Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 07:36 AM EDT

PDB ID	:	3ABO / pdb_00003abo
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

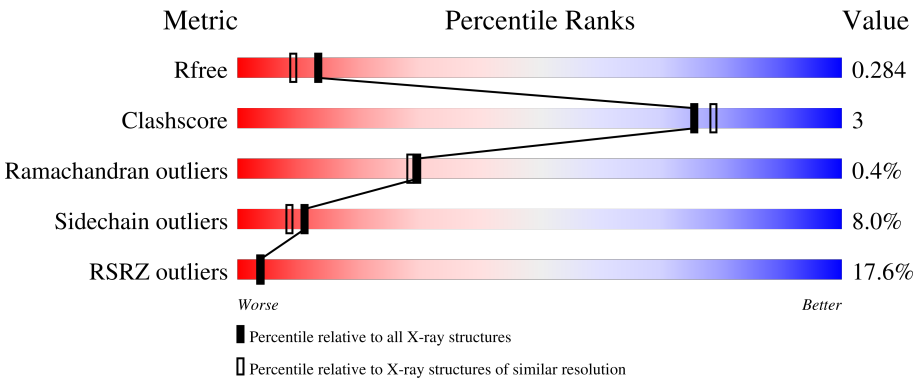
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 93% 7%
1	C	453	5% 91% 8% •
2	B	306	22% 65% 15% • 18%
2	D	306	47% 62% 15% • • 19%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NA	D	1002	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	453	3464	2170	593	679	22	0	0	0
1	C	453	3464	2170	593	679	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	1916	1197	347	362	10	0	0	0
2	D	248	1891	1183	342	357	9	0	0	0

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

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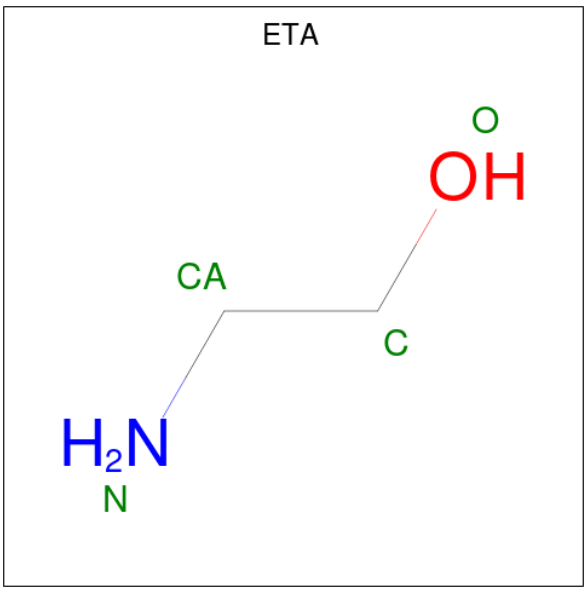
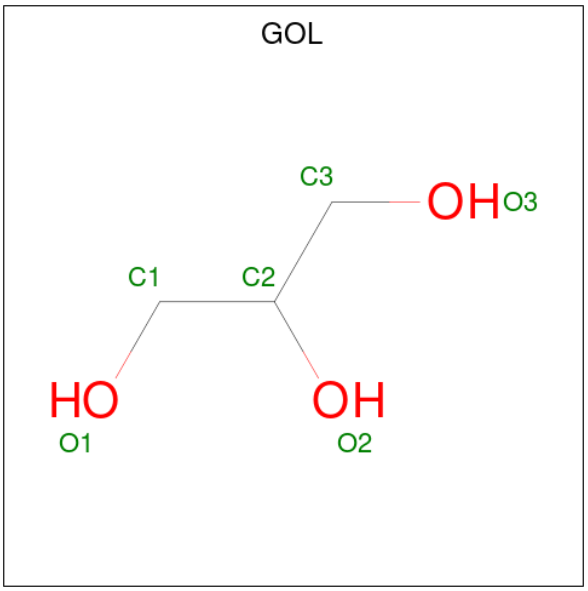
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P19636
D	-4	HIS	-	expression tag	UNP P19636
D	-3	HIS	-	expression tag	UNP P19636
D	-2	HIS	-	expression tag	UNP P19636
D	-1	HIS	-	expression tag	UNP P19636
D	0	HIS	-	expression tag	UNP P19636

- Molecule 3 is ETHANOLAMINE (CCD ID: ETA) (formula: C_2H_7NO).



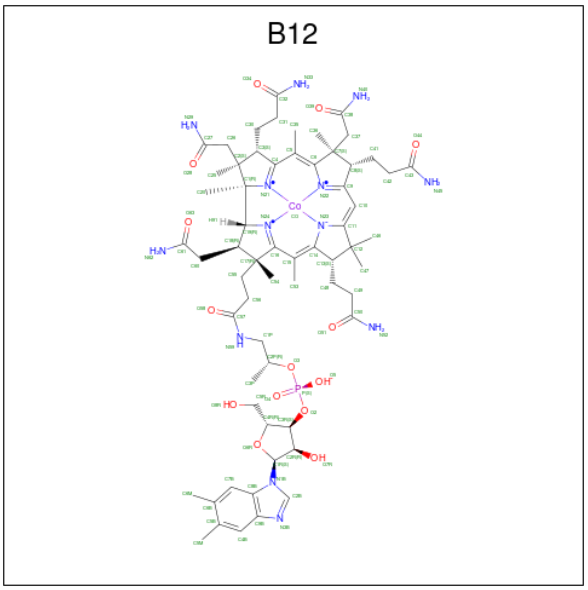
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	4	2	1	1	0	0
			Total	C	N	O		
3	C	1	4	2	1	1	0	0

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



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

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



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is water.

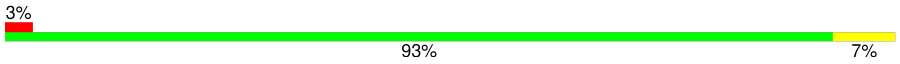
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	322	322	322	0	0
7	B	67	67	67	0	0
7	C	273	273	273	0	0
7	D	45	45	45	0	0

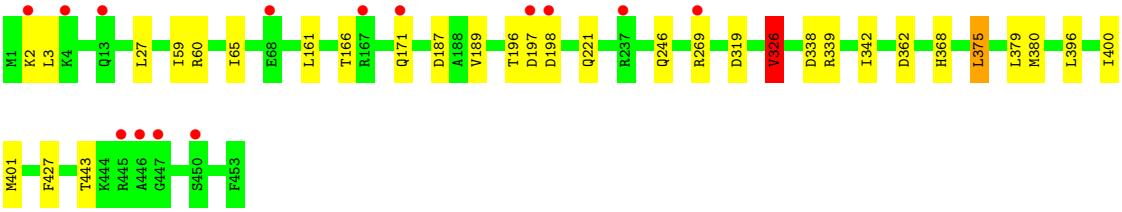
3 Residue-property plots (i)

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 heavy chain

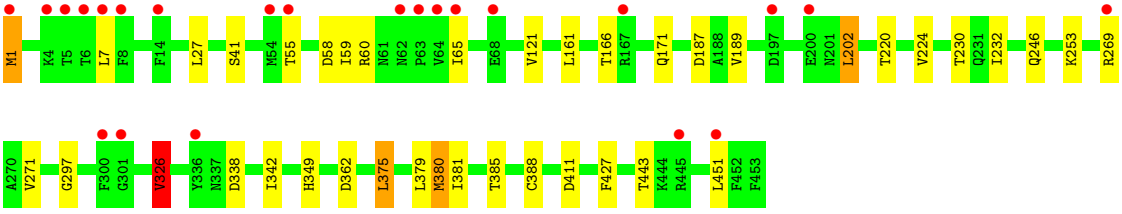
Chain A:





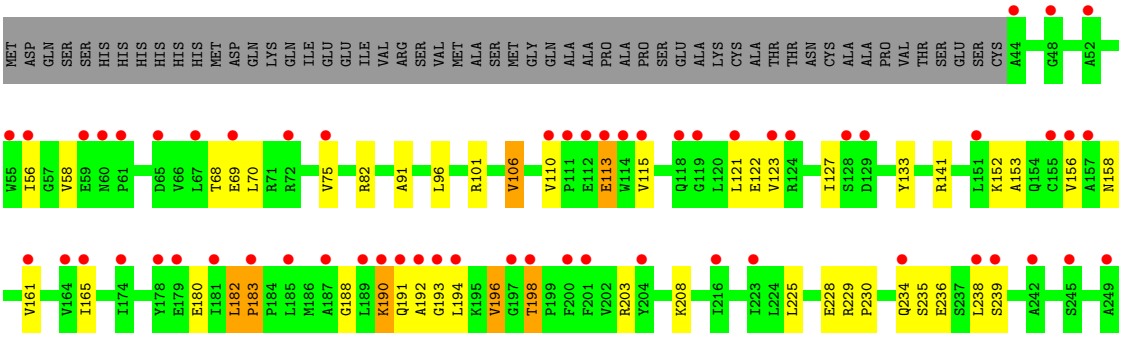
• Molecule 1: Ethanolamine ammonia-lyase heavy chain

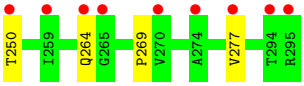
Chain C:



• Molecule 2: Ethanolamine ammonia-lyase light chain

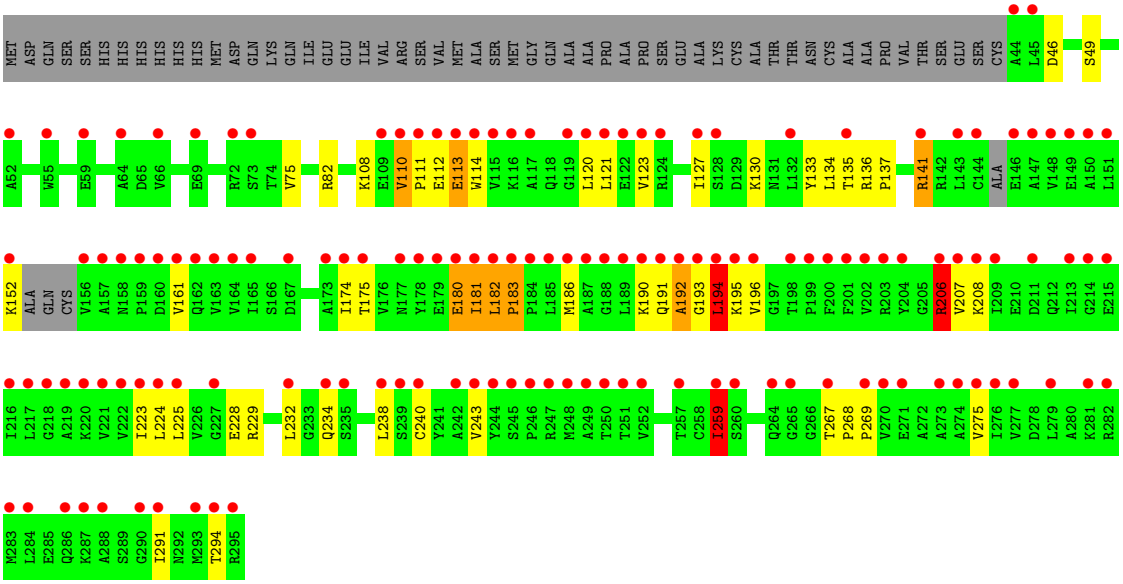
Chain B:





• Molecule 2: Ethanolamine ammonia-lyase light chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	242.76Å 242.76Å 76.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.51 – 2.10 47.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.51-2.10) 97.1 (47.51-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 2.10Å)	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 (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ETA, B12, NA, GOL

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	0.82	2/3518 (0.1%)	0.65	0/4764
1	C	0.81	2/3518 (0.1%)	0.65	0/4764
2	B	0.84	2/1943 (0.1%)	0.67	0/2633
2	D	0.84	3/1916 (0.2%)	0.66	0/2593
All	All	0.82	9/10895 (0.1%)	0.66	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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	183	PRO	CA-C	7.62	1.59	1.52
2	B	183	PRO	CA-C	7.03	1.58	1.52
1	A	319	ASP	N-CA	5.73	1.50	1.46
1	A	189	VAL	CA-CB	5.39	1.61	1.54
2	D	181	ILE	CA-CB	5.28	1.61	1.54
1	C	220	THR	CA-CB	5.26	1.60	1.54
2	B	158	ASN	N-CA	5.23	1.50	1.46
2	D	259	ILE	CA-CB	5.14	1.60	1.54
1	C	189	VAL	CA-CB	5.12	1.61	1.54

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
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 (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	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	0	0	0
3	C	4	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10975	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:H362	5:B:601:B12:H351	1.48	0.92
5:D:601:B12:H362	5:D:601:B12:H351	1.52	0.89
5:B:601:B12:H552	5:B:601:B12:H531	1.57	0.87
5:D:601:B12:H552	5:D:601:B12:H531	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:H601	5:D:601:B12:H262	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:H552	5:D:601:B12:C53	2.35	0.51
5:B:601:B12:H552	5:B:601:B12:C53	2.36	0.50
5:D:601:B12:H362	5:D:601:B12:C35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:PRO:HA	2:D:206:ARG:HD3	1.94	0.48
5:D:601:B12:H541	5:D:601:B12:H602	1.76	0.48
1:C:55:THR:HG22	1:C:58:ASP:CG	2.39	0.47
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
5:B:601:B12:H601	5:B:601:B12:H262	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:OD1	1:A:187:ASP:N	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:H301	5:B:601:B12:H253	1.75	0.43
1:A:342:ILE:HA	1:A:379:LEU:HD13	2.01	0.43
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:OD1	1:C:187:ASP:N	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:115:VAL:HG11	2:B:122:GLU:HG3	2.02	0.41
2:B:127:ILE:HG21	2:B:133:TYR:HB2	2.03	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%)	30	28
1	C	451/453 (100%)	431 (96%)	20 (4%)	0	100	100
2	B	250/306 (82%)	244 (98%)	5 (2%)	1 (0%)	30	28
2	D	242/306 (79%)	234 (97%)	6 (2%)	2 (1%)	16	12
All	All	1394/1518 (92%)	1339 (96%)	50 (4%)	5 (0%)	30	28

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 (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	370/370 (100%)	355 (96%)	15 (4%)	27	29
1	C	370/370 (100%)	353 (95%)	17 (5%)	24	25
2	B	206/251 (82%)	180 (87%)	26 (13%)	4	2
2	D	204/251 (81%)	170 (83%)	34 (17%)	2	1
All	All	1150/1242 (93%)	1058 (92%)	92 (8%)	11	8

All (92) 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	59	ILE
1	A	60	ARG
1	A	65	ILE
1	A	161	LEU
1	A	166	THR
1	A	171	GLN
1	A	221	GLN
1	A	269	ARG
1	A	326	VAL
1	A	339	ARG
1	A	375	LEU
1	A	380	MET
2	B	56	ILE
2	B	68	THR
2	B	69	GLU
2	B	70	LEU
2	B	75	VAL
2	B	96	LEU
2	B	101	ARG
2	B	106	VAL
2	B	113	GLU
2	B	121	LEU
2	B	123	VAL
2	B	152	LYS
2	B	161	VAL
2	B	165	ILE
2	B	182	LEU
2	B	190	LYS
2	B	194	LEU
2	B	196	VAL
2	B	198	THR
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

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Mol	Chain	Res	Type
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	171	GLN
1	C	202	LEU
1	C	230	THR
1	C	253	LYS
1	C	269	ARG
1	C	326	VAL
1	C	375	LEU
1	C	380	MET
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	174	ILE
2	D	175	THR
2	D	180	GLU
2	D	182	LEU
2	D	186	MET
2	D	190	LYS
2	D	191	GLN
2	D	194	LEU
2	D	196	VAL
2	D	206	ARG
2	D	207	VAL
2	D	208	LYS
2	D	223	ILE
2	D	224	LEU

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Mol	Chain	Res	Type
2	D	229	ARG
2	D	232	LEU
2	D	234	GLN
2	D	243	VAL
2	D	259	ILE
2	D	267	THR
2	D	275	VAL
2	D	291	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	227	HIS
1	A	368	HIS
2	B	62	HIS
2	B	131	ASN
2	B	264	GLN
1	C	13	GLN
1	C	87	GLN
1	C	276	ASN
1	C	349	HIS
2	D	234	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	GOL	A	1011	-	5,5,5	0.42	0	5,5,5	0.36	0
4	GOL	A	1012	-	5,5,5	0.34	0	5,5,5	0.32	0
4	GOL	A	1014	-	5,5,5	0.32	0	5,5,5	0.33	0
3	ETA	A	602	-	3,3,3	0.75	0	2,2,2	0.75	0
4	GOL	C	1015	-	5,5,5	0.42	0	5,5,5	0.27	0
5	B12	B	601	-	94,101,101	1.58	16 (17%)	149,166,166	1.27	15 (10%)
4	GOL	C	1013	-	5,5,5	0.39	0	5,5,5	0.24	0
3	ETA	C	602	-	3,3,3	0.74	0	2,2,2	0.70	0
5	B12	D	601	-	94,101,101	1.46	12 (12%)	149,166,166	1.30	19 (12%)

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
4	GOL	A	1011	-	-	4/4/4/4	-
4	GOL	A	1012	-	-	1/4/4/4	-
4	GOL	A	1014	-	-	4/4/4/4	-
3	ETA	A	602	-	-	0/1/1/1	-
4	GOL	C	1015	-	-	2/4/4/4	-
5	B12	B	601	-	-	16/56/223/223	0/3/11/11
4	GOL	C	1013	-	-	0/4/4/4	-
3	ETA	C	602	-	-	0/1/1/1	-
5	B12	D	601	-	-	21/56/223/223	0/3/11/11

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	B12	C19-N24	-7.00	1.40	1.49
5	D	601	B12	C19-N24	-6.70	1.40	1.49
5	B	601	B12	C14-N23	4.33	1.40	1.35
5	B	601	B12	C47-C12	-4.12	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C46-C12	-3.88	1.46	1.54
5	D	601	B12	C8B-C9B	3.86	1.46	1.40
5	D	601	B12	C12-C11	-3.84	1.45	1.52
5	B	601	B12	C6B-C5B	3.73	1.49	1.40
5	D	601	B12	C6B-C5B	3.69	1.49	1.40
5	B	601	B12	C8B-C9B	3.66	1.46	1.40
5	B	601	B12	C9-N22	3.64	1.39	1.30
5	B	601	B12	C46-C12	-3.45	1.47	1.54
5	B	601	B12	C9B-N3B	-3.39	1.33	1.39
5	D	601	B12	C9-N22	3.05	1.38	1.30
5	D	601	B12	C9B-N3B	-2.98	1.34	1.39
5	D	601	B12	C2B-N3B	2.97	1.37	1.31
5	B	601	B12	C2B-N3B	2.87	1.37	1.31
5	B	601	B12	C17-C18	2.73	1.59	1.54
5	D	601	B12	C8B-N1B	-2.63	1.34	1.39
5	B	601	B12	C12-C11	-2.59	1.47	1.52
5	B	601	B12	C8B-N1B	-2.58	1.34	1.39
5	D	601	B12	C14-C15	2.46	1.49	1.38
5	D	601	B12	C10-C11	-2.42	1.30	1.37
5	B	601	B12	C10-C11	-2.32	1.30	1.37
5	B	601	B12	C14-C15	2.28	1.48	1.38
5	D	601	B12	C17-C18	2.25	1.58	1.54
5	B	601	B12	C11-N23	2.10	1.40	1.36
5	B	601	B12	C1-C19	-2.08	1.50	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	B12	C19-N24-C16	5.27	113.05	107.29
5	D	601	B12	C19-N24-C16	4.96	112.71	107.29
5	B	601	B12	C9B-C8B-N1B	3.90	107.03	105.30
5	D	601	B12	C9B-C8B-N1B	3.88	107.03	105.30
5	D	601	B12	C18-C19-N24	3.84	108.10	102.33
5	D	601	B12	C54-C17-C18	-3.67	107.73	112.99
5	B	601	B12	C18-C19-N24	3.45	107.51	102.33
5	B	601	B12	C1-C19-N24	3.18	109.79	106.25
5	B	601	B12	C9B-N3B-C2B	3.17	108.29	104.40
5	D	601	B12	C9B-N3B-C2B	3.13	108.24	104.40
5	B	601	B12	C54-C17-C18	-3.10	108.53	112.99
5	D	601	B12	C8B-C9B-N3B	-3.00	106.76	110.00
5	B	601	B12	C8B-C9B-N3B	-2.98	106.78	110.00
5	D	601	B12	N1B-C2B-N3B	-2.91	109.81	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	601	B12	C47-C12-C46	2.82	114.07	109.41
5	B	601	B12	N1B-C2B-N3B	-2.78	109.98	113.94
5	D	601	B12	C2-C1-C19	2.69	122.80	118.61
5	B	601	B12	C7-C6-C5	-2.69	123.88	128.07
5	D	601	B12	C12-C11-C10	-2.69	119.94	123.40
5	B	601	B12	C20-C1-C19	-2.67	106.78	109.35
5	D	601	B12	C9-N22-C6	2.66	108.48	105.28
5	D	601	B12	C20-C1-C19	-2.65	106.80	109.35
5	B	601	B12	C2-C1-C19	2.63	122.70	118.61
5	B	601	B12	C30-C3-C2	-2.61	113.23	119.00
5	D	601	B12	C30-C3-C2	-2.52	113.43	119.00
5	D	601	B12	C7-C6-C5	-2.51	124.14	128.07
5	D	601	B12	C1-C19-N24	2.18	108.67	106.25
5	B	601	B12	C9-N22-C6	2.09	107.80	105.28
5	D	601	B12	C25-C2-C1	-2.09	110.63	113.75
5	D	601	B12	C8B-N1B-C2B	2.08	108.14	106.26
5	B	601	B12	C25-C2-C1	-2.05	110.69	113.75
5	D	601	B12	C7-C8-C9	2.04	103.48	100.89
5	B	601	B12	C7-C8-C9	2.01	103.44	100.89
5	D	601	B12	C3R-C2R-C1R	2.01	104.31	99.89

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1011	GOL	O1-C1-C2-C3
4	A	1011	GOL	C1-C2-C3-O3
4	A	1014	GOL	C1-C2-C3-O3
4	C	1015	GOL	C1-C2-C3-O3
5	B	601	B12	C38-C37-C7-C36
5	B	601	B12	C42-C41-C8-C9
5	B	601	B12	C2P-O3-P-O5
5	B	601	B12	C2P-O3-P-O2
5	B	601	B12	C2R-C1R-N1B-C8B
5	B	601	B12	O6R-C1R-N1B-C8B
5	D	601	B12	C38-C37-C7-C6
5	D	601	B12	C38-C37-C7-C36
5	D	601	B12	C38-C37-C7-C8
5	D	601	B12	C42-C41-C8-C9
5	D	601	B12	C13-C48-C49-C50
5	D	601	B12	C2P-O3-P-O5
5	D	601	B12	C2P-O3-P-O2

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Mol	Chain	Res	Type	Atoms
5	D	601	B12	O6R-C4R-C5R-O8R
5	D	601	B12	C3R-C4R-C5R-O8R
5	B	601	B12	C13-C48-C49-C50
4	A	1011	GOL	O2-C2-C3-O3
5	D	601	B12	C18-C17-C55-C56
5	B	601	B12	C16-C17-C55-C56
5	D	601	B12	C16-C17-C55-C56
4	A	1014	GOL	O1-C1-C2-C3
5	D	601	B12	O6R-C1R-N1B-C8B
5	B	601	B12	C38-C37-C7-C8
4	C	1015	GOL	O2-C2-C3-O3
5	B	601	B12	C2-C3-C30-C31
5	D	601	B12	C2-C3-C30-C31
5	B	601	B12	C4-C3-C30-C31
5	D	601	B12	C4-C3-C30-C31
4	A	1014	GOL	O1-C1-C2-O2
4	A	1014	GOL	O2-C2-C3-O3
5	B	601	B12	C18-C17-C55-C56
5	D	601	B12	C2R-C1R-N1B-C8B
5	B	601	B12	C38-C37-C7-C6
4	A	1011	GOL	O1-C1-C2-O2
5	D	601	B12	C3P-C2P-O3-P
5	B	601	B12	C2P-O3-P-O4
5	B	601	B12	C3P-C2P-O3-P
5	D	601	B12	C1P-C2P-O3-P
4	A	1012	GOL	O2-C2-C3-O3
5	D	601	B12	C17-C18-C60-C61
5	B	601	B12	C1P-C2P-O3-P
5	D	601	B12	C19-C18-C60-C61
5	D	601	B12	C2P-O3-P-O4
5	D	601	B12	C3R-O2-P-O5

There are no ring outliers.

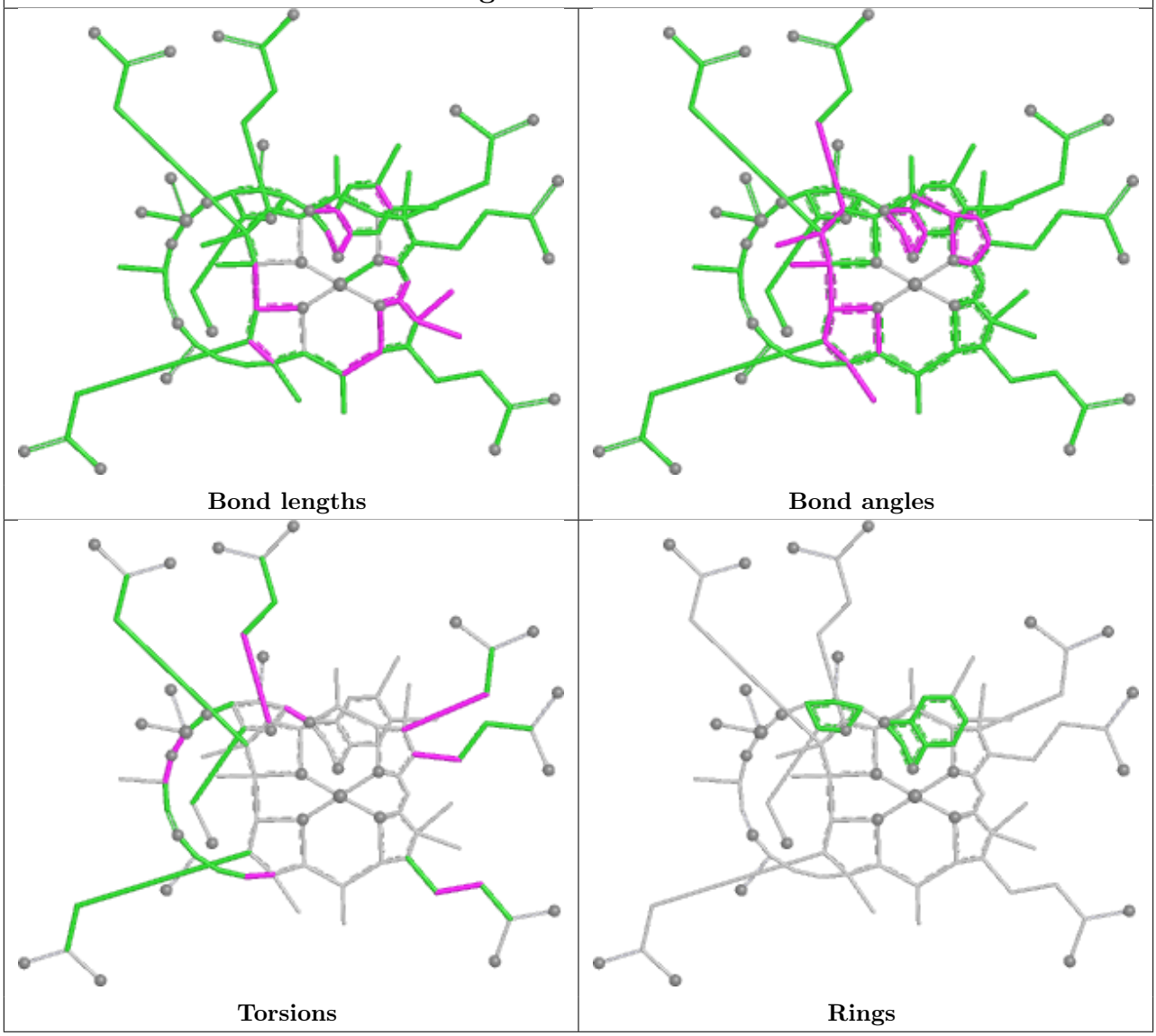
2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	B12	9	0
5	D	601	B12	10	0

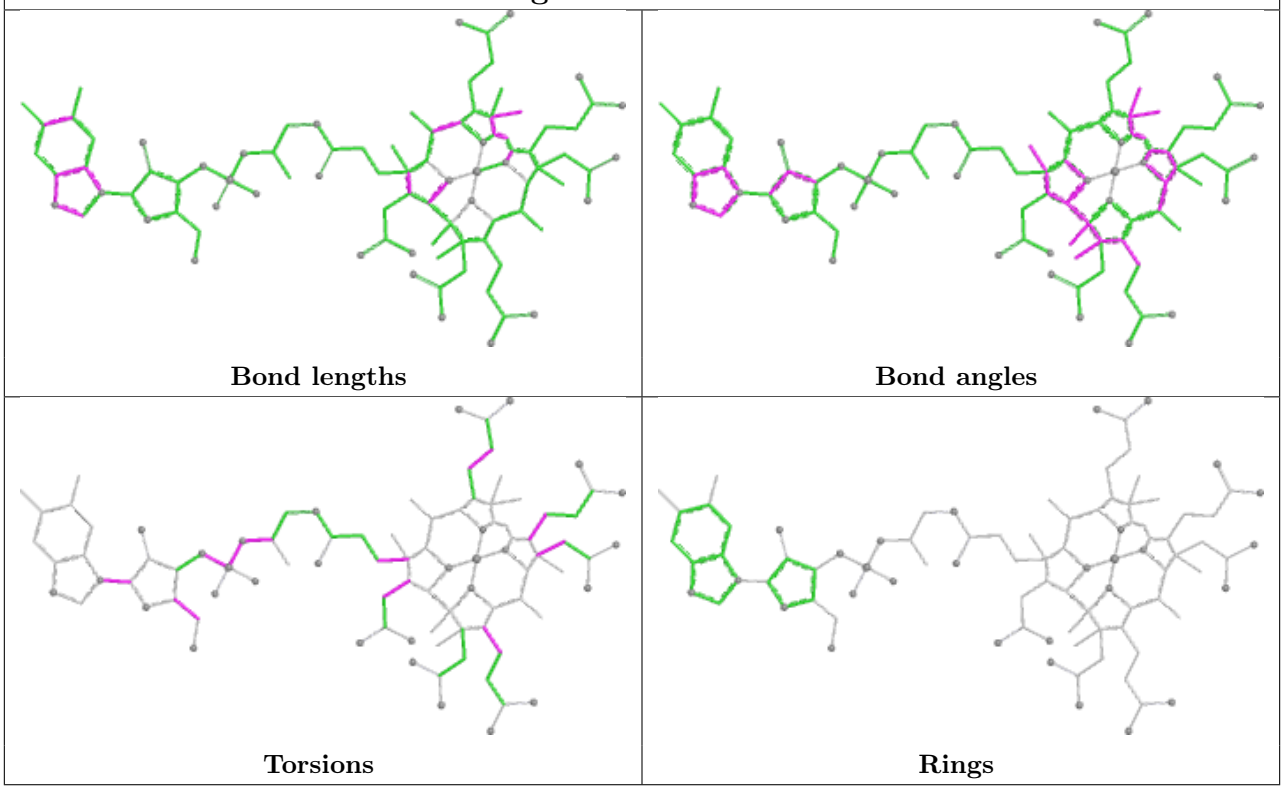
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand B12 B 601



Ligand B12 D 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	453/453 (100%)	0.24	14 (3%) 51 54	18, 30, 48, 61	0
1	C	453/453 (100%)	0.37	23 (5%) 33 35	18, 32, 54, 72	0
2	B	252/306 (82%)	1.54	68 (26%) 1 1	25, 62, 87, 105	0
2	D	248/306 (81%)	2.45	143 (57%) 0 0	23, 80, 128, 139	0
All	All	1406/1518 (92%)	0.91	248 (17%) 4 4	18, 39, 99, 139	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	ALA	8.4
2	D	194	LEU	8.0
2	D	156	VAL	7.8
2	D	123	VAL	6.2
2	B	192	ALA	5.8
2	D	121	LEU	5.6
2	D	198	THR	5.5
2	D	44	ALA	5.4
2	D	275	VAL	5.2
2	B	234	GLN	5.1
2	D	190	LYS	5.1
2	D	161	VAL	5.1
2	D	174	ILE	5.0
2	D	277	VAL	5.0
2	D	220	LYS	5.0
2	D	157	ALA	4.9
2	B	165	ILE	4.9
2	D	110	VAL	4.9
2	D	152	LYS	4.8
2	D	148	VAL	4.8
2	D	193	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	147	ALA	4.5
2	D	151	LEU	4.5
2	D	267	THR	4.4
2	D	181	ILE	4.4
2	D	159	PRO	4.4
2	D	189	LEU	4.4
2	D	111	PRO	4.3
2	D	288	ALA	4.3
2	D	144	CYS	4.3
2	D	214	GLY	4.3
2	D	216	ILE	4.3
2	D	187	ALA	4.2
2	B	44	ALA	4.2
2	D	273	ALA	4.2
2	D	248	MET	4.1
2	D	246	PRO	4.1
2	B	198	THR	4.1
2	D	208	LYS	4.1
2	D	219	ALA	4.0
2	D	291	ILE	4.0
2	D	294	THR	4.0
2	D	178	TYR	4.0
2	D	191	GLN	4.0
2	B	59	GLU	3.9
2	B	55	TRP	3.8
2	D	196	VAL	3.8
2	D	221	VAL	3.8
2	D	200	PHE	3.8
1	A	167	ARG	3.8
2	D	124	ARG	3.8
2	D	150	ALA	3.8
2	B	156	VAL	3.8
2	D	223	ILE	3.8
2	D	295	ARG	3.8
2	D	217	LEU	3.8
2	D	250	THR	3.7
2	D	279	LEU	3.7
2	D	160	ASP	3.7
2	D	206	ARG	3.7
2	D	244	TYR	3.7
2	B	185	LEU	3.6
2	B	295	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	270	VAL	3.6
2	D	175	THR	3.6
2	D	207	VAL	3.5
2	D	245	SER	3.4
2	D	164	VAL	3.4
2	D	183	PRO	3.4
1	A	269	ARG	3.4
2	D	281	LYS	3.4
2	D	251	THR	3.4
2	D	225	LEU	3.4
2	B	111	PRO	3.3
2	B	270	VAL	3.3
2	D	252	VAL	3.3
2	B	191	GLN	3.3
2	D	247	ARG	3.3
2	D	120	LEU	3.3
1	C	4	LYS	3.3
2	D	234	GLN	3.3
2	D	243	VAL	3.3
2	B	157	ALA	3.3
2	D	165	ILE	3.3
2	B	189	LEU	3.3
2	D	73	SER	3.2
2	D	119	GLY	3.2
2	D	218	GLY	3.2
1	C	7	LEU	3.2
2	D	162	GLN	3.2
1	A	197	ASP	3.2
2	B	197	GLY	3.2
2	D	249	ALA	3.2
2	B	216	ILE	3.1
2	D	276	ILE	3.1
1	C	55	THR	3.1
2	B	181	ILE	3.1
2	D	238	LEU	3.1
2	D	128	SER	3.1
2	D	186	MET	3.1
2	B	113	GLU	3.1
2	D	274	ALA	3.1
2	B	294	THR	3.1
2	D	264	GLN	3.1
2	D	222	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	143	LEU	3.1
2	D	284	LEU	3.1
2	D	195	LYS	3.0
2	D	235	SER	3.0
2	B	155	CYS	3.0
2	D	185	LEU	3.0
2	B	200	PHE	3.0
2	B	75	VAL	3.0
2	D	232	LEU	3.0
2	D	127	ILE	3.0
2	D	199	PRO	3.0
2	D	149	GLU	2.9
2	D	209	ILE	2.9
1	A	198	ASP	2.9
2	B	72	ARG	2.9
2	D	203	ARG	2.9
2	D	146	GLU	2.9
2	B	239	SER	2.9
1	C	65	ILE	2.9
2	D	204	TYR	2.9
2	B	190	LYS	2.9
2	D	116	LYS	2.9
2	B	194	LEU	2.9
2	B	277	VAL	2.9
2	D	202	VAL	2.9
2	D	286	GLN	2.9
2	B	274	ALA	2.9
2	D	117	ALA	2.9
2	D	135	THR	2.8
2	D	158	ASN	2.8
2	D	141	ARG	2.8
1	A	447	GLY	2.8
2	B	238	LEU	2.8
2	D	113	GLU	2.8
1	C	269	ARG	2.8
2	D	72	ARG	2.8
2	D	109	GLU	2.8
2	D	215	GLU	2.8
2	D	182	LEU	2.8
2	D	224	LEU	2.8
1	C	64	VAL	2.8
2	D	55	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	282	ARG	2.7
1	C	451	LEU	2.7
2	B	61	PRO	2.7
2	D	269	PRO	2.7
1	C	1	MET	2.7
2	D	180	GLU	2.7
2	B	193	GLY	2.7
1	C	167	ARG	2.7
1	C	197	ASP	2.7
2	B	124	ARG	2.7
2	D	173	ALA	2.6
2	B	179	GLU	2.6
2	D	45	LEU	2.6
2	B	164	VAL	2.6
2	D	132	LEU	2.6
2	B	264	GLN	2.6
2	D	265	GLY	2.6
1	A	450	SER	2.6
2	D	122	GLU	2.5
2	D	213	ILE	2.5
2	B	65	ASP	2.5
1	C	68	GLU	2.5
2	D	179	GLU	2.5
2	D	201	PHE	2.5
2	D	227	GLY	2.5
2	D	59	GLU	2.5
2	D	69	GLU	2.5
2	D	271	GLU	2.5
1	C	14	PHE	2.5
2	D	114	TRP	2.5
1	C	301	GLY	2.5
2	B	123	VAL	2.4
2	D	184	PRO	2.4
2	B	249	ALA	2.4
1	A	4	LYS	2.4
1	A	237	ARG	2.4
2	B	119	GLY	2.4
2	B	115	VAL	2.4
2	D	167	ASP	2.4
1	C	336	TYR	2.4
2	D	239	SER	2.4
1	C	6	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	446	ALA	2.4
1	C	62	ASN	2.4
2	B	178	TYR	2.4
2	B	52	ALA	2.4
1	A	68	GLU	2.4
1	C	5	THR	2.4
2	D	290	GLY	2.3
1	A	445	ARG	2.3
1	C	445	ARG	2.3
2	D	287	LYS	2.3
2	B	56	ILE	2.3
2	D	259	ILE	2.3
2	B	161	VAL	2.3
2	B	187	ALA	2.3
2	D	242	ALA	2.3
1	C	300	PHE	2.3
2	B	174	ILE	2.3
1	A	13	GLN	2.3
1	C	63	PRO	2.3
2	D	52	ALA	2.3
2	D	260	SER	2.3
2	D	177	ASN	2.3
2	B	151	LEU	2.3
1	A	171	GLN	2.2
2	B	128	SER	2.2
2	D	115	VAL	2.2
2	D	211	ASP	2.2
2	B	265	GLY	2.2
2	B	60	ASN	2.2
2	B	110	VAL	2.2
2	B	121	LEU	2.2
2	D	240	CYS	2.2
2	D	257	THR	2.2
2	B	223	ILE	2.1
2	B	250	THR	2.1
2	D	163	VAL	2.1
2	B	183	PRO	2.1
2	B	259	ILE	2.1
2	D	64	ALA	2.1
2	B	67	LEU	2.1
2	B	112	GLU	2.1
2	D	293	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	48	GLY	2.1
2	D	188	GLY	2.1
1	C	8	PHE	2.1
2	B	201	PHE	2.1
2	B	114	TRP	2.1
1	C	54	MET	2.0
1	C	200	GLU	2.0
2	B	245	SER	2.1
2	D	283	MET	2.0
2	B	118	GLN	2.0
1	A	2	LYS	2.0
2	B	69	GLU	2.0
2	D	66	VAL	2.0
2	D	112	GLU	2.0
2	B	242	ALA	2.0
2	B	129	ASP	2.0
2	B	204	TYR	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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	D	1002	1/1	0.55	0.58	94,94,94,94	0
4	GOL	C	1015	6/6	0.80	0.19	56,61,63,66	0
4	GOL	A	1011	6/6	0.84	0.18	36,41,47,54	0
4	GOL	A	1014	6/6	0.89	0.18	29,56,60,67	0
4	GOL	C	1013	6/6	0.90	0.16	44,49,56,57	0
5	B12	D	601	91/91	0.92	0.14	25,43,55,59	0

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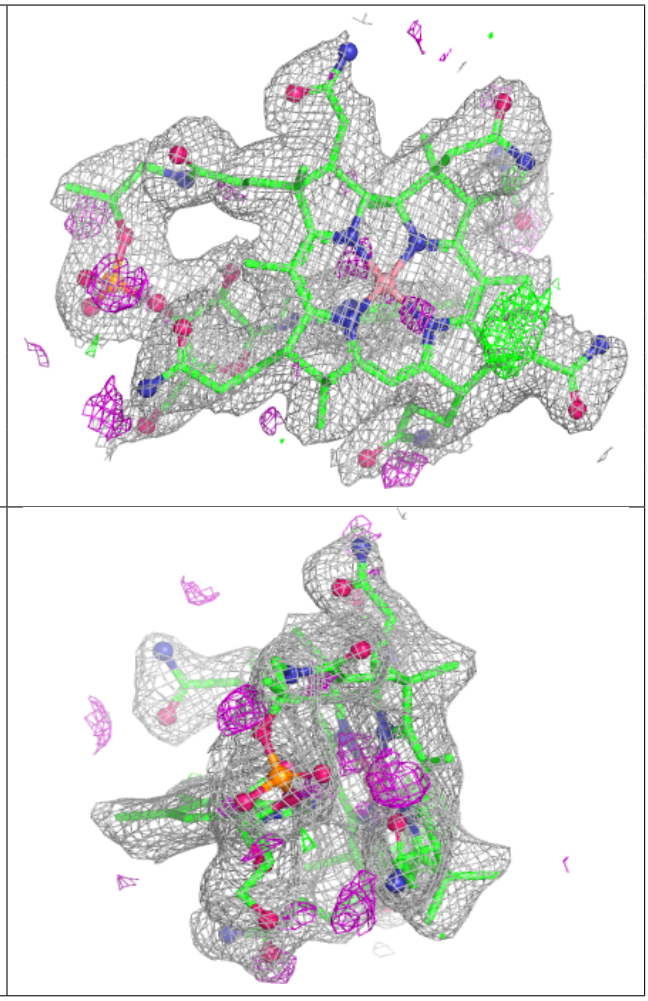
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1012	6/6	0.93	0.12	34,37,43,50	0
6	NA	C	1001	1/1	0.93	0.13	45,45,45,45	0
5	B12	B	601	91/91	0.93	0.13	20,36,44,60	0
3	ETA	C	602	4/4	0.95	0.09	24,25,26,27	0
3	ETA	A	602	4/4	0.95	0.11	25,29,30,32	0

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.

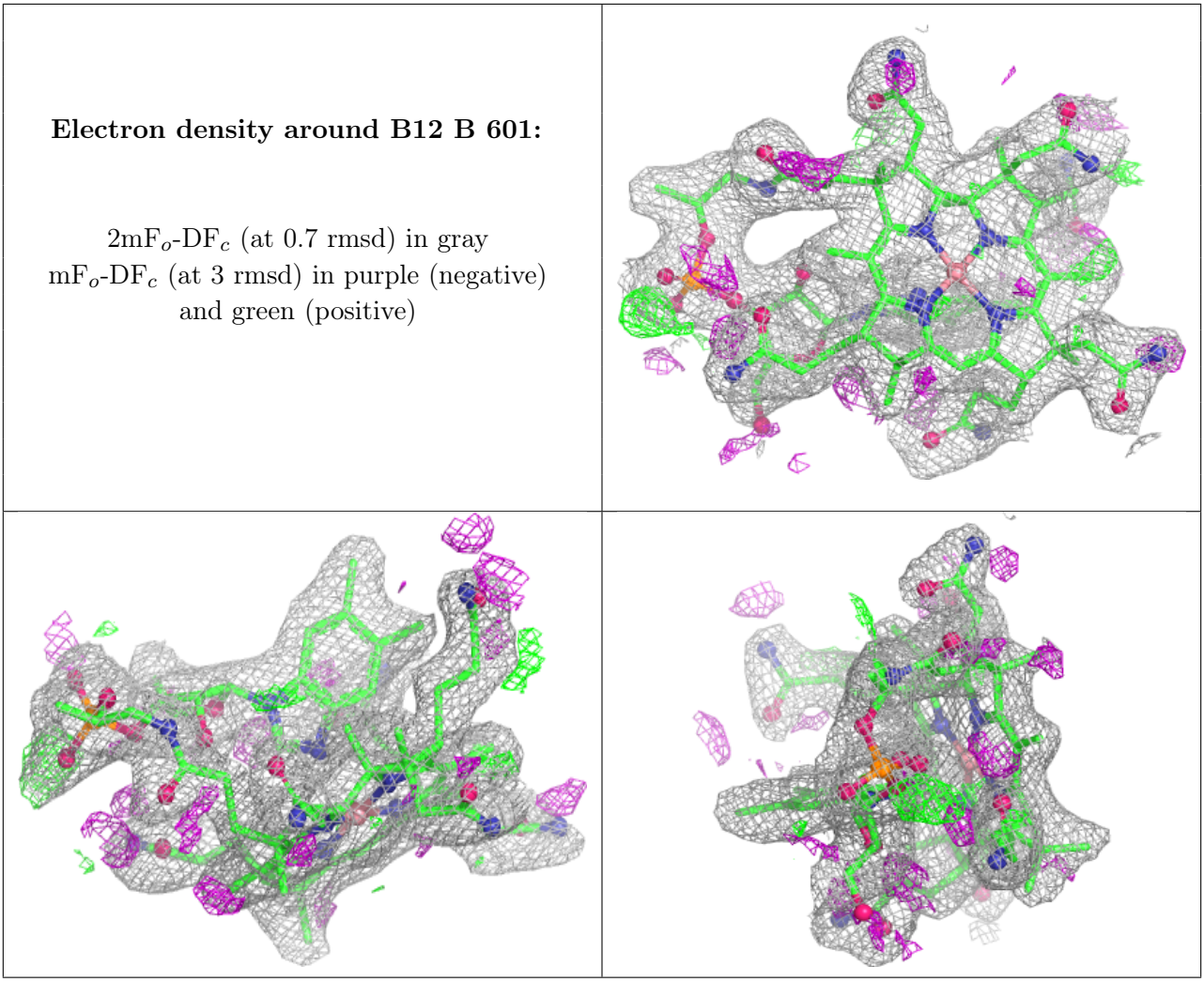
Electron density around B12 D 601:

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 (i)

There are no such residues in this entry.