



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:21 am BST

PDB ID : 5YSN  
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](mailto: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.

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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

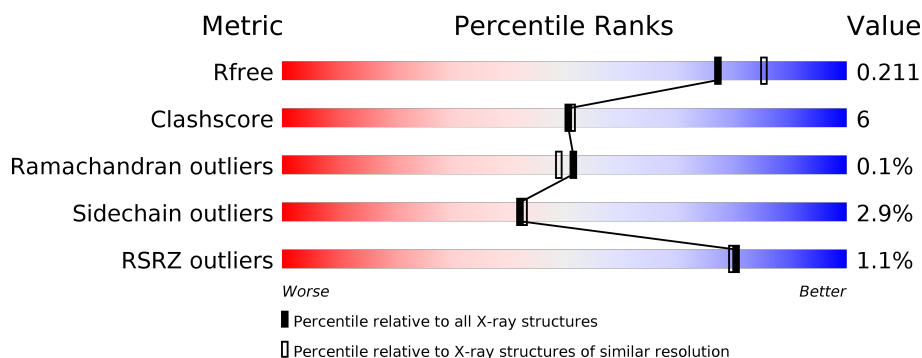
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>
1	C	453	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>
2	B	295	<div> <div style="width: 4%;"></div> <div style="width: 75%;"></div> <div style="width: 9%;"></div> <div style="width: 15%;"></div> </div> <div>% 75% 9% 15%</div>
2	D	295	<div> <div style="width: 4%;"></div> <div style="width: 63%;"></div> <div style="width: 21%;"></div> <div style="width: 15%;"></div> </div> <div>4% 63% 21% 15%</div>

## 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.

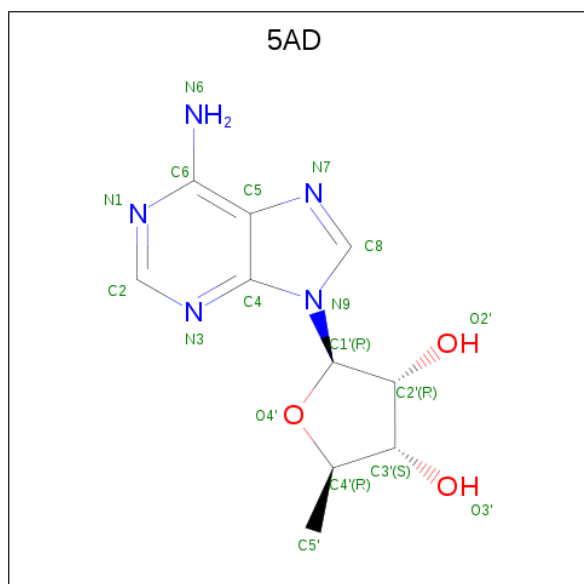
- Molecule 1 is a protein called Ethanolamine ammonia-lyase heavy chain.

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 (three-letter code: 5AD) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



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 (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



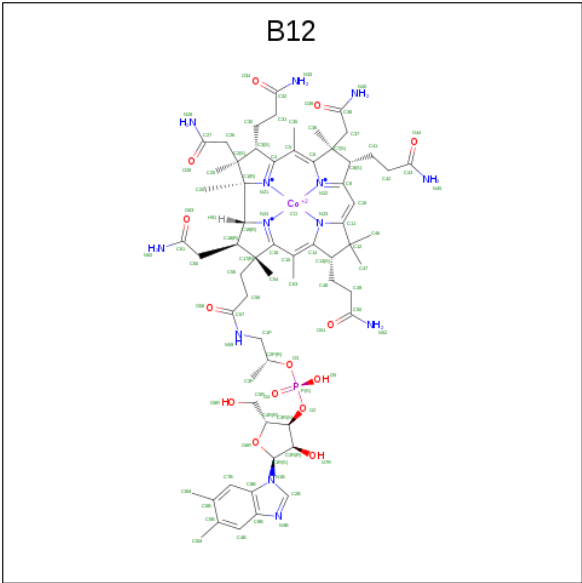
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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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 (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>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		

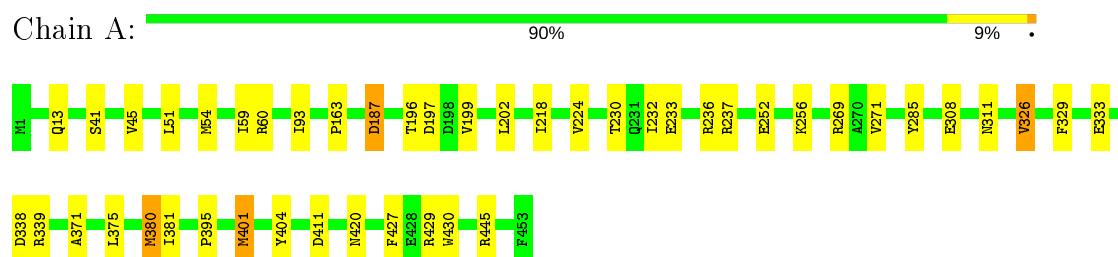
- Molecule 6 is water.

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		

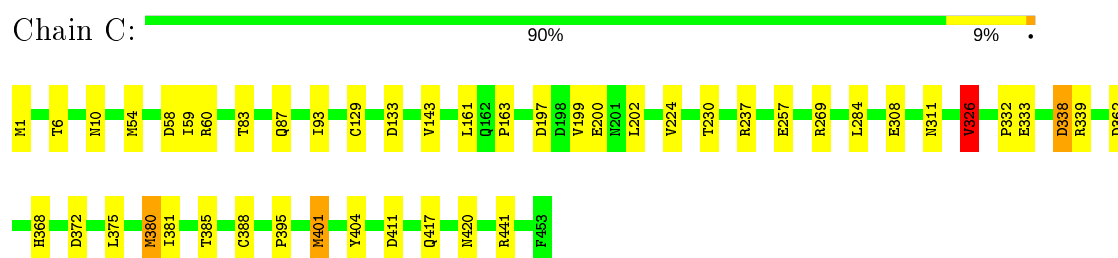
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

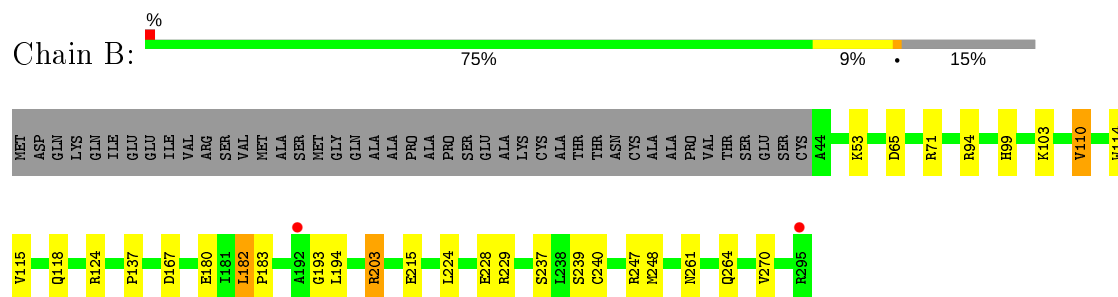
#### • Molecule 1: Ethanolamine ammonia-lyase heavy chain



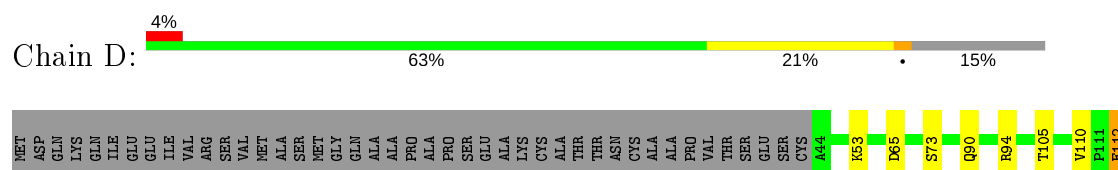
#### • Molecule 1: Ethanolamine ammonia-lyase heavy chain

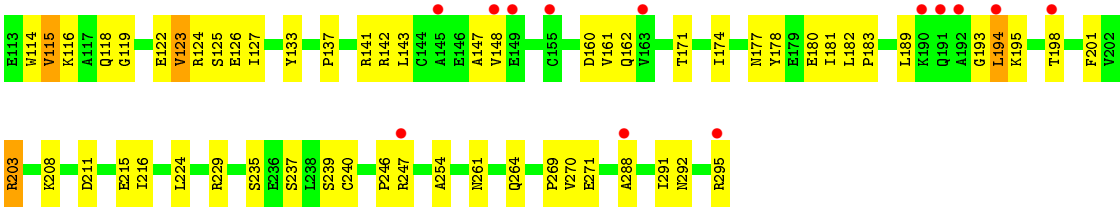


#### • Molecule 2: Ethanolamine ammonia-lyase light chain



#### • 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, $\alpha$ , $\beta$ , $\gamma$	242.72Å 242.72Å 76.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 2.00 48.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.00-2.00) 99.5 (48.22-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.163 , 0.192 0.180 , 0.211	Depositor DCC
$R_{free}$ test set	8636 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 5AD

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	0.46	0/3596	0.62	1/4868 (0.0%)
1	C	0.46	1/3565 (0.0%)	0.60	0/4827
2	B	0.41	0/1960	0.61	0/2655
2	D	0.41	0/1974	0.58	0/2673
All	All	0.44	1/11095 (0.0%)	0.60	1/15023 (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
1	C	0	1
2	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	388	CYS	CB-SG	-5.08	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASP	CB-CG-OD1	5.19	122.97	118.30

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	27	0
1	C	3493	0	3462	28	0
2	B	1927	0	1991	22	0
2	D	1938	0	2007	43	0
3	A	18	0	13	2	0
3	C	18	0	12	0	0
4	A	36	0	48	3	1
4	C	30	0	40	2	0
5	B	91	0	88	7	0
5	D	91	0	88	6	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	128	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 (128) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H531	5:D:601:B12:H552	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:HE2	1:A:401:MET:O	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:N	2:B:65:ASP:OD1	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
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
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
4:A:506:GOL:H11	2:B:103:LYS:HZ1	1.78	0.48
1:C:143:VAL:HG13	4:C:502:GOL:H2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:110:VAL:HB	2:D:171:THR:HG23	1.96	0.47
2:D:182:LEU:HB3	2:D:183:PRO:HD3	1.96	0.47
1:A:380:MET:SD	1:A:411:ASP:HB3	2.55	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:401:MET:HE3	1:C:401:MET:HB2	1.52	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:HB2	1:A:401:MET:HE3	1.75	0.46
2:D:90:GLN:HG2	6:D:719:HOH:O	2.16	0.46
2:B:71:ARG:HD2	2:B:71:ARG:HA	1.83	0.46
2:D:174:ILE:O	2:D:178:TYR:HB2	2.15	0.46
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
4:A:506:GOL:H31	2:B:103:LYS:HZ1	1.81	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:H351	5:B:601:B12:H362	1.99	0.44
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.52	0.44
2:D:53:LYS:HG2	2:D:94:ARG:NH1	2.33	0.44
1:C:257:GLU:OE1	2:D:208:LYS:NZ	2.41	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:112:GLU:H	2:D:112:GLU:HG3	1.59	0.44
1:C:202:LEU:HD22	1:C:224[B]:VAL:HG11	2.00	0.43
1:A:338:ASP:OD1	1:C:339:ARG:NH1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:GLU:HB2	6:D:702:HOH:O	2.18	0.43
5:D:601:B12:H91	5:D:601:B12:H261	1.81	0.43
2:D:105:THR:HG21	2:D:235:SER:OG	2.18	0.43
5:B:601:B12:C55	5:B:601:B12:H531	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
2:D:122:GLU:CD	2:D:203:ARG:HH11	2.22	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:N	2:B:167:ASP:OD1	2.52	0.42
5:D:601:B12:H262	5:D:601:B12:H601	2.02	0.42
1:A:218:ILE:HG12	1:A:430:TRP:CZ2	2.55	0.42
2:B:247:ARG:HA	2:B:247:ARG:HD3	1.82	0.42
2:D:178:TYR:CE1	2:D:182:LEU:HG	2.54	0.42
1:C:129:CYS:HB3	1:C:133:ASP:HB2	2.02	0.42
1:C:83:THR:O	1:C:87:GLN:HG3	2.20	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:381:ILE:O	1:C:385:THR:HG23	2.21	0.41
1:C:1:MET:HB3	1:C:58:ASP:OD2	2.20	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
2:D:123:VAL:HG21	2:D:147:ALA:HA	2.03	0.41
1:C:372:ASP:O	1:C:375:LEU:HB3	2.20	0.41
5:B:601:B12:H361	5:B:601:B12:O39	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
1:A:51:LEU:HA	1:A:54:MET:HE2	2.03	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 symmetry 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%)	47	44
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%)	51	49

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%)	370 (98%)	9 (2%)	49	51
1	C	376/370 (102%)	369 (98%)	7 (2%)	57	61
2	B	208/240 (87%)	201 (97%)	7 (3%)	37	36
2	D	209/240 (87%)	198 (95%)	11 (5%)	22	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1172/1220 (96%)	1138 (97%)	34 (3%)	42	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	60	ARG
1	A	196	THR
1	A	269	ARG
1	A	285	TYR
1	A	380	MET
1	A	401	MET
1	A	404	TYR
1	A	445	ARG
2	B	110	VAL
2	B	115	VAL
2	B	182	LEU
2	B	194	LEU
2	B	203	ARG
2	B	229	ARG
2	B	264	GLN
1	C	54	MET
1	C	60	ARG
1	C	326	VAL
1	C	338	ASP
1	C	380	MET
1	C	401	MET
1	C	404	TYR
2	D	73	SER
2	D	112	GLU
2	D	115	VAL
2	D	123	VAL
2	D	194	LEU
2	D	203	ARG
2	D	229	ARG
2	D	239	SER
2	D	264[A]	GLN
2	D	264[B]	GLN
2	D	295	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
2	B	154	GLN
1	C	171	GLN

### 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](#)

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	-	80,101,101	1.23	7 (8%)	101,166,166	1.33	18 (17%)
4	GOL	C	504	-	5,5,5	0.47	0	5,5,5	0.50	0
4	GOL	A	504	-	5,5,5	0.49	0	5,5,5	0.87	0
3	5AD	C	501	-	17,20,20	1.28	3 (17%)	15,30,30	1.77	3 (20%)
4	GOL	C	505	-	5,5,5	0.49	0	5,5,5	0.35	0
4	GOL	A	502	-	5,5,5	0.41	0	5,5,5	0.39	0
4	GOL	A	505	-	5,5,5	0.56	0	5,5,5	0.60	0
4	GOL	C	502	-	5,5,5	0.41	0	5,5,5	0.16	0
4	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.51	0
4	GOL	C	506	-	5,5,5	0.53	0	5,5,5	0.67	0
5	B12	B	601	-	80,101,101	1.24	8 (10%)	101,166,166	1.34	20 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	503	-	5,5,5	0.53	0	5,5,5	0.57	0
4	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	A	507	-	5,5,5	0.45	0	5,5,5	0.30	0
3	5AD	A	501	-	17,20,20	1.20	2 (11%)	15,30,30	2.01	4 (26%)

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	-	-	15/51/223/223	0/3/11/11
4	GOL	C	504	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
3	5AD	C	501	-	-	0/0/20/20	0/3/3/3
4	GOL	C	505	-	-	2/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-
4	GOL	A	506	-	-	0/4/4/4	-
4	GOL	C	506	-	-	2/4/4/4	-
5	B12	B	601	-	-	13/51/223/223	0/3/11/11
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-
4	GOL	A	507	-	-	0/4/4/4	-
3	5AD	A	501	-	-	0/0/20/20	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	B12	C11-C10	-4.75	1.32	1.40
5	D	601	B12	C8B-C9B	4.74	1.50	1.40
5	B	601	B12	C8B-C9B	4.46	1.49	1.40
5	D	601	B12	C11-C10	-4.37	1.33	1.40
5	B	601	B12	C6B-C5B	3.37	1.49	1.40
5	D	601	B12	C6B-C5B	3.35	1.49	1.40
5	B	601	B12	C2-C3	-3.01	1.53	1.58
5	D	601	B12	C2-C3	-2.90	1.53	1.58
3	C	501	5AD	C5-C4	2.83	1.48	1.40
3	C	501	5AD	O4'-C1'	2.75	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	B12	C14-C15	2.74	1.50	1.40
3	A	501	5AD	C5-C4	2.72	1.48	1.40
5	D	601	B12	C14-C15	2.69	1.50	1.40
5	D	601	B12	CO-N21	-2.49	1.82	1.89
5	B	601	B12	CO-N21	-2.40	1.83	1.89
3	A	501	5AD	O4'-C1'	2.30	1.44	1.41
5	B	601	B12	C1-C2	-2.19	1.53	1.58
5	D	601	B12	O6R-C1R	2.12	1.44	1.41
5	B	601	B12	CO-N23	-2.09	1.84	1.94
3	C	501	5AD	C2-N3	2.07	1.35	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	5AD	C5'-C4'-C3'	-5.44	109.98	115.70
3	C	501	5AD	C5'-C4'-C3'	-4.05	111.44	115.70
5	B	601	B12	C20-C1-C19	-3.97	105.53	109.36
5	B	601	B12	C8-C9-N22	3.47	115.46	111.12
5	B	601	B12	C6-C5-C4	-3.39	118.98	124.27
5	D	601	B12	C6-C5-C4	-3.37	119.01	124.27
5	D	601	B12	C13-C14-C15	-3.33	119.60	131.68
5	B	601	B12	C13-C14-C15	-3.24	119.94	131.68
3	A	501	5AD	N3-C2-N1	-3.18	123.71	128.68
5	D	601	B12	C20-C1-C19	-3.06	106.41	109.36
5	B	601	B12	C25-C2-C3	-3.04	110.94	115.58
3	C	501	5AD	N3-C2-N1	-3.00	123.99	128.68
5	B	601	B12	C30-C3-C2	-2.92	112.93	119.13
5	B	601	B12	C19-C1-N21	2.82	105.05	102.16
5	D	601	B12	C25-C2-C3	-2.81	111.29	115.58
5	B	601	B12	C16-C15-C14	-2.72	120.03	124.27
5	B	601	B12	C26-C2-C3	2.68	112.40	107.47
5	D	601	B12	C3-C4-C5	-2.57	122.36	131.68
5	D	601	B12	C55-C17-C16	2.54	118.40	109.92
5	D	601	B12	C41-C8-C7	-2.53	107.25	114.08
5	B	601	B12	C4B-C9B-N3B	2.48	137.52	130.88
3	C	501	5AD	C4-C5-N7	-2.45	106.85	109.40
5	D	601	B12	C30-C3-C2	-2.44	113.96	119.13
5	D	601	B12	C54-C17-C18	-2.42	109.41	112.98
5	B	601	B12	C3-C4-C5	-2.40	122.99	131.68
5	D	601	B12	C9-C10-C11	-2.38	122.60	130.91
5	B	601	B12	C9-C10-C11	-2.36	122.67	130.91
3	A	501	5AD	C4-C5-N7	-2.35	106.95	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	B12	O6R-C4R-C5R	2.35	114.28	109.21
5	D	601	B12	C2-C26-C27	-2.27	108.83	115.22
5	D	601	B12	C4B-C9B-N3B	2.25	136.90	130.88
5	D	601	B12	C19-C1-N21	2.24	104.46	102.16
5	D	601	B12	C8B-C9B-N3B	-2.23	103.12	107.83
5	B	601	B12	C4B-C9B-C8B	-2.16	118.89	121.10
5	D	601	B12	C60-C18-C17	-2.14	110.59	115.74
5	D	601	B12	C2P-C1P-N59	-2.12	109.81	112.93
5	B	601	B12	C3R-C2R-C1R	2.07	104.47	99.89
5	B	601	B12	C2-C26-C27	-2.06	109.43	115.22
5	B	601	B12	C55-C17-C16	2.06	116.79	109.92
5	B	601	B12	C8B-C9B-N3B	-2.03	103.55	107.83
5	D	601	B12	C16-C15-C14	-2.03	121.11	124.27
5	B	601	B12	O6R-C1R-C2R	-2.02	103.97	106.93
3	A	501	5AD	C3'-C2'-C1'	2.02	104.01	100.98
5	B	601	B12	C3P-C2P-C1P	-2.01	107.49	111.39
5	B	601	B12	P-O2-C3R	2.00	126.70	119.41

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	601	B12	C2P-O3-P-O5
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	C42-C41-C8-C9
5	B	601	B12	C13-C48-C49-C50
5	B	601	B12	C2P-O3-P-O5
4	A	503	GOL	O1-C1-C2-C3
5	D	601	B12	C13-C48-C49-C50
5	D	601	B12	C2-C3-C30-C31
5	B	601	B12	C2-C3-C30-C31
4	C	504	GOL	O1-C1-C2-O2
4	A	505	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
4	C	506	GOL	C1-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	A	503	GOL	O1-C1-C2-O2
5	D	601	B12	C2P-O3-P-O2

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Mol	Chain	Res	Type	Atoms
5	B	601	B12	C2P-O3-P-O2
4	C	502	GOL	O2-C2-C3-O3
5	D	601	B12	C38-C37-C7-C36
5	D	601	B12	C2P-O3-P-O4
5	B	601	B12	C2P-O3-P-O4
5	B	601	B12	C38-C37-C7-C36
5	D	601	B12	C3R-O2-P-O3
5	D	601	B12	C38-C37-C7-C8
5	B	601	B12	C38-C37-C7-C8
5	D	601	B12	C1-C2-C26-C27
5	B	601	B12	C1P-C2P-O3-P
4	C	505	GOL	O2-C2-C3-O3
5	D	601	B12	C25-C2-C26-C27
4	C	506	GOL	O2-C2-C3-O3
5	D	601	B12	C3-C2-C26-C27
5	D	601	B12	C4-C3-C30-C31
5	B	601	B12	C4-C3-C30-C31
5	D	601	B12	C1P-C2P-O3-P
5	D	601	B12	C41-C42-C43-O44
5	D	601	B12	C41-C42-C43-N45

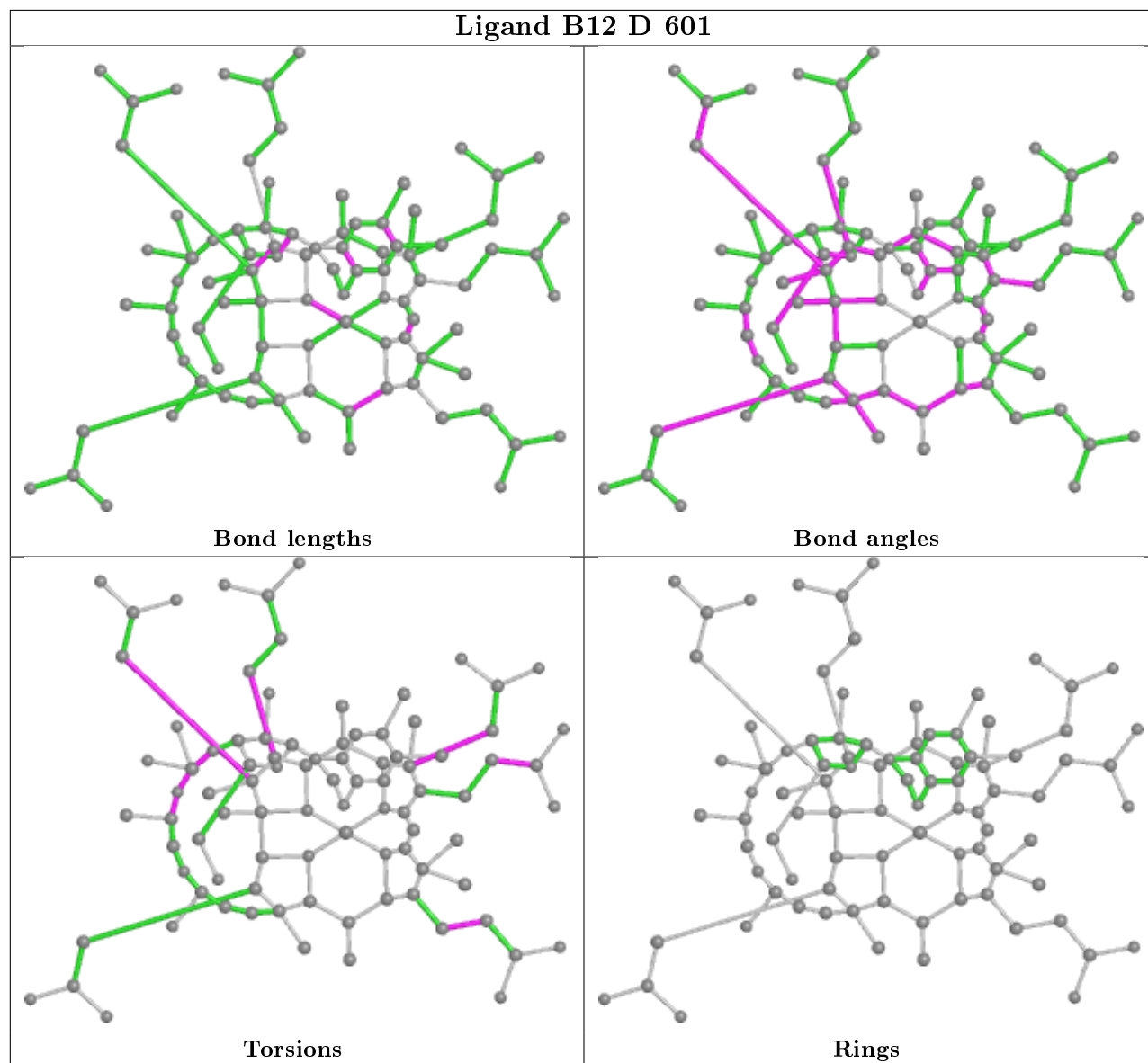
There are no ring outliers.

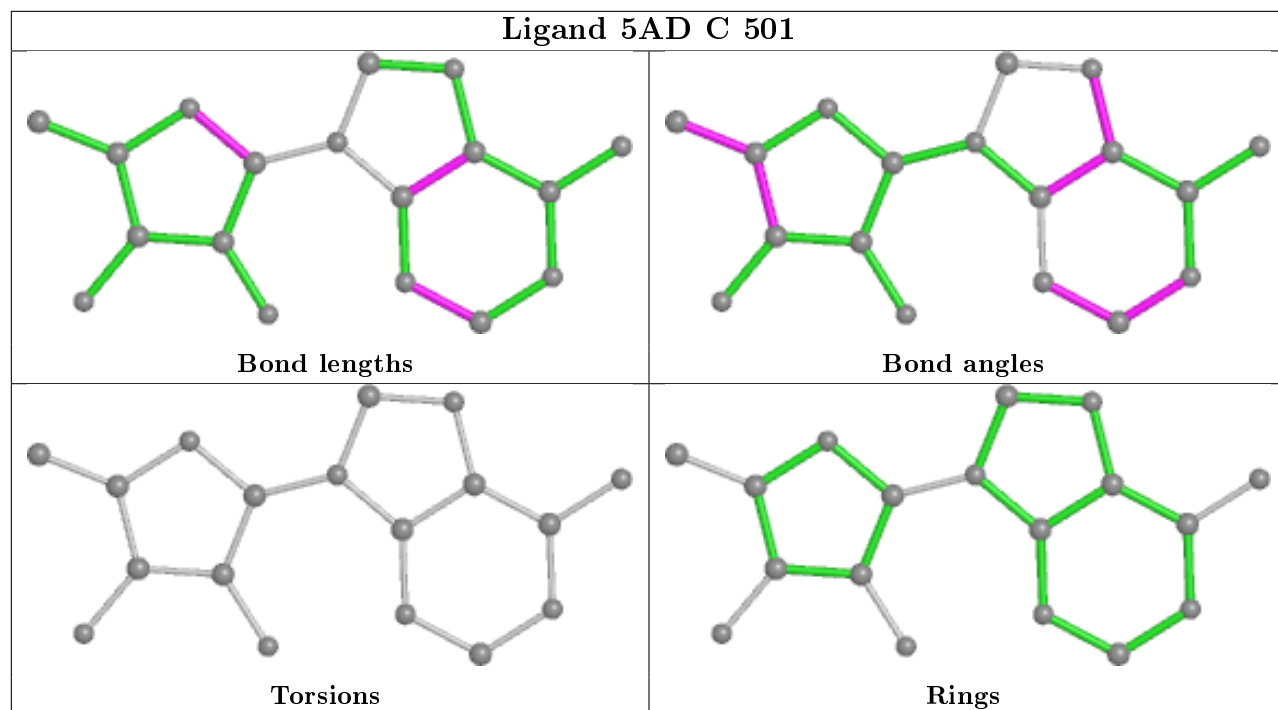
7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	601	B12	6	0
4	C	504	GOL	1	0
4	A	504	GOL	0	1
4	C	502	GOL	1	0
4	A	506	GOL	3	0
5	B	601	B12	7	0
3	A	501	5AD	2	0

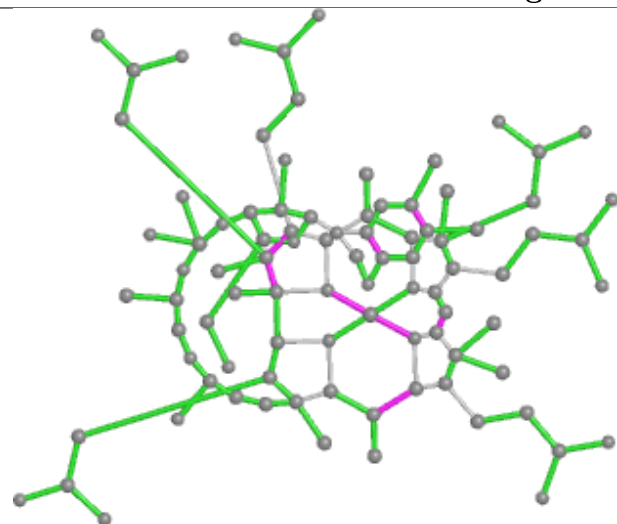
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

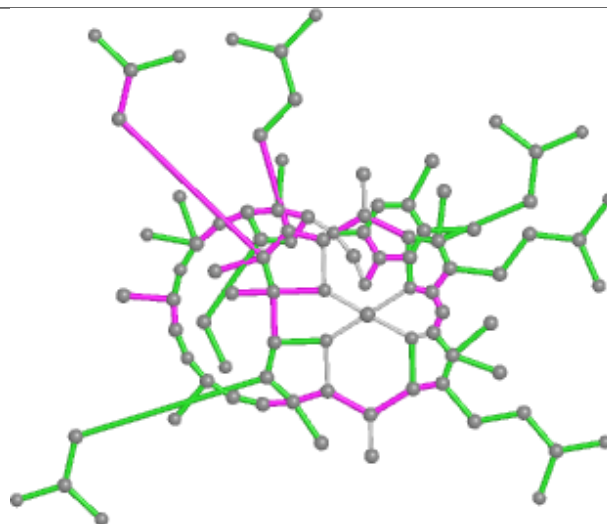




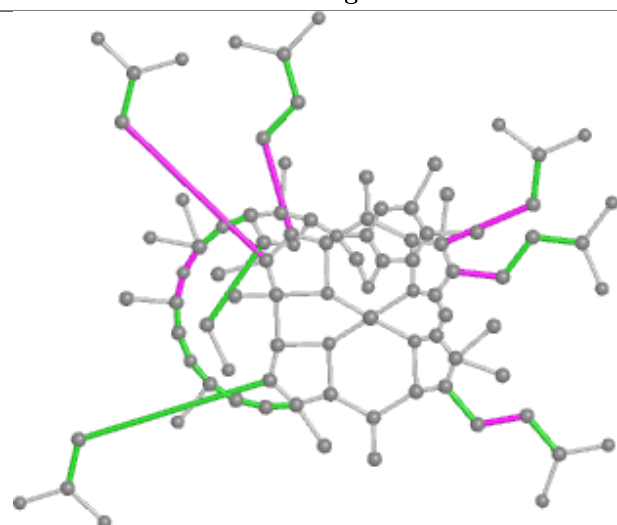
## Ligand B12 B 601



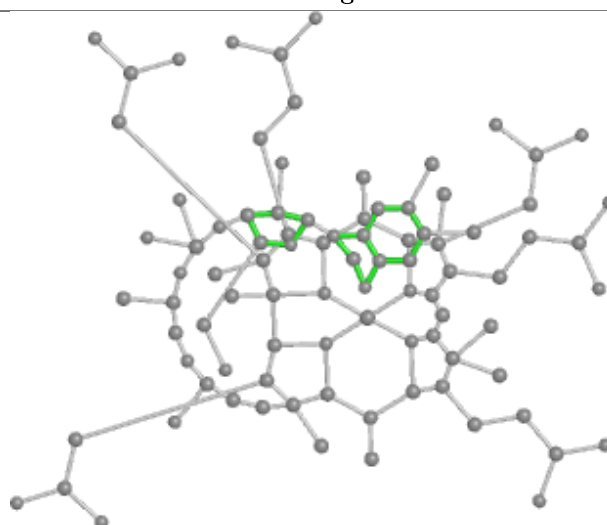
Bond lengths



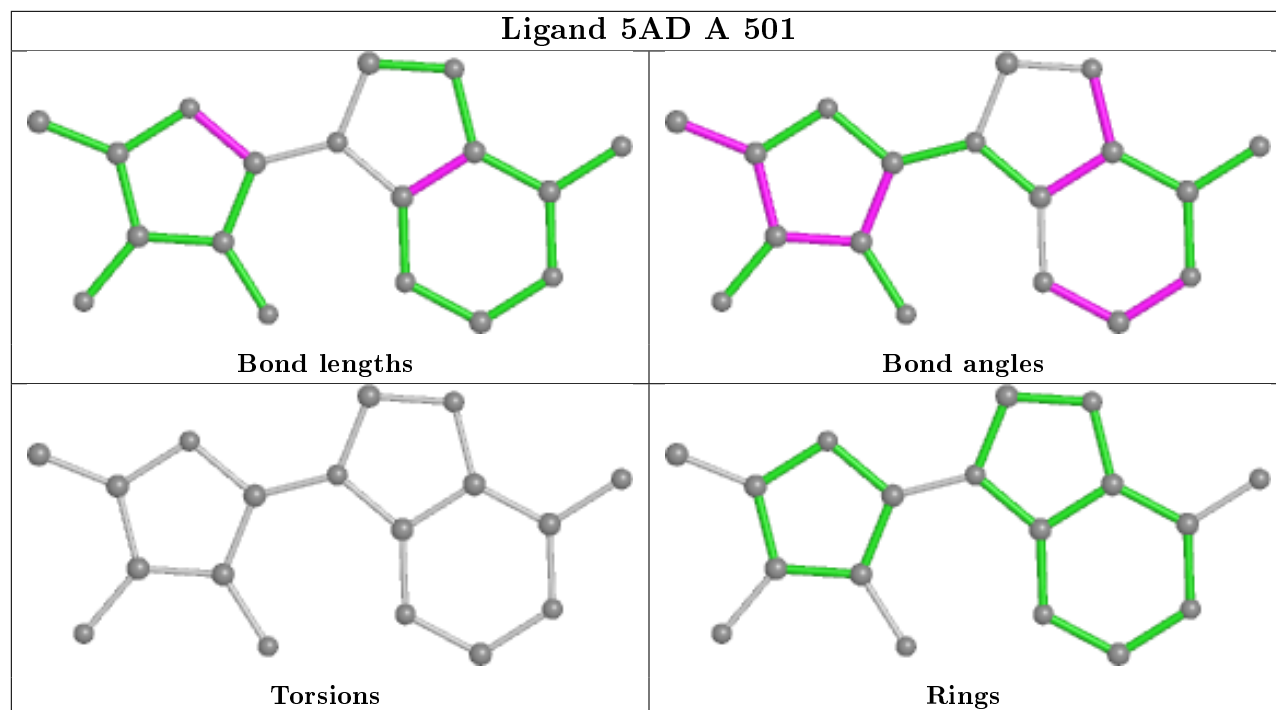
Bond angles



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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	453/453 (100%)	-0.77	0 100 100	13, 23, 37, 61	0
1	C	453/453 (100%)	-0.79	0 100 100	13, 24, 41, 60	0
2	B	252/295 (85%)	-0.50	2 (0%) 86 85	17, 44, 65, 96	0
2	D	252/295 (85%)	0.05	13 (5%) 27 26	15, 52, 87, 122	0
All	All	1410/1496 (94%)	-0.58	15 (1%) 80 79	13, 28, 69, 122	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	ALA	5.7
2	D	194	LEU	3.5
2	D	145	ALA	3.4
2	D	191	GLN	3.0
2	D	148	VAL	3.0
2	D	155	CYS	2.9
2	D	198	THR	2.9
2	B	192	ALA	2.6
2	D	295	ARG	2.6
2	D	288	ALA	2.2
2	D	163	VAL	2.2
2	D	190	LYS	2.2
2	B	295	ARG	2.1
2	D	247	ARG	2.0
2	D	149	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

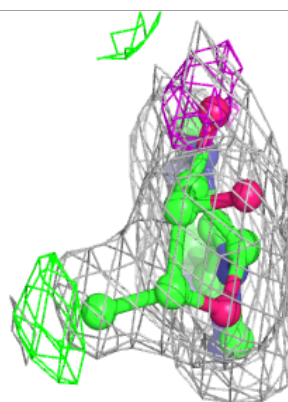
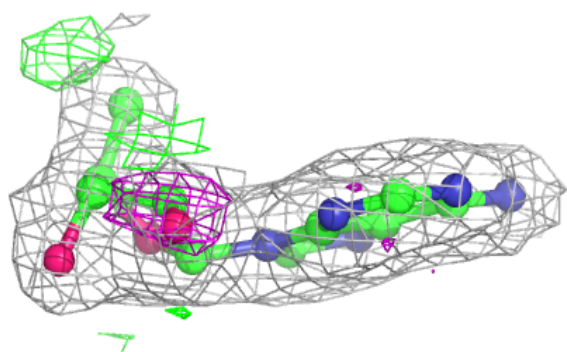
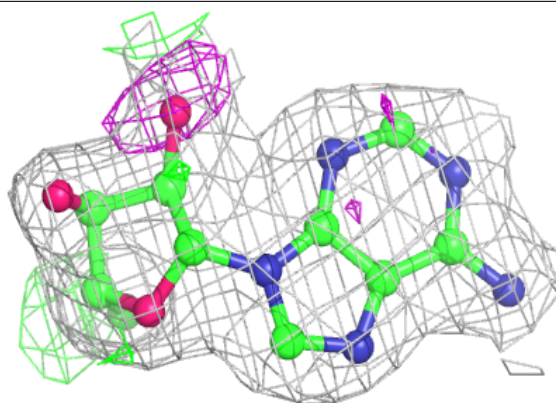
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	504	6/6	0.71	0.24	69,71,71,73	0
4	GOL	A	507	6/6	0.72	0.27	62,69,70,71	0
4	GOL	C	505	6/6	0.81	0.16	39,43,46,48	0
4	GOL	A	506	6/6	0.84	0.23	76,77,78,79	0
4	GOL	A	504	6/6	0.87	0.12	44,49,50,52	0
4	GOL	A	503	6/6	0.91	0.18	27,41,49,54	0
4	GOL	C	502	6/6	0.92	0.12	37,43,46,50	0
3	5AD	C	501	18/18	0.95	0.09	29,32,39,40	0
4	GOL	A	505	6/6	0.96	0.07	26,27,29,29	0
3	5AD	A	501	18/18	0.96	0.07	27,29,33,34	0
4	GOL	C	506	6/6	0.97	0.09	23,30,32,32	0
5	B12	D	601	91/91	0.97	0.09	30,38,44,54	0
4	GOL	C	503	6/6	0.98	0.12	28,31,35,37	0
5	B12	B	601	91/91	0.98	0.08	21,28,35,38	0
4	GOL	A	502	6/6	0.98	0.10	25,28,30,31	0

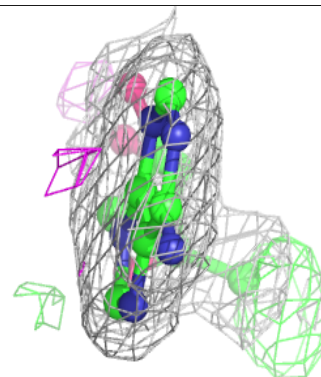
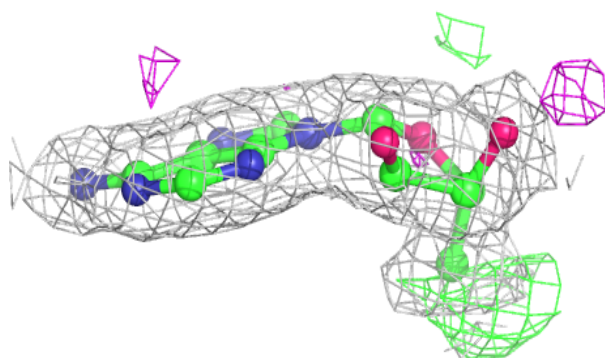
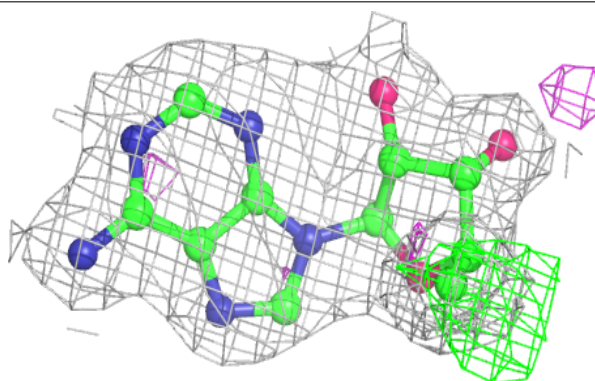
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5AD 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)

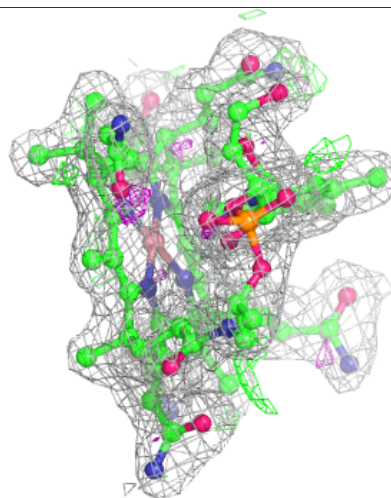
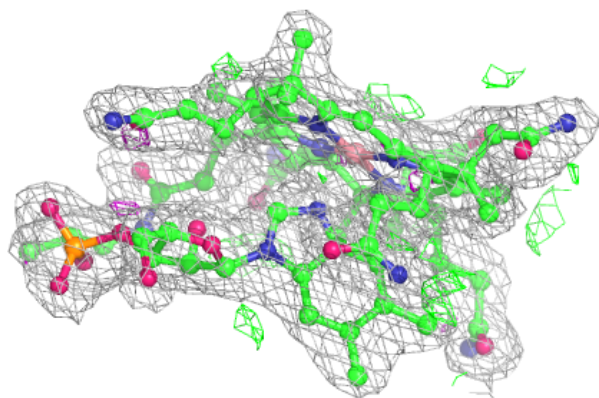
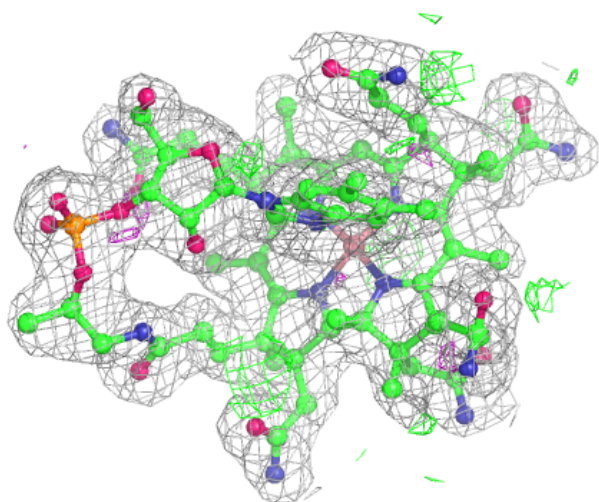
**Electron density around 5AD A 501:**

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



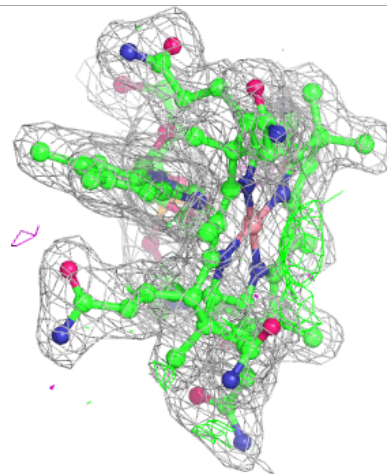
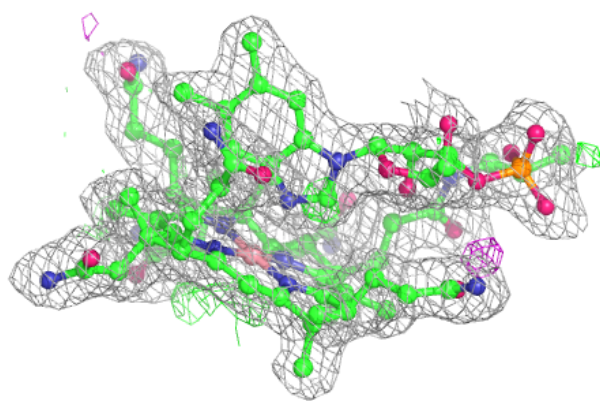
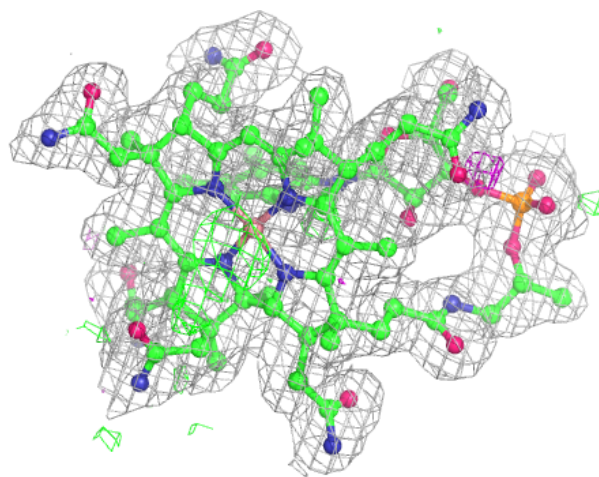
**Electron density around B12 D 601:**

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



**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.