



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:02 AM EDT

PDB ID : 2BB6 / pdb_00002bb6
Title : Structure of Cobalamin-complexed Bovine Transcobalamin in Monoclinic Crystal Form
Authors : Wuerges, J.; Garau, G.; Geremia, S.; Fedosov, S.N.; Petersen, T.E.; Randaccio, L.
Deposited on : 2005-10-17
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) 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

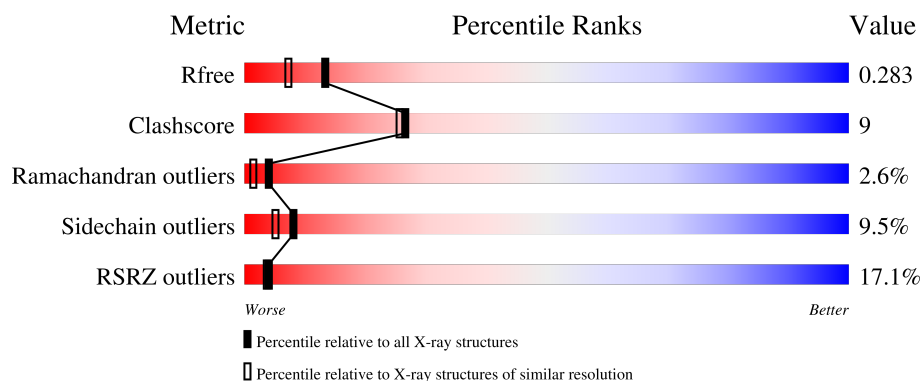
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	18% 80% 15% • •
1	B	414	17% 80% 15% •
1	C	414	18% 80% 16% •
1	D	414	16% 78% 18% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14148 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.

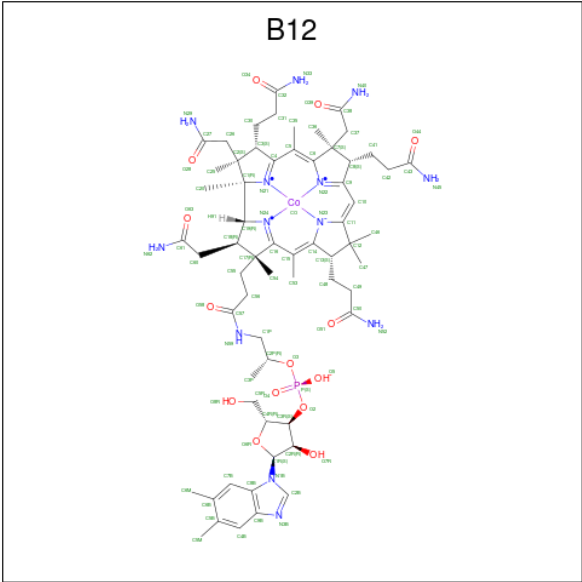
- Molecule 1 is a protein called Transcobalamin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			
1	B	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			
1	C	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			
1	D	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



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

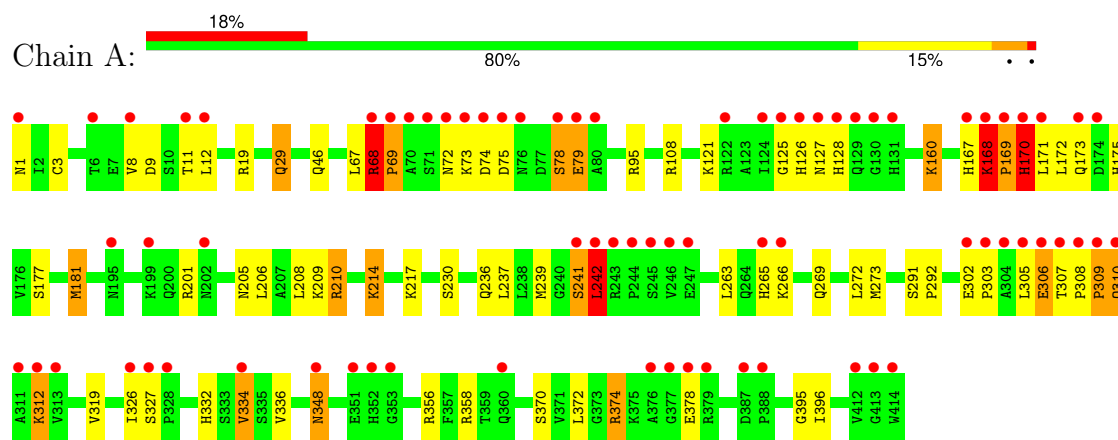
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	204	Total	O	0	0
			204	204		
4	C	198	Total	O	0	0
			198	198		
4	D	181	Total	O	0	0
			181	181		

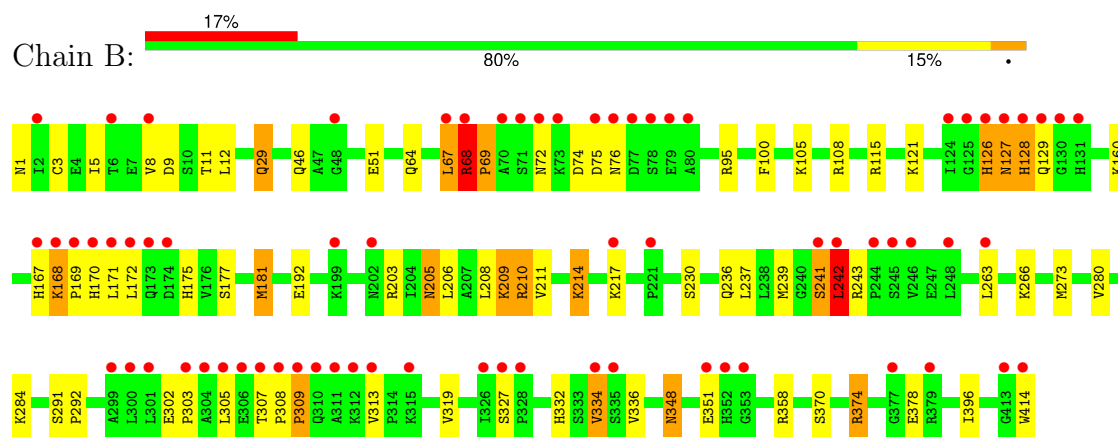
3 Residue-property plots [i](#)

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.

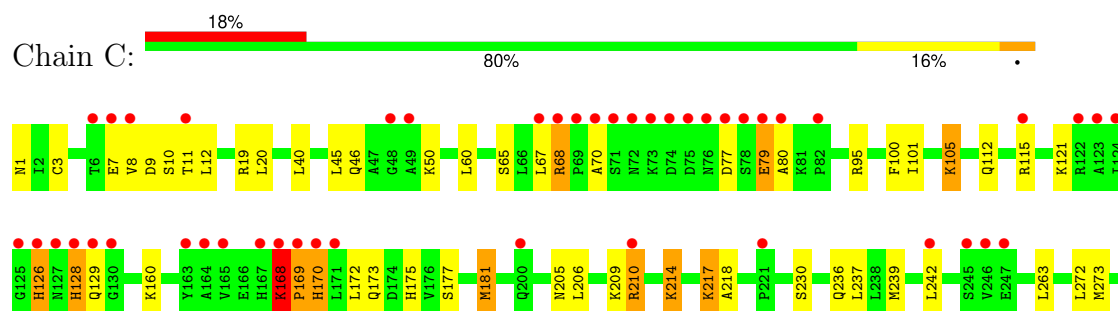
• Molecule 1: Transcobalamin II



• Molecule 1: Transcobalamin II

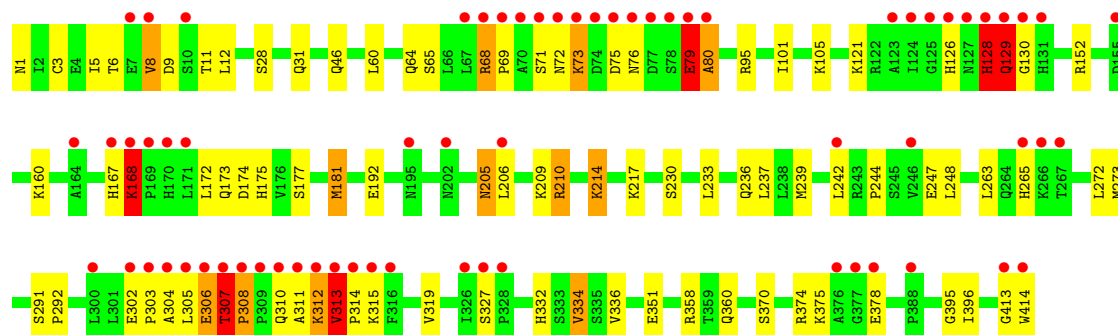
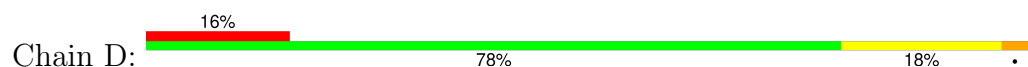


• Molecule 1: Transcobalamin II





● Molecule 1: Transcobalamin II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.83Å 100.66Å 99.14Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	18.00 – 2.00 18.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (18.00-2.00) 96.6 (18.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.280 0.252 , 0.283	Depositor DCC
R_{free} test set	5265 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14148	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0232e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.68	0/3319	0.91	5/4491 (0.1%)
1	B	0.69	0/3319	0.91	3/4491 (0.1%)
1	C	0.70	0/3319	0.90	3/4491 (0.1%)
1	D	0.70	0/3319	0.94	7/4491 (0.2%)
All	All	0.69	0/13276	0.91	18/17964 (0.1%)

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	1
1	B	0	3
1	D	0	4
All	All	0	8

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	SER	CB-CA-C	-7.92	107.44	116.54
1	C	308	PRO	N-CA-C	7.75	120.15	110.70
1	B	167	HIS	N-CA-C	7.11	119.86	108.41
1	A	167	HIS	N-CA-C	6.55	119.51	107.99
1	B	170	HIS	N-CA-C	6.04	119.23	110.42
1	D	68	ARG	CA-C-N	6.01	127.35	119.84
1	D	68	ARG	C-N-CA	6.01	127.35	119.84
1	A	67	LEU	N-CA-C	5.98	118.70	109.07
1	D	314	PRO	N-CA-C	5.67	119.98	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	LYS	CA-C-N	5.65	126.90	119.84
1	C	168	LYS	C-N-CA	5.65	126.90	119.84
1	A	396	ILE	N-CA-C	5.55	116.28	110.62
1	D	396	ILE	N-CA-C	5.55	116.28	110.62
1	D	80	ALA	N-CA-C	-5.50	106.42	113.02
1	B	396	ILE	N-CA-C	5.08	115.80	110.62
1	A	170	HIS	N-CA-C	5.02	117.16	110.53
1	D	307	THR	CA-C-N	5.01	125.55	120.38
1	D	307	THR	C-N-CA	5.01	125.55	120.38

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	ARG	Peptide
1	B	67	LEU	Peptide,Mainchain
1	B	68	ARG	Peptide
1	D	129	GLN	Peptide
1	D	167	HIS	Peptide
1	D	168	LYS	Peptide
1	D	313	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3254	0	3317	55	0
1	B	3254	0	3317	57	0
1	C	3254	0	3317	70	1
1	D	3254	0	3317	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	91	0	88	12	0
3	B	91	0	88	10	0
3	C	91	0	88	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	91	0	88	8	0
4	A	181	0	0	7	0
4	B	204	0	0	15	0
4	C	198	0	0	14	1
4	D	181	0	0	5	0
All	All	14148	0	13620	252	1

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 9.

All (252) 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:10:SER:CB	1:D:129:GLN:HA	1.63	1.29
1:C:10:SER:HB2	1:D:129:GLN:CA	1.66	1.24
1:B:100:PHE:HD2	4:B:1092:HOH:O	0.93	1.20
1:B:100:PHE:CD2	4:B:1092:HOH:O	1.67	1.13
4:C:993:HOH:O	1:D:129:GLN:HB2	1.52	1.06
1:B:68:ARG:HG3	1:B:108:ARG:HH12	1.24	1.02
1:A:306:GLU:HG3	1:B:115:ARG:HH22	1.17	1.02
1:C:168:LYS:HB3	1:C:169:PRO:CD	1.91	0.99
1:C:414:TRP:HZ2	3:C:0:B12:H521	1.04	0.95
1:A:168:LYS:HB3	1:A:169:PRO:HD2	1.49	0.92
1:C:168:LYS:HB3	1:C:169:PRO:HD2	1.51	0.92
3:C:0:B12:H362	3:C:0:B12:H351	1.55	0.88
1:B:5:ILE:HG13	4:B:1038:HOH:O	1.76	0.85
4:A:1069:HOH:O	1:C:217:LYS:HB2	1.77	0.85
1:A:306:GLU:HG3	1:B:115:ARG:NH2	1.90	0.84
1:A:125:GLY:C	1:A:127:ASN:H	1.86	0.84
3:D:0:B12:H362	3:D:0:B12:H351	1.59	0.84
1:A:266:LYS:HG2	1:A:269:GLN:NE2	1.92	0.84
1:A:125:GLY:O	1:A:127:ASN:N	2.11	0.83
3:A:0:B12:H362	3:A:0:B12:H351	1.59	0.82
1:B:280:VAL:HG12	4:B:1038:HOH:O	1.78	0.82
1:C:100:PHE:HB2	4:C:908:HOH:O	1.78	0.82
1:C:9:ASP:HB2	4:C:1034:HOH:O	1.78	0.81
1:C:168:LYS:CB	1:C:169:PRO:HD2	2.10	0.81
3:B:0:B12:H362	3:B:0:B12:H351	1.66	0.78
1:A:241:SER:O	1:A:242:LEU:HB2	1.83	0.77
1:A:332:HIS:HD2	1:A:334:VAL:HG12	1.49	0.76
1:D:332:HIS:HD2	1:D:334:VAL:HG12	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:HIS:HB3	1:A:214:LYS:NZ	2.02	0.74
1:B:68:ARG:HG3	1:B:108:ARG:NH1	2.00	0.74
1:C:332:HIS:HD2	1:C:334:VAL:HG12	1.53	0.74
1:B:332:HIS:HD2	1:B:334:VAL:HG12	1.53	0.73
3:C:0:B12:H531	3:C:0:B12:H552	1.70	0.73
1:C:302:GLU:HG2	1:C:303:PRO:HD2	1.70	0.72
1:C:100:PHE:CD2	4:C:908:HOH:O	2.42	0.72
1:B:208:LEU:HD13	1:B:242:LEU:HD11	1.71	0.71
1:C:100:PHE:HD2	4:C:908:HOH:O	1.72	0.71
1:C:312:LYS:HG3	1:C:313:VAL:H	1.55	0.70
1:A:302:GLU:HG2	1:A:303:PRO:HD2	1.72	0.70
1:B:414:TRP:HZ2	3:B:0:B12:H521	1.37	0.70
1:D:302:GLU:HG2	1:D:303:PRO:HD2	1.72	0.70
1:B:351:GLU:HG3	4:B:911:HOH:O	1.93	0.69
1:A:208:LEU:HD13	1:A:242:LEU:HD11	1.73	0.69
1:D:128:HIS:O	1:D:130:GLY:N	2.26	0.69
1:B:100:PHE:CB	4:B:1092:HOH:O	2.39	0.68
1:B:302:GLU:HG2	1:B:303:PRO:HD2	1.74	0.68
1:D:360:GLN:HB3	4:D:1054:HOH:O	1.93	0.67
1:B:280:VAL:CG1	4:B:1038:HOH:O	2.39	0.67
1:A:170:HIS:HB3	1:A:214:LYS:HZ2	1.59	0.65
1:D:414:TRP:HZ2	3:D:0:B12:H521	1.44	0.65
1:B:100:PHE:HB2	4:B:1092:HOH:O	1.94	0.65
1:D:265:HIS:HD2	4:D:1047:HOH:O	1.80	0.65
1:A:266:LYS:HG2	1:A:269:GLN:HE22	1.60	0.65
1:B:209:LYS:HD3	1:B:243:ARG:HD2	1.79	0.64
1:C:217:LYS:HE3	4:C:1068:HOH:O	1.98	0.64
1:B:241:SER:O	1:B:242:LEU:HB2	1.96	0.64
1:A:68:ARG:HB3	1:A:69:PRO:CD	2.26	0.64
1:D:332:HIS:CD2	1:D:334:VAL:HG12	2.32	0.64
1:C:126:HIS:H	1:C:128:HIS:CE1	2.16	0.63
1:C:10:SER:HB2	1:D:129:GLN:HA	0.76	0.63
1:B:67:LEU:O	1:B:69:PRO:HD2	1.99	0.63
1:A:332:HIS:CD2	1:A:334:VAL:HG12	2.33	0.62
1:B:210:ARG:HD3	1:B:214:LYS:HE2	1.82	0.61
3:B:0:B12:H552	3:B:0:B12:H531	1.83	0.61
1:C:100:PHE:N	4:C:908:HOH:O	2.32	0.61
1:C:332:HIS:CD2	1:C:334:VAL:HG12	2.33	0.61
1:B:168:LYS:HB3	1:B:169:PRO:HD2	1.83	0.61
1:C:210:ARG:HD3	1:C:214:LYS:HE2	1.83	0.61
3:A:0:B12:H531	3:A:0:B12:H552	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ASP:OD2	1:D:11:THR:OG1	2.18	0.60
1:B:319:VAL:HG12	1:B:334:VAL:HG22	1.84	0.60
3:C:0:B12:H353	3:C:0:B12:H302	1.83	0.60
1:B:307:THR:C	1:B:309:PRO:HD3	2.27	0.59
1:D:121:LYS:HG3	1:D:160:LYS:HG3	1.85	0.59
1:A:326:ILE:HD13	4:A:1049:HOH:O	2.03	0.59
1:C:100:PHE:CB	4:C:908:HOH:O	2.40	0.58
1:B:332:HIS:CD2	1:B:334:VAL:HG12	2.36	0.58
1:A:210:ARG:HD3	1:A:214:LYS:HE2	1.86	0.58
1:A:242:LEU:HD13	4:A:1045:HOH:O	2.03	0.58
1:B:121:LYS:HG3	1:B:160:LYS:HG3	1.86	0.58
1:A:319:VAL:HG12	1:A:334:VAL:HG22	1.86	0.58
1:D:306:GLU:O	1:D:307:THR:HB	2.03	0.58
1:D:128:HIS:C	1:D:130:GLY:H	2.12	0.58
1:D:319:VAL:HG12	1:D:334:VAL:HG22	1.85	0.57
1:C:312:LYS:NZ	1:C:312:LYS:HA	2.18	0.57
1:D:414:TRP:HZ2	3:D:0:B12:N52	2.02	0.57
1:A:121:LYS:HG3	1:A:160:LYS:HG3	1.87	0.57
1:C:45:LEU:HD22	4:D:1032:HOH:O	2.03	0.57
1:C:121:LYS:HG3	1:C:160:LYS:HG3	1.87	0.57
1:C:319:VAL:HG12	1:C:334:VAL:HG22	1.86	0.57
1:C:9:ASP:OD2	1:C:11:THR:OG1	2.22	0.57
1:A:201:ARG:HG2	4:A:1055:HOH:O	2.06	0.56
1:D:68:ARG:HB2	4:D:1082:HOH:O	2.05	0.56
1:B:126:HIS:O	1:B:127:ASN:HB2	2.04	0.56
1:B:236:GLN:HA	1:B:239:MET:HE3	1.88	0.56
1:A:236:GLN:HA	1:A:239:MET:HE3	1.86	0.55
1:D:210:ARG:HD3	1:D:214:LYS:HE2	1.88	0.55
1:A:9:ASP:OD2	1:A:11:THR:OG1	2.24	0.55
1:D:302:GLU:CG	1:D:303:PRO:HD2	2.37	0.54
1:B:160:LYS:NZ	4:B:1066:HOH:O	2.40	0.54
1:C:302:GLU:CG	1:C:303:PRO:HD2	2.37	0.54
1:B:9:ASP:OD2	1:B:11:THR:OG1	2.24	0.53
3:A:0:B12:H353	3:A:0:B12:H302	1.90	0.53
1:D:236:GLN:HA	1:D:239:MET:HE3	1.90	0.53
1:A:168:LYS:HB3	1:A:169:PRO:CD	2.31	0.53
1:A:302:GLU:CG	1:A:303:PRO:HD2	2.37	0.53
1:C:20:LEU:HD12	1:C:40:LEU:HD21	1.91	0.52
1:D:168:LYS:HE2	1:D:210:ARG:HH22	1.73	0.52
1:C:351:GLU:OE1	1:C:351:GLU:HA	2.09	0.52
1:B:1:ASN:ND2	1:B:3:CYS:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:THR:O	1:B:309:PRO:HD3	2.10	0.52
1:D:315:LYS:HG2	4:D:1006:HOH:O	2.11	0.51
1:B:175:HIS:HE1	3:B:0:B12:C5	2.23	0.51
3:B:0:B12:H482	3:B:0:B12:H533	1.91	0.51
1:C:168:LYS:C	1:C:170:HIS:H	2.18	0.51
1:A:310:GLN:HB2	1:A:312:LYS:HB2	1.93	0.51
1:C:126:HIS:N	1:C:128:HIS:CE1	2.78	0.51
1:D:79:GLU:CG	1:D:79:GLU:O	2.59	0.51
1:A:1:ASN:ND2	1:A:3:CYS:HB2	2.27	0.50
1:C:168:LYS:C	1:C:170:HIS:N	2.69	0.50
1:D:358:ARG:HB2	1:D:370:SER:HB3	1.94	0.50
1:A:68:ARG:HB3	1:A:69:PRO:HD3	1.94	0.50
1:A:358:ARG:HB2	1:A:370:SER:HB3	1.94	0.50
1:C:9:ASP:HB3	1:C:12:LEU:HD12	1.92	0.50
1:C:236:GLN:HA	1:C:239:MET:HE3	1.93	0.50
1:C:358:ARG:NH1	4:C:1055:HOH:O	2.44	0.50
1:B:334:VAL:HG11	1:B:348:ASN:HD21	1.77	0.50
1:A:175:HIS:HE1	3:A:0:B12:C5	2.25	0.49
1:A:9:ASP:HB3	1:A:12:LEU:HD12	1.94	0.49
1:C:352:HIS:CD2	4:C:992:HOH:O	2.65	0.49
1:D:28:SER:OG	1:D:31:GLN:HG3	2.13	0.49
1:B:302:GLU:CG	1:B:303:PRO:HD2	2.40	0.49
1:C:20:LEU:HD12	1:C:40:LEU:CD2	2.43	0.49
1:D:304:ALA:HB1	1:D:306:GLU:OE1	2.13	0.49
1:D:244:PRO:HB3	1:D:248:LEU:HD23	1.93	0.49
1:B:374:ARG:NH2	4:B:1046:HOH:O	2.01	0.49
1:B:51:GLU:HG2	4:B:1022:HOH:O	2.13	0.48
3:A:0:B12:H491	3:A:0:B12:H471	1.94	0.48
3:D:0:B12:H533	3:D:0:B12:H482	1.94	0.48
1:C:358:ARG:HG3	4:C:1055:HOH:O	2.12	0.48
3:B:0:B12:H471	3:B:0:B12:H491	1.96	0.48
1:A:170:HIS:HB3	1:A:214:LYS:HZ1	1.75	0.48
1:B:9:ASP:HB3	1:B:12:LEU:HD12	1.96	0.48
1:B:358:ARG:HB2	1:B:370:SER:HB3	1.97	0.47
1:C:168:LYS:O	1:C:170:HIS:N	2.47	0.47
1:B:1:ASN:HD21	1:B:3:CYS:HB2	1.78	0.47
1:A:68:ARG:HG3	1:A:108:ARG:HH12	1.78	0.47
1:C:112:GLN:HA	1:C:115:ARG:HG2	1.95	0.47
3:C:0:B12:H351	3:C:0:B12:C36	2.31	0.47
1:D:273:MET:HE2	1:D:273:MET:HA	1.96	0.47
1:A:265:HIS:CD2	4:B:1066:HOH:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:0:B12:H531	3:A:0:B12:H543	1.97	0.47
1:C:68:ARG:HD3	1:C:70:ALA:HB3	1.97	0.47
1:C:177:SER:O	1:C:181:MET:HG3	2.14	0.47
1:C:358:ARG:HB2	1:C:370:SER:HB3	1.97	0.47
1:A:201:ARG:HA	4:A:1064:HOH:O	2.14	0.47
1:B:126:HIS:CD2	1:B:128:HIS:H	2.34	0.46
1:A:273:MET:HE2	1:A:273:MET:HA	1.97	0.46
1:C:10:SER:HB2	1:D:129:GLN:C	2.33	0.46
1:C:67:LEU:HD13	1:C:105:LYS:HD2	1.96	0.46
1:A:334:VAL:HG23	1:A:336:VAL:HG13	1.96	0.46
1:D:1:ASN:ND2	1:D:3:CYS:HB2	2.31	0.46
1:A:1:ASN:HD21	1:A:3:CYS:HB2	1.79	0.46
1:C:311:ALA:O	1:C:312:LYS:HB2	2.15	0.46
1:D:175:HIS:HE1	3:D:0:B12:C5	2.29	0.46
1:C:1:ASN:ND2	1:C:3:CYS:HB2	2.31	0.45
1:C:414:TRP:HZ2	3:C:0:B12:N52	1.89	0.45
1:C:19:ARG:HG2	4:C:1059:HOH:O	2.16	0.45
1:D:312:LYS:O	1:D:313:VAL:HG13	2.16	0.45
1:C:175:HIS:HE1	3:C:0:B12:C5	2.29	0.45
1:C:50:LYS:HE2	4:C:987:HOH:O	2.15	0.45
1:C:68:ARG:HG2	1:C:70:ALA:HB3	1.99	0.45
1:C:126:HIS:H	1:C:128:HIS:HE1	1.65	0.45
1:D:395:GLY:HA3	3:D:0:B12:HM52	1.99	0.45
1:B:74:ASP:OD1	1:B:74:ASP:N	2.49	0.44
1:A:334:VAL:HG11	1:A:348:ASN:HD21	1.83	0.44
1:D:177:SER:O	1:D:181:MET:HG3	2.17	0.44
1:C:168:LYS:CB	1:C:169:PRO:CD	2.67	0.44
1:D:128:HIS:C	1:D:130:GLY:N	2.73	0.44
1:A:29:GLN:HE21	1:A:29:GLN:HB3	1.58	0.44
1:A:68:ARG:H	1:A:108:ARG:HH22	1.66	0.44
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.87	0.44
1:D:378:GLU:CD	1:D:378:GLU:H	2.26	0.44
1:A:175:HIS:CE1	3:A:0:B12:C6	3.01	0.44
1:B:192:GLU:OE1	1:B:205:ASN:ND2	2.51	0.44
1:C:395:GLY:HA3	3:C:0:B12:HM53	2.00	0.44
1:A:374:ARG:NH2	4:A:966:HOH:O	2.26	0.43
3:A:0:B12:H362	3:A:0:B12:C35	2.40	0.43
3:C:0:B12:H482	3:C:0:B12:H533	1.99	0.43
1:A:125:GLY:C	1:A:127:ASN:N	2.59	0.43
1:B:29:GLN:HE21	1:B:29:GLN:HB3	1.63	0.43
1:B:95:ARG:O	1:B:292:PRO:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:THR:HA	1:D:308:PRO:HD2	1.76	0.43
1:B:334:VAL:HG23	1:B:336:VAL:HG13	1.99	0.43
1:D:126:HIS:HB2	1:D:128:HIS:CE1	2.54	0.43
1:A:356:ARG:HG2	1:A:372:LEU:HA	1.99	0.43
1:B:273:MET:HE2	1:B:273:MET:HA	2.00	0.43
1:C:273:MET:HE2	1:C:273:MET:HA	2.00	0.43
1:B:378:GLU:CD	1:B:378:GLU:H	2.27	0.43
1:C:20:LEU:CD1	1:C:40:LEU:CD2	2.97	0.43
1:B:203:ARG:HD2	4:B:1075:HOH:O	2.18	0.42
1:C:10:SER:CB	1:D:129:GLN:CA	2.53	0.42
3:A:0:B12:H482	3:A:0:B12:H533	2.00	0.42
1:A:378:GLU:CD	1:A:378:GLU:H	2.28	0.42
1:B:74:ASP:C	1:B:76:ASN:H	2.27	0.42
3:B:0:B12:H262	3:B:0:B12:H91	1.84	0.42
3:C:0:B12:H362	3:C:0:B12:C35	2.39	0.42
1:D:334:VAL:HG23	1:D:336:VAL:HG13	2.00	0.42
1:A:78:SER:O	1:A:79:GLU:HB3	2.19	0.42
1:A:95:ARG:HA	1:A:95:ARG:HD2	1.88	0.42
1:D:192:GLU:OE1	1:D:205:ASN:ND2	2.52	0.42
1:D:311:ALA:C	1:D:312:LYS:HG3	2.43	0.42
1:D:95:ARG:O	1:D:292:PRO:HG3	2.19	0.42
3:B:0:B12:H491	3:B:0:B12:C47	2.50	0.42
1:B:128:HIS:CG	1:B:129:GLN:N	2.88	0.42
1:B:305:LEU:HB2	4:B:1098:HOH:O	2.20	0.42
1:D:1:ASN:HD21	1:D:3:CYS:HB2	1.84	0.42
3:D:0:B12:H552	3:D:0:B12:H531	2.02	0.42
1:B:177:SER:O	1:B:181:MET:HG3	2.19	0.42
1:B:175:HIS:CE1	3:B:0:B12:C6	3.03	0.42
3:B:0:B12:H353	3:B:0:B12:H302	2.01	0.42
1:C:413:GLY:O	1:C:414:TRP:HB3	2.20	0.42
1:C:327:SER:HB3	4:C:985:HOH:O	2.19	0.41
1:A:19:ARG:HG2	4:A:1054:HOH:O	2.21	0.41
1:C:217:LYS:HE2	1:C:218:ALA:N	2.36	0.41
1:C:378:GLU:H	1:C:378:GLU:CD	2.28	0.41
3:D:0:B12:H362	3:D:0:B12:C35	2.39	0.41
1:C:1:ASN:HD21	1:C:3:CYS:HB2	1.84	0.41
1:C:334:VAL:HG23	1:C:336:VAL:HG13	2.02	0.41
1:D:233:LEU:HD23	1:D:233:LEU:HA	1.95	0.41
1:A:168:LYS:CB	1:A:169:PRO:HD2	2.36	0.41
1:B:181:MET:HE2	1:B:211:VAL:HG22	2.03	0.41
1:C:20:LEU:CD1	1:C:40:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:GLU:CD	1:D:378:GLU:N	2.79	0.41
1:A:395:GLY:HA3	3:A:0:B12:HM53	2.03	0.41
1:B:319:VAL:CG1	1:B:334:VAL:HG22	2.49	0.41
1:B:378:GLU:CD	1:B:378:GLU:N	2.79	0.41
1:A:177:SER:O	1:A:181:MET:HG3	2.20	0.41
3:A:0:B12:C61	3:A:0:B12:H252	2.51	0.41
1:D:95:ARG:HA	1:D:95:ARG:HD2	1.89	0.41
1:D:413:GLY:O	1:D:414:TRP:HB3	2.21	0.41
1:A:319:VAL:CG1	1:A:334:VAL:HG22	2.50	0.41
1:D:5:ILE:HG22	1:D:8:VAL:HG22	2.02	0.41
1:A:95:ARG:O	1:A:292:PRO:HG3	2.21	0.40
1:B:284:LYS:NZ	4:B:1016:HOH:O	2.54	0.40
1:C:95:ARG:HA	1:C:95:ARG:HD2	1.89	0.40
1:C:168:LYS:HB3	1:C:169:PRO:HD3	1.93	0.40
1:C:319:VAL:CG1	1:C:334:VAL:HG22	2.51	0.40
1:D:68:ARG:NH2	1:D:80:ALA:O	2.54	0.40
1:C:68:ARG:NH2	1:C:80:ALA:O	2.54	0.40
3:A:0:B12:H262	3:A:0:B12:H91	2.00	0.40
1:C:175:HIS:CE1	3:C:0:B12:C6	3.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLN:NE2	4:C:1094:HOH:O[2_655]	2.10	0.10

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	412/414 (100%)	388 (94%)	10 (2%)	14 (3%)	3 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/414 (100%)	382 (93%)	21 (5%)	9 (2%)	5	2
1	C	412/414 (100%)	384 (93%)	19 (5%)	9 (2%)	5	2
1	D	412/414 (100%)	388 (94%)	13 (3%)	11 (3%)	4	1
All	All	1648/1656 (100%)	1542 (94%)	63 (4%)	43 (3%)	4	1

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	69	PRO
1	A	72	ASN
1	A	126	HIS
1	A	242	LEU
1	B	69	PRO
1	B	126	HIS
1	B	127	ASN
1	B	242	LEU
1	C	168	LYS
1	C	169	PRO
1	C	170	HIS
1	D	73	LYS
1	D	76	ASN
1	D	129	GLN
1	A	74	ASP
1	A	79	GLU
1	A	307	THR
1	C	128	HIS
1	C	129	GLN
1	D	69	PRO
1	D	71	SER
1	D	72	ASN
1	D	308	PRO
1	A	168	LYS
1	A	78	SER
1	A	128	HIS
1	B	128	HIS
1	C	310	GLN
1	D	79	GLU
1	D	128	HIS
1	D	168	LYS
1	D	307	THR

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Mol	Chain	Res	Type
1	A	75	ASP
1	A	169	PRO
1	B	75	ASP
1	C	79	GLU
1	C	309	PRO
1	B	168	LYS
1	B	309	PRO
1	B	308	PRO
1	C	308	PRO
1	A	309	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/358 (100%)	326 (91%)	32 (9%)	9	6
1	B	358/358 (100%)	330 (92%)	28 (8%)	11	8
1	C	358/358 (100%)	324 (90%)	34 (10%)	8	5
1	D	358/358 (100%)	316 (88%)	42 (12%)	5	3
All	All	1432/1432 (100%)	1296 (90%)	136 (10%)	8	5

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	29	GLN
1	A	46	GLN
1	A	68	ARG
1	A	73	LYS
1	A	160	LYS
1	A	168	LYS
1	A	170	HIS
1	A	171	LEU
1	A	172	LEU
1	A	173	GLN

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Mol	Chain	Res	Type
1	A	181	MET
1	A	205	ASN
1	A	206	LEU
1	A	209	LYS
1	A	210	ARG
1	A	214	LYS
1	A	217	LYS
1	A	230	SER
1	A	237	LEU
1	A	242	LEU
1	A	263	LEU
1	A	272	LEU
1	A	291	SER
1	A	305	LEU
1	A	306	GLU
1	A	310	GLN
1	A	312	LYS
1	A	327	SER
1	A	334	VAL
1	A	348	ASN
1	A	374	ARG
1	B	8	VAL
1	B	29	GLN
1	B	46	GLN
1	B	64	GLN
1	B	68	ARG
1	B	72	ASN
1	B	105	LYS
1	B	171	LEU
1	B	172	LEU
1	B	181	MET
1	B	205	ASN
1	B	206	LEU
1	B	209	LYS
1	B	210	ARG
1	B	214	LYS
1	B	217	LYS
1	B	230	SER
1	B	237	LEU
1	B	241	SER
1	B	242	LEU
1	B	263	LEU

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Mol	Chain	Res	Type
1	B	266	LYS
1	B	291	SER
1	B	313	VAL
1	B	327	SER
1	B	334	VAL
1	B	348	ASN
1	B	374	ARG
1	C	7	GLU
1	C	8	VAL
1	C	46	GLN
1	C	60	LEU
1	C	65	SER
1	C	68	ARG
1	C	77	ASP
1	C	79	GLU
1	C	101	ILE
1	C	105	LYS
1	C	126	HIS
1	C	168	LYS
1	C	172	LEU
1	C	173	GLN
1	C	181	MET
1	C	205	ASN
1	C	206	LEU
1	C	209	LYS
1	C	210	ARG
1	C	214	LYS
1	C	217	LYS
1	C	230	SER
1	C	237	LEU
1	C	242	LEU
1	C	263	LEU
1	C	272	LEU
1	C	291	SER
1	C	305	LEU
1	C	306	GLU
1	C	312	LYS
1	C	327	SER
1	C	334	VAL
1	C	351	GLU
1	C	374	ARG
1	D	6	THR

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Mol	Chain	Res	Type
1	D	8	VAL
1	D	12	LEU
1	D	46	GLN
1	D	60	LEU
1	D	64	GLN
1	D	65	SER
1	D	73	LYS
1	D	75	ASP
1	D	79	GLU
1	D	101	ILE
1	D	105	LYS
1	D	128	HIS
1	D	152	ARG
1	D	168	LYS
1	D	172	LEU
1	D	173	GLN
1	D	174	ASP
1	D	181	MET
1	D	205	ASN
1	D	206	LEU
1	D	209	LYS
1	D	210	ARG
1	D	214	LYS
1	D	217	LYS
1	D	230	SER
1	D	237	LEU
1	D	242	LEU
1	D	247	GLU
1	D	263	LEU
1	D	272	LEU
1	D	291	SER
1	D	305	LEU
1	D	306	GLU
1	D	310	GLN
1	D	312	LYS
1	D	313	VAL
1	D	327	SER
1	D	334	VAL
1	D	351	GLU
1	D	374	ARG
1	D	375	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	53	HIS
1	A	63	GLN
1	A	167	HIS
1	A	200	GLN
1	A	205	ASN
1	A	269	GLN
1	A	348	ASN
1	A	352	HIS
1	A	360	GLN
1	A	383	GLN
1	B	1	ASN
1	B	53	HIS
1	B	63	GLN
1	B	72	ASN
1	B	200	GLN
1	B	348	ASN
1	B	360	GLN
1	C	1	ASN
1	C	31	GLN
1	C	53	HIS
1	C	63	GLN
1	C	128	HIS
1	C	129	GLN
1	C	173	GLN
1	C	200	GLN
1	C	205	ASN
1	C	352	HIS
1	C	360	GLN
1	C	383	GLN
1	D	1	ASN
1	D	31	GLN
1	D	63	GLN
1	D	128	HIS
1	D	200	GLN
1	D	205	ASN
1	D	352	HIS
1	D	360	GLN
1	D	393	GLN
1	D	394	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	B12	B	0	1	94,101,101	0.91	2 (2%)	149,166,166	1.16	9 (6%)
3	B12	C	0	1	94,101,101	0.88	3 (3%)	149,166,166	1.18	11 (7%)
3	B12	D	0	1	94,101,101	0.97	2 (2%)	149,166,166	1.30	17 (11%)
3	B12	A	0	1	94,101,101	0.90	1 (1%)	149,166,166	1.14	11 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	B	0	1	-	1/56/223/223	0/3/11/11
3	B12	C	0	1	-	1/56/223/223	0/3/11/11
3	B12	D	0	1	-	3/56/223/223	0/3/11/11
3	B12	A	0	1	-	1/56/223/223	0/3/11/11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	0	B12	C14-N23	4.67	1.41	1.35
3	A	0	B12	C14-N23	4.41	1.41	1.35
3	B	0	B12	C14-N23	3.63	1.39	1.35
3	C	0	B12	C14-N23	2.89	1.39	1.35
3	C	0	B12	C11-N23	-2.55	1.32	1.36
3	D	0	B12	C4B-C9B	-2.21	1.36	1.40
3	B	0	B12	C11-N23	-2.13	1.32	1.36
3	C	0	B12	P-O5	-2.11	1.45	1.55

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	0	B12	C9-N22-C6	6.14	112.66	105.28
3	A	0	B12	C9-N22-C6	5.91	112.40	105.28
3	B	0	B12	C9-N22-C6	5.31	111.67	105.28
3	C	0	B12	C9-N22-C6	4.66	110.88	105.28
3	A	0	B12	O6R-C1R-N1B	4.39	116.52	108.09
3	B	0	B12	C2R-C1R-N1B	-3.82	103.82	113.30
3	D	0	B12	C20-C1-C2	3.76	119.48	113.28
3	D	0	B12	C2R-C1R-N1B	-3.75	103.98	113.30
3	B	0	B12	O6R-C1R-N1B	3.75	115.28	108.09
3	D	0	B12	O6R-C1R-N1B	3.73	115.26	108.09
3	C	0	B12	C2R-C1R-N1B	-3.72	104.05	113.30
3	C	0	B12	O6R-C1R-N1B	3.69	115.17	108.09
3	B	0	B12	C19-N24-C16	3.68	111.31	107.29
3	B	0	B12	C25-C2-C26	-3.60	102.59	109.74
3	D	0	B12	C19-N24-C16	3.43	111.04	107.29
3	C	0	B12	C19-N24-C16	3.41	111.01	107.29
3	A	0	B12	C2R-C1R-N1B	-3.40	104.85	113.30
3	C	0	B12	C20-C1-C2	3.38	118.86	113.28
3	A	0	B12	C19-N24-C16	3.38	110.98	107.29
3	C	0	B12	C25-C2-C26	-3.12	103.54	109.74
3	D	0	B12	C47-C12-C46	-2.96	104.50	109.41
3	A	0	B12	C25-C2-C26	-2.85	104.07	109.74
3	A	0	B12	C7-C8-C9	2.81	104.45	100.89
3	D	0	B12	C18-C60-C61	2.67	120.84	114.04
3	D	0	B12	C1-C19-N24	2.67	109.22	106.25
3	D	0	B12	C19-C1-N21	2.65	104.87	102.14
3	C	0	B12	C2P-C1P-N59	2.57	116.70	112.92
3	C	0	B12	C19-C1-N21	2.57	104.78	102.14
3	A	0	B12	C26-C2-C1	2.54	113.94	110.00
3	D	0	B12	C26-C2-C1	2.53	113.92	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	0	B12	C1-C19-N24	2.49	109.01	106.25
3	D	0	B12	C25-C2-C26	-2.48	104.82	109.74
3	C	0	B12	C47-C12-C46	-2.47	105.31	109.41
3	C	0	B12	C60-C18-C19	2.40	120.84	114.59
3	D	0	B12	O2-P-O3	-2.37	96.24	102.87
3	D	0	B12	C18-C17-C16	2.33	103.50	100.69
3	D	0	B12	C55-C17-C18	-2.30	106.72	111.12
3	A	0	B12	C2P-C1P-N59	2.28	116.28	112.92
3	A	0	B12	C5R-C4R-C3R	-2.24	107.78	114.84
3	B	0	B12	C60-C18-C19	2.24	120.40	114.59
3	B	0	B12	C4B-C9B-C8B	-2.21	118.13	120.16
3	B	0	B12	C20-C1-C2	2.11	116.75	113.28
3	D	0	B12	C2P-C1P-N59	2.10	116.01	112.92
3	B	0	B12	C36-C7-C8	2.07	115.86	112.05
3	D	0	B12	O28-C27-N29	-2.05	117.06	122.53
3	A	0	B12	C30-C3-C4	2.00	114.36	109.66
3	D	0	B12	C5M-C5B-C4B	-2.00	116.04	119.57
3	C	0	B12	C20-C1-N21	-2.00	106.95	110.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	0	B12	C13-C48-C49-C50
3	D	0	B12	C3R-C4R-C5R-O8R
3	D	0	B12	O6R-C4R-C5R-O8R
3	B	0	B12	C13-C48-C49-C50
3	D	0	B12	C13-C48-C49-C50
3	C	0	B12	C13-C48-C49-C50

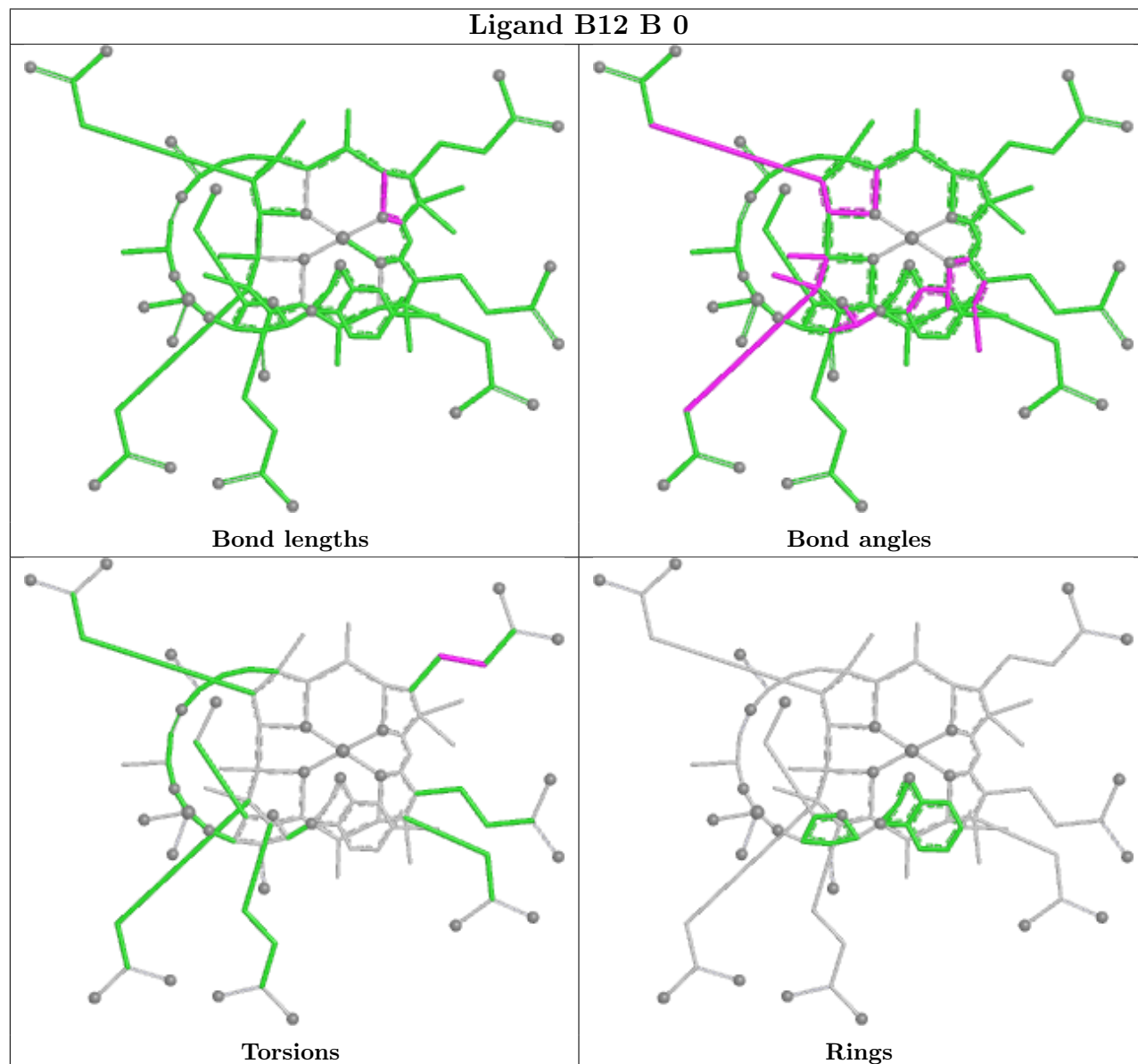
There are no ring outliers.

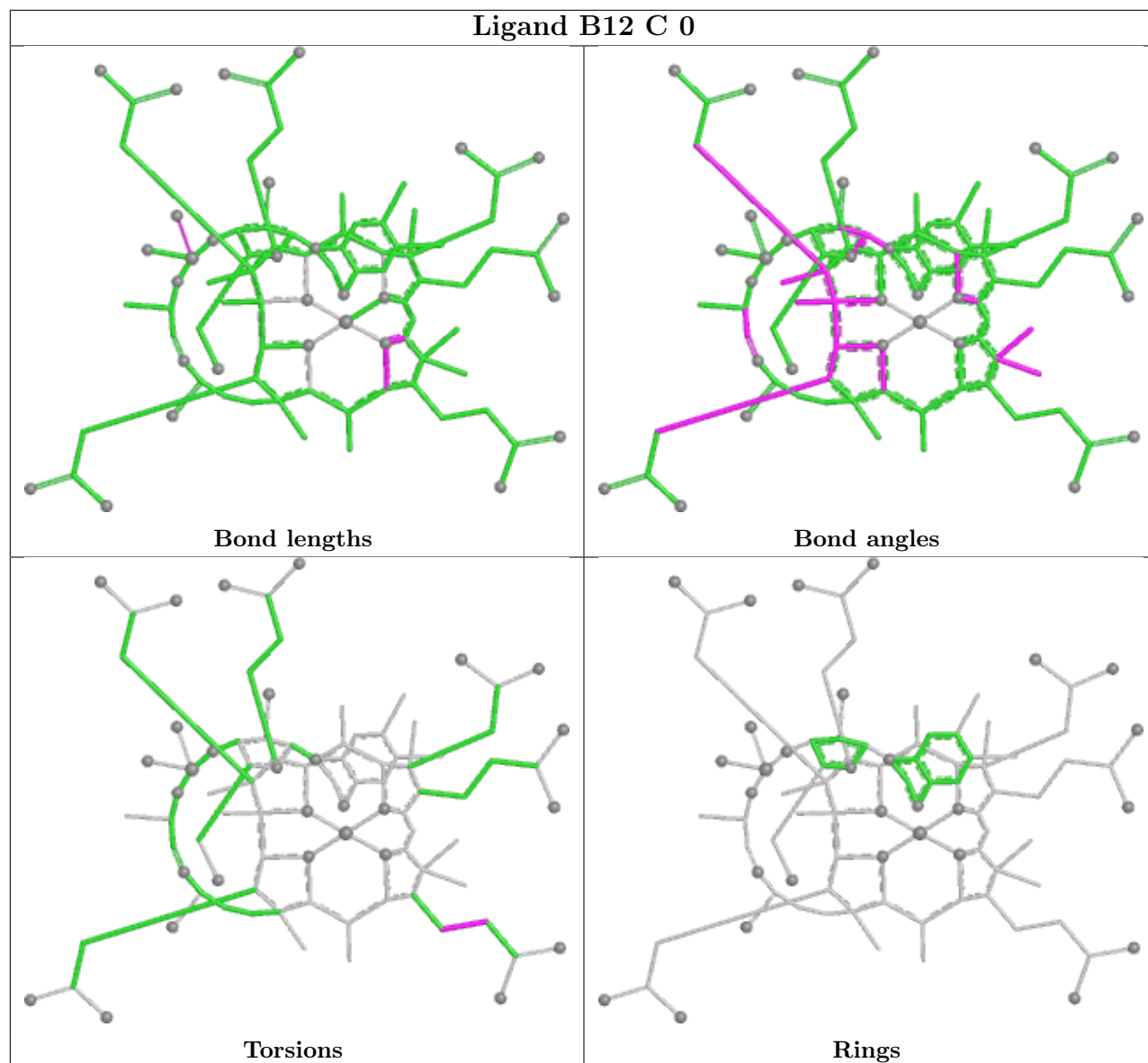
4 monomers are involved in 41 short contacts:

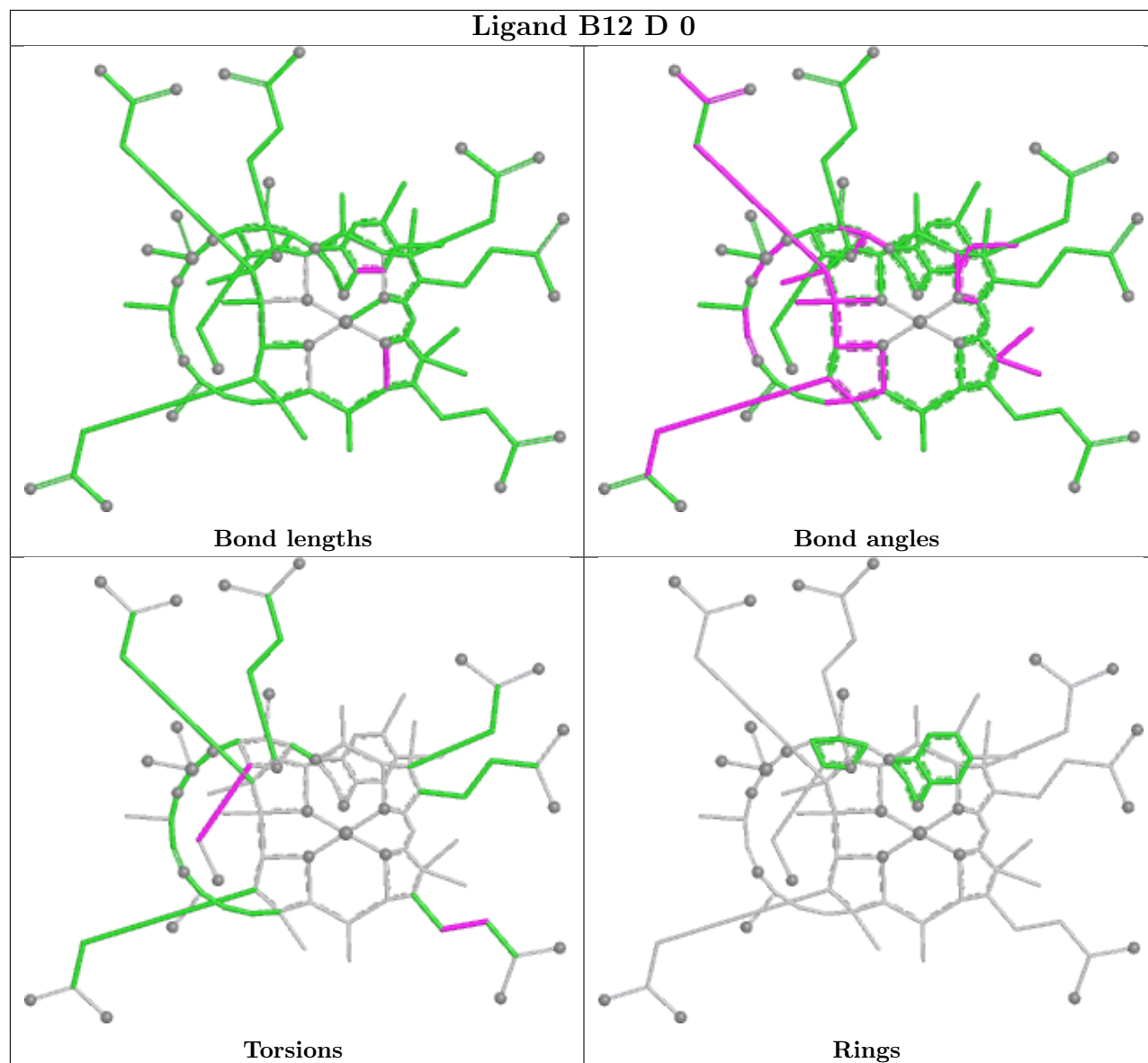
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	0	B12	10	0
3	C	0	B12	11	0
3	D	0	B12	8	0
3	A	0	B12	12	0

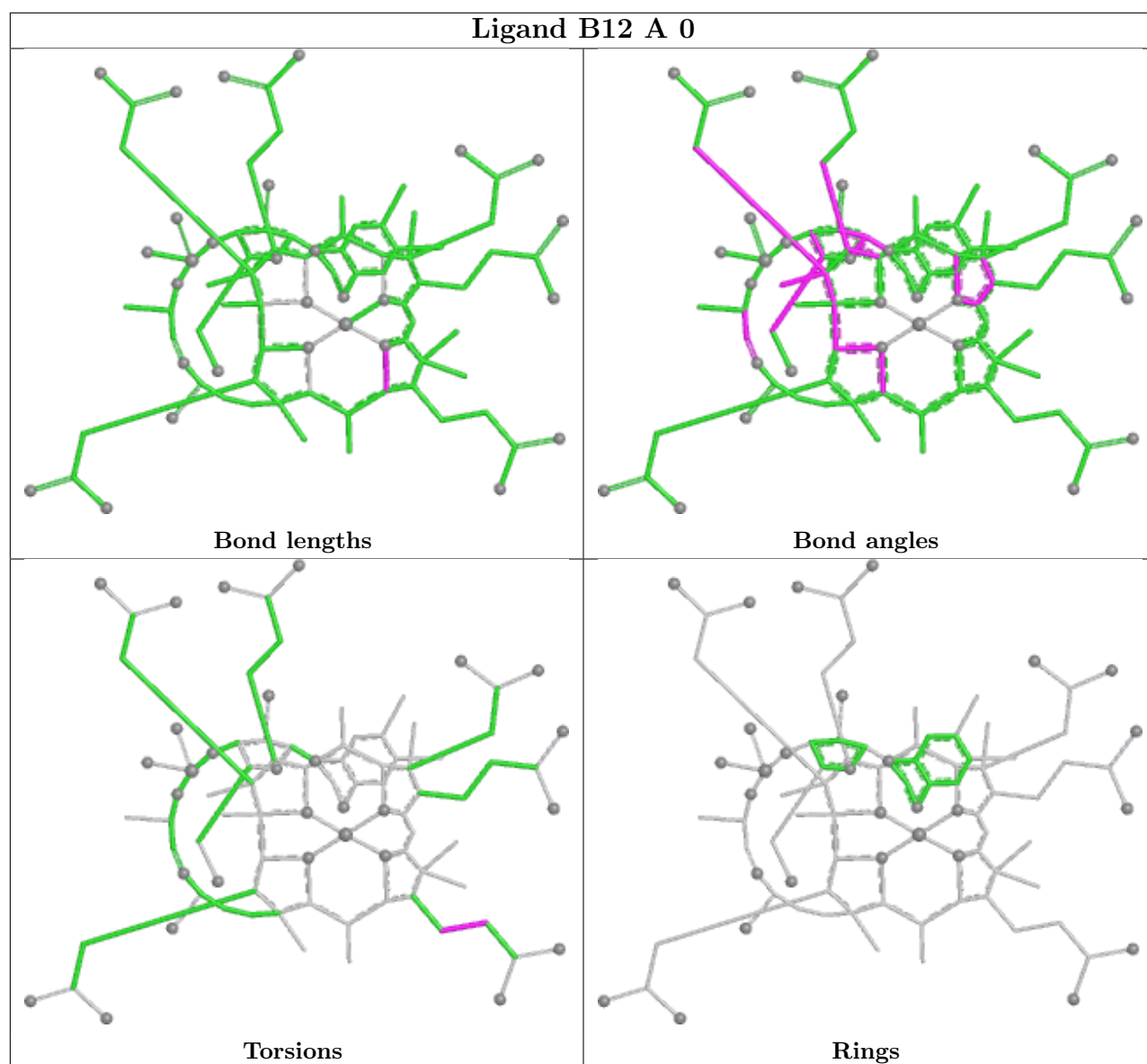
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	414/414 (100%)	0.82	75 (18%) 3 3	8, 30, 77, 151	0
1	B	414/414 (100%)	0.86	70 (16%) 4 4	8, 31, 77, 157	0
1	C	414/414 (100%)	1.01	73 (17%) 4 3	9, 33, 86, 221	0
1	D	414/414 (100%)	0.86	66 (15%) 5 4	11, 31, 79, 151	0
All	All	1656/1656 (100%)	0.89	284 (17%) 4 4	8, 31, 79, 221	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	303	PRO	10.1
1	C	304	ALA	9.4
1	A	305	LEU	8.8
1	C	305	LEU	7.8
1	D	313	VAL	7.3
1	C	71	SER	7.3
1	D	305	LEU	7.0
1	C	309	PRO	6.9
1	B	305	LEU	6.9
1	D	311	ALA	6.7
1	D	70	ALA	6.6
1	C	80	ALA	6.6
1	C	313	VAL	6.5
1	C	307	THR	6.5
1	D	73	LYS	6.5
1	B	303	PRO	6.3
1	D	307	THR	6.1
1	A	311	ALA	6.0
1	C	168	LYS	5.8
1	D	169	PRO	5.7
1	A	169	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	126	HIS	5.6
1	D	80	ALA	5.5
1	D	7	GLU	5.5
1	A	414	TRP	5.2
1	A	327	SER	5.2
1	C	78	SER	5.2
1	B	304	ALA	5.2
1	D	126	HIS	5.2
1	D	72	ASN	5.2
1	C	311	ALA	5.1
1	A	303	PRO	5.1
1	A	241	SER	5.1
1	A	128	HIS	5.1
1	D	309	PRO	5.0
1	B	311	ALA	5.0
1	C	300	LEU	4.9
1	A	70	ALA	4.9
1	A	309	PRO	4.8
1	B	313	VAL	4.8
1	C	308	PRO	4.8
1	B	414	TRP	4.7
1	A	313	VAL	4.7
1	D	308	PRO	4.7
1	A	78	SER	4.5
1	D	8	VAL	4.5
1	C	314	PRO	4.5
1	D	414	TRP	4.5
1	B	328	PRO	4.5
1	A	80	ALA	4.4
1	B	327	SER	4.4
1	D	314	PRO	4.4
1	B	70	ALA	4.4
1	C	328	PRO	4.4
1	D	129	GLN	4.4
1	C	70	ALA	4.3
1	D	75	ASP	4.2
1	A	174	ASP	4.1
1	B	71	SER	4.1
1	C	169	PRO	4.1
1	D	171	LEU	4.1
1	D	327	SER	4.1
1	D	304	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	128	HIS	4.1
1	B	353	GLY	4.0
1	C	7	GLU	4.0
1	A	1	ASN	4.0
1	D	128	HIS	4.0
1	B	307	THR	4.0
1	A	168	LYS	3.9
1	D	69	PRO	3.9
1	C	72	ASN	3.9
1	D	124	ILE	3.8
1	C	124	ILE	3.8
1	D	266	LYS	3.8
1	C	310	GLN	3.8
1	C	312	LYS	3.8
1	B	300	LEU	3.8
1	B	312	LYS	3.7
1	B	174	ASP	3.7
1	C	171	LEU	3.7
1	D	168	LYS	3.7
1	B	308	PRO	3.7
1	A	71	SER	3.7
1	D	131	HIS	3.7
1	A	244	PRO	3.6
1	D	130	GLY	3.6
1	C	327	SER	3.6
1	D	71	SER	3.6
1	C	246	VAL	3.6
1	C	73	LYS	3.6
1	B	169	PRO	3.6
1	A	307	THR	3.6
1	C	68	ARG	3.5
1	C	353	GLY	3.5
1	B	246	VAL	3.5
1	A	73	LYS	3.5
1	A	242	LEU	3.5
1	B	171	LEU	3.5
1	B	242	LEU	3.5
1	C	67	LEU	3.5
1	D	125	GLY	3.5
1	A	246	VAL	3.5
1	D	310	GLN	3.5
1	A	171	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	309	PRO	3.4
1	C	301	LEU	3.4
1	C	8	VAL	3.4
1	D	246	VAL	3.4
1	B	130	GLY	3.4
1	A	167	HIS	3.4
1	A	328	PRO	3.4
1	B	352	HIS	3.4
1	C	167	HIS	3.4
1	C	128	HIS	3.3
1	A	413	GLY	3.3
1	B	8	VAL	3.3
1	C	377	GLY	3.3
1	D	76	ASN	3.3
1	B	78	SER	3.2
1	B	173	GLN	3.2
1	B	126	HIS	3.2
1	B	245	SER	3.2
1	A	353	GLY	3.2
1	A	245	SER	3.2
1	A	304	ALA	3.1
1	B	244	PRO	3.1
1	D	123	ALA	3.1
1	C	115	ARG	3.1
1	A	126	HIS	3.1
1	C	69	PRO	3.1
1	C	77	ASP	3.1
1	D	378	GLU	3.1
1	D	377	GLY	3.0
1	C	127	ASN	3.0
1	B	77	ASP	3.0
1	B	131	HIS	3.0
1	B	168	LYS	3.0
1	A	127	ASN	3.0
1	C	352	HIS	3.0
1	B	301	LEU	3.0
1	C	125	GLY	3.0
1	D	328	PRO	3.0
1	A	74	ASP	3.0
1	C	123	ALA	3.0
1	A	125	GLY	2.9
1	A	124	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	170	HIS	2.9
1	C	76	ASN	2.9
1	D	77	ASP	2.9
1	C	247	GLU	2.9
1	C	75	ASP	2.9
1	C	170	HIS	2.9
1	A	173	GLN	2.8
1	A	131	HIS	2.8
1	A	170	HIS	2.8
1	A	377	GLY	2.8
1	B	80	ALA	2.8
1	A	352	HIS	2.8
1	B	73	LYS	2.8
1	B	72	ASN	2.7
1	C	74	ASP	2.7
1	D	302	GLU	2.7
1	C	48	GLY	2.7
1	C	49	ALA	2.7
1	D	242	LEU	2.7
1	B	167	HIS	2.7
1	D	312	LYS	2.7
1	A	11	THR	2.7
1	D	303	PRO	2.7
1	B	76	ASN	2.7
1	D	388	PRO	2.7
1	D	127	ASN	2.7
1	B	241	SER	2.7
1	A	326	ILE	2.7
1	B	377	GLY	2.7
1	A	69	PRO	2.6
1	A	266	LYS	2.6
1	B	379	ARG	2.6
1	A	310	GLN	2.6
1	C	129	GLN	2.6
1	D	202	ASN	2.6
1	C	82	PRO	2.6
1	D	300	LEU	2.6
1	A	129	GLN	2.6
1	B	310	GLN	2.6
1	C	414	TRP	2.6
1	B	221	PRO	2.6
1	D	316	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	79	GLU	2.6
1	A	130	GLY	2.5
1	B	351	GLU	2.5
1	B	125	GLY	2.5
1	B	75	ASP	2.5
1	C	306	GLU	2.5
1	A	388	PRO	2.5
1	C	122	ARG	2.5
1	C	302	GLU	2.4
1	B	6	THR	2.4
1	C	245	SER	2.4
1	B	48	GLY	2.4
1	C	376	ALA	2.4
1	A	265	HIS	2.4
1	B	172	LEU	2.4
1	B	248	LEU	2.4
1	B	306	GLU	2.4
1	D	74	ASP	2.4
1	C	6	THR	2.4
1	B	299	ALA	2.4
1	D	206	LEU	2.4
1	B	129	GLN	2.4
1	A	75	ASP	2.4
1	A	76	ASN	2.3
1	D	67	LEU	2.3
1	D	195	ASN	2.3
1	B	326	ILE	2.3
1	A	8	VAL	2.3
1	A	79	GLU	2.3
1	D	167	HIS	2.3
1	A	306	GLU	2.3
1	A	122	ARG	2.3
1	B	413	GLY	2.3
1	C	130	GLY	2.3
1	C	163	TYR	2.3
1	A	312	LYS	2.3
1	B	334	VAL	2.3
1	C	165	VAL	2.3
1	C	297	PRO	2.3
1	A	247	GLU	2.2
1	B	335	SER	2.2
1	A	202	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	376	ALA	2.2
1	D	413	GLY	2.2
1	A	12	LEU	2.2
1	A	351	GLU	2.2
1	C	79	GLU	2.2
1	D	170	HIS	2.2
1	D	265	HIS	2.2
1	B	199	LYS	2.2
1	B	315	LYS	2.2
1	D	315	LYS	2.2
1	A	379	ARG	2.2
1	C	351	GLU	2.2
1	C	296	ALA	2.2
1	A	72	ASN	2.2
1	B	124	ILE	2.1
1	C	326	ILE	2.1
1	D	306	GLU	2.1
1	A	412	VAL	2.1
1	A	376	ALA	2.1
1	A	243	ARG	2.1
1	C	210	ARG	2.1
1	C	242	LEU	2.1
1	A	302	GLU	2.1
1	C	11	THR	2.1
1	D	267	THR	2.1
1	A	334	VAL	2.1
1	A	378	GLU	2.1
1	B	79	GLU	2.1
1	A	360	GLN	2.1
1	C	200	GLN	2.1
1	B	68	ARG	2.1
1	D	68	ARG	2.1
1	C	349	ALA	2.1
1	D	164	ALA	2.1
1	B	127	ASN	2.1
1	B	202	ASN	2.1
1	D	155	ASP	2.1
1	C	221	PRO	2.1
1	B	2	ILE	2.1
1	D	326	ILE	2.1
1	C	164	ALA	2.1
1	D	10	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	195	ASN	2.0
1	A	348	ASN	2.0
1	A	68	ARG	2.0
1	A	6	THR	2.0
1	B	217	LYS	2.0
1	D	78	SER	2.0
1	B	67	LEU	2.0
1	B	263	LEU	2.0
1	A	387	ASP	2.0
1	A	199	LYS	2.0
1	A	308	PRO	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](#)

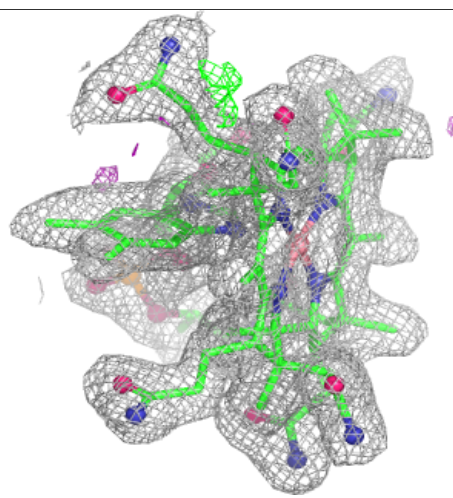
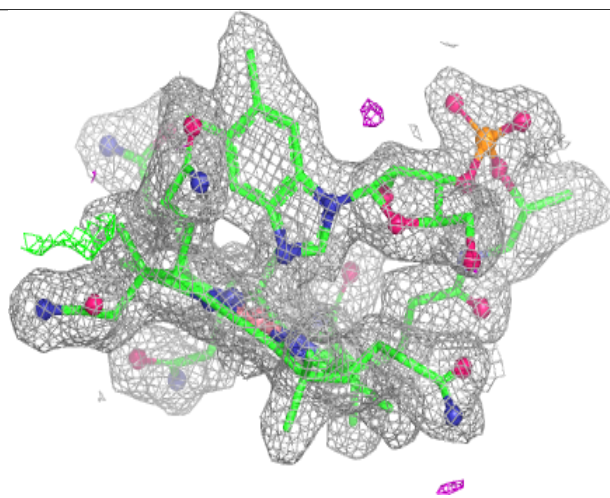
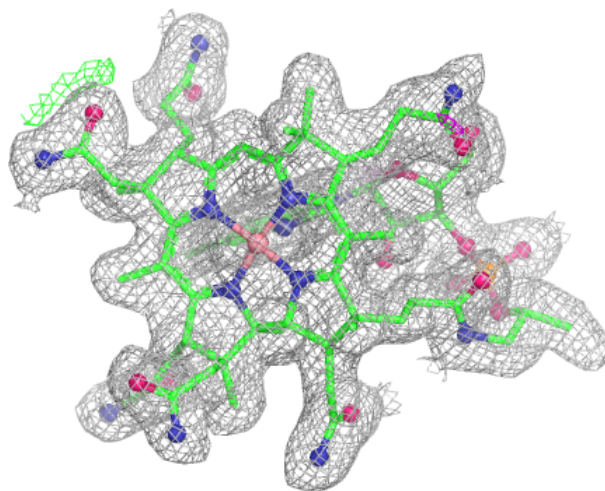
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	B12	A	0	91/91	0.97	0.06	7,13,21,38	0
3	B12	B	0	91/91	0.97	0.06	7,14,27,44	0
3	B12	C	0	91/91	0.97	0.07	7,15,31,44	0
3	B12	D	0	91/91	0.97	0.07	9,15,28,42	0
2	CL	D	903	1/1	0.98	0.03	24,24,24,24	0
2	CL	C	904	1/1	0.99	0.03	23,23,23,23	0
2	CL	B	902	1/1	0.99	0.03	24,24,24,24	0
2	CL	A	901	1/1	1.00	0.05	23,23,23,23	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.

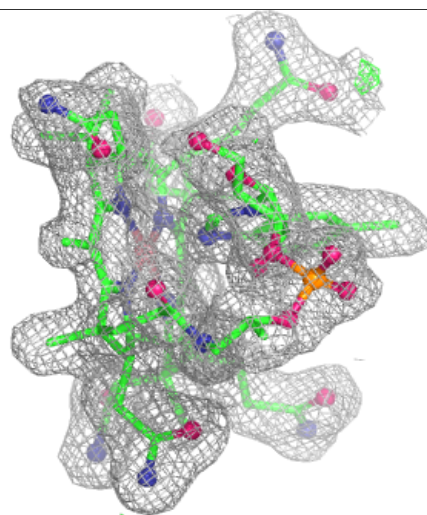
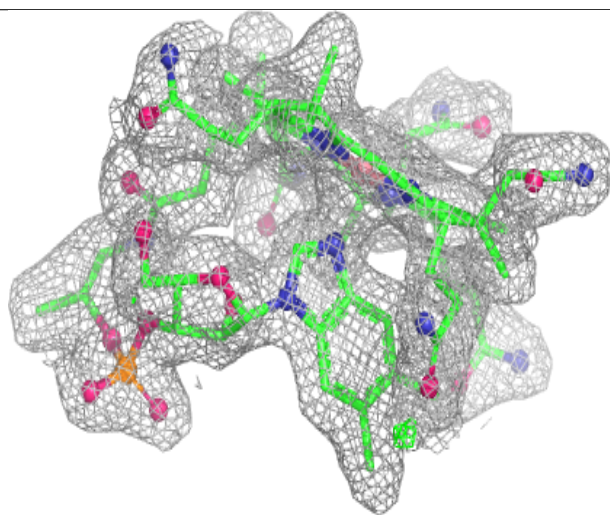
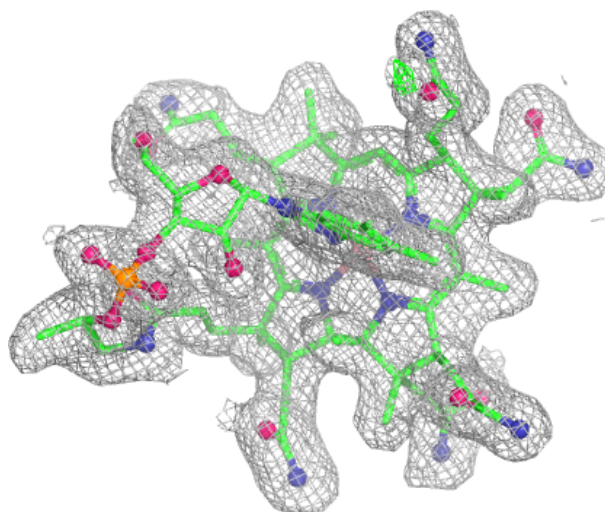
Electron density around B12 A 0:

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



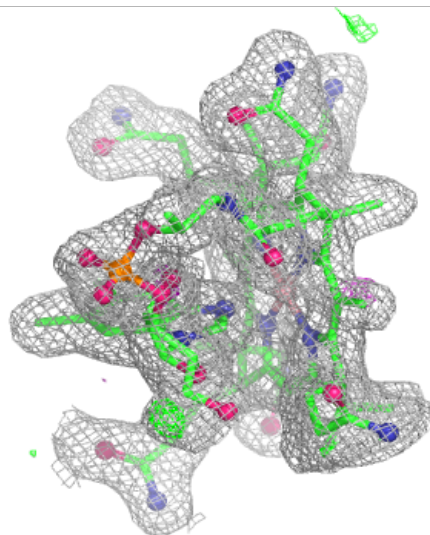
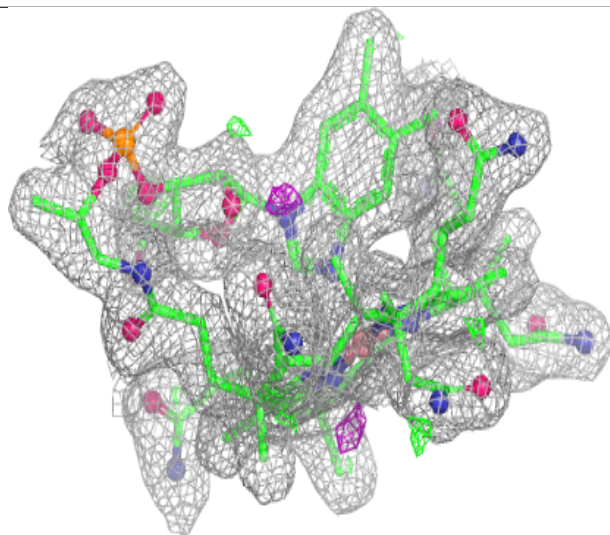
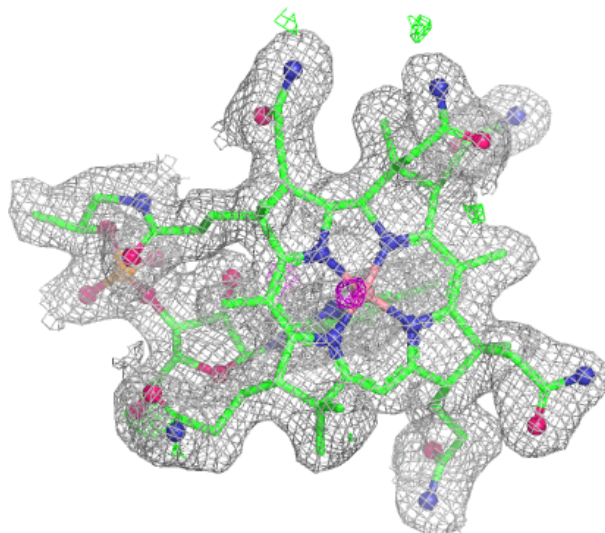
Electron density around B12 B 0:

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



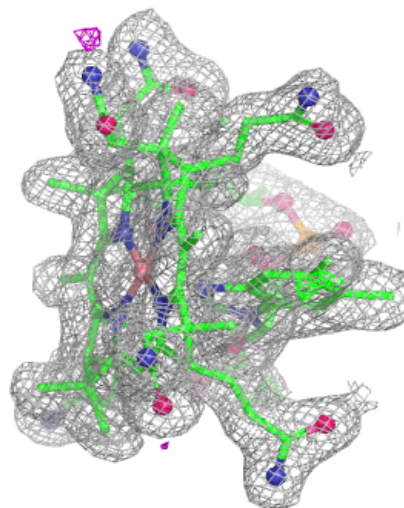
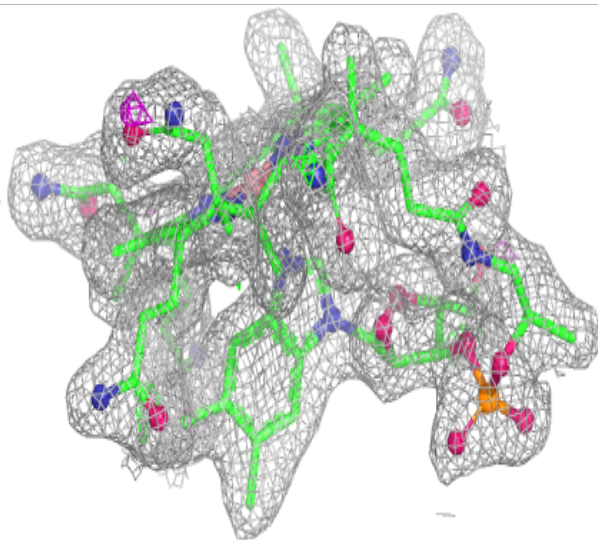
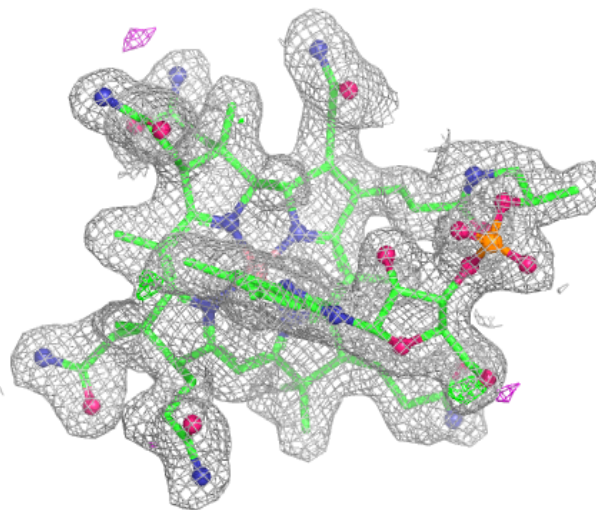
Electron density around B12 C 0:

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



Electron density around B12 D 0:

$2mF_o-DF_c$ (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.