



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:58 pm BST

PDB ID : 1I9C  
Title : GLUTAMATE MUTASE FROM CLOSTRIDIUM COCHLEARIIUM: COM-  
PLEX WITH ADENOSYLCOBALAMIN AND SUBSTRATE  
Authors : Gruber, K.; Kratky, C.  
Deposited on : 2001-03-19  
Resolution : 1.90 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 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

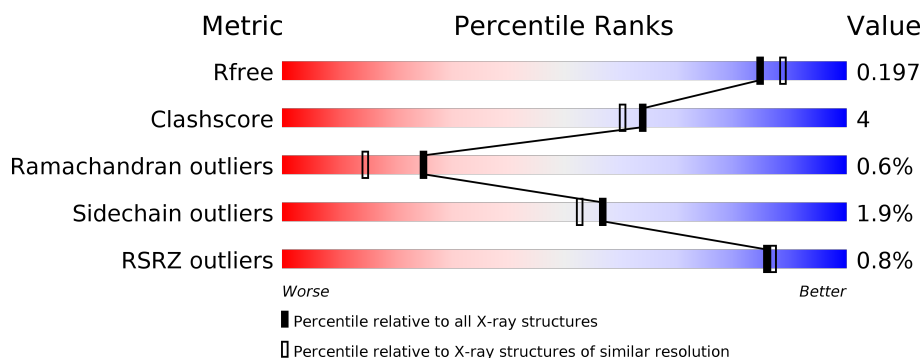
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	137	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>••</div> </div> </div>
1	C	137	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>•</div> </div> </div>
2	B	483	<div> <div></div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
2	D	483	<div> <div></div> <div> <div></div> <div>87%</div> <div>12%</div> <div>•</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLU	B	1305[A]	-	-	X	-
5	GLU	D	1306[A]	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11290 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 GLUTAMATE MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	1	0
			1046	665	177	199	5			
1	C	137	Total	C	N	O	S	0	1	0
			1046	665	177	199	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASN	VAL	SEE REMARK 999	UNP P80078
A	60	VAL	LEU	SEE REMARK 999	UNP P80078
C	45	ASN	VAL	SEE REMARK 999	UNP P80078
C	60	VAL	LEU	SEE REMARK 999	UNP P80078

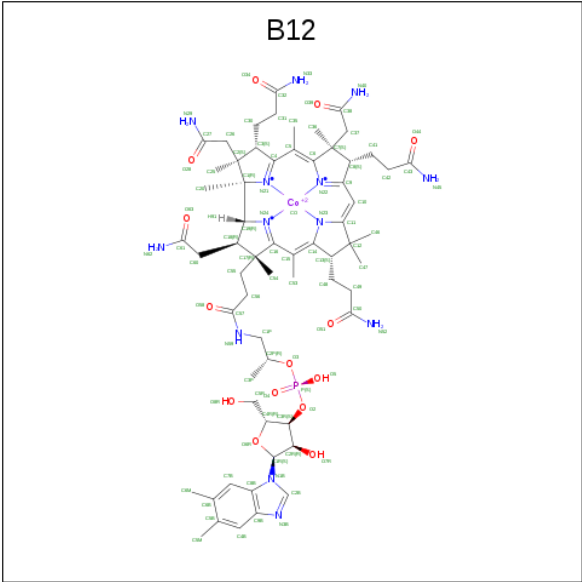
- Molecule 2 is a protein called GLUTAMATE MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	483	Total	C	N	O	S	0	15	0
			3823	2421	652	727	23			
2	D	483	Total	C	N	O	S	0	14	0
			3823	2423	651	726	23			

There are 2 discrepancies between the modelled and reference sequences:

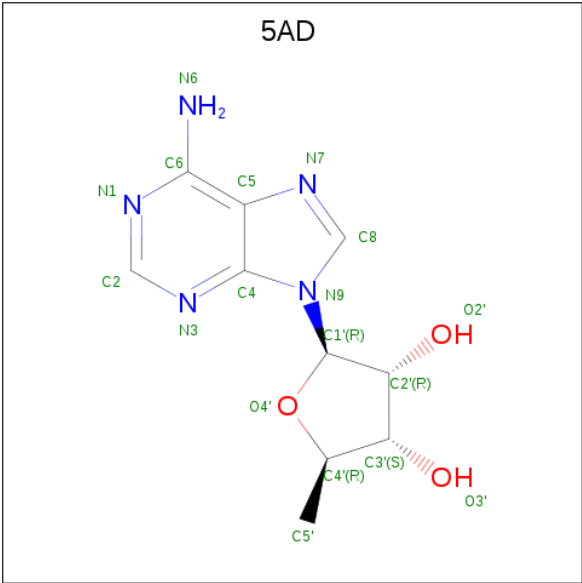
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	PHE	TYR	SEE REMARK 999	UNP P80077
D	130	PHE	TYR	SEE REMARK 999	UNP P80077

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



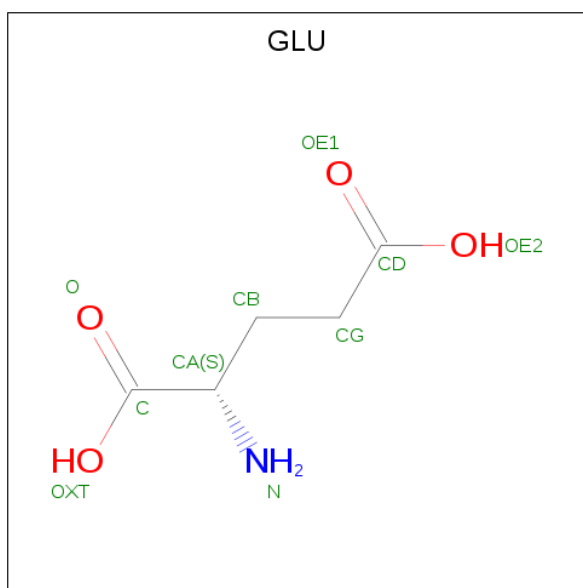
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



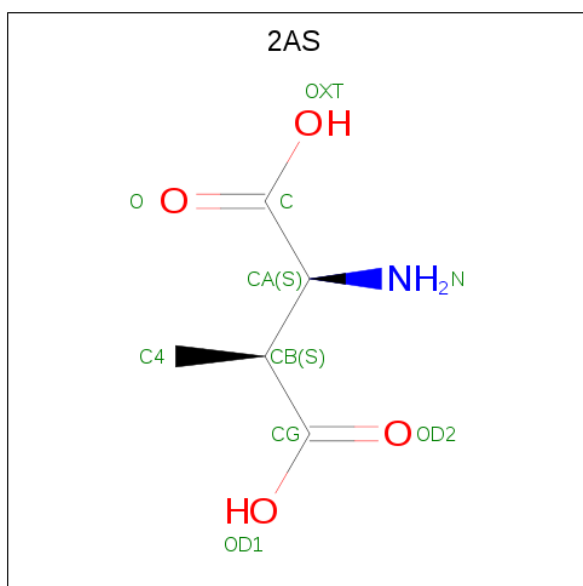
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			36	20	10	6		
4	D	1	Total	C	N	O	0	1
			36	20	10	6		

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	1
			10	5	1	4		
5	D	1	Total	C	N	O	0	1
			10	5	1	4		

- Molecule 6 is (2S,3S)-3-methyl-aspartic acid (three-letter code: 2AS) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	1
			10	5	1	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	1
			10	5	1	4		

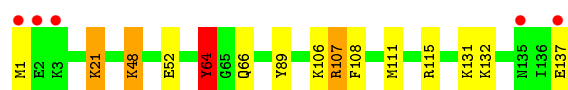
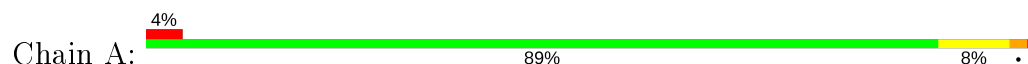
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	125	Total	O	0	0
			125	125		
7	B	494	Total	O	0	0
			494	494		
7	C	125	Total	O	0	0
			125	125		
7	D	514	Total	O	0	0
			514	514		

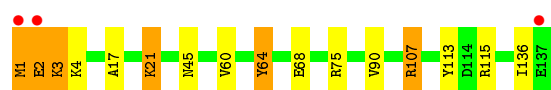
### 3 Residue-property plots [i](#)

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

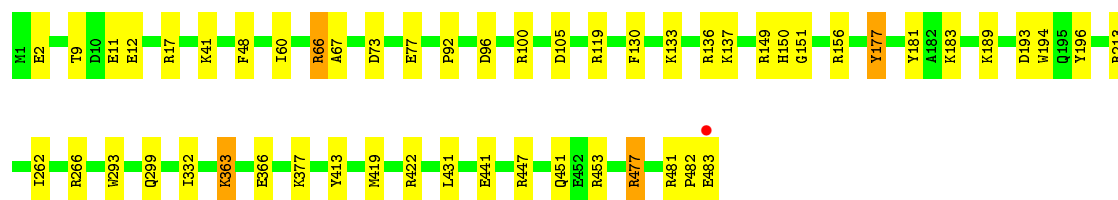
- Molecule 1: GLUTAMATE MUTASE



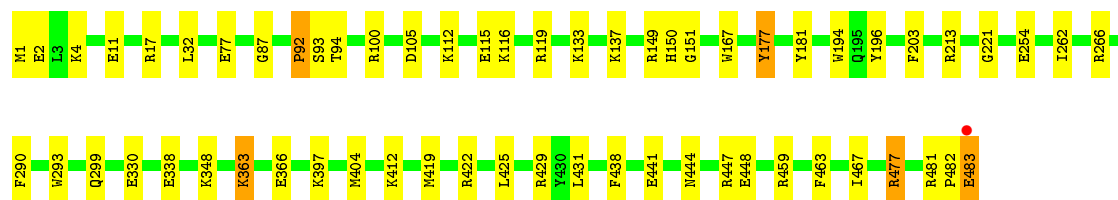
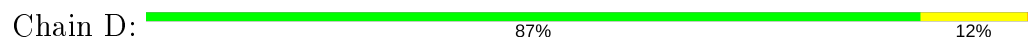
- Molecule 1: GLUTAMATE MUTASE



- Molecule 2: GLUTAMATE MUTASE



- Molecule 2: GLUTAMATE MUTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.35Å 113.14Å 108.44Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.90) 95.4 (29.84-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	32.83 (at 1.89Å)	Xtriage
Refinement program	SHELXL-97, REFMAC	Depositor
R, $R_{free}$	0.168 , 0.221 0.161 , 0.197	Depositor DCC
$R_{free}$ test set	6137 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.0	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: B12, 2AS, 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	0.42	0/1067	1.13	7/1438 (0.5%)
1	C	0.41	0/1067	1.13	7/1438 (0.5%)
2	B	0.43	0/3964	1.15	22/5342 (0.4%)
2	D	0.43	0/3954	1.16	23/5331 (0.4%)
All	All	0.43	0/10052	1.15	59/13549 (0.4%)

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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ARG	CD-NE-CZ	9.99	137.58	123.60
2	B	177	TYR	CB-CG-CD2	9.33	126.60	121.00
2	D	196	TYR	CB-CG-CD2	9.27	126.56	121.00
2	D	17	ARG	NE-CZ-NH1	8.91	124.76	120.30
2	B	413	TYR	CB-CG-CD2	-8.37	115.98	121.00
2	B	156	ARG	NE-CZ-NH2	-8.31	116.14	120.30
2	B	136	ARG	NE-CZ-NH2	-7.98	116.31	120.30
2	B	422	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	D	477[A]	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	D	477[B]	ARG	NE-CZ-NH1	7.60	124.10	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	196	TYR	CG-CD2-CE2	7.54	127.33	121.30
2	D	459	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	B	119	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	B	196	TYR	CG-CD2-CE2	7.33	127.16	121.30
1	A	64	TYR	CB-CG-CD1	7.19	125.31	121.00
2	D	17	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	107	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	B	66	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	89	TYR	CB-CG-CD1	6.81	125.09	121.00
2	B	453	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	D	213	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	B	477[A]	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	477[B]	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	17	ARG	CD-NE-CZ	6.54	132.75	123.60
1	A	115	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	D	11	GLU	C-N-CA	6.30	137.45	121.70
2	B	447	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	89	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	C	113	TYR	CB-CG-CD2	6.17	124.70	121.00
2	D	194	TRP	CA-CB-CG	-6.09	102.12	113.70
2	B	149	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	B	130	PHE	CD1-CE1-CZ	5.99	127.28	120.10
1	C	115	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	B	453	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	D	177	TYR	CB-CG-CD2	5.72	124.43	121.00
2	D	119	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	149	ARG	CD-NE-CZ	5.68	131.55	123.60
2	B	194	TRP	CA-CB-CG	-5.63	103.01	113.70
1	C	64	TYR	CB-CG-CD1	5.62	124.38	121.00
1	A	115	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	113	TYR	CB-CG-CD1	-5.53	117.68	121.00
2	B	11	GLU	C-N-CA	5.51	135.48	121.70
2	D	100	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	D	447	ARG	CD-NE-CZ	5.46	131.24	123.60
2	D	404	MET	CA-CB-CG	5.40	122.48	113.30
1	C	64	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	D	105	ASP	CB-CG-OD1	5.36	123.13	118.30
2	D	441	GLU	C-N-CA	5.34	135.05	121.70
1	C	75	ARG	CD-NE-CZ	5.30	131.02	123.60
2	D	338	GLU	C-N-CA	5.29	134.93	121.70
2	B	213	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	B	105	ASP	CB-CG-OD1	5.21	122.98	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	149	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	D	422	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	D	429	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	64	TYR	CA-CB-CG	5.12	123.12	113.40
2	D	438	PHE	CB-CG-CD1	5.03	124.32	120.80
2	B	66	ARG	CD-NE-CZ	5.02	130.62	123.60
2	D	459	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	92	PRO	Peptide
2	D	92	PRO	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	1046	0	1061	7	0
1	C	1046	0	1061	11	0
2	B	3823	0	3812	25	0
2	D	3823	0	3819	30	0
3	A	91	0	88	1	0
3	C	91	0	88	2	0
4	B	36	0	26	3	0
4	D	36	0	26	4	0
5	B	10	0	5	7	0
5	D	10	0	5	6	0
6	B	10	0	7	1	0
6	D	10	0	7	1	0
7	A	125	0	0	2	0
7	B	494	0	0	9	0
7	C	125	0	0	1	0
7	D	514	0	0	10	0
All	All	11290	0	10005	84	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 4.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLU:O	1:C:2:GLU:HG2	1.43	1.10
2:D:177:TYR:HH	5:D:1306[A]:GLU:N	1.69	0.90
1:C:2:GLU:CG	1:C:2:GLU:O	2.22	0.87
2:B:189:LYS:HE2	2:B:193:ASP:OD2	1.83	0.79
2:D:2:GLU:OE1	2:D:4:LYS:HE3	1.83	0.78
2:B:177:TYR:HH	5:B:1305[A]:GLU:N	1.81	0.78
4:D:1304[A]:5AD:H5'1	5:D:1306[A]:GLU:HG2	1.69	0.74
2:B:41:LYS:HE3	7:B:1617:HOH:O	1.90	0.71
4:B:1303[A]:5AD:H5'1	5:B:1305[A]:GLU:HG2	1.73	0.70
2:D:419:MET:HG3	7:D:1799:HOH:O	1.92	0.69
2:B:73:ASP:O	2:B:77[B]:GLU:HG3	1.93	0.68
2:D:94:THR:HG21	4:D:1304[B]:5AD:N7	2.10	0.66
2:B:377:LYS:HD2	7:B:1666:HOH:O	2.00	0.62
2:D:133:LYS:O	2:D:137:LYS:HG2	1.99	0.62
2:D:477[B]:ARG:NH2	2:D:481:ARG:HG3	2.16	0.60
5:B:1305[A]:GLU:HG3	5:B:1305[A]:GLU:OXT	2.05	0.57
2:D:137:LYS:HE2	7:D:1438:HOH:O	2.05	0.56
2:B:366:GLU:HG2	7:B:1766:HOH:O	2.05	0.55
2:D:330:GLU:OE2	4:D:1304[B]:5AD:H3'	2.07	0.55
2:B:9:THR:OG1	2:B:12:GLU:HG3	2.07	0.54
2:B:189:LYS:HE3	7:B:1672:HOH:O	2.06	0.54
2:D:112:LYS:HE2	2:D:115:GLU:OE1	2.08	0.54
1:C:68:GLU:OE2	1:C:107:ARG:HD3	2.08	0.54
1:C:1:MET:O	1:C:4:LYS:HE2	2.08	0.53
2:B:133:LYS:O	2:B:137:LYS:HG3	2.08	0.53
2:D:363[A]:LYS:HE3	2:D:366:GLU:OE1	2.09	0.52
4:B:1303[A]:5AD:C5'	5:B:1305[A]:GLU:HG2	2.40	0.52
2:B:482:PRO:O	2:B:483:GLU:HB2	2.08	0.51
2:D:32:LEU:HD13	2:D:203:PHE:CE2	2.45	0.51
2:B:2:GLU:OE1	2:B:2:GLU:HA	2.11	0.51
5:D:1306[A]:GLU:HG3	5:D:1306[A]:GLU:OXT	2.11	0.51
2:D:77[B]:GLU:HG3	7:D:1504:HOH:O	2.11	0.50
1:A:1:MET:SD	1:A:131:LYS:HE2	2.50	0.50
2:D:397:LYS:HE3	7:D:1566:HOH:O	2.11	0.49
2:B:181:TYR:HH	5:B:1305[A]:GLU:HB2	1.77	0.49
2:D:482:PRO:O	2:D:483:GLU:O	2.30	0.49
2:D:181:TYR:OH	6:D:1308[B]:2AS:H4B	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLU:HG2	7:A:837:HOH:O	2.12	0.48
2:B:181:TYR:OH	5:B:1305[A]:GLU:HB2	2.13	0.48
4:D:1304[A]:5AD:C5'	5:D:1306[A]:GLU:HG2	2.41	0.48
1:A:132:LYS:HD3	7:A:916:HOH:O	2.13	0.48
2:B:477[B]:ARG:NH2	2:B:481:ARG:HG3	2.29	0.47
1:C:1:MET:CE	1:C:2:GLU:HB3	2.44	0.47
1:A:48:LYS:O	1:A:52:GLU:HG3	2.15	0.47
1:C:60:VAL:O	1:C:90:VAL:HA	2.14	0.47
2:D:116:LYS:HE3	7:D:1775:HOH:O	2.15	0.47
2:B:66:ARG:O	2:B:67:ALA:HB2	2.16	0.46
2:D:254:GLU:HB2	2:D:290:PHE:CZ	2.50	0.46
1:C:17:ALA:O	1:C:21[A]:LYS:HD2	2.16	0.46
2:B:266:ARG:HD2	7:B:1659:HOH:O	2.15	0.46
1:C:1:MET:HB3	1:C:136:ILE:CG2	2.46	0.46
2:B:451[A]:GLN:NE2	7:B:1501:HOH:O	2.50	0.45
2:B:96:ASP:O	2:B:100:ARG:HG3	2.17	0.45
3:C:800:B12:H372	3:C:800:B12:H351	1.98	0.45
2:B:262:ILE:O	2:B:266:ARG:HG3	2.17	0.45
2:B:66:ARG:HD3	4:B:1303[A]:5AD:O4'	2.16	0.45
2:D:419:MET:SD	2:D:431:LEU:HD23	2.57	0.45
2:D:299:GLN:HG3	7:D:1529:HOH:O	2.16	0.45
5:D:1306[A]:GLU:HG3	7:D:1325:HOH:O	2.17	0.45
2:D:77[B]:GLU:HG2	7:D:1575:HOH:O	2.17	0.44
2:D:181:TYR:OH	5:D:1306[A]:GLU:HB2	2.17	0.44
2:D:444[A]:ASN:ND2	2:D:448:GLU:OE2	2.50	0.44
2:B:181:TYR:OH	6:B:1307[B]:2AS:H4B	2.17	0.44
2:B:299:GLN:CG	2:B:332:ILE:HD11	2.46	0.44
2:B:419:MET:SD	2:B:431:LEU:HD23	2.58	0.44
2:B:441[B]:GLU:HG3	7:B:1514:HOH:O	2.16	0.44
1:C:45:ASN:ND2	7:C:918:HOH:O	2.50	0.44
2:D:221:GLY:HA2	7:D:1466:HOH:O	2.17	0.44
3:C:800:B12:O39	3:C:800:B12:H361	2.18	0.43
2:D:482:PRO:O	2:D:483:GLU:HG3	2.18	0.43
3:A:800:B12:H372	3:A:800:B12:H351	2.00	0.43
2:D:87:GLY:O	2:D:348:LYS:HD2	2.19	0.43
1:C:1:MET:HE2	1:C:2:GLU:HB3	2.01	0.42
2:D:262:ILE:O	2:D:266:ARG:HG3	2.19	0.42
1:A:64:TYR:CE1	1:A:66:GLN:HB2	2.56	0.41
1:C:1:MET:HB3	1:C:136:ILE:HG21	2.02	0.41
2:D:463:PHE:CE2	2:D:467:ILE:HD11	2.56	0.41
1:A:108:PHE:O	1:A:111:MET:HB2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:SER:HB2	2:D:167:TRP:CZ3	2.56	0.41
2:D:1:MET:HG3	7:D:1819:HOH:O	2.20	0.40
5:B:1305[A]:GLU:HG3	7:B:1315:HOH:O	2.21	0.40
2:B:363[A]:LYS:NZ	7:B:1766:HOH:O	2.53	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	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
1	C	136/137 (99%)	131 (96%)	4 (3%)	1 (1%)	22	12
2	B	496/483 (103%)	487 (98%)	6 (1%)	3 (1%)	25	15
2	D	495/483 (102%)	487 (98%)	5 (1%)	3 (1%)	25	15
All	All	1263/1240 (102%)	1238 (98%)	18 (1%)	7 (1%)	25	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	293	TRP
1	C	3	LYS
2	D	150	HIS
2	B	150	HIS
2	D	151	GLY
2	B	151	GLY
2	D	293	TRP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/111 (101%)	106 (95%)	6 (5%)	22	13
1	C	112/111 (101%)	106 (95%)	6 (5%)	22	13
2	B	411/396 (104%)	406 (99%)	5 (1%)	71	70
2	D	410/396 (104%)	403 (98%)	7 (2%)	60	57
All	All	1045/1014 (103%)	1021 (98%)	24 (2%)	57	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21[A]	LYS
1	A	21[B]	LYS
1	A	48	LYS
1	A	64	TYR
1	A	106	LYS
1	A	107	ARG
2	B	48	PHE
2	B	60	ILE
2	B	183	LYS
2	B	363[A]	LYS
2	B	363[B]	LYS
1	C	1	MET
1	C	2	GLU
1	C	3	LYS
1	C	21[A]	LYS
1	C	21[B]	LYS
1	C	64	TYR
2	D	92	PRO
2	D	363[A]	LYS
2	D	363[B]	LYS
2	D	412	LYS
2	D	425[A]	LEU
2	D	425[B]	LEU
2	D	483	GLU



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

Mol	Chain	Res	Type
2	B	23	GLN
1	C	33	ASN
2	D	23	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](#)

10 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
3	B12	A	800	1	80,101,101	0.80	0	101,166,166	1.33	16 (15%)
3	B12	C	800	1	80,101,101	0.86	2 (2%)	101,166,166	1.37	19 (18%)
4	5AD	B	1303[A]	-	17,20,20	1.40	3 (17%)	15,30,30	2.02	5 (33%)
4	5AD	B	1303[B]	-	17,20,20	1.52	3 (17%)	15,30,30	1.95	6 (40%)
6	2AS	B	1307[B]	-	3,9,9	1.41	0	2,12,12	1.61	1 (50%)
6	2AS	D	1308[B]	-	3,9,9	0.98	0	2,12,12	0.71	0
4	5AD	D	1304[A]	-	17,20,20	1.25	2 (11%)	15,30,30	1.92	5 (33%)
4	5AD	D	1304[B]	-	17,20,20	1.49	4 (23%)	15,30,30	1.88	7 (46%)

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	B12	A	800	1	-	13/51/223/223	0/3/11/11
3	B12	C	800	1	-	13/51/223/223	0/3/11/11
4	5AD	B	1303[A]	-	-	0/0/20/20	0/3/3/3
4	5AD	B	1303[B]	-	-	0/0/20/20	0/3/3/3
6	2AS	B	1307[B]	-	-	3/4/12/12	-
6	2AS	D	1308[B]	-	-	2/4/12/12	-
4	5AD	D	1304[A]	-	-	0/0/20/20	0/3/3/3
4	5AD	D	1304[B]	-	-	0/0/20/20	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1303[B]	5AD	O4'-C1'	3.71	1.46	1.41
4	D	1304[B]	5AD	O4'-C1'	3.38	1.45	1.41
4	B	1303[A]	5AD	O4'-C1'	3.13	1.45	1.41
3	C	800	B12	C2-C3	-2.78	1.53	1.58
4	B	1303[B]	5AD	C8-N7	-2.61	1.30	1.34
4	D	1304[A]	5AD	O4'-C1'	2.58	1.44	1.41
4	B	1303[A]	5AD	C8-N7	-2.56	1.30	1.34
4	D	1304[B]	5AD	C3'-C4'	2.50	1.56	1.52
4	B	1303[B]	5AD	C3'-C4'	2.44	1.56	1.52
4	D	1304[B]	5AD	C8-N7	-2.43	1.30	1.34
4	D	1304[A]	5AD	C8-N7	-2.14	1.30	1.34
3	C	800	B12	P-O5	-2.07	1.45	1.55
4	D	1304[B]	5AD	C5-C4	-2.06	1.35	1.40
4	B	1303[A]	5AD	O3'-C3'	-2.01	1.38	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1303[A]	5AD	C5'-C4'-C3'	-4.26	111.23	115.70
4	B	1303[B]	5AD	O4'-C1'-C2'	-3.87	101.27	106.93
4	D	1304[A]	5AD	C5-C6-N6	3.81	126.15	120.35
4	D	1304[B]	5AD	C5-C6-N6	3.45	125.59	120.35
4	B	1303[A]	5AD	C5-C6-N6	3.28	125.33	120.35
3	C	800	B12	C2-C3-C4	3.27	105.10	101.67
4	B	1303[B]	5AD	C5'-C4'-C3'	-3.20	112.34	115.70
3	A	800	B12	C2-C3-C4	3.17	105.00	101.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1304[A]	5AD	C5'-C4'-C3'	-3.17	112.37	115.70
3	C	800	B12	C18-C60-C61	3.09	121.69	113.97
4	B	1303[A]	5AD	C4-C5-N7	3.07	112.60	109.40
3	A	800	B12	O6R-C1R-C2R	-3.05	102.47	106.93
3	A	800	B12	C55-C17-C16	3.04	120.06	109.92
4	B	1303[B]	5AD	C4-C5-N7	2.94	112.46	109.40
4	D	1304[B]	5AD	O4'-C1'-C2'	-2.92	102.67	106.93
3	C	800	B12	C8-C9-N22	2.87	114.71	111.12
4	B	1303[B]	5AD	C5-C6-N6	2.84	124.67	120.35
3	A	800	B12	C18-C60-C61	2.79	120.92	113.97
4	D	1304[B]	5AD	C4-C5-N7	2.76	112.28	109.40
3	A	800	B12	C5M-C5B-C6B	2.73	126.34	120.74
3	A	800	B12	C8-C9-N22	2.73	114.53	111.12
4	D	1304[A]	5AD	C4-C5-N7	2.72	112.23	109.40
3	C	800	B12	C55-C17-C16	2.71	118.95	109.92
3	C	800	B12	C6M-C6B-C7B	-2.63	114.05	120.34
4	B	1303[A]	5AD	O3'-C3'-C2'	2.63	120.32	111.82
4	D	1304[B]	5AD	C5'-C4'-C3'	-2.59	112.98	115.70
3	C	800	B12	C5M-C5B-C6B	2.55	125.95	120.74
3	C	800	B12	C6M-C6B-C5B	2.47	125.80	120.74
3	A	800	B12	C6M-C6B-C7B	-2.46	114.45	120.34
3	C	800	B12	C55-C17-C18	-2.45	106.41	111.14
3	C	800	B12	C37-C38-N40	2.44	124.26	116.52
4	B	1303[B]	5AD	C3'-C2'-C1'	-2.35	97.44	100.98
3	A	800	B12	C13-C14-C15	-2.32	123.25	131.68
3	C	800	B12	C5M-C5B-C4B	-2.31	114.81	120.34
3	C	800	B12	O5-P-O4	2.30	123.64	112.24
4	B	1303[A]	5AD	C5-C6-N1	-2.29	115.16	120.35
6	B	1307[B]	2AS	C4-CB-CA	2.27	114.65	111.34
3	C	800	B12	C4B-C9B-C8B	-2.21	118.84	121.10
3	A	800	B12	C1-C19-N24	2.21	108.72	106.24
4	D	1304[A]	5AD	C5-C6-N1	-2.19	115.39	120.35
3	C	800	B12	C41-C8-C7	2.17	119.96	114.08
3	A	800	B12	C5M-C5B-C4B	-2.17	115.16	120.34
4	D	1304[B]	5AD	C5-C6-N1	-2.16	115.45	120.35
3	C	800	B12	C36-C7-C37	-2.16	107.14	110.83
3	A	800	B12	O7R-C2R-C3R	2.13	117.21	111.17
3	C	800	B12	C1-C19-N24	2.12	108.62	106.24
4	D	1304[A]	5AD	O2'-C2'-C3'	2.11	118.65	111.82
3	A	800	B12	C5-C6-N22	2.11	128.65	124.81
3	C	800	B12	C30-C31-C32	2.10	119.72	112.59
3	C	800	B12	C48-C49-C50	-2.09	105.50	112.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C5-C6-N22	2.09	128.61	124.81
4	B	1303[B]	5AD	C5-C6-N1	-2.07	115.65	120.35
4	D	1304[B]	5AD	C3'-C2'-C1'	-2.07	97.86	100.98
3	A	800	B12	O5-P-O4	2.07	122.46	112.24
3	A	800	B12	C20-C1-C19	2.07	111.34	109.36
3	A	800	B12	C6M-C6B-C5B	2.05	124.93	120.74
3	A	800	B12	C55-C17-C18	-2.05	107.19	111.14
3	C	800	B12	C25-C2-C1	2.02	116.81	113.80
4	D	1304[B]	5AD	C1'-N9-C4	-2.02	123.10	126.64

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	B12	C38-C37-C7-C36
3	A	800	B12	C38-C37-C7-C8
3	A	800	B12	C1P-C2P-O3-P
3	A	800	B12	C3P-C2P-O3-P
3	C	800	B12	C38-C37-C7-C36
3	C	800	B12	C38-C37-C7-C8
3	C	800	B12	C1P-C2P-O3-P
3	C	800	B12	C3P-C2P-O3-P
6	B	1307[B]	2AS	C-CA-CB-CG
6	B	1307[B]	2AS	N-CA-CB-CG
3	C	800	B12	C8-C41-C42-C43
3	C	800	B12	C2P-O3-P-O2
3	A	800	B12	C8-C41-C42-C43
6	B	1307[B]	2AS	C-CA-CB-C4
3	A	800	B12	C2P-O3-P-O2
3	C	800	B12	C30-C31-C32-N33
3	C	800	B12	C30-C31-C32-O34
3	A	800	B12	C4-C3-C30-C31
3	A	800	B12	C55-C56-C57-O58
3	A	800	B12	C18-C60-C61-O63
3	C	800	B12	C18-C60-C61-O63
3	C	800	B12	C18-C60-C61-N62
3	A	800	B12	C30-C31-C32-O34
3	C	800	B12	C55-C56-C57-O58
3	A	800	B12	C18-C60-C61-N62
6	D	1308[B]	2AS	C-CA-CB-C4
3	A	800	B12	C30-C31-C32-N33
3	A	800	B12	C55-C56-C57-N59

*Continued on next page...*

*Continued from previous page...*

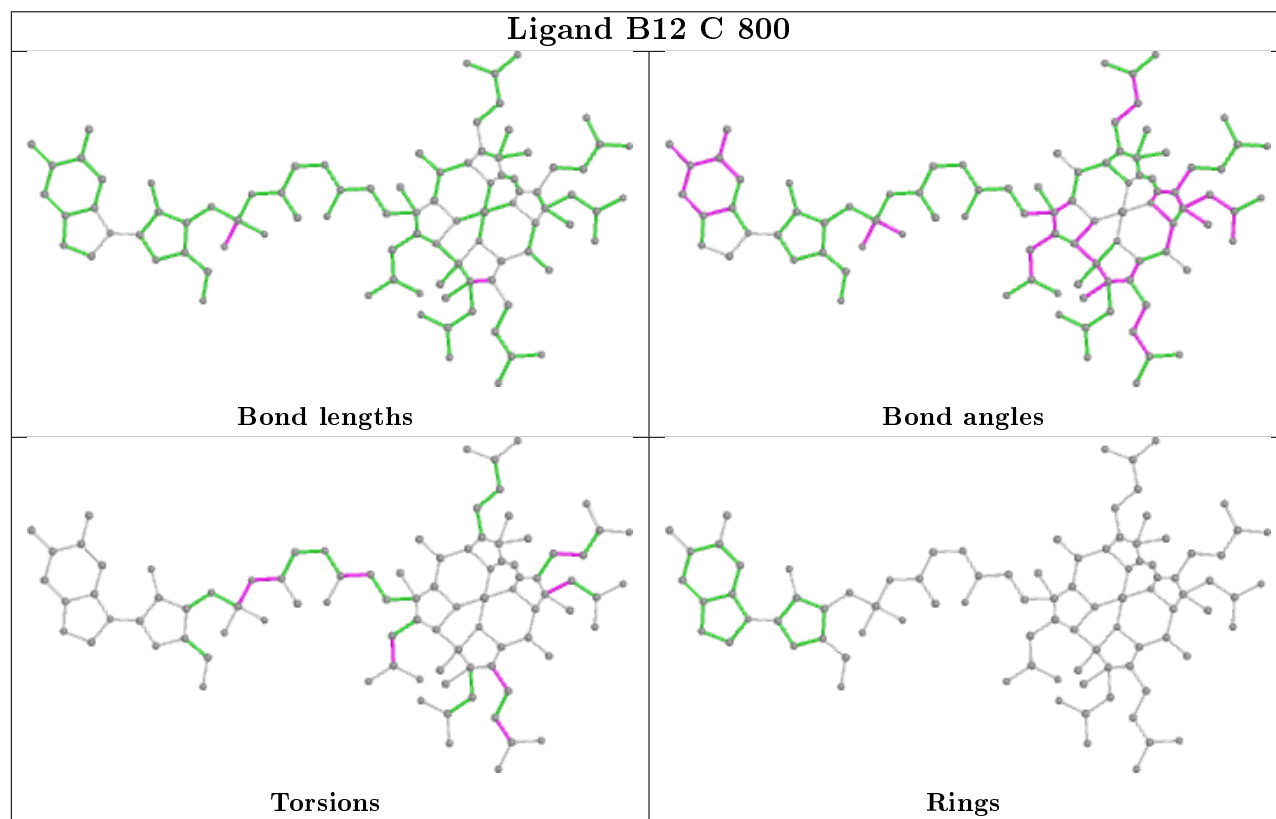
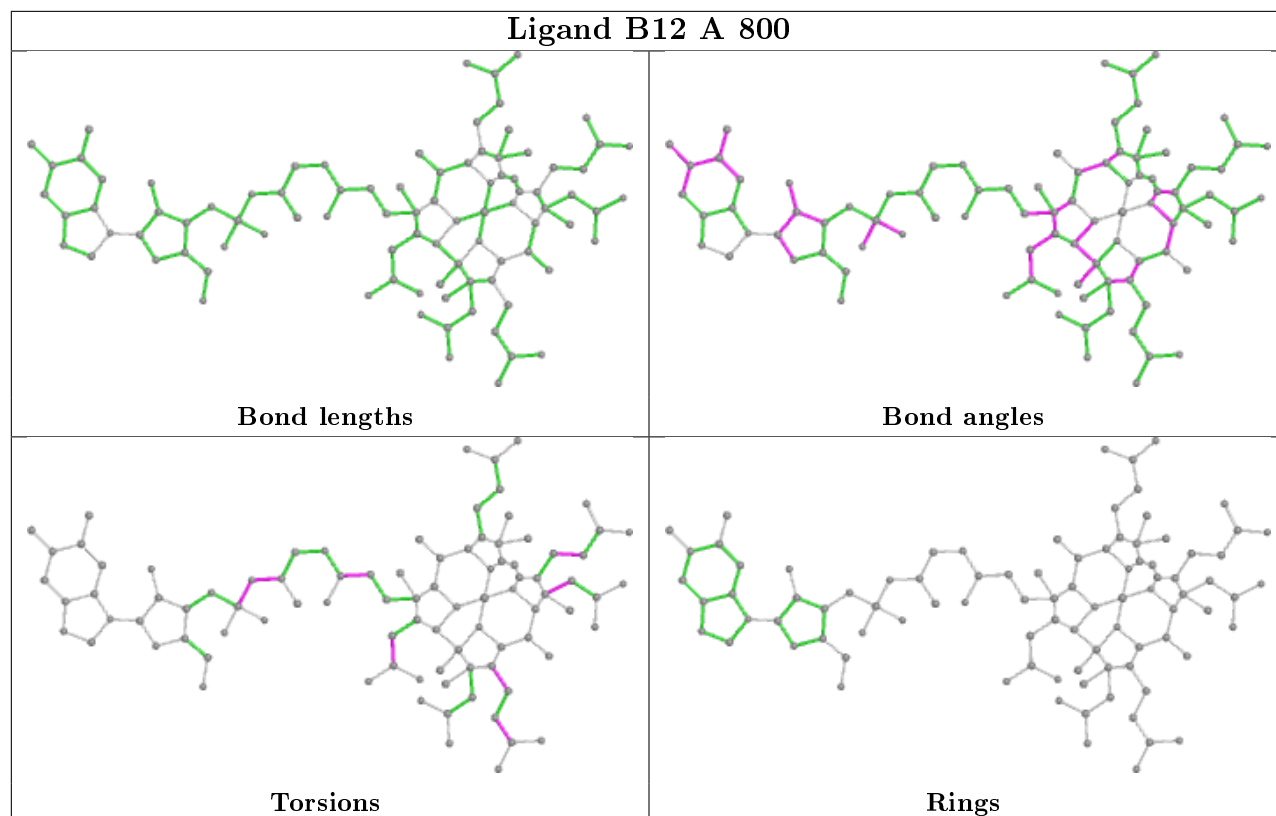
Mol	Chain	Res	Type	Atoms
3	C	800	B12	C55-C56-C57-N59
6	D	1308[B]	2AS	N-CA-CB-CG
3	C	800	B12	C4-C3-C30-C31

There are no ring outliers.

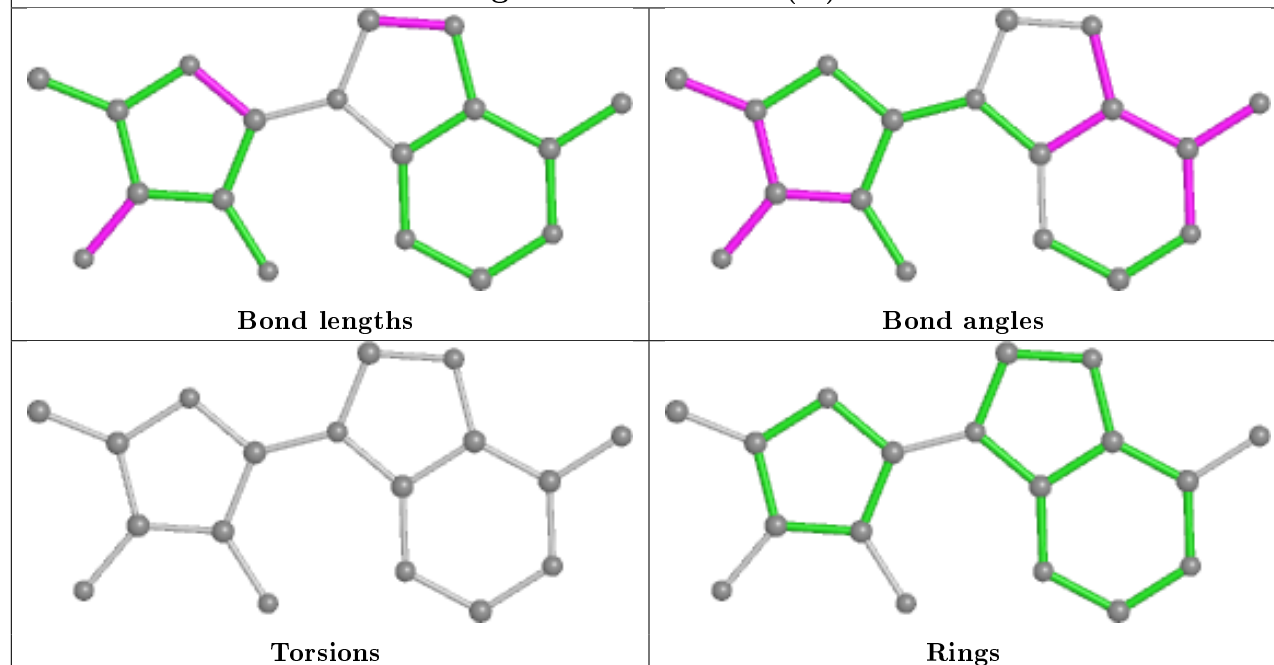
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	1	0
3	C	800	B12	2	0
4	B	1303[A]	5AD	3	0
6	B	1307[B]	2AS	1	0
6	D	1308[B]	2AS	1	0
4	D	1304[A]	5AD	2	0
4	D	1304[B]	5AD	2	0

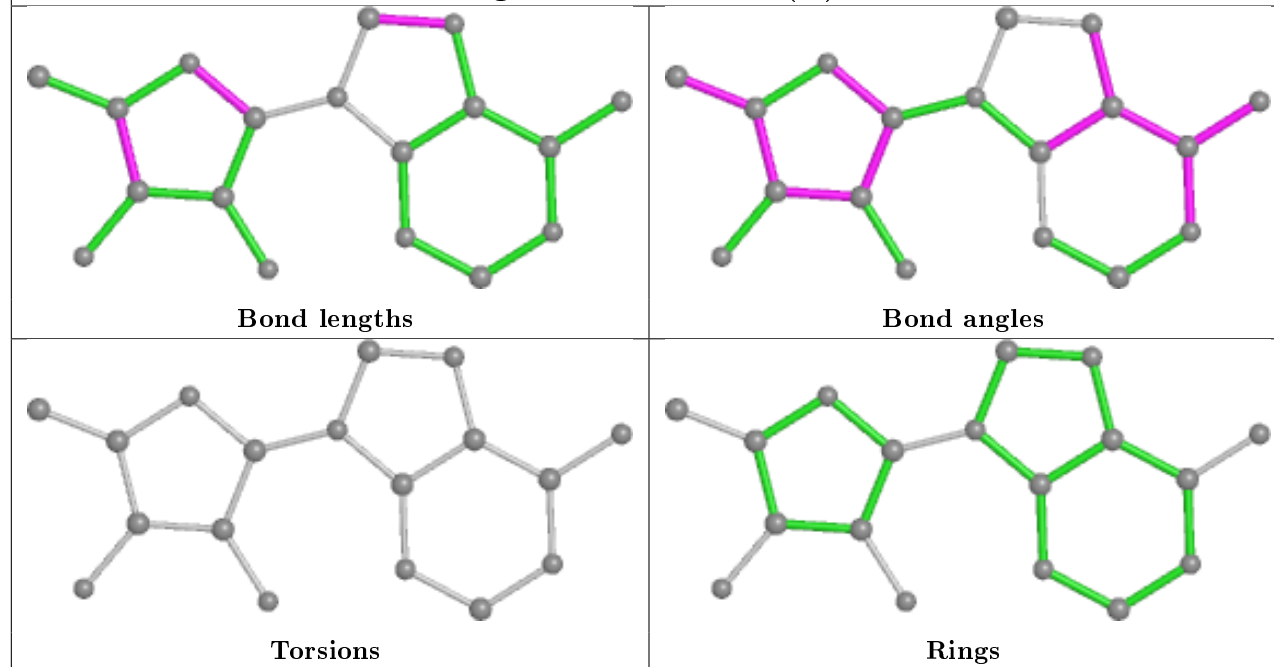
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

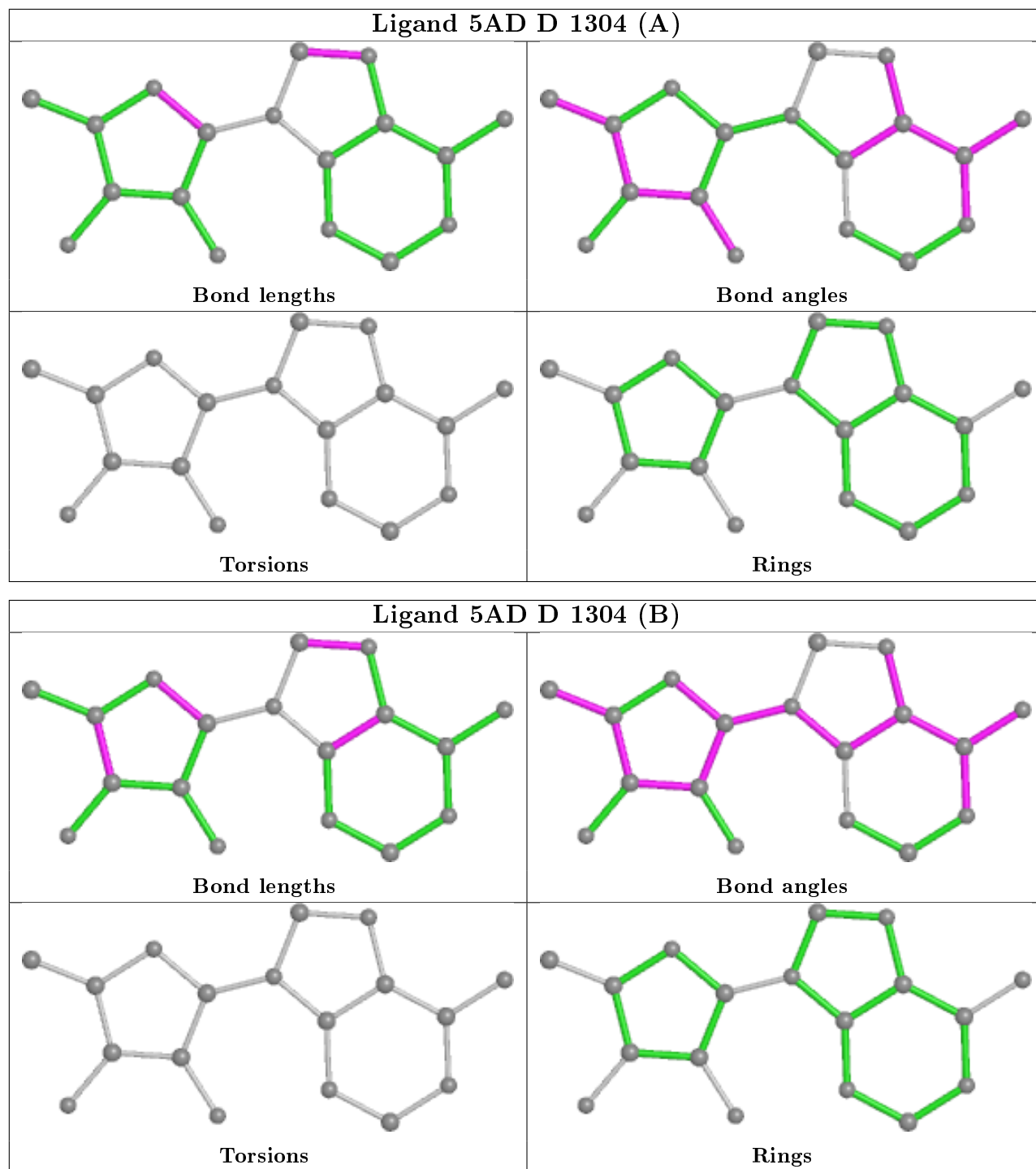


## Ligand 5AD B 1303 (A)



## Ligand 5AD B 1303 (B)





## 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, 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	137/137 (100%)	-0.13	5 (3%) 42 45	5, 14, 33, 56	0
1	C	137/137 (100%)	-0.11	3 (2%) 62 64	7, 13, 33, 67	0
2	B	483/483 (100%)	-0.44	1 (0%) 95 95	4, 9, 20, 67	0
2	D	483/483 (100%)	-0.42	1 (0%) 95 95	4, 9, 21, 68	0
All	All	1240/1240 (100%)	-0.36	10 (0%) 86 87	4, 10, 23, 68	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	6.6
1	C	2	GLU	5.5
2	D	483	GLU	5.2
1	A	1	MET	3.8
1	A	135	ASN	3.6
2	B	483	GLU	3.5
1	A	137	GLU	3.2
1	C	137	GLU	3.1
1	A	2	GLU	2.8
1	A	3	LYS	2.5

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

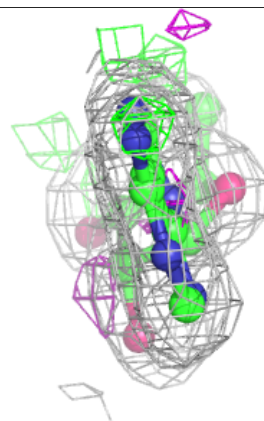
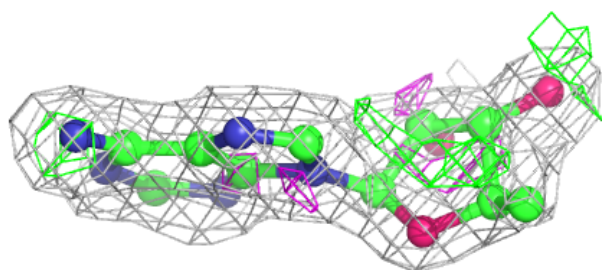
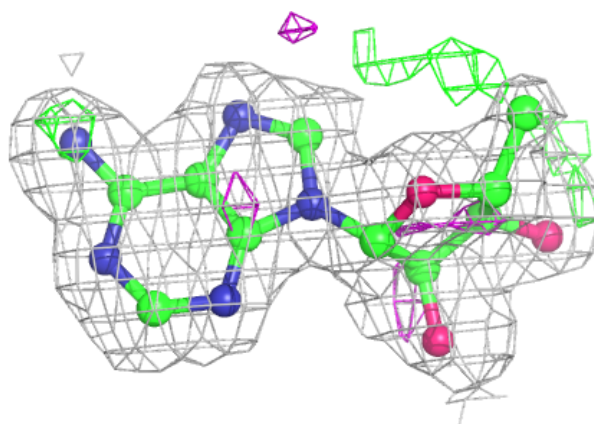
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	5AD	B	1303[A]	18/18	0.92	0.15	12,12,12,12	18
4	5AD	B	1303[B]	18/18	0.92	0.15	12,12,12,12	18
4	5AD	D	1304[A]	18/18	0.92	0.15	12,12,12,12	18
4	5AD	D	1304[B]	18/18	0.92	0.15	12,12,12,12	18
6	2AS	B	1307[B]	10/10	0.97	0.10	7,7,7,7	10
6	2AS	D	1308[B]	10/10	0.97	0.11	7,7,7,7	10
5	GLU	D	1306[A]	10/10	0.97	0.11	7,7,7,7	10
3	B12	C	800	91/91	0.97	0.09	2,7,13,19	0
5	GLU	B	1305[A]	10/10	0.98	0.09	7,7,7,7	10
3	B12	A	800	91/91	0.98	0.08	0,7,13,20	0

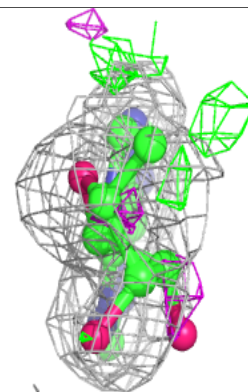
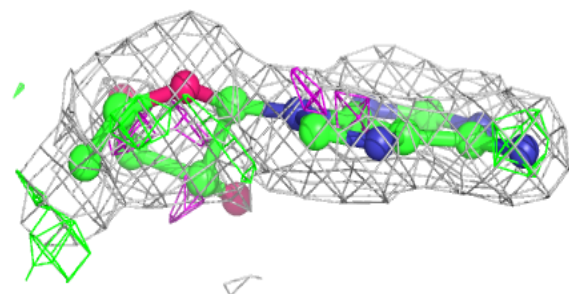
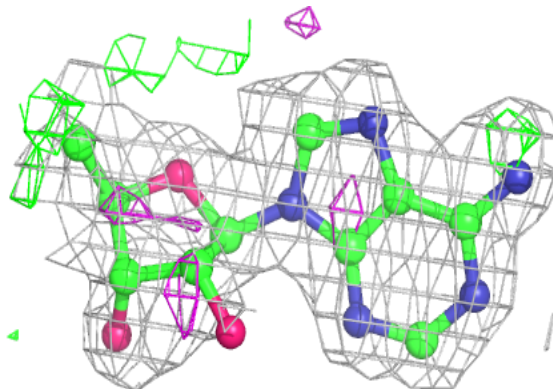
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5AD B 1303 (A):**

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

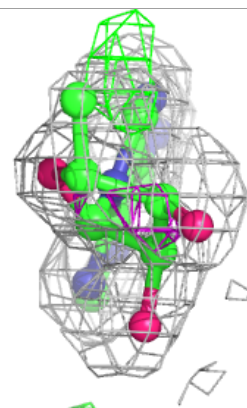
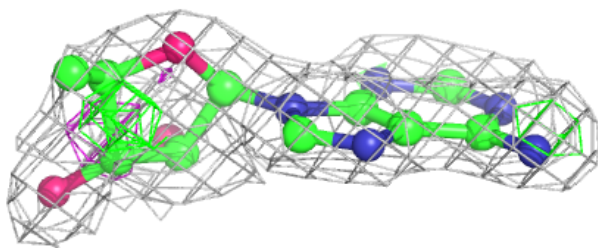
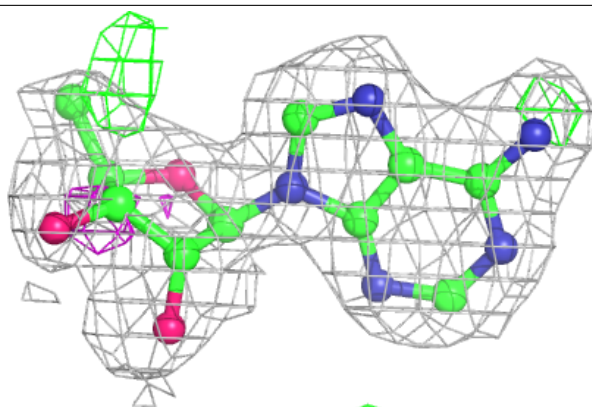
**Electron density around 5AD B 1303 (B):**

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

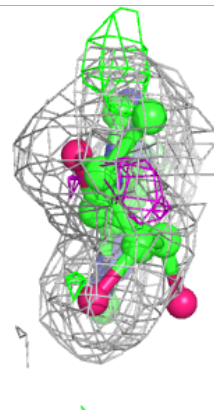
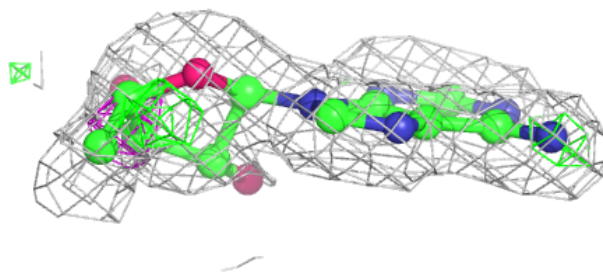
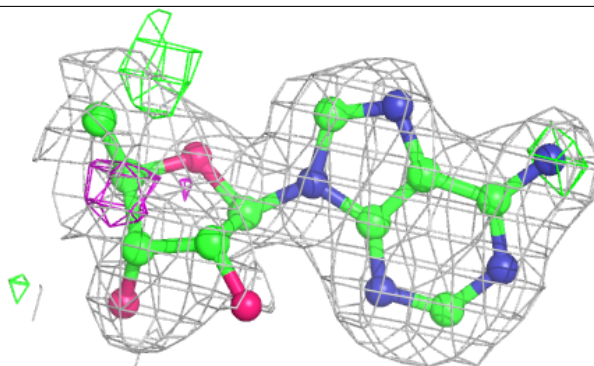


**Electron density around 5AD D 1304 (A):**

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

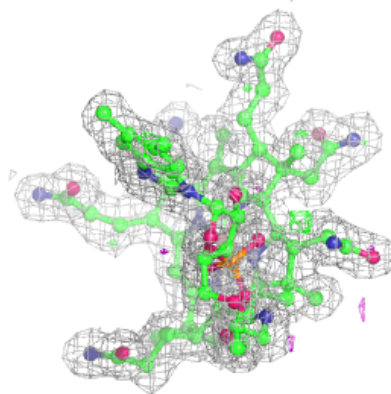
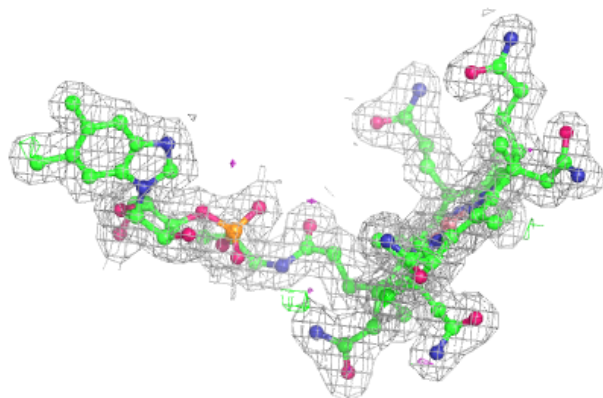
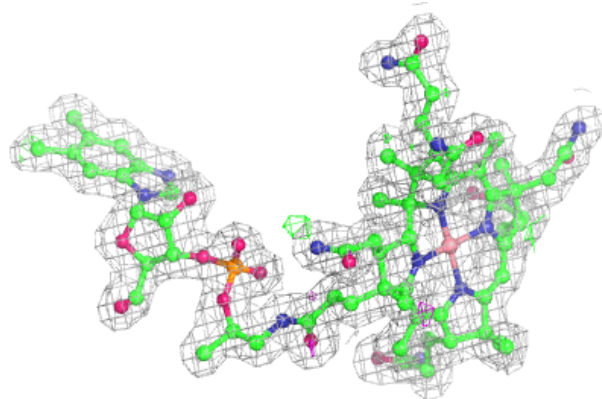
**Electron density around 5AD D 1304 (B):**

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

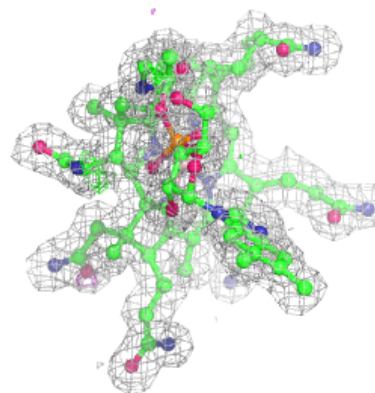
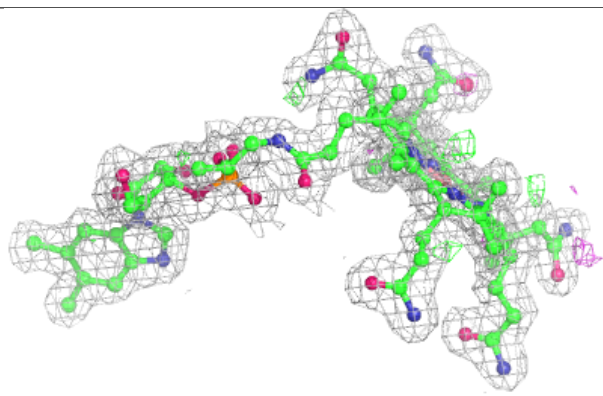
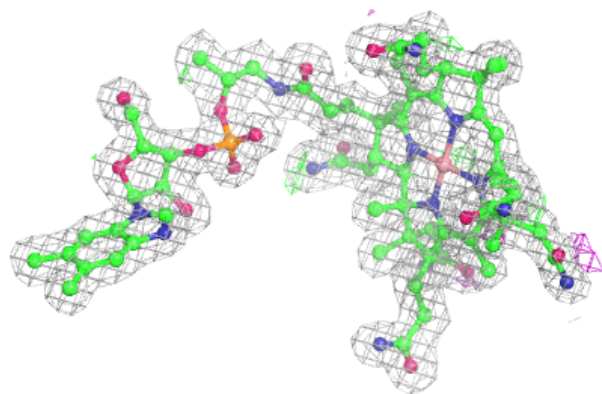


**Electron density around B12 C 800:**

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

**Electron density around B12 A 800:**

$2mF_o-DF_c$  (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.