Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 11:44 PM EDT

PDB ID	:	3ANY
Title	:	Crystal structure of ethanolamine ammonia-lyase from escherichia coli complexed with CN-CBL and (R)-2-amino-1-propanol
Authors	:	Shibata, N.
Deposited on	:	2010-09-16
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:

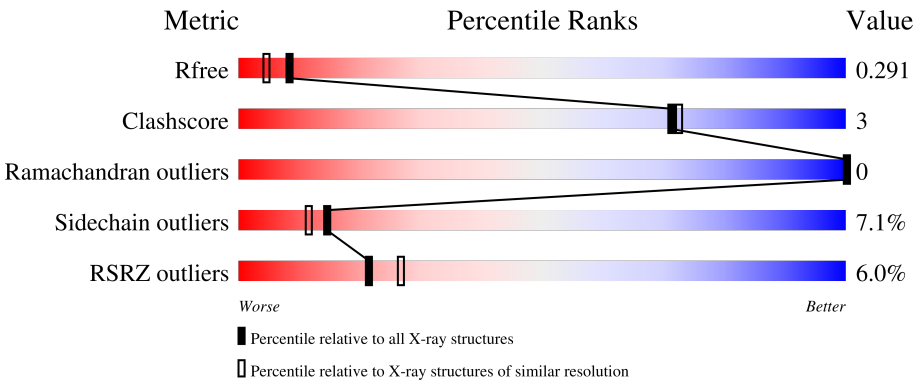
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (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}	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 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	92% 7%
1	C	453	91% 9% •
2	B	263	9% 82% 13% • •
2	D	263	23% 79% 15% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11700 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	3470	2174	593	681	22	0	2	0
1	C	453	3495	2192	599	682	22	0	6	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	252	1916	1197	347	362	10	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

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

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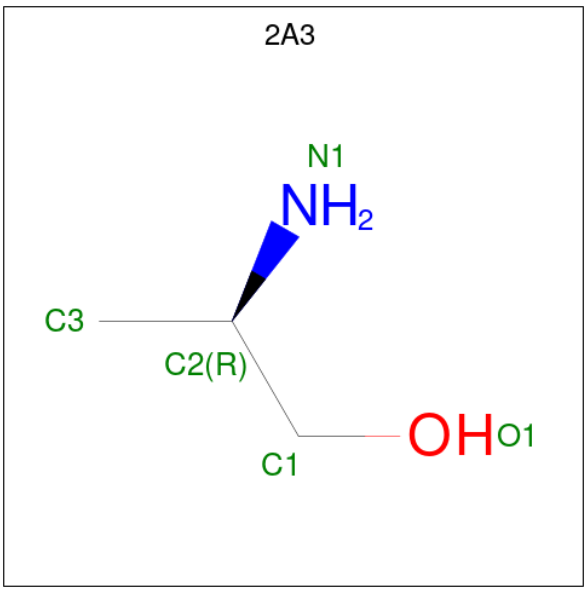
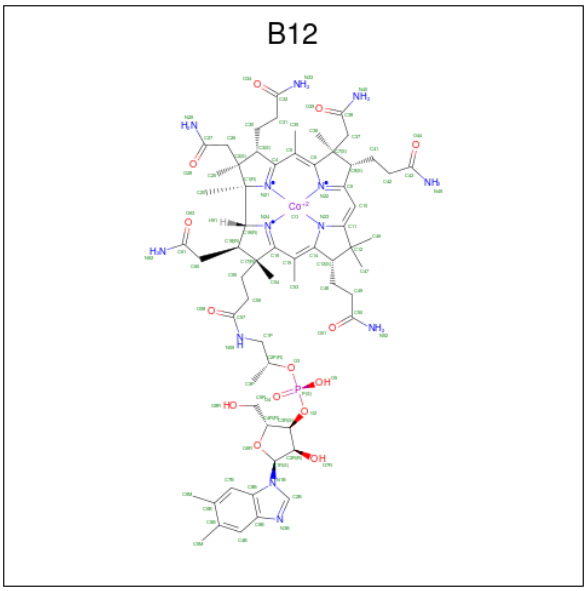
Chain	Residue	Modelled	Actual	Comment	Reference
D	38	HIS	-	expression tag	UNP P19636
D	39	HIS	-	expression tag	UNP P19636
D	40	HIS	-	expression tag	UNP P19636
D	41	HIS	-	expression tag	UNP P19636
D	42	HIS	-	expression tag	UNP P19636
D	43	HIS	-	expression tag	UNP P19636

- Molecule 3 is (2R)-2-aminopropan-1-ol (three-letter code: 2A3) (formula: C_3H_9NO).



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

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 5 is water.

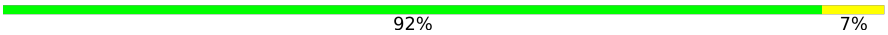
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	274	274	274	0	0
5	B	75	75	75	0	0
5	C	272	272	272	0	0
5	D	90	90	90	0	0

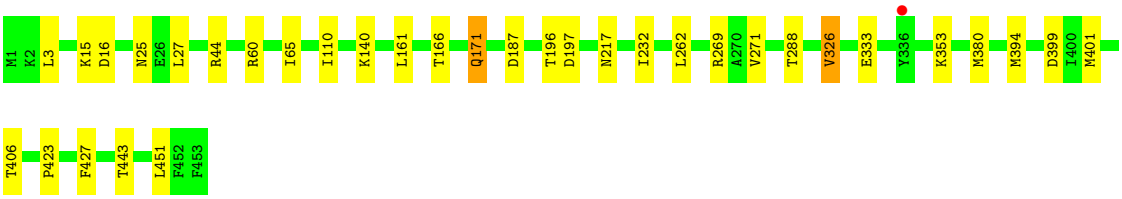
3 Residue-property plots (i)

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

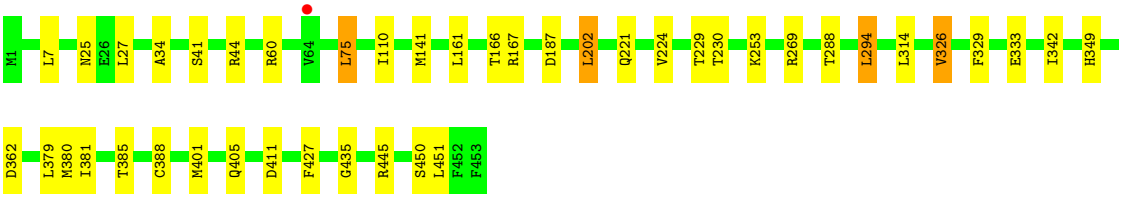
Chain A:





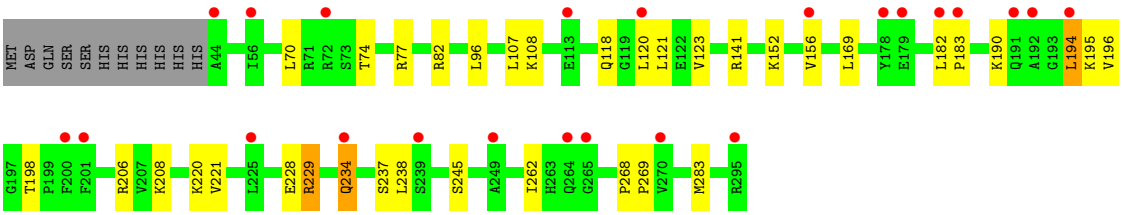
• Molecule 1: Ethanolamine ammonia-lyase heavy chain

Chain C:



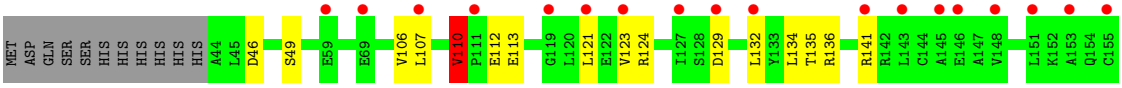
• Molecule 2: Ethanolamine ammonia-lyase light chain

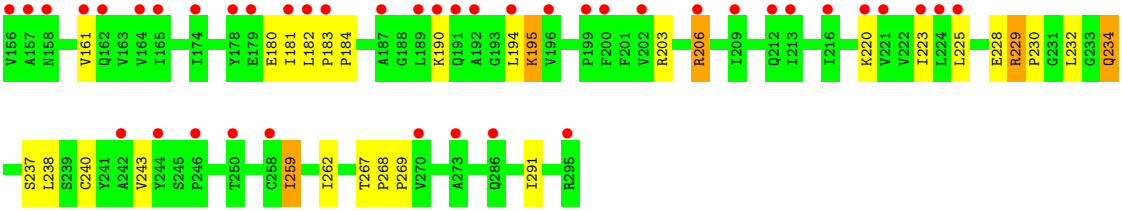
Chain B:



• Molecule 2: Ethanolamine ammonia-lyase light chain

Chain D:




V156 A157 N158 V161 Q162 V163 V164 I165 I174 Y178 E179 E180 I181 L182 P183 P184 A187 G188 L189 K190 Q191 A192 G193 L194 K195 V196 P199 F200 F201 V202 R203 R206 I209 Q212 I213 I216 K220 V221 V222 I223 L224 L225 E228 R229 P230 G231 L232 G233 Q234
S237 L238 S239 C240 Y241 A242 V243 Y244 S245 P246 T250 C258 I259 I262 T267 P268 P269 V270 A273 Q286 I291 R295

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	244.07Å 244.07Å 76.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.84 – 2.10 47.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.8 (47.84-2.10) 92.8 (47.82-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.246 , 0.276 0.260 , 0.291	Depositor DCC
R_{free} test set	7043 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 16.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: 2A3, B12

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	0.56	0/3530	0.34	0/4780
1	C	0.57	0/3567	0.35	0/4829
2	B	0.53	0/1943	0.34	0/2633
2	D	0.53	0/1943	0.34	0/2633
All	All	0.55	0/10983	0.34	0/14875

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	2
1	C	0	1
2	B	0	2
2	D	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	VAL	Peptide
1	A	423	PRO	Peptide
2	B	120	LEU	Peptide
2	B	206	ARG	Peptide
1	C	326	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	D	110	VAL	Peptide
2	D	206	ARG	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	3470	0	3429	11	0
1	C	3495	0	3471	19	0
2	B	1916	0	1973	11	0
2	D	1916	0	1973	16	0
3	A	5	0	9	0	0
3	C	5	0	9	0	0
4	B	91	0	88	11	0
4	D	91	0	88	13	0
5	A	274	0	0	0	0
5	B	75	0	0	0	0
5	C	272	0	0	0	0
5	D	90	0	0	0	0
All	All	11700	0	11040	76	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 (76) 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:269[B]:ARG:HH11	1:C:269[B]:ARG:HG3	1.09	1.18
1:C:269[B]:ARG:HH11	1:C:269[B]:ARG:CG	1.83	0.90
4:B:601:B12:H552	4:B:601:B12:H531	1.58	0.86
4:B:601:B12:H362	4:B:601:B12:H351	1.56	0.85
4:D:601:B12:H552	4:D:601:B12:H531	1.63	0.81
4:D:601:B12:H362	4:D:601:B12:H351	1.67	0.77
1:C:329:PHE:O	2:D:229:ARG:NH2	2.20	0.70
1:C:269[B]:ARG:HG3	1:C:269[B]:ARG:NH1	1.91	0.67
2:B:234:GLN:HE22	2:B:237:SER:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ALA:HB2	1:C:294:LEU:HD11	1.88	0.55
1:C:75:LEU:HD22	1:C:314:LEU:HD12	1.88	0.55
1:C:269[B]:ARG:CG	1:C:269[B]:ARG:NH1	2.50	0.55
2:D:240:CYS:HB3	2:D:259:ILE:HG23	1.88	0.55
4:D:601:B12:H601	4:D:601:B12:H262	1.87	0.55
2:B:156:VAL:HG22	2:B:198:THR:HG22	1.90	0.54
4:B:601:B12:H601	4:B:601:B12:H262	1.89	0.53
4:D:601:B12:H552	4:D:601:B12:C53	2.36	0.53
4:B:601:B12:H482	4:B:601:B12:H2B	1.89	0.53
4:B:601:B12:H362	4:B:601:B12:C35	2.32	0.53
1:C:342:ILE:HA	1:C:379:LEU:HD13	1.91	0.53
1:C:202:LEU:HD22	1:C:224:VAL:HG11	1.90	0.52
2:B:229:ARG:NH1	4:B:601:B12:H543	2.25	0.52
2:D:228:GLU:HA	4:D:601:B12:H1P2	1.92	0.52
2:D:135:THR:HG23	2:D:136:ARG:HG2	1.93	0.51
2:D:106:VAL:HG12	2:D:230:PRO:HG2	1.92	0.50
2:D:225:LEU:HB3	2:D:238:LEU:HD21	1.93	0.50
2:B:228:GLU:HA	4:B:601:B12:H1P2	1.94	0.50
1:A:394:MET:HE1	1:A:399:ASP:HB2	1.93	0.50
4:B:601:B12:H552	4:B:601:B12:C53	2.36	0.49
1:C:288:THR:O	1:C:326:VAL:HG22	2.11	0.49
4:D:601:B12:H362	4:D:601:B12:C35	2.40	0.49
1:A:25:ASN:O	1:A:44:ARG:HD3	2.12	0.49
1:A:326:VAL:HG23	1:A:326:VAL:O	2.13	0.49
2:D:234:GLN:HE22	2:D:237:SER:HB2	1.75	0.49
4:D:601:B12:H2B	4:D:601:B12:H482	1.93	0.49
2:B:238:LEU:HB3	2:B:262:ILE:HB	1.94	0.49
2:D:46:ASP:HB3	2:D:49:SER:HB3	1.95	0.48
1:C:25:ASN:O	1:C:44:ARG:HD3	2.13	0.48
2:D:180:GLU:HB3	2:D:269:PRO:HB2	1.95	0.47
1:C:380:MET:SD	1:C:411:ASP:HB3	2.54	0.47
4:D:601:B12:H541	4:D:601:B12:H602	1.78	0.47
1:A:288:THR:O	1:A:326:VAL:HG22	2.14	0.47
1:C:435:GLY:HA3	1:C:445:ARG:HH22	1.79	0.47
1:C:326:VAL:O	1:C:326:VAL:HG23	2.15	0.47
2:D:183:PRO:HB2	2:D:184:PRO:HD3	1.97	0.47
4:B:601:B12:H481	4:B:601:B12:H473	1.52	0.46
1:C:349:HIS:CE1	1:C:388:CYS:HA	2.50	0.46
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.51	0.46
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.51	0.45
2:D:181:ILE:HG12	2:D:269:PRO:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:601:B12:H473	4:D:601:B12:H481	1.63	0.45
2:B:221:VAL:HG13	2:B:283:MET:HE1	1.99	0.44
4:B:601:B12:H261	4:B:601:B12:H91	1.92	0.44
4:D:601:B12:H472	4:D:601:B12:H10	1.79	0.44
2:B:169:LEU:HD13	2:B:229:ARG:HB3	1.99	0.44
2:D:110:VAL:O	2:D:203:ARG:NH2	2.46	0.44
2:D:181:ILE:HD11	2:D:262:ILE:HG21	2.00	0.44
4:D:601:B12:H301	4:D:601:B12:H253	1.79	0.43
1:C:326:VAL:HA	1:C:362:ASP:HB3	2.01	0.42
1:A:171:GLN:H	1:A:171:GLN:HG2	1.58	0.42
2:B:141:ARG:HG2	2:B:208:LYS:HB2	2.02	0.42
1:A:187:ASP:OD1	1:A:187:ASP:N	2.51	0.42
2:D:190:LYS:HA	2:D:190:LYS:HD3	1.88	0.42
1:C:381:ILE:O	1:C:385:THR:HG23	2.20	0.42
1:A:443:THR:O	2:B:82:ARG:NH1	2.52	0.42
1:C:110:ILE:HD13	1:C:141:MET:HG2	2.02	0.42
1:A:394:MET:HE2	1:A:406:THR:CG2	2.50	0.41
2:B:194:LEU:HB2	2:B:195:LYS:H	1.72	0.41
4:D:601:B12:H261	4:D:601:B12:H91	1.93	0.41
4:B:601:B12:H481	4:B:601:B12:H521	1.45	0.41
4:D:601:B12:H562	4:D:601:B12:H18	1.86	0.41
2:D:194:LEU:HB3	2:D:195:LYS:H	1.61	0.41
2:D:268:PRO:HA	2:D:269:PRO:HD3	1.79	0.41
1:A:232:ILE:HG23	1:A:271:VAL:HG21	2.03	0.40
2:B:268:PRO:HA	2:B:269:PRO:HD3	1.84	0.40
1:A:353:LYS:HD2	1:A:353:LYS:HA	1.77	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	453/453 (100%)	436 (96%)	17 (4%)	0	100	100
1	C	457/453 (101%)	438 (96%)	19 (4%)	0	100	100
2	B	250/263 (95%)	243 (97%)	7 (3%)	0	100	100
2	D	250/263 (95%)	243 (97%)	7 (3%)	0	100	100
All	All	1410/1432 (98%)	1360 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	372/370 (100%)	352 (95%)	20 (5%)	22	20
1	C	376/370 (102%)	357 (95%)	19 (5%)	24	22
2	B	206/217 (95%)	187 (91%)	19 (9%)	9	6
2	D	206/217 (95%)	182 (88%)	24 (12%)	5	3
All	All	1160/1174 (99%)	1078 (93%)	82 (7%)	14	11

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	15	LYS
1	A	16	ASP
1	A	27	LEU
1	A	60	ARG
1	A	65	ILE
1	A	110	ILE
1	A	140	LYS
1	A	161	LEU
1	A	166	THR
1	A	171	GLN
1	A	196	THR
1	A	197	ASP

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	262	LEU
1	A	269	ARG
1	A	333	GLU
1	A	380	MET
1	A	401	MET
1	A	451	LEU
2	B	70	LEU
2	B	74	THR
2	B	77	ARG
2	B	96	LEU
2	B	107	LEU
2	B	108	LYS
2	B	118	GLN
2	B	121	LEU
2	B	123	VAL
2	B	152	LYS
2	B	182	LEU
2	B	183	PRO
2	B	190	LYS
2	B	194	LEU
2	B	196	VAL
2	B	220	LYS
2	B	229	ARG
2	B	234	GLN
2	B	245	SER
1	C	7	LEU
1	C	27	LEU
1	C	41	SER
1	C	60	ARG
1	C	75	LEU
1	C	161	LEU
1	C	166	THR
1	C	167	ARG
1	C	202	LEU
1	C	221	GLN
1	C	229	THR
1	C	230	THR
1	C	253	LYS
1	C	294	LEU
1	C	333	GLU
1	C	401	MET

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Mol	Chain	Res	Type
1	C	405	GLN
1	C	450	SER
1	C	451	LEU
2	D	107	LEU
2	D	110	VAL
2	D	112	GLU
2	D	113	GLU
2	D	121	LEU
2	D	123	VAL
2	D	124	ARG
2	D	129	ASP
2	D	132	LEU
2	D	134	LEU
2	D	141	ARG
2	D	161	VAL
2	D	182	LEU
2	D	195	LYS
2	D	206	ARG
2	D	220	LYS
2	D	223	ILE
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	291	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
2	B	99	HIS
2	B	131	ASN
2	B	234	GLN
1	C	349	HIS
2	D	99	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	B12	B	601	-	90,101,101	1.40	14 (15%)	137,166,166	1.07	11 (8%)
4	B12	D	601	-	90,101,101	1.32	11 (12%)	137,166,166	1.10	11 (8%)
3	2A3	A	602	-	4,4,4	0.55	0	3,4,4	0.84	0
3	2A3	C	602	-	4,4,4	0.61	0	3,4,4	0.76	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
4	B12	B	601	-	-	19/52/223/223	0/3/11/11
4	B12	D	601	-	-	20/52/223/223	0/3/11/11
3	2A3	A	602	-	-	0/2/2/2	-
3	2A3	C	602	-	-	0/2/2/2	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	B12	C19-N24	-5.26	1.39	1.48
4	D	601	B12	C19-N24	-5.11	1.39	1.48
4	D	601	B12	C12-C11	-4.31	1.44	1.52
4	B	601	B12	C14-N23	4.17	1.40	1.35
4	B	601	B12	C47-C12	-3.65	1.46	1.54
4	B	601	B12	C9-N22	3.65	1.40	1.30
4	D	601	B12	C46-C12	-3.64	1.46	1.54
4	D	601	B12	C6B-C5B	3.54	1.49	1.40
4	B	601	B12	C6B-C5B	3.51	1.49	1.40
4	B	601	B12	C46-C12	-3.16	1.47	1.54
4	D	601	B12	C8B-C9B	3.09	1.46	1.40
4	D	601	B12	C9-N22	3.08	1.38	1.30
4	B	601	B12	C8B-C9B	2.75	1.46	1.40
4	B	601	B12	C12-C11	-2.55	1.47	1.52
4	D	601	B12	C10-C11	-2.54	1.30	1.38
4	D	601	B12	O6R-C1R	2.46	1.44	1.41
4	B	601	B12	C16-C15	-2.38	1.38	1.44
4	B	601	B12	C11-N23	2.36	1.41	1.37
4	B	601	B12	C14-C15	2.27	1.48	1.38
4	B	601	B12	O6R-C1R	2.21	1.44	1.41
4	B	601	B12	C10-C11	-2.20	1.31	1.38
4	D	601	B12	C14-C15	2.19	1.47	1.38
4	D	601	B12	C17-C18	2.16	1.58	1.54
4	B	601	B12	C17-C18	2.11	1.58	1.54
4	D	601	B12	C14-N23	2.04	1.37	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	601	B12	C18-C19-N24	3.80	108.10	102.31
4	B	601	B12	C1-C19-N24	3.78	110.49	106.24
4	B	601	B12	C18-C19-N24	3.51	107.66	102.31
4	D	601	B12	C47-C12-C46	3.01	114.43	109.35
4	D	601	B12	C54-C17-C18	-2.99	108.57	112.98
4	D	601	B12	C12-C11-C10	-2.76	119.77	123.37
4	B	601	B12	C54-C17-C18	-2.74	108.94	112.98
4	B	601	B12	C30-C3-C2	-2.69	113.39	119.09
4	D	601	B12	C30-C3-C2	-2.61	113.57	119.09
4	B	601	B12	C7-C6-C5	-2.45	124.21	128.07
4	D	601	B12	C7-C6-C5	-2.41	124.28	128.07
4	D	601	B12	C1-C19-N24	2.32	108.85	106.24
4	D	601	B12	C19-C1-N21	2.25	104.47	102.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	B12	C9-C10-C11	-2.21	122.78	125.97
4	D	601	B12	C20-C1-C19	-2.20	107.24	109.36
4	B	601	B12	C19-C1-N21	2.15	104.36	102.16
4	D	601	B12	C15-C14-N23	-2.12	123.67	126.26
4	B	601	B12	C25-C2-C1	-2.11	110.60	113.78
4	B	601	B12	C48-C13-C12	-2.09	110.76	116.63
4	B	601	B12	C47-C12-C46	2.09	112.89	109.35
4	B	601	B12	C20-C1-C19	-2.07	107.36	109.36
4	D	601	B12	C3R-C2R-C1R	2.06	104.45	99.89

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	B12	C38-C37-C7-C6
4	B	601	B12	C38-C37-C7-C36
4	B	601	B12	C38-C37-C7-C8
4	B	601	B12	C42-C41-C8-C9
4	B	601	B12	C2P-O3-P-O5
4	D	601	B12	C38-C37-C7-C6
4	D	601	B12	C38-C37-C7-C36
4	D	601	B12	C38-C37-C7-C8
4	D	601	B12	C42-C41-C8-C9
4	D	601	B12	C13-C48-C49-C50
4	D	601	B12	C16-C17-C55-C56
4	D	601	B12	C2P-O3-P-O5
4	D	601	B12	O6R-C4R-C5R-O8R
4	D	601	B12	C3R-C4R-C5R-O8R
4	B	601	B12	O6R-C4R-C5R-O8R
4	B	601	B12	C14-C13-C48-C49
4	B	601	B12	C13-C48-C49-C50
4	B	601	B12	C3R-C4R-C5R-O8R
4	D	601	B12	C18-C17-C55-C56
4	B	601	B12	C2-C3-C30-C31
4	D	601	B12	C2-C3-C30-C31
4	B	601	B12	C16-C17-C55-C56
4	B	601	B12	C12-C13-C48-C49
4	B	601	B12	C18-C17-C55-C56
4	D	601	B12	C12-C13-C48-C49
4	B	601	B12	C4-C3-C30-C31
4	B	601	B12	C2P-O3-P-O4
4	D	601	B12	C2P-O3-P-O4

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Mol	Chain	Res	Type	Atoms
4	D	601	B12	C4-C3-C30-C31
4	B	601	B12	C2P-O3-P-O2
4	D	601	B12	C2P-O3-P-O2
4	B	601	B12	C48-C49-C50-N52
4	B	601	B12	C48-C49-C50-O51
4	D	601	B12	C25-C2-C26-C27
4	D	601	B12	C17-C18-C60-C61
4	D	601	B12	C14-C13-C48-C49
4	B	601	B12	C25-C2-C26-C27
4	D	601	B12	C3-C2-C26-C27
4	D	601	B12	C19-C18-C60-C61

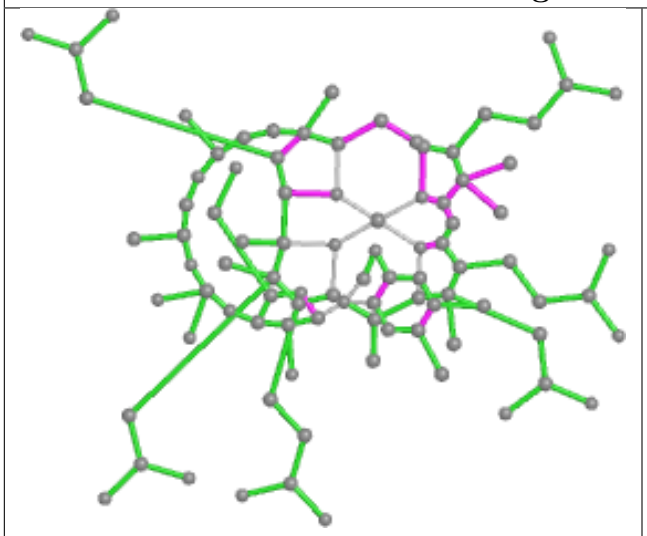
There are no ring outliers.

2 monomers are involved in 24 short contacts:

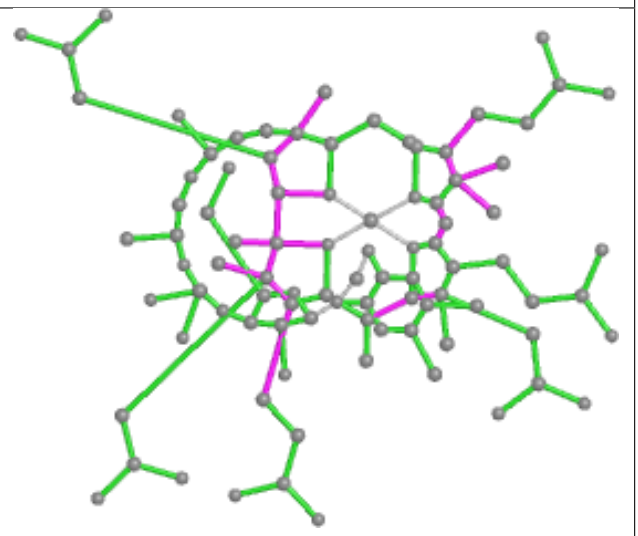
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	B12	11	0
4	D	601	B12	13	0

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.

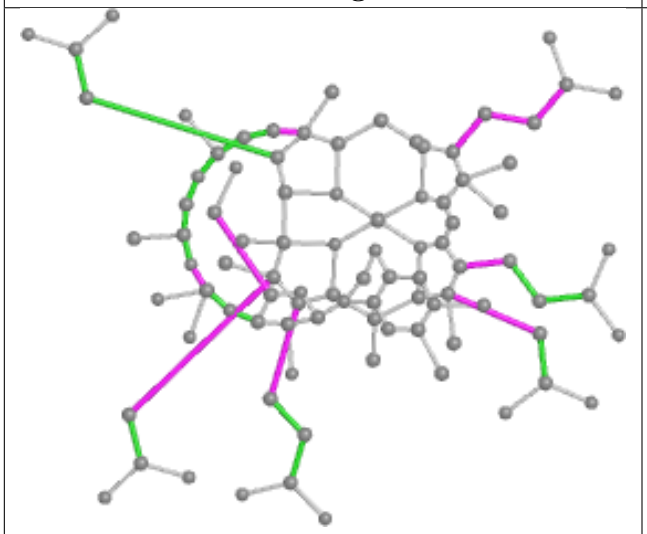
Ligand B12 B 601



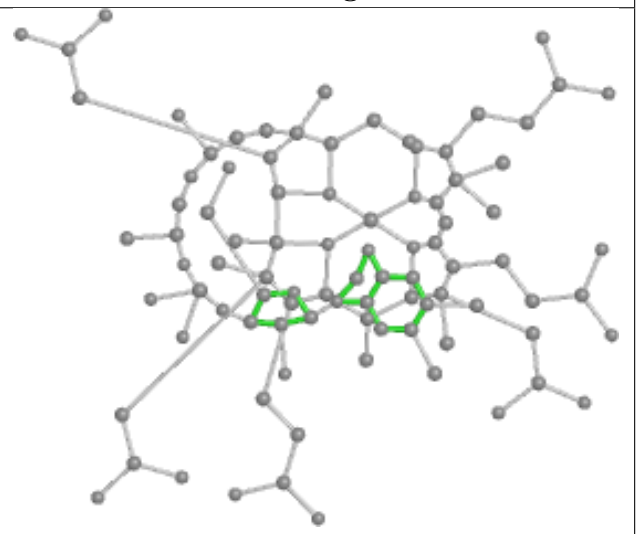
Bond lengths



Bond angles

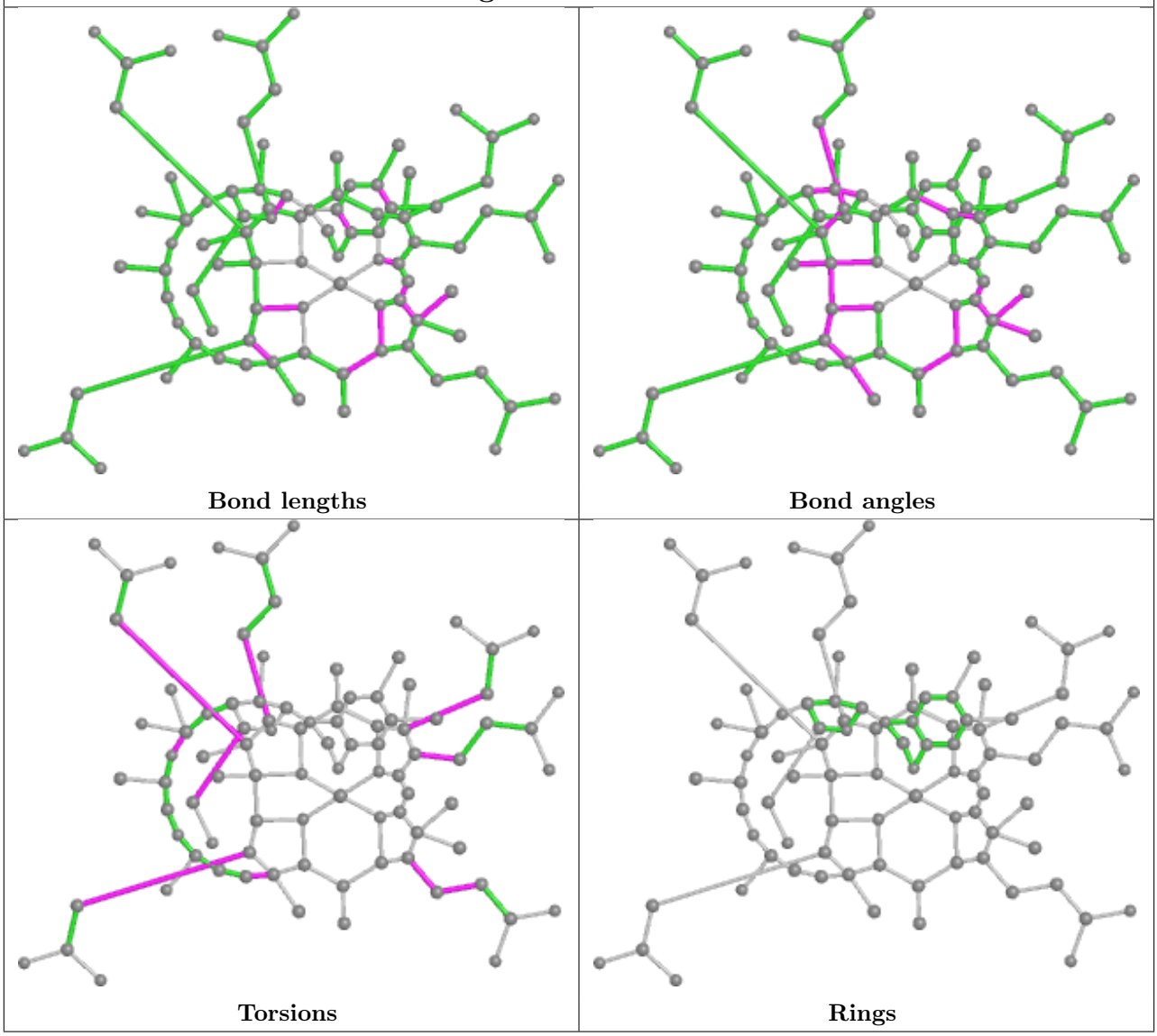


Torsions



Rings

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%)	0.12	1 (0%)	95	95	18, 31, 49, 59	0
1	C	453/453 (100%)	0.10	1 (0%)	95	95	16, 31, 54, 67	0
2	B	252/263 (95%)	0.74	23 (9%)	9	12	26, 60, 85, 98	0
2	D	252/263 (95%)	1.26	60 (23%)	0	0	21, 72, 110, 122	0
All	All	1410/1432 (98%)	0.43	85 (6%)	21	27	16, 39, 90, 122	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	161	VAL	7.4
2	D	123	VAL	6.1
2	D	148	VAL	6.1
2	D	200	PHE	6.0
2	D	153	ALA	5.9
2	D	145	ALA	5.2
2	D	111	PRO	5.0
2	D	216	ILE	4.8
2	D	192	ALA	4.6
2	D	187	ALA	4.5
2	D	156	VAL	4.4
2	D	202	VAL	4.3
2	D	119	GLY	4.3
2	D	191	GLN	3.8
2	B	270	VAL	3.8
2	D	190	LYS	3.7
2	B	249	ALA	3.6
2	B	191	GLN	3.6
2	D	194	LEU	3.5
2	D	174	ILE	3.5
2	D	189	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	192	ALA	3.4
2	D	165	ILE	3.3
2	D	244	TYR	3.3
2	B	72	ARG	3.3
2	D	196	VAL	3.2
2	D	273	ALA	3.2
2	D	107	LEU	3.2
2	D	181	ILE	3.1
2	D	155	CYS	3.1
2	B	113	GLU	3.0
2	D	121	LEU	3.0
2	D	164	VAL	3.0
2	D	246	PRO	3.0
2	D	225	LEU	2.9
2	D	157	ALA	2.9
2	B	183	PRO	2.8
2	B	44	ALA	2.8
2	D	158	ASN	2.8
2	D	295	ARG	2.8
2	D	220	LYS	2.7
2	D	213	ILE	2.7
2	D	178	TYR	2.6
2	B	56	ILE	2.6
2	D	129	ASP	2.6
2	D	146	GLU	2.6
2	B	194	LEU	2.6
2	D	151	LEU	2.6
2	D	223	ILE	2.5
2	B	265	GLY	2.5
2	D	212	GLN	2.5
2	D	224	LEU	2.5
2	D	143	LEU	2.5
2	B	156	VAL	2.4
2	D	69	GLU	2.4
2	D	242	ALA	2.4
2	B	295	ARG	2.4
2	D	127	ILE	2.4
2	D	258	CYS	2.4
2	B	120	LEU	2.4
2	B	201	PHE	2.4
2	D	59	GLU	2.4
2	D	183	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	162	GLN	2.3
2	D	209	ILE	2.3
2	B	178	TYR	2.3
2	B	179	GLU	2.3
2	D	141	ARG	2.3
2	B	200	PHE	2.3
2	D	179	GLU	2.3
2	D	132	LEU	2.2
1	C	64	VAL	2.2
2	D	206	ARG	2.2
2	D	270	VAL	2.2
2	B	239	SER	2.2
1	A	336	TYR	2.2
2	B	234	GLN	2.1
2	B	225	LEU	2.1
2	D	199	PRO	2.1
2	B	182	LEU	2.1
2	D	182	LEU	2.1
2	D	286	GLN	2.1
2	B	264	GLN	2.0
2	D	221	VAL	2.0
2	D	250	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	2A3	A	602	5/5	0.90	0.14	24,24,30,30	0

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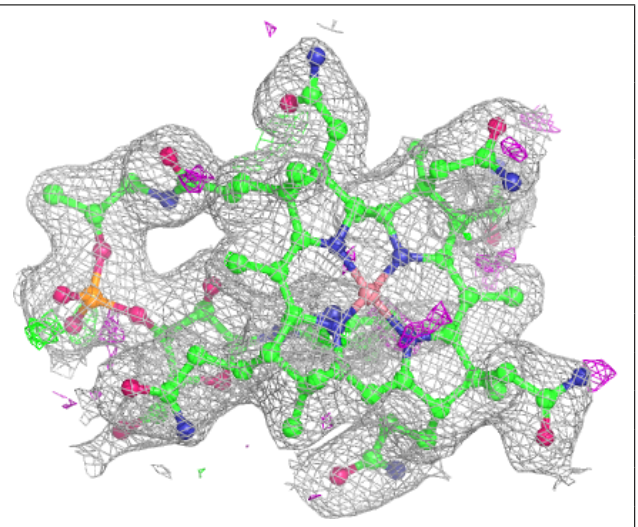
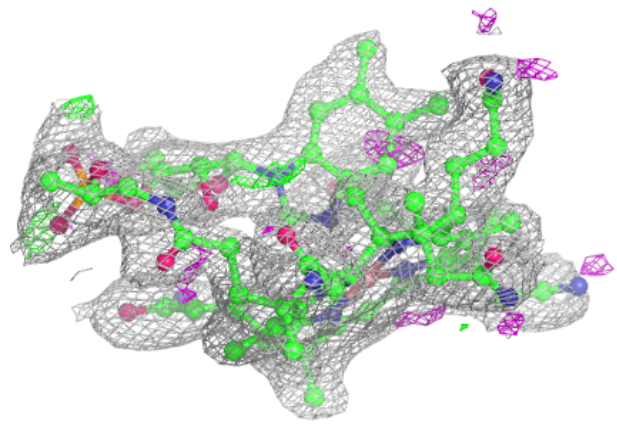
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	B12	B	601	91/91	0.94	0.15	28,35,45,53	0
4	B12	D	601	91/91	0.94	0.17	29,44,52,59	0
3	2A3	C	602	5/5	0.96	0.11	23,26,29,29	0

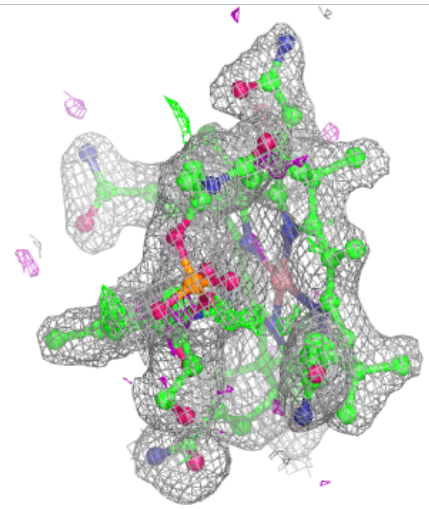
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 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)

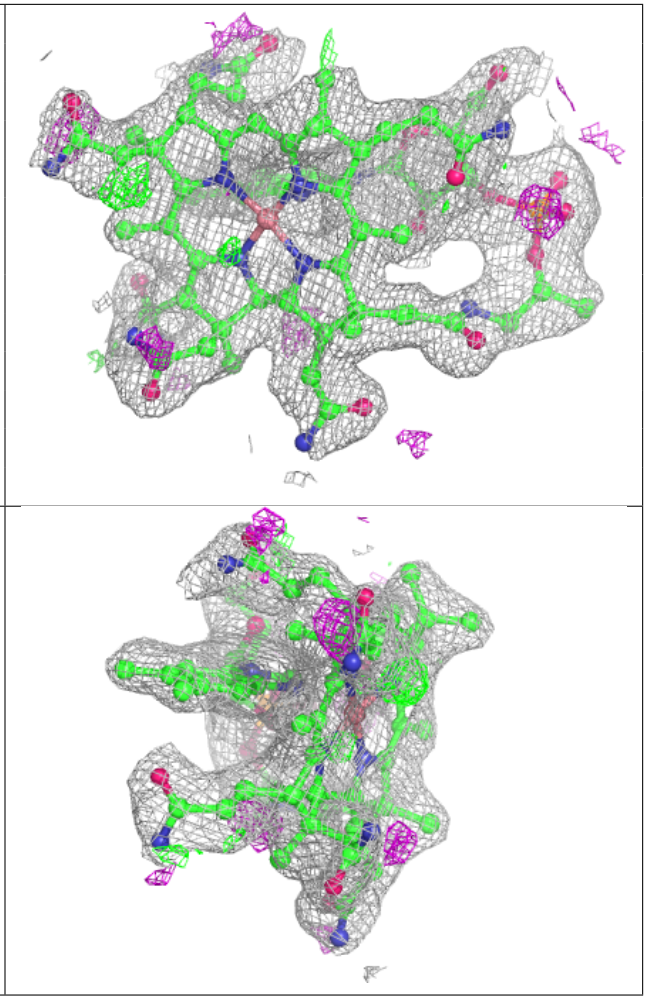






Electron density around B12 D 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.