



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:00 am BST

PDB ID : 3ABO  
Title : Crystal structure of ethanolamine ammonia-lyase from Escherichia coli complexed with CN-Cbl and ethanolamine  
Authors : Shibata, N.  
Deposited on : 2009-12-21  
Resolution : 2.10 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

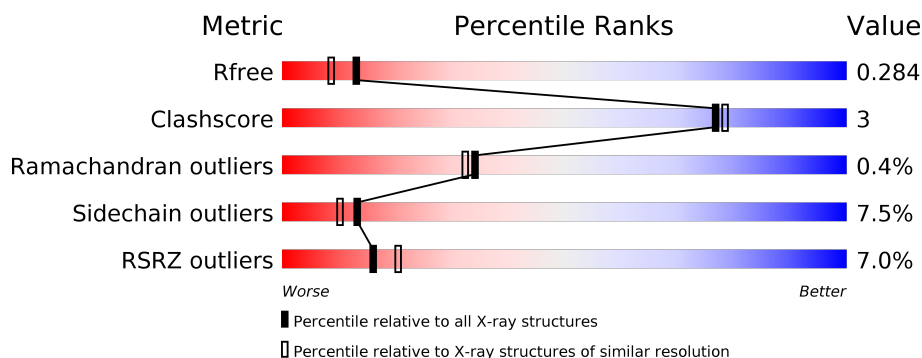
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> <div>•</div> </div>
1	C	453	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>•</div> </div>
2	B	306	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>18%</div> </div> <div>•</div> </div>
2	D	306	<div> <div>22%</div> <div> <div></div> <div>64%</div> <div>14%</div> <div>19%</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
6	NA	D	1002	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11664 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	0	0
			3464	2170	593	679	22			
1	C	453	Total	C	N	O	S	0	0	0
			3464	2170	593	679	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	0	0
			1916	1197	347	362	10			
2	D	248	Total	C	N	O	S	0	0	0
			1891	1183	342	357	9			

There are 22 discrepancies between the modelled and reference sequences:

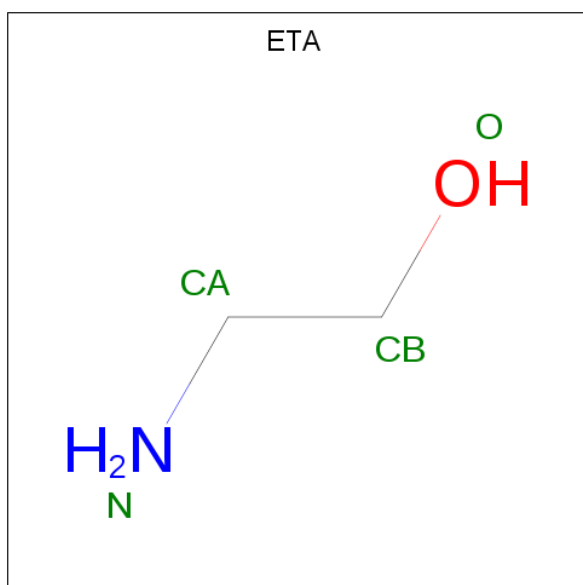
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	EXPRESSION TAG	UNP P19636
B	-9	ASP	-	EXPRESSION TAG	UNP P19636
B	-8	GLN	-	EXPRESSION TAG	UNP P19636
B	-7	SER	-	EXPRESSION TAG	UNP P19636
B	-6	SER	-	EXPRESSION TAG	UNP P19636
B	-5	HIS	-	EXPRESSION TAG	UNP P19636
B	-4	HIS	-	EXPRESSION TAG	UNP P19636
B	-3	HIS	-	EXPRESSION TAG	UNP P19636
B	-2	HIS	-	EXPRESSION TAG	UNP P19636
B	-1	HIS	-	EXPRESSION TAG	UNP P19636
B	0	HIS	-	EXPRESSION TAG	UNP P19636
D	-10	MET	-	EXPRESSION TAG	UNP P19636
D	-9	ASP	-	EXPRESSION TAG	UNP P19636
D	-8	GLN	-	EXPRESSION TAG	UNP P19636
D	-7	SER	-	EXPRESSION TAG	UNP P19636
D	-6	SER	-	EXPRESSION TAG	UNP P19636

*Continued on next page...*

Continued from previous page...

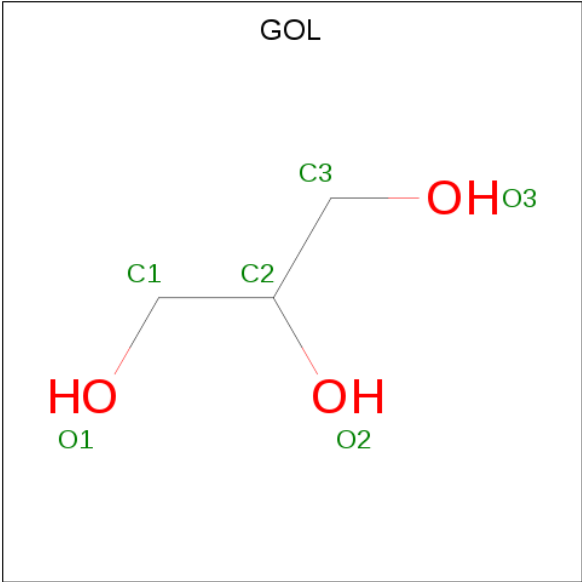
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP P19636
D	-4	HIS	-	EXPRESSION TAG	UNP P19636
D	-3	HIS	-	EXPRESSION TAG	UNP P19636
D	-2	HIS	-	EXPRESSION TAG	UNP P19636
D	-1	HIS	-	EXPRESSION TAG	UNP P19636
D	0	HIS	-	EXPRESSION TAG	UNP P19636

- Molecule 3 is ETHANOLAMINE (three-letter code: ETA) (formula:  $C_2H_7NO$ ).



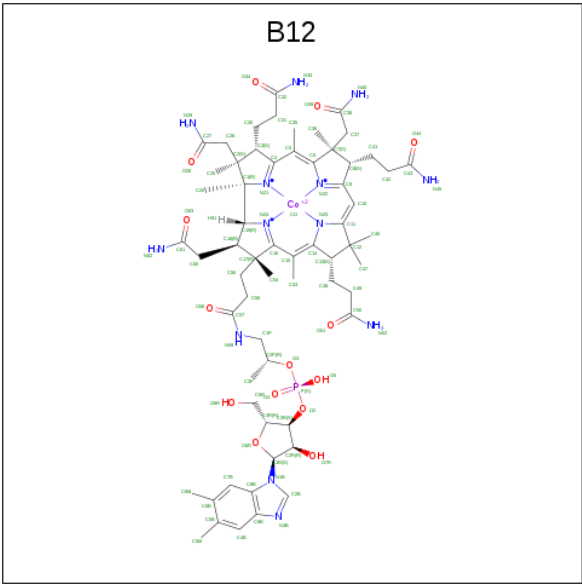
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			4	2	1	1		
3	C	1	Total	C	N	O	0	0
			4	2	1	1		

- 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	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Na		
			1	1	0	0
6	C	1	Total	Na		
			1	1	0	0

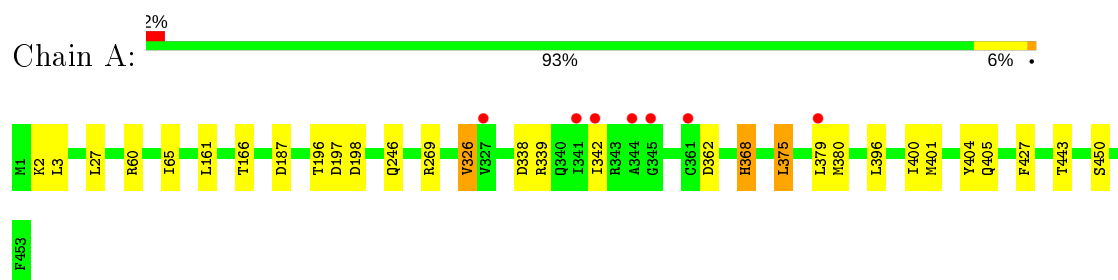
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	322	Total	O		
			322	322	0	0
7	B	67	Total	O		
			67	67	0	0
7	C	273	Total	O		
			273	273	0	0
7	D	45	Total	O		
			45	45	0	0

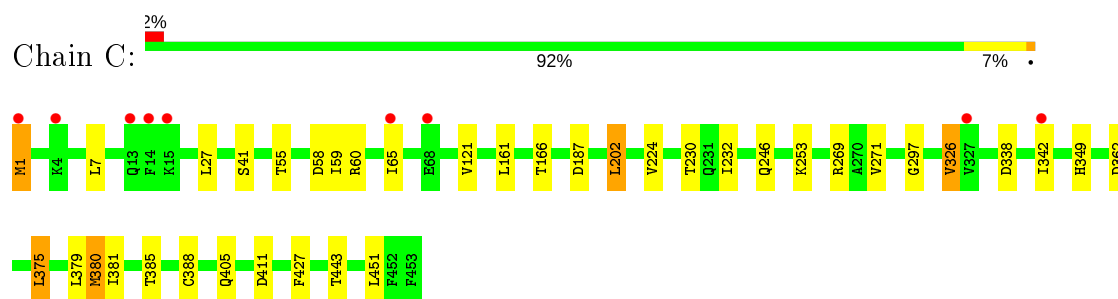
### 3 Residue-property plots [i](#)

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

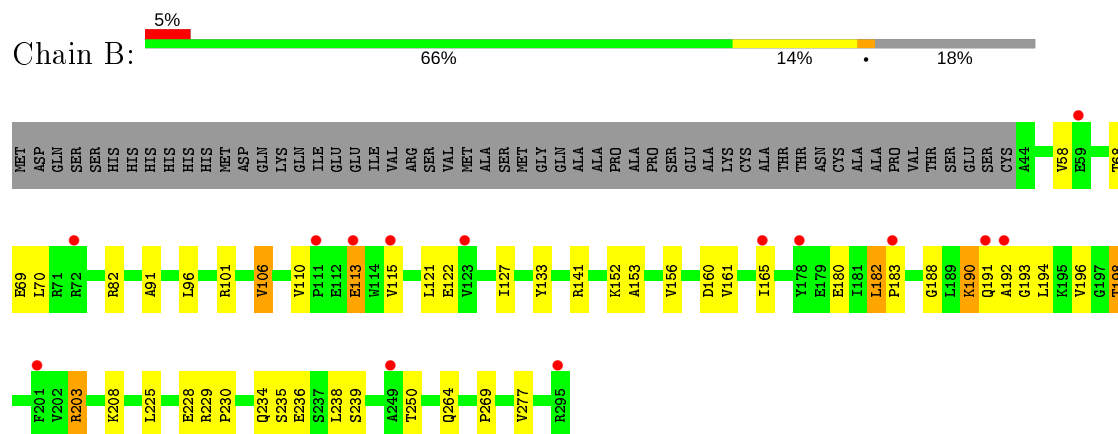
- Molecule 1: Ethanolamine ammonia-lyase heavy chain



- Molecule 1: Ethanolamine ammonia-lyase heavy chain



- Molecule 2: Ethanolamine ammonia-lyase light chain



- Molecule 2: Ethanolamine ammonia-lyase light chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	242.76 Å   242.76 Å   76.46 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	47.51 – 2.10 46.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.51-2.10) 97.2 (46.37-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.240 , 0.266 0.255 , 0.284	Depositor DCC
$R_{free}$ test set	7304 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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, ETA, B12, NA

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	0.58	0/3518	0.34	0/4764
1	C	0.58	0/3518	0.34	0/4764
2	B	0.55	0/1943	0.34	0/2633
2	D	0.54	0/1916	0.34	0/2593
All	All	0.57	0/10895	0.34	0/14754

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	4
1	C	0	3
2	B	0	4
2	D	0	6
All	All	0	17

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	THR	Peptide
1	A	197	ASP	Peptide
1	A	326	VAL	Peptide
1	A	400	ILE	Peptide
2	B	153	ALA	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	B	191	GLN	Peptide
2	B	193	GLY	Peptide
2	B	58	VAL	Peptide
1	C	1	MET	Peptide
1	C	297	GLY	Peptide
1	C	326	VAL	Peptide
2	D	110	VAL	Peptide
2	D	120	LEU	Peptide
2	D	192	ALA	Peptide
2	D	194	LEU	Peptide
2	D	206	ARG	Peptide
2	D	294	THR	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	3464	0	3419	9	0
1	C	3464	0	3419	14	0
2	B	1916	0	1973	15	0
2	D	1891	0	1948	16	0
3	A	4	0	7	0	0
3	C	4	0	7	0	0
4	A	18	0	24	0	0
4	C	12	0	16	0	0
5	B	91	0	88	9	0
5	D	91	0	88	10	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	322	0	0	0	0
7	B	67	0	0	0	0
7	C	273	0	0	0	0
7	D	45	0	0	0	0
All	All	11664	0	10989	66	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 3.

All (66) 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)
5:B:601:B12:H351	5:B:601:B12:H362	1.48	0.92
5:D:601:B12:H351	5:D:601:B12:H362	1.52	0.89
5:B:601:B12:H552	5:B:601:B12:H531	1.57	0.87
5:D:601:B12:H531	5:D:601:B12:H552	1.59	0.84
2:D:228:GLU:HA	5:D:601:B12:H1P2	1.81	0.61
2:B:110:VAL:O	2:B:203:ARG:NH2	2.32	0.60
2:B:106:VAL:HG12	2:B:230:PRO:HG2	1.83	0.60
5:B:601:B12:H362	5:B:601:B12:C35	2.29	0.58
5:B:601:B12:H351	5:B:601:B12:C36	2.26	0.57
5:D:601:B12:H262	5:D:601:B12:H601	1.87	0.56
5:D:601:B12:H351	5:D:601:B12:C36	2.29	0.56
2:B:156:VAL:HG22	2:B:198:THR:HG22	1.87	0.55
2:D:180:GLU:HB3	2:D:269:PRO:HB2	1.88	0.55
2:B:180:GLU:HB3	2:B:269:PRO:HB2	1.89	0.54
2:D:135:THR:HG23	2:D:136:ARG:HG2	1.92	0.51
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.46	0.51
1:A:246:GLN:NE2	5:B:601:B12:O39	2.43	0.51
1:C:349:HIS:CE1	1:C:388:CYS:HA	2.46	0.51
5:D:601:B12:C53	5:D:601:B12:H552	2.35	0.51
5:B:601:B12:C53	5:B:601:B12:H552	2.36	0.50
5:D:601:B12:C35	5:D:601:B12:H362	2.32	0.50
2:B:141:ARG:HG2	2:B:208:LYS:HB2	1.94	0.50
2:B:228:GLU:HA	5:B:601:B12:H1P2	1.93	0.50
2:D:127:ILE:HG21	2:D:133:TYR:HB2	1.94	0.49
1:C:326:VAL:HA	1:C:362:ASP:HB3	1.94	0.49
2:D:240:CYS:HB3	2:D:259:ILE:HG23	1.95	0.49
1:A:326:VAL:HA	1:A:362:ASP:HB3	1.95	0.49
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.48	0.48
1:C:202:LEU:HD22	1:C:224:VAL:HG11	1.93	0.48
2:D:137:PRO:HA	2:D:206:ARG:HD3	1.94	0.48
5:D:601:B12:H602	5:D:601:B12:H541	1.76	0.48
1:C:338:ASP:HA	1:C:375:LEU:HD13	1.96	0.47
2:D:182:LEU:HB3	2:D:183:PRO:HD3	1.97	0.47
2:D:111:PRO:HB2	2:D:114:TRP:H	1.80	0.46
2:B:225:LEU:HB3	2:B:238:LEU:HD21	1.96	0.46
2:D:113:GLU:H	2:D:113:GLU:HG2	1.46	0.46
1:C:342:ILE:HA	1:C:379:LEU:HD13	1.97	0.46
5:D:601:B12:H473	5:D:601:B12:H481	1.77	0.45
2:D:46:ASP:HB3	2:D:49:SER:HB3	1.96	0.45
2:D:194:LEU:HB3	2:D:195:LYS:H	1.61	0.45
1:C:443:THR:O	2:D:82:ARG:NH2	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:B12:H262	5:B:601:B12:H601	1.98	0.45
2:B:182:LEU:HB3	2:B:183:PRO:HD3	1.99	0.45
1:C:246:GLN:NE2	5:D:601:B12:O39	2.50	0.44
1:A:187:ASP:N	1:A:187:ASP:OD1	2.50	0.44
1:A:368:HIS:H	1:A:368:HIS:CD2	2.36	0.43
2:B:188:GLY:HA3	2:B:277:VAL:HG21	1.99	0.43
1:C:381:ILE:O	1:C:385:THR:HG23	2.19	0.43
2:B:113:GLU:H	2:B:113:GLU:HG2	1.47	0.43
5:B:601:B12:H253	5:B:601:B12:H301	1.75	0.43
1:A:342:ILE:HA	1:A:379:LEU:HD13	2.01	0.43
1:C:55:THR:HG22	1:C:58:ASP:CG	2.39	0.42
2:D:268:PRO:HA	2:D:269:PRO:HD3	1.91	0.42
1:A:338:ASP:HA	1:A:375:LEU:HD13	2.00	0.42
1:C:380:MET:SD	1:C:411:ASP:HB3	2.59	0.42
1:A:443:THR:O	2:B:82:ARG:NH1	2.51	0.42
2:D:225:LEU:HB3	2:D:238:LEU:HD21	2.01	0.42
1:C:187:ASP:N	1:C:187:ASP:OD1	2.52	0.41
2:D:141:ARG:HE	2:D:141:ARG:HB3	1.50	0.41
1:C:59:ILE:HB	1:C:121:VAL:HG22	2.03	0.41
1:C:232:ILE:HG23	1:C:271:VAL:HG21	2.01	0.41
2:B:127:ILE:HG21	2:B:133:TYR:HB2	2.03	0.41
2:B:115:VAL:HG11	2:B:122:GLU:HG3	2.02	0.41
1:A:396:LEU:HD11	2:B:91:ALA:HB1	2.03	0.41
2:B:190:LYS:HG2	2:B:196:VAL:HG21	2.04	0.40
2:D:181:ILE:HB	2:D:269:PRO:HB3	2.04	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	451/453 (100%)	430 (95%)	19 (4%)	2 (0%)	34 32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	451/453 (100%)	431 (96%)	20 (4%)	0	100	100
2	B	250/306 (82%)	244 (98%)	5 (2%)	1 (0%)	34	32
2	D	242/306 (79%)	234 (97%)	6 (2%)	2 (1%)	19	15
All	All	1394/1518 (92%)	1339 (96%)	50 (4%)	5 (0%)	34	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	192	ALA
2	B	192	ALA
1	A	401	MET
1	A	198	ASP
2	D	193	GLY

### 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	370/370 (100%)	355 (96%)	15 (4%)	30	31
1	C	370/370 (100%)	354 (96%)	16 (4%)	29	29
2	B	206/251 (82%)	182 (88%)	24 (12%)	5	3
2	D	204/251 (81%)	173 (85%)	31 (15%)	3	1
All	All	1150/1242 (93%)	1064 (92%)	86 (8%)	13	10

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	LEU
1	A	27	LEU
1	A	60	ARG
1	A	65	ILE
1	A	161	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	166	THR
1	A	269	ARG
1	A	339	ARG
1	A	368	HIS
1	A	375	LEU
1	A	380	MET
1	A	404	TYR
1	A	405	GLN
1	A	450	SER
2	B	68	THR
2	B	69	GLU
2	B	70	LEU
2	B	96	LEU
2	B	101	ARG
2	B	106	VAL
2	B	113	GLU
2	B	121	LEU
2	B	152	LYS
2	B	160	ASP
2	B	161	VAL
2	B	165	ILE
2	B	182	LEU
2	B	190	LYS
2	B	194	LEU
2	B	198	THR
2	B	203	ARG
2	B	229	ARG
2	B	234	GLN
2	B	235	SER
2	B	236	GLU
2	B	239	SER
2	B	250	THR
2	B	264	GLN
1	C	1	MET
1	C	7	LEU
1	C	27	LEU
1	C	41	SER
1	C	60	ARG
1	C	65	ILE
1	C	161	LEU
1	C	166	THR
1	C	202	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	230	THR
1	C	253	LYS
1	C	269	ARG
1	C	375	LEU
1	C	380	MET
1	C	405	GLN
1	C	451	LEU
2	D	75	VAL
2	D	108	LYS
2	D	110	VAL
2	D	112	GLU
2	D	113	GLU
2	D	121	LEU
2	D	123	VAL
2	D	130	LYS
2	D	134	LEU
2	D	141	ARG
2	D	152	LYS
2	D	161	VAL
2	D	180	GLU
2	D	182	LEU
2	D	190	LYS
2	D	191	GLN
2	D	194	LEU
2	D	203	ARG
2	D	206	ARG
2	D	223	ILE
2	D	224	LEU
2	D	229	ARG
2	D	232	LEU
2	D	234	GLN
2	D	240	CYS
2	D	243	VAL
2	D	247	ARG
2	D	259	ILE
2	D	267	THR
2	D	275	VAL
2	D	291	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
5	B12	D	601	-	80,101,101	1.21	6 (7%)	101,166,166	1.17	14 (13%)
5	B12	B	601	-	80,101,101	1.28	9 (11%)	101,166,166	1.15	12 (11%)
4	GOL	C	1015	-	5,5,5	0.42	0	5,5,5	0.24	0
4	GOL	A	1011	-	5,5,5	0.41	0	5,5,5	0.32	0
3	ETA	C	602	-	3,3,3	0.72	0	2,2,2	0.72	0
4	GOL	A	1012	-	5,5,5	0.33	0	5,5,5	0.28	0
3	ETA	A	602	-	3,3,3	0.74	0	2,2,2	0.77	0
4	GOL	C	1013	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	A	1014	-	5,5,5	0.32	0	5,5,5	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	B12	D	601	-	-	17/51/223/223	0/3/11/11
5	B12	B	601	-	-	13/51/223/223	0/3/11/11
4	GOL	C	1015	-	-	2/4/4/4	-
4	GOL	A	1011	-	-	4/4/4/4	-
3	ETA	C	602	-	-	0/1/1/1	-
4	GOL	A	1012	-	-	1/4/4/4	-
3	ETA	A	602	-	-	0/1/1/1	-
4	GOL	C	1013	-	-	0/4/4/4	-
4	GOL	A	1014	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C11-C10	-6.27	1.30	1.40
5	B	601	B12	C11-C10	-6.08	1.30	1.40
5	B	601	B12	C17-C18	4.06	1.59	1.54
5	B	601	B12	C6B-C5B	3.63	1.49	1.40
5	D	601	B12	C6B-C5B	3.59	1.49	1.40
5	D	601	B12	C17-C18	3.40	1.58	1.54
5	D	601	B12	C8B-C9B	3.00	1.46	1.40
5	B	601	B12	C8B-C9B	2.85	1.46	1.40
5	B	601	B12	O6R-C1R	2.44	1.44	1.41
5	D	601	B12	O6R-C1R	2.39	1.44	1.41
5	B	601	B12	C2-C3	2.39	1.62	1.58
5	D	601	B12	C14-C15	2.35	1.49	1.40
5	B	601	B12	C14-C15	2.14	1.48	1.40
5	B	601	B12	CO-N21	-2.10	1.83	1.89
5	B	601	B12	C1-C19	-2.06	1.50	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	B12	C54-C17-C18	-3.56	107.73	112.98
5	B	601	B12	C1-C19-N24	3.16	109.79	106.24
5	B	601	B12	C54-C17-C18	-3.02	108.53	112.98
5	B	601	B12	C30-C3-C2	-2.78	113.23	119.13
5	D	601	B12	C12-C11-C10	-2.77	119.94	124.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	B12	C30-C3-C2	-2.69	113.43	119.13
5	B	601	B12	C20-C1-C19	-2.68	106.78	109.36
5	D	601	B12	C2-C1-C19	2.66	122.80	118.60
5	D	601	B12	C20-C1-C19	-2.65	106.80	109.36
5	B	601	B12	C25-C2-C3	-2.61	111.60	115.58
5	B	601	B12	C2-C1-C19	2.60	122.70	118.60
5	B	601	B12	C16-C15-C14	-2.48	120.40	124.27
5	D	601	B12	C16-C15-C14	-2.44	120.47	124.27
5	D	601	B12	C25-C2-C3	-2.38	111.95	115.58
5	B	601	B12	C9-C10-C11	-2.23	123.14	130.91
5	B	601	B12	C6-C5-C4	-2.21	120.83	124.27
5	D	601	B12	C6-C5-C4	-2.17	120.89	124.27
5	D	601	B12	C1-C19-N24	2.16	108.67	106.24
5	B	601	B12	C13-C14-C15	-2.14	123.91	131.68
5	D	601	B12	C25-C2-C1	-2.14	110.63	113.80
5	B	601	B12	C12-C11-C10	-2.12	121.05	124.64
5	D	601	B12	C9-C10-C11	-2.12	123.51	130.91
5	B	601	B12	C25-C2-C1	-2.10	110.69	113.80
5	D	601	B12	C3-C4-C5	-2.09	124.10	131.68
5	D	601	B12	C47-C12-C46	2.07	114.07	109.73
5	D	601	B12	C13-C14-C15	-2.06	124.20	131.68

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	601	B12	C38-C37-C7-C36
5	D	601	B12	C38-C37-C7-C8
5	D	601	B12	C13-C48-C49-C50
5	D	601	B12	C2P-O3-P-O4
5	D	601	B12	C2P-O3-P-O5
5	B	601	B12	C38-C37-C7-C36
5	B	601	B12	C2P-O3-P-O5
4	C	1015	GOL	C1-C2-C3-O3
4	A	1011	GOL	O1-C1-C2-C3
4	A	1011	GOL	C1-C2-C3-O3
4	A	1014	GOL	C1-C2-C3-O3
5	D	601	B12	O6R-C4R-C5R-O8R
5	D	601	B12	C3R-C4R-C5R-O8R
5	B	601	B12	C13-C48-C49-C50
5	B	601	B12	C2-C3-C30-C31
4	A	1011	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	601	B12	C18-C17-C55-C56
5	D	601	B12	C2-C3-C30-C31
5	D	601	B12	C16-C17-C55-C56
5	B	601	B12	C16-C17-C55-C56
5	B	601	B12	C38-C37-C7-C8
4	A	1014	GOL	O1-C1-C2-C3
4	C	1015	GOL	O2-C2-C3-O3
5	B	601	B12	C18-C17-C55-C56
5	D	601	B12	C2P-O3-P-O2
5	B	601	B12	C2P-O3-P-O2
4	A	1014	GOL	O1-C1-C2-O2
4	A	1014	GOL	O2-C2-C3-O3
5	B	601	B12	C2P-O3-P-O4
4	A	1011	GOL	O1-C1-C2-O2
5	D	601	B12	C3P-C2P-O3-P
5	D	601	B12	C42-C41-C8-C9
5	B	601	B12	C42-C41-C8-C9
5	D	601	B12	C1P-C2P-O3-P
5	B	601	B12	C3P-C2P-O3-P
5	D	601	B12	C17-C18-C60-C61
4	A	1012	GOL	O2-C2-C3-O3
5	B	601	B12	C1P-C2P-O3-P
5	D	601	B12	C19-C18-C60-C61
5	D	601	B12	C4-C3-C30-C31
5	B	601	B12	C4-C3-C30-C31

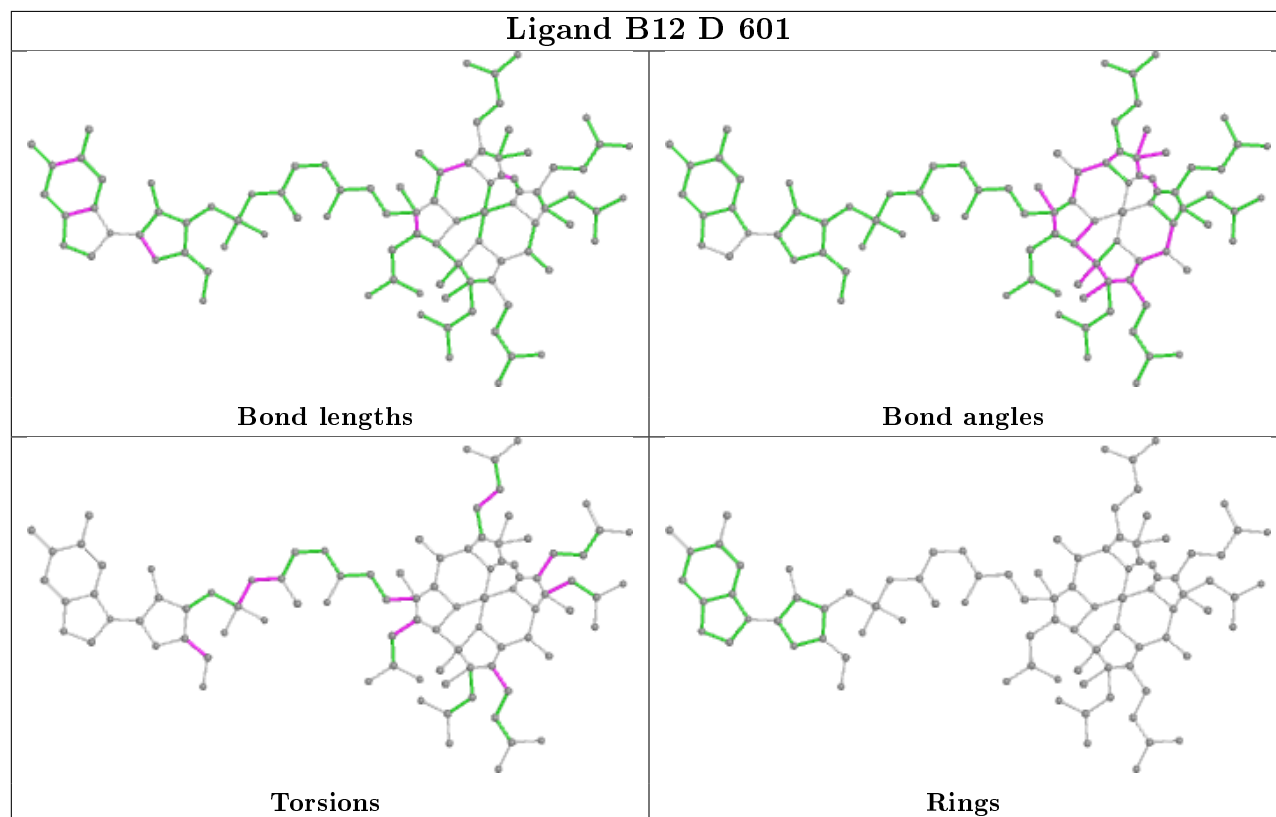
There are no ring outliers.

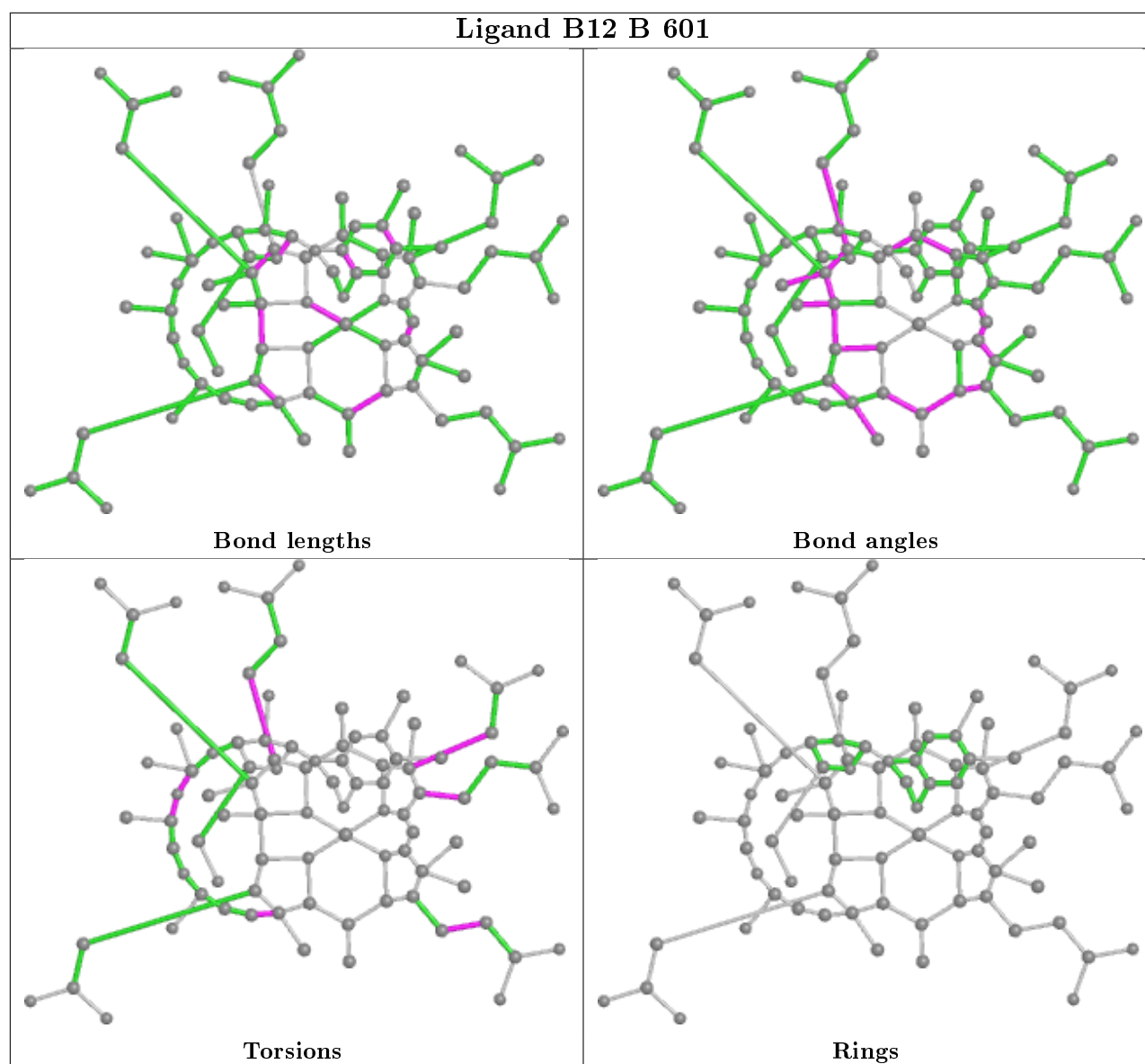
2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	601	B12	10	0
5	B	601	B12	9	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%)	0.02	7 (1%) 73 77	18, 30, 48, 61	0
1	C	453/453 (100%)	0.03	9 (1%) 65 69	18, 32, 54, 72	0
2	B	252/306 (82%)	0.44	14 (5%) 24 29	25, 62, 87, 105	0
2	D	248/306 (81%)	1.36	68 (27%) 0 0	23, 80, 128, 139	0
All	All	1406/1518 (92%)	0.33	98 (6%) 16 20	18, 39, 99, 139	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	ALA	11.2
2	D	123	VAL	8.3
2	D	156	VAL	7.9
2	B	192	ALA	6.9
2	D	151	LEU	6.4
2	D	161	VAL	6.2
2	D	221	VAL	5.3
2	D	187	ALA	5.3
2	D	191	GLN	5.2
2	D	148	VAL	5.2
2	D	111	PRO	5.2
2	D	200	PHE	4.6
2	D	273	ALA	4.3
2	D	162	GLN	4.2
2	D	178	TYR	4.2
2	D	157	ALA	4.1
2	D	196	VAL	4.1
2	D	183	PRO	4.0
2	B	191	GLN	3.9
2	D	174	ILE	3.8
2	D	288	ALA	3.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	194	LEU	3.8
2	D	121	LEU	3.7
2	D	119	GLY	3.6
1	C	4	LYS	3.6
2	D	190	LYS	3.6
2	D	199	PRO	3.5
2	D	193	GLY	3.5
2	B	295	ARG	3.3
2	D	198	THR	3.3
2	D	186	MET	3.3
2	D	149	GLU	3.3
1	C	14	PHE	3.3
2	D	201	PHE	3.2
2	D	120	LEU	3.2
2	D	225	LEU	3.2
1	C	13	GLN	3.1
2	D	276	ILE	3.1
2	D	202	VAL	3.1
2	B	115	VAL	3.0
2	D	245	SER	3.0
2	B	113	GLU	3.0
2	D	118	GLN	2.9
2	D	275	VAL	2.9
2	D	284	LEU	2.9
2	B	111	PRO	2.9
2	D	244	TYR	2.9
1	A	379	LEU	2.8
1	C	15	LYS	2.8
2	D	184	PRO	2.8
2	D	286	GLN	2.8
2	D	223	ILE	2.8
2	D	271	GLU	2.8
2	D	246	PRO	2.7
1	A	327	VAL	2.7
1	A	341	ILE	2.6
2	D	217	LEU	2.6
2	B	201	PHE	2.6
1	C	1	MET	2.6
2	D	216	ILE	2.6
1	A	344	ALA	2.5
2	B	59	GLU	2.5
2	B	123	VAL	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	132	LEU	2.5
2	D	143	LEU	2.5
2	D	218	GLY	2.5
2	D	127	ILE	2.4
2	D	213	ILE	2.4
2	D	124	ARG	2.4
2	D	281	LYS	2.3
2	D	287	LYS	2.3
2	D	110	VAL	2.3
2	D	165	ILE	2.3
2	D	215	GLU	2.3
2	D	158	ASN	2.3
1	A	342	ILE	2.3
2	B	178	TYR	2.2
2	D	270	VAL	2.2
2	B	249	ALA	2.2
2	D	267	THR	2.2
2	D	128	SER	2.2
2	D	147	ALA	2.2
2	D	181	ILE	2.2
2	D	209	ILE	2.2
2	D	277	VAL	2.2
1	C	65	ILE	2.1
1	C	342	ILE	2.1
2	D	189	LEU	2.1
1	A	345	GLY	2.1
2	D	220	LYS	2.1
2	B	72	ARG	2.1
1	C	327	VAL	2.1
2	D	160	ASP	2.0
1	A	361	CYS	2.0
2	B	183	PRO	2.0
2	B	165	ILE	2.0
1	C	68	GLU	2.0
2	D	164	VAL	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 ⓘ

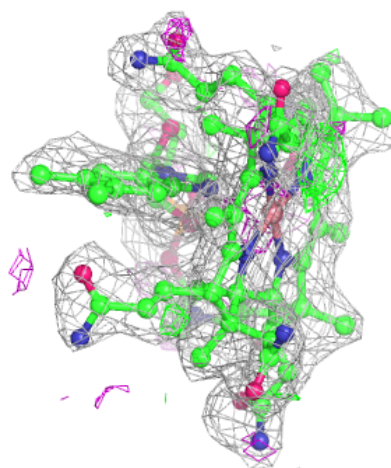
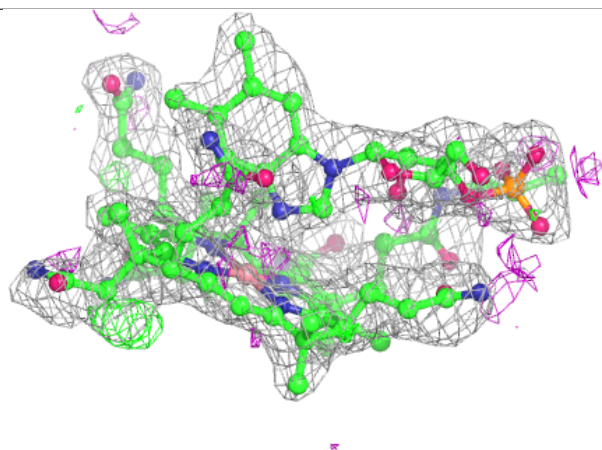
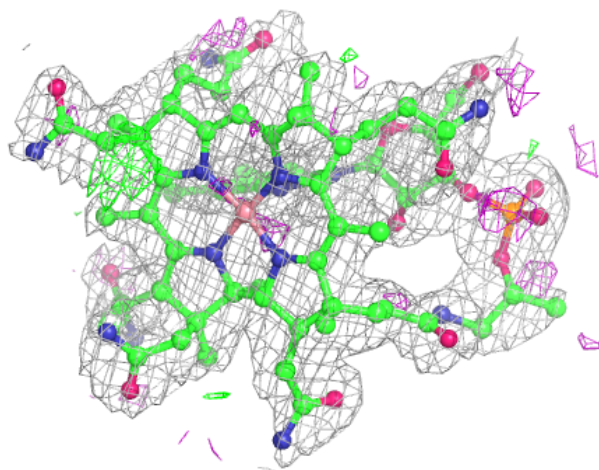
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	D	1002	1/1	0.03	0.83	94,94,94,94	0
4	GOL	C	1015	6/6	0.78	0.25	56,61,63,66	0
4	GOL	A	1011	6/6	0.83	0.17	36,41,47,54	0
6	NA	C	1001	1/1	0.87	0.19	45,45,45,45	0
4	GOL	C	1013	6/6	0.87	0.15	44,49,56,57	0
4	GOL	A	1012	6/6	0.91	0.14	34,37,43,50	0
5	B12	D	601	91/91	0.92	0.15	25,43,55,59	0
4	GOL	A	1014	6/6	0.92	0.18	29,56,60,67	0
5	B12	B	601	91/91	0.94	0.15	20,36,44,60	0
3	ETA	A	602	4/4	0.96	0.28	25,29,30,32	0
3	ETA	C	602	4/4	0.96	0.23	24,25,26,27	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.

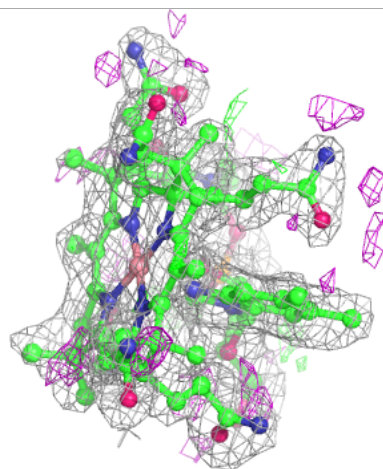
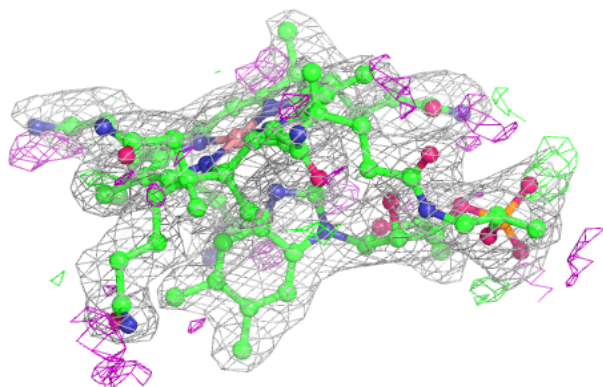
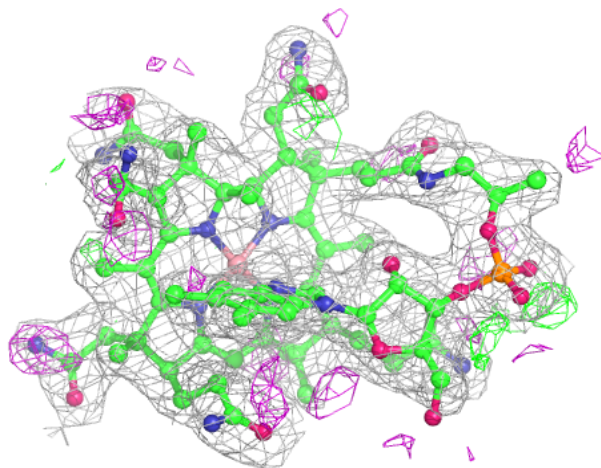
**Electron density around B12 D 601:**

$2mF_o-DF_c$  (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.