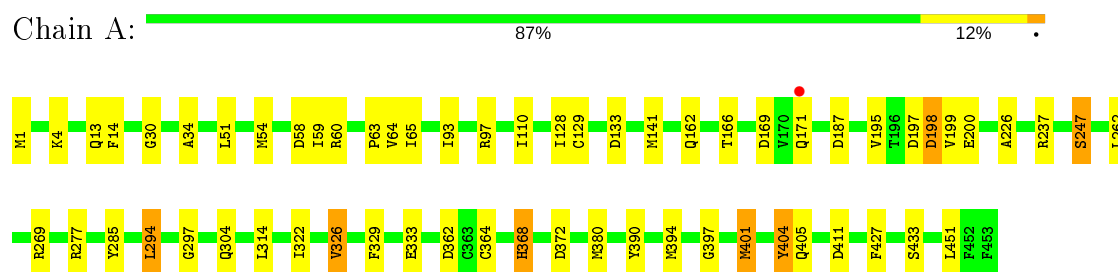
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	421	Total O 421 421	0	0
6	B	129	Total O 129 129	0	0
6	C	349	Total O 349 349	0	0
6	D	101	Total O 101 101	0	0

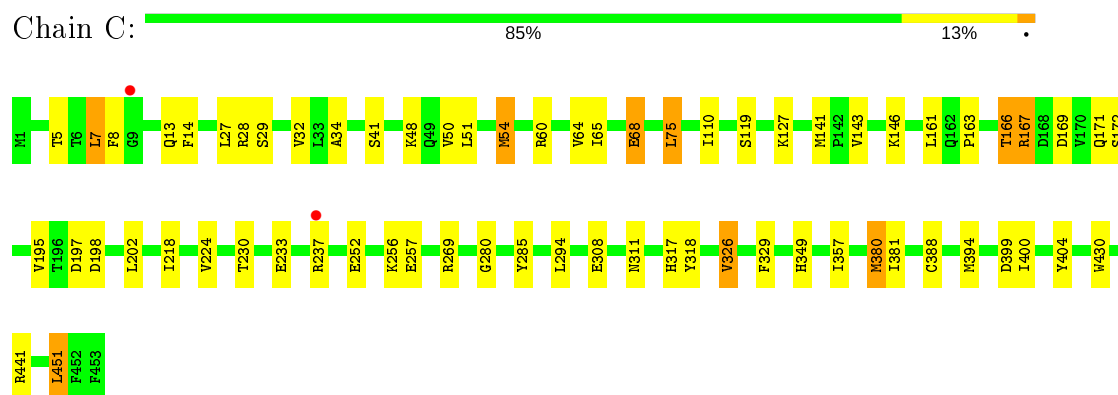
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

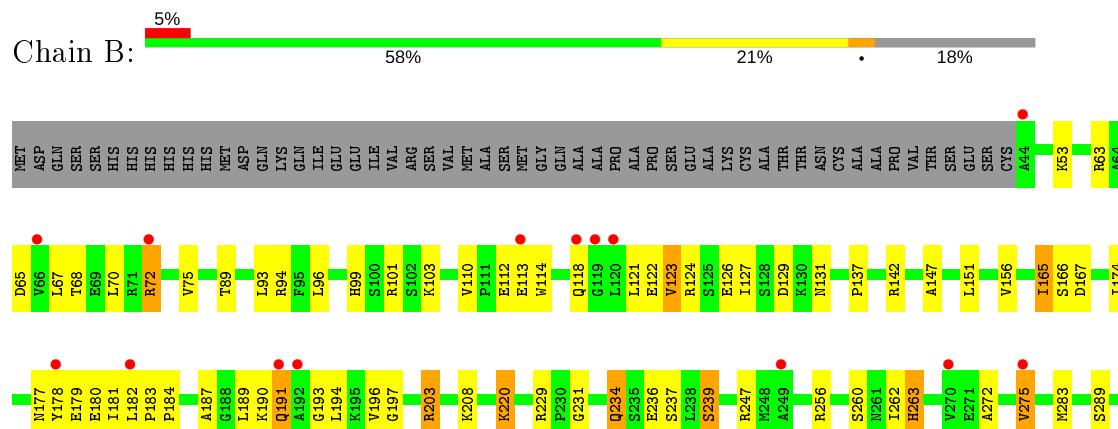
- Molecule 1: Ethanolamine ammonia-lyase heavy chain



- Molecule 1: Ethanolamine ammonia-lyase heavy chain

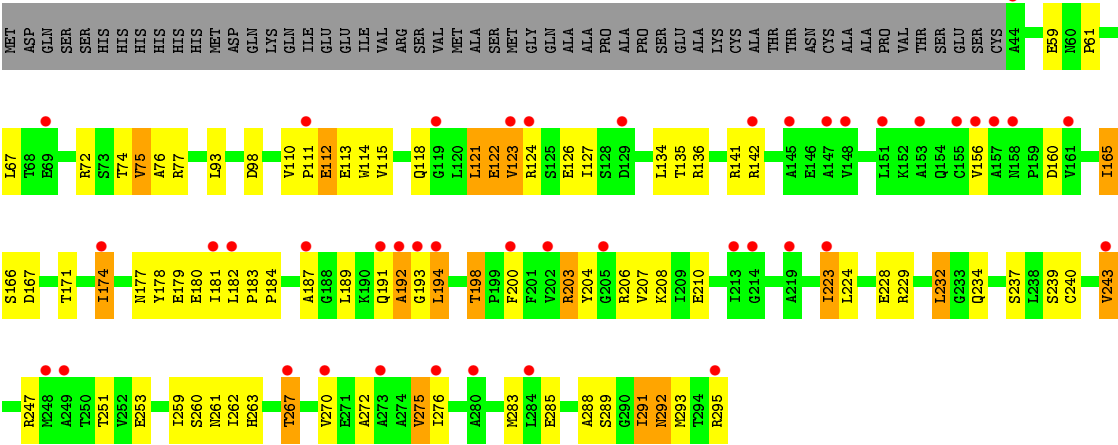


- Molecule 2: Ethanolamine ammonia-lyase light chain





● Molecule 2: Ethanolamine ammonia-lyase light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	244.12Å 244.12Å 77.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.29 – 2.10 42.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (42.29-2.10) 94.5 (42.28-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0087	Depositor
R, R_{free}	0.248 , 0.285 0.238 , 0.258	Depositor DCC
R_{free} test set	7300 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 7.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.109 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11985	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/3518	0.47	0/4764
1	C	0.34	0/3518	0.47	0/4764
2	B	0.28	0/1943	0.44	0/2633
2	D	0.26	0/1943	0.44	0/2633
All	All	0.32	0/10922	0.46	0/14794

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	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	VAL	Peptide
1	C	326	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3464	0	3418	44	0
1	C	3464	0	3419	52	0
2	B	1916	0	1973	56	0
2	D	1916	0	1973	76	0
3	A	18	0	24	2	0
3	C	18	0	24	2	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	B	91	0	88	22	0
5	D	91	0	88	28	0
6	A	421	0	0	7	1
6	B	129	0	0	5	0
6	C	349	0	0	4	1
6	D	101	0	0	4	0
All	All	11985	0	11007	270	1

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 12.

All (270) 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:D:601:B12:H533	5:D:601:B12:N52	1.32	1.38
5:D:601:B12:H521	5:D:601:B12:C53	1.49	1.24
1:C:269:ARG:NH2	1:C:318:TYR:O	1.81	1.14
2:B:239:SER:HB3	2:B:260:SER:HA	1.30	1.12
2:B:165:ILE:HD11	2:B:174:ILE:HG23	1.28	1.07
2:D:167:ASP:HA	2:D:174:ILE:HD11	1.32	1.07
1:C:451:LEU:O	1:C:451:LEU:HD12	1.55	1.05
1:C:202:LEU:CD1	1:C:230:THR:HG22	1.89	1.02
5:D:601:B12:H552	5:D:601:B12:H531	1.42	1.01
5:B:601:B12:H552	5:B:601:B12:H531	1.42	1.00
5:B:601:B12:H351	5:B:601:B12:H362	1.40	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:HD12	1:C:230:THR:HG22	1.43	1.00
5:D:601:B12:H491	5:D:601:B12:H4R	1.49	0.94
5:D:601:B12:H362	5:D:601:B12:H351	1.50	0.93
2:D:74:THR:HG22	2:D:76:ALA:H	1.28	0.93
2:D:247:ARG:O	2:D:251:THR:HG22	1.70	0.92
2:B:189:LEU:O	2:B:193:GLY:HA3	1.70	0.92
2:B:110:VAL:O	2:B:203:ARG:NH2	2.03	0.92
1:C:202:LEU:HD22	1:C:224:VAL:HG11	1.52	0.91
2:D:110:VAL:O	2:D:203:ARG:NH2	2.06	0.88
2:D:240:CYS:HB3	2:D:259:ILE:HG22	1.57	0.86
2:D:167:ASP:HA	2:D:174:ILE:CD1	2.07	0.84
2:D:141:ARG:NH2	5:D:601:B12:O8R	2.12	0.83
1:A:51:LEU:HA	1:A:54:MET:HE2	1.61	0.82
2:B:165:ILE:HD11	2:B:174:ILE:CG2	2.11	0.78
5:D:601:B12:H421	5:D:601:B12:H363	1.67	0.77
1:A:197:ASP:OD1	1:A:226:ALA:HB1	1.86	0.76
2:D:174:ILE:O	2:D:178:TYR:HB2	1.84	0.76
2:D:223:ILE:HD12	2:D:276:ILE:HG21	1.66	0.75
1:C:202:LEU:CD1	1:C:230:THR:CG2	2.64	0.74
5:B:601:B12:C35	5:B:601:B12:H362	2.17	0.74
1:A:326:VAL:HG12	1:A:329:PHE:HB2	1.69	0.74
2:D:223:ILE:HD12	2:D:276:ILE:CG2	2.18	0.73
1:C:202:LEU:HD11	1:C:230:THR:CG2	2.19	0.73
1:C:202:LEU:CD2	1:C:224:VAL:HG11	2.18	0.72
1:C:202:LEU:HD22	1:C:224:VAL:CG1	2.19	0.72
5:D:601:B12:N52	5:D:601:B12:C53	2.26	0.72
1:C:29:SER:O	1:C:32:VAL:HG22	1.90	0.71
2:B:272:ALA:O	2:B:275:VAL:HG12	1.89	0.71
2:D:240:CYS:HB3	2:D:259:ILE:CG2	2.20	0.71
1:C:202:LEU:HD11	1:C:230:THR:HG22	1.73	0.70
2:D:191:GLN:O	2:D:192:ALA:HB3	1.91	0.70
1:A:200:GLU:HB2	6:A:740:HOH:O	1.91	0.70
1:C:269:ARG:NH2	1:C:318:TYR:C	2.45	0.70
5:D:601:B12:C4R	5:D:601:B12:H491	2.23	0.69
1:C:172:SER:OG	2:D:74:THR:HG23	1.93	0.69
2:D:182:LEU:HB3	2:D:183:PRO:HD3	1.76	0.67
2:D:283:MET:HE3	2:D:289:SER:HB3	1.77	0.66
1:A:4:LYS:HD3	1:A:13:GLN:OE1	1.95	0.66
2:B:101:ARG:NH1	6:B:317:HOH:O	2.24	0.65
1:A:51:LEU:HD12	1:A:54:MET:HE3	1.77	0.65
5:B:601:B12:H552	5:B:601:B12:C53	2.20	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:601:B12:H202	5:D:601:B12:N3B	2.12	0.65
5:D:601:B12:H552	5:D:601:B12:C53	2.22	0.64
1:C:7:LEU:HD22	1:C:8:PHE:CD1	2.33	0.63
1:C:5:THR:HG23	1:C:50:VAL:HG22	1.81	0.63
5:B:601:B12:H203	5:B:601:B12:H301	1.80	0.62
2:B:179:GLU:HA	2:B:179:GLU:OE1	1.99	0.62
2:B:187:ALA:O	2:B:191:GLN:HB2	2.00	0.61
2:D:156:VAL:HG13	2:D:198:THR:HG22	1.82	0.61
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.36	0.60
1:C:166:THR:O	1:C:195:VAL:HG21	2.01	0.60
2:D:98:ASP:HB3	2:D:232:LEU:HD22	1.83	0.60
1:C:51:LEU:HA	1:C:54:MET:HG3	1.82	0.60
2:B:234:GLN:NE2	2:B:236:GLU:H	2.00	0.60
2:D:259:ILE:HG23	2:D:259:ILE:O	2.02	0.60
2:B:182:LEU:HB3	2:B:183:PRO:HD3	1.82	0.60
1:C:110:ILE:HD12	1:C:141:MET:HG2	1.83	0.59
2:B:123:VAL:CG1	2:B:147:ALA:HB1	2.32	0.59
5:B:601:B12:C36	5:B:601:B12:H351	2.18	0.59
5:B:601:B12:H401	5:B:601:B12:H8	1.66	0.59
2:D:288:ALA:HB1	2:D:292:ASN:HB2	1.83	0.59
2:B:53:LYS:HG2	2:B:94:ARG:NH1	2.18	0.58
1:C:257:GLU:CD	2:D:253:GLU:HB2	2.23	0.58
1:C:326:VAL:HG12	1:C:329:PHE:HB2	1.84	0.58
1:A:51:LEU:HD12	1:A:54:MET:CE	2.34	0.58
5:B:601:B12:H533	5:B:601:B12:H492	1.84	0.58
1:A:198:ASP:OD1	6:A:841:HOH:O	2.17	0.58
1:C:167:ARG:NH1	6:C:875:HOH:O	2.36	0.58
2:D:191:GLN:O	2:D:192:ALA:CB	2.52	0.58
2:B:190:LYS:HG2	2:B:196:VAL:HG21	1.86	0.57
1:C:169:ASP:OD2	1:C:171:GLN:HB2	2.04	0.57
5:D:601:B12:H351	5:D:601:B12:C36	2.28	0.57
2:B:123:VAL:HG11	2:B:147:ALA:HB1	1.88	0.56
1:A:247:SER:OG	5:B:601:B12:N40	2.38	0.56
2:D:135:THR:HG23	2:D:136:ARG:HG2	1.86	0.56
1:A:401:MET:O	1:A:401:MET:HG2	2.05	0.56
5:D:601:B12:H601	5:D:601:B12:H262	1.88	0.55
1:A:59:ILE:HD12	1:A:93:ILE:HD11	1.89	0.55
1:A:110:ILE:HD12	1:A:141:MET:HG2	1.87	0.55
5:D:601:B12:H301	5:D:601:B12:H203	1.88	0.55
1:A:372:ASP:HB2	6:A:538:HOH:O	2.06	0.55
2:B:147:ALA:O	2:B:151:LEU:HD13	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:GLU:HG2	2:D:237:SER:O	2.07	0.55
2:B:234:GLN:OE1	2:B:237:SER:HB2	2.06	0.54
2:B:190:LYS:HG2	2:B:196:VAL:CG2	2.37	0.54
1:C:143:VAL:HG13	3:C:2004:GOL:H12	1.89	0.54
2:B:262:ILE:O	2:B:263:HIS:HB3	2.06	0.54
1:C:349:HIS:CE1	1:C:388:CYS:HA	2.43	0.54
5:D:601:B12:C4	5:D:601:B12:H4B	2.37	0.54
1:C:441:ARG:NH1	6:C:703:HOH:O	2.41	0.53
2:B:123:VAL:HG13	2:B:147:ALA:CB	2.38	0.53
1:A:277:ARG:HB3	3:A:2006:GOL:H31	1.90	0.53
2:D:223:ILE:CD1	2:D:276:ILE:HG21	2.36	0.53
2:B:114:TRP:O	2:B:118:GLN:HG2	2.09	0.53
1:C:68:GLU:H	1:C:68:GLU:CD	2.08	0.53
2:D:166:SER:O	2:D:174:ILE:HD12	2.08	0.53
2:D:61:PRO:HB3	2:D:67:LEU:HD11	1.91	0.53
2:D:285:GLU:HB3	6:D:815:HOH:O	2.07	0.53
2:B:220:LYS:N	2:B:220:LYS:HD3	2.24	0.53
5:D:601:B12:H362	5:D:601:B12:C35	2.32	0.53
2:B:99:HIS:O	2:B:103:LYS:HG2	2.09	0.53
2:B:123:VAL:CG1	2:B:124:ARG:N	2.72	0.52
2:B:234:GLN:HE22	2:B:236:GLU:N	2.08	0.52
1:C:218:ILE:HG12	1:C:430:TRP:CZ2	2.44	0.52
1:C:308:GLU:O	1:C:311:ASN:HB2	2.10	0.52
2:B:65:ASP:OD2	2:B:65:ASP:N	2.43	0.52
2:D:187:ALA:O	2:D:191:GLN:HB2	2.10	0.52
1:C:451:LEU:O	1:C:451:LEU:CD1	2.45	0.51
2:B:234:GLN:HE22	2:B:236:GLU:H	1.58	0.51
5:B:601:B12:C55	5:B:601:B12:H531	2.23	0.51
2:D:224:LEU:O	2:D:240:CYS:HA	2.11	0.51
5:B:601:B12:H2B	5:B:601:B12:O7R	2.11	0.51
1:A:368:HIS:CD2	1:A:368:HIS:H	2.29	0.51
1:A:51:LEU:CD1	1:A:54:MET:HE3	2.41	0.51
2:B:112:GLU:H	2:B:112:GLU:CD	2.13	0.50
2:D:114:TRP:O	2:D:118:GLN:HG2	2.11	0.50
2:D:165:ILE:HG22	2:D:200:PHE:O	2.11	0.50
1:A:64:VAL:HG23	1:A:65:ILE:HG13	1.94	0.50
1:C:75:LEU:HD21	1:C:317:HIS:CB	2.42	0.50
5:D:601:B12:O34	5:D:601:B12:HM53	2.10	0.50
1:A:187:ASP:HB3	1:A:427:PHE:CD1	2.47	0.49
2:D:123:VAL:HG13	2:D:124:ARG:N	2.26	0.49
1:C:75:LEU:HD21	1:C:317:HIS:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:ASN:O	2:D:181:ILE:HG22	2.12	0.49
2:B:177:ASN:O	2:B:181:ILE:HG22	2.12	0.49
1:C:167:ARG:NH2	6:C:678:HOH:O	2.46	0.49
5:B:601:B12:H8	5:B:601:B12:N40	2.28	0.48
2:D:110:VAL:HG12	2:D:203:ARG:HH22	1.78	0.48
1:A:34:ALA:HB2	1:A:294:LEU:HD22	1.95	0.48
2:B:112:GLU:OE2	6:B:325:HOH:O	2.20	0.48
2:D:267:THR:HG23	2:D:272:ALA:HB2	1.95	0.48
5:D:601:B12:C42	5:D:601:B12:H363	2.35	0.48
1:A:166:THR:O	1:A:195:VAL:HG21	2.13	0.48
1:C:202:LEU:HD11	1:C:230:THR:HG21	1.95	0.48
2:D:121:LEU:HD22	2:D:122:GLU:N	2.29	0.48
1:A:199:VAL:HG21	1:A:237:ARG:HH11	1.79	0.48
2:B:247:ARG:NH2	6:B:823:HOH:O	2.47	0.48
1:C:202:LEU:HD12	1:C:230:THR:CG2	2.27	0.48
1:A:322:ILE:HB	1:A:390:TYR:CE1	2.49	0.47
2:D:180:GLU:HG2	2:D:270:VAL:HG23	1.96	0.47
1:A:326:VAL:CG1	1:A:329:PHE:HB2	2.40	0.47
5:B:601:B12:H473	5:B:601:B12:H481	1.52	0.47
5:B:601:B12:C2B	5:B:601:B12:O7R	2.62	0.47
1:A:169:ASP:OD2	1:A:171:GLN:HB2	2.15	0.47
2:B:156:VAL:CG2	2:B:197:GLY:HA2	2.45	0.47
2:D:203:ARG:HG2	2:D:204:TYR:CD2	2.50	0.47
1:A:13:GLN:HG3	1:A:14:PHE:N	2.29	0.47
1:C:34:ALA:HB2	1:C:294:LEU:HD22	1.95	0.47
2:D:239:SER:OG	2:D:260:SER:HA	2.14	0.47
5:D:601:B12:H302	5:D:601:B12:H4B	1.95	0.47
1:C:64:VAL:HG23	1:C:65:ILE:HG13	1.97	0.47
1:C:161:LEU:O	1:C:163:PRO:HD3	2.15	0.47
5:D:601:B12:H531	5:D:601:B12:C55	2.21	0.47
2:D:295:ARG:HB3	2:D:295:ARG:NH1	2.30	0.47
1:C:48:LYS:NZ	1:C:127:LYS:O	2.48	0.47
2:D:267:THR:CG2	2:D:267:THR:O	2.63	0.47
5:D:601:B12:H301	5:D:601:B12:H253	1.66	0.47
1:A:333:GLU:HG3	2:B:137:PRO:HG3	1.97	0.46
2:B:256:ARG:HB2	5:B:601:B12:HM61	1.96	0.46
2:D:110:VAL:HG23	2:D:171:THR:HG23	1.97	0.46
2:D:189:LEU:O	2:D:193:GLY:HA3	2.15	0.46
2:D:160:ASP:OD1	2:D:194:LEU:HB3	2.14	0.46
2:D:291:ILE:O	2:D:291:ILE:HG23	2.15	0.46
2:B:126:GLU:OE1	2:B:142:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:PRO:HG2	2:D:114:TRP:HB2	1.96	0.46
1:A:277:ARG:NH2	6:A:546:HOH:O	2.49	0.46
2:B:89:THR:O	2:B:93:LEU:HG	2.14	0.46
1:C:218:ILE:HG12	1:C:430:TRP:CE2	2.50	0.46
5:B:601:B12:H533	5:B:601:B12:C49	2.46	0.46
1:C:326:VAL:CG1	1:C:329:PHE:HB2	2.44	0.46
2:D:77:ARG:NH2	2:D:232:LEU:HD13	2.31	0.46
1:A:51:LEU:CD1	1:A:54:MET:CE	2.93	0.46
1:A:63:PRO:HD2	6:A:693:HOH:O	2.15	0.46
2:D:207:VAL:O	2:D:210:GLU:HG2	2.16	0.46
2:D:262:ILE:O	2:D:263:HIS:HB3	2.16	0.46
2:B:166:SER:O	2:B:174:ILE:HD11	2.16	0.46
1:A:364:CYS:HB2	1:A:404:TYR:CD2	2.52	0.45
2:B:247:ARG:HG3	6:B:550:HOH:O	2.15	0.45
2:D:112:GLU:HA	2:D:115:VAL:HG22	1.98	0.45
1:C:197:ASP:OD1	1:C:230:THR:HG21	2.17	0.45
1:A:30:GLY:HA3	1:A:304:GLN:OE1	2.17	0.45
3:C:2003:GOL:H12	6:C:936:HOH:O	2.17	0.45
2:D:295:ARG:CZ	2:D:295:ARG:HB3	2.47	0.45
1:A:364:CYS:HB2	1:A:404:TYR:CE2	2.52	0.45
2:B:208:LYS:HG2	2:B:256:ARG:HH21	1.82	0.45
2:B:165:ILE:HG13	2:B:166:SER:N	2.31	0.44
2:D:259:ILE:HD13	2:D:275:VAL:HG21	1.99	0.44
2:D:75:VAL:CG1	2:D:75:VAL:O	2.65	0.44
2:D:126:GLU:OE1	2:D:142:ARG:NH1	2.50	0.44
2:D:179:GLU:OE1	2:D:179:GLU:HA	2.17	0.44
2:B:129:ASP:OD1	2:B:131:ASN:HB2	2.16	0.44
2:B:208:LYS:HE2	5:B:601:B12:O8R	2.17	0.44
1:C:27:LEU:HD13	1:C:28:ARG:N	2.32	0.44
1:A:368:HIS:H	1:A:368:HIS:HD2	1.64	0.44
1:A:1:MET:HB3	1:A:58:ASP:OD2	2.18	0.44
1:C:34:ALA:HB2	1:C:294:LEU:CD2	2.47	0.44
5:D:601:B12:O7R	5:D:601:B12:C2B	2.65	0.44
1:A:380:MET:SD	1:A:411:ASP:HB3	2.58	0.44
5:D:601:B12:O7R	5:D:601:B12:H2B	2.17	0.44
1:C:27:LEU:HD13	1:C:27:LEU:C	2.38	0.44
2:D:141:ARG:NH2	5:D:601:B12:H0R8	2.14	0.44
2:D:124:ARG:HD2	2:D:127:ILE:O	2.17	0.44
2:B:123:VAL:HG13	2:B:124:ARG:N	2.33	0.43
5:B:601:B12:C8	5:B:601:B12:N40	2.81	0.43
1:C:13:GLN:HG3	1:C:14:PHE:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:B12:H301	5:B:601:B12:H253	1.76	0.43
2:B:123:VAL:HG13	2:B:147:ALA:HB1	1.99	0.43
2:D:74:THR:HG21	2:D:76:ALA:HB3	1.99	0.43
2:B:123:VAL:HG13	2:B:147:ALA:HB2	2.01	0.43
2:D:141:ARG:HG2	2:D:208:LYS:HB2	2.00	0.43
2:D:261:ASN:ND2	6:D:410:HOH:O	2.15	0.43
2:B:183:PRO:N	2:B:184:PRO:HD2	2.33	0.43
1:C:252:GLU:O	1:C:256:LYS:HG3	2.19	0.43
1:C:380:MET:HG2	1:C:381:ILE:N	2.33	0.43
2:D:110:VAL:HG13	2:D:111:PRO:O	2.19	0.43
2:B:72:ARG:HB2	2:B:72:ARG:HE	1.45	0.43
2:D:112:GLU:CD	2:D:112:GLU:H	2.22	0.43
1:C:400:ILE:HG21	2:D:75:VAL:HG12	2.00	0.42
2:D:171:THR:O	2:D:174:ILE:HG12	2.20	0.42
1:A:277:ARG:HE	3:A:2006:GOL:H31	1.85	0.42
2:B:124:ARG:HD2	2:B:127:ILE:O	2.20	0.42
1:A:162:GLN:HB3	1:A:394:MET:HG2	2.02	0.42
2:D:183:PRO:N	2:D:184:PRO:HD2	2.34	0.42
1:A:397:GLY:O	1:A:405:GLN:HA	2.20	0.42
5:B:601:B12:H521	5:B:601:B12:H481	1.20	0.42
2:D:123:VAL:CG1	2:D:124:ARG:N	2.83	0.42
2:D:210:GLU:OE2	2:D:243:VAL:HG22	2.20	0.42
2:D:237:SER:OG	2:D:261:ASN:HA	2.20	0.42
6:A:661:HOH:O	2:B:231:GLY:HA3	2.19	0.42
2:D:259:ILE:O	2:D:259:ILE:CG2	2.68	0.42
5:D:601:B12:O28	5:D:601:B12:H3	2.19	0.42
2:B:167:ASP:HA	2:B:174:ILE:HG13	2.02	0.41
1:C:394:MET:HE1	1:C:399:ASP:HA	2.01	0.41
2:D:289:SER:HA	2:D:293:MET:SD	2.61	0.41
2:D:59:GLU:HG3	6:D:669:HOH:O	2.19	0.41
5:D:601:B12:H482	5:D:601:B12:H473	1.70	0.41
2:B:283:MET:CE	2:B:289:SER:HB3	2.50	0.41
1:A:97:ARG:HD2	1:A:128:ILE:HG13	2.02	0.41
5:B:601:B12:H351	5:B:601:B12:H371	2.01	0.41
1:C:233:GLU:O	1:C:237:ARG:HG3	2.20	0.41
2:B:220:LYS:HE2	6:B:719:HOH:O	2.19	0.41
1:A:129:CYS:HB3	1:A:133:ASP:HB2	2.03	0.41
1:C:146:LYS:HG3	1:C:280:GLY:HA3	2.03	0.41
2:B:75:VAL:CG1	2:B:75:VAL:O	2.69	0.41
2:D:203:ARG:HG2	2:D:204:TYR:CE2	2.56	0.41
2:D:180:GLU:HG2	2:D:270:VAL:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:VAL:HG21	2:D:122:GLU:OE2	2.22	0.40
2:D:207:VAL:HG23	2:D:208:LYS:N	2.36	0.40
1:A:326:VAL:HA	1:A:362:ASP:HB3	2.02	0.40
2:B:178:TYR:C	2:B:180:GLU:H	2.23	0.40
2:B:67:LEU:HA	2:B:67:LEU:HD23	1.91	0.40
1:C:143:VAL:HG11	1:C:357:ILE:C	2.42	0.40
5:D:601:B12:H602	5:D:601:B12:H541	1.83	0.40
1:A:294:LEU:O	1:A:294:LEU:HD12	2.21	0.40
2:B:289:SER:HA	2:B:293:MET:SD	2.62	0.40
5:B:601:B12:H203	5:B:601:B12:C30	2.48	0.40
2:D:206:ARG:HD2	6:D:321:HOH:O	2.20	0.40
5:D:601:B12:H2B	5:D:601:B12:H492	2.02	0.40
1:A:297:GLY:HA2	6:A:611:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:763:HOH:O	6:C:562:HOH:O[2_545]	2.11	0.09

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	451/453 (100%)	433 (96%)	18 (4%)	0	100	100
1	C	451/453 (100%)	437 (97%)	14 (3%)	0	100	100
2	B	250/306 (82%)	240 (96%)	8 (3%)	2 (1%)	19	15
2	D	250/306 (82%)	237 (95%)	11 (4%)	2 (1%)	19	15
All	All	1402/1518 (92%)	1347 (96%)	51 (4%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	63	ARG
2	B	263	HIS
2	D	194	LEU
2	D	192	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	357 (96%)	13 (4%)	36	38
1	C	370/370 (100%)	356 (96%)	14 (4%)	33	34
2	B	206/251 (82%)	188 (91%)	18 (9%)	10	7
2	D	206/251 (82%)	184 (89%)	22 (11%)	6	3
All	All	1152/1242 (93%)	1085 (94%)	67 (6%)	20	17

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	198	ASP
1	A	247	SER
1	A	262	LEU
1	A	269	ARG
1	A	285	TYR
1	A	294	LEU
1	A	314	LEU
1	A	368	HIS
1	A	401	MET
1	A	404	TYR
1	A	433	SER
1	A	451	LEU
2	B	68	THR
2	B	70	LEU
2	B	72	ARG
2	B	96	LEU
2	B	113	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	121	LEU
2	B	122	GLU
2	B	123	VAL
2	B	165	ILE
2	B	191	GLN
2	B	194	LEU
2	B	203	ARG
2	B	220	LYS
2	B	229	ARG
2	B	234	GLN
2	B	239	SER
2	B	275	VAL
2	B	295	ARG
1	C	7	LEU
1	C	41	SER
1	C	54	MET
1	C	60	ARG
1	C	68	GLU
1	C	75	LEU
1	C	119	SER
1	C	166	THR
1	C	167	ARG
1	C	198	ASP
1	C	285	TYR
1	C	380	MET
1	C	404	TYR
1	C	451	LEU
2	D	72	ARG
2	D	75	VAL
2	D	93	LEU
2	D	112	GLU
2	D	113	GLU
2	D	121	LEU
2	D	122	GLU
2	D	123	VAL
2	D	134	LEU
2	D	165	ILE
2	D	174	ILE
2	D	198	THR
2	D	203	ARG
2	D	223	ILE
2	D	229	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	232	LEU
2	D	234	GLN
2	D	243	VAL
2	D	267	THR
2	D	275	VAL
2	D	291	ILE
2	D	292	ASN

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

Mol	Chain	Res	Type
1	A	368	HIS
2	B	234	GLN
1	C	349	HIS
2	D	99	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	GOL	C	2003	-	5,5,5	0.37	0	5,5,5	0.45	0
3	GOL	A	2002	-	5,5,5	0.29	0	5,5,5	0.64	0
3	GOL	A	2006	-	5,5,5	0.17	0	5,5,5	0.44	0
3	GOL	A	2001	-	5,5,5	0.29	0	5,5,5	0.52	0
5	B12	B	601	-	80,101,101	1.07	5 (6%)	101,166,166	1.32	17 (16%)
3	GOL	C	2005	-	5,5,5	0.30	0	5,5,5	0.61	0
5	B12	D	601	-	80,101,101	1.07	5 (6%)	101,166,166	1.52	18 (17%)
3	GOL	C	2004	-	5,5,5	0.28	0	5,5,5	1.00	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
3	GOL	C	2003	-	-	4/4/4/4	-
3	GOL	A	2002	-	-	2/4/4/4	-
3	GOL	A	2006	-	-	4/4/4/4	-
3	GOL	A	2001	-	-	3/4/4/4	-
5	B12	B	601	-	-	20/51/223/223	0/3/11/11
3	GOL	C	2005	-	-	3/4/4/4	-
5	B12	D	601	-	-	15/51/223/223	0/3/11/11
3	GOL	C	2004	-	-	4/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C11-C10	-4.14	1.33	1.40
5	B	601	B12	C11-C10	-3.96	1.34	1.40
5	B	601	B12	C8B-C9B	3.88	1.48	1.40
5	D	601	B12	C8B-C9B	3.75	1.48	1.40
5	B	601	B12	C6B-C5B	3.44	1.49	1.40
5	D	601	B12	C6B-C5B	3.21	1.48	1.40
5	D	601	B12	C1-C2	-2.48	1.53	1.58
5	B	601	B12	O6R-C1R	2.39	1.44	1.41
5	D	601	B12	O6R-C1R	2.13	1.44	1.41
5	B	601	B12	C1-C2	-2.13	1.53	1.58

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	B12	C47-C12-C46	5.47	121.20	109.73
5	D	601	B12	C2-C1-C19	4.11	125.08	118.60
5	B	601	B12	C2-C1-C19	4.08	125.03	118.60
5	D	601	B12	C54-C17-C18	-4.01	107.07	112.98
5	D	601	B12	C20-C1-C2	-3.33	107.81	113.32
5	D	601	B12	C30-C3-C2	-3.28	112.17	119.13
5	B	601	B12	C25-C2-C3	-3.20	110.69	115.58
5	D	601	B12	C19-C1-N21	3.12	105.36	102.16
5	D	601	B12	C25-C2-C3	-3.08	110.89	115.58
5	D	601	B12	C20-C1-C19	-3.03	106.43	109.36
5	B	601	B12	C20-C1-C19	-2.99	106.47	109.36
5	D	601	B12	C48-C13-C12	-2.96	108.37	116.59
5	B	601	B12	C54-C17-C18	-2.83	108.81	112.98
5	D	601	B12	C25-C2-C1	-2.82	109.61	113.80
5	D	601	B12	C1-C2-C3	2.81	105.10	101.59
5	B	601	B12	C30-C3-C2	-2.77	113.27	119.13
5	D	601	B12	C12-C11-C10	-2.75	119.98	124.64
5	B	601	B12	C55-C56-C57	-2.67	105.41	111.23
5	D	601	B12	C26-C2-C3	2.66	112.36	107.47
5	D	601	B12	C55-C17-C18	2.63	116.22	111.14
5	B	601	B12	C1-C2-C3	2.62	104.87	101.59
5	B	601	B12	C9-C10-C11	-2.53	122.06	130.91
5	D	601	B12	C9-C10-C11	-2.43	122.44	130.91
5	B	601	B12	C16-C15-C14	-2.42	120.50	124.27
5	D	601	B12	C16-C15-C14	-2.35	120.60	124.27
5	D	601	B12	C37-C7-C8	-2.34	102.09	108.37
5	B	601	B12	C20-C1-C2	-2.29	109.53	113.32
5	B	601	B12	O6R-C1R-C2R	-2.26	103.63	106.93
5	B	601	B12	C6-C5-C4	-2.23	120.80	124.27
5	D	601	B12	C2P-C1P-N59	-2.22	109.66	112.93
5	B	601	B12	C5R-C4R-C3R	-2.18	107.91	114.85
5	B	601	B12	C55-C17-C18	2.16	115.32	111.14
5	B	601	B12	C47-C12-C46	2.06	114.04	109.73
5	B	601	B12	C1-C19-N24	2.02	108.51	106.24
5	B	601	B12	C12-C11-C10	-2.01	121.24	124.64

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	B12	C4-C3-C30-C31
5	B	601	B12	C2P-O3-P-O4
5	B	601	B12	C2P-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2002	GOL	C1-C2-C3-O3
3	A	2006	GOL	O1-C1-C2-C3
3	C	2005	GOL	O1-C1-C2-O2
3	C	2005	GOL	O1-C1-C2-C3
5	D	601	B12	C38-C37-C7-C36
5	D	601	B12	C38-C37-C7-C8
5	D	601	B12	C2P-O3-P-O5
5	D	601	B12	O6R-C4R-C5R-O8R
3	C	2004	GOL	C1-C2-C3-O3
5	B	601	B12	O6R-C4R-C5R-O8R
5	B	601	B12	C3R-C4R-C5R-O8R
5	D	601	B12	C3R-C4R-C5R-O8R
5	B	601	B12	C13-C48-C49-C50
3	C	2004	GOL	O2-C2-C3-O3
5	B	601	B12	C18-C17-C55-C56
5	B	601	B12	C16-C17-C55-C56
5	D	601	B12	C16-C17-C55-C56
5	D	601	B12	C25-C2-C26-C27
3	C	2003	GOL	O1-C1-C2-C3
3	C	2003	GOL	C1-C2-C3-O3
3	A	2006	GOL	C1-C2-C3-O3
3	C	2004	GOL	O1-C1-C2-C3
3	A	2006	GOL	O1-C1-C2-O2
3	A	2006	GOL	O2-C2-C3-O3
5	B	601	B12	C48-C49-C50-O51
5	B	601	B12	C12-C13-C48-C49
5	B	601	B12	C48-C49-C50-N52
5	D	601	B12	C18-C17-C55-C56
5	B	601	B12	C2P-O3-P-O2
5	D	601	B12	C2P-O3-P-O2
3	C	2003	GOL	O1-C1-C2-O2
3	C	2004	GOL	O1-C1-C2-O2
5	B	601	B12	C2-C3-C30-C31
5	D	601	B12	C2P-O3-P-O4
3	A	2002	GOL	O2-C2-C3-O3
5	B	601	B12	C1P-C2P-O3-P
5	B	601	B12	C3P-C2P-O3-P
5	D	601	B12	C3-C2-C26-C27
5	D	601	B12	C2-C3-C30-C31
5	B	601	B12	C38-C37-C7-C36
3	A	2001	GOL	O1-C1-C2-O2
5	B	601	B12	C42-C41-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	601	B12	C4-C3-C30-C31
3	A	2001	GOL	C1-C2-C3-O3
3	C	2003	GOL	O2-C2-C3-O3
5	B	601	B12	C7-C37-C38-N40
5	B	601	B12	C7-C37-C38-O39
5	B	601	B12	C18-C60-C61-O63
3	C	2005	GOL	O2-C2-C3-O3
3	A	2001	GOL	O1-C1-C2-C3
5	D	601	B12	C1P-C2P-O3-P
5	D	601	B12	C42-C41-C8-C7

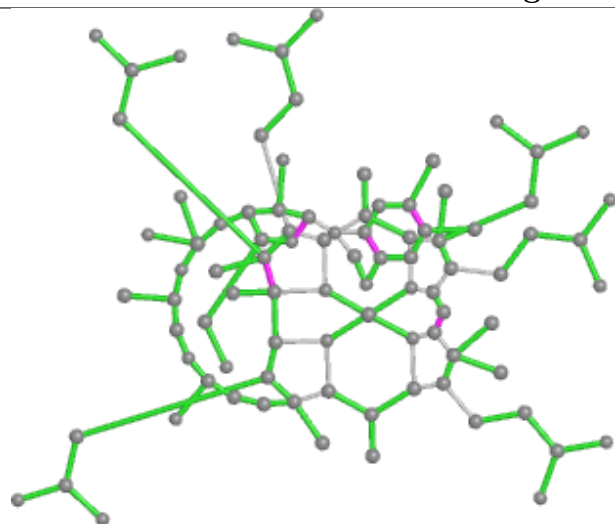
There are no ring outliers.

5 monomers are involved in 54 short contacts:

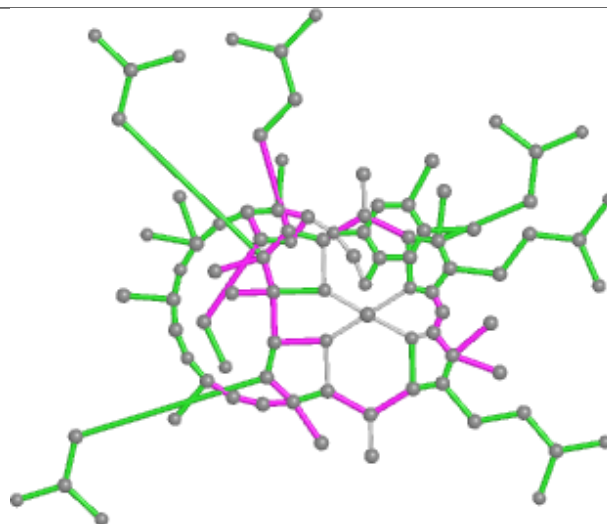
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2003	GOL	1	0
3	A	2006	GOL	2	0
5	B	601	B12	22	0
5	D	601	B12	28	0
3	C	2004	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

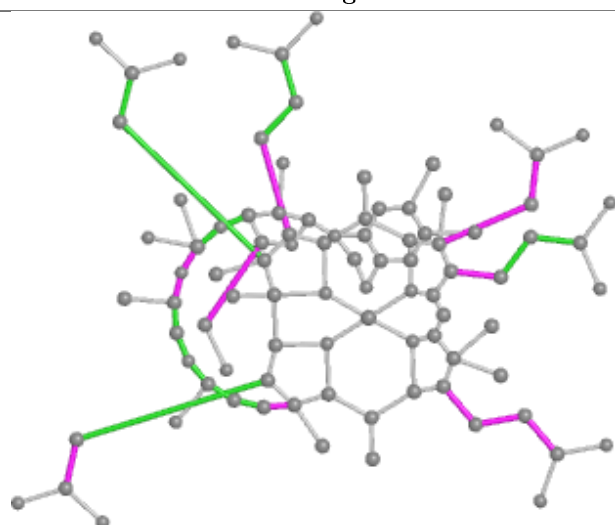
Ligand B12 B 601



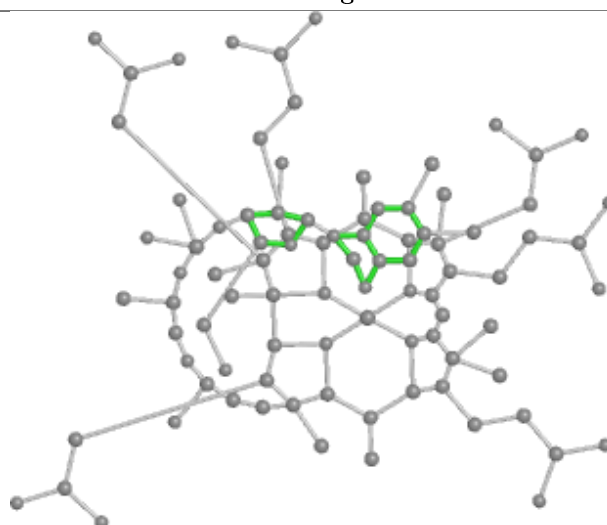
Bond lengths



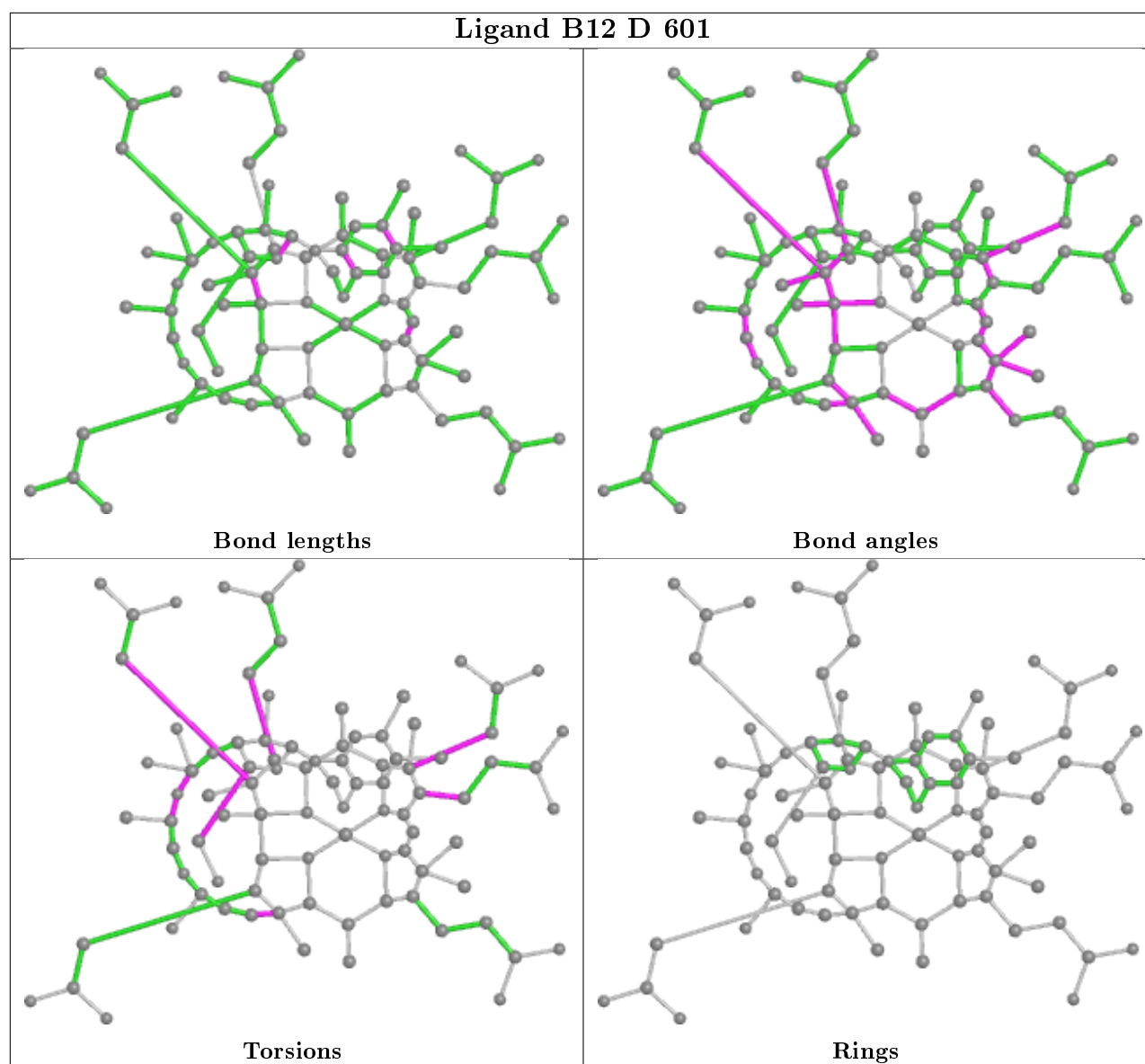
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	453/453 (100%)	-0.00	1 (0%) 95 95	15, 27, 41, 50	0
1	C	453/453 (100%)	-0.06	2 (0%) 92 93	15, 26, 44, 63	0
2	B	252/306 (82%)	0.55	15 (5%) 21 27	25, 50, 73, 82	0
2	D	252/306 (82%)	1.04	43 (17%) 1 1	19, 63, 105, 118	0
All	All	1410/1518 (92%)	0.26	61 (4%) 35 41	15, 33, 80, 118	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	ALA	7.0
2	D	153	ALA	6.7
2	D	123	VAL	5.4
2	B	119	GLY	5.3
2	D	270	VAL	5.0
2	D	119	GLY	4.8
2	D	273	ALA	4.5
2	D	191	GLN	4.0
2	D	148	VAL	3.9
2	D	156	VAL	3.9
2	D	161	VAL	3.8
2	B	113	GLU	3.8
2	D	200	PHE	3.7
2	D	295	ARG	3.3
1	A	171	GLN	3.2
2	D	145	ALA	3.1
2	B	178	TYR	3.1
2	B	44	ALA	3.1
2	D	147	ALA	3.1
2	D	158	ASN	2.9
2	B	270	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	191	GLN	2.8
2	D	193	GLY	2.8
2	B	192	ALA	2.8
2	D	151	LEU	2.8
2	D	219	ALA	2.8
2	D	187	ALA	2.8
2	D	111	PRO	2.7
2	D	157	ALA	2.7
2	D	284	LEU	2.7
2	B	72	ARG	2.6
2	B	249	ALA	2.6
2	B	120	LEU	2.6
2	D	174	ILE	2.6
2	D	267	THR	2.6
2	D	243	VAL	2.5
2	B	295	ARG	2.5
2	D	194	LEU	2.5
2	D	276	ILE	2.5
2	D	205	GLY	2.5
2	D	44	ALA	2.4
2	D	248	MET	2.4
1	C	9	GLY	2.4
2	D	202	VAL	2.3
2	D	280	ALA	2.2
2	D	129	ASP	2.2
2	D	223	ILE	2.2
2	D	142	ARG	2.1
2	B	118	GLN	2.1
2	D	124	ARG	2.1
2	B	66	VAL	2.1
2	D	214	GLY	2.1
2	D	181	ILE	2.1
2	D	155	CYS	2.1
2	D	182	LEU	2.0
2	D	213	ILE	2.0
2	B	275	VAL	2.0
2	D	249	ALA	2.0
2	D	69	GLU	2.0
2	B	182	LEU	2.0
1	C	237	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

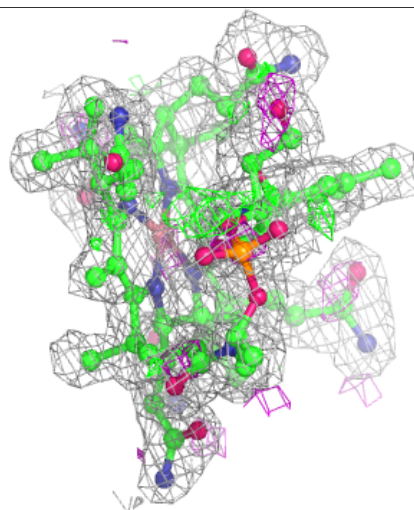
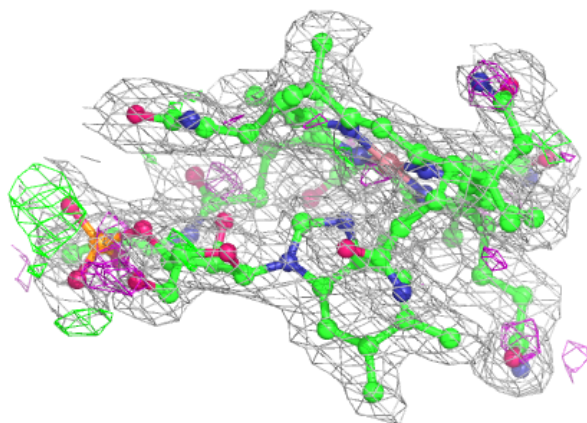
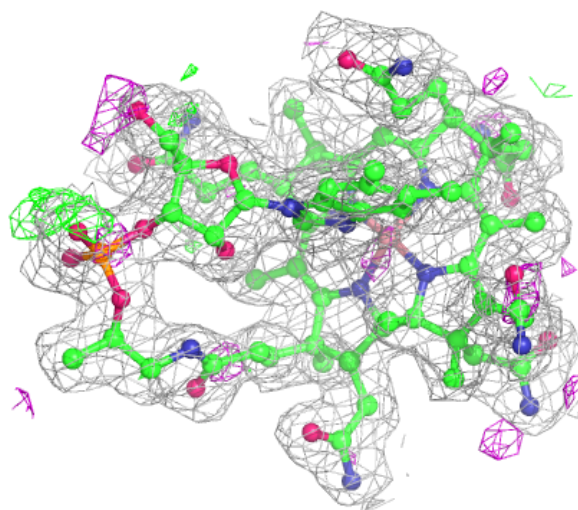
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	C	3007	1/1	0.88	0.17	24,24,24,24	0
3	GOL	A	2006	6/6	0.88	0.25	21,21,21,21	0
3	GOL	A	2001	6/6	0.88	0.16	19,19,20,20	0
4	NA	A	3005	1/1	0.88	0.19	22,22,22,22	0
3	GOL	A	2002	6/6	0.91	0.16	19,19,19,19	0
3	GOL	C	2003	6/6	0.92	0.26	20,20,20,20	0
4	NA	A	3004	1/1	0.93	0.07	19,19,19,19	0
5	B12	B	601	91/91	0.94	0.13	17,18,18,19	0
5	B12	D	601	91/91	0.94	0.12	18,18,19,19	0
3	GOL	C	2004	6/6	0.94	0.15	20,20,21,21	0
4	NA	B	3002	1/1	0.95	0.06	20,20,20,20	0
3	GOL	C	2005	6/6	0.95	0.21	20,20,20,21	0
4	NA	D	3003	1/1	0.97	0.09	21,21,21,21	0
4	NA	D	3006	1/1	0.97	0.17	20,20,20,20	0
4	NA	A	3001	1/1	0.99	0.15	20,20,20,20	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.

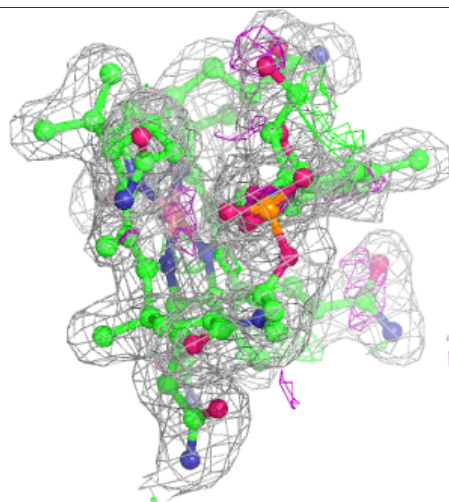
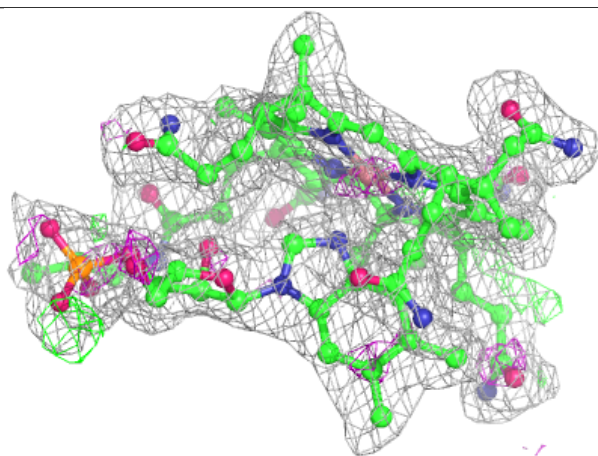
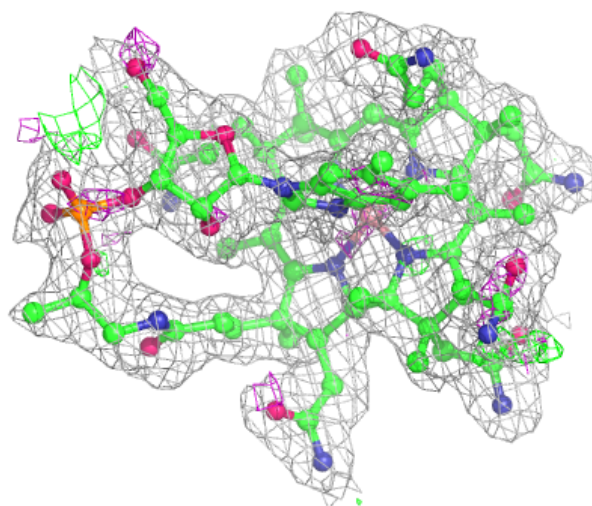
Electron density around B12 B 601:

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



Electron density around B12 D 601:

$2mF_o-DF_c$ (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.