



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:39 PM JST

PDB ID : 7XRM  
Title : Ethanolamine ammonia-lyase complexed with AdoMeCbl  
Authors : Shibata, N.; Toraya, T.  
Deposited on : 2022-05-10  
Resolution : 2.13 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.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

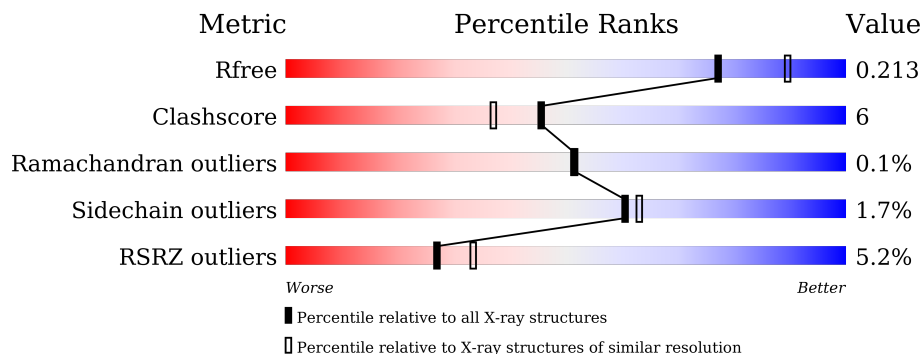
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 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	 88% 12%
1	C	453	 89% 11% .
2	B	263	 3% 78% 17% . .
2	D	263	 25% 76% 20% .

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11814 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 large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	453	Total 3484	C 2184	N 597	O 681	S 22	0	4	0
1	C	453	Total 3492	C 2190	N 599	O 680	S 23	0	5	0

- Molecule 2 is a protein called Ethanolamine ammonia-lyase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	253	Total 1943	C 1213	N 354	O 366	S 10	0	2	0
2	D	252	Total 1956	C 1222	N 351	O 373	S 10	0	6	0

There are 22 discrepancies between the modelled and reference sequences:

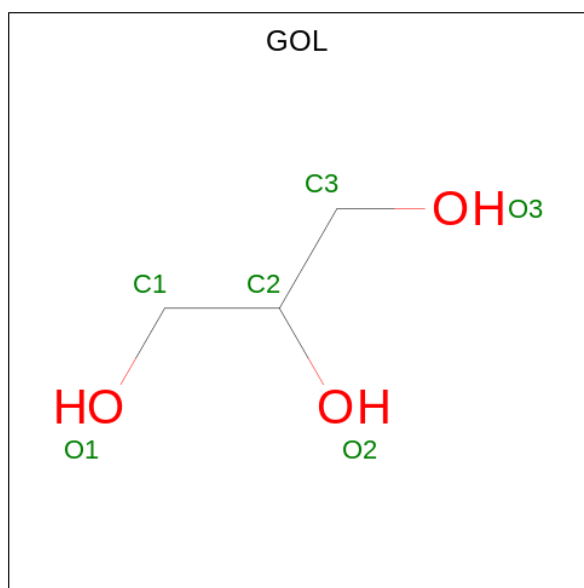
Chain	Residue	Modelled	Actual	Comment	Reference
B	33	MET	-	initiating methionine	UNP P19636
B	34	ASP	-	expression tag	UNP P19636
B	35	GLN	-	expression tag	UNP P19636
B	36	SER	-	expression tag	UNP P19636
B	37	SER	-	expression tag	UNP P19636
B	38	HIS	-	expression tag	UNP P19636
B	39	HIS	-	expression tag	UNP P19636
B	40	HIS	-	expression tag	UNP P19636
B	41	HIS	-	expression tag	UNP P19636
B	42	HIS	-	expression tag	UNP P19636
B	43	HIS	-	expression tag	UNP P19636
D	33	MET	-	initiating methionine	UNP P19636
D	34	ASP	-	expression tag	UNP P19636
D	35	GLN	-	expression tag	UNP P19636
D	36	SER	-	expression tag	UNP P19636
D	37	SER	-	expression tag	UNP P19636

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Chain	Residue	Modelled	Actual	Comment	Reference
D	38	HIS	-	expression tag	UNP P19636
D	39	HIS	-	expression tag	UNP P19636
D	40	HIS	-	expression tag	UNP P19636
D	41	HIS	-	expression tag	UNP P19636
D	42	HIS	-	expression tag	UNP P19636
D	43	HIS	-	expression tag	UNP P19636

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



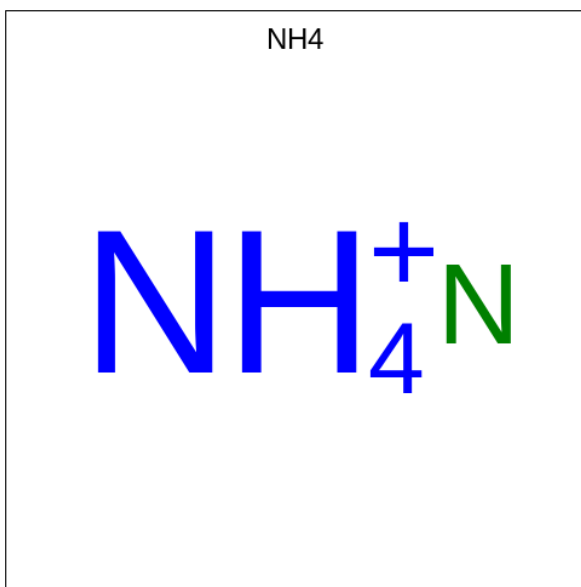
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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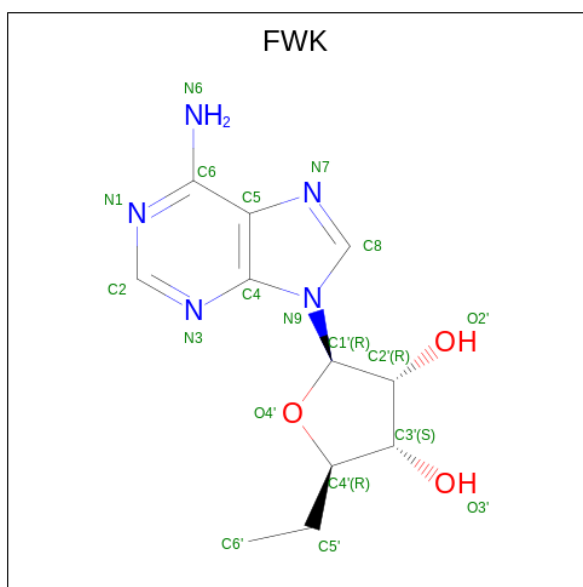
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



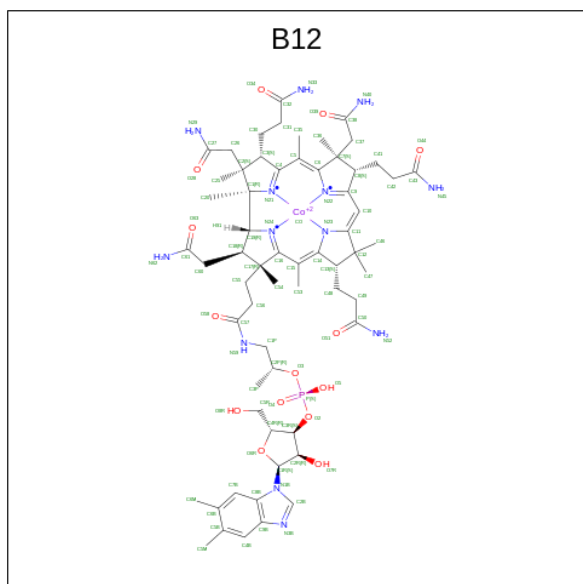
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 1 1	0	0
4	C	1	Total N 1 1	0	0

- Molecule 5 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-ethyl-oxolane-3,4-diol (three-letter code: FWK) (formula: C<sub>11</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	19	11	5	3	0	0
5	C	1	19	11	5	3	0	0

- Molecule 6 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ) (labeled as "Ligand of Interest" by depositor).



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

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

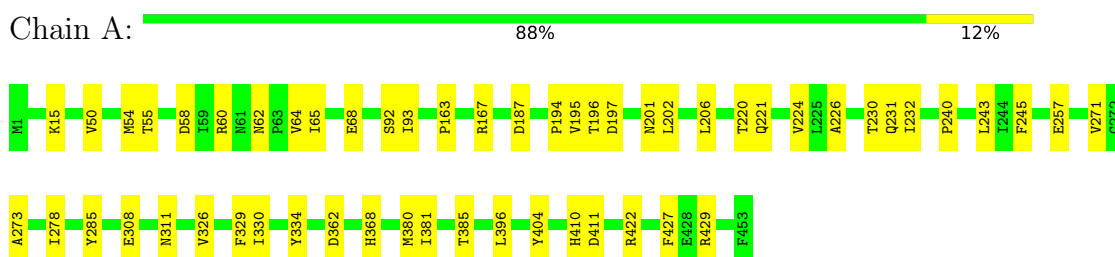
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	286	Total 286	O 286	0	0
7	B	72	Total 72	O 72	0	0
7	C	259	Total 259	O 259	0	0
7	D	34	Total 34	O 34	0	0

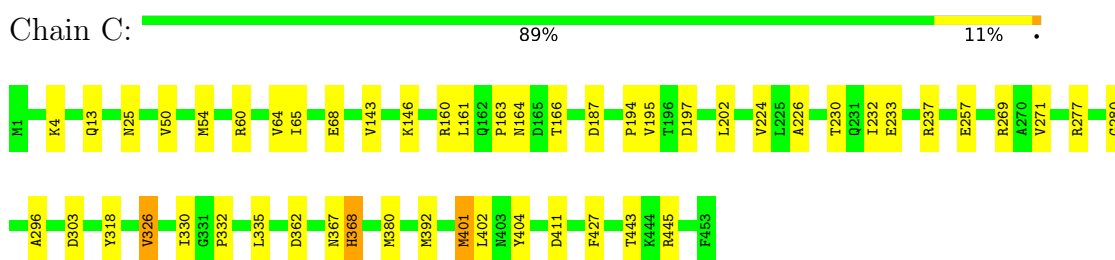
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

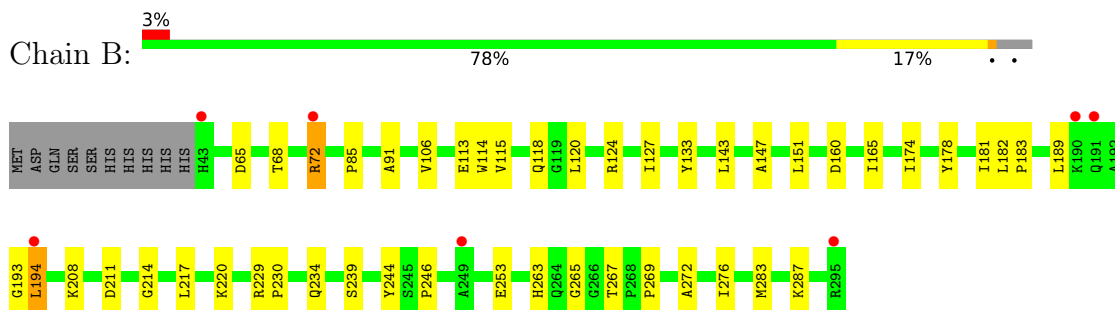
- Molecule 1: Ethanolamine ammonia-lyase large subunit



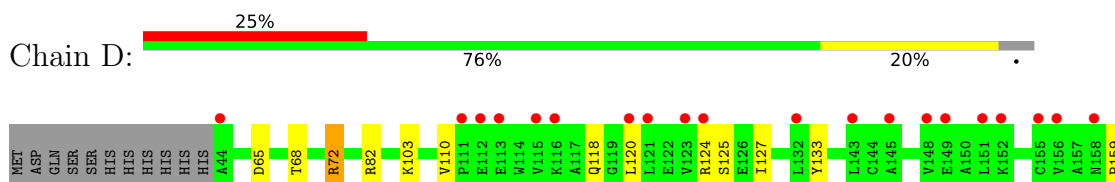
- Molecule 1: Ethanolamine ammonia-lyase large subunit



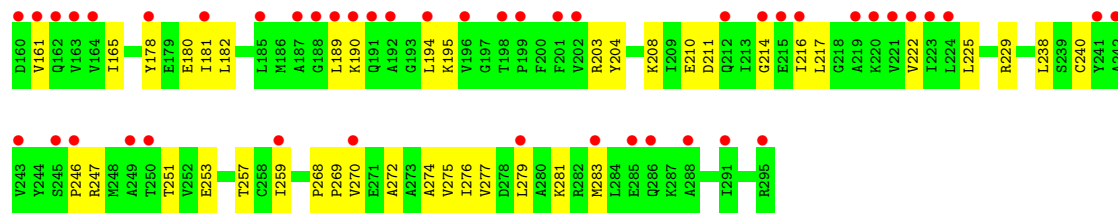
- Molecule 2: Ethanolamine ammonia-lyase small subunit



- Molecule 2: Ethanolamine ammonia-lyase small subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	242.88Å 242.88Å 76.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.42 – 2.13 46.42 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.42-2.13) 99.2 (46.42-2.13)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.14Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.194 , 0.220 0.195 , 0.213	Depositor DCC
$R_{free}$ test set	7190 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.085 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B12, FWK, GOL, NH4

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	0.26	0/3550	0.48	0/4807
1	C	0.26	0/3561	0.48	0/4820
2	B	0.28	0/1974	0.55	0/2674
2	D	0.25	0/1992	0.56	0/2699
All	All	0.26	0/11077	0.51	0/15000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3484	0	3452	36	0
1	C	3492	0	3468	31	0
2	B	1943	0	1998	29	0
2	D	1956	0	2012	37	0
3	A	24	0	32	3	0
3	C	42	0	56	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	19	0	0	0	0
6	B	91	0	88	9	0
6	D	91	0	88	8	0
7	A	286	0	0	5	0
7	B	72	0	0	0	0
7	C	259	0	0	0	0
7	D	34	0	0	0	0
All	All	11814	0	11194	144	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 (144) 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:B:160:ASP:HB2	2:B:194:LEU:HD13	1.60	0.82
2:D:216:ILE:HG22	2:D:217:LEU:HD23	1.71	0.73
1:C:269[B]:ARG:NH1	1:C:318:TYR:O	2.26	0.68
1:A:202:LEU:HD22	1:A:224[A]:VAL:HG21	1.77	0.66
2:B:113:GLU:N	2:B:113:GLU:OE1	2.29	0.65
2:B:118:GLN:HB2	2:B:120:LEU:HD12	1.79	0.63
1:A:64:VAL:HG23	1:A:65:ILE:HG13	1.81	0.62
1:C:64:VAL:HG23	1:C:65:ILE:HG13	1.80	0.61
1:A:429:ARG:NH2	7:A:605:HOH:O	2.32	0.61
2:D:68:THR:O	2:D:72:ARG:HG2	2.01	0.60
2:B:165:ILE:HD11	2:B:174:ILE:HG23	1.84	0.60
2:B:272:ALA:O	2:B:276:ILE:HG13	2.01	0.60
6:D:301:B12:H601	6:D:301:B12:H262	1.82	0.60
2:B:68:THR:O	2:B:72:ARG:HG2	2.01	0.59
2:D:247:ARG:O	2:D:251:THR:HG22	2.03	0.59
2:B:244:TYR:OH	2:B:287:LYS:HG2	2.02	0.58
2:D:225:LEU:HD13	2:D:238:LEU:HD21	1.85	0.58
2:D:208:LYS:HE2	2:D:253:GLU:OE1	2.04	0.58
1:A:380:MET:SD	1:A:411:ASP:HB3	2.45	0.57
2:B:127:ILE:HG21	2:B:133:TYR:HB2	1.86	0.57
1:C:232:ILE:HG23	1:C:271:VAL:HG21	1.87	0.56
1:A:68:GLU:OE2	7:A:601:HOH:O	2.18	0.56
1:C:164:ASN:HB3	1:C:401[B]:MET:HG2	1.88	0.55
1:C:233:GLU:O	1:C:237:ARG:HG3	2.07	0.55
6:B:301:B12:H552	6:B:301:B12:H531	1.90	0.53
2:D:124:ARG:NH1	2:D:125:SER:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD22	1:A:224[B]:VAL:HG11	1.89	0.53
1:A:206:LEU:HB3	1:A:240:PRO:HG2	1.89	0.53
1:C:443:THR:O	2:D:82:ARG:NH2	2.42	0.53
1:A:194:PRO:HG3	1:A:226:ALA:HB2	1.90	0.53
1:A:187:ASP:OD1	1:A:187:ASP:N	2.42	0.53
1:A:232:ILE:HG23	1:A:271:VAL:HG21	1.91	0.52
2:D:178:TYR:CE1	2:D:182:LEU:HD12	2.44	0.52
6:D:301:B12:H552	6:D:301:B12:H531	1.92	0.52
2:D:272:ALA:O	2:D:276:ILE:HD12	2.09	0.52
1:A:326:VAL:HA	1:A:362:ASP:HB3	1.91	0.52
2:B:211:ASP:HA	2:B:246:PRO:HB2	1.92	0.52
2:B:114:TRP:O	2:B:118:GLN:HG2	2.10	0.52
2:D:180[A]:GLU:HG2	2:D:270:VAL:HG13	1.90	0.52
1:C:143:VAL:HG13	3:C:501:GOL:H11	1.93	0.51
2:D:127:ILE:HG21	2:D:133:TYR:HB2	1.92	0.51
2:B:65:ASP:N	2:B:65:ASP:OD1	2.42	0.51
2:B:214:GLY:HA3	2:B:246:PRO:HG2	1.93	0.51
1:C:277:ARG:HE	3:C:505:GOL:H32	1.75	0.51
2:B:120:LEU:HD11	2:B:178:TYR:OH	2.11	0.50
1:C:25:ASN:ND2	1:C:303:ASP:OD2	2.38	0.50
2:D:274:ALA:O	2:D:277:VAL:HG12	2.11	0.50
2:D:277:VAL:O	2:D:281:LYS:HG3	2.11	0.50
1:C:257:GLU:OE2	2:D:253:GLU:N	2.40	0.50
1:A:368:HIS:H	1:A:368:HIS:CD2	2.30	0.49
1:C:4:LYS:HB2	1:C:13:GLN:HE22	1.77	0.49
2:B:253:GLU:HB3	6:B:301:B12:H452	1.77	0.49
2:D:203:ARG:HG2	2:D:204:TYR:CD1	2.47	0.49
6:B:301:B12:H601	6:B:301:B12:H262	1.94	0.49
2:D:240:CYS:HB3	2:D:259:ILE:HB	1.94	0.49
1:C:4:LYS:HB2	1:C:13:GLN:NE2	2.28	0.48
2:D:181[A]:ILE:HB	2:D:269:PRO:HB3	1.95	0.48
2:D:181[B]:ILE:HB	2:D:269:PRO:HB3	1.95	0.48
1:A:196:THR:OG1	1:A:201:ASN:ND2	2.45	0.48
1:A:326:VAL:HG12	1:A:329:PHE:HB2	1.96	0.48
2:D:118:GLN:HB2	2:D:120:LEU:HD12	1.96	0.48
6:D:301:B12:C4	6:D:301:B12:H4B	2.43	0.48
6:B:301:B12:H533	6:B:301:B12:H521	1.77	0.48
1:C:257:GLU:HG3	1:C:296:ALA:HB1	1.95	0.47
2:D:120:LEU:HD11	2:D:178:TYR:OH	2.15	0.47
1:A:58:ASP:O	1:A:62:ASN:ND2	2.42	0.47
6:D:301:B12:H261	6:D:301:B12:H91	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ARG:NH2	7:A:613:HOH:O	2.41	0.47
1:C:326:VAL:HA	1:C:362:ASP:HB3	1.95	0.47
2:D:110:VAL:O	2:D:203:ARG:NH2	2.48	0.47
2:D:65:ASP:OD1	2:D:65:ASP:N	2.46	0.46
2:D:165:ILE:HG12	2:D:225:LEU:HB2	1.97	0.46
2:B:120:LEU:HD11	2:B:178:TYR:CZ	2.51	0.46
1:C:380:MET:SD	1:C:411:ASP:HB3	2.56	0.46
2:B:208:LYS:NZ	2:B:211:ASP:OD2	2.48	0.46
6:B:301:B12:H363	6:B:301:B12:H412	1.53	0.46
2:D:214:GLY:HA3	2:D:246:PRO:HG2	1.98	0.46
1:A:50:VAL:O	1:A:54:MET:HG3	2.16	0.45
1:A:278:ILE:HB	3:A:503:GOL:H31	1.98	0.45
1:C:332:PRO:HA	1:C:335:LEU:O	2.17	0.45
1:A:257:GLU:OE2	2:B:253:GLU:N	2.50	0.45
1:C:187:ASP:OD1	1:C:187:ASP:N	2.41	0.45
1:C:197:ASP:OD2	1:C:230:THR:HG21	2.17	0.45
2:D:178:TYR:CZ	2:D:182:LEU:HD12	2.52	0.45
1:A:273:ALA:HA	3:A:503:GOL:H12	1.99	0.45
1:C:160:ARG:HD3	1:C:392:MET:SD	2.57	0.45
1:C:445:ARG:NH1	1:C:445:ARG:HG2	2.31	0.45
2:B:263:HIS:HD1	2:B:265:GLY:H	1.64	0.45
2:B:151:LEU:HB3	2:B:217:LEU:HD21	1.98	0.44
2:D:210:GLU:HB2	2:D:222:VAL:HG11	1.99	0.44
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.53	0.44
2:D:159:PRO:HA	2:D:195:LYS:HG2	1.99	0.44
6:D:301:B12:H521	6:D:301:B12:H482	1.62	0.44
2:B:181:ILE:HB	2:B:269:PRO:HB3	1.98	0.44
1:A:220:THR:OG1	1:A:221:GLN:N	2.50	0.44
1:A:330:ILE:HG21	1:A:334:TYR:CE2	2.53	0.44
1:C:50:VAL:O	1:C:54:MET:HG3	2.17	0.44
6:D:301:B12:H253	6:D:301:B12:H301	1.74	0.44
6:B:301:B12:H2B	6:B:301:B12:H482	1.99	0.43
1:C:367:ASN:O	2:D:103:LYS:HE3	2.18	0.43
6:D:301:B12:H372	6:D:301:B12:H351	2.00	0.43
1:A:381:ILE:O	1:A:385:THR:HG23	2.18	0.43
2:B:106:VAL:HG22	2:B:230:PRO:HG2	1.99	0.43
1:C:368:HIS:CD2	1:C:368:HIS:H	2.36	0.43
1:A:429:ARG:NH2	7:A:623:HOH:O	2.51	0.43
1:A:197:ASP:OD2	1:A:230:THR:HG21	2.19	0.43
6:B:301:B12:H91	6:B:301:B12:H261	1.39	0.43
1:C:194:PRO:HG3	1:C:226:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ARG:HG2	1:C:445:ARG:HH11	1.84	0.42
1:C:161:LEU:O	1:C:163:PRO:HD3	2.20	0.42
2:D:211:ASP:HA	2:D:246:PRO:HB2	2.01	0.42
2:D:272:ALA:O	2:D:275:VAL:N	2.50	0.42
2:B:267:THR:HG22	2:B:272:ALA:HB2	2.01	0.42
1:A:308:GLU:O	1:A:311:ASN:HB2	2.20	0.42
2:D:257:THR:HG21	2:D:279:LEU:HD11	2.00	0.42
2:D:279:LEU:O	2:D:283:MET:HG3	2.19	0.42
3:A:501:GOL:H12	7:A:734:HOH:O	2.20	0.42
1:A:410:HIS:HB3	2:B:85:PRO:O	2.19	0.42
6:D:301:B12:H412	6:D:301:B12:C4B	2.50	0.42
2:B:189:LEU:O	2:B:193:GLY:HA3	2.19	0.42
1:A:54:MET:O	1:A:93:ILE:HG12	2.20	0.41
1:C:401[B]:MET:HG3	1:C:402:LEU:N	2.34	0.41
2:D:165:ILE:HD12	2:D:182:LEU:HD11	2.02	0.41
2:D:268:PRO:HA	2:D:269:PRO:HD3	1.96	0.41
1:A:330:ILE:HG21	1:A:334:TYR:HE2	1.85	0.41
1:A:396:LEU:HD11	2:B:91:ALA:HB1	2.01	0.41
1:C:202:LEU:HG	1:C:224[A]:VAL:HG21	2.01	0.41
1:A:231:GLN:NE2	1:A:245:PHE:O	2.53	0.41
2:B:244:TYR:HB2	2:B:283:MET:HE3	2.02	0.41
2:D:161:VAL:HG21	2:D:189:LEU:HD13	2.02	0.41
2:D:194:LEU:HB3	2:D:195:LYS:H	1.56	0.41
2:B:182:LEU:HB3	2:B:183:PRO:CD	2.51	0.41
6:B:301:B12:H18	6:B:301:B12:H562	1.84	0.41
1:C:166:THR:O	1:C:195:VAL:HG21	2.21	0.41
2:B:143:LEU:HB3	2:B:147:ALA:HB3	2.02	0.41
1:A:55:THR:HA	1:A:92:SER:HA	2.04	0.40
1:A:195:VAL:HG12	1:A:196:THR:HG23	2.04	0.40
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.57	0.40
1:A:221:GLN:HG3	1:A:243:LEU:HG	2.04	0.40
1:A:245:PHE:HA	1:A:285:TYR:O	2.20	0.40
6:B:301:B12:H253	6:B:301:B12:H301	1.73	0.40
2:D:272:ALA:O	2:D:275:VAL:HG22	2.20	0.40
2:B:115:VAL:HG23	2:B:120:LEU:HB2	2.04	0.40
1:C:146:LYS:HG3	1:C:280:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/453 (100%)	438 (96%)	16 (4%)	1 (0%)	47	45
1	C	456/453 (101%)	437 (96%)	18 (4%)	1 (0%)	47	45
2	B	253/263 (96%)	245 (97%)	8 (3%)	0	100	100
2	D	256/263 (97%)	242 (94%)	14 (6%)	0	100	100
All	All	1420/1432 (99%)	1362 (96%)	56 (4%)	2 (0%)	51	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO
1	C	330	ILE

### 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	374/370 (101%)	370 (99%)	4 (1%)	73	76
1	C	375/370 (101%)	368 (98%)	7 (2%)	57	59
2	B	209/217 (96%)	202 (97%)	7 (3%)	38	35
2	D	212/217 (98%)	209 (99%)	3 (1%)	67	70
All	All	1170/1174 (100%)	1149 (98%)	21 (2%)	60	60

All (21) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	15	LYS
1	A	60	ARG
1	A	167	ARG
1	A	404	TYR
2	B	72	ARG
2	B	124	ARG
2	B	194	LEU
2	B	220	LYS
2	B	229	ARG
2	B	234	GLN
2	B	239	SER
1	C	60	ARG
1	C	68	GLU
1	C	326	VAL
1	C	368	HIS
1	C	401[A]	MET
1	C	401[B]	MET
1	C	404	TYR
2	D	72	ARG
2	D	190	LYS
2	D	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	368	HIS
2	B	154	GLN
2	B	261	ASN
1	C	10	ASN
1	C	13	GLN
1	C	61	ASN
1	C	368	HIS
2	D	191	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are modelled with single atom - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	C	501	-	5,5,5	0.91	0	5,5,5	0.97	0
3	GOL	C	504	-	5,5,5	0.98	0	5,5,5	0.96	0
6	B12	D	301	-	90,101,101	1.34	10 (11%)	137,166,166	1.21	11 (8%)
5	FWK	A	506	-	18,21,21	1.07	1 (5%)	17,31,31	1.38	3 (17%)
3	GOL	C	502	-	5,5,5	0.86	0	5,5,5	1.01	0
3	GOL	C	506	-	5,5,5	0.92	0	5,5,5	0.98	0
3	GOL	A	502	-	5,5,5	0.89	0	5,5,5	0.94	0
3	GOL	C	503	-	5,5,5	0.92	0	5,5,5	0.95	0
3	GOL	A	501	-	5,5,5	0.96	0	5,5,5	0.97	0
3	GOL	C	505	-	5,5,5	0.96	0	5,5,5	0.93	0
5	FWK	C	509	-	18,21,21	1.06	1 (5%)	17,31,31	1.36	3 (17%)
3	GOL	A	504	-	5,5,5	0.92	0	5,5,5	0.91	0
3	GOL	C	507	-	5,5,5	1.01	0	5,5,5	0.82	0
6	B12	B	301	-	90,101,101	1.33	11 (12%)	137,166,166	1.18	14 (10%)
3	GOL	A	503	-	5,5,5	0.96	0	5,5,5	1.11	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '·' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	501	-	-	3/4/4/4	-
3	GOL	C	504	-	-	1/4/4/4	-
6	B12	D	301	-	-	21/52/223/223	0/3/11/11
5	FWK	A	506	-	-	0/2/22/22	0/3/3/3
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	C	506	-	-	4/4/4/4	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	C	503	-	-	3/4/4/4	-
3	GOL	A	501	-	-	2/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
5	FWK	C	509	-	-	1/2/22/22	0/3/3/3
3	GOL	A	504	-	-	0/4/4/4	-
3	GOL	C	507	-	-	0/4/4/4	-
6	B12	B	301	-	-	22/52/223/223	0/3/11/11
3	GOL	A	503	-	-	1/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	B12	C14-N23	-5.19	1.28	1.35
6	B	301	B12	C14-N23	-5.08	1.28	1.35
6	D	301	B12	C11-N23	4.29	1.45	1.37
6	D	301	B12	C8B-C9B	4.18	1.49	1.40
6	B	301	B12	C8B-C9B	4.15	1.49	1.40
6	B	301	B12	C11-N23	4.05	1.44	1.37
6	B	301	B12	C16-C15	-4.03	1.33	1.44
6	D	301	B12	C16-C15	-3.79	1.34	1.44
6	B	301	B12	C6B-C5B	3.39	1.49	1.40
6	D	301	B12	C6B-C5B	3.37	1.49	1.40
6	D	301	B12	C14-C15	2.89	1.50	1.38
6	B	301	B12	C14-C15	2.76	1.50	1.38
6	B	301	B12	C10-C9	2.63	1.46	1.39
5	A	506	FWK	C5-C4	2.56	1.47	1.40
6	D	301	B12	C10-C9	2.50	1.46	1.39
5	C	509	FWK	C5-C4	2.50	1.47	1.40
6	B	301	B12	C19-N24	-2.47	1.44	1.48
6	B	301	B12	C1-C2	-2.26	1.53	1.58
6	D	301	B12	C19-N24	-2.22	1.44	1.48
6	D	301	B12	C1-C2	-2.22	1.53	1.58
6	B	301	B12	C1-C19	-2.14	1.50	1.55
6	B	301	B12	O6R-C1R	2.14	1.44	1.41
6	D	301	B12	C1-C19	-2.06	1.50	1.55

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301	B12	C9-C10-C11	-4.74	119.11	125.97
6	D	301	B12	C17-C16-C15	3.91	132.43	126.26
6	B	301	B12	C17-C16-C15	3.62	131.97	126.26
6	B	301	B12	C9-C10-C11	-3.41	121.04	125.97
6	B	301	B12	C13-C14-N23	3.31	113.61	109.10
5	C	509	FWK	N3-C2-N1	-3.30	123.53	128.68
6	D	301	B12	C20-C1-N21	3.14	115.42	110.27
6	D	301	B12	C54-C17-C18	-3.10	108.41	112.98
5	A	506	FWK	N3-C2-N1	-3.10	123.84	128.68
6	D	301	B12	C13-C14-N23	2.98	113.15	109.10
6	B	301	B12	C20-C1-N21	2.95	115.10	110.27
6	B	301	B12	C54-C17-C18	-2.91	108.68	112.98
6	B	301	B12	C13-C14-C15	-2.87	119.94	124.32
6	D	301	B12	C18-C17-C16	2.79	104.06	100.67
6	D	301	B12	C17-C16-N24	-2.75	106.91	111.15
5	A	506	FWK	C3'-C2'-C1'	2.56	104.83	100.98
5	A	506	FWK	C4-C5-N7	-2.49	106.81	109.40
6	D	301	B12	C2P-C1P-N59	-2.47	109.30	112.93
6	B	301	B12	C2P-C1P-N59	-2.43	109.35	112.93
6	B	301	B12	C18-C17-C16	2.40	103.58	100.67
6	B	301	B12	C30-C3-C2	-2.39	114.04	119.09
6	B	301	B12	C17-C16-N24	-2.34	107.54	111.15
5	C	509	FWK	C3'-C2'-C1'	2.28	104.41	100.98
6	B	301	B12	C60-C18-C19	-2.24	108.78	114.62
5	C	509	FWK	C4-C5-N7	-2.24	107.07	109.40
6	D	301	B12	C60-C18-C19	-2.17	108.97	114.62
6	D	301	B12	C13-C14-C15	-2.17	121.01	124.32
6	B	301	B12	C41-C8-C9	2.12	114.93	111.19
6	D	301	B12	C3R-C2R-C1R	2.10	104.55	99.89
6	B	301	B12	C53-C15-C16	2.07	123.94	120.38
6	B	301	B12	C2-C1-C19	-2.06	115.35	118.60
3	A	503	GOL	C3-C2-C1	-2.00	103.91	111.70

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	GOL	O1-C1-C2-C3
3	C	505	GOL	O1-C1-C2-O2
3	C	505	GOL	O1-C1-C2-C3
3	C	506	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	301	B12	C1-C2-C26-C27
6	B	301	B12	C25-C2-C26-C27
6	B	301	B12	C3-C2-C26-C27
6	B	301	B12	C2P-O3-P-O5
6	D	301	B12	C2P-O3-P-O5
6	B	301	B12	C13-C48-C49-C50
6	B	301	B12	C2-C3-C30-C31
6	D	301	B12	C2-C3-C30-C31
6	D	301	B12	C4-C3-C30-C31
3	C	503	GOL	O1-C1-C2-O2
6	B	301	B12	C4-C3-C30-C31
6	B	301	B12	C42-C41-C8-C9
6	D	301	B12	C13-C48-C49-C50
6	B	301	B12	C16-C17-C55-C56
6	D	301	B12	C16-C17-C55-C56
6	D	301	B12	C1-C2-C26-C27
6	D	301	B12	C25-C2-C26-C27
6	D	301	B12	C3-C2-C26-C27
3	A	501	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-C3
3	C	506	GOL	O1-C1-C2-C3
6	B	301	B12	C42-C41-C8-C7
3	C	506	GOL	O2-C2-C3-O3
6	B	301	B12	C18-C17-C55-C56
6	D	301	B12	C3R-O2-P-O3
3	C	501	GOL	O1-C1-C2-O2
3	C	501	GOL	C1-C2-C3-O3
6	D	301	B12	C41-C42-C43-O44
6	B	301	B12	C2P-O3-P-O4
6	D	301	B12	C2P-O3-P-O4
3	C	506	GOL	O1-C1-C2-O2
6	D	301	B12	C41-C42-C43-N45
6	D	301	B12	C18-C17-C55-C56
5	C	509	FWK	O4'-C4'-C5'-C6'
3	A	503	GOL	O2-C2-C3-O3
6	B	301	B12	C2P-O3-P-O2
6	D	301	B12	C2P-O3-P-O2
3	A	501	GOL	O1-C1-C2-O2
6	B	301	B12	C1P-C2P-O3-P
6	B	301	B12	C3P-C2P-O3-P
6	B	301	B12	C38-C37-C7-C36
6	D	301	B12	C38-C37-C7-C36

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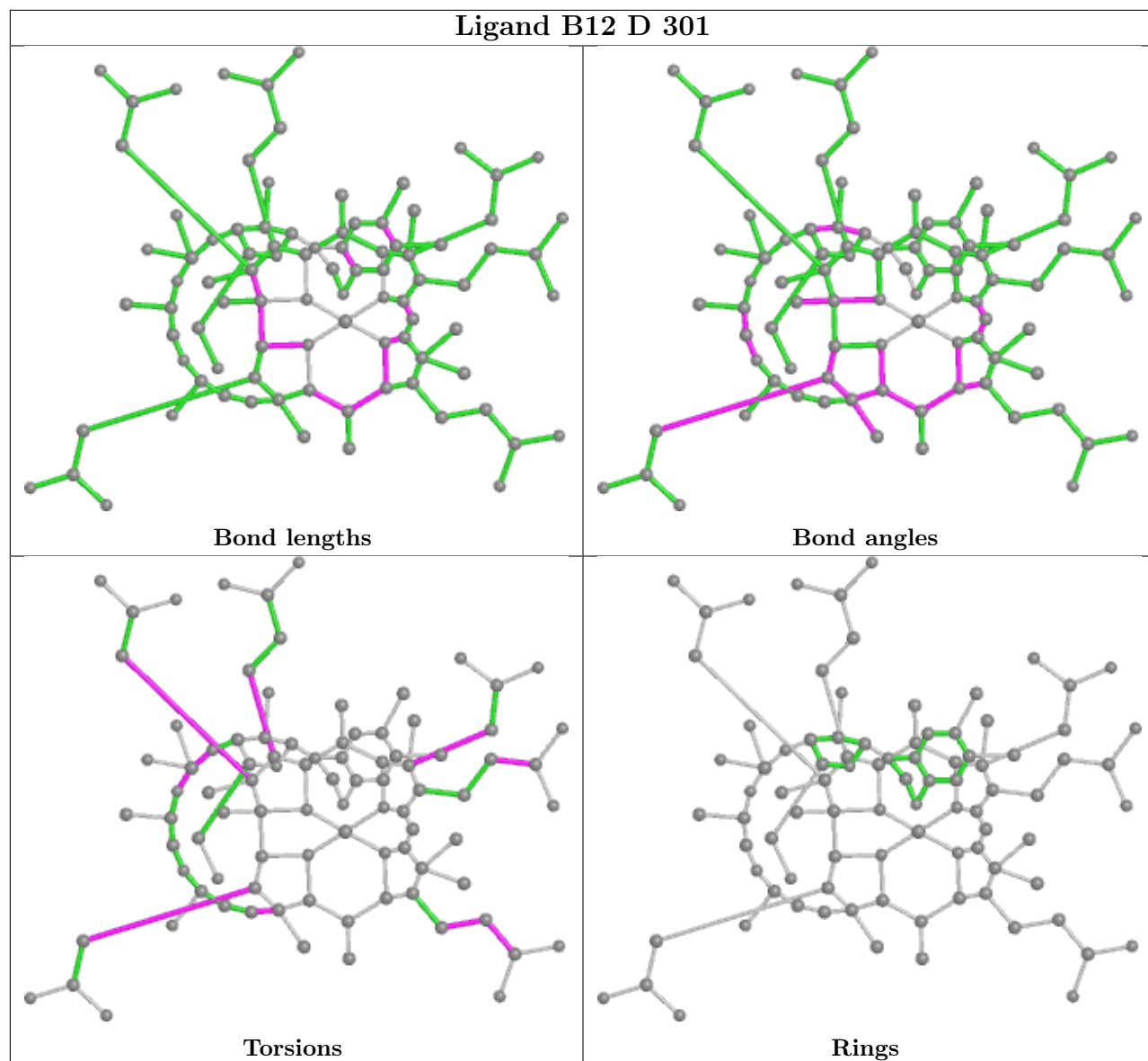
Mol	Chain	Res	Type	Atoms
6	D	301	B12	C38-C37-C7-C8
6	D	301	B12	C48-C49-C50-O51
6	D	301	B12	C3R-O2-P-O5
6	D	301	B12	C48-C49-C50-N52
6	B	301	B12	C38-C37-C7-C8
3	C	503	GOL	C1-C2-C3-O3
3	C	504	GOL	C1-C2-C3-O3
6	B	301	B12	C18-C60-C61-O63
6	D	301	B12	C17-C18-C60-C61
6	D	301	B12	C19-C18-C60-C61
6	B	301	B12	C3R-O2-P-O3
6	B	301	B12	C17-C18-C60-C61
6	B	301	B12	C48-C49-C50-O51
6	B	301	B12	C48-C49-C50-N52

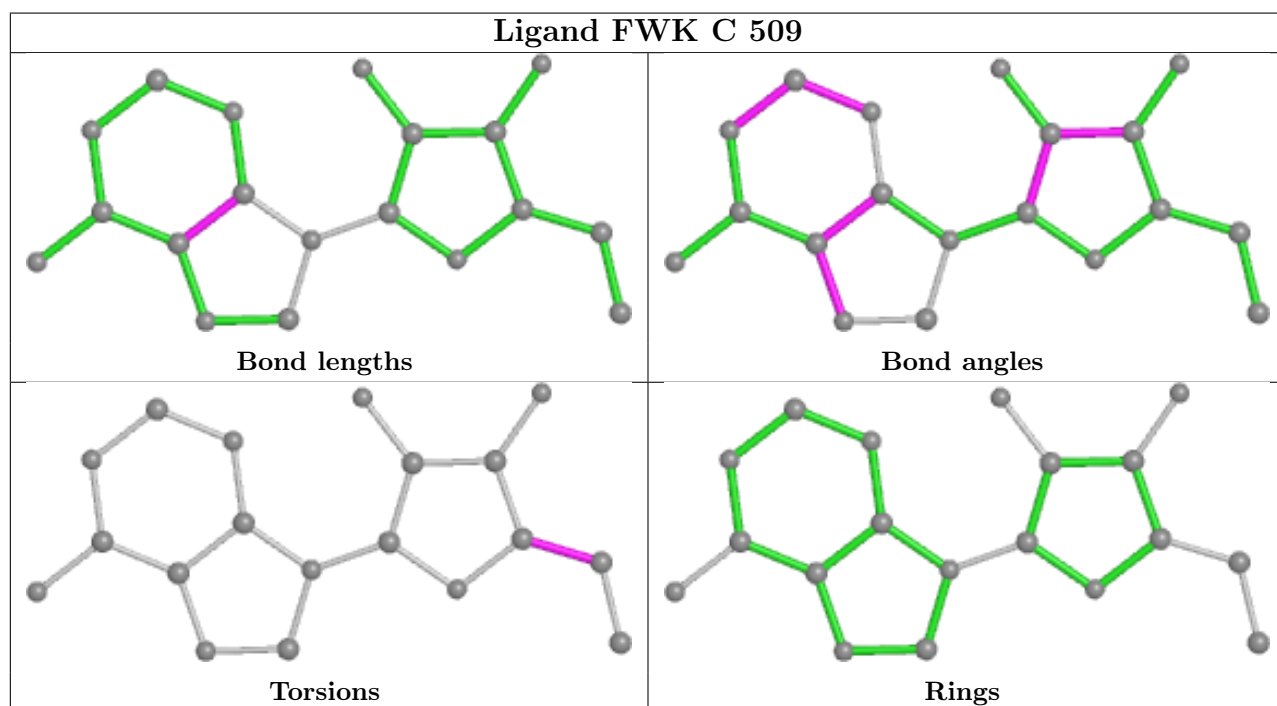
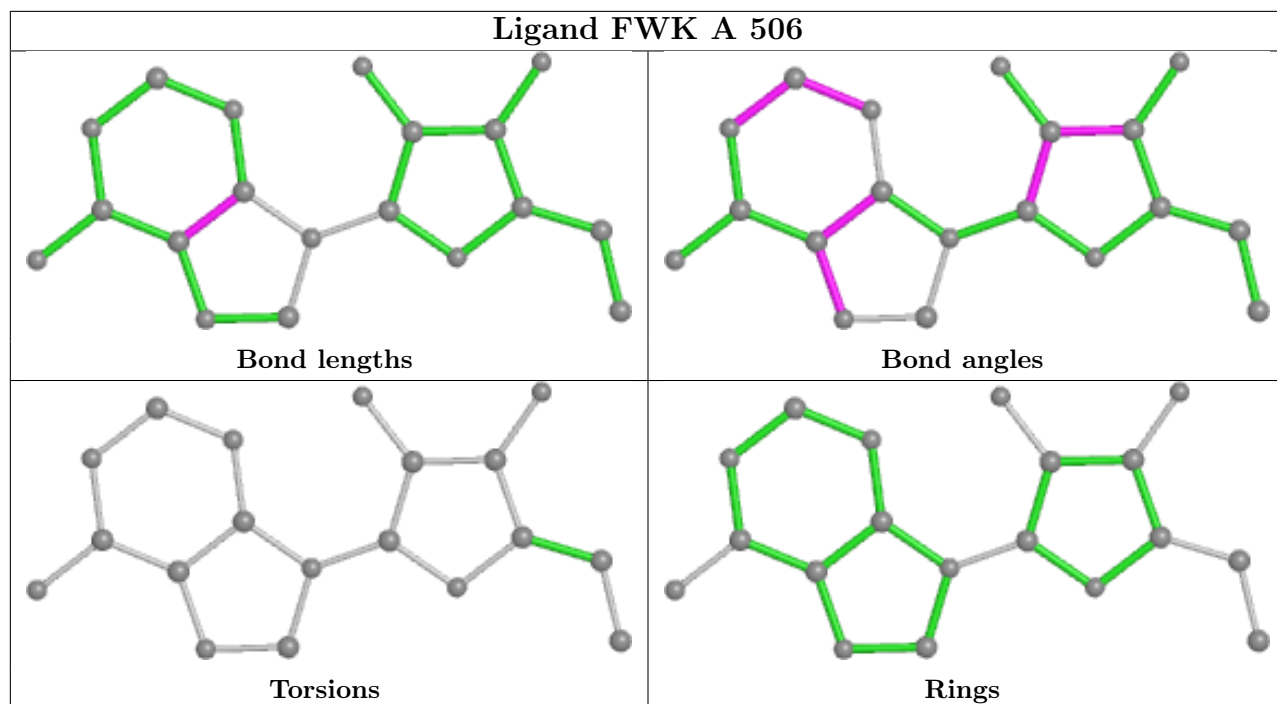
There are no ring outliers.

6 monomers are involved in 22 short contacts:

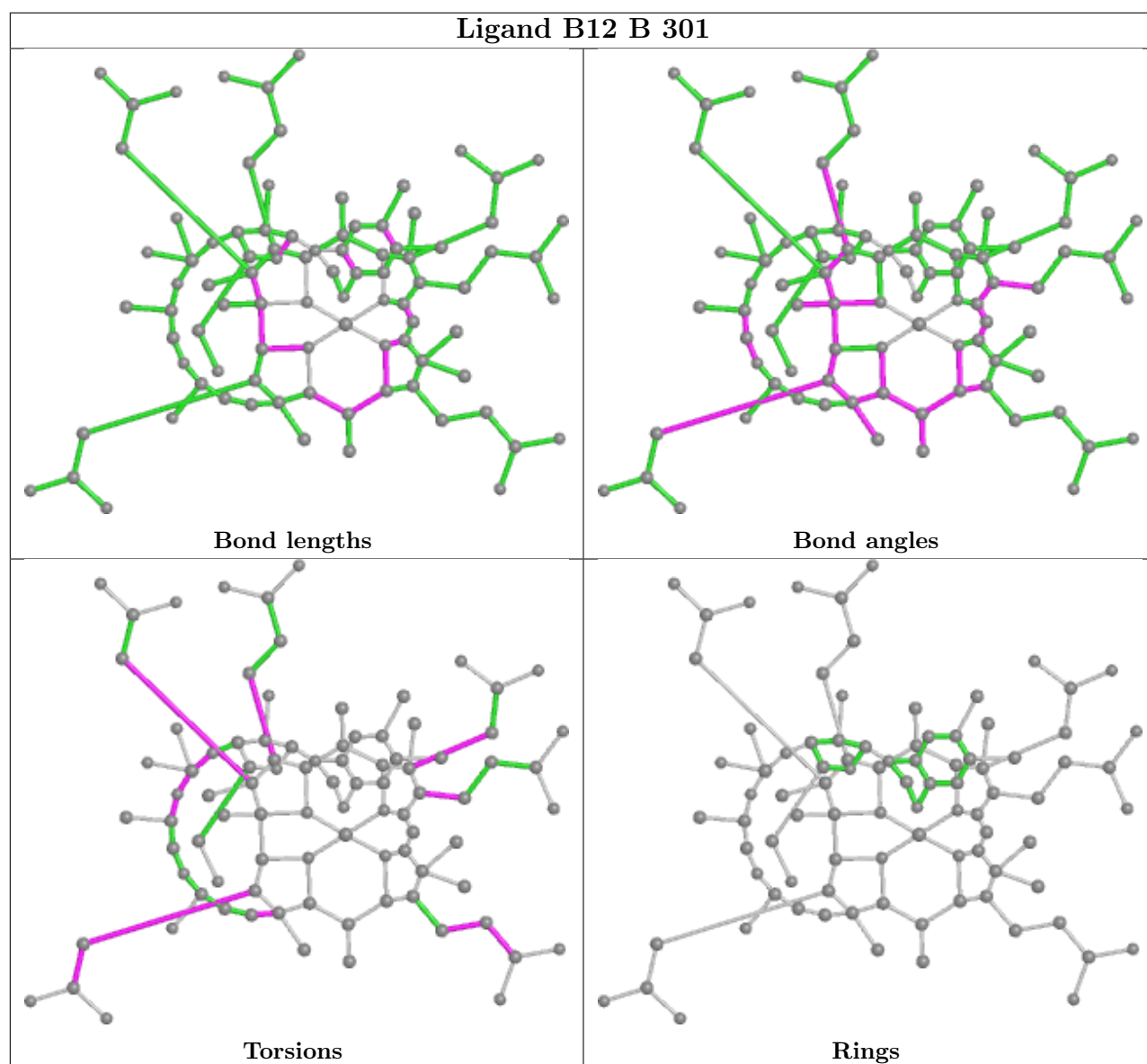
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	GOL	1	0
6	D	301	B12	8	0
3	A	501	GOL	1	0
3	C	505	GOL	1	0
6	B	301	B12	9	0
3	A	503	GOL	2	0

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.









## 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%)	-0.11	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	21, 34, 51, 74	0
1	C	453/453 (100%)	-0.14	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	20, 35, 55, 75	0
2	B	253/263 (96%)	0.17	7 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">61</span>	29, 58, 77, 107	0
2	D	252/263 (95%)	1.32	66 (26%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	28, 82, 124, 156	0
All	All	1411/1432 (98%)	0.19	73 (5%) <span style="border: 1px solid red; padding: 2px;">27</span> <span style="border: 1px solid red; padding: 2px;">33</span>	20, 41, 101, 156	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	121	LEU	9.2
2	D	148	VAL	9.0
2	D	161	VAL	8.7
2	D	192	ALA	8.4
2	D	189	LEU	6.8
2	D	145	ALA	6.7
2	D	216	ILE	5.7
2	D	152	LYS	5.6
2	D	286	GLN	5.5
2	D	151	LEU	5.5
2	D	246	PRO	5.0
2	D	202	VAL	5.0
2	D	164	VAL	4.7
2	D	222	VAL	4.6
2	D	188	GLY	4.1
2	D	120	LEU	4.1
2	D	178	TYR	4.1
2	D	160	ASP	4.0
2	D	223	ILE	4.0
2	D	132	LEU	3.9
2	D	221	VAL	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	163	VAL	3.7
2	D	143	LEU	3.7
2	D	243	VAL	3.6
2	D	215	GLU	3.5
2	D	245	SER	3.4
2	D	259	ILE	3.4
2	D	155	CYS	3.4
2	D	158	ASN	3.3
2	B	295	ARG	3.3
2	D	112	GLU	3.3
2	D	115	VAL	3.2
2	D	214	GLY	3.1
2	D	198	THR	3.1
2	D	212	GLN	3.0
2	B	190	LYS	2.9
2	D	116	LYS	2.9
2	D	201	PHE	2.9
2	D	285	GLU	2.9
2	D	220	LYS	2.9
2	D	196	VAL	2.8
2	D	187	ALA	2.7
2	B	191	GLN	2.7
2	D	194	LEU	2.7
2	D	279	LEU	2.7
2	D	199	PRO	2.7
2	D	242	ALA	2.7
2	D	111	PRO	2.6
2	D	250	THR	2.5
2	D	270	VAL	2.5
2	D	124	ARG	2.5
2	D	185	LEU	2.5
2	B	72	ARG	2.4
2	D	123	VAL	2.4
2	D	156	VAL	2.4
2	D	219	ALA	2.4
2	D	191	GLN	2.3
2	D	241	TYR	2.3
2	D	291	ILE	2.3
2	D	44	ALA	2.2
2	D	283	MET	2.2
2	D	224	LEU	2.2
2	D	149	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	249	ALA	2.2
2	D	181[A]	ILE	2.2
2	B	43	HIS	2.2
2	D	190	LYS	2.1
2	D	162	GLN	2.1
2	D	249	ALA	2.1
2	D	288	ALA	2.1
2	D	113	GLU	2.0
2	D	295	ARG	2.0
2	B	194	LEU	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 monosaccharides 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, 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.

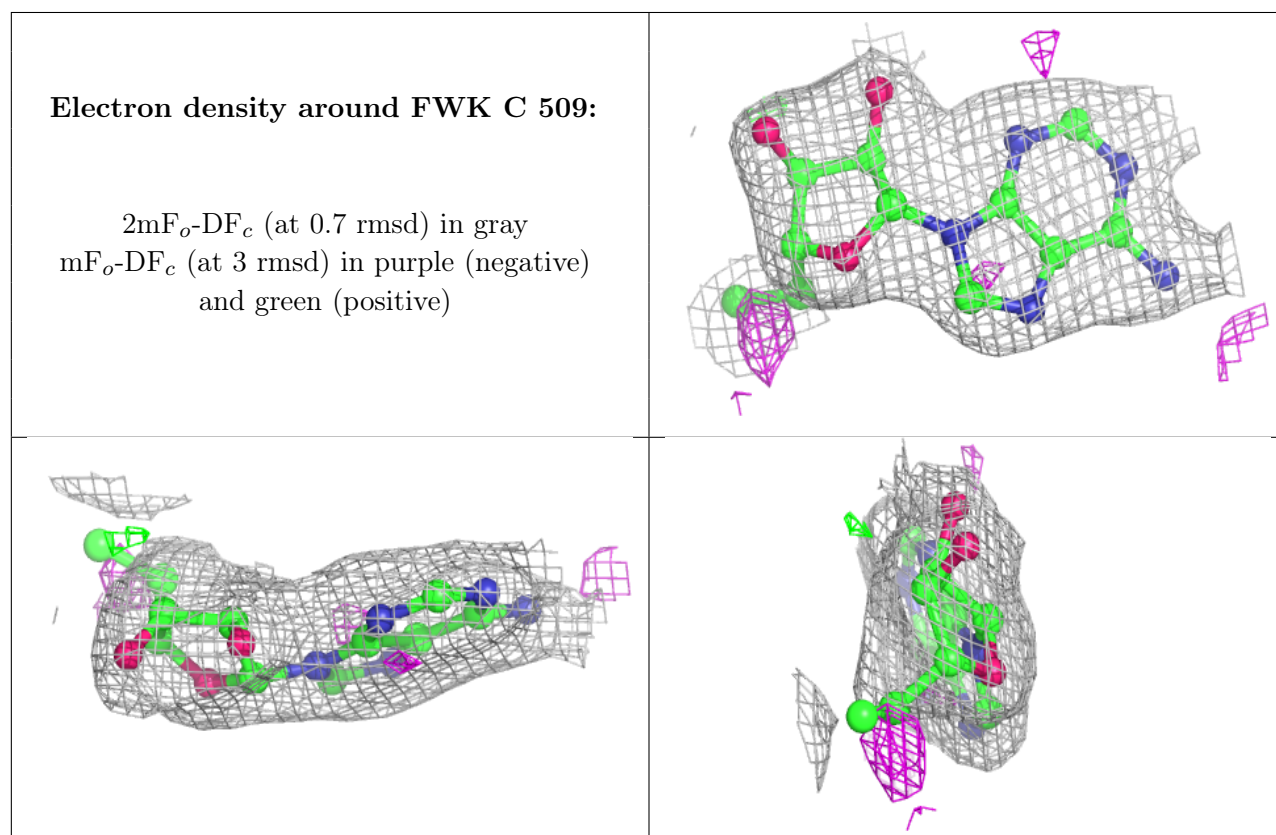
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	507	6/6	0.70	0.25	48,61,69,72	0
3	GOL	C	504	6/6	0.76	0.27	40,45,46,47	0
3	GOL	A	502	6/6	0.77	0.26	51,55,57,61	0
3	GOL	C	506	6/6	0.78	0.30	46,56,58,60	0
3	GOL	A	504	6/6	0.80	0.20	37,45,47,49	0
3	GOL	C	503	6/6	0.81	0.36	46,47,52,58	0
3	GOL	C	505	6/6	0.81	0.18	38,47,49,53	0
3	GOL	A	501	6/6	0.89	0.15	36,39,41,54	0
3	GOL	C	502	6/6	0.93	0.25	40,46,46,48	0
3	GOL	C	501	6/6	0.93	0.15	36,41,48,51	0
5	FWK	C	509	19/19	0.94	0.14	39,40,55,59	0
3	GOL	A	503	6/6	0.95	0.15	34,37,42,42	0
6	B12	D	301	91/91	0.95	0.15	47,62,71,76	0

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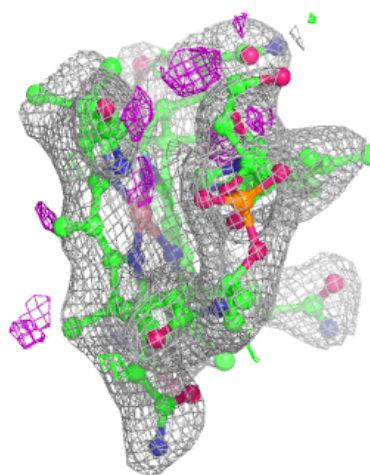
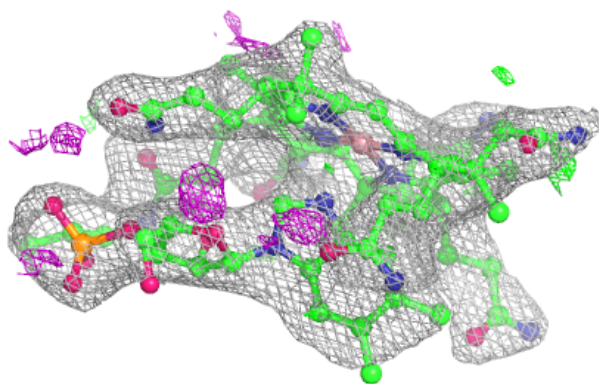
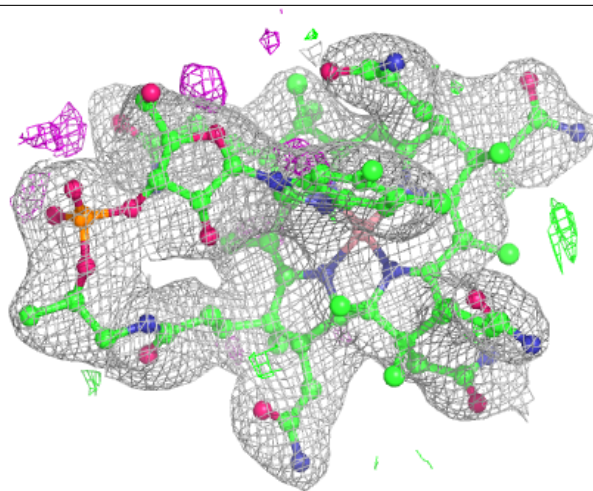
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NH4	C	508	1/1	0.96	0.29	35,35,35,35	0
6	B12	B	301	91/91	0.97	0.12	33,41,49,55	0
5	FWK	A	506	19/19	0.98	0.11	29,35,40,42	0
4	NH4	A	505	1/1	0.99	0.18	27,27,27,27	0

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.



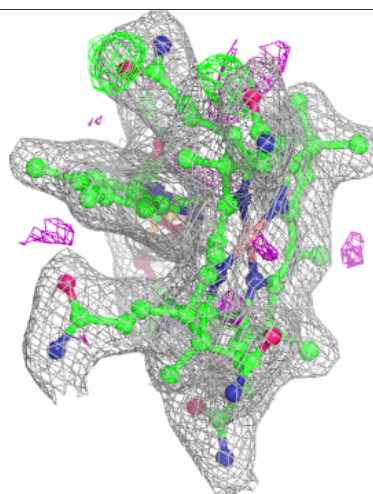
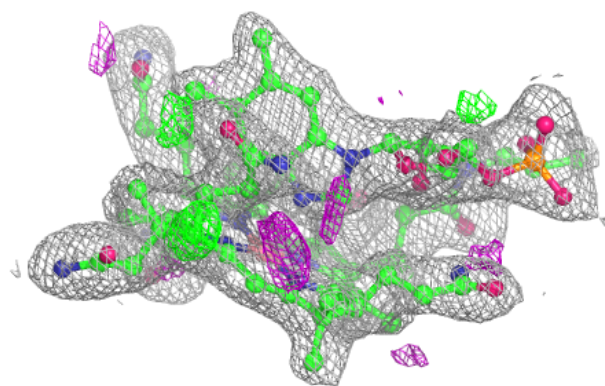
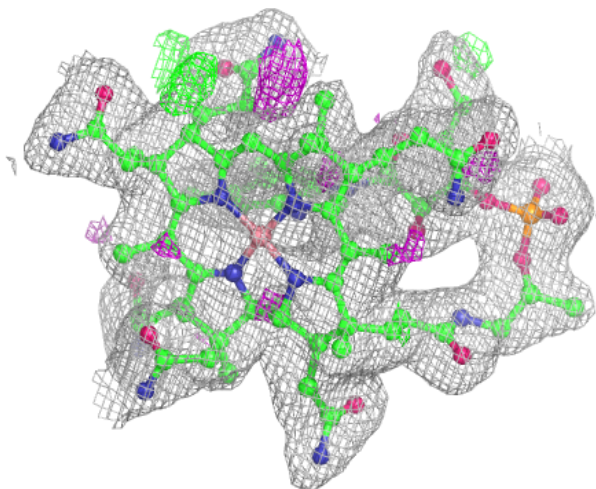
**Electron density around B12 D 301:**

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

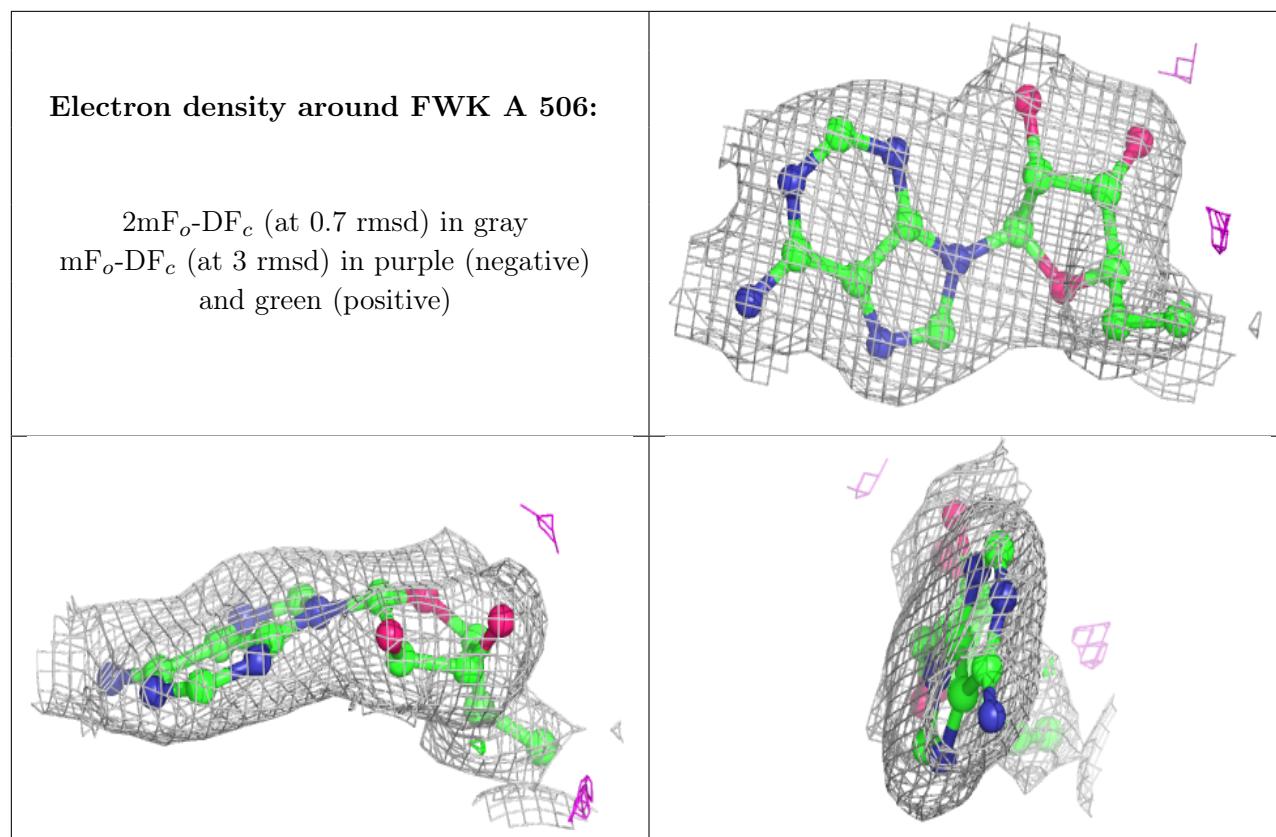


**Electron density around B12 B 301:**

$2mF_o-DF_c$  (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.