Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2023 – 07:43 pm BST

PDB ID	:	8C37
Title	:	An intermediate light exposed 2.15 Angstrom crystal structure of H132A variant of cobalamin binding domain belonging to a light-dependent transcription regulator TtCarH obtained under anaerobic conditions
Authors	:	Poddar, H.; Leys, D.
Deposited on	:	2022-12-23
Resolution	:	2.15 Å(reported)

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

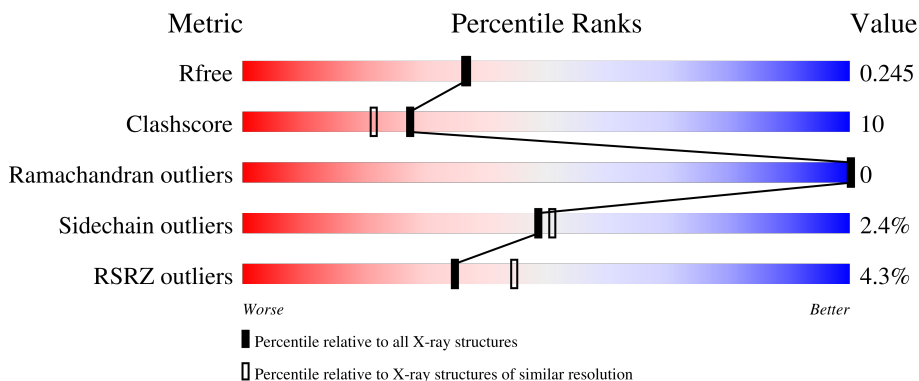|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.15 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		2.4%
RSRZ outliers		4.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	215	2% / 84% / 7% / 9%
1	B	215	80% / 10% · 9%
1	C	215	7% / 83% / 8% · 8%
1	D	215	7% / 82% / 8% · 9%

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
2	B12	A	301	X	-	-	-
2	B12	B	301	X	-	-	-
2	B12	C	301	X	-	-	-
2	B12	D	301[A]	X	-	X	-
2	B12	D	301[B]	X	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6726 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 Probable transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	1	0
			1476	947	265	262	2			
1	B	196	Total	C	N	O	S	0	0	0
			1478	949	266	261	2			
1	C	197	Total	C	N	O	S	0	1	0
			1494	958	270	264	2			
1	D	195	Total	C	N	O	S	0	1	0
			1482	954	266	260	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	HIS	engineered mutation	UNP Q746J7
A	286	GLY	-	expression tag	UNP Q746J7
A	287	HIS	-	expression tag	UNP Q746J7
A	288	HIS	-	expression tag	UNP Q746J7
A	289	HIS	-	expression tag	UNP Q746J7
A	290	HIS	-	expression tag	UNP Q746J7
A	291	HIS	-	expression tag	UNP Q746J7
A	292	HIS	-	expression tag	UNP Q746J7
B	132	ALA	HIS	engineered mutation	UNP Q746J7
B	286	GLY	-	expression tag	UNP Q746J7
B	287	HIS	-	expression tag	UNP Q746J7
B	288	HIS	-	expression tag	UNP Q746J7
B	289	HIS	-	expression tag	UNP Q746J7
B	290	HIS	-	expression tag	UNP Q746J7
B	291	HIS	-	expression tag	UNP Q746J7
B	292	HIS	-	expression tag	UNP Q746J7
C	132	ALA	HIS	engineered mutation	UNP Q746J7
C	286	GLY	-	expression tag	UNP Q746J7
C	287	HIS	-	expression tag	UNP Q746J7
C	288	HIS	-	expression tag	UNP Q746J7
C	289	HIS	-	expression tag	UNP Q746J7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	290	HIS	-	expression tag	UNP Q746J7
C	291	HIS	-	expression tag	UNP Q746J7
C	292	HIS	-	expression tag	UNP Q746J7
D	132	ALA	HIS	engineered mutation	UNP Q746J7
D	286	GLY	-	expression tag	UNP Q746J7
D	287	HIS	-	expression tag	UNP Q746J7
D	288	HIS	-	expression tag	UNP Q746J7
D	289	HIS	-	expression tag	UNP Q746J7
D	290	HIS	-	expression tag	UNP Q746J7
D	291	HIS	-	expression tag	UNP Q746J7
D	292	HIS	-	expression tag	UNP Q746J7

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).
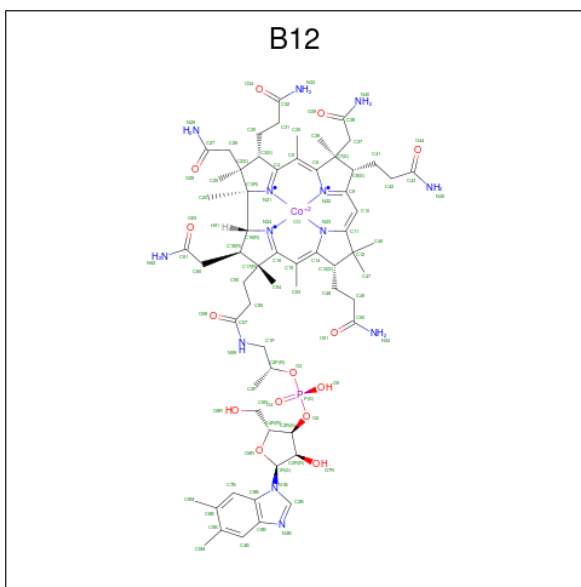
B12

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	D	1	Total	C	Co	N	O	P	0	1
			182	124	2	26	28	2		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total 94	O 94	0	0
3	B	87	Total 87	O 87	0	0
3	C	87	Total 87	O 87	0	0
3	D	73	Total 73	O 73	0	0

3 Residue-property plots ⓘ

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.
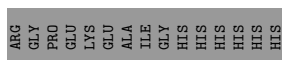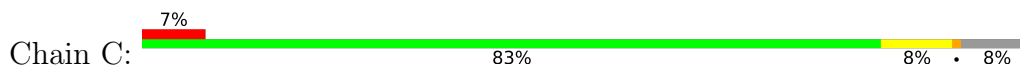
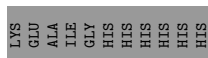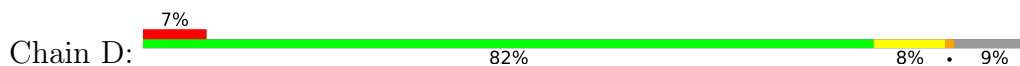• Molecule 1: Probable transcriptional regulator
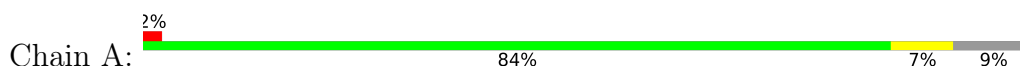
• Molecule 1: Probable transcriptional regulator
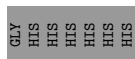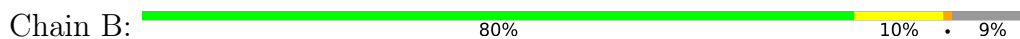
• Molecule 1: Probable transcriptional regulator

• Molecule 1: Probable transcriptional regulator

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.82Å 69.68Å 201.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.18 – 2.15 61.82 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.18-2.15) 100.0 (61.82-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.193 , 0.230 0.216 , 0.245	Depositor DCC
R_{free} test set	2416 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6726	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/1513	0.66	0/2057
1	B	0.48	0/1512	0.71	0/2057
1	C	0.48	0/1531	0.72	0/2082
1	D	0.46	0/1520	0.72	0/2068
All	All	0.46	0/6076	0.70	0/8264

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	3
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	15

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	176	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	257	ARG	Sidechain
1	B	93	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	176	ARG	Sidechain
1	C	213	ARG	Sidechain
1	C	93	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	176	ARG	Sidechain
1	D	189	ARG	Sidechain
1	D	93	ARG	Sidechain

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	1476	0	1512	7	0
1	B	1478	0	1516	13	0
1	C	1494	0	1533	10	0
1	D	1482	0	1519	16	0
2	A	91	0	86	8	0
2	B	91	0	87	14	0
2	C	91	0	87	12	0
2	D	182	0	174	66	0
3	A	94	0	0	1	0
3	B	87	0	0	0	0
3	C	87	0	0	3	0
3	D	73	0	0	0	0
All	All	6726	0	6514	129	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 10.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301[B]:B12:O44	2:D:301[B]:B12:H10	1.38	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301[B]:B12:H253	2:D:301[B]:B12:O63	1.44	1.16
2:D:301[A]:B12:H4R	2:D:301[A]:B12:C3P	1.75	1.15
2:D:301[B]:B12:H491	2:D:301[B]:B12:H533	1.14	1.13
2:D:301[A]:B12:H561	2:D:301[A]:B12:O63	1.51	1.10
2:D:301[A]:B12:H351	2:D:301[A]:B12:H362	1.13	1.07
2:D:301[B]:B12:O34	2:D:301[B]:B12:C26	1.88	1.06
2:D:301[B]:B12:H362	2:D:301[B]:B12:H351	1.38	1.04
2:D:301[B]:B12:O34	2:D:301[B]:B12:H261	1.28	1.04
2:D:301[A]:B12:H3P2	2:D:301[A]:B12:C4R	1.86	1.04
2:D:301[B]:B12:H491	2:D:301[B]:B12:C53	1.88	1.03
2:D:301[B]:B12:H543	2:D:301[B]:B12:H531	1.38	1.02
2:A:301:B12:H362	2:A:301:B12:H351	1.42	1.02
2:D:301[B]:B12:H10	2:D:301[B]:B12:C43	1.90	1.02
2:D:301[B]:B12:C53	2:D:301[B]:B12:H561	1.90	1.00
2:D:301[A]:B12:H351	2:D:301[A]:B12:C36	1.93	0.96
2:D:301[A]:B12:H4R	2:D:301[A]:B12:H3P2	0.97	0.94
2:D:301[A]:B12:H1P1	2:D:301[A]:B12:O5	1.68	0.93
2:D:301[A]:B12:H561	2:D:301[A]:B12:C61	1.99	0.93
2:D:301[B]:B12:O44	2:D:301[B]:B12:C10	2.22	0.87
2:D:301[A]:B12:O63	2:D:301[A]:B12:C56	2.23	0.86
2:D:301[B]:B12:H533	2:D:301[B]:B12:C49	2.03	0.85
2:B:301:B12:H463	2:B:301:B12:C49	2.08	0.83
2:D:301[B]:B12:H312	2:D:301[B]:B12:H291	1.43	0.83
2:D:301[B]:B12:H531	2:D:301[B]:B12:H561	1.61	0.80
2:D:301[B]:B12:H351	2:D:301[B]:B12:C36	2.13	0.77
2:D:301[A]:B12:H531	2:D:301[A]:B12:H551	1.68	0.76
2:B:301:B12:H463	2:B:301:B12:C50	2.16	0.76
2:D:301[B]:B12:H533	2:D:301[B]:B12:H561	1.68	0.75
2:D:301[A]:B12:H561	2:D:301[A]:B12:C60	2.15	0.74
2:B:301:B12:H552	2:B:301:B12:H531	1.68	0.74
2:C:301:B12:H551	2:C:301:B12:H531	1.71	0.73
2:D:301[B]:B12:C53	2:D:301[B]:B12:C49	2.66	0.71
2:A:301:B12:H351	2:A:301:B12:C36	2.20	0.71
2:D:301[B]:B12:O63	2:D:301[B]:B12:C25	2.34	0.70
2:D:301[B]:B12:H2B	2:D:301[B]:B12:O2	1.92	0.70
2:B:301:B12:H533	2:B:301:B12:H492	1.73	0.69
1:A:121:LEU:HD21	1:A:183:LEU:HD11	1.74	0.69
1:B:225:LEU:HD11	2:B:301:B12:H422	1.74	0.67
2:B:301:B12:C49	2:B:301:B12:H533	2.26	0.66
2:D:301[A]:B12:O5	2:D:301[A]:B12:C1P	2.39	0.66
2:D:301[A]:B12:H203	2:D:301[A]:B12:H302	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:B12:H362	2:C:301:B12:H351	1.79	0.64
2:C:301:B12:H3	2:C:301:B12:H291	1.64	0.62
2:B:301:B12:H8	2:B:301:B12:O39	1.99	0.61
1:B:264:MET:HB2	2:B:301:B12:HM63	1.83	0.61
1:D:177:HIS:HD2	2:D:301[A]:B12:C48	2.14	0.61
2:D:301[A]:B12:H531	2:D:301[A]:B12:C55	2.29	0.60
2:B:301:B12:H532	2:B:301:B12:H481	1.83	0.60
1:D:113:GLU:OE2	1:D:190:ARG:HD2	2.01	0.60
1:D:125:ARG:NH2	2:D:301[A]:B12:O5	2.35	0.60
2:D:301[A]:B12:H362	2:D:301[A]:B12:C35	2.08	0.59
1:C:141:GLU:OE2	2:C:301:B12:H532	2.03	0.59
2:C:301:B12:H482	2:C:301:B12:H533	1.85	0.58
2:C:301:B12:H531	2:C:301:B12:C55	2.31	0.58
2:A:301:B12:H353	2:A:301:B12:H302	1.85	0.58
2:D:301[B]:B12:H531	2:D:301[B]:B12:C54	2.19	0.58
2:B:301:B12:H362	2:B:301:B12:H351	1.86	0.58
2:B:301:B12:H531	2:B:301:B12:C55	2.34	0.58
2:D:301[B]:B12:O63	2:D:301[B]:B12:C19	2.52	0.58
2:A:301:B12:H562	2:A:301:B12:H531	1.85	0.57
2:D:301[B]:B12:H362	2:D:301[B]:B12:C35	2.23	0.57
2:D:301[A]:B12:O63	2:D:301[A]:B12:C57	2.53	0.57
2:C:301:B12:C55	2:C:301:B12:C53	2.83	0.56
2:D:301[A]:B12:H353	2:D:301[A]:B12:H311	1.88	0.56
2:D:301[A]:B12:H203	2:D:301[A]:B12:C30	2.36	0.56
2:B:301:B12:C48	2:B:301:B12:C53	2.85	0.54
2:B:301:B12:H481	2:B:301:B12:C53	2.36	0.54
2:D:301[B]:B12:H8	2:D:301[B]:B12:O39	2.07	0.54
1:D:177:HIS:NE2	2:D:301[A]:B12:N23	2.57	0.53
1:A:140:GLU:HG2	1:B:210:LEU:HD13	1.91	0.53
2:C:301:B12:H601	2:C:301:B12:H262	1.91	0.53
1:B:245:PHE:CD1	1:B:264:MET:HG3	2.44	0.52
2:D:301[B]:B12:H312	2:D:301[B]:B12:N29	1.93	0.52
2:D:301[B]:B12:O5	2:D:301[B]:B12:H3P1	2.09	0.52
1:D:177:HIS:HD2	2:D:301[A]:B12:H482	1.74	0.51
1:A:162:PRO:HB3	1:C:192:GLY:HA3	1.92	0.51
1:D:248:GLY:HA2	2:D:301[A]:B12:O7R	2.11	0.51
1:D:141:GLU:OE1	2:D:301[A]:B12:H462	2.11	0.51
2:D:301[B]:B12:C53	2:D:301[B]:B12:H543	2.27	0.51
2:D:301[B]:B12:C35	2:D:301[B]:B12:H301	2.42	0.50
1:C:220:VAL:HG13	2:C:301:B12:HM52	1.94	0.50
2:D:301[A]:B12:O63	2:D:301[A]:B12:O58	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:HIS:CD2	1:B:268:LYS:HD3	2.48	0.48
1:D:254:GLU:CD	1:D:254:GLU:H	2.15	0.48
2:D:301[A]:B12:C36	2:D:301[A]:B12:C35	2.76	0.48
1:C:213:ARG:NH2	1:D:92:LEU:O	2.46	0.48
1:B:245:PHE:HD1	1:B:264:MET:HG3	1.77	0.47
1:A:121:LEU:HB2	1:A:122:PRO:HD3	1.96	0.47
2:D:301[B]:B12:H291	2:D:301[B]:B12:C31	2.20	0.47
2:D:301[B]:B12:H301	2:D:301[B]:B12:H352	1.96	0.47
1:D:121:LEU:HD21	1:D:183:LEU:HD11	1.98	0.46
1:B:121:LEU:HD21	1:B:183:LEU:HD11	1.98	0.46
2:C:301:B12:H3	2:C:301:B12:N29	2.30	0.46
2:A:301:B12:H561	3:A:470:HOH:O	2.15	0.46
1:C:184:ALA:HA	1:C:267:LEU:HD22	1.98	0.45
2:D:301[A]:B12:H3P2	2:D:301[A]:B12:C5R	2.44	0.45
2:B:301:B12:H463	2:B:301:B12:H491	1.98	0.44
1:D:177:HIS:CD2	2:D:301[A]:B12:C48	2.99	0.44
1:A:198:LEU:O	1:B:142:HIS:HB3	2.17	0.44
1:C:143:LEU:HD12	3:C:468:HOH:O	2.17	0.44
1:B:83:LEU:HD13	1:B:110:TRP:HH2	1.82	0.44
2:C:301:B12:H353	2:C:301:B12:H302	1.99	0.44
1:B:184:ALA:HA	1:B:267:LEU:HD22	2.00	0.44
1:D:230:ARG:HG2	1:D:230:ARG:NH1	2.33	0.44
1:D:177:HIS:NE2	2:D:301[A]:B12:N22	2.66	0.43
2:C:301:B12:H562	2:C:301:B12:O63	2.19	0.43
2:A:301:B12:H601	2:A:301:B12:H262	1.99	0.43
2:D:301[A]:B12:C55	2:D:301[A]:B12:C53	2.95	0.43
2:D:301[B]:B12:H261	2:D:301[B]:B12:H203	1.85	0.43
1:D:230:ARG:HG2	1:D:230:ARG:HH11	1.83	0.42
2:A:301:B12:C10	2:A:301:B12:H421	2.50	0.42
1:A:124:LEU:HG	1:A:148:LEU:HD13	2.02	0.42
1:B:177:HIS:ND1	1:B:224:VAL:HG11	2.33	0.42
2:D:301[A]:B12:H253	2:D:301[A]:B12:H301	1.49	0.42
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.85	0.41
1:D:184:ALA:HA	1:D:267:LEU:HD22	2.00	0.41
2:D:301[B]:B12:O2	2:D:301[B]:B12:C2B	2.66	0.41
2:A:301:B12:H531	2:A:301:B12:C56	2.49	0.41
2:D:301[A]:B12:H481	2:D:301[A]:B12:H473	1.81	0.41
1:A:254:GLU:H	1:A:254:GLU:CD	2.24	0.41
2:D:301[B]:B12:H59	2:D:301[B]:B12:H552	1.62	0.41
1:C:265:GLU:HA	3:C:433:HOH:O	2.20	0.41
1:D:177:HIS:CD2	2:D:301[A]:B12:H481	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:HIS:HE1	3:C:443:HOH:O	2.04	0.41
1:C:227:GLU:HB2	1:C:228:PRO:HD3	2.03	0.41
2:D:301[B]:B12:C43	2:D:301[B]:B12:C10	2.79	0.40
1:C:197:TYR:CZ	1:C:199:GLY:HA2	2.56	0.40
1:B:162:PRO:O	1:B:194:PRO:HB3	2.21	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	194/215 (90%)	190 (98%)	4 (2%)	0	100	100
1	B	194/215 (90%)	190 (98%)	4 (2%)	0	100	100
1	C	196/215 (91%)	191 (97%)	5 (3%)	0	100	100
1	D	194/215 (90%)	191 (98%)	3 (2%)	0	100	100
All	All	778/860 (90%)	762 (98%)	16 (2%)	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	144/160 (90%)	142 (99%)	2 (1%)	67	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	144/160 (90%)	140 (97%)	4 (3%)	43	44
1	C	146/160 (91%)	142 (97%)	4 (3%)	44	46
1	D	144/160 (90%)	140 (97%)	4 (3%)	43	44
All	All	578/640 (90%)	564 (98%)	14 (2%)	49	51

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	239	ASP
1	B	100	GLU
1	B	142	HIS
1	B	176	ARG
1	B	272	GLU
1	C	142	HIS
1	C	176	ARG
1	C	179	ILE
1	C	249	GLN
1	D	124	LEU
1	D	142	HIS
1	D	254	GLU
1	D	274	LEU

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

Mol	Chain	Res	Type
1	A	187	HIS
1	B	187	HIS
1	C	249	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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
2	B12	D	301[A]	1	90,101,101	1.30	9 (10%)	137,166,166	1.97	25 (18%)
2	B12	B	301	-	90,101,101	1.50	12 (13%)	137,166,166	2.50	30 (21%)
2	B12	A	301	-	90,101,101	1.40	11 (12%)	137,166,166	2.37	31 (22%)
2	B12	C	301	1	90,101,101	1.30	13 (14%)	137,166,166	2.12	26 (18%)
2	B12	D	301[B]	-	90,101,101	1.37	9 (10%)	137,166,166	2.94	35 (25%)

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
2	B12	D	301[A]	1	1/1/36/38	24/52/223/223	0/3/11/11
2	B12	B	301	-	1/1/36/38	13/52/223/223	0/3/11/11
2	B12	A	301	-	1/1/36/38	14/52/223/223	0/3/11/11
2	B12	C	301	1	1/1/36/38	20/52/223/223	0/3/11/11
2	B12	D	301[B]	-	2/2/36/38	23/52/223/223	0/3/11/11

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	B12	C14-N23	-6.84	1.26	1.35
2	D	301[B]	B12	C14-N23	-6.28	1.27	1.35
2	A	301	B12	C14-N23	-5.55	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	B12	C9-N22	4.71	1.43	1.30
2	B	301	B12	C9-N22	4.69	1.43	1.30
2	D	301[B]	B12	C9-N22	4.66	1.42	1.30
2	B	301	B12	C12-C11	-4.31	1.44	1.52
2	C	301	B12	C8B-C9B	4.25	1.49	1.40
2	D	301[A]	B12	C9-N22	4.24	1.41	1.30
2	D	301[B]	B12	C16-C15	-4.01	1.33	1.44
2	A	301	B12	C9-N22	3.89	1.40	1.30
2	A	301	B12	C19-N24	-3.87	1.41	1.48
2	D	301[B]	B12	C8B-C9B	3.75	1.48	1.40
2	D	301[A]	B12	C16-C15	-3.73	1.34	1.44
2	A	301	B12	C6B-C5B	3.73	1.50	1.40
2	D	301[A]	B12	C14-N23	-3.70	1.30	1.35
2	D	301[A]	B12	C8B-C9B	3.70	1.48	1.40
2	D	301[B]	B12	C19-N24	-3.45	1.42	1.48
2	D	301[A]	B12	C6B-C5B	3.44	1.49	1.40
2	C	301	B12	C14-N23	-3.44	1.30	1.35
2	D	301[A]	B12	C19-N24	-3.42	1.42	1.48
2	A	301	B12	C8B-C9B	3.42	1.47	1.40
2	B	301	B12	C6B-C5B	3.39	1.49	1.40
2	A	301	B12	C16-C15	-3.29	1.35	1.44
2	D	301[B]	B12	C6B-C5B	3.29	1.49	1.40
2	C	301	B12	C6B-C5B	3.21	1.48	1.40
2	A	301	B12	C1-C19	-3.10	1.48	1.55
2	B	301	B12	C19-N24	-3.03	1.43	1.48
2	C	301	B12	C19-N24	-3.01	1.43	1.48
2	B	301	B12	C16-C15	-2.93	1.36	1.44
2	B	301	B12	C10-C11	-2.75	1.29	1.38
2	D	301[A]	B12	C1-C19	-2.70	1.49	1.55
2	B	301	B12	C2R-C1R	-2.57	1.49	1.53
2	C	301	B12	O6R-C1R	2.56	1.44	1.41
2	C	301	B12	C16-C15	-2.55	1.37	1.44
2	D	301[B]	B12	C10-C9	2.54	1.46	1.39
2	B	301	B12	C8B-C9B	2.51	1.45	1.40
2	C	301	B12	C14-C15	2.51	1.49	1.38
2	D	301[A]	B12	C14-C15	2.51	1.49	1.38
2	D	301[A]	B12	C10-C9	2.51	1.46	1.39
2	C	301	B12	C1-C2	-2.38	1.53	1.58
2	C	301	B12	C10-C9	2.35	1.45	1.39
2	C	301	B12	O3-C2P	-2.35	1.39	1.45
2	B	301	B12	O6R-C1R	2.24	1.44	1.41
2	A	301	B12	C10-C9	2.22	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	B12	C4B-C9B	-2.20	1.38	1.41
2	D	301[B]	B12	O6R-C1R	2.20	1.44	1.41
2	D	301[B]	B12	C1-C19	-2.12	1.50	1.55
2	B	301	B12	C11-N23	-2.10	1.33	1.37
2	A	301	B12	C1-C2	-2.10	1.54	1.58
2	B	301	B12	C14-C15	2.09	1.47	1.38
2	A	301	B12	C4B-C9B	-2.09	1.38	1.41
2	C	301	B12	C18-C19	-2.04	1.49	1.53
2	A	301	B12	O3-C2P	-2.01	1.40	1.45

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[B]	B12	C25-C2-C3	-12.88	80.02	112.96
2	B	301	B12	C12-C11-C10	-12.53	107.06	123.37
2	D	301[B]	B12	C1-C19-N24	11.31	118.97	106.24
2	C	301	B12	C1-C19-N24	11.24	118.89	106.24
2	A	301	B12	C18-C19-N24	10.36	118.07	102.31
2	A	301	B12	C54-C17-C55	10.27	126.20	109.25
2	D	301[A]	B12	C18-C19-N24	10.14	117.74	102.31
2	D	301[A]	B12	C1-C19-N24	10.07	117.58	106.24
2	B	301	B12	C1-C19-N24	9.83	117.30	106.24
2	A	301	B12	C1-C19-N24	9.62	117.06	106.24
2	C	301	B12	C18-C19-N24	9.35	116.53	102.31
2	D	301[B]	B12	C26-C2-C3	-9.11	91.30	107.41
2	B	301	B12	C13-C12-C11	-8.93	90.86	100.97
2	B	301	B12	C18-C19-N24	8.69	115.53	102.31
2	D	301[B]	B12	C18-C19-N24	8.65	115.48	102.31
2	D	301[B]	B12	C47-C12-C46	8.39	123.53	109.35
2	C	301	B12	C54-C17-C55	7.99	122.43	109.25
2	A	301	B12	C55-C17-C18	-7.89	95.89	111.15
2	B	301	B12	C12-C11-N23	7.75	122.63	111.83
2	D	301[B]	B12	C13-C12-C11	-7.17	92.85	100.97
2	D	301[B]	B12	C46-C12-C13	-7.07	83.95	112.72
2	D	301[B]	B12	C47-C12-C13	-7.01	84.19	112.72
2	A	301	B12	C20-C1-C19	-6.73	102.87	109.36
2	D	301[B]	B12	C25-C2-C1	6.59	123.72	113.78
2	D	301[A]	B12	C20-C1-C19	-6.39	103.20	109.36
2	D	301[B]	B12	C12-C11-C10	-5.97	115.59	123.37
2	C	301	B12	C55-C17-C16	-5.94	104.92	116.65
2	B	301	B12	C20-C1-C19	-5.86	103.70	109.36
2	A	301	B12	C18-C17-C16	5.80	107.71	100.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[B]	B12	C25-C2-C26	5.57	120.97	109.71
2	D	301[B]	B12	C2-C3-C4	5.32	107.68	101.63
2	C	301	B12	C20-C1-C19	-5.29	104.26	109.36
2	D	301[B]	B12	C1-C2-C3	-5.18	94.97	101.60
2	B	301	B12	C47-C12-C46	5.18	118.10	109.35
2	D	301[B]	B12	C2-C26-C27	-4.88	101.50	115.22
2	A	301	B12	C56-C57-N59	-4.71	108.49	116.42
2	D	301[B]	B12	C7-C6-N22	4.69	116.51	107.94
2	D	301[B]	B12	C3-C4-C5	4.63	131.61	123.81
2	D	301[B]	B12	C7-C6-C5	-4.57	120.89	128.07
2	D	301[B]	B12	C12-C11-N23	4.47	118.07	111.83
2	B	301	B12	C41-C8-C7	4.45	126.39	114.14
2	D	301[B]	B12	C2-C1-N21	4.45	107.97	101.77
2	D	301[A]	B12	C30-C3-C2	-4.18	110.24	119.09
2	A	301	B12	C48-C13-C14	-4.15	98.15	108.49
2	D	301[A]	B12	C56-C55-C17	-4.14	107.53	115.52
2	D	301[A]	B12	C18-C17-C16	4.14	105.70	100.67
2	D	301[B]	B12	C2P-C1P-N59	-4.11	106.88	112.93
2	B	301	B12	C9-C10-C11	-4.07	120.08	125.97
2	A	301	B12	C56-C55-C17	4.00	123.21	115.52
2	D	301[B]	B12	C3-C4-N21	-3.91	107.07	111.97
2	A	301	B12	C7-C6-N22	3.90	115.07	107.94
2	A	301	B12	C13-C12-C11	-3.88	96.58	100.97
2	B	301	B12	C2-C1-C19	3.84	124.66	118.60
2	D	301[A]	B12	C54-C17-C55	3.83	115.57	109.25
2	B	301	B12	C42-C41-C8	3.83	125.78	114.73
2	B	301	B12	C12-C13-C14	3.77	108.56	102.26
2	A	301	B12	C17-C18-C19	-3.76	96.62	102.36
2	C	301	B12	C18-C17-C16	3.72	105.19	100.67
2	A	301	B12	C60-C18-C19	3.69	124.26	114.62
2	A	301	B12	C19-C1-N21	3.68	105.93	102.16
2	C	301	B12	O2-P-O4	-3.66	95.73	109.47
2	C	301	B12	C2-C3-C4	3.59	105.71	101.63
2	C	301	B12	C56-C55-C17	3.57	122.40	115.52
2	A	301	B12	C7-C6-C5	-3.48	122.59	128.07
2	B	301	B12	C8-C9-N22	3.45	117.64	110.77
2	D	301[A]	B12	C54-C17-C18	-3.41	107.95	112.98
2	D	301[B]	B12	C12-C13-C14	3.37	107.89	102.26
2	D	301[A]	B12	C55-C56-C57	3.34	118.53	111.23
2	B	301	B12	C2P-C1P-N59	-3.33	108.03	112.93
2	D	301[B]	B12	C26-C2-C1	3.29	115.13	110.01
2	C	301	B12	C2-C1-N21	3.27	106.33	101.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301[B]	B12	C6-C5-C4	-3.27	115.69	121.54
2	D	301[A]	B12	C9-C10-C11	-3.23	121.30	125.97
2	B	301	B12	C10-C11-N23	3.19	129.89	124.43
2	C	301	B12	C13-C14-N23	3.17	113.42	109.10
2	C	301	B12	C54-C17-C18	-3.14	108.34	112.98
2	B	301	B12	C46-C12-C11	3.13	121.33	110.08
2	D	301[A]	B12	C7-C6-N22	3.05	113.51	107.94
2	D	301[B]	B12	C35-C5-C4	3.04	122.99	116.79
2	D	301[A]	B12	C30-C3-C4	2.99	116.60	109.63
2	D	301[A]	B12	C13-C14-N23	2.98	113.16	109.10
2	B	301	B12	C26-C2-C3	2.97	112.67	107.41
2	C	301	B12	C56-C57-N59	2.97	121.42	116.42
2	B	301	B12	C2-C1-N21	2.91	105.83	101.77
2	A	301	B12	C25-C2-C1	-2.88	109.44	113.78
2	D	301[A]	B12	C7-C6-C5	-2.88	123.54	128.07
2	D	301[B]	B12	C8-C9-N22	2.88	116.51	110.77
2	A	301	B12	C8-C9-C10	-2.85	117.17	123.32
2	A	301	B12	C2-C1-N21	2.83	105.71	101.77
2	D	301[A]	B12	C3R-C2R-C1R	2.79	106.08	99.89
2	A	301	B12	C55-C17-C16	-2.79	111.14	116.65
2	C	301	B12	C30-C31-C32	-2.78	103.16	112.59
2	D	301[B]	B12	C46-C12-C11	2.78	120.08	110.08
2	C	301	B12	O5-P-O4	2.77	125.92	112.24
2	B	301	B12	C46-C12-C13	-2.75	101.52	112.72
2	D	301[A]	B12	C17-C18-C19	-2.73	98.19	102.36
2	B	301	B12	C42-C43-N45	2.72	124.97	116.51
2	C	301	B12	C7-C6-N22	2.68	112.84	107.94
2	A	301	B12	C35-C5-C6	2.67	126.69	122.43
2	C	301	B12	C2-C1-C19	2.67	122.81	118.60
2	B	301	B12	C8-C9-C10	-2.66	117.57	123.32
2	A	301	B12	O58-C57-N59	2.63	127.98	123.01
2	D	301[A]	B12	C12-C11-C10	-2.63	119.95	123.37
2	A	301	B12	C8-C9-N22	2.60	115.95	110.77
2	A	301	B12	C49-C48-C13	2.59	122.21	114.73
2	D	301[A]	B12	C1-C2-C3	-2.59	98.29	101.60
2	B	301	B12	C2R-C3R-C4R	2.58	107.80	103.22
2	B	301	B12	C1-C19-C18	2.58	126.11	121.88
2	D	301[A]	B12	O51-C50-C49	2.58	128.64	121.07
2	B	301	B12	C48-C13-C14	2.57	114.90	108.49
2	A	301	B12	C53-C15-C16	2.56	124.79	120.38
2	C	301	B12	C12-C11-C10	-2.56	120.03	123.37
2	B	301	B12	C5-C6-N22	-2.56	119.96	123.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	B12	C37-C7-C8	2.56	115.24	108.39
2	D	301[B]	B12	C9-C10-C11	-2.55	122.28	125.97
2	D	301[A]	B12	C55-C17-C18	-2.49	106.33	111.15
2	C	301	B12	C7-C6-C5	-2.49	124.15	128.07
2	A	301	B12	C20-C1-N21	-2.49	106.19	110.27
2	C	301	B12	C3P-C2P-C1P	2.45	116.15	111.39
2	D	301[B]	B12	O3-C2P-C1P	2.36	111.62	106.92
2	D	301[B]	B12	C17-C16-N24	2.33	114.73	111.15
2	B	301	B12	C47-C12-C13	-2.32	103.26	112.72
2	C	301	B12	C9-C10-C11	-2.32	122.61	125.97
2	D	301[A]	B12	C48-C13-C14	2.29	114.21	108.49
2	D	301[A]	B12	O6R-C4R-C5R	-2.25	104.34	109.21
2	B	301	B12	C7-C6-N22	2.25	112.05	107.94
2	D	301[A]	B12	C60-C18-C19	2.25	120.50	114.62
2	D	301[B]	B12	C7-C8-C9	2.25	103.78	100.90
2	C	301	B12	C54-C17-C16	-2.22	100.89	112.40
2	B	301	B12	C18-C17-C16	2.20	103.35	100.67
2	C	301	B12	C2R-C3R-C4R	2.20	107.12	103.22
2	A	301	B12	C20-C1-C2	2.19	116.94	113.28
2	D	301[A]	B12	C48-C49-C50	2.18	120.00	112.59
2	B	301	B12	C4B-C9B-C8B	-2.18	118.86	121.10
2	C	301	B12	C1-C2-C3	-2.18	98.81	101.60
2	A	301	B12	C48-C49-C50	-2.11	105.44	112.59
2	D	301[A]	B12	C19-C1-N21	2.09	104.31	102.16
2	D	301[B]	B12	C30-C31-C32	-2.07	105.57	112.59
2	D	301[B]	B12	P-O2-C3R	2.05	126.88	119.41
2	D	301[B]	B12	C42-C41-C8	-2.05	108.81	114.73
2	D	301[B]	B12	C1-C19-C18	2.04	125.23	121.88
2	A	301	B12	C60-C61-N62	2.04	121.12	116.21
2	A	301	B12	C9-C10-C11	-2.03	123.03	125.97
2	A	301	B12	C53-C15-C14	-2.02	114.36	118.43
2	A	301	B12	C6-C5-C4	-2.02	117.93	121.54
2	C	301	B12	O58-C57-C56	-2.01	118.34	122.02
2	B	301	B12	C3-C4-C5	2.00	127.18	123.81

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	B12	C19
2	B	301	B12	C19
2	C	301	B12	C19
2	D	301[A]	B12	C19

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Mol	Chain	Res	Type	Atom
2	D	301[B]	B12	C19
2	D	301[B]	B12	C2

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	B12	C16-C17-C55-C56
2	A	301	B12	C54-C17-C55-C56
2	B	301	B12	C25-C2-C26-C27
2	B	301	B12	C3-C2-C26-C27
2	B	301	B12	C42-C41-C8-C7
2	C	301	B12	C38-C37-C7-C6
2	C	301	B12	C38-C37-C7-C36
2	C	301	B12	C38-C37-C7-C8
2	C	301	B12	C16-C17-C55-C56
2	C	301	B12	C54-C17-C55-C56
2	C	301	B12	C18-C17-C55-C56
2	C	301	B12	N59-C1P-C2P-C3P
2	C	301	B12	N59-C1P-C2P-O3
2	D	301[A]	B12	C25-C2-C26-C27
2	D	301[A]	B12	C3-C2-C26-C27
2	D	301[A]	B12	C16-C17-C55-C56
2	D	301[A]	B12	N59-C1P-C2P-C3P
2	D	301[A]	B12	N59-C1P-C2P-O3
2	D	301[A]	B12	C1P-C2P-O3-P
2	D	301[A]	B12	C3P-C2P-O3-P
2	D	301[A]	B12	C2P-O3-P-O5
2	D	301[A]	B12	C3R-O2-P-O5
2	D	301[B]	B12	C1-C2-C26-C27
2	D	301[B]	B12	C3-C2-C26-C27
2	D	301[B]	B12	C2-C3-C30-C31
2	D	301[B]	B12	C19-C18-C60-C61
2	D	301[B]	B12	N59-C1P-C2P-C3P
2	D	301[B]	B12	N59-C1P-C2P-O3
2	D	301[B]	B12	C3P-C2P-O3-P
2	D	301[B]	B12	C3R-O2-P-O5
2	C	301	B12	C56-C57-N59-C1P
2	B	301	B12	C13-C48-C49-C50
2	D	301[B]	B12	C3-C30-C31-C32
2	D	301[B]	B12	C42-C41-C8-C7
2	B	301	B12	C42-C41-C8-C9
2	D	301[A]	B12	C4-C3-C30-C31

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Mol	Chain	Res	Type	Atoms
2	C	301	B12	O58-C57-N59-C1P
2	D	301[A]	B12	C4R-C3R-O2-P
2	D	301[B]	B12	C2P-O3-P-O2
2	D	301[B]	B12	C42-C41-C8-C9
2	D	301[A]	B12	C2-C3-C30-C31
2	D	301[B]	B12	C55-C56-C57-N59
2	D	301[A]	B12	C1-C2-C26-C27
2	D	301[B]	B12	C55-C56-C57-O58
2	D	301[A]	B12	C2R-C3R-O2-P
2	C	301	B12	C2-C26-C27-N29
2	A	301	B12	C41-C42-C43-O44
2	D	301[A]	B12	C18-C17-C55-C56
2	B	301	B12	C2P-O3-P-O2
2	D	301[A]	B12	C2P-O3-P-O2
2	D	301[A]	B12	C3R-O2-P-O3
2	C	301	B12	C3-C30-C31-C32
2	A	301	B12	C17-C55-C56-C57
2	D	301[B]	B12	C17-C55-C56-C57
2	D	301[B]	B12	O6R-C4R-C5R-O8R
2	D	301[B]	B12	C14-C13-C48-C49
2	B	301	B12	C55-C56-C57-O58
2	D	301[B]	B12	C3R-O2-P-O3
2	C	301	B12	C2-C26-C27-O28
2	D	301[A]	B12	C2P-O3-P-O4
2	D	301[A]	B12	C3R-O2-P-O4
2	D	301[B]	B12	C2P-O3-P-O4
2	D	301[B]	B12	C3R-O2-P-O4
2	A	301	B12	C41-C42-C43-N45
2	B	301	B12	C1-C2-C26-C27
2	B	301	B12	C48-C49-C50-O51
2	D	301[B]	B12	C12-C13-C48-C49
2	A	301	B12	C7-C37-C38-O39
2	A	301	B12	C18-C60-C61-O63
2	A	301	B12	C18-C60-C61-N62
2	B	301	B12	C55-C56-C57-N59
2	B	301	B12	C48-C49-C50-N52
2	D	301[A]	B12	C17-C18-C60-C61
2	C	301	B12	C4-C3-C30-C31
2	C	301	B12	C3P-C2P-O3-P
2	A	301	B12	C2P-O3-P-O2
2	C	301	B12	C2P-O3-P-O2
2	A	301	B12	C18-C17-C55-C56

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Mol	Chain	Res	Type	Atoms
2	D	301[B]	B12	C18-C17-C55-C56
2	A	301	B12	C7-C37-C38-N40
2	D	301[A]	B12	C55-C56-C57-O58
2	D	301[B]	B12	C2P-O3-P-O5
2	C	301	B12	C17-C18-C60-C61
2	C	301	B12	C19-C18-C60-C61
2	D	301[A]	B12	C54-C17-C55-C56
2	D	301[A]	B12	C19-C18-C60-C61
2	B	301	B12	N59-C1P-C2P-O3
2	C	301	B12	C1P-C2P-O3-P
2	A	301	B12	C56-C57-N59-C1P
2	A	301	B12	C42-C41-C8-C9
2	A	301	B12	C38-C37-C7-C8
2	C	301	B12	C2-C3-C30-C31
2	D	301[A]	B12	C55-C56-C57-N59
2	B	301	B12	C1P-C2P-O3-P

There are no ring outliers.

5 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301[A]	B12	33	0
2	B	301	B12	14	0
2	A	301	B12	8	0
2	C	301	B12	12	0
2	D	301[B]	B12	33	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 D 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 D 301 (B)

Bond lengths

Bond angles

Torsions

Rings
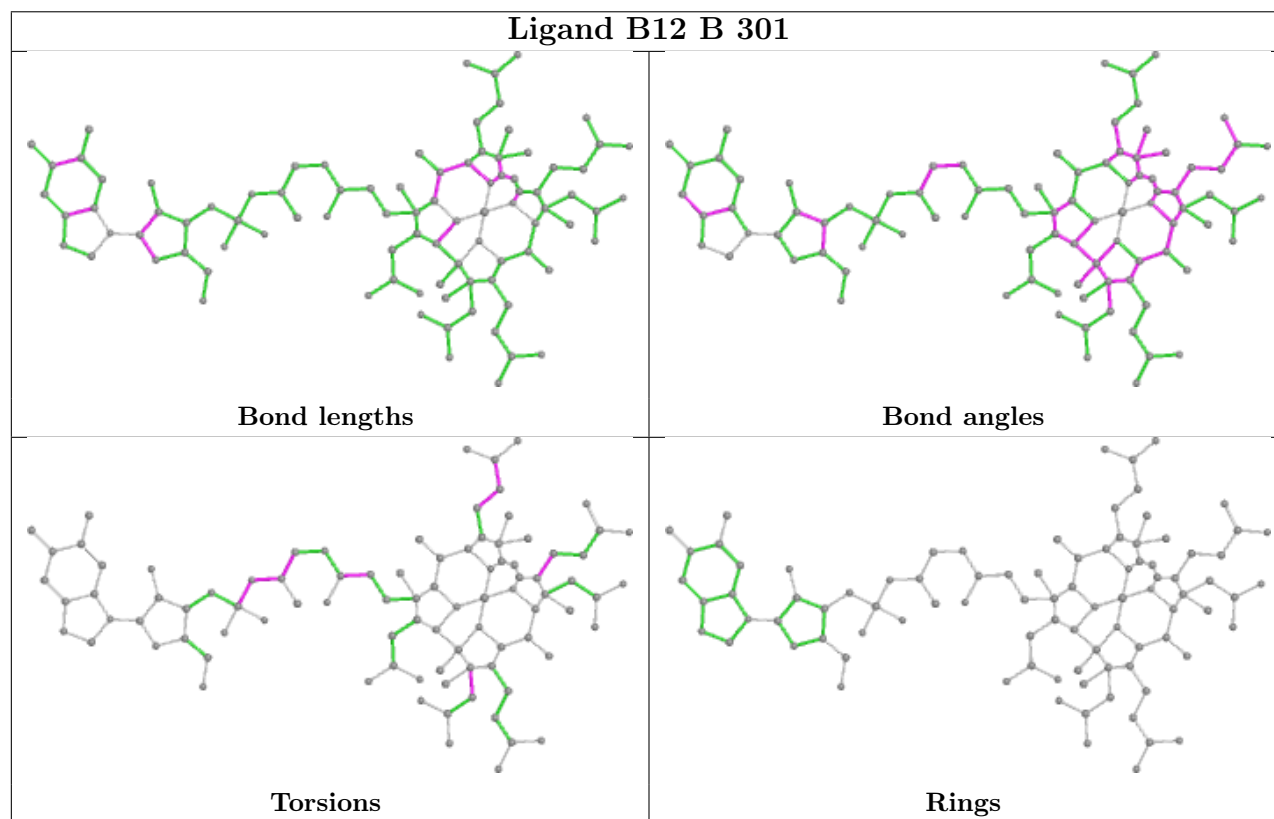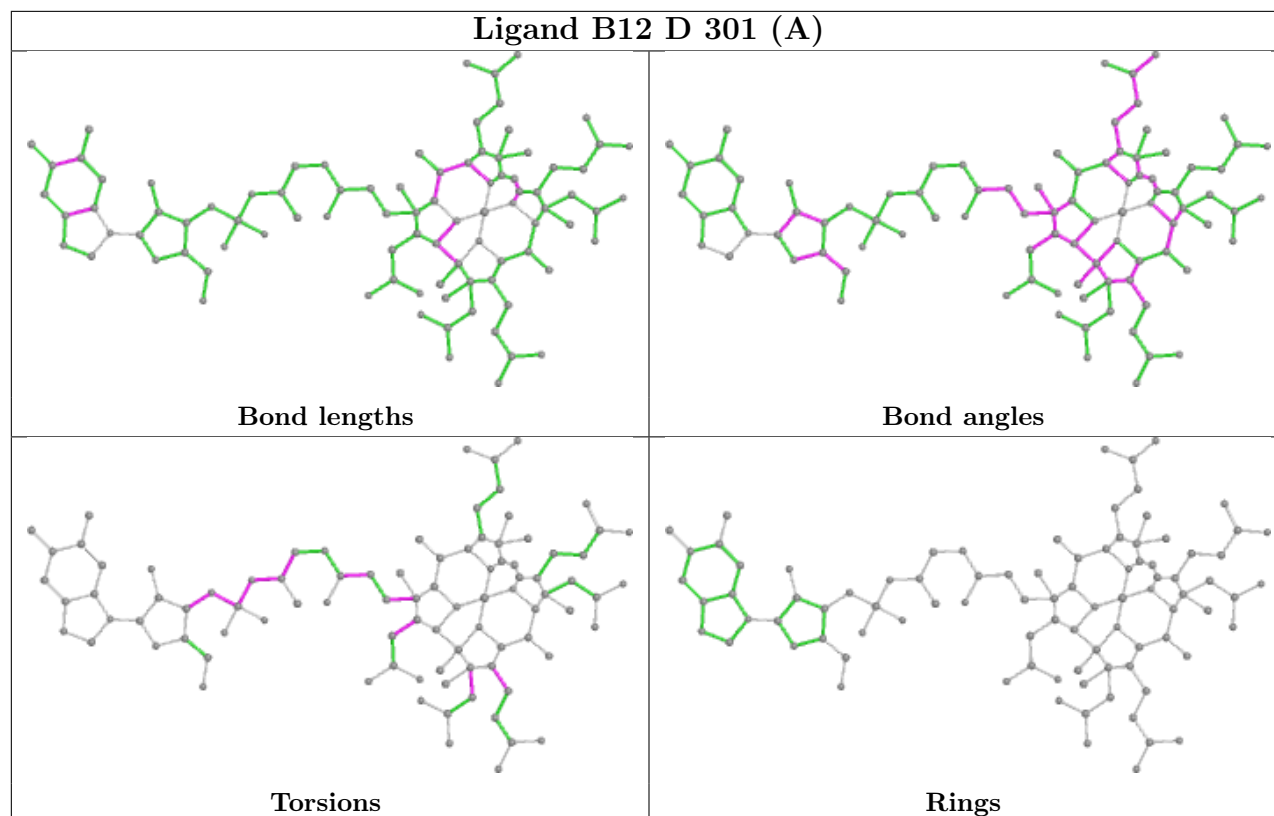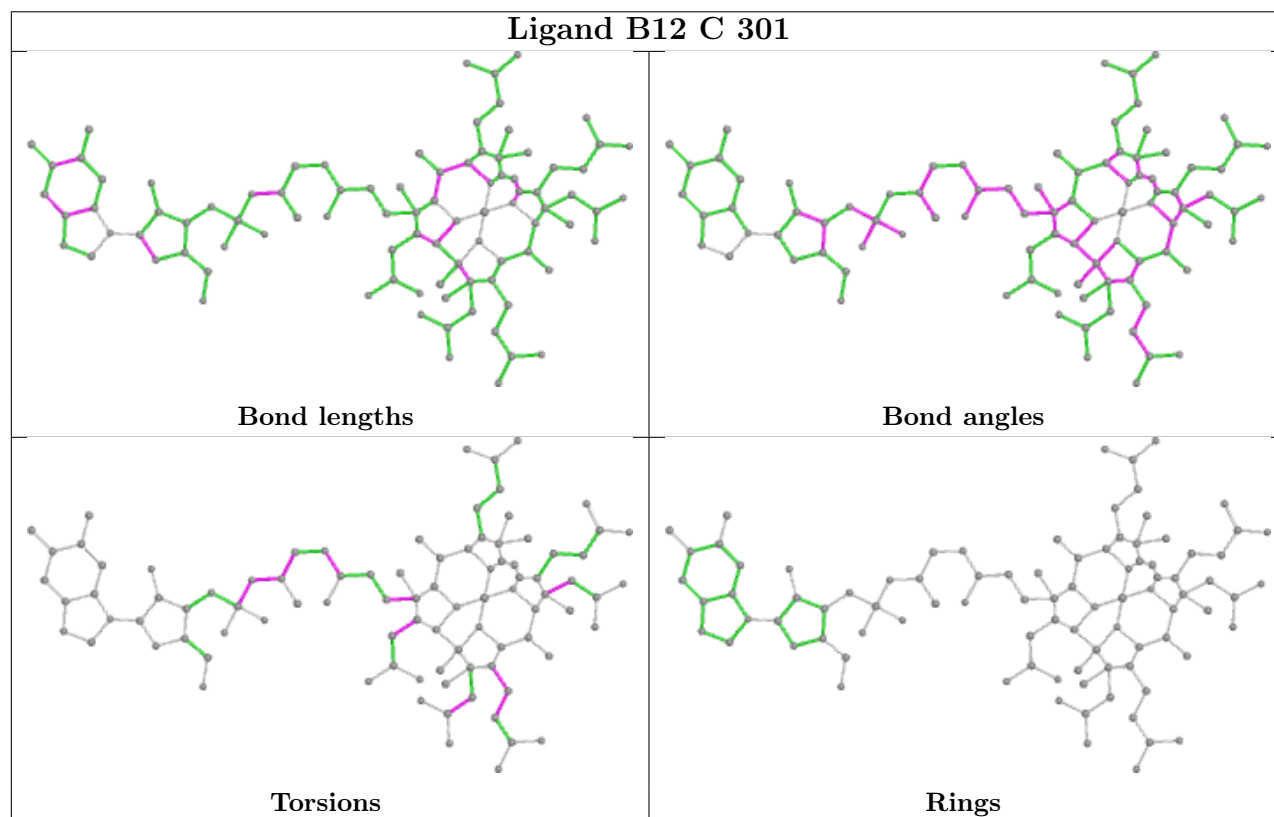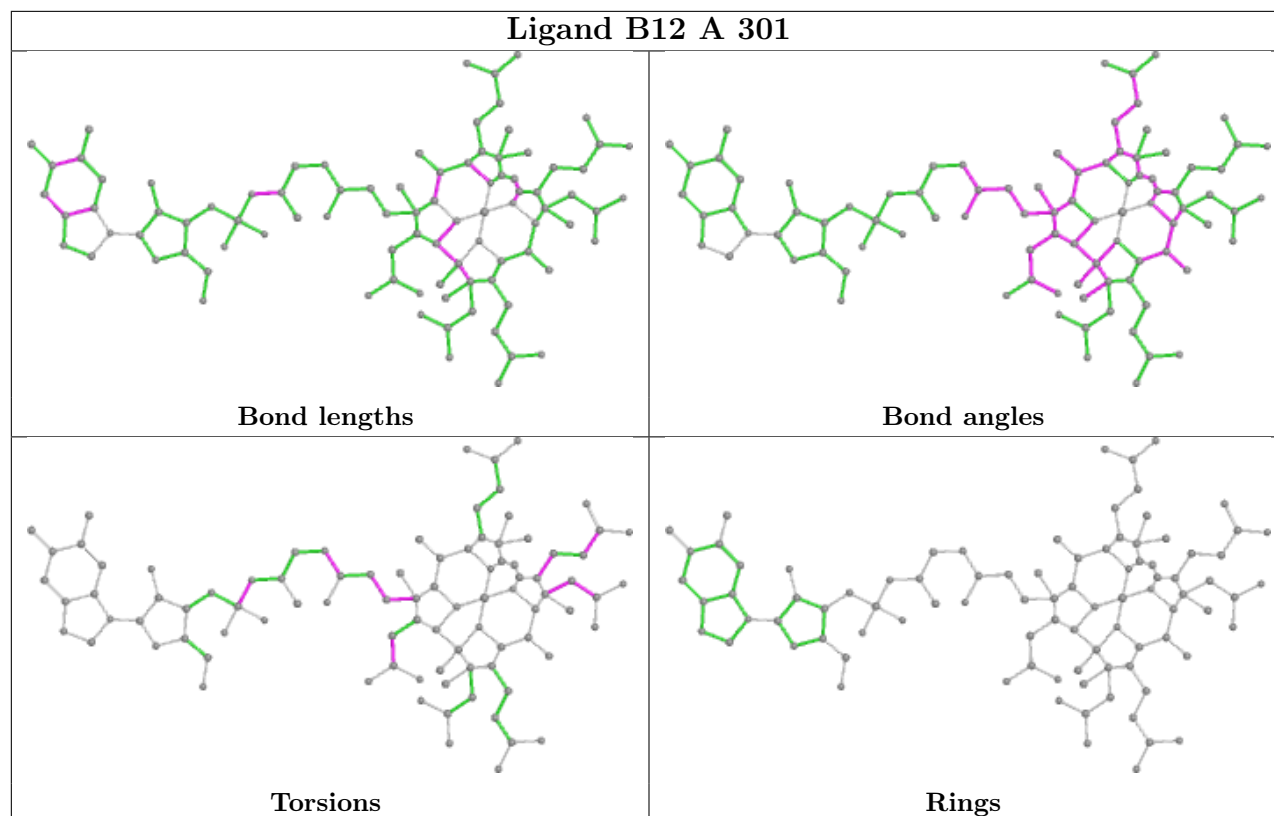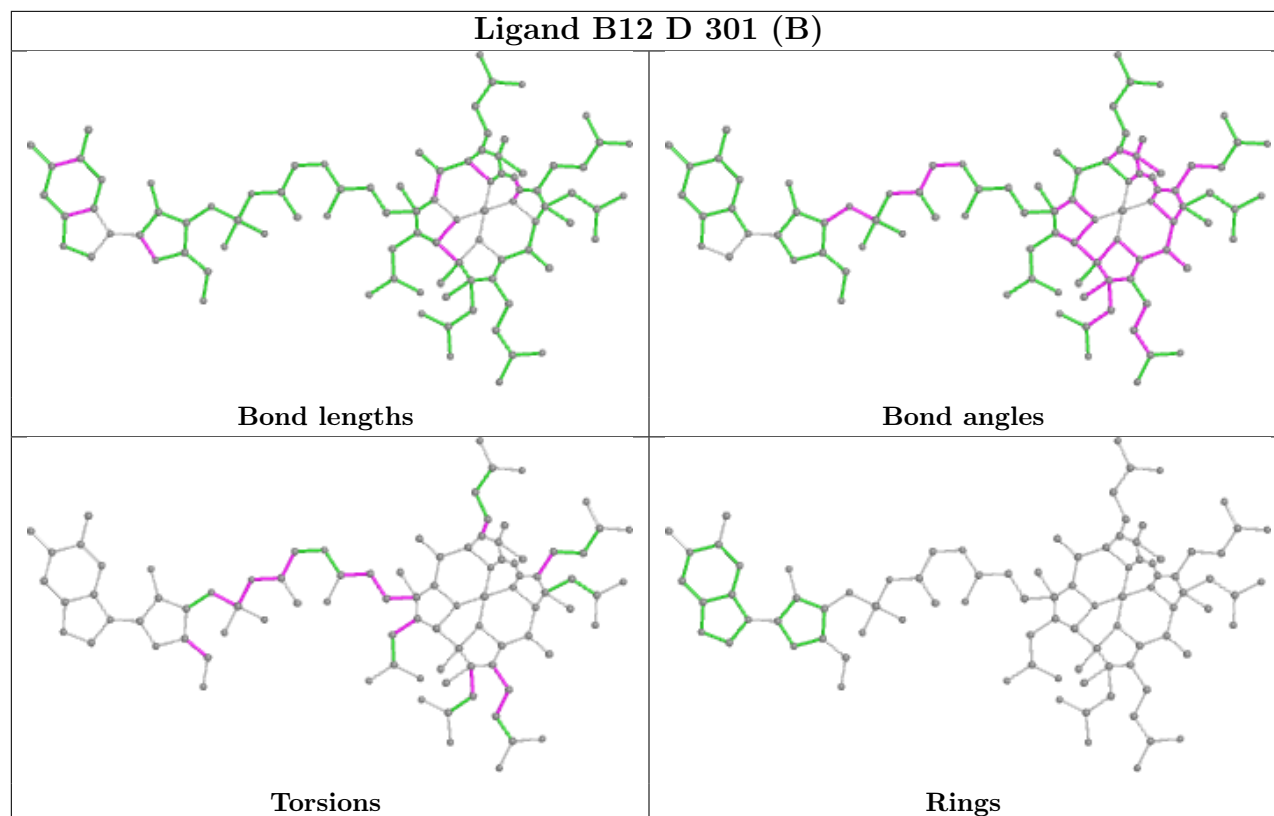
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	195/215 (90%)	0.25	4 (2%)	63	71	37, 51, 83, 102	0
1	B	196/215 (91%)	0.26	1 (0%)	91	93	34, 51, 84, 95	0
1	C	197/215 (91%)	0.40	15 (7%)	13	19	36, 50, 76, 89	0
1	D	195/215 (90%)	0.56	14 (7%)	15	21	34, 51, 78, 94	0
All	All	783/860 (91%)	0.37	34 (4%)	35	45	34, 51, 80, 102	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	131	TRP	4.4
1	C	238	LYS	4.4
1	A	238	LYS	4.0
1	C	212	ARG	4.0
1	D	132	ALA	3.9
1	C	274	LEU	3.4
1	D	230	ARG	3.3
1	D	82	ASP	3.2
1	C	249	GLN	3.1
1	D	213	ARG	3.0
1	C	264	MET	3.0
1	D	96	LEU	3.0
1	D	137	GLY	2.8
1	C	240	LEU	2.8
1	C	254	GLU	2.7
1	C	272	GLU	2.7
1	C	161	PHE	2.6
1	A	264	MET	2.6
1	C	239	ASP	2.5
1	D	266	ASP	2.4
1	D	249	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	164	GLY	2.4
1	C	257	ARG	2.4
1	C	268	LYS	2.4
1	D	238	LYS	2.2
1	D	257	ARG	2.2
1	A	212	ARG	2.2
1	D	268	LYS	2.2
1	B	118	HIS	2.1
1	D	92	LEU	2.1
1	C	208	ARG	2.1
1	A	266	ASP	2.1
1	D	176	ARG	2.1
1	C	266	ASP	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 monosaccharides 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, 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
2	B12	C	301	91/91	0.82	0.20	46,64,77,90	0
2	B12	D	301[A]	91/91	0.83	0.27	34,61,72,81	91
2	B12	D	301[B]	91/91	0.83	0.27	49,81,91,94	91
2	B12	B	301	91/91	0.90	0.17	43,70,90,97	0
2	B12	A	301	91/91	0.94	0.13	46,56,65,76	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 C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
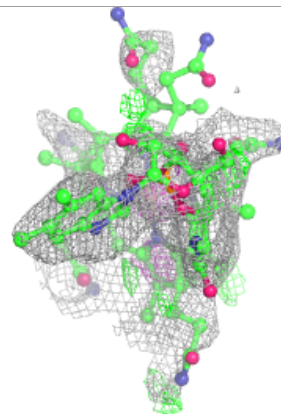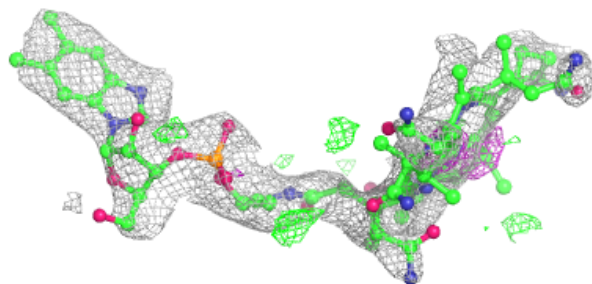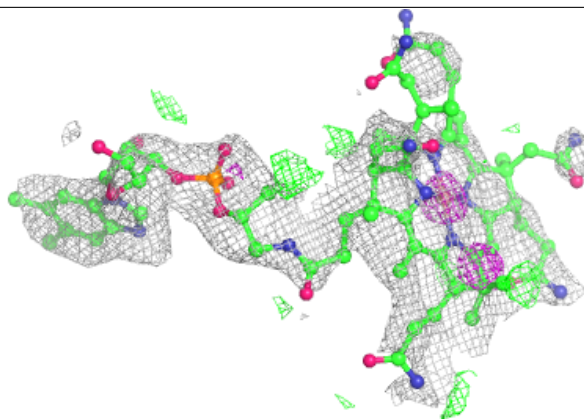mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
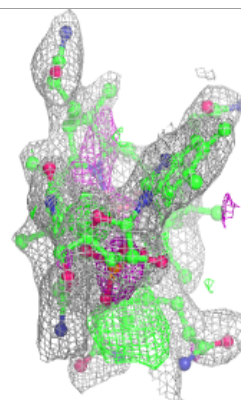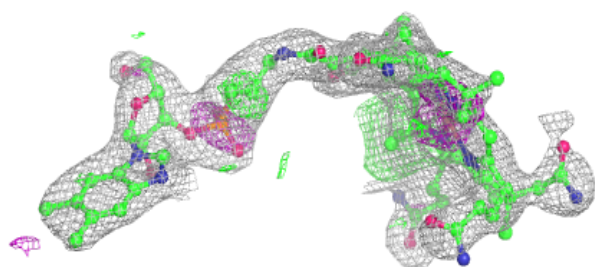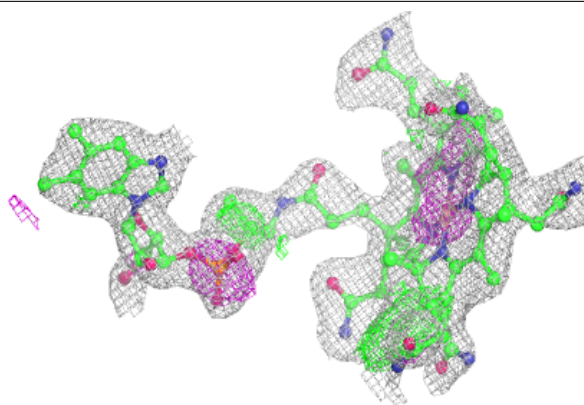
Electron density around B12 D 301 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
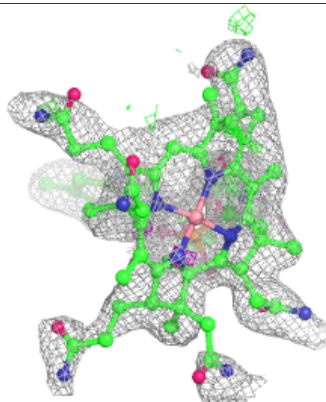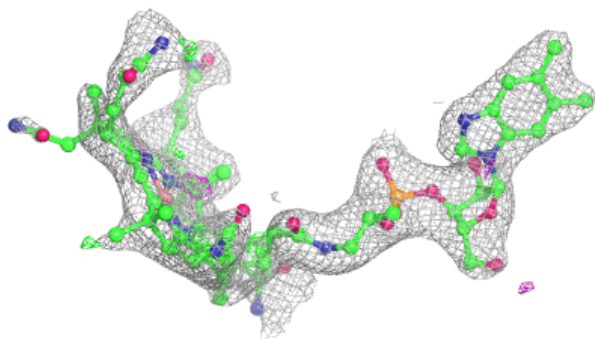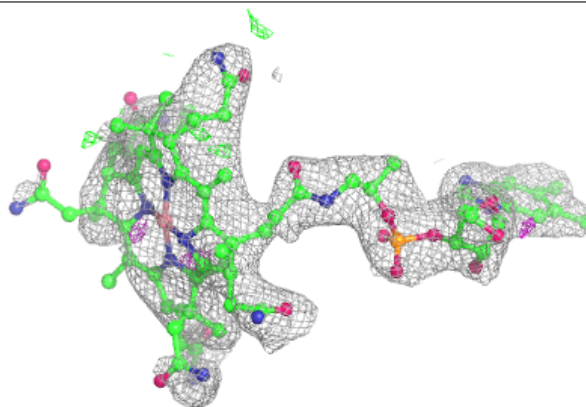mF_o-DF_c (at 3 rmsd) in purple (negative)
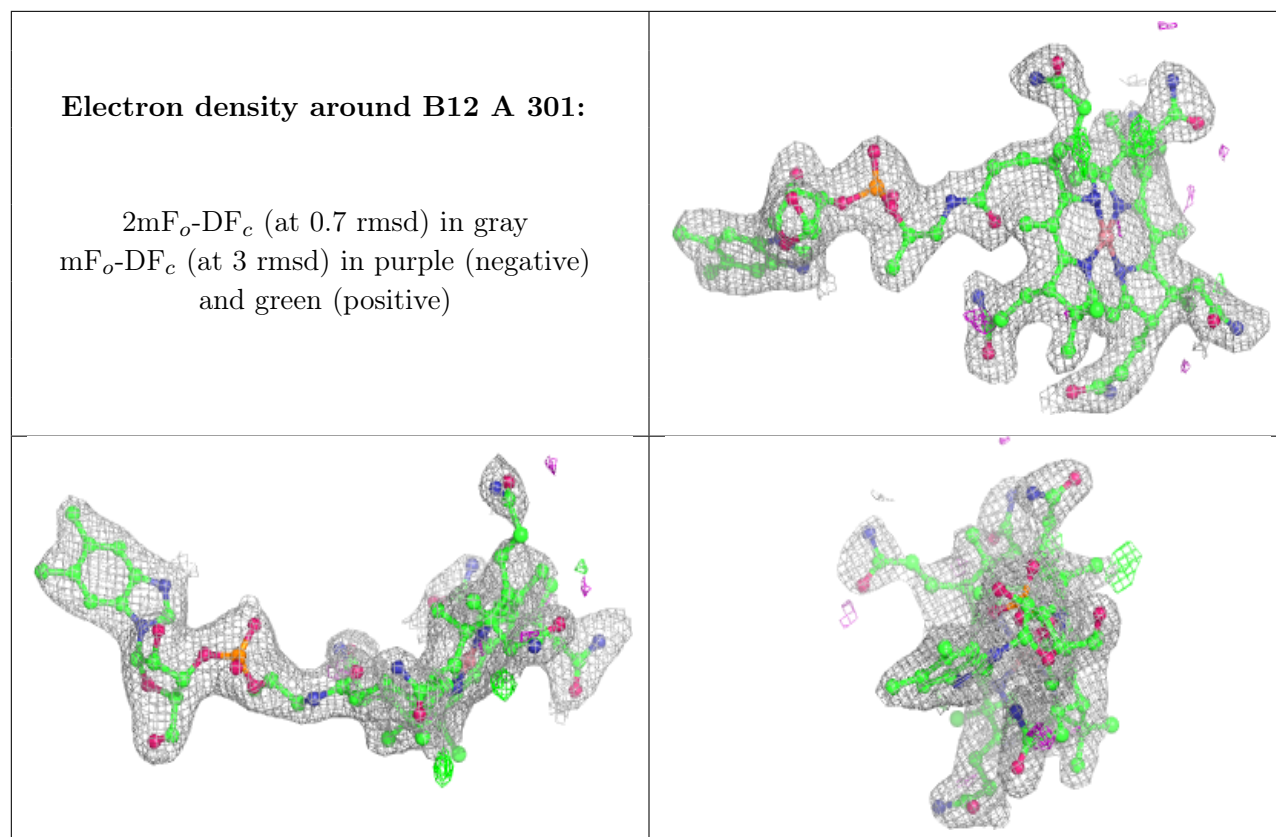and green (positive)
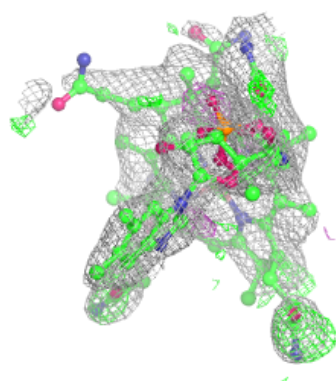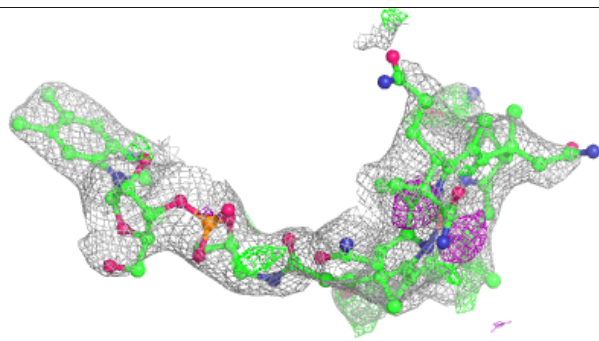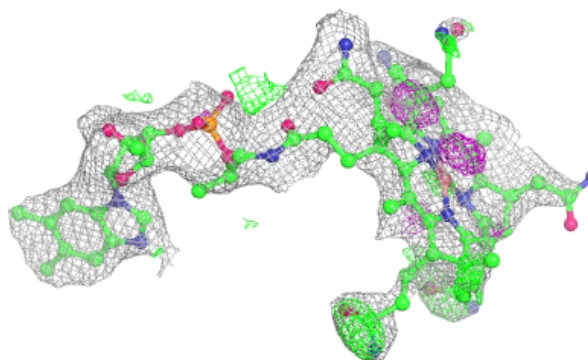
Electron density around B12 D 301 (B):

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

Electron density around B12 B 301:

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

Electron density around B12 A 301:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.