



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:56 PM EDT

PDB ID : 9MRS / pdb_00009mrs
Title : Crystal structure of human MMACHC in complex with MMADHC and B12
Authors : Mascarenhas, R.; Banerjee, R.
Deposited on : 2025-01-08
Resolution : 3.40 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

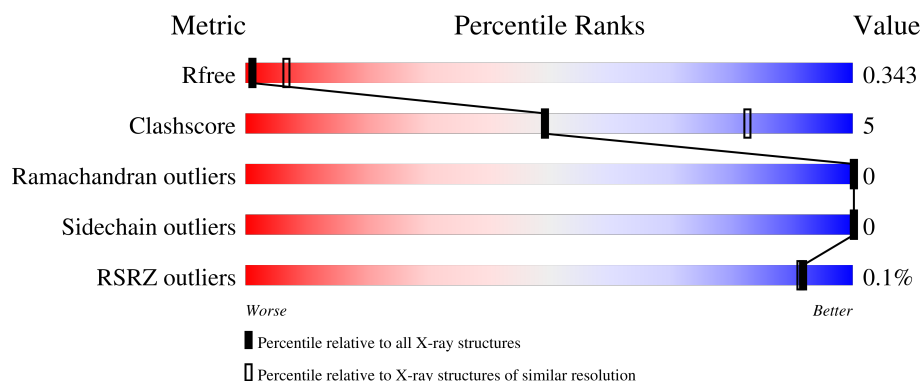
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

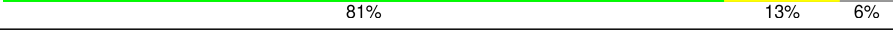
The reported resolution of this entry is 3.40 Å.

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.



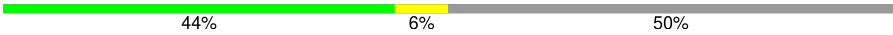
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	223	 79% 15% 6%
1	B	223	 77% 18% 5%
1	E	223	 80% 14% 6%
1	G	223	 81% 13% 6%
2	C	296	 44% 51%

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Mol	Chain	Length	Quality of chain
2	D	296	 44% 6% 50%
2	F	296	 44% 5% 51%
2	H	296	 44% 5% 51%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11661 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 Cyanocobalamin reductase / alkylcobalamin dealkylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	1	0
			1653	1071	280	297	5			
1	B	211	Total	C	N	O	S	0	1	0
			1699	1109	287	298	5			
1	E	210	Total	C	N	O	S	0	1	0
			1669	1088	281	295	5			
1	G	210	Total	C	N	O	S	0	1	0
			1694	1099	293	296	6			

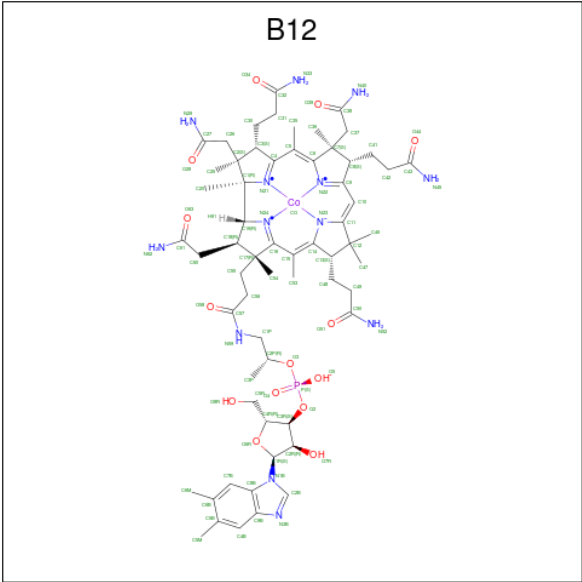
- Molecule 2 is a protein called Cobalamin trafficking protein CblD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	148	Total	C	N	O	S	0	0	0
			1158	742	189	220	7			
2	F	144	Total	C	N	O	S	0	0	0
			1141	731	185	219	6			
2	C	144	Total	C	N	O	S	0	0	0
			1139	729	185	219	6			
2	H	144	Total	C	N	O	S	0	0	0
			1144	733	185	219	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	262	SER	CYS	conflict	UNP Q9H3L0
F	262	SER	CYS	conflict	UNP Q9H3L0
C	262	SER	CYS	conflict	UNP Q9H3L0
H	262	SER	CYS	conflict	UNP Q9H3L0

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).

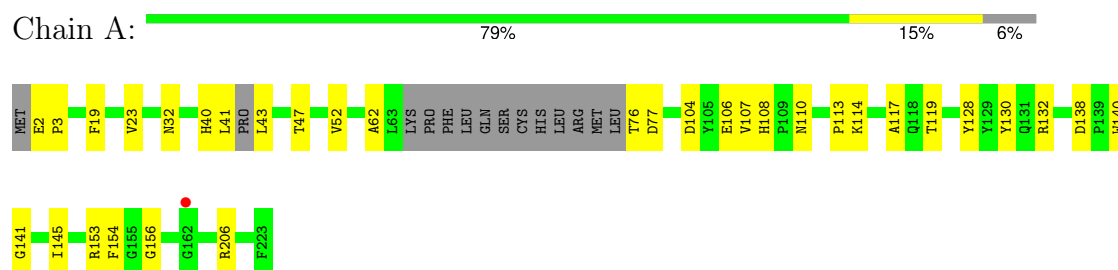


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	G	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

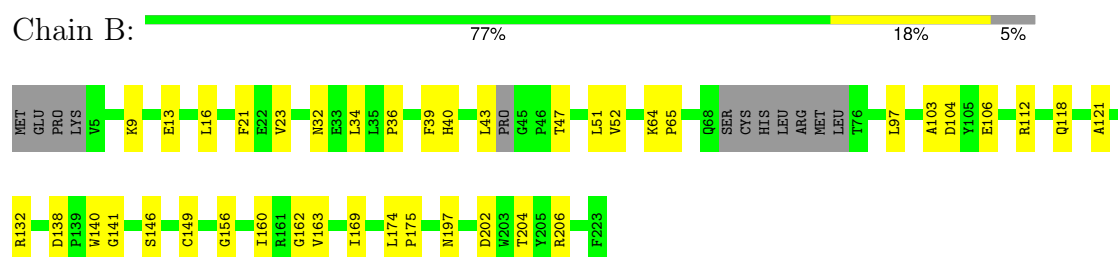
3 Residue-property plots

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.

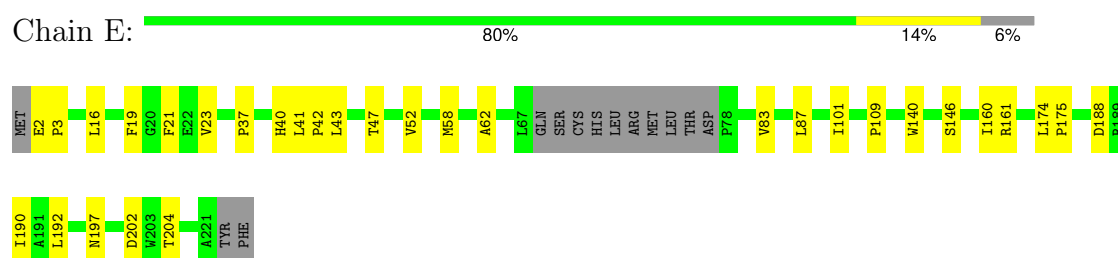
- Molecule 1: Cyanocobalamin reductase / alkylcobalamin dealkylase



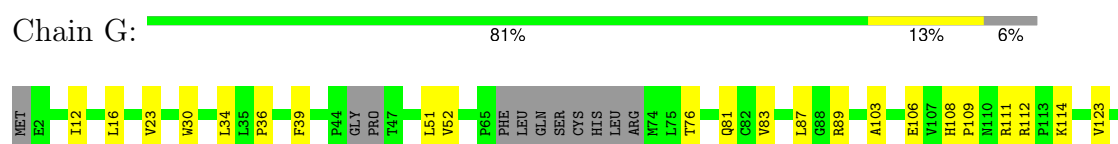
- Molecule 1: Cyanocobalamin reductase / alkylcobalamin dealkylase



- Molecule 1: Cyanocobalamin reductase / alkylcobalamin dealkylase



- Molecule 1: Cyanocobalamin reductase / alkylcobalamin dealkylase



MET	THR
ALA	MET
ASN	GLY
VAL	PRO
LEU	PHE
CYS	GLY
ASN	PRO
ARG	GLN
ALA	ASP
ARG	GLN
LEU	ARG
VAL	PHE
SER	GLN
TYR	LEU
LEU	PRO
GLY	GLY
PHE	ILE
CYS	ASN
SER	GLY
LEU	PHE
VAL	ASP
LYS	CYS
ARG	HIS
VAL	LEU
VAL	ALA
VAL	ASN
ASN	GLY
PRO	THR
LYS	ALA
ALA	SER
PHE	GLN
SER	LYS
THR	LYS
ALA	SER
GLY	LEU
SER	VAL
GLY	HIS
SER	LYS
GLY	THR
SER	LEU
ASP	PRO
GLU	ASP
VAL	VAL
SER	LEU
HIS	ALA
VAL	ALA
ALA	PRO
ALA	LEU
PRO	SER
PRO	SER
ASP	GLU
ASP	ILE
ARG	CYS
THR	HIS
VAL	GLU
VAL	PHE
TRP	THR
PRO	VAL
ASP	MET
GLU	ALA
	GLN
	TYR
	VAL
ASN	
GLU	
PHE	
GLN	
GLY	
ASN	
ASP	
ALA	
PRO	
VAL	
GLU	
GLN	
GLU	
ILE	
ASN	
SER	
ALA	
GLU	
THR	
TYR	
PHE	
GLU	
SER	
ALA	
ARG	
V146	
I150	
P166	
E167	
VAL	
ALA	
ASN	
GLY	
K172	
L176	
M186	
T187	
R197	
R216	
I225	
S228	
F234	
G235	
P236	
L242	
R250	
V256	
V264	
L293	
SER	
GLY	
ASN	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.76Å 67.98Å 192.66Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	41.24 – 3.40 41.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	53.2 (41.24-3.40) 53.6 (41.24-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.300 , 0.357 0.306 , 0.343	Depositor DCC
R_{free} test set	673 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 122.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11661	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.09	0/1709	0.24	0/2340
1	B	0.08	0/1759	0.24	0/2407
1	E	0.09	0/1729	0.25	0/2370
1	G	0.09	0/1750	0.26	0/2390
2	C	0.07	0/1163	0.20	0/1574
2	D	0.07	0/1182	0.21	0/1600
2	F	0.07	0/1165	0.21	0/1577
2	H	0.07	0/1168	0.21	0/1580
All	All	0.08	0/11625	0.23	0/15838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1653	0	1569	20	0
1	B	1699	0	1635	25	0
1	E	1669	0	1604	21	0
1	G	1694	0	1644	19	0
2	C	1139	0	1102	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1158	0	1124	9	0
2	F	1141	0	1109	8	0
2	H	1144	0	1116	11	0
3	A	91	0	88	7	0
3	B	91	0	88	8	0
3	E	91	0	88	4	0
3	G	91	0	88	2	0
All	All	11661	0	11255	124	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 5.

All (124) 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:B:149:CYS:H	3:B:301:B12:H332	1.40	0.67
2:F:255:SER:HB2	2:F:266:ARG:HB2	1.78	0.65
2:D:290:MET:HA	2:D:293:LEU:HD23	1.79	0.64
1:E:160:ILE:O	3:E:301:B12:N29	2.32	0.62
1:B:118:GLN:HE21	3:B:301:B12:H331	1.48	0.61
1:G:23:VAL:HG12	1:G:52:VAL:HG22	1.83	0.59
2:F:166:PRO:HG3	2:F:236:PRO:HD2	1.86	0.57
1:B:9:LYS:NZ	1:B:13:GLU:OE2	2.34	0.57
3:E:301:B12:H601	3:E:301:B12:H262	1.87	0.57
1:B:23:VAL:HG12	1:B:52:VAL:HG22	1.85	0.57
1:E:19:PHE:HB3	1:E:62:ALA:HB2	1.88	0.56
1:A:110:ASN:HA	2:D:197:ARG:HD2	1.87	0.55
1:B:32:ASN:O	1:B:40:HIS:NE2	2.39	0.55
1:G:109:PRO:HB3	2:H:228:SER:HA	1.87	0.55
1:G:192:LEU:HD13	1:G:208:ALA:HB2	1.87	0.55
1:A:32:ASN:O	1:A:40:HIS:NE2	2.39	0.55
1:E:202:ASP:OD2	1:E:204:THR:OG1	2.21	0.54
2:D:186:MET:HG2	2:D:273:HIS:HA	1.88	0.54
2:F:187:THR:HG22	2:F:264:VAL:HG21	1.90	0.54
1:B:43:LEU:HD22	1:B:47:THR:HG21	1.89	0.53
2:C:166:PRO:HG3	2:C:236:PRO:HD2	1.91	0.53
1:B:36:PRO:HG2	1:B:39:PHE:HD2	1.74	0.52
1:B:104:ASP:OD2	3:B:301:B12:N29	2.40	0.52
3:B:301:B12:H552	3:B:301:B12:H531	1.91	0.52
1:B:132:ARG:NH2	1:B:141:GLY:O	2.42	0.52
1:E:37:PRO:HA	1:E:40:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:225:ILE:HG13	2:F:242:LEU:HD23	1.92	0.52
1:E:174:LEU:HD12	1:E:175:PRO:HD2	1.90	0.52
1:E:42:PRO:HB3	2:H:216:ARG:HH22	1.75	0.51
3:A:401:B12:H531	3:A:401:B12:H552	1.91	0.51
1:B:174:LEU:HD12	1:B:175:PRO:HD2	1.91	0.51
2:H:166:PRO:HG3	2:H:236:PRO:HD2	1.93	0.51
1:E:58:MET:HG2	1:E:62:ALA:HB3	1.93	0.50
2:D:258:ASP:HA	2:D:263:LYS:HG2	1.93	0.50
1:A:41:LEU:O	1:A:43:LEU:N	2.45	0.50
1:B:146:SER:N	1:B:197:ASN:OD1	2.40	0.50
2:D:165:PHE:HB3	2:D:221:TRP:HH2	1.77	0.50
1:G:76:THR:OG1	1:G:81:GLN:OE1	2.27	0.50
1:E:87:LEU:HB3	1:E:101:ILE:HD13	1.93	0.50
1:E:109:PRO:HB3	2:F:228:SER:HA	1.94	0.50
2:C:225:ILE:HG13	2:C:242:LEU:HD23	1.94	0.49
1:A:19:PHE:HB3	1:A:62:ALA:HB2	1.94	0.49
1:G:16:LEU:HD23	1:G:52:VAL:HG11	1.93	0.49
1:G:83:VAL:HG11	1:G:161:ARG:HB3	1.95	0.49
2:H:187:THR:HG22	2:H:264:VAL:HG11	1.96	0.48
3:E:301:B12:H552	3:E:301:B12:H531	1.96	0.48
3:A:401:B12:H601	3:A:401:B12:H262	1.96	0.48
2:D:187:THR:HG22	2:D:264:VAL:HG21	1.96	0.48
1:E:21:PHE:HE1	1:E:161:ARG:HG3	1.79	0.48
1:A:23:VAL:HG12	1:A:52:VAL:HG22	1.95	0.47
1:E:43:LEU:HD13	1:E:47:THR:HG21	1.96	0.47
1:B:103:ALA:HB3	1:B:106:GLU:HG3	1.96	0.47
2:D:150:ILE:HG12	2:D:176:LEU:HG	1.96	0.47
2:H:250:ARG:HB3	2:H:256:VAL:HG23	1.97	0.47
1:E:23:VAL:HG12	1:E:52:VAL:HG22	1.96	0.47
1:G:51:LEU:HD23	1:G:163:VAL:HG22	1.94	0.47
1:G:108:HIS:HB2	1:G:112:ARG:HB2	1.95	0.47
1:A:138:ASP:HB2	1:A:140:TRP:CE3	2.48	0.47
1:G:34:LEU:HD13	3:G:301:B12:HM53	1.97	0.47
1:B:103:ALA:HA	1:B:162:GLY:HA3	1.97	0.47
1:A:2:GLU:HB3	1:A:3:PRO:HD3	1.97	0.47
2:H:187:THR:HG22	2:H:264:VAL:HG21	1.96	0.46
1:B:112:ARG:HG3	2:C:194:GLU:CD	2.41	0.46
1:E:41:LEU:O	1:E:43:LEU:N	2.46	0.46
2:C:187:THR:HG22	2:C:264:VAL:HG21	1.96	0.46
1:G:174:LEU:HD12	1:G:175:PRO:HD2	1.98	0.46
1:E:188:ASP:O	1:E:192:LEU:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HD2	1:A:145:ILE:HB	1.99	0.45
2:C:161:PHE:HD1	2:C:164:LEU:HD12	1.82	0.45
2:C:223:ASP:OD2	2:C:235:GLY:N	2.49	0.44
1:A:43:LEU:HD13	1:A:47:THR:HG21	1.99	0.44
1:B:156:GLY:HA3	1:B:206:ARG:HA	1.99	0.44
1:G:103:ALA:HB3	1:G:106:GLU:HG3	1.98	0.44
1:G:12:ILE:HG22	1:G:23:VAL:HG11	1.99	0.44
1:G:36:PRO:HG2	1:G:39:PHE:HD2	1.81	0.44
1:A:156:GLY:HA3	1:A:206:ARG:HA	1.99	0.44
1:B:138:ASP:HB2	1:B:140:TRP:CE3	2.52	0.44
1:B:51:LEU:HG	1:B:121:ALA:HA	2.00	0.44
1:E:2:GLU:HB2	1:E:3:PRO:HD3	2.00	0.43
1:A:104:ASP:OD2	3:A:401:B12:N29	2.50	0.43
2:F:150:ILE:HG12	2:F:176:LEU:HG	1.99	0.43
2:F:161:PHE:HD1	2:F:164:LEU:HD12	1.83	0.43
3:A:401:B12:H473	3:A:401:B12:H482	1.92	0.43
1:E:87:LEU:HD13	1:E:101:ILE:HG21	2.00	0.43
1:A:107:VAL:HG12	1:A:113:PRO:HA	2.00	0.43
1:A:108:HIS:CE1	1:A:114:LYS:HG2	2.54	0.43
2:H:186:MET:HE3	2:H:197:ARG:CZ	2.49	0.43
1:B:34:LEU:HD13	3:B:301:B12:HM62	2.01	0.42
1:E:146:SER:N	1:E:197:ASN:OD1	2.51	0.42
3:B:301:B12:H601	3:B:301:B12:H262	2.01	0.42
1:A:76:THR:OG1	1:A:77:ASP:N	2.52	0.42
3:B:301:B12:H451	3:B:301:B12:H411	1.70	0.42
1:E:16:LEU:HB3	1:E:21:PHE:HB2	2.01	0.42
1:A:106:GLU:HB3	1:A:114:LYS:HD2	2.02	0.42
2:F:223:ASP:OD2	2:F:235:GLY:N	2.50	0.42
2:H:150:ILE:HG12	2:H:176:LEU:HG	2.01	0.42
2:H:225:ILE:HG13	2:H:242:LEU:HD23	2.02	0.42
1:B:16:LEU:HB3	1:B:21:PHE:HB2	2.01	0.42
1:B:64:LYS:HB3	1:B:65:PRO:HD3	2.02	0.41
1:B:202:ASP:OD2	1:B:204:THR:OG1	2.25	0.41
1:E:83:VAL:HG21	1:E:161:ARG:HD2	2.02	0.41
1:A:132:ARG:NH2	1:A:141:GLY:O	2.35	0.41
1:B:65:PRO:HG3	1:G:89:ARG:NH2	2.35	0.41
1:B:97:LEU:HD22	1:B:169:ILE:HD11	2.01	0.41
1:G:30:TRP:HB3	1:G:123:VAL:HG11	2.03	0.41
1:A:128:TYR:HB3	1:A:130:TYR:CE2	2.55	0.41
1:A:153:ARG:HD2	1:A:154:PHE:CE2	2.56	0.41
1:B:160:ILE:O	3:B:301:B12:N29	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:LEU:HD21	1:G:87:LEU:HD23	2.01	0.41
2:D:266:ARG:HG2	2:D:272:THR:HG22	2.03	0.41
2:C:265:ILE:HD13	2:C:276:VAL:HG21	2.03	0.41
1:A:117:ALA:H	3:A:401:B12:H622	1.68	0.41
2:D:174:MET:HB2	2:D:281:THR:HG23	2.03	0.41
3:A:401:B12:H621	3:A:401:B12:H18	1.48	0.41
1:G:106:GLU:HB3	1:G:114:LYS:HD2	2.01	0.41
2:C:187:THR:HG22	2:C:264:VAL:HG11	2.02	0.41
1:A:119:THR:HG23	3:A:401:B12:HM63	2.03	0.41
3:E:301:B12:H253	3:E:301:B12:H301	1.91	0.40
1:G:132:ARG:HB2	1:G:145:ILE:HB	2.03	0.40
1:B:51:LEU:HD23	1:B:163:VAL:HG22	2.04	0.40
1:E:42:PRO:HB3	2:H:234:PHE:HB3	2.03	0.40
1:E:140:TRP:CZ2	1:E:190:ILE:HG23	2.57	0.40
1:G:111:ARG:HD2	2:H:197:ARG:NH2	2.37	0.40
3:G:301:B12:H552	3:G:301:B12:H531	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	204/223 (92%)	195 (96%)	9 (4%)	0	100	100
1	B	206/223 (92%)	200 (97%)	6 (3%)	0	100	100
1	E	207/223 (93%)	197 (95%)	10 (5%)	0	100	100
1	G	203/223 (91%)	194 (96%)	9 (4%)	0	100	100
2	C	140/296 (47%)	138 (99%)	2 (1%)	0	100	100
2	D	144/296 (49%)	136 (94%)	8 (6%)	0	100	100
2	F	140/296 (47%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	140/296 (47%)	136 (97%)	4 (3%)	0	100	100
All	All	1384/2076 (67%)	1330 (96%)	54 (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	169/192 (88%)	169 (100%)	0	100	100
1	B	176/192 (92%)	176 (100%)	0	100	100
1	E	172/192 (90%)	172 (100%)	0	100	100
1	G	176/192 (92%)	176 (100%)	0	100	100
2	C	125/256 (49%)	125 (100%)	0	100	100
2	D	126/256 (49%)	126 (100%)	0	100	100
2	F	126/256 (49%)	126 (100%)	0	100	100
2	H	127/256 (50%)	127 (100%)	0	100	100
All	All	1197/1792 (67%)	1197 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
2	F	288	HIS
1	G	131	GLN
2	C	288	HIS
2	H	251	HIS

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](#)

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	$\# Z > 2$
3	B12	G	301	-	94,101,101	1.03	6 (6%)	149,166,166	1.68	26 (17%)
3	B12	B	301	-	94,101,101	1.04	5 (5%)	149,166,166	1.69	28 (18%)
3	B12	E	301	-	94,101,101	1.04	5 (5%)	149,166,166	1.73	27 (18%)
3	B12	A	401	-	94,101,101	1.04	4 (4%)	149,166,166	1.72	27 (18%)

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	G	301	-	-	25/56/223/223	0/3/11/11
3	B12	B	301	-	-	26/56/223/223	0/3/11/11
3	B12	E	301	-	-	17/56/223/223	0/3/11/11
3	B12	A	401	-	-	18/56/223/223	0/3/11/11

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	B12	C54-C17	2.78	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	B12	C54-C17	2.75	1.59	1.54
3	E	301	B12	C14-N23	2.73	1.38	1.35
3	E	301	B12	C54-C17	2.72	1.59	1.54
3	A	401	B12	C54-C17	2.69	1.59	1.54
3	A	401	B12	C14-N23	2.67	1.38	1.35
3	B	301	B12	C14-N23	2.65	1.38	1.35
3	G	301	B12	C35-C5	2.62	1.56	1.50
3	A	401	B12	C35-C5	2.60	1.56	1.50
3	B	301	B12	C35-C5	2.59	1.56	1.50
3	E	301	B12	C35-C5	2.57	1.56	1.50
3	G	301	B12	C14-N23	2.33	1.38	1.35
3	B	301	B12	C2B-N1B	-2.29	1.33	1.37
3	E	301	B12	C2B-N1B	-2.27	1.33	1.37
3	G	301	B12	C2B-N1B	-2.26	1.33	1.37
3	A	401	B12	C2B-N1B	-2.25	1.33	1.37
3	E	301	B12	C6B-C5B	2.07	1.45	1.40
3	G	301	B12	C6B-C5B	2.04	1.45	1.40
3	G	301	B12	C30-C3	2.03	1.59	1.54
3	B	301	B12	C6B-C5B	2.02	1.45	1.40

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	B12	C19-N24-C16	7.71	115.72	107.29
3	E	301	B12	C19-N24-C16	7.32	115.29	107.29
3	B	301	B12	C19-N24-C16	7.13	115.08	107.29
3	G	301	B12	C19-N24-C16	6.63	114.54	107.29
3	B	301	B12	C9-N22-C6	5.36	111.73	105.28
3	E	301	B12	C9-N22-C6	5.34	111.71	105.28
3	A	401	B12	C9-N22-C6	5.34	111.70	105.28
3	G	301	B12	C16-C15-C14	-5.20	113.33	121.26
3	G	301	B12	C9-N22-C6	5.13	111.45	105.28
3	A	401	B12	C55-C17-C16	5.01	126.38	116.59
3	B	301	B12	C18-C17-C16	4.87	106.56	100.69
3	E	301	B12	C55-C17-C16	4.70	125.78	116.59
3	E	301	B12	C18-C17-C16	4.64	106.29	100.69
3	G	301	B12	C18-C17-C16	4.52	106.14	100.69
3	B	301	B12	C54-C17-C18	-4.48	106.56	112.99
3	A	401	B12	C18-C17-C16	4.46	106.07	100.69
3	B	301	B12	C16-C15-C14	-4.28	114.74	121.26
3	G	301	B12	C54-C17-C18	-4.16	107.02	112.99
3	E	301	B12	C16-C15-C14	-4.15	114.94	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	B12	C16-C15-C14	-4.11	115.00	121.26
3	A	401	B12	C1P-N59-C57	-4.06	113.97	122.69
3	E	301	B12	C54-C17-C18	-4.02	107.22	112.99
3	B	301	B12	C55-C17-C16	4.02	124.45	116.59
3	A	401	B12	C54-C17-C16	-3.96	91.91	112.41
3	G	301	B12	C54-C17-C16	-3.93	92.04	112.41
3	E	301	B12	C54-C17-C16	-3.92	92.09	112.41
3	E	301	B12	C1P-N59-C57	-3.86	114.42	122.69
3	B	301	B12	C54-C17-C16	-3.79	92.75	112.41
3	B	301	B12	C1P-N59-C57	-3.78	114.57	122.69
3	E	301	B12	C53-C15-C16	3.78	126.78	120.36
3	A	401	B12	C54-C17-C18	-3.63	107.77	112.99
3	G	301	B12	C1P-N59-C57	-3.61	114.95	122.69
3	A	401	B12	C53-C15-C16	3.58	126.44	120.36
3	G	301	B12	C55-C17-C16	3.52	123.47	116.59
3	A	401	B12	C17-C16-N24	-3.48	105.86	111.17
3	G	301	B12	C15-C16-N24	3.37	127.22	122.42
3	B	301	B12	C53-C15-C16	3.30	125.97	120.36
3	E	301	B12	C17-C16-N24	-3.24	106.22	111.17
3	E	301	B12	C18-C19-N24	3.24	107.20	102.33
3	B	301	B12	C15-C16-N24	3.24	127.03	122.42
3	B	301	B12	C13-C14-C15	-3.21	119.44	124.32
3	B	301	B12	C17-C16-N24	-3.06	106.49	111.17
3	A	401	B12	C55-C56-C57	-3.04	104.48	111.25
3	E	301	B12	C15-C16-N24	3.01	126.71	122.42
3	G	301	B12	C17-C16-N24	-2.97	106.63	111.17
3	B	301	B12	C18-C19-N24	2.97	106.80	102.33
3	G	301	B12	C55-C17-C18	2.97	116.79	111.12
3	G	301	B12	C53-C15-C16	2.95	125.37	120.36
3	G	301	B12	C18-C19-N24	2.94	106.75	102.33
3	E	301	B12	C55-C56-C57	-2.91	104.76	111.25
3	A	401	B12	C18-C19-N24	2.87	106.65	102.33
3	E	301	B12	C9B-C8B-N1B	2.87	106.58	105.30
3	B	301	B12	C9B-C8B-N1B	2.85	106.57	105.30
3	B	301	B12	C5M-C5B-C6B	-2.82	114.99	120.76
3	A	401	B12	C1-C19-N24	-2.79	103.14	106.25
3	A	401	B12	C15-C16-N24	2.79	126.39	122.42
3	E	301	B12	C5M-C5B-C6B	-2.78	115.07	120.76
3	E	301	B12	C7B-C8B-C9B	2.77	125.79	122.47
3	B	301	B12	C7B-C8B-C9B	2.76	125.78	122.47
3	A	401	B12	C5M-C5B-C6B	-2.74	115.17	120.76
3	E	301	B12	C19-C1-N21	-2.72	99.34	102.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	B12	C13-C14-C15	-2.69	120.22	124.32
3	G	301	B12	C5M-C5B-C6B	-2.69	115.27	120.76
3	A	401	B12	C3R-C2R-C1R	2.63	105.68	99.89
3	B	301	B12	C55-C56-C57	-2.63	105.39	111.25
3	A	401	B12	C4B-C5B-C6B	2.62	123.53	119.69
3	E	301	B12	C4B-C5B-C6B	2.62	123.53	119.69
3	B	301	B12	C4B-C5B-C6B	2.59	123.48	119.69
3	G	301	B12	C4B-C5B-C6B	2.58	123.47	119.69
3	B	301	B12	O28-C27-N29	-2.58	115.65	122.53
3	A	401	B12	O28-C27-N29	-2.54	115.74	122.53
3	A	401	B12	C7B-C8B-C9B	2.53	125.51	122.47
3	G	301	B12	O28-C27-N29	-2.53	115.77	122.53
3	G	301	B12	C55-C56-C57	-2.53	105.61	111.25
3	E	301	B12	O28-C27-N29	-2.52	115.79	122.53
3	E	301	B12	C1-C19-N24	-2.43	103.55	106.25
3	A	401	B12	C13-C14-C15	-2.42	120.64	124.32
3	A	401	B12	C9B-C8B-N1B	2.40	106.37	105.30
3	G	301	B12	C9B-C8B-N1B	2.38	106.36	105.30
3	B	301	B12	C1-C19-C18	-2.35	118.09	121.90
3	G	301	B12	C7B-C8B-C9B	2.35	125.29	122.47
3	B	301	B12	C8B-C9B-N3B	-2.33	107.48	110.00
3	E	301	B12	C8B-C9B-N3B	-2.32	107.49	110.00
3	B	301	B12	C55-C17-C18	2.28	115.48	111.12
3	A	401	B12	C19-C1-N21	-2.24	99.84	102.14
3	G	301	B12	C37-C7-C8	-2.22	102.50	108.37
3	B	301	B12	O2-C3R-C2R	2.21	119.62	111.68
3	G	301	B12	O2-C3R-C2R	2.18	119.49	111.68
3	G	301	B12	C8B-C9B-N3B	-2.17	107.65	110.00
3	G	301	B12	C13-C14-C15	-2.15	121.05	124.32
3	B	301	B12	C37-C7-C8	-2.15	102.70	108.37
3	A	401	B12	C8B-C9B-N3B	-2.15	107.68	110.00
3	E	301	B12	C9B-C4B-C5B	-2.12	116.89	120.83
3	E	301	B12	O28-C27-C26	2.11	128.53	121.98
3	B	301	B12	O28-C27-C26	2.11	128.52	121.98
3	A	401	B12	C9B-C4B-C5B	-2.11	116.92	120.83
3	A	401	B12	O28-C27-C26	2.09	128.47	121.98
3	G	301	B12	O28-C27-C26	2.09	128.46	121.98
3	B	301	B12	C9B-C4B-C5B	-2.09	116.96	120.83
3	G	301	B12	C9B-C4B-C5B	-2.07	116.99	120.83
3	A	401	B12	C37-C7-C8	-2.07	102.91	108.37
3	A	401	B12	O6R-C1R-N1B	-2.07	104.12	108.09
3	G	301	B12	C2P-C1P-N59	-2.05	109.90	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	B12	C2-C3-C4	2.04	103.94	101.64
3	E	301	B12	O2-C3R-C2R	2.04	118.98	111.68
3	B	301	B12	C35-C5-C4	-2.03	112.69	116.79
3	B	301	B12	C13-C14-N23	2.01	111.81	109.09
3	E	301	B12	C31-C32-N33	2.00	122.90	116.49

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	B12	C38-C37-C7-C6
3	A	401	B12	C38-C37-C7-C36
3	A	401	B12	C38-C37-C7-C8
3	A	401	B12	C42-C41-C8-C9
3	A	401	B12	C14-C13-C48-C49
3	A	401	B12	C18-C60-C61-O63
3	A	401	B12	C18-C60-C61-N62
3	B	301	B12	C38-C37-C7-C6
3	B	301	B12	C38-C37-C7-C36
3	B	301	B12	C38-C37-C7-C8
3	B	301	B12	C42-C41-C8-C9
3	B	301	B12	C3R-O2-P-O3
3	B	301	B12	C3R-O2-P-O5
3	E	301	B12	C38-C37-C7-C6
3	E	301	B12	C38-C37-C7-C36
3	E	301	B12	C38-C37-C7-C8
3	E	301	B12	C42-C41-C8-C9
3	E	301	B12	C14-C13-C48-C49
3	G	301	B12	C4-C3-C30-C31
3	G	301	B12	C38-C37-C7-C6
3	G	301	B12	C38-C37-C7-C36
3	G	301	B12	C38-C37-C7-C8
3	G	301	B12	C42-C41-C8-C9
3	G	301	B12	C16-C17-C55-C56
3	G	301	B12	N59-C1P-C2P-O3
3	G	301	B12	C2P-O3-P-O4
3	G	301	B12	C2P-O3-P-O2
3	G	301	B12	C3R-O2-P-O3
3	G	301	B12	C3R-O2-P-O5
3	B	301	B12	C8-C41-C42-C43
3	G	301	B12	C8-C41-C42-C43
3	A	401	B12	C4-C3-C30-C31

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Mol	Chain	Res	Type	Atoms
3	E	301	B12	C4-C3-C30-C31
3	E	301	B12	C8-C41-C42-C43
3	G	301	B12	C2-C3-C30-C31
3	A	401	B12	C13-C48-C49-C50
3	E	301	B12	C13-C48-C49-C50
3	B	301	B12	C3R-C4R-C5R-O8R
3	A	401	B12	C3R-C4R-C5R-O8R
3	G	301	B12	C2R-C3R-O2-P
3	B	301	B12	O6R-C4R-C5R-O8R
3	B	301	B12	C16-C17-C55-C56
3	G	301	B12	N59-C1P-C2P-C3P
3	B	301	B12	C13-C48-C49-C50
3	A	401	B12	O6R-C4R-C5R-O8R
3	A	401	B12	C2-C3-C30-C31
3	G	301	B12	C4R-C3R-O2-P
3	E	301	B12	C2-C3-C30-C31
3	G	301	B12	C18-C17-C55-C56
3	A	401	B12	O6R-C1R-N1B-C8B
3	G	301	B12	C2R-C1R-N1B-C8B
3	E	301	B12	C30-C31-C32-N33
3	B	301	B12	C2R-C3R-O2-P
3	E	301	B12	C30-C31-C32-O34
3	B	301	B12	O6R-C1R-N1B-C8B
3	B	301	B12	C41-C42-C43-N45
3	B	301	B12	C3R-O2-P-O4
3	G	301	B12	C3-C30-C31-C32
3	G	301	B12	C17-C18-C60-C61
3	A	401	B12	C2R-C1R-N1B-C8B
3	E	301	B12	C2P-C1P-N59-C57
3	B	301	B12	C41-C42-C43-O44
3	B	301	B12	C4-C3-C30-C31
3	E	301	B12	C41-C42-C43-N45
3	B	301	B12	C4R-C3R-O2-P
3	E	301	B12	C3-C30-C31-C32
3	B	301	B12	C2P-C1P-N59-C57
3	B	301	B12	C1P-C2P-O3-P
3	B	301	B12	C3P-C2P-O3-P
3	E	301	B12	C41-C42-C43-O44
3	G	301	B12	C30-C31-C32-N33
3	A	401	B12	C17-C18-C60-C61
3	A	401	B12	C19-C18-C60-C61
3	A	401	B12	C2P-C1P-N59-C57

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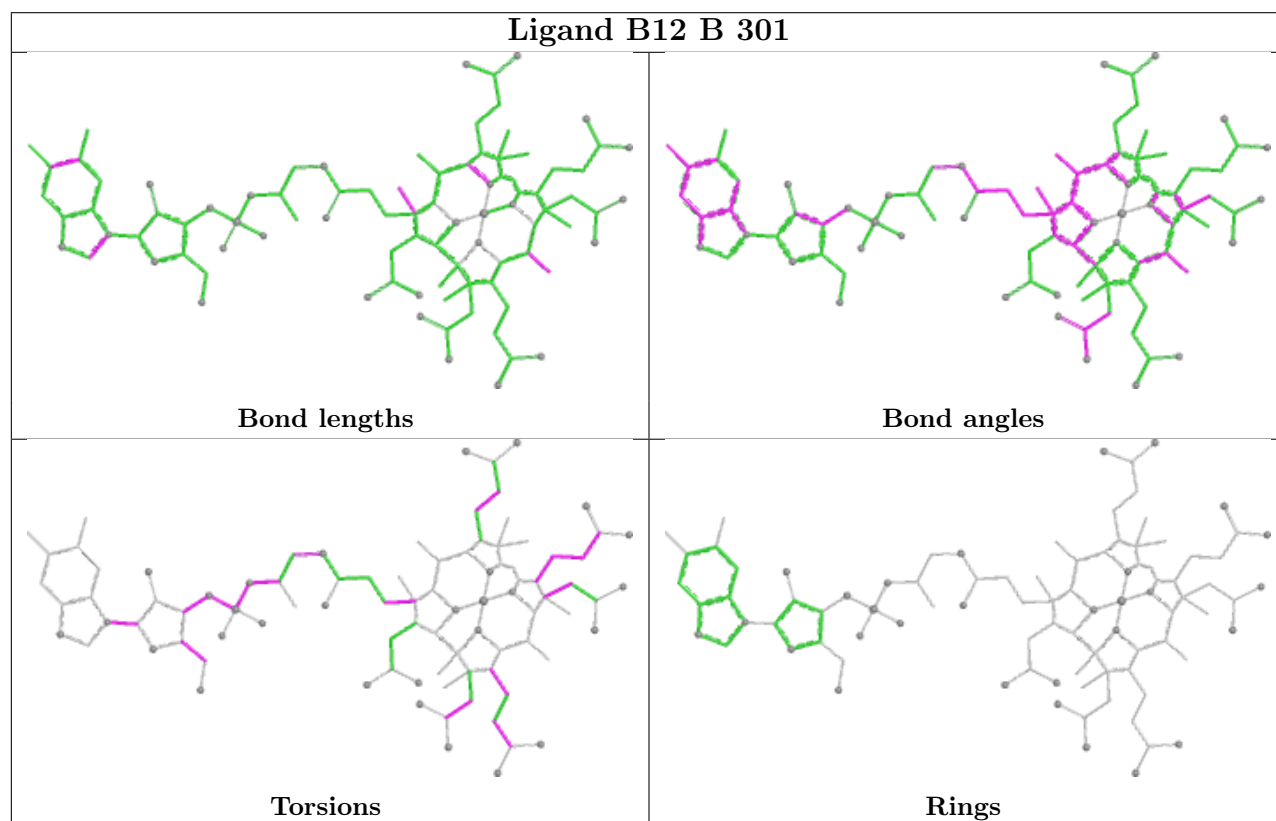
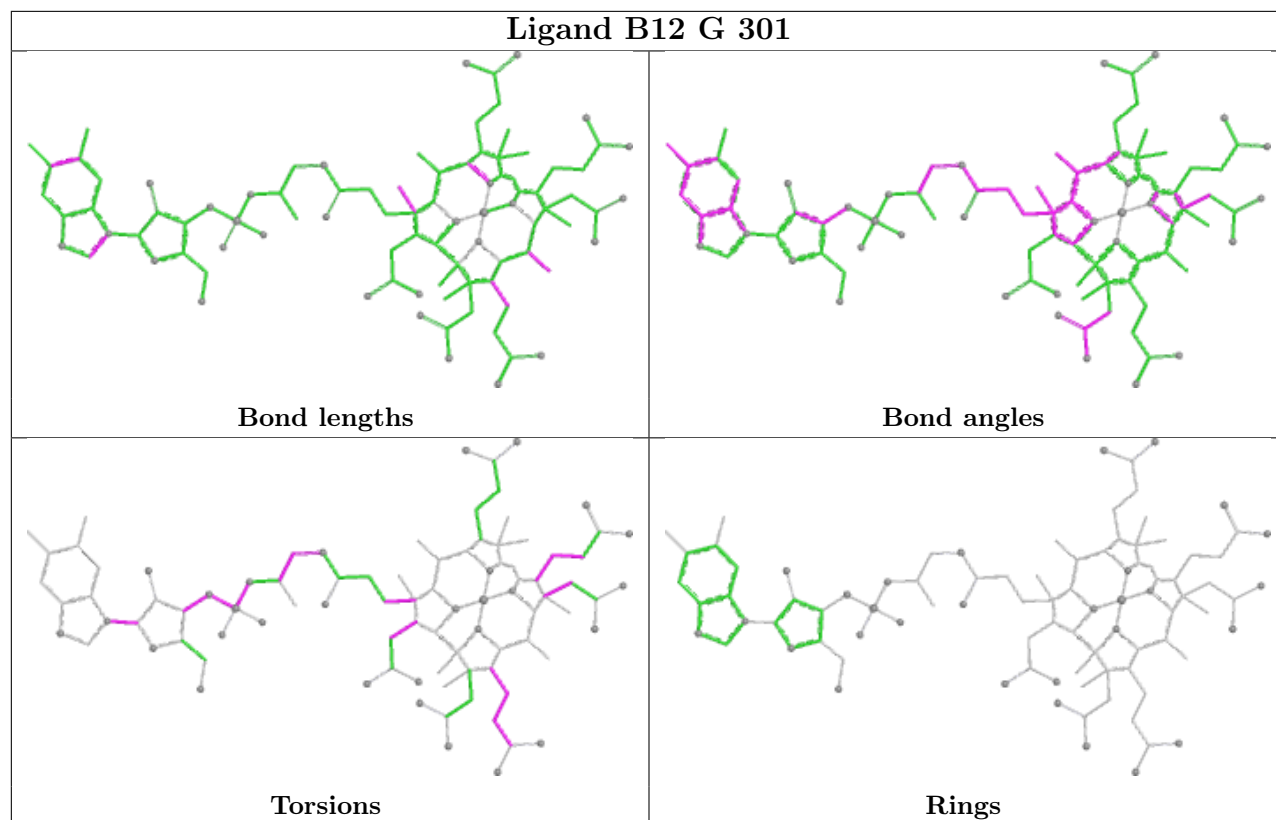
Mol	Chain	Res	Type	Atoms
3	B	301	B12	C2-C26-C27-N29
3	B	301	B12	C2P-O3-P-O4
3	B	301	B12	C2P-O3-P-O5
3	E	301	B12	C2P-O3-P-O4
3	E	301	B12	C2P-O3-P-O5
3	G	301	B12	C2P-O3-P-O5
3	G	301	B12	C3R-O2-P-O4
3	B	301	B12	C2-C3-C30-C31
3	A	401	B12	C1P-C2P-O3-P
3	G	301	B12	C30-C31-C32-O34
3	B	301	B12	C30-C31-C32-N33
3	G	301	B12	C2P-C1P-N59-C57

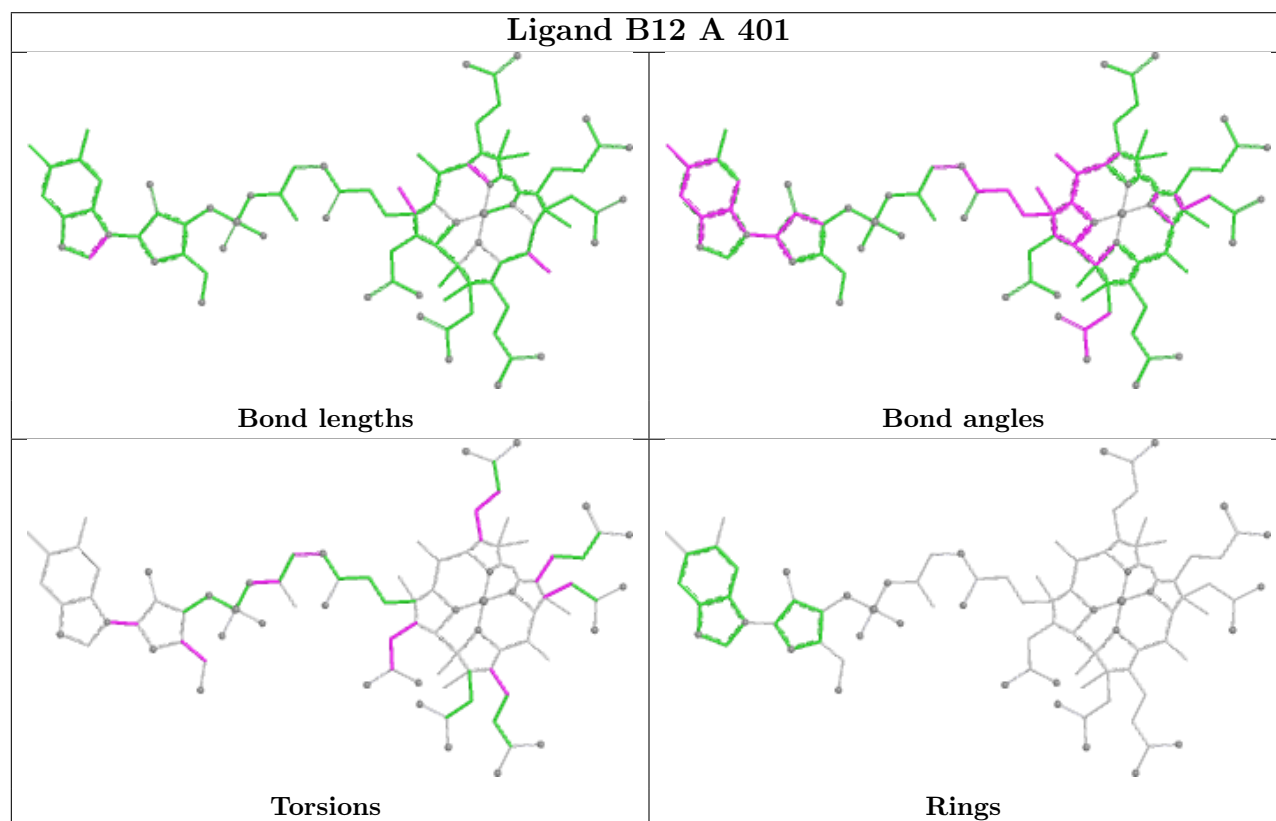
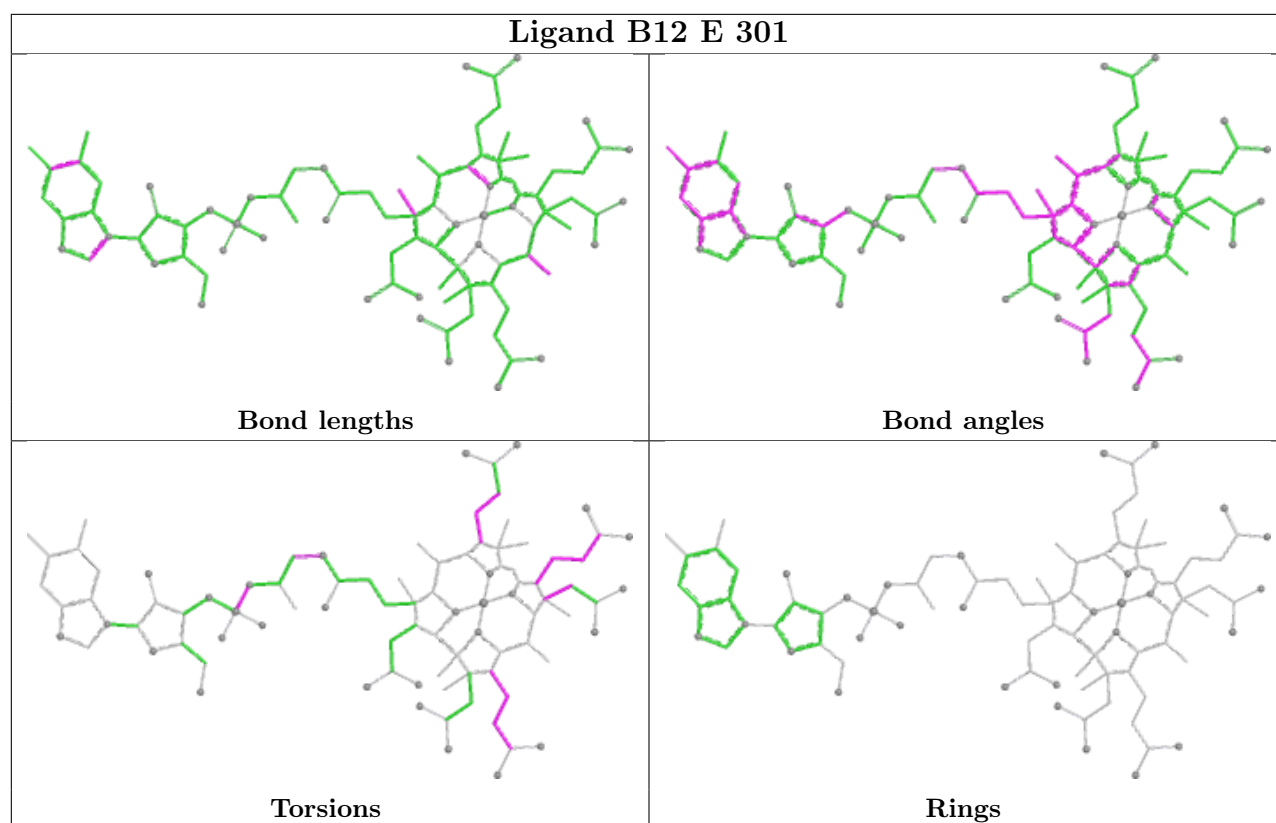
There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	B12	2	0
3	B	301	B12	8	0
3	E	301	B12	4	0
3	A	401	B12	7	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 [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	209/223 (93%)	-1.23	1 (0%) 87 78	43, 60, 63, 64	1 (0%)
1	B	211/223 (94%)	-1.23	0 100 100	47, 64, 69, 74	1 (0%)
1	E	210/223 (94%)	-1.14	0 100 100	40, 71, 79, 83	1 (0%)
1	G	210/223 (94%)	-1.07	0 100 100	53, 86, 94, 100	1 (0%)
2	C	144/296 (48%)	-1.23	0 100 100	61, 68, 74, 78	0
2	D	148/296 (50%)	-1.23	0 100 100	58, 62, 68, 71	0
2	F	144/296 (48%)	-1.19	0 100 100	72, 76, 83, 86	0
2	H	144/296 (48%)	-1.06	0 100 100	79, 88, 93, 94	0
All	All	1420/2076 (68%)	-1.17	1 (0%) 92 91	40, 69, 92, 100	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	GLY	2.4

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,

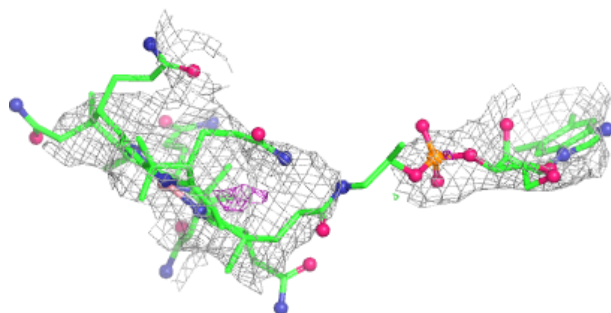
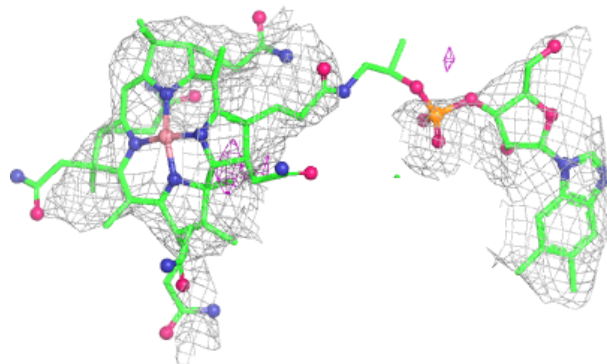
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	B12	G	301	91/91	0.98	0.06	84,91,93,94	0
3	B12	B	301	91/91	0.99	0.05	58,63,64,65	0
3	B12	E	301	91/91	0.99	0.05	70,74,75,75	0
3	B12	A	401	91/91	0.99	0.04	56,59,59,60	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.

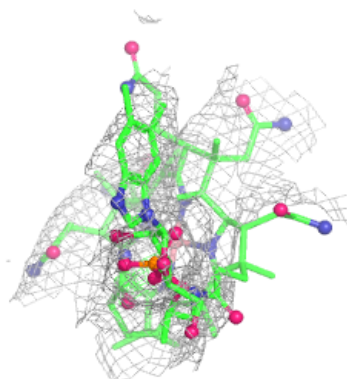
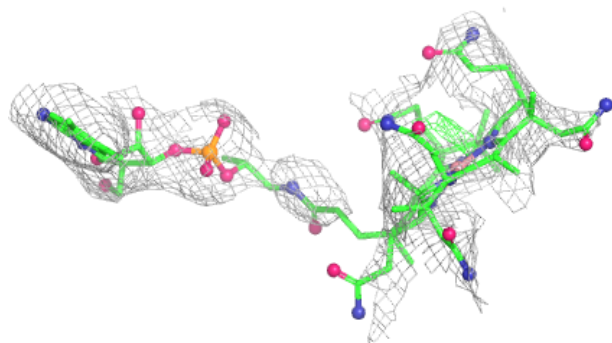
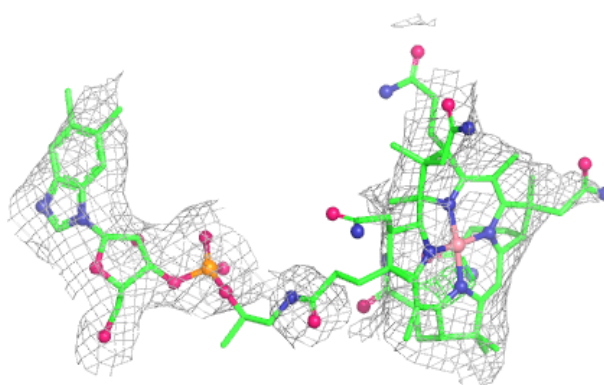
Electron density around B12 G 301:

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

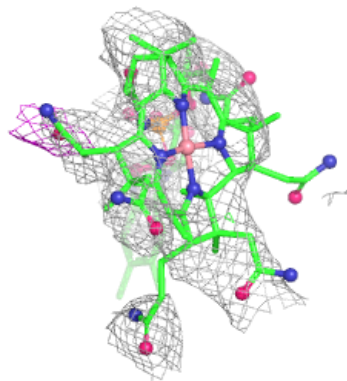
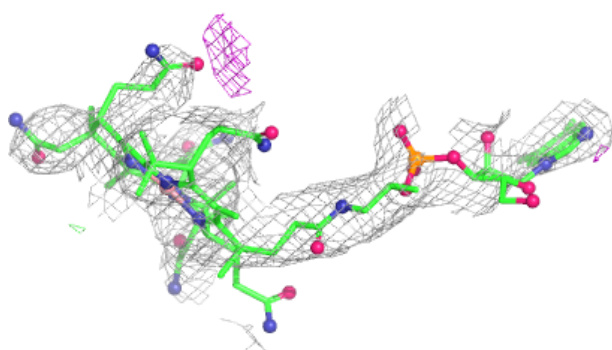
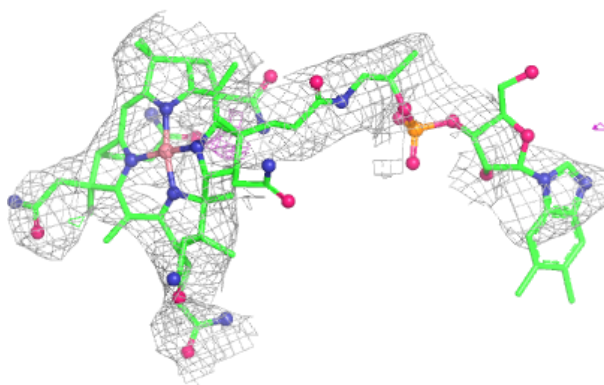


Electron density around B12 B 301:

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

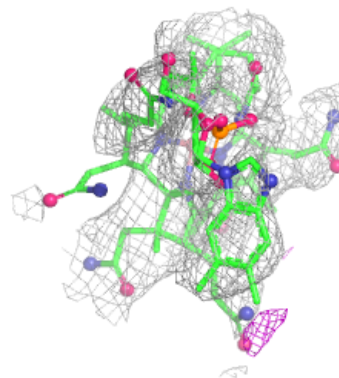
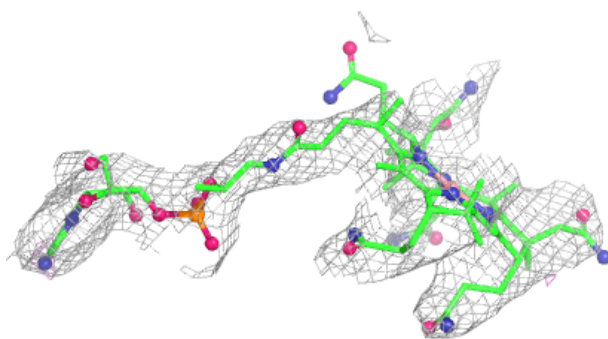
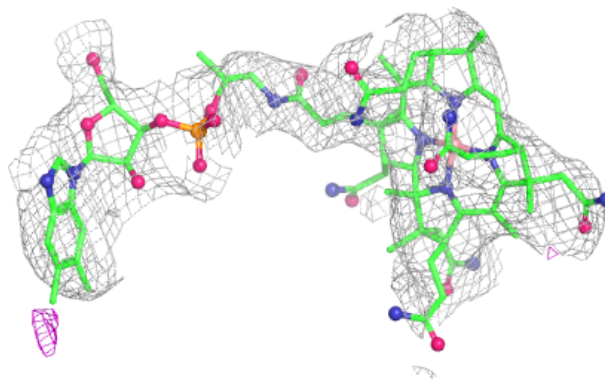
**Electron density around B12 E 301:**

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



Electron density around B12 A 401:

$2mF_o-DF_c$ (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.