



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:07 PM UTC

PDB ID : 5YSN / pdb_00005ysn
Title : Ethanolamine ammonia-lyase, AdoCbl/substrate-free
Authors : Shibata, N.
Deposited on : 2017-11-14
Resolution : 2.00 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

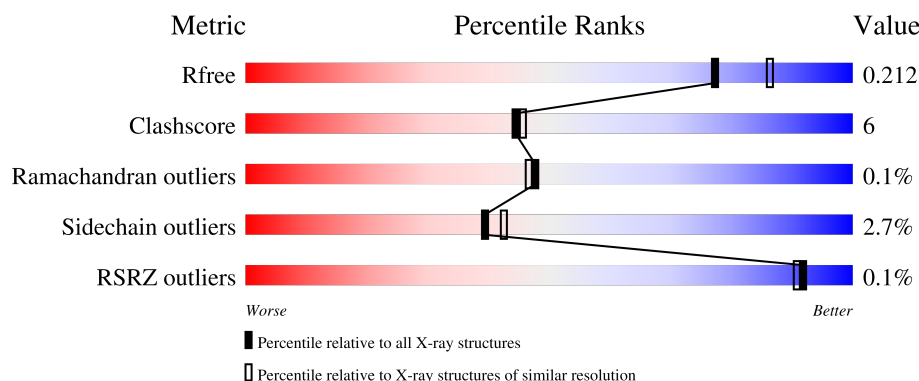
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	453	90% 10%
1	C	453	89% 9% .
2	B	295	74% 11% . 15%
2	D	295	63% 21% . 15%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12142 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.

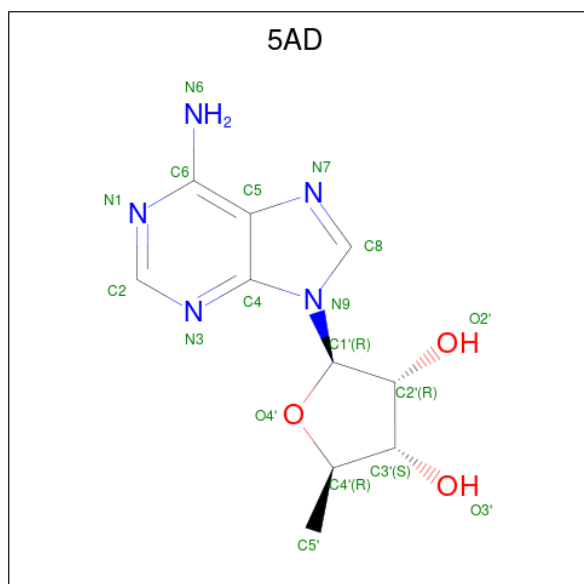
- Molecule 1 is a protein called Ethanolamine ammonia-lyase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	9	0
			3515	2204	604	685	22			
1	C	453	Total	C	N	O	S	0	6	0
			3493	2190	597	684	22			

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

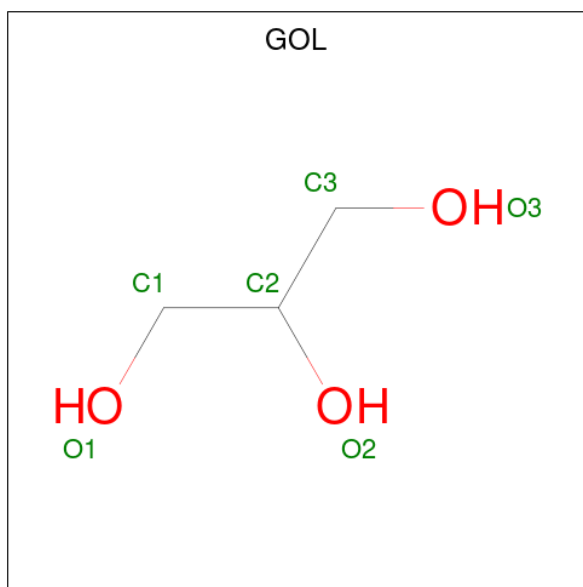
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	2	0
			1927	1204	350	363	10			
2	D	252	Total	C	N	O	S	0	3	0
			1938	1211	354	363	10			

- Molecule 3 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		
3	C	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



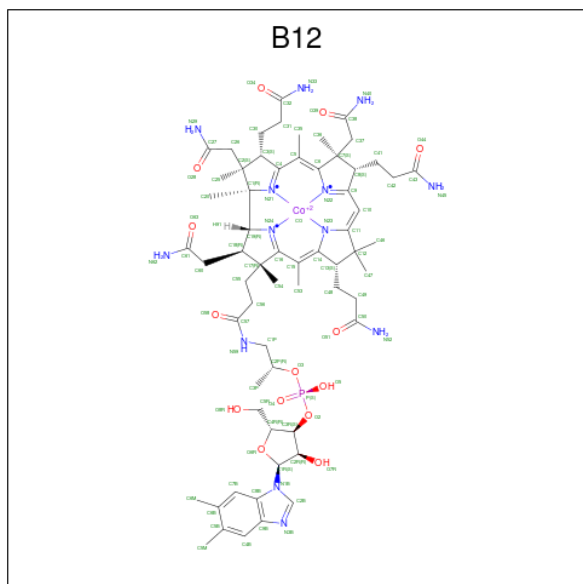
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is COBALAMIN (CCD ID: 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		

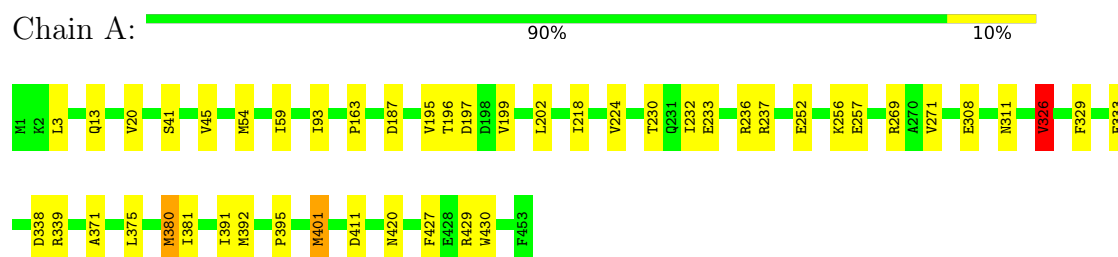
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	400	Total	O	0	0
			400	400		
6	B	135	Total	O	0	0
			135	135		
6	C	370	Total	O	0	0
			370	370		
6	D	80	Total	O	0	0
			80	80		

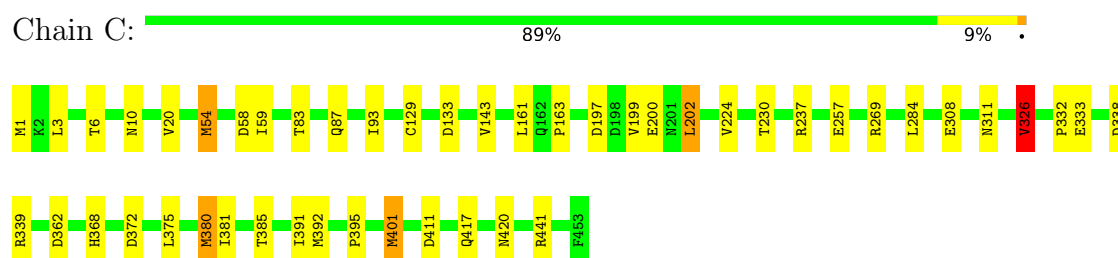
3 Residue-property plots

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.

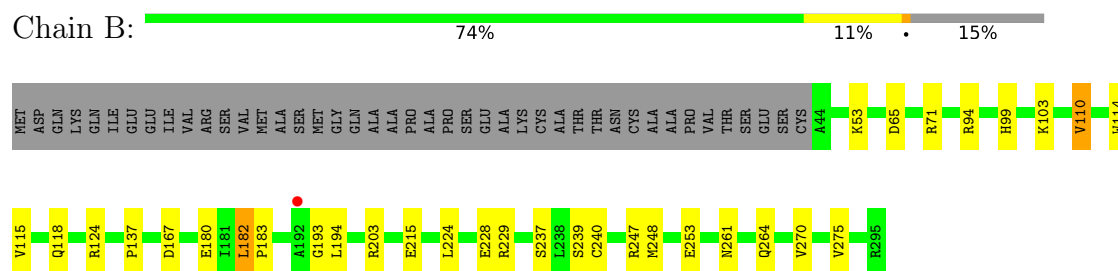
- Molecule 1: Ethanolamine ammonia-lyase heavy chain



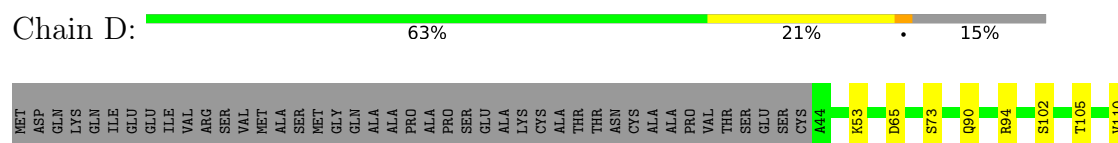
- Molecule 1: Ethanolamine ammonia-lyase heavy chain

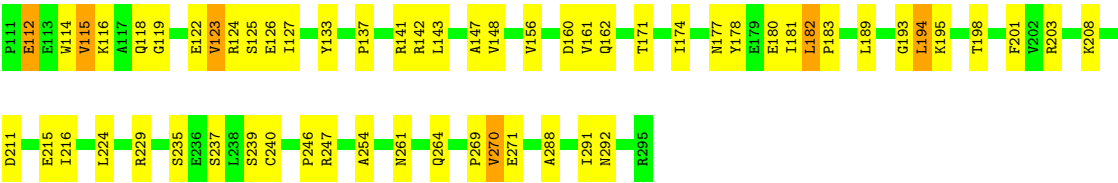


- Molecule 2: Ethanolamine ammonia-lyase light chain



- 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	242.72Å 242.72Å 76.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 2.00 48.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.00-2.00) 99.5 (48.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.163 , 0.192 0.181 , 0.212	Depositor DCC
R_{free} test set	8636 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12142	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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, 5AD, B12

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3596	0.59	0/4868
1	C	0.40	0/3565	0.59	0/4827
2	B	0.36	0/1960	0.59	0/2655
2	D	0.35	0/1974	0.56	0/2673
All	All	0.39	0/11095	0.59	0/15023

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
2	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	VAL	Peptide
2	B	193	GLY	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	3515	0	3497	30	0
1	C	3493	0	3462	32	0
2	B	1927	0	1991	22	0
2	D	1938	0	2007	44	0
3	A	18	0	13	2	0
3	C	18	0	12	0	0
4	A	36	0	48	2	1
4	C	30	0	40	2	0
5	B	91	0	88	7	0
5	D	91	0	88	7	0
6	A	400	0	0	3	0
6	B	135	0	0	2	0
6	C	370	0	0	4	1
6	D	80	0	0	2	0
All	All	12142	0	11246	135	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 6.

All (135) 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)
2:D:110:VAL:O	2:D:203:ARG:NH2	2.04	0.89
2:B:110:VAL:O	2:B:203:ARG:NH2	2.09	0.85
1:C:1:MET:HE3	1:C:3:LEU:HD21	1.60	0.82
2:B:180:GLU:HG2	2:B:270:VAL:HG23	1.66	0.77
1:C:269:ARG:HG2	1:C:284:LEU:HD11	1.71	0.72
1:A:420[A]:ASN:OD1	6:A:601:HOH:O	2.08	0.72
2:D:126:GLU:OE1	2:D:142:ARG:NH1	2.24	0.71
2:D:122:GLU:HG3	2:D:201:PHE:HD2	1.54	0.70
1:A:197:ASP:OD2	1:A:230[A]:THR:HG21	1.96	0.63
1:A:252:GLU:HG2	1:A:256:LYS:HE3	1.81	0.63
1:A:59:ILE:HD12	1:A:93:ILE:HD11	1.83	0.61
2:D:114:TRP:O	2:D:118:GLN:HG2	2.01	0.60
4:A:506:GOL:H11	2:B:103:LYS:HZ1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:TRP:O	2:B:118:GLN:HG2	2.01	0.59
1:A:395:PRO:HD3	6:A:697:HOH:O	2.04	0.58
5:D:601:B12:H552	5:D:601:B12:H531	1.85	0.58
2:D:141:ARG:HD3	2:D:208:LYS:HD2	1.86	0.57
4:A:506:GOL:H11	2:B:103:LYS:NZ	2.18	0.56
1:C:417:GLN:O	4:C:504:GOL:O2	2.23	0.56
5:B:601:B12:H552	5:B:601:B12:H531	1.85	0.56
1:A:329:PHE:CD2	3:A:501:5AD:H8	2.41	0.56
2:D:148:VAL:HG13	2:D:216:ILE:HD13	1.88	0.56
2:D:115:VAL:HG21	2:D:122:GLU:HB2	1.88	0.56
1:A:401:MET:O	1:A:401:MET:HE2	2.06	0.55
2:D:211:ASP:HA	2:D:246:PRO:HB2	1.90	0.54
2:D:122:GLU:HG3	2:D:201:PHE:CD2	2.40	0.53
1:A:326:VAL:HG12	1:A:329:PHE:HB2	1.91	0.53
1:C:326:VAL:HA	1:C:362:ASP:HB3	1.91	0.53
2:D:161:VAL:HG21	2:D:189:LEU:HD13	1.91	0.53
2:D:65:ASP:OD1	2:D:65:ASP:N	2.41	0.52
2:B:65:ASP:OD1	2:B:65:ASP:N	2.42	0.52
1:A:202:LEU:HD22	1:A:224[A]:VAL:HG21	1.92	0.52
1:A:429[A]:ARG:NH1	6:A:604:HOH:O	2.42	0.52
2:B:228:GLU:OE1	2:B:239:SER:HB3	2.10	0.52
2:D:124[A]:ARG:NH1	2:D:125:SER:O	2.40	0.51
2:D:180:GLU:HG2	2:D:270:VAL:HG23	1.91	0.51
1:A:391:ILE:C	1:A:392:MET:HE2	2.35	0.51
2:D:189:LEU:O	2:D:193:GLY:HA3	2.11	0.50
2:D:162:GLN:NE2	2:D:198:THR:O	2.32	0.50
2:D:215:GLU:HG2	2:D:247:ARG:HH11	1.76	0.50
1:C:380:MET:HG2	1:C:381:ILE:N	2.26	0.50
2:D:177:ASN:O	2:D:181:ILE:HG22	2.11	0.50
1:C:20:VAL:HG11	1:C:54:MET:HE2	1.94	0.49
2:B:53:LYS:HG2	2:B:94:ARG:NH1	2.27	0.49
2:B:215:GLU:HG2	2:B:247:ARG:HH11	1.77	0.49
1:C:197:ASP:OD2	1:C:230:THR:HG21	2.13	0.49
2:D:143:LEU:HB3	2:D:147:ALA:HB3	1.95	0.49
1:C:395:PRO:HD3	6:C:632:HOH:O	2.13	0.48
1:A:333:GLU:HG3	2:B:137:PRO:HG3	1.95	0.48
1:A:199:VAL:HG11	1:A:237[B]:ARG:HD3	1.94	0.48
1:C:143:VAL:HG13	4:C:502:GOL:H2	1.96	0.48
1:A:339:ARG:NH1	1:C:338:ASP:OD1	2.44	0.48
1:A:41:SER:O	1:A:45:VAL:HG23	2.14	0.47
1:A:233[A]:GLU:OE2	1:A:237[A]:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:VAL:HB	2:D:171:THR:HG23	1.96	0.47
2:D:122:GLU:CD	2:D:203:ARG:HH11	2.22	0.47
1:A:380:MET:SD	1:A:411:ASP:HB3	2.55	0.47
2:D:182:LEU:HB3	2:D:183:PRO:HD3	1.96	0.47
2:D:116:LYS:O	2:D:119:GLY:N	2.36	0.47
1:A:371:ALA:HB1	1:A:375:LEU:HD23	1.97	0.47
1:C:420[A]:ASN:OD1	6:C:601:HOH:O	2.20	0.47
2:B:215:GLU:OE1	2:B:248:MET:N	2.46	0.46
2:D:127:ILE:HD12	2:D:133:TYR:HA	1.96	0.46
2:D:181:ILE:HB	2:D:269:PRO:HB3	1.97	0.46
1:A:232:ILE:HG23	1:A:271:VAL:HG21	1.98	0.46
1:A:401:MET:HE3	1:A:401:MET:HB2	1.75	0.46
2:D:90:GLN:HG2	6:D:719:HOH:O	2.16	0.46
2:B:71:ARG:HA	2:B:71:ARG:HD2	1.83	0.46
2:D:174:ILE:O	2:D:178:TYR:HB2	2.15	0.46
1:C:391:ILE:C	1:C:392:MET:HE2	2.41	0.45
5:B:601:B12:H363	5:B:601:B12:H421	1.98	0.45
2:B:261:ASN:ND2	6:B:705:HOH:O	2.35	0.45
1:C:257:GLU:OE1	2:D:208:LYS:NZ	2.41	0.45
1:A:308:GLU:O	1:A:311:ASN:HB2	2.16	0.45
1:C:6:THR:HA	1:C:10:ASN:O	2.17	0.45
1:C:332:PRO:HG3	1:C:368:HIS:O	2.17	0.45
5:B:601:B12:H261	5:B:601:B12:H91	1.59	0.45
1:C:380:MET:SD	1:C:411:ASP:HB3	2.56	0.45
2:D:288:ALA:HB1	2:D:292:ASN:HB2	1.98	0.45
1:C:308:GLU:O	1:C:311:ASN:HB2	2.17	0.45
2:D:224:LEU:O	2:D:240:CYS:HA	2.17	0.45
5:D:601:B12:H362	5:D:601:B12:H351	1.98	0.45
5:B:601:B12:H362	5:B:601:B12:H351	1.99	0.44
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.52	0.44
1:C:401:MET:HE2	1:C:401:MET:O	2.17	0.44
2:D:53:LYS:HG2	2:D:94:ARG:NH1	2.33	0.44
2:D:254:ALA:O	2:D:291:ILE:HG23	2.17	0.44
1:C:441:ARG:NH1	6:C:618:HOH:O	2.49	0.44
2:D:102:SER:O	2:D:105:THR:OG1	2.33	0.44
2:D:112:GLU:H	2:D:112:GLU:HG3	1.59	0.44
1:A:338:ASP:OD1	1:C:339:ARG:NH1	2.51	0.43
1:C:202:LEU:HD22	1:C:224[B]:VAL:HG11	2.00	0.43
2:B:124[B]:ARG:HB3	2:B:203:ARG:HB3	1.99	0.43
2:D:160:ASP:HB2	2:D:194:LEU:HD13	2.00	0.43
2:D:271:GLU:HB2	6:D:702:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:601:B12:H261	5:D:601:B12:H91	1.81	0.43
2:D:105:THR:HG21	2:D:235:SER:OG	2.18	0.43
5:B:601:B12:H531	5:B:601:B12:C55	2.49	0.43
2:B:99:HIS:O	2:B:103:LYS:HG2	2.18	0.43
1:C:161:LEU:O	1:C:163:PRO:HD3	2.18	0.42
1:C:199:VAL:HG11	1:C:237:ARG:HD2	2.01	0.42
1:C:401:MET:HE1	5:D:601:B12:H291	1.84	0.42
1:A:257:GLU:CD	2:B:253:GLU:HB2	2.44	0.42
1:A:401:MET:HE2	1:A:401:MET:C	2.44	0.42
2:B:224:LEU:O	2:B:240:CYS:HA	2.19	0.42
2:D:237:SER:OG	2:D:261:ASN:HA	2.18	0.42
2:B:167:ASP:OD1	2:B:167:ASP:N	2.52	0.42
5:D:601:B12:H601	5:D:601:B12:H262	2.02	0.42
1:A:218:ILE:HG12	1:A:430:TRP:CZ2	2.55	0.42
2:B:247:ARG:HD3	2:B:247:ARG:HA	1.82	0.42
2:D:178:TYR:CE1	2:D:182:LEU:HG	2.54	0.42
1:C:83:THR:O	1:C:87:GLN:HG3	2.20	0.42
1:C:129:CYS:HB3	1:C:133:ASP:HB2	2.02	0.42
5:D:601:B12:H412	5:D:601:B12:H363	1.77	0.42
1:A:380:MET:HG2	1:A:381:ILE:N	2.35	0.41
1:A:329:PHE:CG	3:A:501:5AD:H8	2.55	0.41
2:B:182:LEU:HB3	2:B:183:PRO:HD3	2.03	0.41
2:D:122:GLU:OE2	2:D:203:ARG:NH1	2.53	0.41
2:D:123:VAL:CG2	2:D:147:ALA:HA	2.51	0.41
5:B:601:B12:H253	5:B:601:B12:H301	1.64	0.41
1:C:200:GLU:HB2	6:C:764:HOH:O	2.19	0.41
5:D:601:B12:O39	5:D:601:B12:H361	2.20	0.41
1:C:1:MET:HB3	1:C:58:ASP:OD2	2.20	0.41
1:C:381:ILE:O	1:C:385:THR:HG23	2.21	0.41
2:D:125:SER:HB2	2:D:142:ARG:O	2.21	0.41
1:A:232:ILE:O	1:A:236:ARG:HG3	2.21	0.41
1:C:59:ILE:HD12	1:C:93:ILE:HD11	2.03	0.41
1:C:372:ASP:O	1:C:375:LEU:HB3	2.20	0.41
2:D:123:VAL:HG21	2:D:147:ALA:HA	2.03	0.41
1:A:20:VAL:HG11	1:A:54:MET:HE2	2.02	0.41
5:B:601:B12:O39	5:B:601:B12:H361	2.21	0.40
2:D:194:LEU:HB2	2:D:195:LYS:H	1.65	0.40
2:B:71:ARG:NE	6:B:720:HOH:O	2.55	0.40
2:B:237:SER:OG	2:B:261:ASN:HA	2.21	0.40
1:C:333:GLU:HG3	2:D:137:PRO:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:504:GOL:O1	6:C:854:HOH:O[3_655]	2.16	0.04

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	460/453 (102%)	448 (97%)	11 (2%)	1 (0%)	43	42
1	C	457/453 (101%)	443 (97%)	14 (3%)	0	100	100
2	B	252/295 (85%)	248 (98%)	4 (2%)	0	100	100
2	D	253/295 (86%)	244 (96%)	9 (4%)	0	100	100
All	All	1422/1496 (95%)	1383 (97%)	38 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO

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	379/370 (102%)	371 (98%)	8 (2%)	47	52
1	C	376/370 (102%)	371 (99%)	5 (1%)	61	68
2	B	208/240 (87%)	201 (97%)	7 (3%)	32	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	209/240 (87%)	197 (94%)	12 (6%)	18	15
All	All	1172/1220 (96%)	1140 (97%)	32 (3%)	39	42

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	13	GLN
1	A	195	VAL
1	A	196	THR
1	A	269	ARG
1	A	326	VAL
1	A	380	MET
1	A	401	MET
2	B	110	VAL
2	B	115	VAL
2	B	182	LEU
2	B	194	LEU
2	B	229	ARG
2	B	264	GLN
2	B	275	VAL
1	C	54	MET
1	C	202	LEU
1	C	326	VAL
1	C	380	MET
1	C	401	MET
2	D	73	SER
2	D	112	GLU
2	D	115	VAL
2	D	123	VAL
2	D	156	VAL
2	D	182	LEU
2	D	194	LEU
2	D	229	ARG
2	D	239	SER
2	D	264[A]	GLN
2	D	264[B]	GLN
2	D	270	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	C	87	GLN
1	C	171	GLN
2	D	60	ASN
2	D	177	ASN
2	D	261	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	$\# Z > 2$
5	B12	D	601	-	94,101,101	2.13	11 (11%)	149,166,166	1.60	22 (14%)
4	GOL	C	502	-	5,5,5	0.42	0	5,5,5	0.18	0
4	GOL	A	504	-	5,5,5	0.52	0	5,5,5	0.90	0
4	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.27	0
3	5AD	A	501	-	20,20,20	1.60	4 (20%)	28,30,30	2.50	9 (32%)
5	B12	B	601	-	94,101,101	2.09	12 (12%)	149,166,166	1.49	21 (14%)
4	GOL	A	505	-	5,5,5	0.57	0	5,5,5	0.65	0
4	GOL	A	503	-	5,5,5	0.54	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.54	0
4	GOL	C	504	-	5,5,5	0.49	0	5,5,5	0.52	0
3	5AD	C	501	-	20,20,20	1.65	3 (15%)	28,30,30	2.41	9 (32%)
4	GOL	C	506	-	5,5,5	0.55	0	5,5,5	0.72	0
4	GOL	A	507	-	5,5,5	0.47	0	5,5,5	0.29	0
4	GOL	C	505	-	5,5,5	0.52	0	5,5,5	0.35	0
4	GOL	A	502	-	5,5,5	0.41	0	5,5,5	0.44	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
5	B12	D	601	-	-	15/56/223/223	0/3/11/11
4	GOL	C	502	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-
3	5AD	A	501	-	-	2/4/20/20	0/3/3/3
5	B12	B	601	-	-	15/56/223/223	0/3/11/11
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	A	506	-	-	0/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
3	5AD	C	501	-	-	2/4/20/20	0/3/3/3
4	GOL	C	506	-	-	2/4/4/4	-
4	GOL	A	507	-	-	0/4/4/4	-
4	GOL	C	505	-	-	2/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C19-N24	-16.21	1.28	1.49
5	B	601	B12	C19-N24	-15.87	1.28	1.49
5	D	601	B12	C8B-C9B	6.08	1.50	1.40
5	B	601	B12	C8B-C9B	5.72	1.49	1.40
3	C	501	5AD	C5-C4	5.23	1.48	1.39
3	A	501	5AD	C5-C4	5.06	1.48	1.39
5	D	601	B12	C11-N23	4.24	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	B12	C11-N23	4.04	1.44	1.36
5	B	601	B12	C14-N23	-3.91	1.30	1.35
5	D	601	B12	C16-C15	-3.48	1.34	1.44
5	B	601	B12	C6B-C5B	3.47	1.49	1.40
5	D	601	B12	C6B-C5B	3.45	1.49	1.40
5	D	601	B12	C14-N23	-3.36	1.30	1.35
5	B	601	B12	C16-C15	-3.14	1.35	1.44
5	D	601	B12	C10-C9	2.94	1.47	1.39
5	B	601	B12	C14-C15	2.81	1.50	1.38
5	D	601	B12	C14-C15	2.76	1.50	1.38
3	C	501	5AD	C5-C6	2.56	1.48	1.41
5	D	601	B12	C9B-N3B	-2.54	1.35	1.39
5	B	601	B12	C10-C9	2.52	1.46	1.39
3	C	501	5AD	C8-N7	2.49	1.36	1.31
5	B	601	B12	C8B-N1B	-2.46	1.34	1.39
3	A	501	5AD	C5-C6	2.45	1.47	1.41
5	D	601	B12	C8B-N1B	-2.44	1.34	1.39
3	A	501	5AD	C8-N7	2.40	1.36	1.31
5	B	601	B12	C1-C2	-2.21	1.53	1.58
5	B	601	B12	C9B-N3B	-2.12	1.35	1.39
3	A	501	5AD	C5-N7	-2.04	1.35	1.39
5	B	601	B12	CO-N22	-2.04	1.86	1.96
5	D	601	B12	CO-N22	-2.02	1.86	1.96

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	5AD	C5-C4-N3	-6.60	117.62	126.72
5	D	601	B12	C8B-C9B-N3B	-6.36	103.12	110.00
3	C	501	5AD	C5-C4-N3	-6.23	118.13	126.72
5	D	601	B12	C9B-C8B-N1B	6.16	108.03	105.30
5	B	601	B12	C8B-C9B-N3B	-5.97	103.55	110.00
5	D	601	B12	C18-C19-N24	5.95	111.27	102.33
3	A	501	5AD	C5'-C4'-C3'	-5.44	109.98	115.70
3	A	501	5AD	N3-C4-N9	5.44	136.42	127.17
3	C	501	5AD	N3-C4-N9	5.34	136.24	127.17
5	B	601	B12	C18-C19-N24	5.34	110.35	102.33
5	B	601	B12	C9B-C8B-N1B	4.97	107.51	105.30
5	D	601	B12	C9B-N3B-C2B	4.88	110.39	104.40
5	B	601	B12	C9B-N3B-C2B	4.46	109.87	104.40
5	B	601	B12	C4B-C9B-N3B	4.17	137.52	130.51
5	D	601	B12	C13-C14-N23	4.11	114.66	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	5AD	C5'-C4'-C3'	-4.05	111.44	115.70
5	B	601	B12	C20-C1-C19	-3.97	105.53	109.35
3	A	501	5AD	C2-N3-C4	3.87	121.28	111.83
5	D	601	B12	C4B-C9B-N3B	3.80	136.90	130.51
3	C	501	5AD	C2-N3-C4	3.75	120.99	111.83
5	B	601	B12	C7-C8-C9	3.36	105.15	100.89
5	B	601	B12	C13-C14-N23	3.29	113.55	109.09
3	C	501	5AD	C4-C5-N7	-3.26	106.85	110.58
3	A	501	5AD	N3-C2-N1	-3.22	123.71	128.58
3	A	501	5AD	C4-C5-N7	-3.17	106.95	110.58
5	D	601	B12	C13-C14-C15	-3.10	119.60	124.32
5	D	601	B12	C20-C1-N21	3.10	115.38	110.26
5	D	601	B12	C20-C1-C19	-3.06	106.41	109.35
3	C	501	5AD	N3-C2-N1	-3.03	123.99	128.58
5	D	601	B12	C7-C8-C9	3.01	104.71	100.89
3	C	501	5AD	C4-N9-C8	2.91	108.79	105.74
5	B	601	B12	C13-C14-C15	-2.88	119.94	124.32
5	B	601	B12	C26-C2-C3	2.85	112.40	107.42
5	B	601	B12	C19-C1-N21	2.82	105.05	102.14
5	B	601	B12	C30-C3-C2	-2.75	112.93	119.00
3	C	501	5AD	C5-N7-C8	2.68	107.67	103.45
5	D	601	B12	C17-C16-C15	2.61	130.40	126.26
5	B	601	B12	C17-C16-C15	2.58	130.35	126.26
5	D	601	B12	C41-C8-C7	-2.52	107.25	114.19
5	D	601	B12	C54-C17-C18	-2.50	109.41	112.99
3	A	501	5AD	C5-N7-C8	2.42	107.25	103.45
5	B	601	B12	C19-N24-C16	2.40	109.91	107.29
5	D	601	B12	O6R-C4R-C5R	2.40	114.28	109.22
5	B	601	B12	C8-C9-N22	2.38	115.46	110.77
5	B	601	B12	C2R-C1R-N1B	2.36	119.17	113.30
5	D	601	B12	C9-C10-C11	-2.35	122.60	125.97
5	B	601	B12	C9-C10-C11	-2.31	122.67	125.97
5	D	601	B12	C2-C26-C27	-2.29	108.83	115.19
5	D	601	B12	C30-C3-C2	-2.28	113.96	119.00
5	D	601	B12	C19-N24-C16	2.27	109.77	107.29
5	D	601	B12	C19-C1-N21	2.25	104.46	102.14
5	D	601	B12	C2P-C1P-N59	-2.11	109.81	112.92
5	B	601	B12	C8-C9-C10	-2.09	118.88	123.33
5	B	601	B12	C3R-C2R-C1R	2.08	104.47	99.89
5	B	601	B12	C2-C26-C27	-2.07	109.43	115.19
5	D	601	B12	C48-C13-C14	2.07	113.64	108.51
3	A	501	5AD	C4-N9-C8	2.05	107.89	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	B12	C3P-C2P-C1P	-2.04	107.49	111.42
5	D	601	B12	N1B-C2B-N3B	-2.02	111.06	113.94
3	C	501	5AD	N9-C8-N7	-2.02	111.07	113.94
3	A	501	5AD	C2'-C1'-N9	-2.02	108.29	113.30

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-C3
4	C	504	GOL	O1-C1-C2-C3
4	C	505	GOL	C1-C2-C3-O3
5	B	601	B12	C1-C2-C26-C27
5	B	601	B12	C25-C2-C26-C27
5	B	601	B12	C3-C2-C26-C27
5	B	601	B12	C13-C48-C49-C50
5	B	601	B12	C2P-O3-P-O5
5	B	601	B12	C2P-O3-P-O2
5	B	601	B12	O6R-C1R-N1B-C8B
5	D	601	B12	C2P-O3-P-O5
5	D	601	B12	C2R-C1R-N1B-C8B
5	D	601	B12	O6R-C1R-N1B-C8B
5	D	601	B12	C13-C48-C49-C50
4	C	504	GOL	O1-C1-C2-O2
5	D	601	B12	C4-C3-C30-C31
5	B	601	B12	C2-C3-C30-C31
5	D	601	B12	C2-C3-C30-C31
5	B	601	B12	C4-C3-C30-C31
4	A	505	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
4	C	506	GOL	C1-C2-C3-O3
5	B	601	B12	C2R-C1R-N1B-C8B
4	A	503	GOL	O1-C1-C2-O2
4	A	505	GOL	O2-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
5	D	601	B12	C38-C37-C7-C36
5	B	601	B12	C38-C37-C7-C36
5	B	601	B12	C2P-O3-P-O4
5	D	601	B12	C2P-O3-P-O4
5	B	601	B12	C38-C37-C7-C8
5	D	601	B12	C38-C37-C7-C8
5	D	601	B12	C1-C2-C26-C27

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Mol	Chain	Res	Type	Atoms
4	C	505	GOL	O2-C2-C3-O3
4	C	506	GOL	O2-C2-C3-O3
5	B	601	B12	C1P-C2P-O3-P
5	D	601	B12	C25-C2-C26-C27
3	A	501	5AD	C2'-C1'-N9-C8
5	B	601	B12	C3R-O2-P-O5
5	D	601	B12	C3R-O2-P-O4
5	D	601	B12	C3R-O2-P-O5
5	D	601	B12	C3-C2-C26-C27
3	A	501	5AD	C2'-C1'-N9-C4
3	C	501	5AD	C2'-C1'-N9-C4
5	D	601	B12	C1P-C2P-O3-P
3	C	501	5AD	C2'-C1'-N9-C8

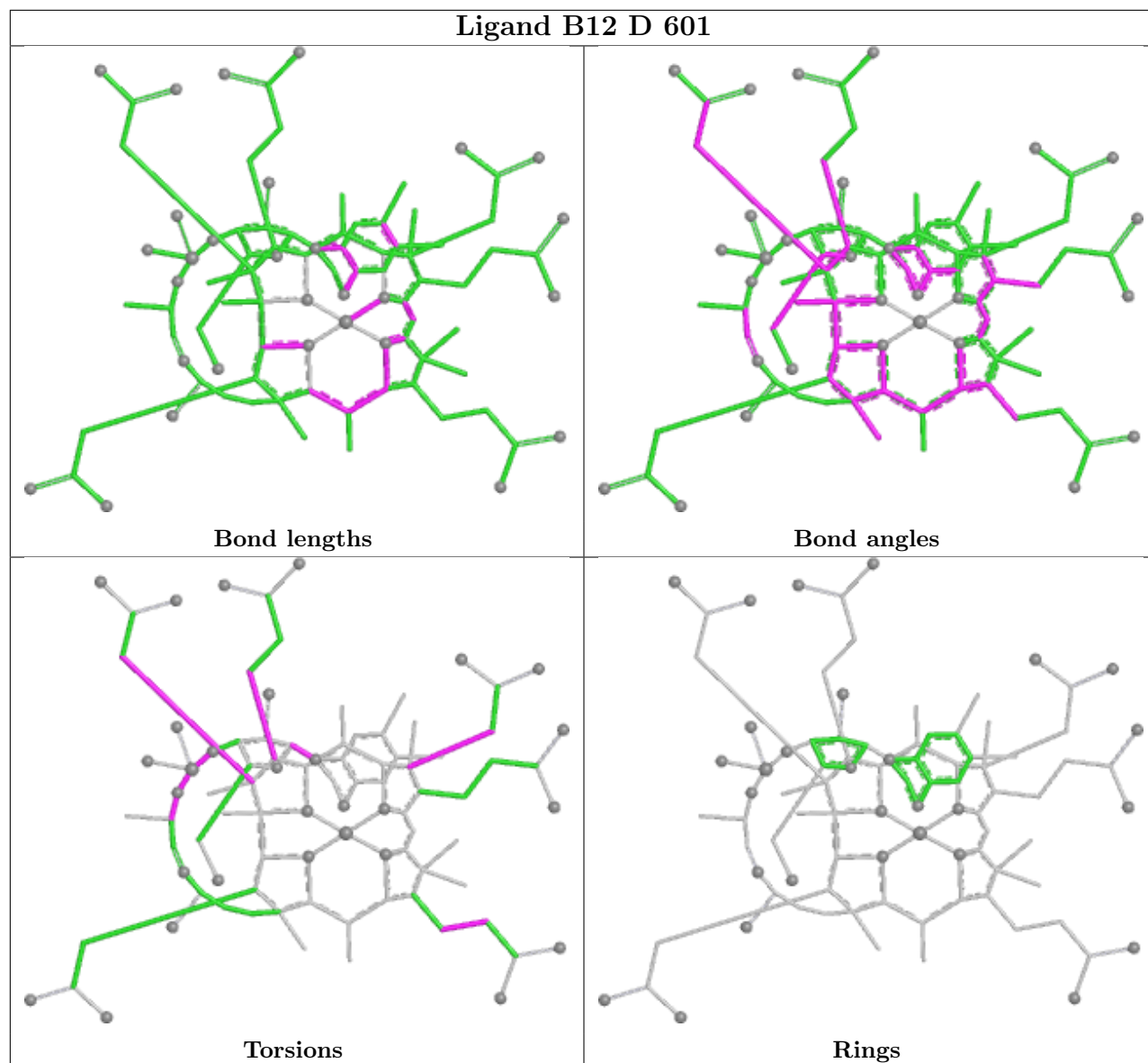
There are no ring outliers.

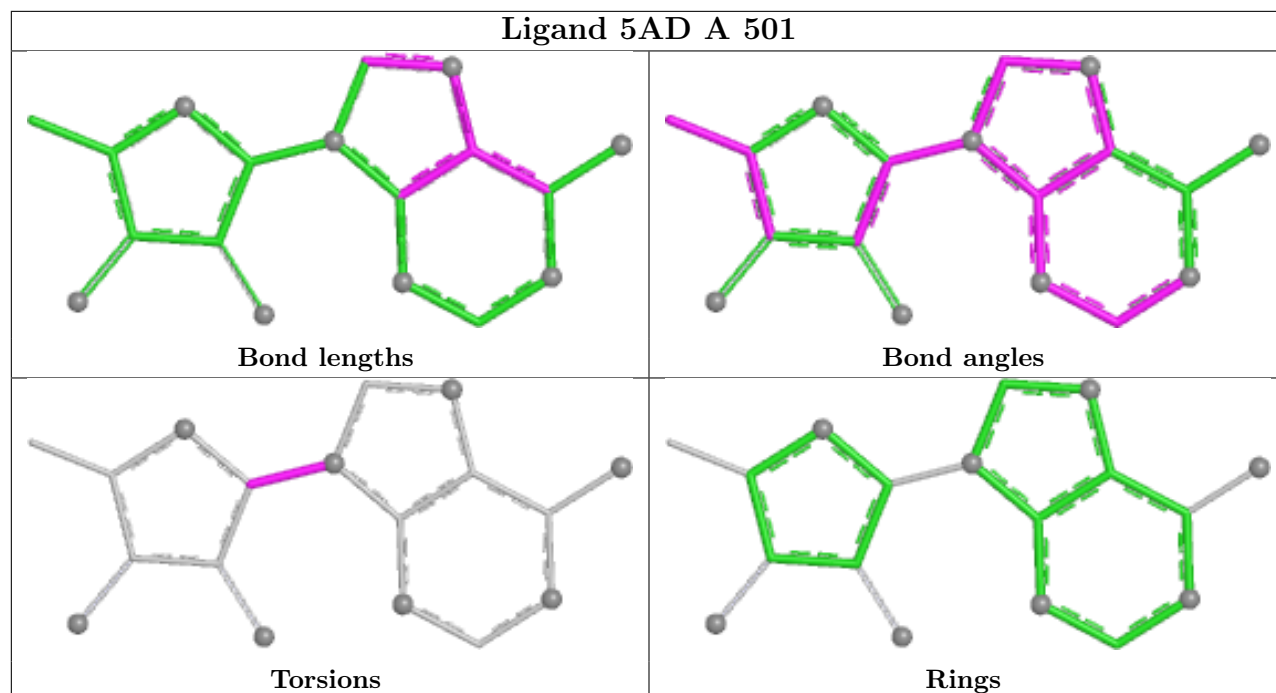
7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	601	B12	7	0
4	C	502	GOL	1	0
4	A	504	GOL	0	1
3	A	501	5AD	2	0
5	B	601	B12	7	0
4	A	506	GOL	2	0
4	C	504	GOL	1	0

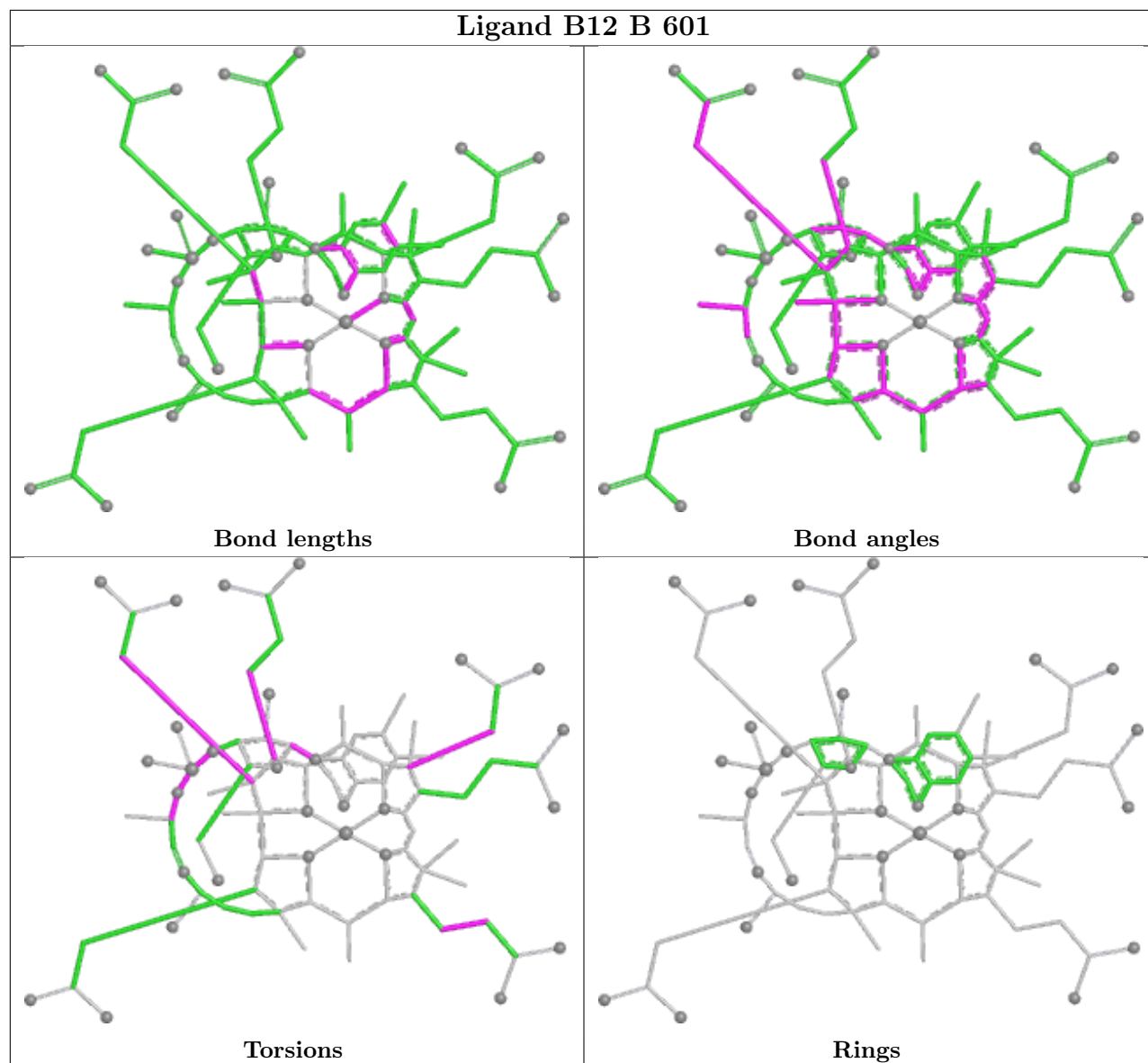
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

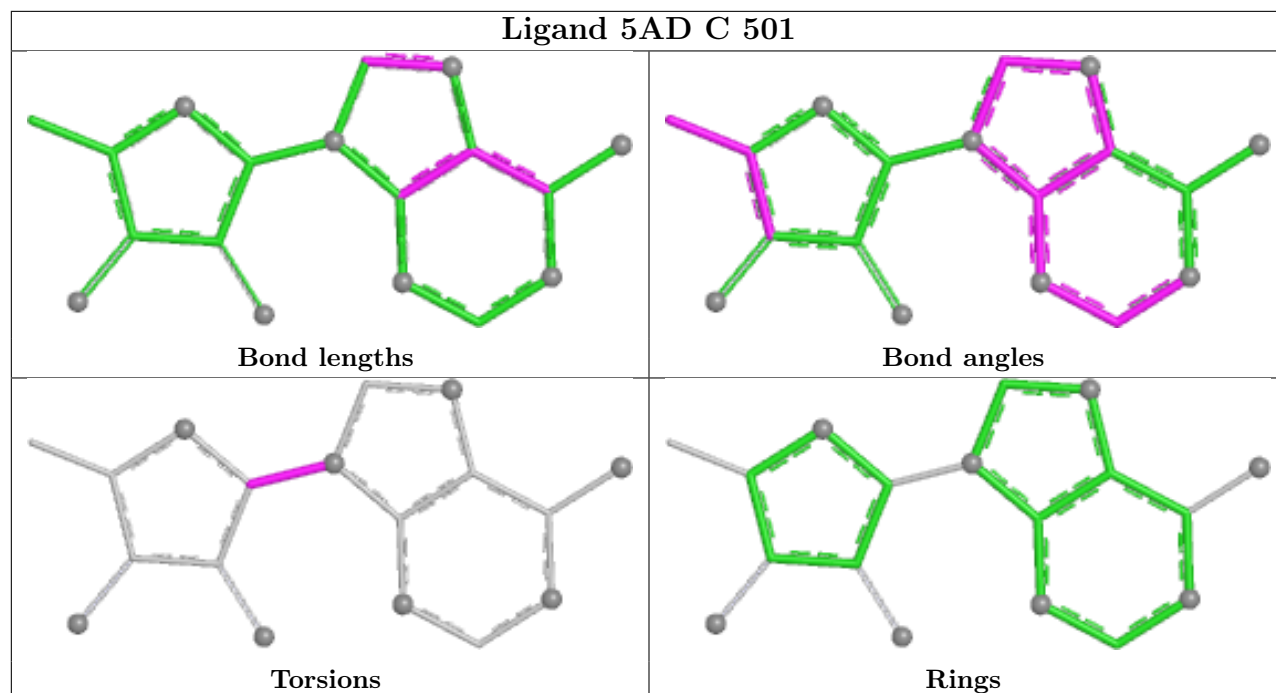
Ligand B12 D 601





Ligand B12 B 601





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	453/453 (100%)	-1.78	0	100 100	10, 22, 37, 61	9 (1%)
1	C	453/453 (100%)	-1.77	0	100 100	9, 24, 41, 60	6 (1%)
2	B	252/295 (85%)	-1.36	1 (0%)	88 88	17, 44, 65, 96	2 (0%)
2	D	252/295 (85%)	-1.13	0	100 100	15, 52, 87, 122	3 (1%)
All	All	1410/1496 (94%)	-1.58	1 (0%)	92 91	9, 28, 69, 122	20 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	192	ALA	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
3	5AD	A	501	18/18	0.99	0.03	27,29,33,34	0

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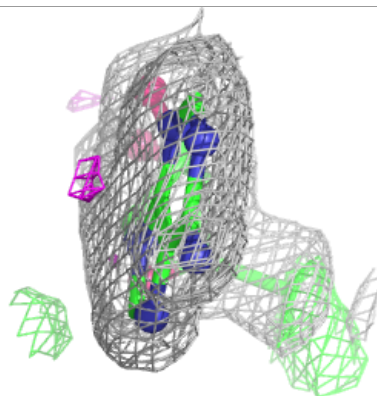
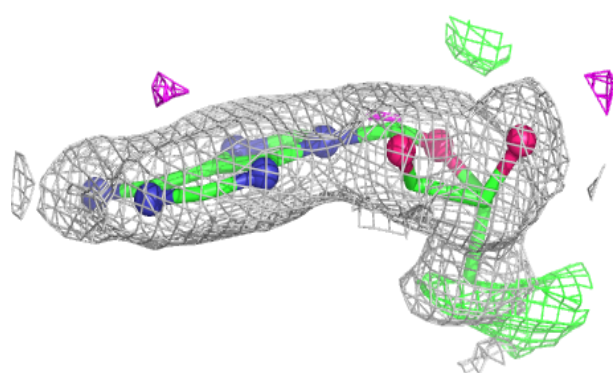
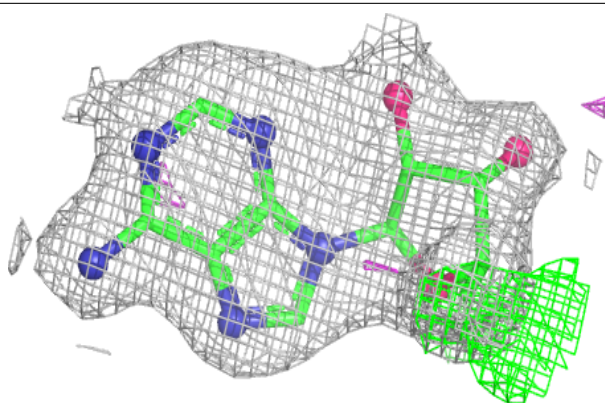
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	503	6/6	0.99	0.05	27,41,49,54	0
4	GOL	A	504	6/6	0.99	0.05	44,49,50,52	0
4	GOL	A	506	6/6	0.99	0.07	76,77,78,79	0
4	GOL	A	507	6/6	0.99	0.06	62,69,70,71	0
4	GOL	C	504	6/6	0.99	0.07	69,71,71,73	0
4	GOL	C	505	6/6	0.99	0.04	39,43,46,48	0
4	GOL	A	502	6/6	1.00	0.03	25,28,30,31	0
4	GOL	C	502	6/6	1.00	0.03	37,43,46,50	0
4	GOL	C	503	6/6	1.00	0.04	28,31,35,37	0
4	GOL	A	505	6/6	1.00	0.03	26,27,29,29	0
3	5AD	C	501	18/18	1.00	0.03	29,32,39,40	0
4	GOL	C	506	6/6	1.00	0.03	23,30,32,32	0
5	B12	B	601	91/91	1.00	0.02	21,28,35,38	0
5	B12	D	601	91/91	1.00	0.02	30,38,44,54	0

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

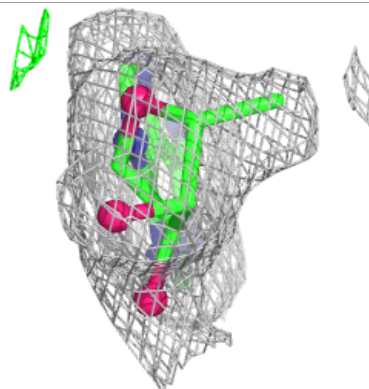
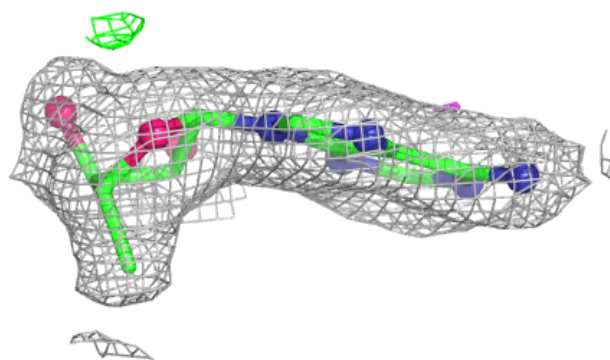
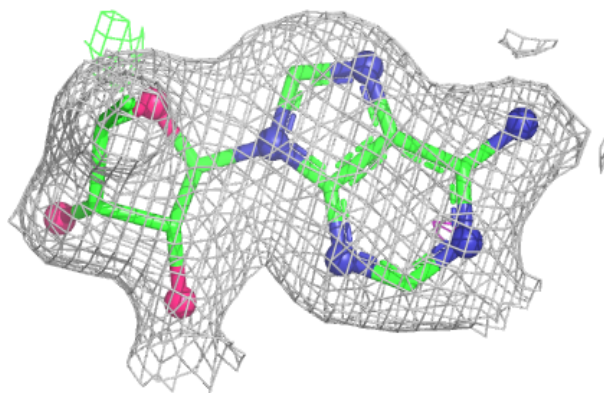
Electron density around 5AD A 501:

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



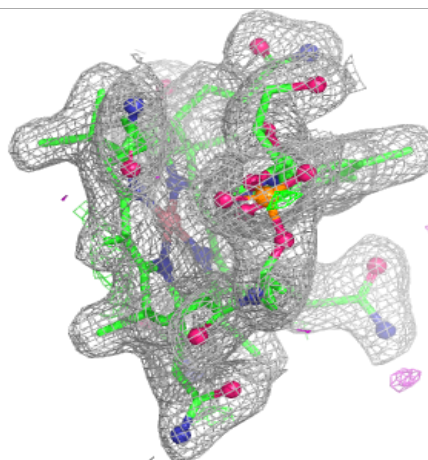
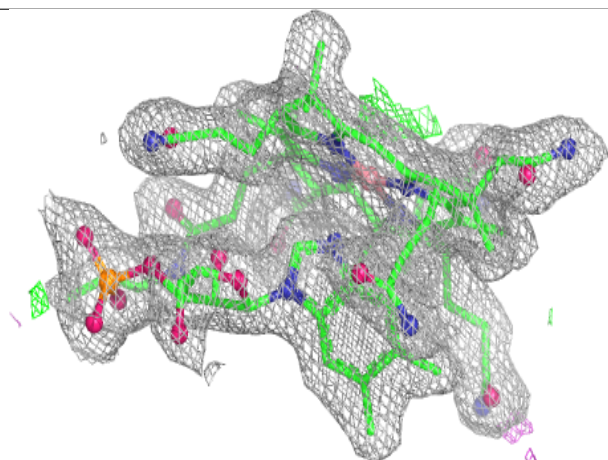
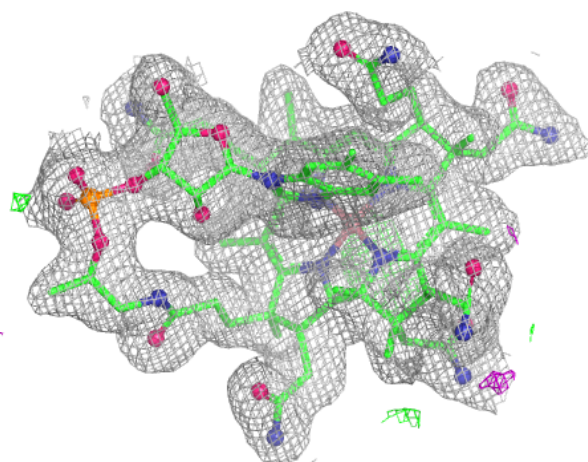
Electron density around 5AD C 501:

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



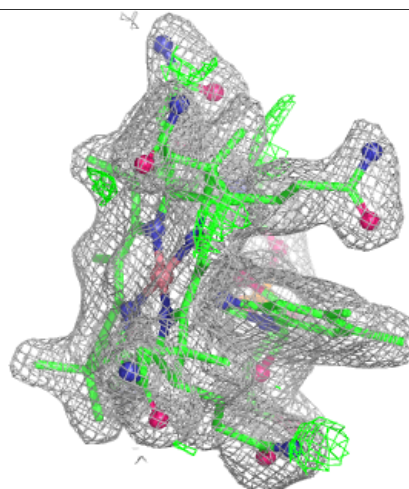
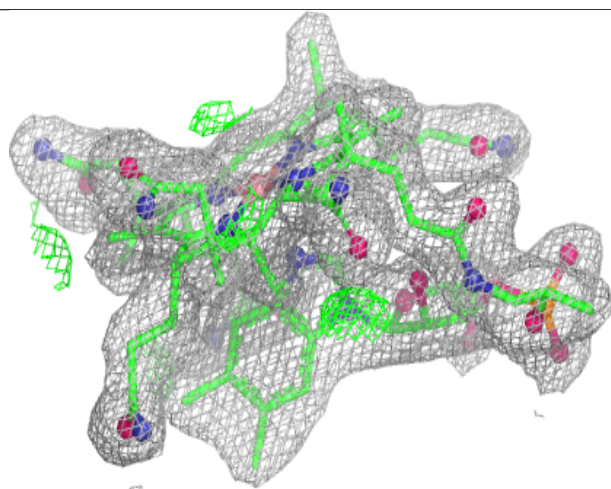
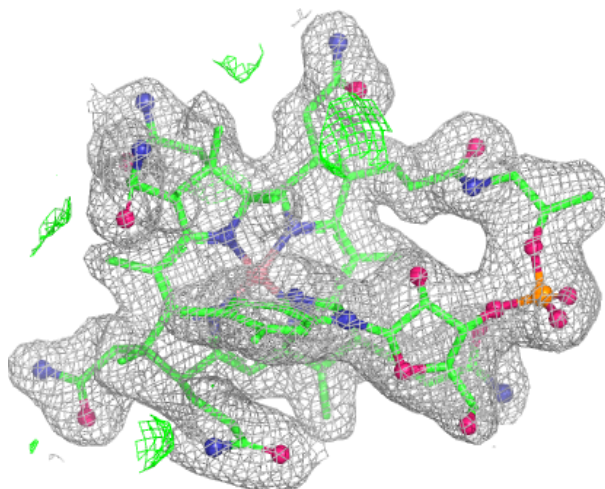
Electron density around B12 B 601:

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



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.