



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:35 pm BST

PDB ID : 3ABQ
Title : Crystal structure of ethanolamine ammonia-lyase from Escherichia coli complexed with CN-Cbl and 2-amino-1-propanol
Authors : Shibata, N.
Deposited on : 2009-12-21
Resolution : 2.05 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

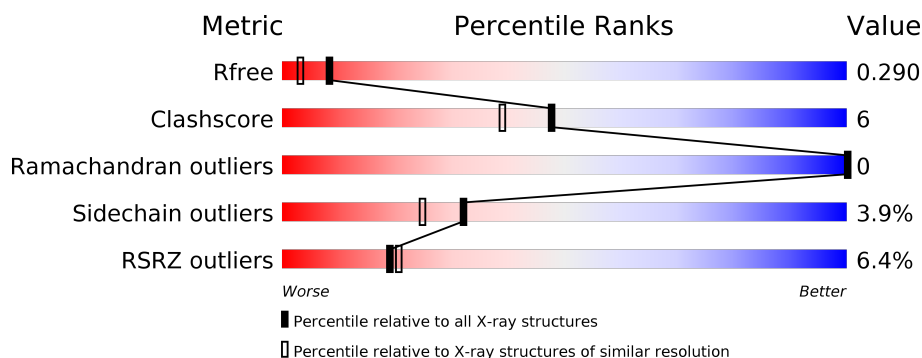
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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>%</div> <div> <div></div> <div>94%</div> <div>6%</div> <div>.</div> </div> </div>
1	C	453	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
2	B	306	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>11%</div> <div>18%</div> </div> </div>
2	D	306	<div> <div>23%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>19%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12057 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	7	0
			3500	2197	599	681	23			
1	C	453	Total	C	N	O	S	8	6	0
			3497	2194	599	680	24			

- 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	248	Total	C	N	O	S	0	0	0
			1891	1183	342	357	9			

There are 22 discrepancies between the modelled and reference sequences:

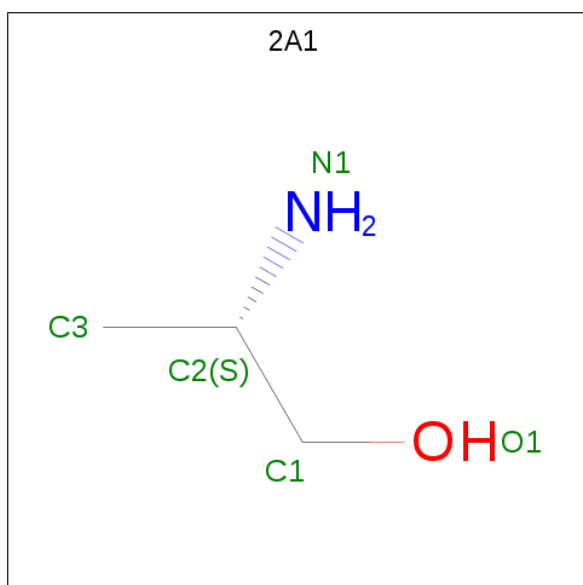
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	EXPRESSION TAG	UNP P19636
B	-9	ASP	-	EXPRESSION TAG	UNP P19636
B	-8	GLN	-	EXPRESSION TAG	UNP P19636
B	-7	SER	-	EXPRESSION TAG	UNP P19636
B	-6	SER	-	EXPRESSION TAG	UNP P19636
B	-5	HIS	-	EXPRESSION TAG	UNP P19636
B	-4	HIS	-	EXPRESSION TAG	UNP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

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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 (2S)-2-aminopropan-1-ol (three-letter code: 2A1) (formula: C₃H₉NO).



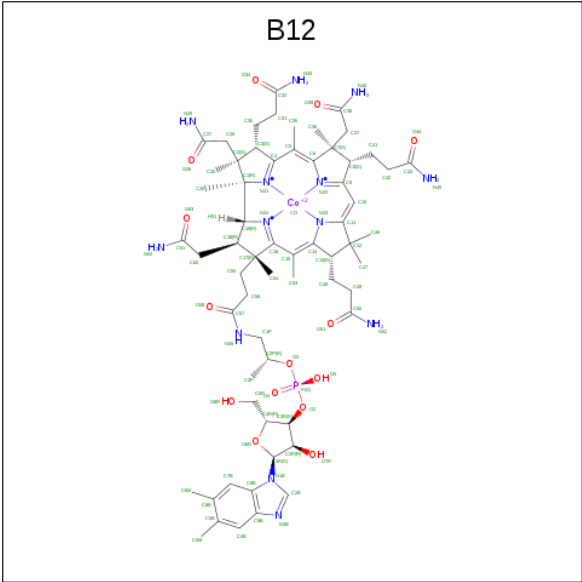
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is GLYCEROL (three-letter code: 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	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- 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	1
			94	63	1	14	15	1		

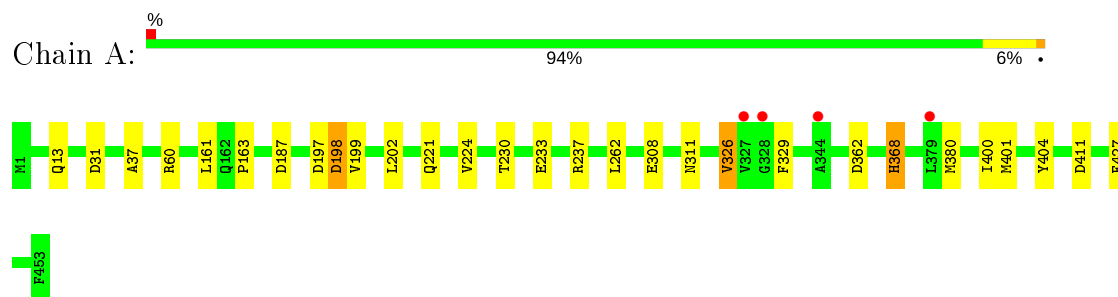
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	422	Total	O	0	0
			422	422		
6	B	124	Total	O	0	0
			124	124		
6	C	377	Total	O	0	0
			377	377		
6	D	87	Total	O	0	0
			87	87		

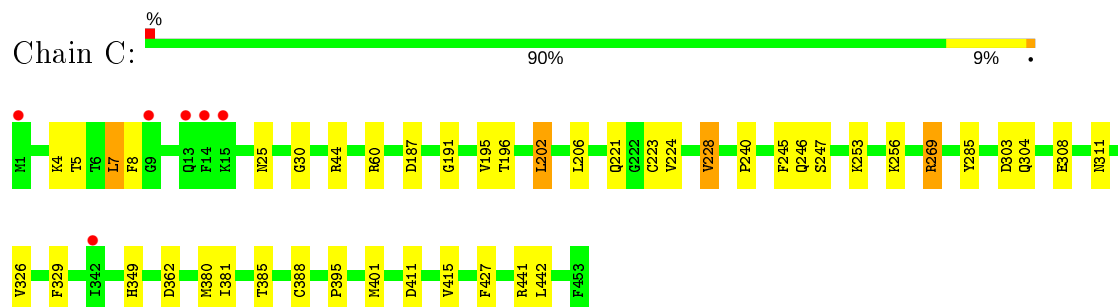
3 Residue-property plots [i](#)

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.

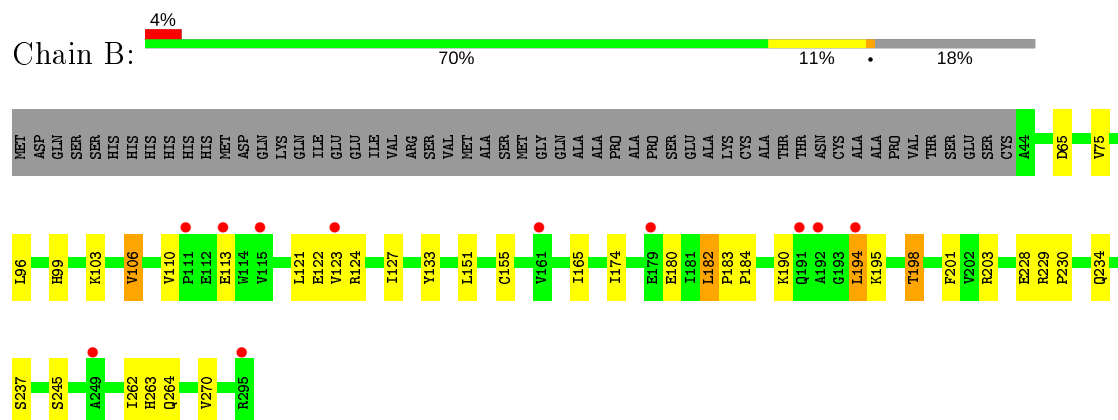
- Molecule 1: Ethanolamine ammonia-lyase heavy chain



- Molecule 1: Ethanolamine ammonia-lyase heavy chain

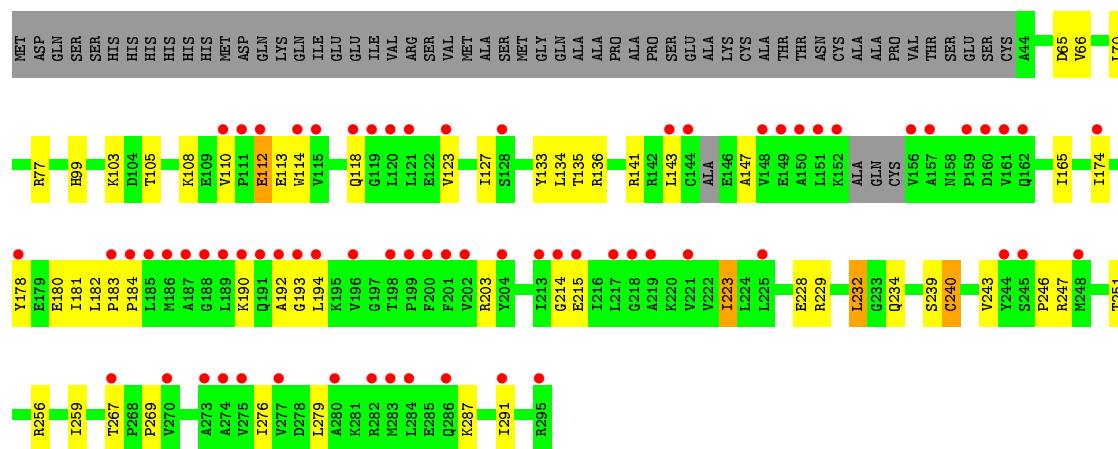


- Molecule 2: Ethanolamine ammonia-lyase light chain



- 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	241.87Å 241.87Å 76.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.05 46.22 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.05) 99.5 (46.22-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0087	Depositor
R, R_{free}	0.230 , 0.269 0.255 , 0.290	Depositor DCC
R_{free} test set	7958 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12057	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, B12, 2A1

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	0.24	0/3575	0.38	0/4839
1	C	0.26	0/3569	0.41	2/4830 (0.0%)
2	B	0.21	0/1943	0.37	0/2633
2	D	0.20	0/1916	0.36	0/2593
All	All	0.23	0/11003	0.39	2/14895 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	269[A]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	269[B]	ARG	NE-CZ-NH1	5.62	123.11	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	3500	0	3484	17	0
1	C	3497	0	3477	42	0
2	B	1916	0	1973	19	0
2	D	1891	0	1948	26	0
3	A	5	0	9	0	0
3	C	5	0	9	0	0
4	A	24	0	32	0	0
4	C	24	0	32	5	0
5	B	91	0	88	16	0
5	D	94	0	8	3	0
6	A	422	0	0	2	0
6	B	124	0	0	0	0
6	C	377	0	0	2	0
6	D	87	0	0	1	0
All	All	12057	0	11060	121	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 6.

All (121) 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:C:195[B]:VAL:HG12	1:C:401[B]:MET:CE	1.37	1.51
1:C:195[B]:VAL:CG1	1:C:401[B]:MET:CE	2.11	1.28
1:C:195[B]:VAL:HG12	1:C:401[B]:MET:HE1	1.17	1.16
5:B:601:B12:H351	5:B:601:B12:H362	1.34	1.05
1:C:195[B]:VAL:CG1	1:C:401[B]:MET:HE3	1.84	1.04
5:B:601:B12:H552	5:B:601:B12:H531	1.49	0.94
1:C:195[B]:VAL:HG12	1:C:401[B]:MET:HE2	1.47	0.93
1:C:195[B]:VAL:CG1	1:C:401[B]:MET:HE1	1.85	0.92
5:B:601:B12:H362	5:B:601:B12:C35	2.13	0.78
1:A:197:ASP:OD2	1:A:230:THR:HG21	1.82	0.77
2:B:110:VAL:O	2:B:203:ARG:NH2	2.16	0.76
2:D:182:LEU:HB3	2:D:183:PRO:HD3	1.71	0.72
1:C:195[A]:VAL:HG22	1:C:401[A]:MET:CE	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:THR:HA	2:D:108:LYS:HD2	1.72	0.70
2:B:165:ILE:HD11	2:B:174:ILE:HG23	1.72	0.70
1:C:228:VAL:HG13	1:C:246:GLN:HB2	1.77	0.67
5:B:601:B12:H473	5:B:601:B12:C49	2.25	0.66
2:D:240:CYS:HB3	2:D:259:ILE:HG23	1.80	0.64
2:D:223:ILE:HD12	2:D:276:ILE:HG21	1.79	0.63
2:B:106:VAL:HG12	2:B:230:PRO:HG2	1.80	0.62
5:B:601:B12:C47	5:B:601:B12:C49	2.77	0.61
5:B:601:B12:H351	5:B:601:B12:C36	2.13	0.60
2:B:182:LEU:HB3	2:B:183:PRO:HD3	1.83	0.60
1:C:202:LEU:HD22	1:C:224:VAL:HG11	1.84	0.60
1:C:195[B]:VAL:HG13	1:C:401[B]:MET:CE	2.24	0.60
1:C:195[A]:VAL:CG2	1:C:401[A]:MET:HE3	2.32	0.59
2:B:228:GLU:HA	5:B:601:B12:H1P2	1.85	0.59
1:C:246:GLN:NE2	5:D:601[B]:B12:O39	2.36	0.58
2:D:135:THR:HG23	2:D:136:ARG:HG2	1.87	0.57
5:B:601:B12:C53	5:B:601:B12:H552	2.29	0.57
5:B:601:B12:H533	5:B:601:B12:H521	1.70	0.57
1:C:195[A]:VAL:CG2	1:C:401[A]:MET:CE	2.84	0.55
2:B:122:GLU:HG3	2:B:201:PHE:HD1	1.70	0.55
1:C:380[B]:MET:SD	1:C:415:VAL:HG23	2.47	0.54
1:C:44:ARG:HH22	4:C:2008:GOL:H11	1.73	0.54
2:D:192:ALA:N	2:D:193:GLY:HA3	2.22	0.54
1:A:326:VAL:HG12	1:A:329:PHE:HB2	1.90	0.54
5:B:601:B12:C47	5:B:601:B12:H491	2.38	0.54
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.43	0.54
1:C:195[A]:VAL:HG22	1:C:401[A]:MET:HE3	1.90	0.53
1:C:349:HIS:CE1	1:C:388:CYS:HA	2.44	0.53
1:C:380[B]:MET:SD	1:C:415:VAL:CG2	2.96	0.53
1:C:195[B]:VAL:HG23	1:C:196:THR:HG23	1.90	0.53
1:C:4:LYS:HG2	1:C:5:THR:N	2.24	0.53
1:C:441:ARG:NH2	6:C:703:HOH:O	2.43	0.52
2:B:123:VAL:CG1	2:B:124:ARG:N	2.73	0.51
2:D:77:ARG:NH2	2:D:232:LEU:HD13	2.25	0.51
1:C:326:VAL:HG12	1:C:329:PHE:HB2	1.93	0.51
2:D:127:ILE:HG21	2:D:133:TYR:HB2	1.93	0.50
2:D:181:ILE:HB	2:D:269:PRO:HB3	1.92	0.50
1:C:247:SER:OG	5:D:601[A]:B12:N40	2.45	0.50
1:C:7:LEU:HD22	1:C:8:PHE:CD1	2.47	0.50
1:C:195[B]:VAL:HG13	1:C:401[B]:MET:HE3	1.83	0.50
2:D:165:ILE:HD13	2:D:178:TYR:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:B12:H471	5:B:601:B12:H491	1.92	0.49
2:D:110:VAL:O	2:D:203:ARG:NH2	2.29	0.49
2:B:228:GLU:HG2	2:B:237:SER:O	2.12	0.49
5:B:601:B12:C36	5:B:601:B12:C35	2.84	0.49
1:C:442:LEU:O	4:C:2005:GOL:H12	2.12	0.49
1:A:380:MET:SD	1:A:411:ASP:HB3	2.53	0.48
1:C:195[A]:VAL:HG22	1:C:401[A]:MET:HE2	1.94	0.48
2:B:65:ASP:OD2	2:B:65:ASP:N	2.44	0.48
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.49	0.48
2:D:228:GLU:OE1	2:D:239:SER:OG	2.26	0.48
1:C:308:GLU:O	1:C:311:ASN:HB2	2.14	0.47
1:A:233:GLU:OE2	1:A:237[A]:ARG:NH2	2.47	0.47
1:A:161:LEU:O	1:A:163:PRO:HD3	2.15	0.46
5:B:601:B12:H253	5:B:601:B12:H301	1.68	0.46
1:A:237[A]:ARG:NH2	6:A:888:HOH:O	2.49	0.46
2:B:180:GLU:HG2	2:B:270:VAL:HG23	1.98	0.46
2:D:65:ASP:OD2	2:D:65:ASP:N	2.48	0.45
2:B:194:LEU:HB2	2:B:195:LYS:H	1.65	0.45
1:A:199:VAL:HG11	1:A:237[A]:ARG:HD2	1.99	0.45
1:C:381:ILE:O	1:C:385:THR:HG23	2.17	0.45
1:A:326:VAL:CG1	1:A:329:PHE:HB2	2.47	0.44
1:C:380[A]:MET:SD	1:C:411:ASP:HB3	2.56	0.44
2:D:143:LEU:HB3	2:D:147:ALA:HB3	1.99	0.44
1:C:25:ASN:ND2	1:C:303:ASP:OD2	2.48	0.44
2:D:215:GLU:HG2	2:D:247:ARG:HH11	1.82	0.43
2:B:127:ILE:HG21	2:B:133:TYR:HB2	2.01	0.43
2:D:112:GLU:CD	2:D:112:GLU:H	2.21	0.43
2:D:174:ILE:O	2:D:178:TYR:HB2	2.18	0.43
2:B:99:HIS:O	2:B:103:LYS:HG2	2.19	0.43
1:A:326:VAL:HA	1:A:362:ASP:HB3	2.01	0.43
1:C:30:GLY:HA3	1:C:304:GLN:OE1	2.19	0.43
5:B:601:B12:C55	5:B:601:B12:H531	2.29	0.43
2:D:183:PRO:HB2	2:D:184:PRO:HD3	2.00	0.43
1:A:31:ASP:HB3	1:A:37:ALA:HB2	2.01	0.43
2:D:66:VAL:O	2:D:70:LEU:HG	2.18	0.43
2:D:99:HIS:O	2:D:103:LYS:HG2	2.19	0.42
1:C:206:LEU:HB3	1:C:240:PRO:HG2	2.01	0.42
2:D:287:LYS:HE2	2:D:287:LYS:HB3	1.84	0.42
2:B:75:VAL:O	2:B:75:VAL:HG12	2.20	0.42
1:C:395:PRO:HD3	6:C:804:HOH:O	2.19	0.42
1:A:187:ASP:N	1:A:187:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:ILE:O	2:B:263:HIS:HB3	2.20	0.42
1:A:198:ASP:O	1:A:202:LEU:HG	2.20	0.41
2:D:194:LEU:HD12	2:D:194:LEU:HA	1.91	0.41
2:D:214:GLY:HA3	2:D:246:PRO:HG2	2.02	0.41
1:C:441:ARG:NE	4:C:2005:GOL:O2	2.38	0.41
1:C:44:ARG:HH12	4:C:2008:GOL:C3	2.34	0.41
5:B:601:B12:N29	5:B:601:B12:H3	2.35	0.41
2:B:75:VAL:CG1	2:B:75:VAL:O	2.69	0.41
1:C:326:VAL:CG1	1:C:329:PHE:HB2	2.50	0.41
1:A:368:HIS:H	1:A:368:HIS:CD2	2.39	0.41
2:B:183:PRO:HB2	2:B:184:PRO:HD3	2.03	0.41
2:B:155:CYS:HA	2:B:198:THR:HG21	2.02	0.41
5:B:601:B12:H301	5:B:601:B12:H203	2.03	0.41
1:C:44:ARG:NH2	4:C:2008:GOL:H11	2.37	0.40
2:D:114:TRP:O	2:D:118:GLN:HG2	2.21	0.40
1:A:400:ILE:HG12	6:A:554:HOH:O	2.21	0.40
2:B:165:ILE:HG23	2:B:201:PHE:HA	2.04	0.40
1:C:245:PHE:HA	1:C:285:TYR:O	2.22	0.40
1:C:326:VAL:HA	1:C:362:ASP:HB3	2.03	0.40
1:A:308:GLU:O	1:A:311:ASN:HB2	2.21	0.40
1:C:191:GLY:HA2	1:C:223:CYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/453 (101%)	443 (97%)	15 (3%)	0	100	100
1	C	457/453 (101%)	444 (97%)	13 (3%)	0	100	100
2	B	250/306 (82%)	245 (98%)	5 (2%)	0	100	100
2	D	242/306 (79%)	236 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1407/1518 (93%)	1368 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/370 (102%)	369 (98%)	8 (2%)	53	48
1	C	376/370 (102%)	367 (98%)	9 (2%)	49	42
2	B	206/251 (82%)	193 (94%)	13 (6%)	18	9
2	D	204/251 (81%)	188 (92%)	16 (8%)	12	5
All	All	1163/1242 (94%)	1117 (96%)	46 (4%)	32	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	60	ARG
1	A	198	ASP
1	A	221	GLN
1	A	262	LEU
1	A	368	HIS
1	A	401	MET
1	A	404	TYR
2	B	96	LEU
2	B	106	VAL
2	B	113	GLU
2	B	121	LEU
2	B	151	LEU
2	B	182	LEU
2	B	190	LYS
2	B	194	LEU
2	B	198	THR

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Mol	Chain	Res	Type
2	B	229	ARG
2	B	234	GLN
2	B	245	SER
2	B	264	GLN
1	C	7	LEU
1	C	60	ARG
1	C	202	LEU
1	C	221	GLN
1	C	228	VAL
1	C	253	LYS
1	C	256	LYS
1	C	269[A]	ARG
1	C	269[B]	ARG
2	D	112	GLU
2	D	113	GLU
2	D	123	VAL
2	D	134	LEU
2	D	180	GLU
2	D	190	LYS
2	D	223	ILE
2	D	229	ARG
2	D	232	LEU
2	D	234	GLN
2	D	240	CYS
2	D	243	VAL
2	D	251	THR
2	D	267	THR
2	D	279	LEU
2	D	291	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	HIS
2	B	131	ASN
1	C	349	HIS
2	D	99	HIS
2	D	234	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	2006	-	5,5,5	0.37	0	5,5,5	0.28	0
5	B12	B	601	-	80,101,101	1.07	4 (5%)	101,166,166	1.19	13 (12%)
4	GOL	A	2007	-	5,5,5	0.35	0	5,5,5	0.31	0
4	GOL	A	2002	-	5,5,5	0.40	0	5,5,5	0.36	0
5	B12	D	601[A]	-	80,101,101	1.06	5 (6%)	101,166,166	1.38	16 (15%)
3	2A1	C	602	-	4,4,4	0.66	0	3,4,4	1.16	0
3	2A1	A	602	-	4,4,4	0.65	0	3,4,4	1.30	0
4	GOL	C	2003	-	5,5,5	0.35	0	5,5,5	0.36	0
4	GOL	C	2004	-	5,5,5	0.37	0	5,5,5	0.28	0
4	GOL	C	2005	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	C	2008	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	A	2001	-	5,5,5	0.36	0	5,5,5	0.26	0
5	B12	D	601[B]	-	80,101,101	1.06	5 (6%)	101,166,166	1.38	16 (15%)

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	2006	-	-	2/4/4/4	-
5	B12	B	601	-	-	17/51/223/223	0/3/11/11
4	GOL	A	2007	-	-	0/4/4/4	-
4	GOL	A	2002	-	-	2/4/4/4	-
5	B12	D	601[A]	-	-	16/51/223/223	0/3/11/11
3	2A1	C	602	-	-	0/2/2/2	-
3	2A1	A	602	-	-	1/2/2/2	-
4	GOL	C	2003	-	-	3/4/4/4	-
4	GOL	C	2004	-	-	2/4/4/4	-
4	GOL	C	2005	-	-	2/4/4/4	-
4	GOL	C	2008	-	-	2/4/4/4	-
4	GOL	A	2001	-	-	2/4/4/4	-
5	B12	D	601[B]	-	-	17/51/223/223	0/3/11/11

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601[A]	B12	C11-C10	-4.06	1.34	1.40
5	D	601[B]	B12	C11-C10	-4.06	1.34	1.40
5	B	601	B12	C11-C10	-3.91	1.34	1.40
5	B	601	B12	C8B-C9B	3.91	1.48	1.40
5	D	601[A]	B12	C8B-C9B	3.88	1.48	1.40
5	D	601[B]	B12	C8B-C9B	3.88	1.48	1.40
5	B	601	B12	C6B-C5B	3.44	1.49	1.40
5	D	601[A]	B12	C6B-C5B	3.40	1.49	1.40
5	D	601[B]	B12	C6B-C5B	3.40	1.49	1.40
5	B	601	B12	C1-C2	-2.42	1.53	1.58
5	D	601[A]	B12	C1-C2	-2.15	1.53	1.58
5	D	601[B]	B12	C1-C2	-2.15	1.53	1.58
5	D	601[A]	B12	C2-C3	-2.07	1.55	1.58
5	D	601[B]	B12	C2-C3	-2.07	1.55	1.58

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601[A]	B12	C47-C12-C46	5.28	120.79	109.73
5	D	601[B]	B12	C47-C12-C46	5.28	120.79	109.73
5	D	601[A]	B12	C54-C17-C18	-4.28	106.66	112.98
5	D	601[B]	B12	C54-C17-C18	-4.28	106.66	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601[A]	B12	C2-C1-C19	4.10	125.06	118.60
5	D	601[B]	B12	C2-C1-C19	4.10	125.06	118.60
5	B	601	B12	C2-C1-C19	3.25	123.72	118.60
5	B	601	B12	C54-C17-C18	-3.24	108.20	112.98
5	D	601[A]	B12	C20-C1-C19	-3.12	106.34	109.36
5	D	601[B]	B12	C20-C1-C19	-3.12	106.34	109.36
5	B	601	B12	C25-C2-C3	-2.97	111.05	115.58
5	D	601[A]	B12	C1-C2-C3	2.94	105.27	101.59
5	D	601[B]	B12	C1-C2-C3	2.94	105.27	101.59
5	D	601[A]	B12	C12-C11-C10	-2.79	119.91	124.64
5	D	601[B]	B12	C12-C11-C10	-2.79	119.91	124.64
5	D	601[A]	B12	C25-C2-C1	-2.76	109.70	113.80
5	D	601[B]	B12	C25-C2-C1	-2.76	109.70	113.80
5	D	601[A]	B12	C25-C2-C3	-2.76	111.38	115.58
5	D	601[B]	B12	C25-C2-C3	-2.76	111.38	115.58
5	D	601[A]	B12	C20-C1-C2	-2.68	108.88	113.32
5	D	601[B]	B12	C20-C1-C2	-2.68	108.88	113.32
5	B	601	B12	C9-C10-C11	-2.61	121.79	130.91
5	B	601	B12	C1-C2-C3	2.59	104.83	101.59
5	D	601[A]	B12	C19-C1-N21	2.59	104.81	102.16
5	D	601[B]	B12	C19-C1-N21	2.59	104.81	102.16
5	B	601	B12	C30-C3-C2	-2.57	113.68	119.13
5	B	601	B12	C16-C15-C14	-2.54	120.31	124.27
5	B	601	B12	C20-C1-C19	-2.49	106.96	109.36
5	D	601[A]	B12	C9-C10-C11	-2.45	122.34	130.91
5	D	601[B]	B12	C9-C10-C11	-2.45	122.34	130.91
5	B	601	B12	C47-C12-C46	2.39	114.75	109.73
5	B	601	B12	C25-C2-C1	-2.36	110.30	113.80
5	D	601[A]	B12	C16-C15-C14	-2.26	120.74	124.27
5	D	601[B]	B12	C16-C15-C14	-2.26	120.74	124.27
5	B	601	B12	C1-C19-N24	2.25	108.77	106.24
5	B	601	B12	C6-C5-C4	-2.21	120.82	124.27
5	D	601[A]	B12	C30-C3-C2	-2.20	114.47	119.13
5	D	601[B]	B12	C30-C3-C2	-2.20	114.47	119.13
5	D	601[A]	B12	C2P-C1P-N59	-2.14	109.77	112.93
5	D	601[B]	B12	C2P-C1P-N59	-2.14	109.77	112.93
5	B	601	B12	C2P-C1P-N59	-2.09	109.85	112.93
5	D	601[A]	B12	C6-C5-C4	-2.09	121.01	124.27
5	D	601[B]	B12	C6-C5-C4	-2.09	121.01	124.27
5	D	601[A]	B12	C55-C17-C18	2.06	115.13	111.14
5	D	601[B]	B12	C55-C17-C18	2.06	115.13	111.14

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	B12	C2-C3-C30-C31
5	B	601	B12	C38-C37-C7-C36
5	B	601	B12	C38-C37-C7-C8
5	B	601	B12	C13-C48-C49-C50
5	B	601	B12	C2P-O3-P-O4
5	B	601	B12	C2P-O3-P-O5
4	A	2002	GOL	O1-C1-C2-O2
4	A	2002	GOL	O1-C1-C2-C3
5	D	601[A]	B12	C4-C3-C30-C31
5	D	601[A]	B12	C2P-O3-P-O4
5	D	601[A]	B12	C2P-O3-P-O5
4	C	2004	GOL	C1-C2-C3-O3
4	C	2005	GOL	O1-C1-C2-O2
4	C	2005	GOL	O1-C1-C2-C3
5	D	601[B]	B12	C4-C3-C30-C31
5	D	601[B]	B12	C38-C37-C7-C36
5	D	601[B]	B12	C38-C37-C7-C8
5	D	601[B]	B12	C2P-O3-P-O4
5	D	601[B]	B12	C2P-O3-P-O5
5	B	601	B12	O6R-C4R-C5R-O8R
5	D	601[A]	B12	O6R-C4R-C5R-O8R
5	D	601[B]	B12	O6R-C4R-C5R-O8R
5	B	601	B12	C3R-C4R-C5R-O8R
4	C	2004	GOL	O2-C2-C3-O3
5	D	601[A]	B12	C3R-C4R-C5R-O8R
5	D	601[B]	B12	C3R-C4R-C5R-O8R
5	B	601	B12	C16-C17-C55-C56
5	D	601[A]	B12	C16-C17-C55-C56
5	D	601[B]	B12	C16-C17-C55-C56
4	A	2006	GOL	O1-C1-C2-C3
4	C	2003	GOL	C1-C2-C3-O3
4	C	2008	GOL	O1-C1-C2-C3
4	C	2008	GOL	O1-C1-C2-O2
5	B	601	B12	C2P-O3-P-O2
5	D	601[A]	B12	C2P-O3-P-O2
5	D	601[B]	B12	C2P-O3-P-O2
4	C	2003	GOL	O2-C2-C3-O3
4	A	2006	GOL	O1-C1-C2-O2
4	A	2001	GOL	O1-C1-C2-O2
5	B	601	B12	C18-C17-C55-C56
5	D	601[A]	B12	C48-C49-C50-O51
5	D	601[B]	B12	C48-C49-C50-O51

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Mol	Chain	Res	Type	Atoms
5	B	601	B12	C1P-C2P-O3-P
5	B	601	B12	C3P-C2P-O3-P
5	D	601[A]	B12	C1P-C2P-O3-P
5	D	601[A]	B12	C3P-C2P-O3-P
5	D	601[B]	B12	C1P-C2P-O3-P
5	D	601[B]	B12	C3P-C2P-O3-P
5	D	601[A]	B12	C2-C3-C30-C31
5	D	601[B]	B12	C2-C3-C30-C31
5	B	601	B12	C42-C41-C8-C9
5	D	601[A]	B12	C42-C41-C8-C9
5	D	601[B]	B12	C42-C41-C8-C9
3	A	602	2A1	O1-C1-C2-N1
4	C	2003	GOL	O1-C1-C2-C3
5	D	601[A]	B12	C48-C49-C50-N52
5	D	601[B]	B12	C48-C49-C50-N52
5	B	601	B12	C48-C49-C50-O51
5	B	601	B12	C48-C49-C50-N52
5	D	601[A]	B12	C18-C17-C55-C56
5	D	601[B]	B12	C18-C17-C55-C56
5	D	601[A]	B12	C13-C48-C49-C50
5	D	601[B]	B12	C13-C48-C49-C50
5	D	601[A]	B12	C38-C37-C7-C36
4	A	2001	GOL	O1-C1-C2-C3
5	B	601	B12	C4-C3-C30-C31

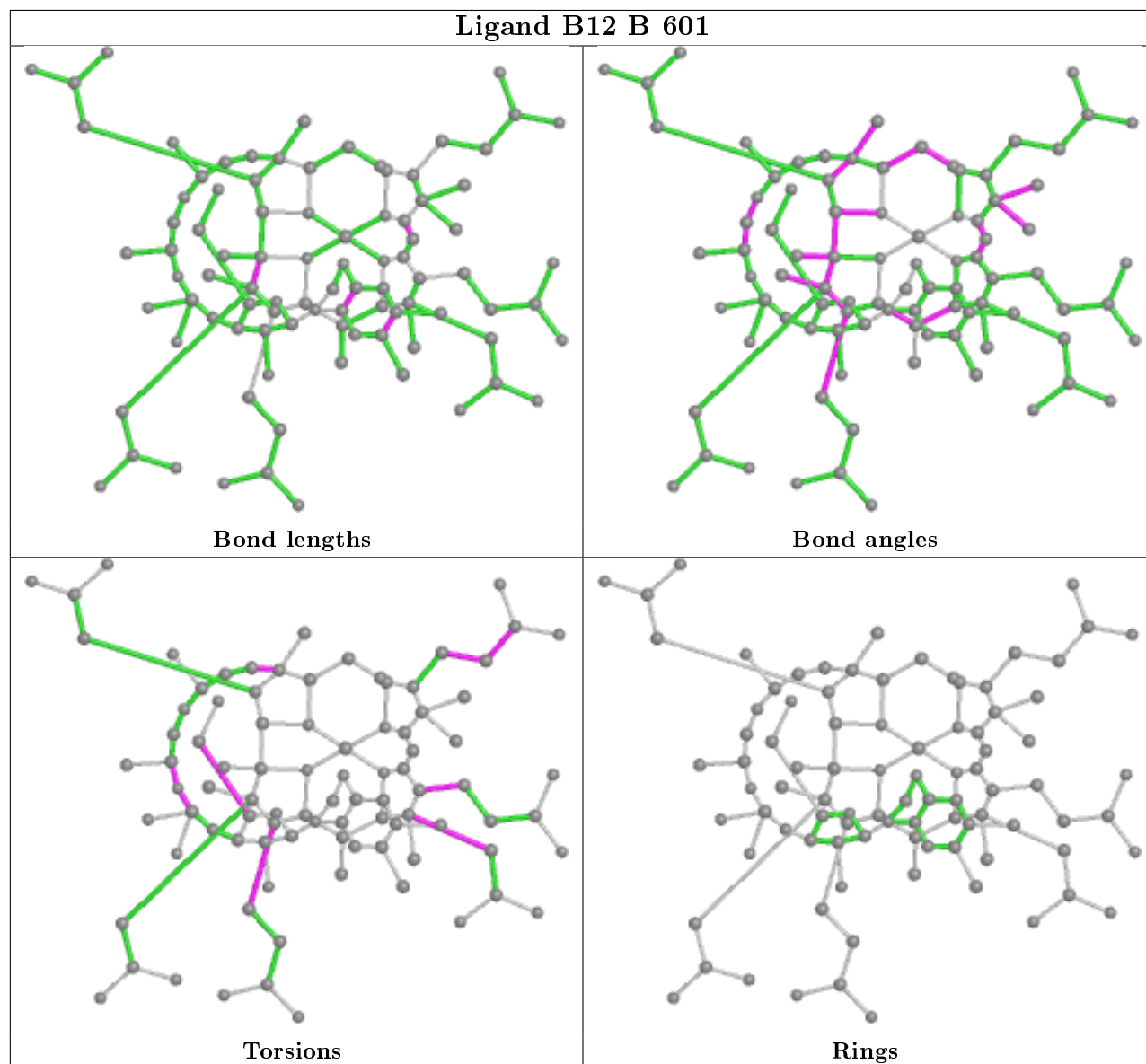
There are no ring outliers.

5 monomers are involved in 24 short contacts:

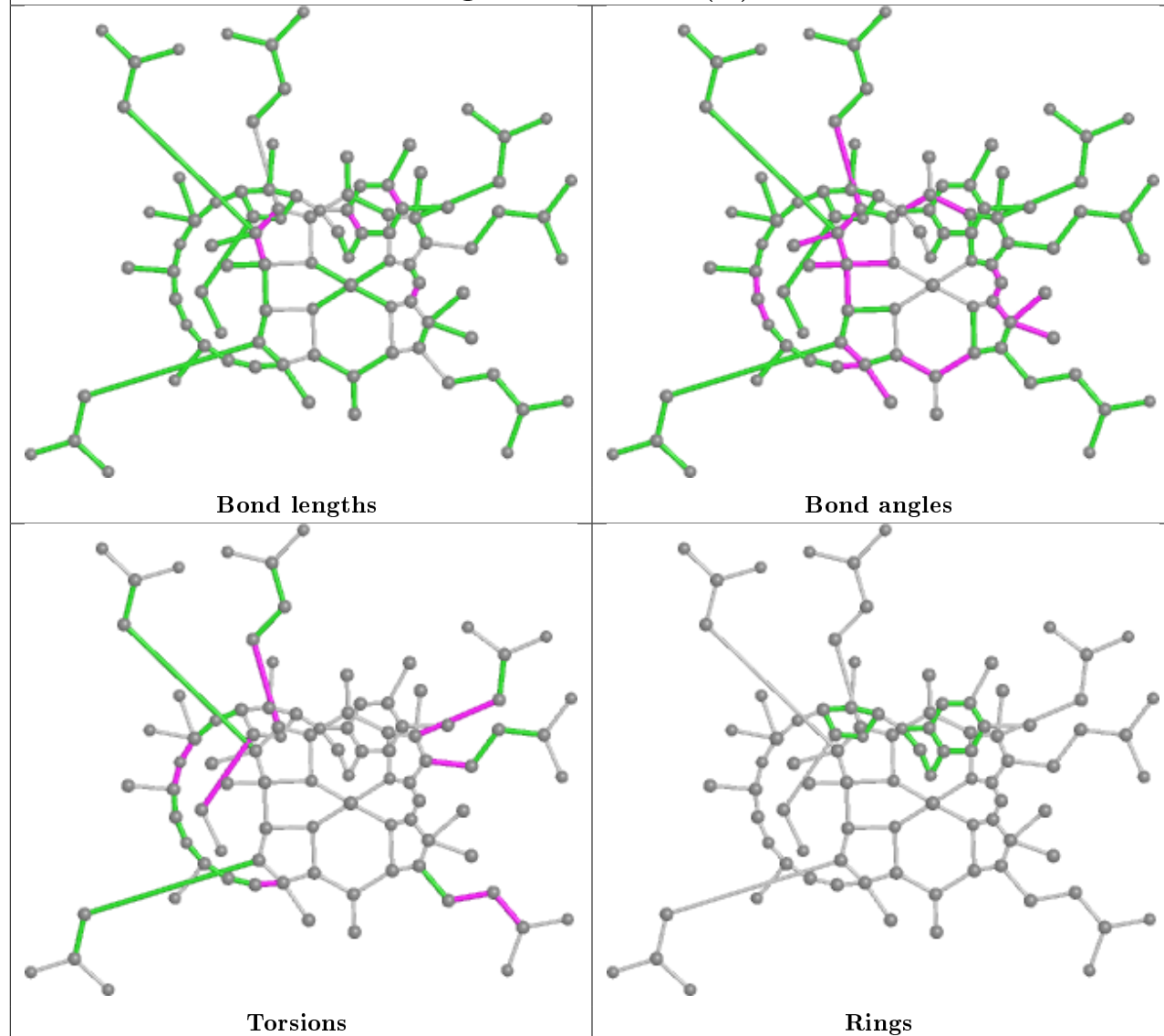
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	B12	16	0
5	D	601[A]	B12	2	0
4	C	2005	GOL	2	0
4	C	2008	GOL	3	0
5	D	601[B]	B12	1	0

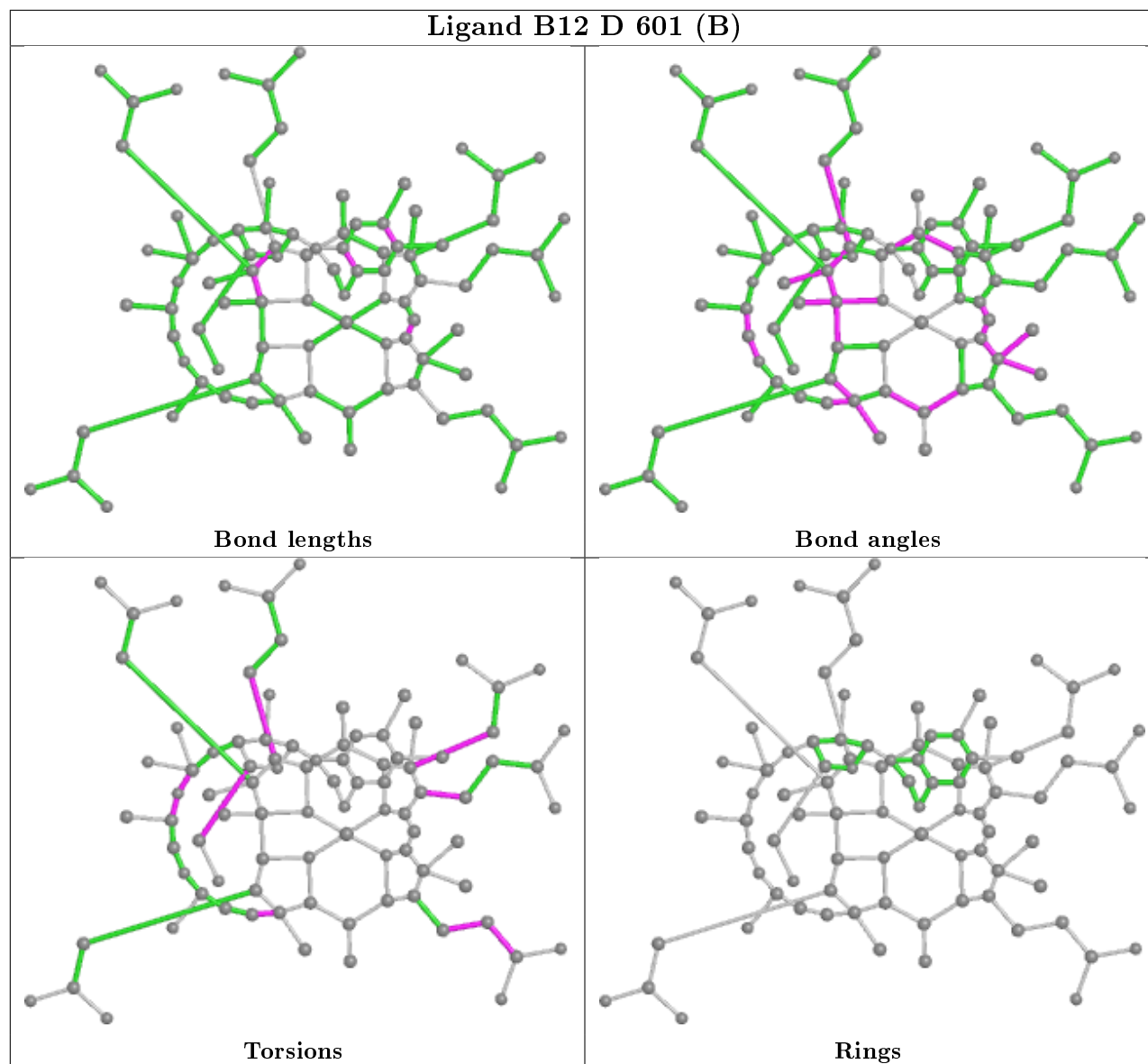
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 D 601 (A)





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%)	-0.02	4 (0%) 84 86	15, 27, 46, 63	0
1	C	453/453 (100%)	-0.01	6 (1%) 77 79	13, 29, 52, 75	0
2	B	252/306 (82%)	0.32	11 (4%) 34 37	21, 53, 77, 100	0
2	D	248/306 (81%)	1.28	69 (27%) 0 0	18, 75, 120, 146	0
All	All	1406/1518 (92%)	0.27	90 (6%) 19 21	13, 35, 95, 146	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	ALA	8.9
2	D	151	LEU	8.1
2	D	156	VAL	7.3
2	D	148	VAL	6.3
2	B	192	ALA	6.2
2	D	123	VAL	5.7
2	D	200	PHE	5.4
2	D	191	GLN	5.4
2	D	187	ALA	5.3
2	D	157	ALA	4.8
2	D	196	VAL	4.6
2	D	202	VAL	4.4
2	D	194	LEU	4.2
2	D	161	VAL	4.2
2	D	120	LEU	4.2
2	D	149	GLU	4.1
2	D	193	GLY	4.1
2	D	119	GLY	4.0
2	D	110	VAL	4.0
2	D	178	TYR	4.0
2	B	194	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	244	TYR	3.8
2	D	183	PRO	3.8
2	D	162	GLN	3.7
2	D	128	SER	3.6
2	D	143	LEU	3.5
2	D	284	LEU	3.5
2	B	191	GLN	3.5
2	D	217	LEU	3.5
2	D	186	MET	3.3
2	D	275	VAL	3.2
2	D	118	GLN	3.2
2	D	291	ILE	3.2
2	D	144	CYS	3.1
2	D	111	PRO	3.1
2	B	295	ARG	3.1
2	B	111	PRO	3.0
2	D	245	SER	3.0
2	D	174	ILE	3.0
2	D	188	GLY	3.0
2	D	201	PHE	3.0
2	D	274	ALA	3.0
2	D	114	TRP	3.0
2	B	179	GLU	2.9
2	D	225	LEU	2.9
2	D	199	PRO	2.9
2	D	189	LEU	2.9
2	D	198	THR	2.9
2	D	190	LYS	2.9
2	D	273	ALA	2.8
2	B	113	GLU	2.8
1	C	1	MET	2.8
2	D	204	TYR	2.7
2	D	185	LEU	2.7
2	D	213	ILE	2.7
2	D	295	ARG	2.7
2	D	277	VAL	2.7
2	D	283	MET	2.7
2	D	248	MET	2.6
1	C	15	LYS	2.6
2	D	159	PRO	2.5
2	D	286	GLN	2.5
2	D	184	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	112	GLU	2.4
2	B	115	VAL	2.4
2	D	160	ASP	2.4
1	C	14	PHE	2.4
2	D	221	VAL	2.4
1	A	344	ALA	2.4
1	A	379	LEU	2.3
1	C	13	GLN	2.3
2	D	115	VAL	2.3
2	B	161	VAL	2.2
2	D	150	ALA	2.2
2	D	280	ALA	2.2
2	D	121	LEU	2.2
2	D	214	GLY	2.2
2	D	215	GLU	2.2
1	C	9	GLY	2.2
2	B	249	ALA	2.2
2	D	270	VAL	2.1
2	D	267	THR	2.1
2	D	282	ARG	2.1
1	A	328	GLY	2.1
2	D	218	GLY	2.1
1	C	342	ILE	2.0
2	D	219	ALA	2.0
2	B	123	VAL	2.0
2	D	152	LYS	2.0
1	A	327	VAL	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,

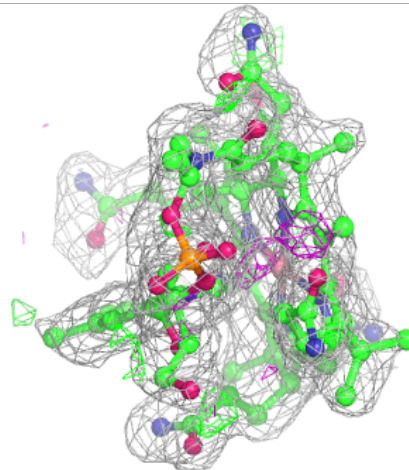
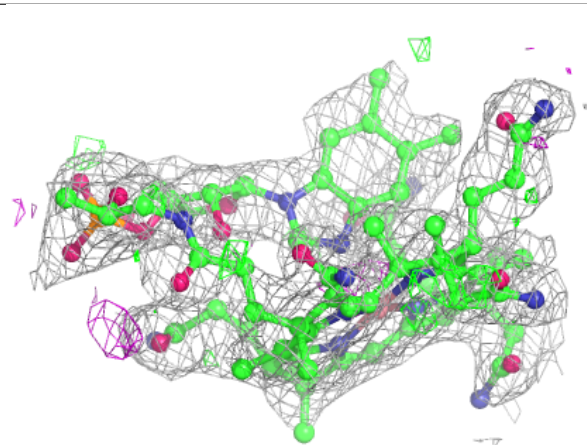
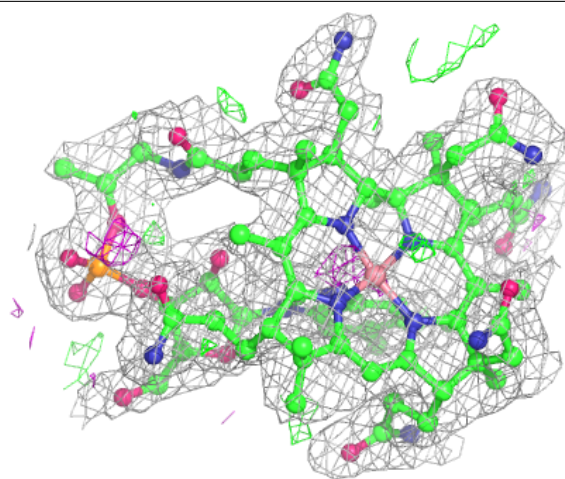
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	2008	6/6	0.79	0.17	37,44,47,57	0
4	GOL	A	2002	6/6	0.89	0.14	27,36,40,43	0
4	GOL	C	2004	6/6	0.90	0.24	45,46,52,54	0
3	2A1	C	602	5/5	0.91	0.21	23,23,34,41	0
4	GOL	A	2001	6/6	0.91	0.12	25,28,32,39	0
4	GOL	C	2003	6/6	0.92	0.14	30,37,44,48	0
4	GOL	A	2006	6/6	0.94	0.16	27,40,46,46	0
3	2A1	A	602	5/5	0.94	0.27	22,22,37,41	0
5	B12	D	601[A]	91/91	0.94	0.14	14,37,51,57	3
5	B12	D	601[B]	91/91	0.94	0.14	14,37,51,57	3
5	B12	B	601	91/91	0.95	0.12	18,28,40,49	0
4	GOL	C	2005	6/6	0.96	0.20	31,39,47,60	0
4	GOL	A	2007	6/6	0.97	0.09	19,24,24,37	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.

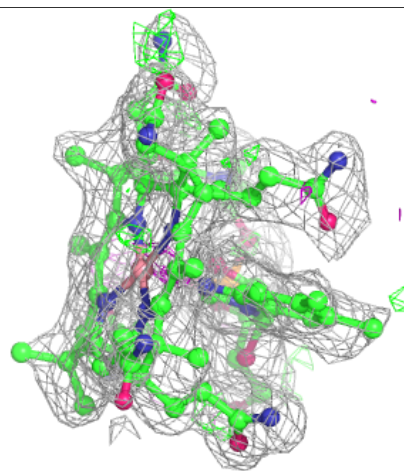
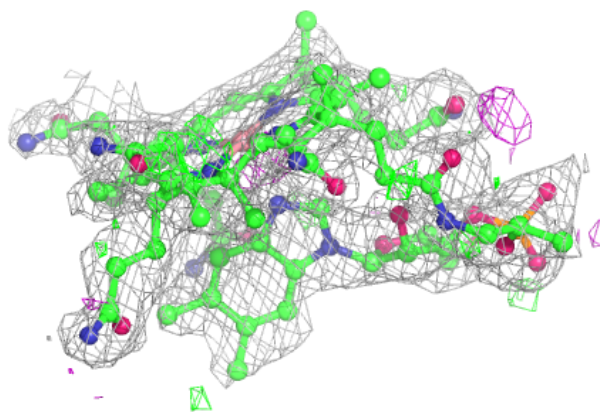
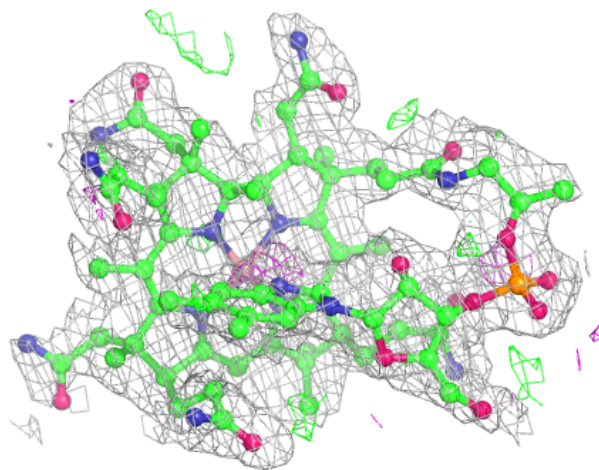
Electron density around B12 D 601 (A):

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



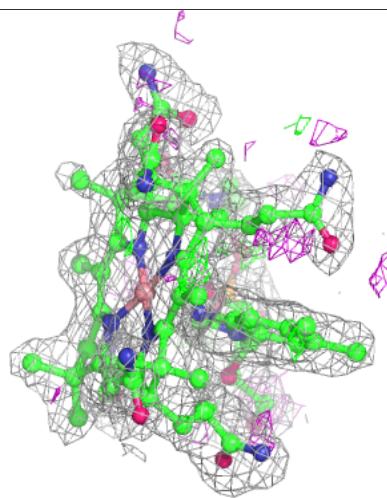
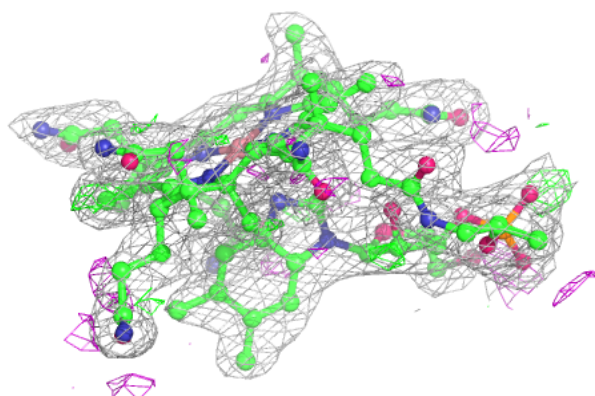
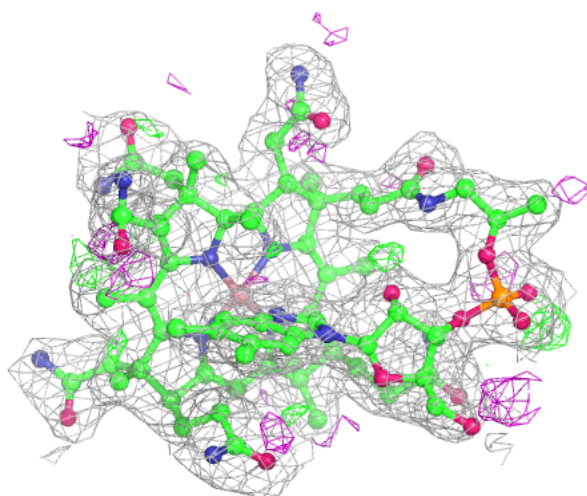
Electron density around B12 D 601 (B):

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



Electron density around B12 B 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 ⓘ

There are no such residues in this entry.