



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 8SSE / pdb_00008sse
Title : Methionine synthase, C-terminal fragment, Cobalamin and Reactivation Domains from *Thermus thermophilus* HB8
Authors : Yamada, K.; Mendoza, J.; Koutmos, M.
Deposited on : 2023-05-08
Resolution : 3.15 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

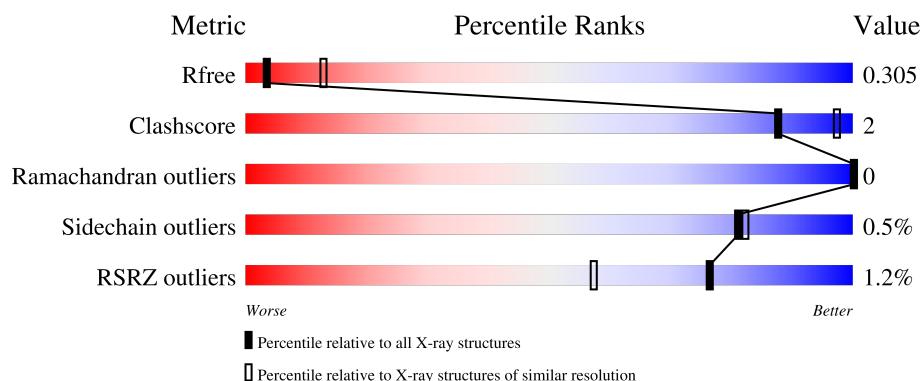
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	523	89% 7% .
1	B	523	89% 7% .
1	C	523	89% 8% .
1	D	523	89% 7% .
1	E	523	89% 8% .

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Mol	Chain	Length	Quality of chain
1	F	523	2% 88% 8%

2 Entry composition [i](#)

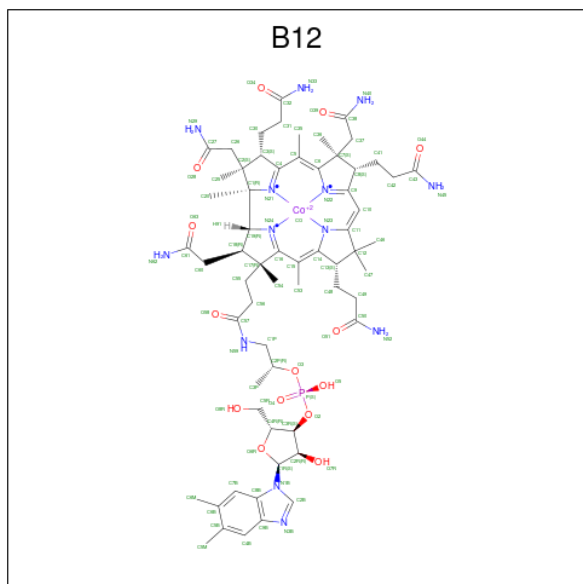
There are 3 unique types of molecules in this entry. The entry contains 24880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4012	2572	705	719	16			
1	B	506	Total	C	N	O	S	0	0	0
			4005	2567	704	718	16			
1	C	507	Total	C	N	O	S	0	0	0
			4012	2572	705	719	16			
1	D	506	Total	C	N	O	S	0	0	0
			4005	2567	704	718	16			
1	E	507	Total	C	N	O	S	0	0	0
			4012	2572	705	719	16			
1	F	505	Total	C	N	O	S	0	0	0
			3994	2561	700	717	16			

- Molecule 2 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
2	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	E	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	F	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

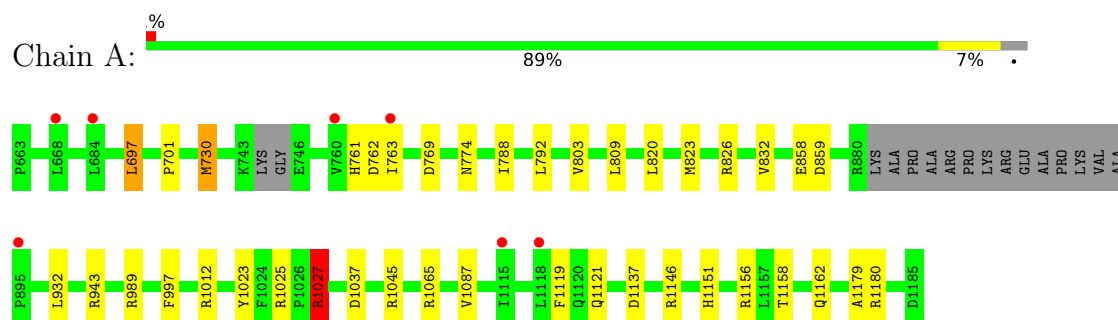
- Molecule 3 is water.

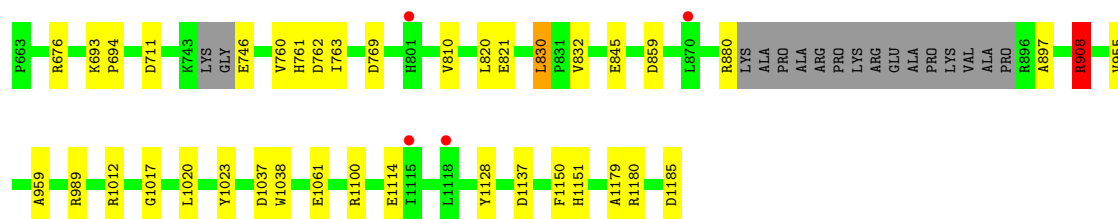
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	40	Total	O	0	0
			40	40		
3	C	62	Total	O	0	0
			62	62		
3	D	40	Total	O	0	0
			40	40		
3	E	55	Total	O	0	0
			55	55		
3	F	50	Total	O	0	0
			50	50		

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.

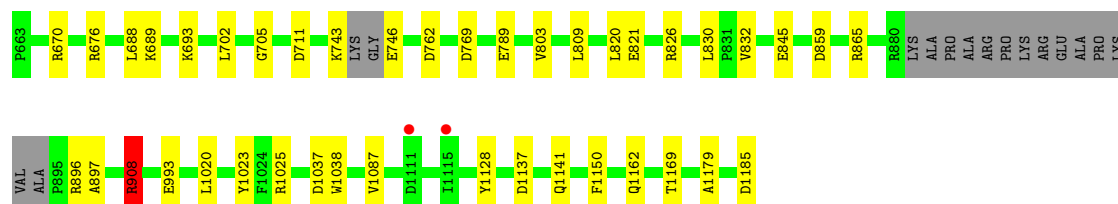
• Molecule 1: Methionine synthase





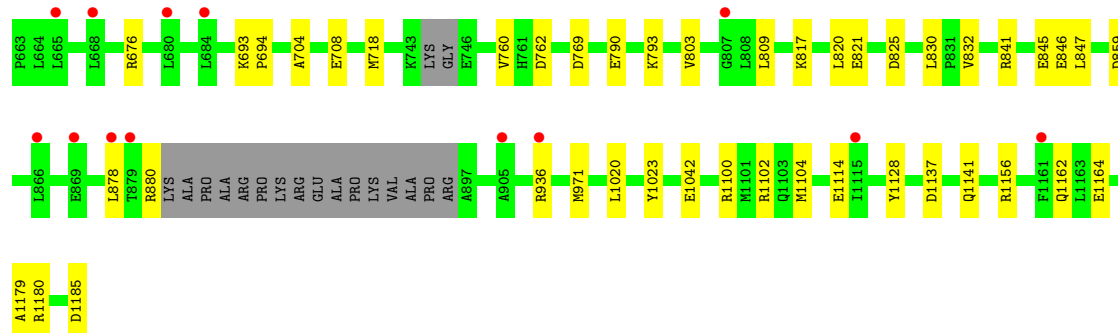
• Molecule 1: Methionine synthase

Chain E: 89% 8% .



• Molecule 1: Methionine synthase

Chain F: 88% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.13Å 95.84Å 238.75Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	49.30 – 3.15 49.30 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.30-3.15) 98.7 (49.30-3.15)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.245 , 0.307 0.246 , 0.305	Depositor DCC
R_{free} test set	3279 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.006 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24880	wwPDB-VP
Average B, all atoms (Å ²)	83.0	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 39.99 % 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 2.9241e-04. 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: 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	0.80	0/4107	1.40	11/5548 (0.2%)
1	B	0.75	0/4099	1.36	13/5537 (0.2%)
1	C	0.80	2/4107 (0.0%)	1.42	14/5548 (0.3%)
1	D	0.74	0/4099	1.36	15/5537 (0.3%)
1	E	0.80	0/4107	1.40	14/5548 (0.3%)
1	F	0.74	0/4088	1.36	11/5523 (0.2%)
All	All	0.77	2/24607 (0.0%)	1.38	78/33241 (0.2%)

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	9
1	B	0	9
1	C	0	6
1	D	0	7
1	E	0	8
1	F	0	3
All	All	0	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1140	ASP	CG-OD2	5.19	1.35	1.25
1	C	1095	GLU	CD-OE2	5.08	1.34	1.25

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	THR	OG1-CB-CG2	-8.09	93.13	109.30
1	E	1037	ASP	CA-CB-CG	7.80	120.40	112.60
1	B	859	ASP	CA-CB-CG	7.04	119.64	112.60
1	B	1185	ASP	CA-CB-CG	6.96	119.56	112.60
1	B	1027	ARG	CG-CD-NE	6.82	127.01	112.00
1	B	1037	ASP	CA-CB-CG	6.67	119.27	112.60
1	D	769	ASP	CA-CB-CG	6.53	119.13	112.60
1	E	1150	PHE	CA-CB-CG	6.53	120.33	113.80
1	F	821	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	711	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	1037	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	1146	ARG	CG-CD-NE	6.30	125.87	112.00
1	D	1185	ASP	CA-CB-CG	6.27	118.87	112.60
1	F	769	ASP	CA-CB-CG	6.25	118.85	112.60
1	E	769	ASP	CA-CB-CG	6.21	118.81	112.60
1	F	1185	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	769	ASP	CA-CB-CG	6.08	118.68	112.60
1	E	1137	ASP	CA-CB-CG	6.03	118.63	112.60
1	E	1185	ASP	CA-CB-CG	6.01	118.61	112.60
1	C	1185	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	1137	ASP	CA-CB-CG	5.95	118.55	112.60
1	C	769	ASP	CA-CB-CG	5.93	118.53	112.60
1	D	1037	ASP	CA-CB-CG	5.93	118.53	112.60
1	E	845	GLU	CB-CG-CD	5.92	122.67	112.60
1	D	830	LEU	CB-CA-C	5.90	117.95	109.11
1	F	845	GLU	CB-CG-CD	5.74	122.36	112.60
1	D	859	ASP	CA-CB-CG	5.74	118.34	112.60
1	F	762	ASP	CA-CB-CG	5.72	118.33	112.60
1	F	1042	GLU	CB-CG-CD	5.71	122.31	112.60
1	C	845	GLU	CB-CG-CD	5.70	122.28	112.60
1	A	859	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	769	ASP	CA-CB-CG	5.65	118.25	112.60
1	F	859	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	821	GLU	CB-CG-CD	5.54	122.02	112.60
1	D	845	GLU	CB-CG-CD	5.49	121.94	112.60
1	B	1111	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	908	ARG	N-CA-CB	5.43	118.27	109.90
1	C	1137	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	1137	ASP	CA-CB-CG	5.42	118.02	112.60
1	F	825	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	902	GLU	N-CA-CB	5.39	117.94	110.17
1	E	711	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	1027	ARG	NE-CZ-NH1	-5.36	116.14	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	762	ASP	CA-CB-CG	5.36	117.95	112.60
1	F	1114	GLU	CB-CG-CD	5.35	121.69	112.60
1	C	762	ASP	CA-CB-CG	5.34	117.94	112.60
1	E	993	GLU	CB-CA-C	5.34	118.96	109.72
1	B	1150	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	868	GLU	CB-CG-CD	5.34	121.67	112.60
1	C	740	HIS	CA-CB-CG	5.32	119.12	113.80
1	F	1137	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	789	GLU	CB-CG-CD	5.28	121.58	112.60
1	F	1141	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	E	859	ASP	CA-CB-CG	5.25	117.85	112.60
1	D	711	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	859	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	908	ARG	CB-CG-CD	-5.21	99.33	111.30
1	D	1114	GLU	CB-CG-CD	5.21	121.45	112.60
1	B	958	GLU	CB-CG-CD	5.20	121.44	112.60
1	E	789	GLU	CB-CG-CD	5.20	121.44	112.60
1	C	1176	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	B	1151	HIS	CA-CB-CG	5.10	118.90	113.80
1	E	821	GLU	CB-CG-CD	5.10	121.27	112.60
1	D	1151	HIS	CA-CB-CG	5.10	118.90	113.80
1	C	711	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	936	ARG	CA-CB-CG	5.08	124.26	114.10
1	D	1150	PHE	CA-CB-CG	5.08	118.88	113.80
1	D	1061	GLU	CB-CG-CD	5.08	121.23	112.60
1	E	1169	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	762	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	943	ARG	CG-CD-NE	5.06	123.12	112.00
1	E	762	ASP	CA-CB-CG	5.05	117.66	112.60
1	B	1000	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	858	GLU	CB-CG-CD	5.04	121.18	112.60
1	A	730	MET	CB-CG-SD	5.04	127.82	112.70
1	E	693	LYS	CB-CA-C	5.03	118.56	109.45
1	A	1151	HIS	CA-CB-CG	5.01	118.81	113.80
1	D	762	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1012	ARG	Sidechain
1	A	1025	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1027	ARG	Sidechain
1	A	1045	ARG	Sidechain
1	A	1065	ARG	Sidechain
1	A	1119	PHE	Mainchain
1	A	1156	ARG	Sidechain
1	A	826	ARG	Sidechain
1	A	989	ARG	Sidechain
1	B	1027	ARG	Sidechain
1	B	1102	ARG	Sidechain
1	B	1180	ARG	Sidechain
1	B	676	ARG	Sidechain
1	B	824	ARG	Sidechain
1	B	896	ARG	Sidechain
1	B	898	ARG	Sidechain
1	B	948	ARG	Sidechain
1	B	989	ARG	Sidechain
1	C	1012	ARG	Sidechain
1	C	1180	ARG	Sidechain
1	C	670	ARG	Sidechain
1	C	676	ARG	Sidechain
1	C	943	ARG	Sidechain
1	C	948	ARG	Sidechain
1	D	1012	ARG	Sidechain
1	D	1100	ARG	Sidechain
1	D	1180	ARG	Sidechain
1	D	676	ARG	Sidechain
1	D	880	ARG	Sidechain
1	D	908	ARG	Sidechain
1	D	989	ARG	Sidechain
1	E	1025	ARG	Sidechain
1	E	670	ARG	Sidechain
1	E	676	ARG	Sidechain
1	E	826	ARG	Sidechain
1	E	865	ARG	Sidechain
1	E	896	ARG	Peptide,Sidechain
1	E	908	ARG	Sidechain
1	F	1102	ARG	Sidechain
1	F	1180	ARG	Sidechain
1	F	676	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	4012	0	4013	16	0
1	B	4005	0	4005	9	0
1	C	4012	0	4013	14	0
1	D	4005	0	4005	11	0
1	E	4012	0	4013	15	0
1	F	3994	0	3992	15	0
2	A	91	0	88	6	0
2	B	91	0	88	2	0
2	C	91	0	88	7	0
2	D	91	0	88	5	0
2	E	91	0	88	4	0
2	F	91	0	88	3	0
3	A	47	0	0	1	0
3	B	40	0	0	0	0
3	C	62	0	0	1	0
3	D	40	0	0	1	0
3	E	55	0	0	1	0
3	F	50	0	0	1	0
All	All	24880	0	24569	100	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 2.

All (100) 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:E:688:LEU:HD11	1:E:689:LYS:NZ	2.03	0.74
1:F:760:VAL:HG22	3:F:1301:HOH:O	1.88	0.74
1:A:697:LEU:HA	1:A:701:PRO:HD2	1.75	0.68
1:C:1058:THR:HG22	1:C:1060:GLY:H	1.59	0.66
1:A:803:VAL:HG21	1:A:823:MET:HE1	1.77	0.66
1:A:788:ILE:HD11	1:A:823:MET:HE3	1.79	0.63
1:F:841:ARG:HD2	1:F:880:ARG:HB3	1.82	0.62
1:E:688:LEU:HD12	1:E:689:LYS:N	2.15	0.61
1:A:820:LEU:HD21	1:A:832:VAL:HG11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:LEU:CD1	1:A:943:ARG:HH12	2.15	0.59
1:C:820:LEU:HD21	1:C:832:VAL:HG11	1.84	0.59
1:D:820:LEU:HD21	1:D:832:VAL:HG11	1.85	0.58
2:C:1201:B12:H362	2:C:1201:B12:H351	1.84	0.58
1:E:688:LEU:HD11	1:E:689:LYS:HZ2	1.69	0.58
1:B:896:ARG:HH21	1:F:846:GLU:HG2	1.68	0.58
1:E:820:LEU:HD21	1:E:832:VAL:HG11	1.85	0.57
1:F:820:LEU:HD21	1:F:832:VAL:HG11	1.87	0.57
1:D:760:VAL:HG22	3:D:1305:HOH:O	2.04	0.56
1:C:810:VAL:HG13	3:C:1313:HOH:O	2.06	0.55
1:A:932:LEU:HD11	1:A:943:ARG:HH12	1.72	0.55
1:A:761:HIS:CE1	1:A:763:ILE:HG22	2.43	0.54
2:D:1201:B12:H362	2:D:1201:B12:H351	1.89	0.54
2:E:1201:B12:H362	2:E:1201:B12:H351	1.90	0.53
1:E:809:LEU:HD12	1:E:1162:GLN:HG2	1.91	0.53
1:B:820:LEU:HD21	1:B:832:VAL:HG11	1.90	0.52
1:B:809:LEU:HD12	1:B:1162:GLN:HG2	1.91	0.52
1:C:809:LEU:HD12	1:C:1162:GLN:HG2	1.91	0.52
1:E:688:LEU:HD11	1:E:689:LYS:HZ3	1.73	0.52
2:F:1201:B12:H543	2:F:1201:B12:H531	1.91	0.52
1:D:908:ARG:HB3	1:D:1038:TRP:CE2	2.45	0.51
1:B:809:LEU:HD13	1:B:1138:LEU:HD21	1.92	0.51
1:A:809:LEU:HD12	1:A:1162:GLN:HG2	1.93	0.51
1:F:809:LEU:HD12	1:F:1162:GLN:HG2	1.93	0.51
1:C:803:VAL:HG11	1:C:823:MET:HE1	1.93	0.49
2:C:1201:B12:H353	2:C:1201:B12:H311	1.94	0.49
2:E:1201:B12:H552	2:E:1201:B12:H531	1.96	0.48
1:D:897:ALA:HB2	1:D:1017:GLY:HA2	1.94	0.48
1:E:702:LEU:O	1:E:705:GLY:N	2.48	0.47
1:C:1087:VAL:CG1	2:C:1201:B12:H533	2.45	0.47
1:C:810:VAL:HG23	2:C:1201:B12:N33	2.30	0.47
2:B:1201:B12:H91	2:B:1201:B12:H262	1.63	0.47
2:A:1201:B12:H362	2:A:1201:B12:H351	1.97	0.47
1:F:841:ARG:CD	1:F:880:ARG:HB3	2.44	0.46
1:B:908:ARG:HG2	1:B:1038:TRP:CZ2	2.50	0.46
1:C:694:PRO:HB2	1:C:741:MET:HE3	1.97	0.46
1:D:761:HIS:CE1	1:D:763:ILE:HG22	2.50	0.46
1:E:897:ALA:HB3	3:E:1345:HOH:O	2.14	0.46
1:F:1156:ARG:HG2	1:F:1164:GLU:HB3	1.97	0.46
1:C:1058:THR:HG22	1:C:1060:GLY:N	2.29	0.46
1:E:803:VAL:HG23	1:E:830:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:PHE:HE2	1:A:1027:ARG:HH21	1.65	0.45
1:F:704:ALA:O	1:F:708:GLU:N	2.44	0.45
2:D:1201:B12:H262	2:D:1201:B12:H91	1.73	0.44
2:D:1201:B12:H552	2:D:1201:B12:H531	1.99	0.44
1:E:1087:VAL:HG13	2:E:1201:B12:H13	1.99	0.44
1:B:1020:LEU:HD21	1:B:1128:TYR:CG	2.52	0.44
1:D:1020:LEU:HD21	1:D:1128:TYR:CG	2.53	0.44
1:D:1023:TYR:CZ	1:D:1179:ALA:HA	2.53	0.44
1:E:1020:LEU:HD21	1:E:1128:TYR:CG	2.52	0.44
1:A:1121:GLN:HG2	1:A:1180:ARG:HD2	1.99	0.44
1:B:1023:TYR:CZ	1:B:1179:ALA:HA	2.53	0.44
1:C:1023:TYR:CZ	1:C:1179:ALA:HA	2.52	0.44
1:A:943:ARG:HB2	1:A:943:ARG:HH11	1.83	0.44
2:E:1201:B12:H262	2:E:1201:B12:H91	1.82	0.44
1:F:790:GLU:HA	1:F:793:LYS:HE2	1.99	0.44
1:A:1023:TYR:CZ	1:A:1179:ALA:HA	2.53	0.44
2:A:1201:B12:H473	2:A:1201:B12:H481	1.85	0.44
1:F:1020:LEU:HD21	1:F:1128:TYR:CG	2.53	0.44
1:F:1023:TYR:CZ	1:F:1179:ALA:HA	2.53	0.43
1:A:1087:VAL:CG1	2:A:1201:B12:H533	2.48	0.43
2:A:1201:B12:H601	2:A:1201:B12:H262	2.00	0.43
1:F:803:VAL:HG23	1:F:830:LEU:HD23	2.00	0.43
1:C:1020:LEU:HD21	1:C:1128:TYR:CG	2.54	0.43
1:E:908:ARG:HG2	1:E:1038:TRP:CE2	2.53	0.43
1:E:1023:TYR:CZ	1:E:1179:ALA:HA	2.54	0.43
1:B:722:PHE:HA	1:B:725:GLN:HB2	2.00	0.43
1:D:693:LYS:HE3	1:D:694:PRO:HD2	2.00	0.43
1:D:908:ARG:HB3	1:D:1038:TRP:CZ2	2.53	0.43
2:A:1201:B12:H562	2:A:1201:B12:H621	1.83	0.42
1:C:817:LYS:HG3	1:C:847:LEU:HD22	2.01	0.42
1:E:688:LEU:HD12	1:E:688:LEU:C	2.45	0.42
1:A:792:LEU:HD21	1:A:823:MET:HE2	2.01	0.42
2:B:1201:B12:H621	2:B:1201:B12:H562	1.84	0.42
1:A:730:MET:SD	1:A:774:ASN:O	2.77	0.42
1:C:1013:GLN:O	1:C:1016:GLY:O	2.38	0.42
2:D:1201:B12:H311	2:D:1201:B12:H353	2.02	0.41
1:B:1132:TYR:HB3	1:B:1133:PRO:HD2	2.02	0.41
2:F:1201:B12:H362	2:F:1201:B12:H351	2.02	0.41
2:C:1201:B12:H601	2:C:1201:B12:H262	2.02	0.41
1:A:943:ARG:HD2	3:A:1330:HOH:O	2.20	0.41
2:A:1201:B12:H262	2:A:1201:B12:H91	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1132:TYR:CD1	2:C:1201:B12:H352	2.54	0.41
1:F:693:LYS:HG2	1:F:694:PRO:HD2	2.03	0.41
1:F:1100:ARG:O	1:F:1104:MET:HG2	2.20	0.41
1:E:743:LYS:HB3	1:E:746:GLU:HG3	2.04	0.40
2:C:1201:B12:H552	2:C:1201:B12:H531	2.03	0.40
1:D:810:VAL:H	2:D:1201:B12:H332	1.69	0.40
1:D:955:VAL:HA	1:D:959:ALA:HB3	2.04	0.40
1:F:817:LYS:HG3	1:F:847:LEU:HD22	2.03	0.40
2:F:1201:B12:H91	2:F:1201:B12:H262	1.66	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	501/523 (96%)	489 (98%)	12 (2%)	0	100	100
1	B	500/523 (96%)	488 (98%)	12 (2%)	0	100	100
1	C	501/523 (96%)	490 (98%)	11 (2%)	0	100	100
1	D	500/523 (96%)	490 (98%)	10 (2%)	0	100	100
1	E	501/523 (96%)	491 (98%)	10 (2%)	0	100	100
1	F	499/523 (95%)	491 (98%)	8 (2%)	0	100	100
All	All	3002/3138 (96%)	2939 (98%)	63 (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	408/419 (97%)	407 (100%)	1 (0%)	87	87
1	B	407/419 (97%)	404 (99%)	3 (1%)	76	80
1	C	408/419 (97%)	407 (100%)	1 (0%)	87	87
1	D	407/419 (97%)	405 (100%)	2 (0%)	81	82
1	E	408/419 (97%)	406 (100%)	2 (0%)	81	82
1	F	406/419 (97%)	402 (99%)	4 (1%)	68	76
All	All	2444/2514 (97%)	2431 (100%)	13 (0%)	81	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	697	LEU
1	B	814	LEU
1	B	918	GLU
1	B	1003	GLU
1	C	936	ARG
1	D	746	GLU
1	D	830	LEU
1	E	908	ARG
1	E	1141	GLN
1	F	718	MET
1	F	878	LEU
1	F	936	ARG
1	F	971	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	761	HIS
1	A	774	ASN
1	A	1055	GLN
1	A	1077	GLN
1	A	1121	GLN
1	A	1124	GLN
1	A	1162	GLN
1	B	692	HIS
1	B	774	ASN

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Mol	Chain	Res	Type
1	B	927	HIS
1	B	1055	GLN
1	B	1162	GLN
1	C	775	ASN
1	C	801	HIS
1	C	927	HIS
1	C	1055	GLN
1	C	1109	HIS
1	C	1110	GLN
1	C	1160	ASN
1	C	1162	GLN
1	D	719	GLN
1	D	725	GLN
1	D	761	HIS
1	D	853	ASN
1	D	927	HIS
1	D	1055	GLN
1	D	1109	HIS
1	D	1110	GLN
1	D	1120	GLN
1	D	1121	GLN
1	E	699	ASN
1	E	761	HIS
1	E	927	HIS
1	E	1055	GLN
1	E	1120	GLN
1	E	1124	GLN
1	E	1162	GLN
1	F	692	HIS
1	F	725	GLN
1	F	775	ASN
1	F	952	GLN
1	F	1055	GLN
1	F	1077	GLN
1	F	1120	GLN
1	F	1151	HIS
1	F	1160	ASN
1	F	1162	GLN
1	F	1167	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	C	1201	-	94,101,101	1.20	8 (8%)	149,166,166	1.70	35 (23%)
2	B12	E	1201	-	94,101,101	1.21	9 (9%)	149,166,166	1.71	29 (19%)
2	B12	B	1201	-	94,101,101	1.23	8 (8%)	149,166,166	1.76	31 (20%)
2	B12	A	1201	-	94,101,101	1.11	7 (7%)	149,166,166	1.85	36 (24%)
2	B12	D	1201	-	94,101,101	1.20	6 (6%)	149,166,166	1.80	36 (24%)
2	B12	F	1201	-	94,101,101	1.27	8 (8%)	149,166,166	1.64	32 (21%)

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	C	1201	-	-	27/56/223/223	0/3/11/11
2	B12	E	1201	-	-	28/56/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B12	B	1201	-	-	25/56/223/223	0/3/11/11
2	B12	A	1201	-	-	24/56/223/223	0/3/11/11
2	B12	D	1201	-	-	20/56/223/223	0/3/11/11
2	B12	F	1201	-	-	26/56/223/223	0/3/11/11

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	B12	C19-N24	-5.21	1.42	1.49
2	F	1201	B12	C19-N24	-5.13	1.42	1.49
2	E	1201	B12	C19-N24	-5.11	1.42	1.49
2	B	1201	B12	C19-N24	-4.98	1.42	1.49
2	C	1201	B12	C19-N24	-4.76	1.43	1.49
2	A	1201	B12	C19-N24	-4.52	1.43	1.49
2	D	1201	B12	C20-C1	3.48	1.60	1.53
2	C	1201	B12	O51-C50	3.24	1.33	1.23
2	E	1201	B12	C18-C19	-3.19	1.47	1.53
2	F	1201	B12	C6B-C5B	3.14	1.48	1.40
2	F	1201	B12	C18-C19	-3.13	1.47	1.53
2	A	1201	B12	O44-C43	2.86	1.32	1.23
2	D	1201	B12	C6B-C5B	2.84	1.47	1.40
2	B	1201	B12	C6B-C5B	2.62	1.47	1.40
2	F	1201	B12	C54-C17	2.62	1.58	1.54
2	A	1201	B12	C6B-C5B	2.61	1.47	1.40
2	E	1201	B12	C53-C15	-2.58	1.45	1.50
2	C	1201	B12	C37-C38	2.58	1.60	1.51
2	F	1201	B12	C35-C5	-2.54	1.45	1.50
2	C	1201	B12	C6B-C5B	2.51	1.47	1.40
2	D	1201	B12	C18-C19	-2.51	1.48	1.53
2	D	1201	B12	C46-C12	2.45	1.59	1.54
2	F	1201	B12	C36-C7	2.43	1.58	1.54
2	F	1201	B12	C46-C12	2.41	1.58	1.54
2	B	1201	B12	C47-C12	2.35	1.58	1.54
2	E	1201	B12	C35-C5	-2.28	1.46	1.50
2	C	1201	B12	C2B-N1B	-2.26	1.33	1.37
2	E	1201	B12	C26-C2	2.24	1.60	1.55
2	B	1201	B12	C18-C19	-2.24	1.49	1.53
2	A	1201	B12	C18-C19	-2.23	1.49	1.53
2	C	1201	B12	P-O4	-2.23	1.43	1.50
2	E	1201	B12	C31-C32	2.22	1.60	1.51
2	D	1201	B12	C54-C17	2.22	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1201	B12	C6B-C5B	2.20	1.46	1.40
2	E	1201	B12	O34-C32	2.20	1.30	1.23
2	B	1201	B12	C26-C2	2.20	1.60	1.55
2	C	1201	B12	C18-C19	-2.17	1.49	1.53
2	C	1201	B12	C7B-C6B	2.13	1.42	1.39
2	A	1201	B12	C2R-C3R	-2.13	1.48	1.53
2	F	1201	B12	O28-C27	2.11	1.30	1.23
2	B	1201	B12	C7B-C6B	2.08	1.42	1.39
2	A	1201	B12	O7R-C2R	-2.07	1.37	1.43
2	B	1201	B12	C60-C61	2.06	1.57	1.51
2	E	1201	B12	C2R-C3R	-2.05	1.48	1.53
2	B	1201	B12	C54-C17	2.03	1.57	1.54
2	A	1201	B12	C43-N45	2.00	1.39	1.32

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	B12	C9B-C8B-N1B	7.87	108.79	105.30
2	A	1201	B12	C41-C8-C9	-7.37	98.32	111.19
2	E	1201	B12	C19-N24-C16	6.87	114.80	107.29
2	D	1201	B12	C19-N24-C16	6.47	114.36	107.29
2	F	1201	B12	C9B-C8B-N1B	6.05	107.98	105.30
2	E	1201	B12	O34-C32-N33	-5.81	107.03	122.53
2	A	1201	B12	C19-N24-C16	5.60	113.42	107.29
2	B	1201	B12	O58-C57-C56	-5.60	111.87	122.02
2	F	1201	B12	C9-N22-C6	5.40	111.78	105.28
2	E	1201	B12	C9-N22-C6	5.19	111.52	105.28
2	A	1201	B12	O58-C57-C56	-5.04	112.88	122.02
2	E	1201	B12	C41-C8-C9	-4.96	102.53	111.19
2	C	1201	B12	C35-C5-C6	-4.93	114.47	122.41
2	C	1201	B12	C19-N24-C16	4.92	112.67	107.29
2	D	1201	B12	C12-C13-C14	-4.80	94.36	102.26
2	A	1201	B12	C9-N22-C6	4.72	110.96	105.28
2	D	1201	B12	O63-C61-C60	-4.64	111.17	120.87
2	D	1201	B12	C9-N22-C6	4.58	110.79	105.28
2	B	1201	B12	C19-N24-C16	4.57	112.29	107.29
2	F	1201	B12	C19-N24-C16	4.50	112.21	107.29
2	E	1201	B12	O58-C57-C56	-4.42	114.01	122.02
2	A	1201	B12	C60-C61-N62	4.42	126.76	116.19
2	A	1201	B12	O34-C32-N33	-4.36	110.90	122.53
2	C	1201	B12	C9-N22-C6	4.36	110.52	105.28
2	D	1201	B12	C9B-C8B-N1B	4.17	107.15	105.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	B12	O58-C57-C56	-4.13	114.53	122.02
2	C	1201	B12	C2-C3-C4	3.98	106.12	101.64
2	A	1201	B12	C2-C3-C4	3.97	106.11	101.64
2	A	1201	B12	C55-C17-C16	3.95	124.32	116.59
2	B	1201	B12	C9-N22-C6	3.91	109.98	105.28
2	B	1201	B12	C41-C8-C9	-3.91	104.37	111.19
2	C	1201	B12	C2P-C1P-N59	-3.89	107.20	112.92
2	D	1201	B12	C55-C17-C16	3.87	124.16	116.59
2	D	1201	B12	C20-C1-C2	3.78	119.52	113.28
2	B	1201	B12	O63-C61-N62	-3.75	112.52	122.53
2	A	1201	B12	C47-C12-C46	-3.64	103.38	109.41
2	A	1201	B12	C15-C14-N23	-3.51	122.02	126.26
2	D	1201	B12	C13-C14-C15	-3.47	119.04	124.32
2	B	1201	B12	O58-C57-N59	3.47	129.84	123.03
2	E	1201	B12	C55-C17-C16	3.44	123.32	116.59
2	D	1201	B12	O51-C50-C49	-3.39	110.81	121.04
2	B	1201	B12	C60-C61-N62	3.38	124.28	116.19
2	D	1201	B12	O34-C32-N33	-3.35	113.59	122.53
2	E	1201	B12	C30-C3-C4	3.34	117.49	109.66
2	C	1201	B12	C13-C12-C11	-3.32	97.26	100.97
2	B	1201	B12	C54-C17-C16	-3.31	95.28	112.41
2	E	1201	B12	O34-C32-C31	3.30	131.02	121.04
2	F	1201	B12	C55-C17-C16	3.28	123.01	116.59
2	C	1201	B12	C54-C17-C18	-3.27	108.29	112.99
2	A	1201	B12	C2P-C1P-N59	-3.26	108.12	112.92
2	C	1201	B12	C5-C6-N22	-3.26	118.95	123.88
2	B	1201	B12	O34-C32-N33	-3.25	113.84	122.53
2	D	1201	B12	C60-C61-N62	3.24	123.94	116.19
2	F	1201	B12	C54-C17-C16	-3.24	95.65	112.41
2	A	1201	B12	C9B-C8B-N1B	3.22	106.73	105.30
2	E	1201	B12	C47-C12-C46	-3.21	104.08	109.41
2	D	1201	B12	C36-C7-C37	3.19	116.16	110.74
2	B	1201	B12	C18-C19-N24	3.17	107.10	102.33
2	F	1201	B12	C60-C61-N62	3.17	123.78	116.19
2	C	1201	B12	O58-C57-N59	3.15	129.21	123.03
2	C	1201	B12	O63-C61-N62	-3.14	114.16	122.53
2	A	1201	B12	C35-C5-C6	-3.08	117.46	122.41
2	D	1201	B12	C2-C3-C4	3.07	105.10	101.64
2	E	1201	B12	C19-C1-N21	-3.07	98.98	102.14
2	C	1201	B12	C60-C61-N62	3.06	123.51	116.19
2	D	1201	B12	C4B-C5B-C6B	3.01	124.10	119.69
2	A	1201	B12	C3-C4-N21	-3.00	108.25	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1201	B12	C2P-C1P-N59	-2.99	108.52	112.92
2	B	1201	B12	C31-C32-N33	2.98	126.05	116.49
2	F	1201	B12	O58-C57-C56	-2.96	116.65	122.02
2	E	1201	B12	C60-C61-N62	2.95	123.26	116.19
2	E	1201	B12	C54-C17-C16	-2.94	97.17	112.41
2	F	1201	B12	C13-C12-C11	-2.93	97.70	100.97
2	B	1201	B12	C49-C50-N52	2.89	125.77	116.49
2	F	1201	B12	C12-C13-C14	-2.89	97.51	102.26
2	F	1201	B12	C18-C19-N24	2.87	106.65	102.33
2	A	1201	B12	C10-C11-N23	-2.85	119.58	124.42
2	C	1201	B12	C55-C17-C16	2.85	122.16	116.59
2	D	1201	B12	C36-C7-C8	2.84	117.29	112.05
2	F	1201	B12	C53-C15-C16	2.84	125.19	120.36
2	E	1201	B12	C12-C11-C10	2.84	127.06	123.40
2	F	1201	B12	O34-C32-N33	-2.83	114.98	122.53
2	D	1201	B12	C1P-N59-C57	-2.82	116.64	122.69
2	A	1201	B12	C12-C11-C10	2.81	127.03	123.40
2	D	1201	B12	C20-C1-N21	-2.78	105.66	110.26
2	A	1201	B12	C36-C7-C37	2.76	115.42	110.74
2	A	1201	B12	C31-C32-N33	2.75	125.31	116.49
2	A	1201	B12	C54-C17-C16	-2.75	98.16	112.41
2	A	1201	B12	O58-C57-N59	2.74	128.42	123.03
2	C	1201	B12	O7R-C2R-C3R	2.74	118.86	111.19
2	B	1201	B12	C16-C15-C14	-2.74	117.09	121.26
2	C	1201	B12	O28-C27-C26	2.71	130.38	121.98
2	D	1201	B12	C49-C50-N52	2.70	125.16	116.49
2	C	1201	B12	C9B-C8B-N1B	2.68	106.49	105.30
2	B	1201	B12	C2P-C1P-N59	-2.67	109.00	112.92
2	D	1201	B12	C17-C16-N24	-2.65	107.12	111.17
2	C	1201	B12	C20-C1-C19	-2.63	106.82	109.35
2	F	1201	B12	O7R-C2R-C3R	2.62	118.53	111.19
2	B	1201	B12	C8B-C9B-N3B	-2.61	107.17	110.00
2	D	1201	B12	C1-C19-N24	-2.60	103.35	106.25
2	A	1201	B12	O7R-C2R-C3R	2.60	118.47	111.19
2	F	1201	B12	C20-C1-C2	2.60	117.57	113.28
2	C	1201	B12	C47-C12-C11	2.60	119.36	110.08
2	E	1201	B12	C10-C11-N23	-2.60	120.02	124.42
2	F	1201	B12	C31-C32-N33	2.60	124.81	116.49
2	E	1201	B12	C9B-C8B-N1B	2.57	106.44	105.30
2	F	1201	B12	C12-C11-C10	2.57	126.71	123.40
2	B	1201	B12	C36-C7-C37	2.56	115.08	110.74
2	B	1201	B12	C55-C17-C16	2.55	121.58	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1201	B12	C35-C5-C6	-2.54	118.32	122.41
2	A	1201	B12	C4B-C5B-C6B	2.53	123.40	119.69
2	F	1201	B12	C8B-C9B-N3B	-2.52	107.27	110.00
2	C	1201	B12	O34-C32-N33	-2.51	115.84	122.53
2	F	1201	B12	O58-C57-N59	2.50	127.94	123.03
2	B	1201	B12	O6R-C1R-N1B	-2.50	103.28	108.09
2	C	1201	B12	C2R-C3R-C4R	2.50	107.61	103.24
2	E	1201	B12	C36-C7-C37	2.50	114.98	110.74
2	B	1201	B12	C47-C12-C11	2.49	118.98	110.08
2	C	1201	B12	C47-C12-C46	-2.49	105.28	109.41
2	D	1201	B12	O6R-C1R-N1B	-2.48	103.33	108.09
2	D	1201	B12	C3-C4-N21	-2.48	108.90	111.98
2	A	1201	B12	C19-C1-N21	-2.47	99.59	102.14
2	D	1201	B12	C20-C1-C19	2.47	111.73	109.35
2	F	1201	B12	C16-C15-C14	-2.47	117.50	121.26
2	D	1201	B12	C7B-C6B-C5B	-2.46	116.08	119.69
2	B	1201	B12	O7R-C2R-C3R	2.46	118.06	111.19
2	C	1201	B12	C19-C1-N21	-2.45	99.61	102.14
2	E	1201	B12	O58-C57-N59	2.45	127.84	123.03
2	A	1201	B12	O5-P-O4	2.45	123.84	112.44
2	C	1201	B12	C3-C4-N21	-2.45	108.94	111.98
2	B	1201	B12	C8B-N1B-C2B	-2.42	104.07	106.26
2	A	1201	B12	O2-C3R-C2R	2.41	120.32	111.68
2	F	1201	B12	C36-C7-C37	2.40	114.81	110.74
2	B	1201	B12	C55-C56-C57	2.39	116.58	111.25
2	A	1201	B12	C9B-C4B-C5B	-2.38	116.41	120.83
2	A	1201	B12	C10-C9-N22	2.38	128.46	125.74
2	C	1201	B12	C48-C49-C50	-2.37	104.50	112.55
2	B	1201	B12	C4B-C5B-C6B	2.37	123.17	119.69
2	B	1201	B12	C13-C12-C11	-2.37	98.32	100.97
2	B	1201	B12	O51-C50-N52	-2.37	116.21	122.53
2	C	1201	B12	C12-C13-C14	-2.36	98.38	102.26
2	D	1201	B12	O6R-C4R-C5R	2.35	114.19	109.22
2	F	1201	B12	C4B-C5B-C6B	2.35	123.13	119.69
2	D	1201	B12	C31-C32-N33	2.34	124.00	116.49
2	E	1201	B12	C12-C13-C14	-2.34	98.42	102.26
2	F	1201	B12	C49-C50-N52	2.34	123.98	116.49
2	C	1201	B12	O28-C27-N29	-2.33	116.31	122.53
2	D	1201	B12	C6M-C6B-C5B	2.31	125.48	120.76
2	F	1201	B12	C8-C9-C10	-2.31	118.42	123.33
2	A	1201	B12	O63-C61-N62	-2.30	116.39	122.53
2	D	1201	B12	C54-C17-C16	-2.28	100.61	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	B12	C12-C13-C14	-2.27	98.53	102.26
2	D	1201	B12	C55-C56-C57	2.27	116.31	111.25
2	A	1201	B12	C47-C12-C11	2.26	118.16	110.08
2	D	1201	B12	C5M-C5B-C6B	-2.26	116.15	120.76
2	E	1201	B12	C4B-C5B-C6B	2.25	123.00	119.69
2	C	1201	B12	C8B-C9B-N3B	-2.25	107.57	110.00
2	C	1201	B12	C7-C8-C9	-2.24	98.05	100.89
2	D	1201	B12	C12-C11-C10	-2.24	120.52	123.40
2	D	1201	B12	C37-C7-C8	-2.23	102.49	108.37
2	B	1201	B12	C20-C1-C2	2.23	116.95	113.28
2	C	1201	B12	C10-C9-N22	2.22	128.28	125.74
2	E	1201	B12	O63-C61-N62	-2.20	116.65	122.53
2	B	1201	B12	C5M-C5B-C6B	-2.19	116.28	120.76
2	F	1201	B12	C6M-C6B-C5B	2.19	125.24	120.76
2	E	1201	B12	C20-C1-N21	2.19	113.88	110.26
2	D	1201	B12	C47-C12-C11	2.18	117.87	110.08
2	F	1201	B12	C2-C3-C4	2.18	104.09	101.64
2	F	1201	B12	C3-C4-C5	2.17	127.45	123.82
2	C	1201	B12	C31-C32-N33	2.17	123.44	116.49
2	D	1201	B12	O2-C3R-C2R	2.17	119.45	111.68
2	E	1201	B12	O51-C50-N52	-2.15	116.78	122.53
2	E	1201	B12	C47-C12-C11	2.14	117.72	110.08
2	C	1201	B12	C55-C56-C57	2.13	116.01	111.25
2	A	1201	B12	C18-C19-N24	2.13	105.52	102.33
2	A	1201	B12	C25-C2-C1	2.12	116.93	113.75
2	D	1201	B12	C30-C3-C2	2.12	123.67	119.00
2	E	1201	B12	C9B-C4B-C5B	-2.11	116.92	120.83
2	C	1201	B12	O5-P-O4	2.10	122.22	112.44
2	A	1201	B12	C8B-C9B-N3B	-2.10	107.73	110.00
2	F	1201	B12	C10-C11-N23	-2.09	120.87	124.42
2	A	1201	B12	O6R-C1R-N1B	-2.09	104.08	108.09
2	A	1201	B12	C1-C2-C3	-2.09	98.97	101.60
2	D	1201	B12	O8R-C5R-C4R	-2.09	104.23	111.33
2	A	1201	B12	O6R-C4R-C5R	2.08	113.62	109.22
2	C	1201	B12	C60-C18-C19	2.08	120.00	114.59
2	C	1201	B12	C4B-C5B-C6B	2.08	122.74	119.69
2	A	1201	B12	C3-C4-C5	2.07	127.29	123.82
2	F	1201	B12	C35-C5-C4	-2.06	112.61	116.79
2	E	1201	B12	O6R-C4R-C5R	2.05	113.56	109.22
2	E	1201	B12	O2-C3R-C2R	2.05	119.04	111.68
2	B	1201	B12	C3-C4-N21	-2.05	109.43	111.98
2	C	1201	B12	C54-C17-C16	-2.04	101.86	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1201	B12	C20-C1-N21	-2.03	106.91	110.26
2	B	1201	B12	O2-C3R-C2R	2.02	118.93	111.68
2	E	1201	B12	O7R-C2R-C3R	2.01	116.83	111.19
2	F	1201	B12	C2P-C1P-N59	-2.01	109.96	112.92
2	F	1201	B12	C1R-N1B-C2B	2.01	131.56	127.09
2	F	1201	B12	C47-C12-C11	2.01	117.26	110.08

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	B12	C4-C3-C30-C31
2	A	1201	B12	C38-C37-C7-C36
2	A	1201	B12	C38-C37-C7-C8
2	A	1201	B12	C18-C60-C61-O63
2	A	1201	B12	C18-C60-C61-N62
2	B	1201	B12	C18-C60-C61-O63
2	B	1201	B12	C18-C60-C61-N62
2	C	1201	B12	C4-C3-C30-C31
2	C	1201	B12	C38-C37-C7-C36
2	C	1201	B12	C38-C37-C7-C8
2	C	1201	B12	C18-C60-C61-O63
2	C	1201	B12	C18-C60-C61-N62
2	C	1201	B12	N59-C1P-C2P-O3
2	D	1201	B12	C18-C60-C61-O63
2	D	1201	B12	C18-C60-C61-N62
2	E	1201	B12	C13-C48-C49-C50
2	E	1201	B12	C18-C60-C61-O63
2	E	1201	B12	C18-C60-C61-N62
2	F	1201	B12	C18-C60-C61-O63
2	F	1201	B12	C18-C60-C61-N62
2	E	1201	B12	C8-C41-C42-C43
2	A	1201	B12	C14-C13-C48-C49
2	B	1201	B12	C4-C3-C30-C31
2	C	1201	B12	C14-C13-C48-C49
2	D	1201	B12	C4-C3-C30-C31
2	E	1201	B12	C4-C3-C30-C31
2	F	1201	B12	C4-C3-C30-C31
2	A	1201	B12	C13-C48-C49-C50
2	C	1201	B12	C8-C41-C42-C43
2	A	1201	B12	C12-C13-C48-C49
2	C	1201	B12	C12-C13-C48-C49

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Mol	Chain	Res	Type	Atoms
2	E	1201	B12	C12-C13-C48-C49
2	D	1201	B12	C3-C2-C26-C27
2	B	1201	B12	C7-C37-C38-N40
2	E	1201	B12	C7-C37-C38-N40
2	A	1201	B12	C8-C41-C42-C43
2	B	1201	B12	C8-C41-C42-C43
2	E	1201	B12	C38-C37-C7-C36
2	E	1201	B12	C38-C37-C7-C8
2	F	1201	B12	C48-C49-C50-N52
2	E	1201	B12	C14-C13-C48-C49
2	F	1201	B12	C48-C49-C50-O51
2	C	1201	B12	C1P-C2P-O3-P
2	C	1201	B12	C3P-C2P-O3-P
2	B	1201	B12	C7-C37-C38-O39
2	D	1201	B12	C7-C37-C38-N40
2	F	1201	B12	C7-C37-C38-N40
2	C	1201	B12	C2-C3-C30-C31
2	B	1201	B12	C13-C48-C49-C50
2	A	1201	B12	C42-C41-C8-C9
2	F	1201	B12	C3-C2-C26-C27
2	A	1201	B12	C2-C3-C30-C31
2	B	1201	B12	C2-C3-C30-C31
2	B	1201	B12	C12-C13-C48-C49
2	D	1201	B12	C2-C3-C30-C31
2	C	1201	B12	C30-C31-C32-N33
2	F	1201	B12	C13-C48-C49-C50
2	A	1201	B12	C38-C37-C7-C6
2	C	1201	B12	C38-C37-C7-C6
2	C	1201	B12	C48-C49-C50-O51
2	C	1201	B12	C48-C49-C50-N52
2	E	1201	B12	C48-C49-C50-O51
2	D	1201	B12	C7-C37-C38-O39
2	F	1201	B12	C8-C41-C42-C43
2	E	1201	B12	C3P-C2P-O3-P
2	F	1201	B12	C7-C37-C38-O39
2	C	1201	B12	C13-C48-C49-C50
2	A	1201	B12	C2R-C1R-N1B-C8B
2	D	1201	B12	C48-C49-C50-O51
2	E	1201	B12	C42-C41-C8-C9
2	B	1201	B12	C2R-C1R-N1B-C2B
2	C	1201	B12	C2R-C1R-N1B-C2B
2	F	1201	B12	C2R-C1R-N1B-C2B

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Mol	Chain	Res	Type	Atoms
2	A	1201	B12	C48-C49-C50-O51
2	B	1201	B12	C42-C41-C8-C9
2	E	1201	B12	C2-C3-C30-C31
2	F	1201	B12	C2-C3-C30-C31
2	B	1201	B12	C3-C30-C31-C32
2	E	1201	B12	C48-C49-C50-N52
2	D	1201	B12	C17-C55-C56-C57
2	D	1201	B12	C25-C2-C26-C27
2	C	1201	B12	N59-C1P-C2P-C3P
2	C	1201	B12	C19-C18-C60-C61
2	D	1201	B12	C19-C18-C60-C61
2	A	1201	B12	O6R-C1R-N1B-C8B
2	B	1201	B12	C2R-C1R-N1B-C8B
2	B	1201	B12	O6R-C1R-N1B-C8B
2	C	1201	B12	C2R-C1R-N1B-C8B
2	C	1201	B12	O6R-C1R-N1B-C8B
2	D	1201	B12	C2R-C1R-N1B-C8B
2	D	1201	B12	O6R-C1R-N1B-C8B
2	E	1201	B12	C2R-C1R-N1B-C8B
2	E	1201	B12	O6R-C1R-N1B-C8B
2	F	1201	B12	C2R-C1R-N1B-C8B
2	F	1201	B12	O6R-C1R-N1B-C8B
2	A	1201	B12	C48-C49-C50-N52
2	E	1201	B12	C1P-C2P-O3-P
2	E	1201	B12	C30-C31-C32-O34
2	D	1201	B12	C38-C37-C7-C8
2	F	1201	B12	C38-C37-C7-C36
2	F	1201	B12	C38-C37-C7-C8
2	D	1201	B12	C48-C49-C50-N52
2	D	1201	B12	C2R-C1R-N1B-C2B
2	B	1201	B12	C3-C2-C26-C27
2	E	1201	B12	C7-C37-C38-O39
2	A	1201	B12	C17-C18-C60-C61
2	A	1201	B12	C19-C18-C60-C61
2	B	1201	B12	C19-C18-C60-C61
2	C	1201	B12	C17-C18-C60-C61
2	D	1201	B12	C17-C18-C60-C61
2	E	1201	B12	C17-C18-C60-C61
2	E	1201	B12	C19-C18-C60-C61
2	F	1201	B12	O6R-C1R-N1B-C2B
2	B	1201	B12	C30-C31-C32-N33
2	F	1201	B12	C55-C56-C57-O58

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Mol	Chain	Res	Type	Atoms
2	A	1201	B12	C1P-C2P-O3-P
2	A	1201	B12	C3P-C2P-O3-P
2	B	1201	B12	C48-C49-C50-O51
2	B	1201	B12	C48-C49-C50-N52
2	E	1201	B12	C55-C56-C57-O58
2	C	1201	B12	C30-C31-C32-O34
2	B	1201	B12	C17-C18-C60-C61
2	E	1201	B12	C2R-C1R-N1B-C2B
2	A	1201	B12	C30-C31-C32-N33
2	F	1201	B12	C30-C31-C32-N33
2	B	1201	B12	O6R-C1R-N1B-C2B
2	D	1201	B12	C30-C31-C32-N33
2	A	1201	B12	C2R-C1R-N1B-C2B
2	A	1201	B12	C2P-O3-P-O4
2	A	1201	B12	C2P-O3-P-O5
2	B	1201	B12	C2P-O3-P-O4
2	C	1201	B12	C2P-O3-P-O4
2	C	1201	B12	C2P-O3-P-O5
2	D	1201	B12	C2P-O3-P-O5
2	E	1201	B12	C2P-O3-P-O4
2	E	1201	B12	C2P-O3-P-O5
2	F	1201	B12	N59-C1P-C2P-O3
2	F	1201	B12	C2P-O3-P-O4
2	F	1201	B12	C2P-O3-P-O5
2	B	1201	B12	C55-C56-C57-O58
2	B	1201	B12	C25-C2-C26-C27
2	F	1201	B12	C25-C2-C26-C27
2	F	1201	B12	C55-C56-C57-N59
2	F	1201	B12	C17-C18-C60-C61
2	F	1201	B12	C19-C18-C60-C61
2	B	1201	B12	C30-C31-C32-O34
2	E	1201	B12	C30-C31-C32-N33
2	C	1201	B12	O6R-C1R-N1B-C2B
2	D	1201	B12	C2P-C1P-N59-C57
2	E	1201	B12	C38-C37-C7-C6

There are no ring outliers.

6 monomers are involved in 27 short contacts:

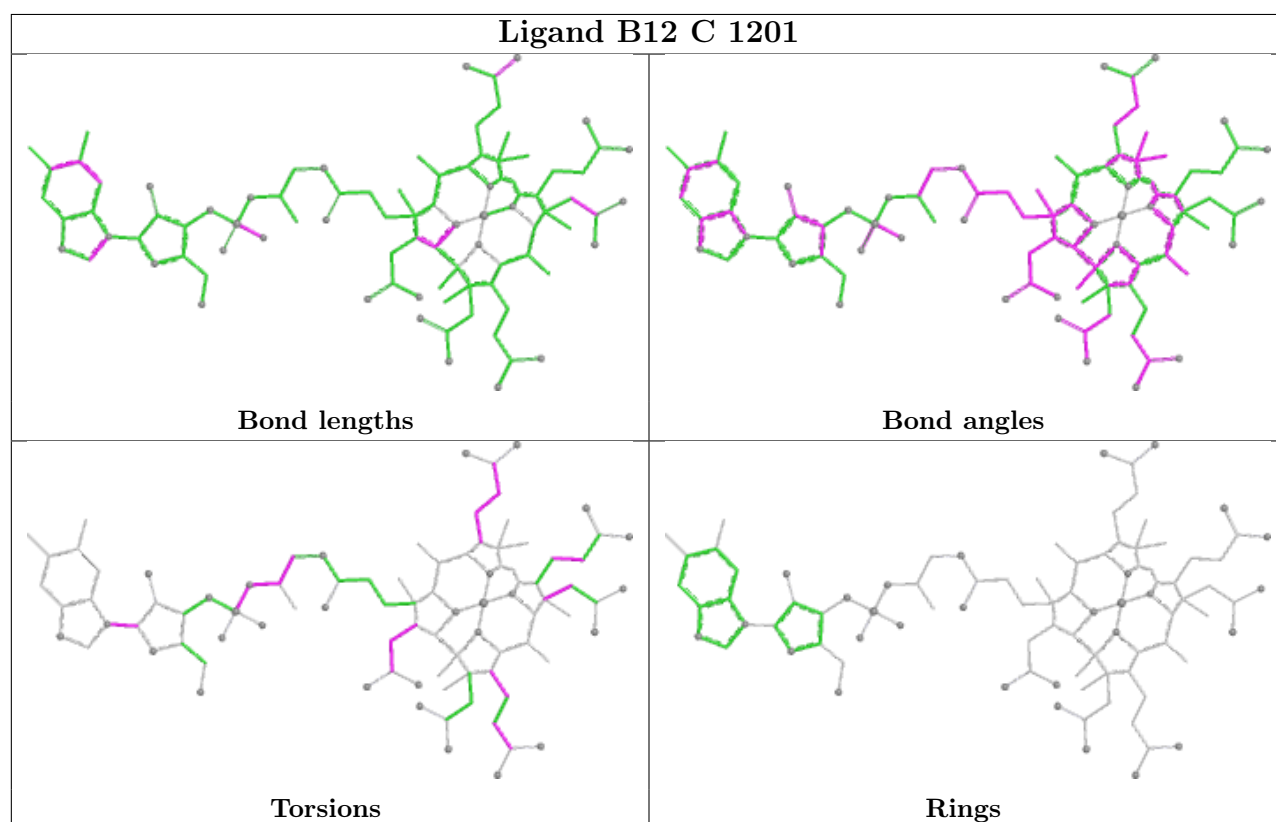
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	B12	7	0
2	E	1201	B12	4	0

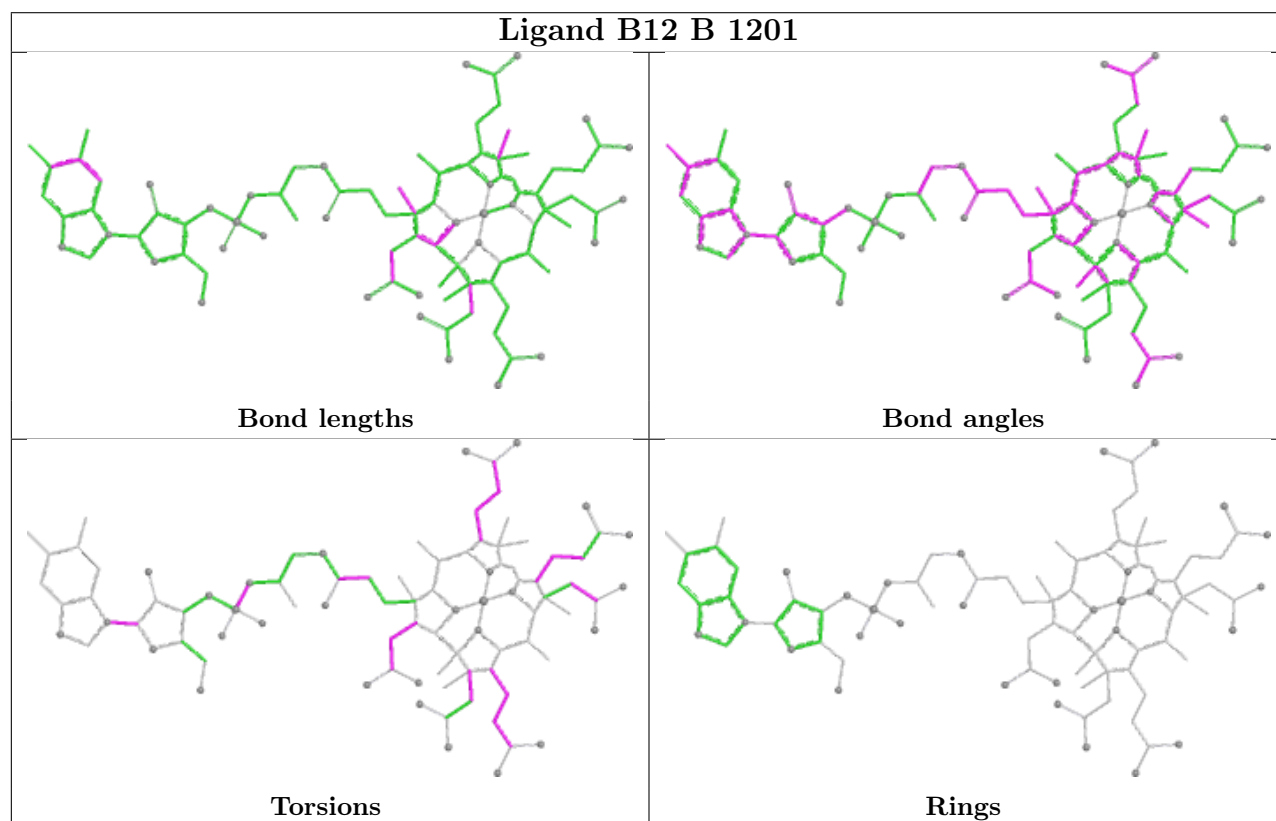
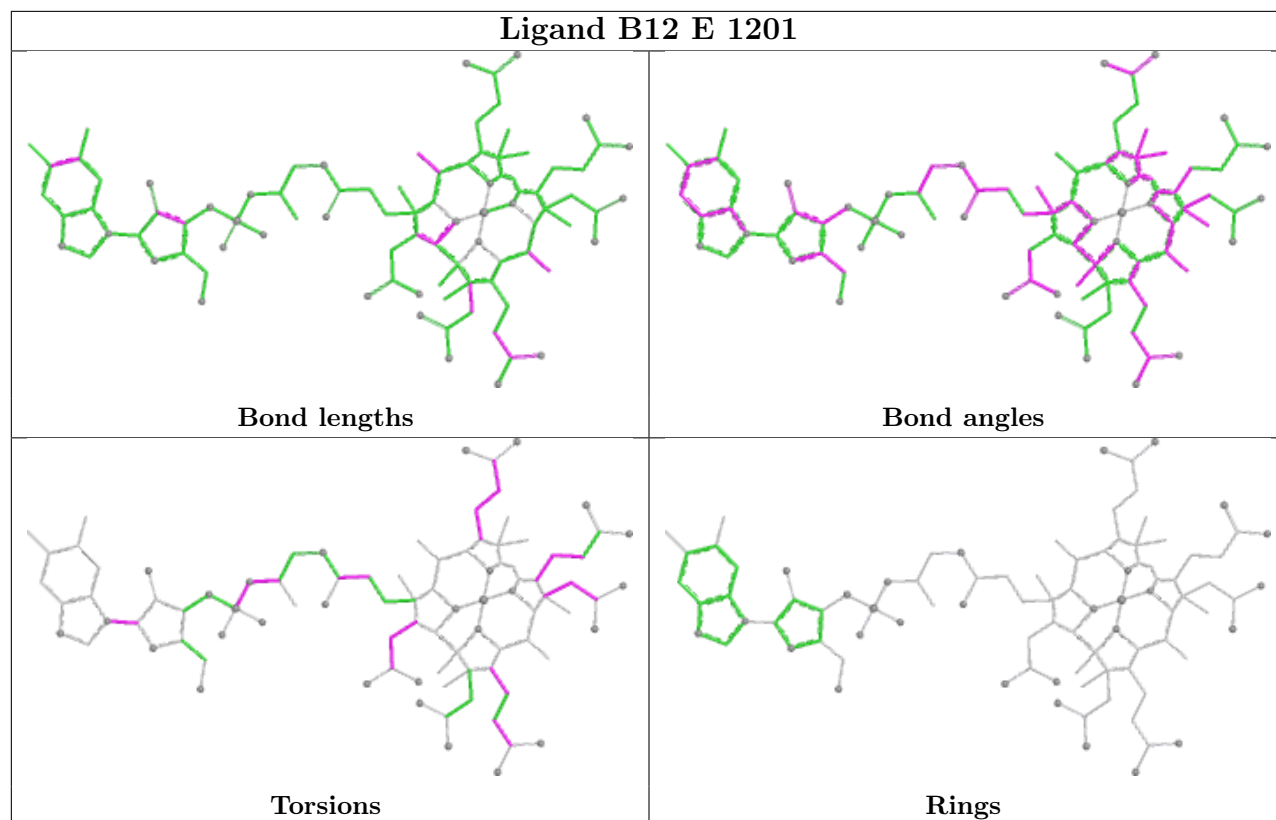
Continued on next page...

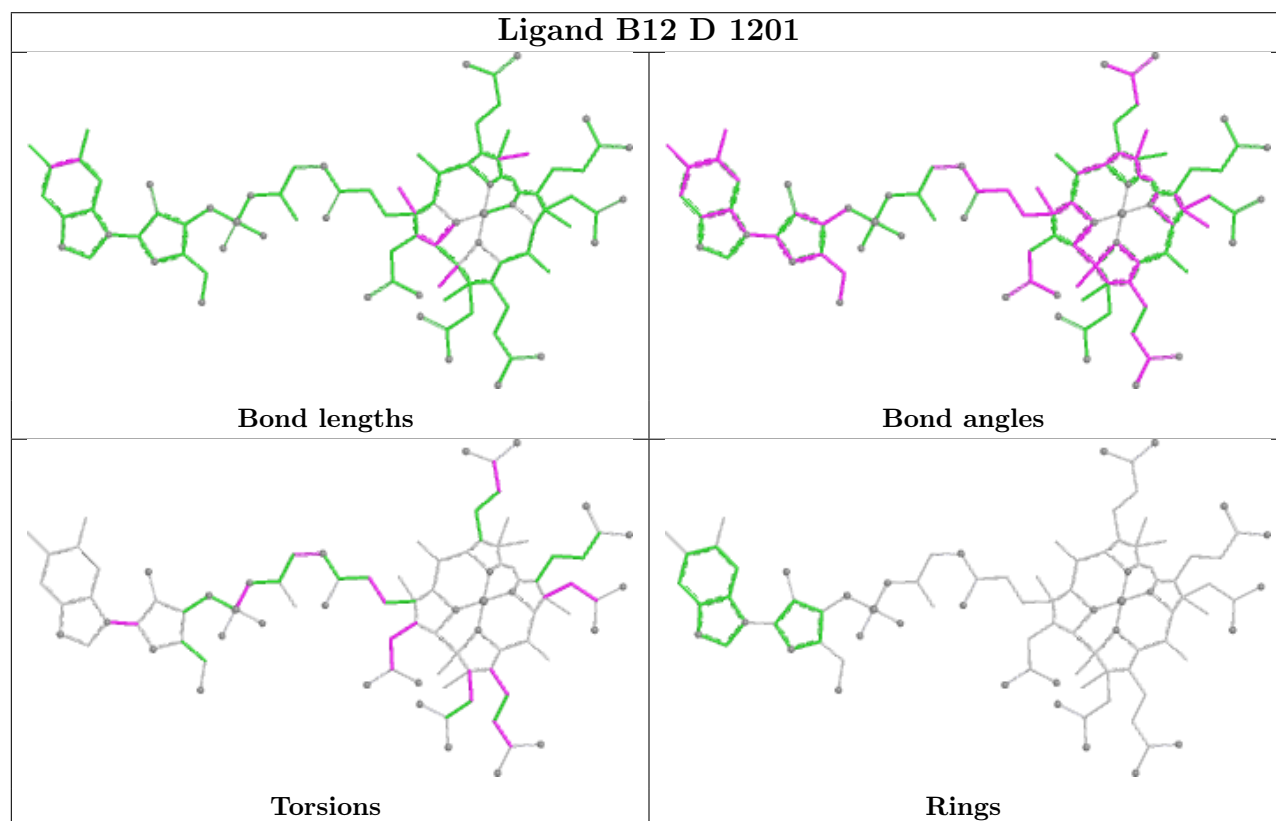
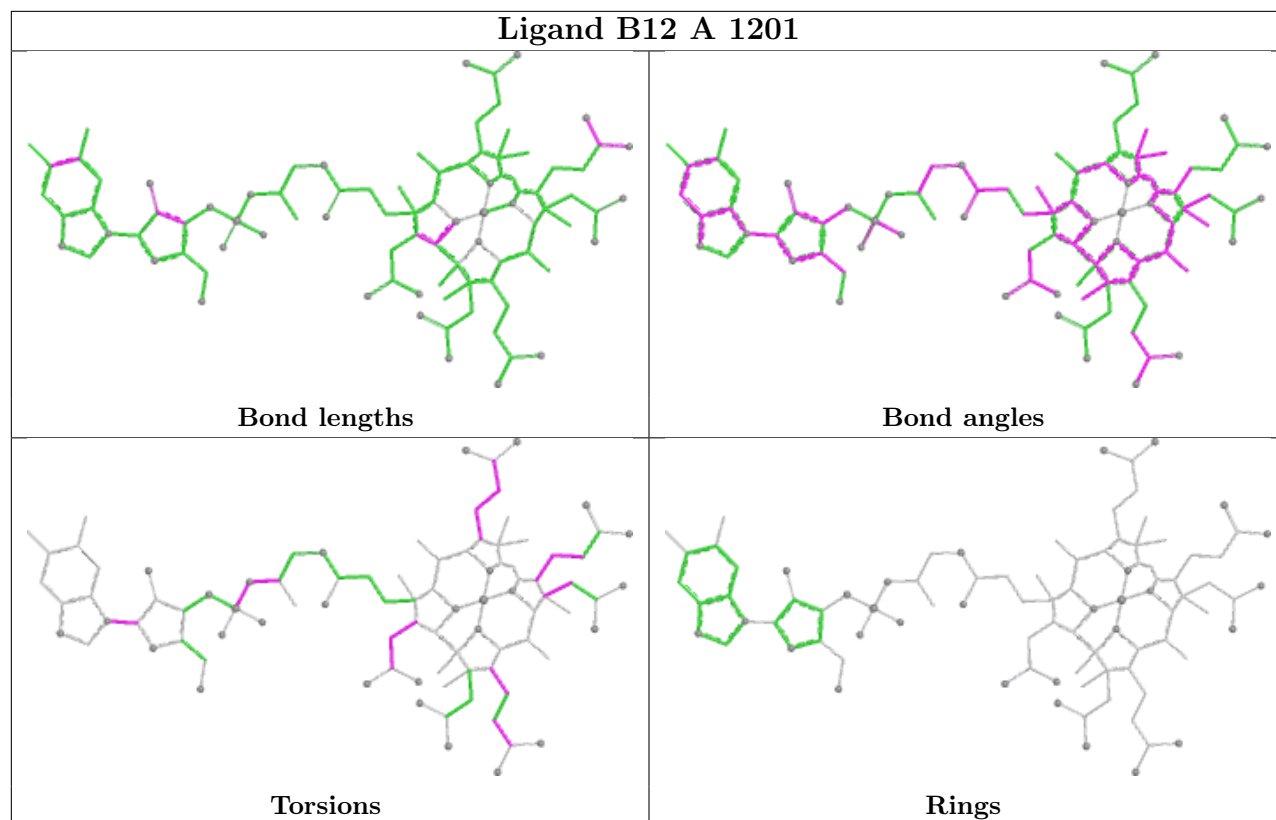
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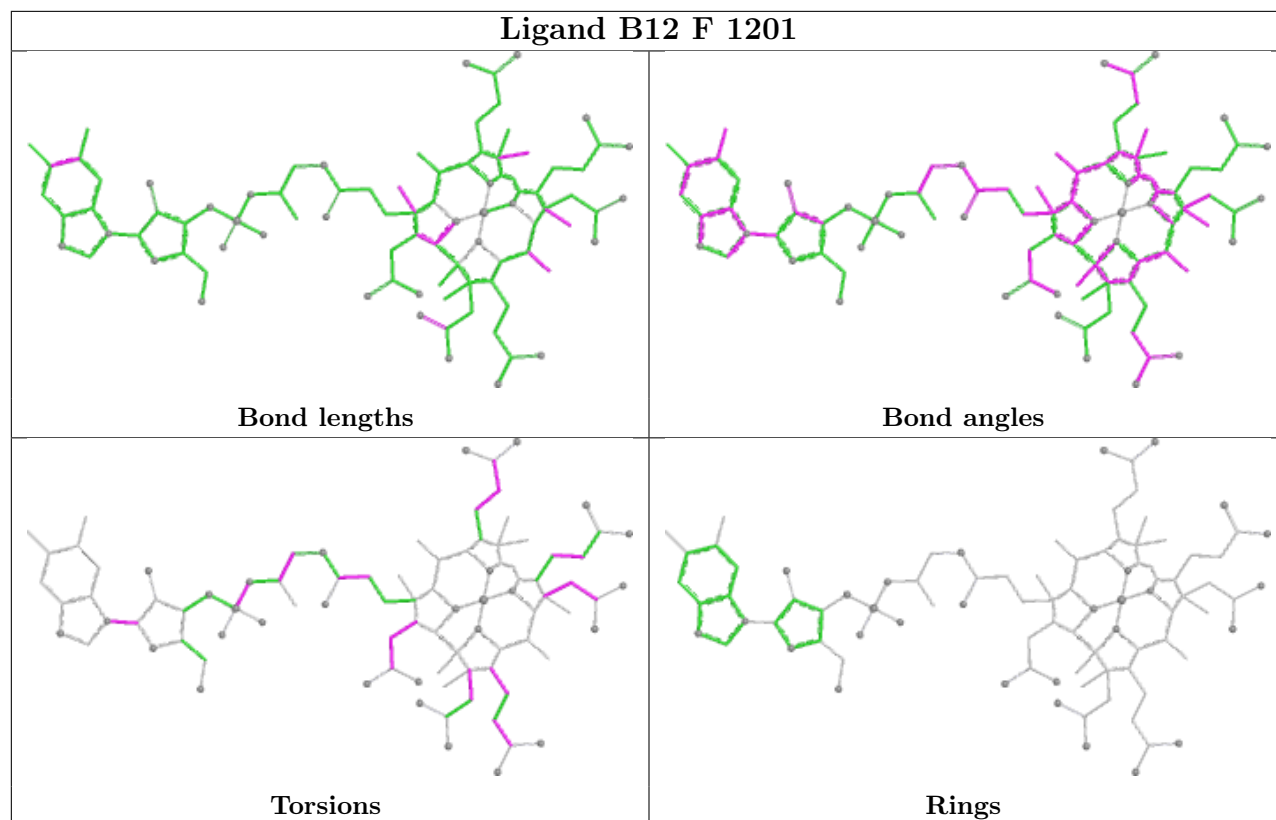
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	B12	2	0
2	A	1201	B12	6	0
2	D	1201	B12	5	0
2	F	1201	B12	3	0

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	507/523 (96%)	0.03	7 (1%) 73 53	30, 65, 160, 219	0
1	B	506/523 (96%)	0.24	6 (1%) 76 57	49, 86, 163, 226	0
1	C	507/523 (96%)	0.01	3 (0%) 85 72	30, 65, 151, 220	0
1	D	506/523 (96%)	0.24	4 (0%) 82 66	45, 86, 147, 211	0
1	E	507/523 (96%)	0.01	2 (0%) 88 78	30, 63, 133, 176	0
1	F	505/523 (96%)	0.24	13 (2%) 57 36	46, 86, 156, 271	0
All	All	3038/3138 (96%)	0.13	35 (1%) 76 57	30, 77, 154, 271	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	908	ARG	2.9
1	C	1115	ILE	2.9
1	F	905	ALA	2.8
1	B	1115	ILE	2.7
1	E	1115	ILE	2.6
1	D	1115	ILE	2.5
1	F	1161	PHE	2.5
1	B	834	LEU	2.4
1	F	866	LEU	2.4
1	F	879	THR	2.4
1	E	1111	ASP	2.4
1	F	936	ARG	2.4
1	F	665	LEU	2.4
1	A	760	VAL	2.4
1	D	1118	LEU	2.3
1	F	878	LEU	2.3
1	A	668	LEU	2.3
1	F	680	LEU	2.3
1	A	763	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	665	LEU	2.3
1	D	870	LEU	2.3
1	A	895	PRO	2.2
1	A	1118	LEU	2.2
1	C	905	ALA	2.2
1	A	684	LEU	2.2
1	B	905	ALA	2.2
1	F	869	GLU	2.1
1	F	684	LEU	2.1
1	F	807	GLY	2.1
1	A	1115	ILE	2.1
1	B	1118	LEU	2.1
1	B	1173	VAL	2.0
1	F	1115	ILE	2.0
1	D	801	HIS	2.0
1	F	668	LEU	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](#)

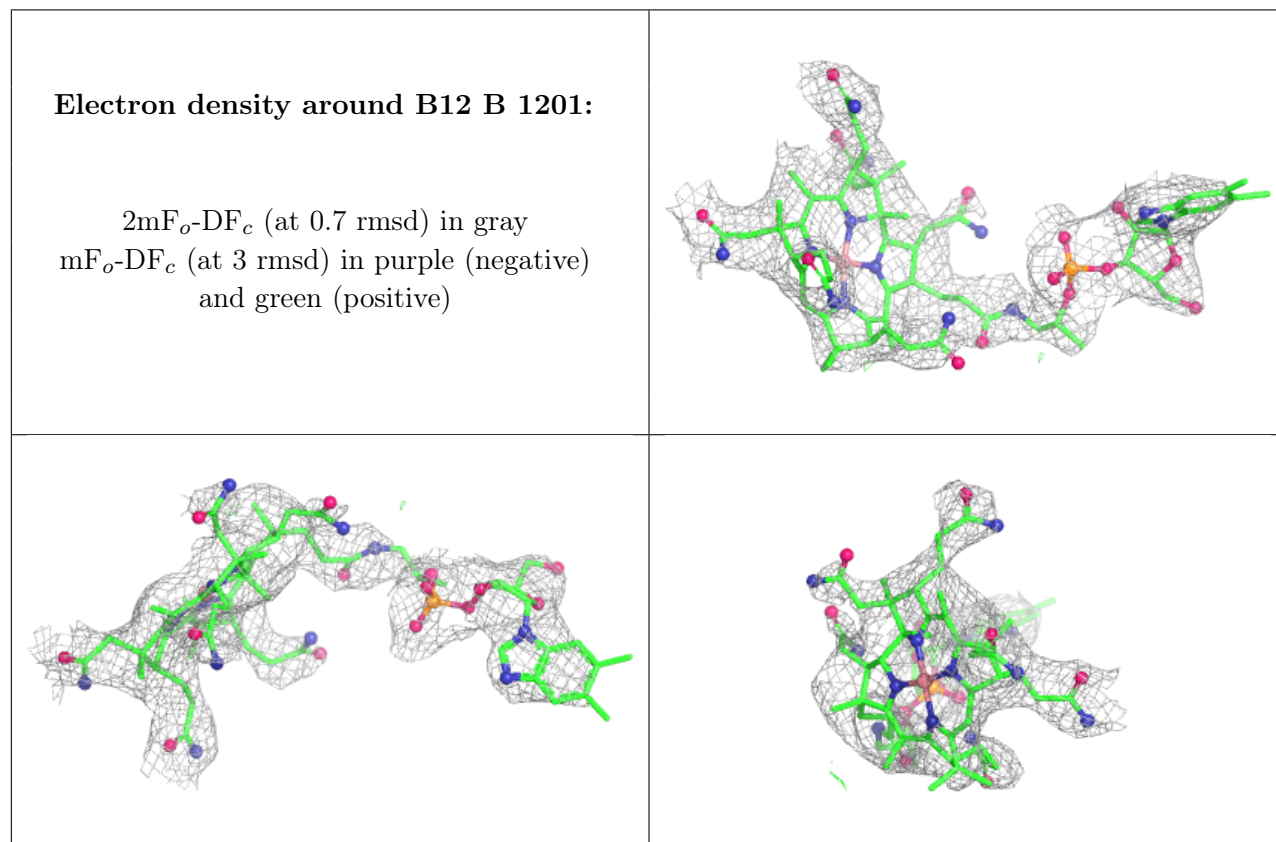
There are no oligosaccharides in this entry.

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.

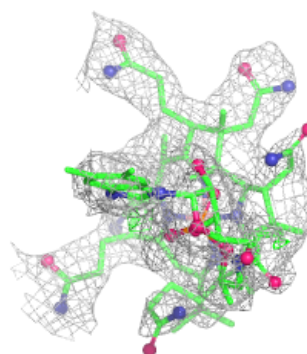
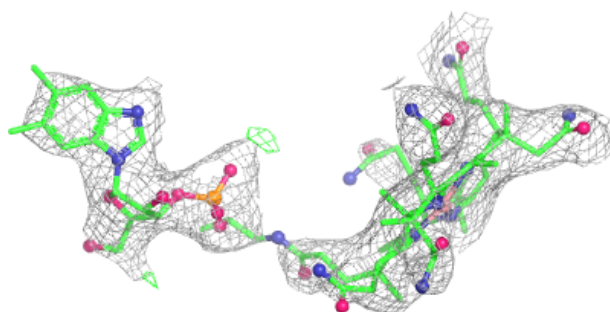
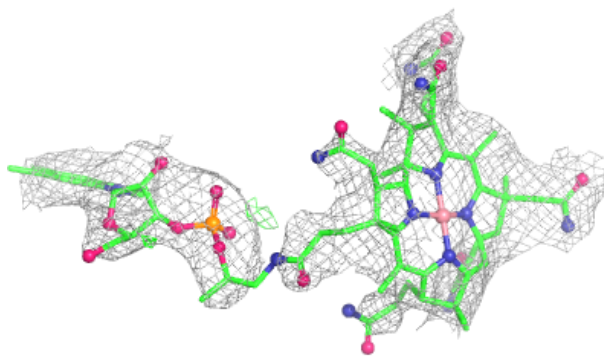
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B12	B	1201	91/91	0.91	0.12	56,80,101,115	0
2	B12	D	1201	91/91	0.93	0.10	53,78,104,119	0
2	B12	C	1201	91/91	0.94	0.10	41,56,79,94	0
2	B12	A	1201	91/91	0.94	0.10	34,54,86,103	0
2	B12	F	1201	91/91	0.94	0.11	49,83,119,134	0
2	B12	E	1201	91/91	0.95	0.10	36,52,80,93	0

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

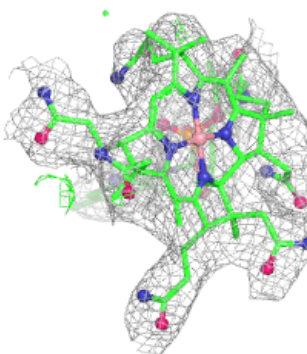
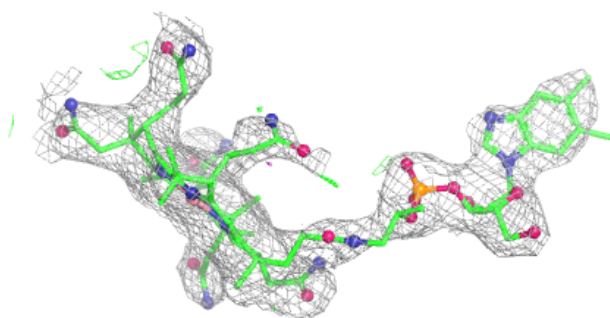
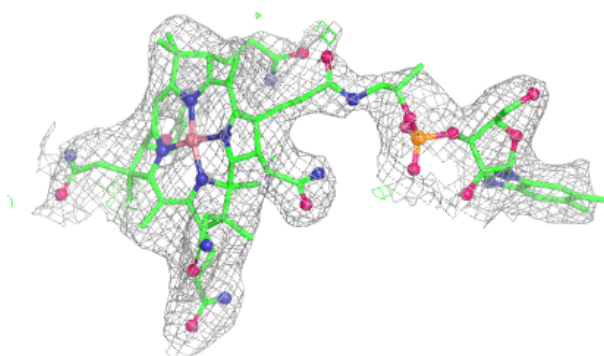


Electron density around B12 D 1201:

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

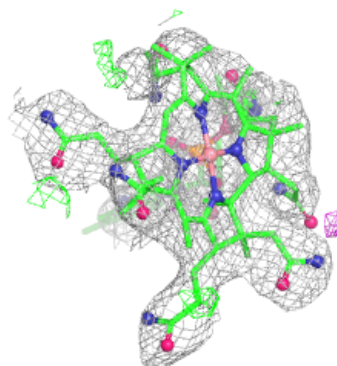
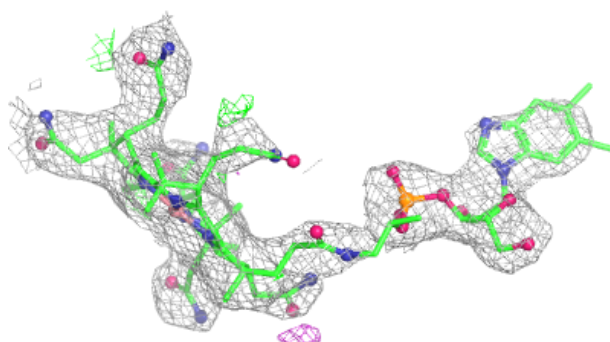
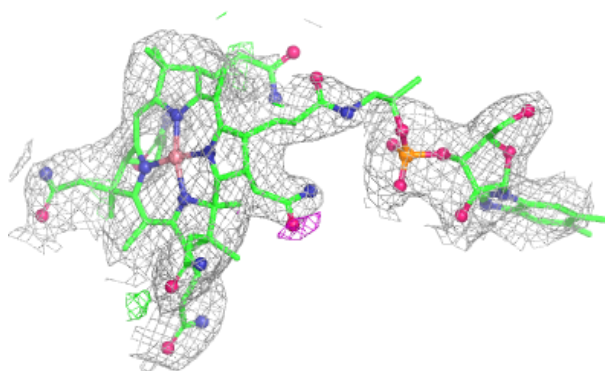
**Electron density around B12 C 1201:**

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

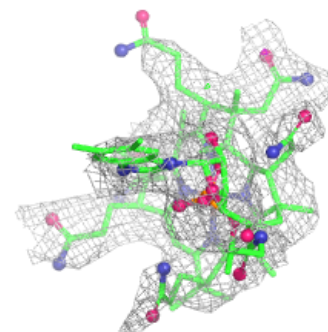
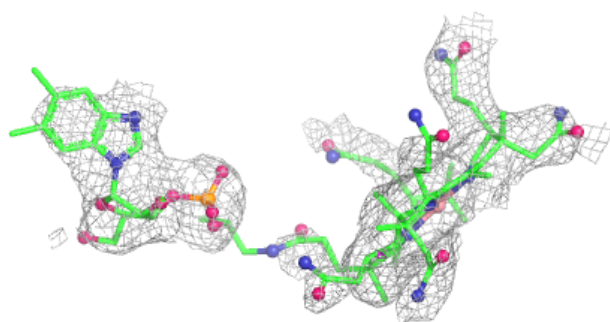
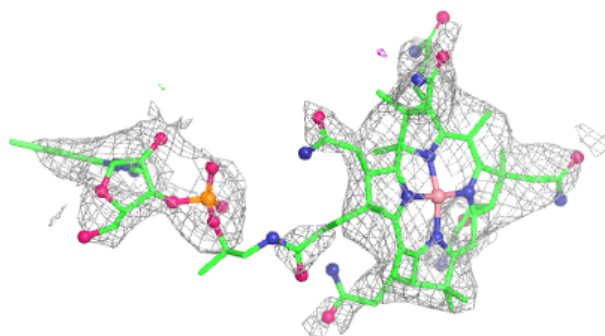


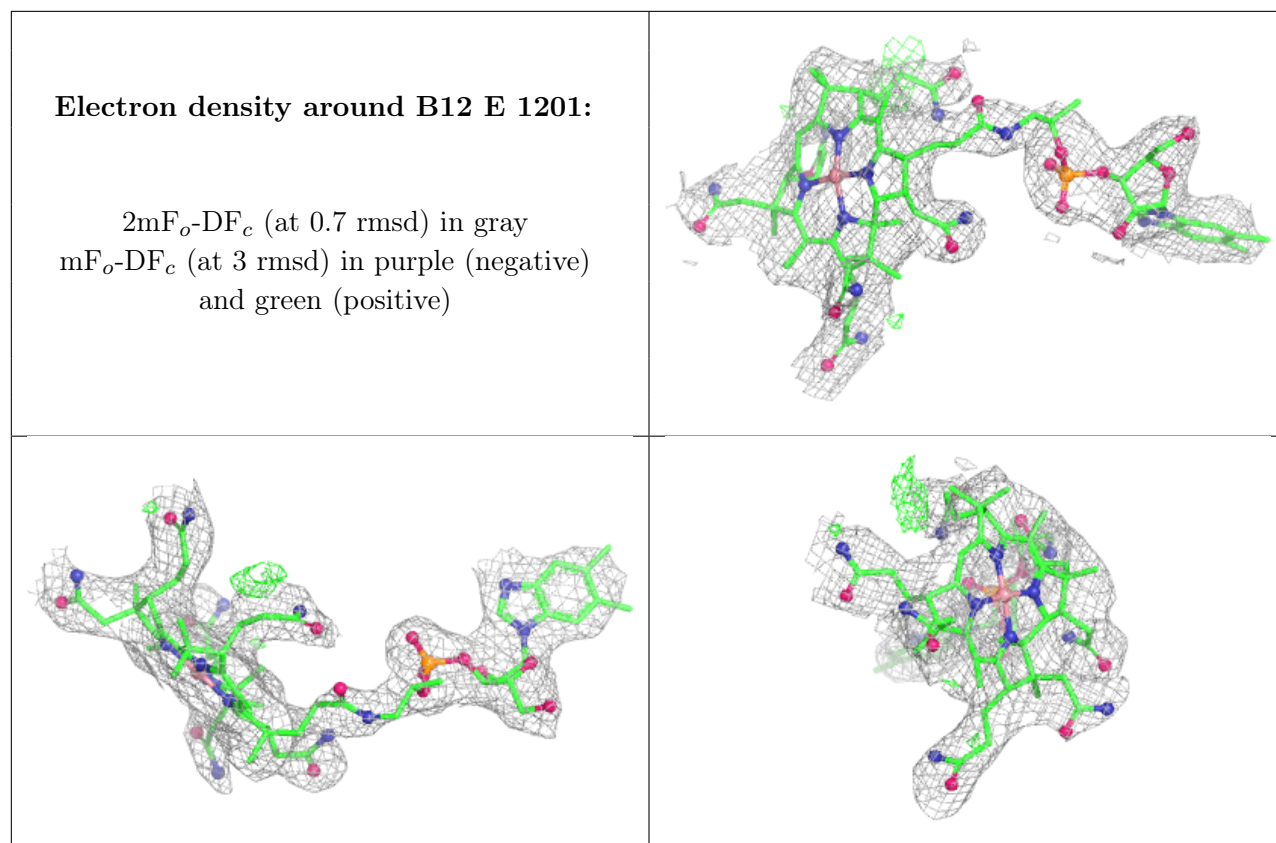
Electron density around B12 A 1201:

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

**Electron density around B12 F 1201:**

$2mF_o-DF_c$ (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.