



Full wwPDB X-ray Structure Validation Report i

Oct 6, 2023 – 04:46 AM EDT

PDB ID : 8SSE
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 i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

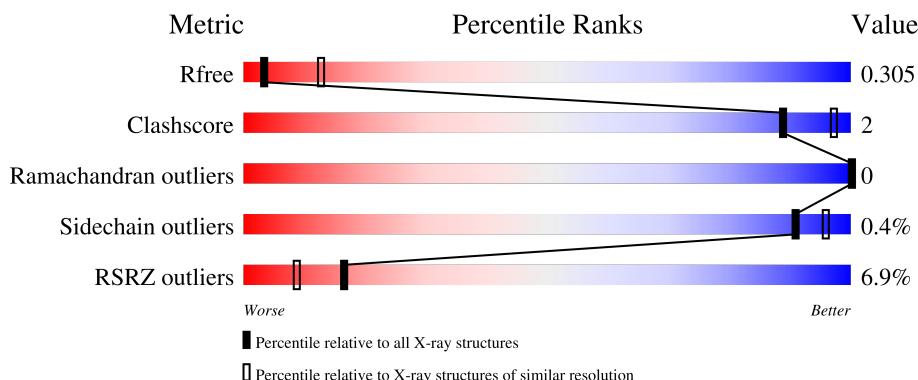
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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.



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Mol	Chain	Length	Quality of chain
1	F	523	<div style="width: 90%;"><div style="width: 8%;">8%</div><div style="width: 90%;">90%</div><div style="width: 7%;">7%</div></div>

2 Entry composition [\(i\)](#)

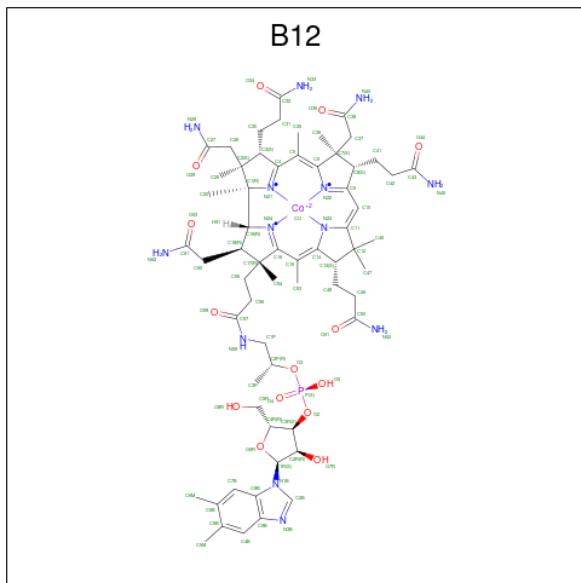
There are 3 unique types of molecules in this entry. The entry contains 24880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P) (labeled as "Ligand of Interest" by depositor).



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

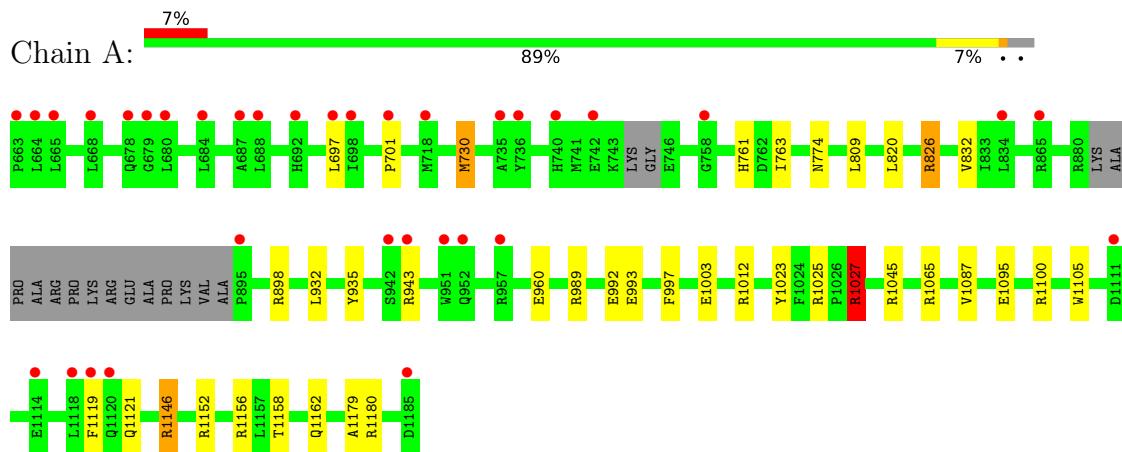
- Molecule 3 is water.

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		

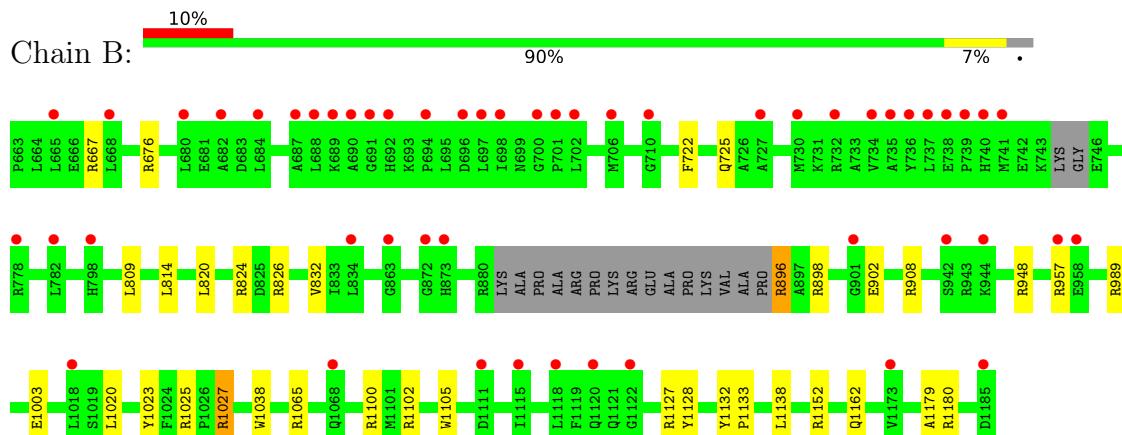
3 Residue-property plots (i)

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.

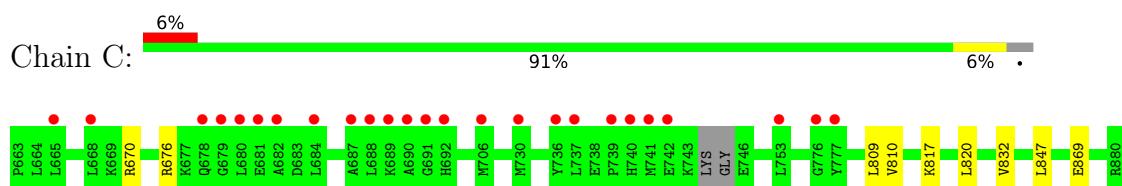
- Molecule 1: Methionine synthase



- Molecule 1: Methionine synthase

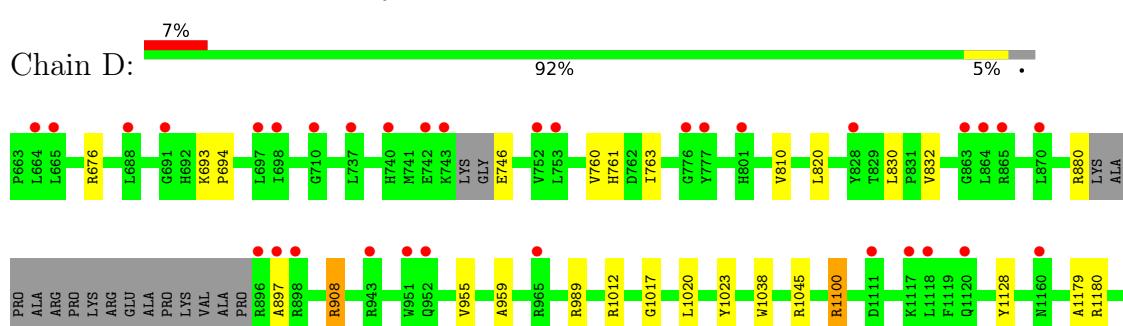


- Molecule 1: Methionine synthase

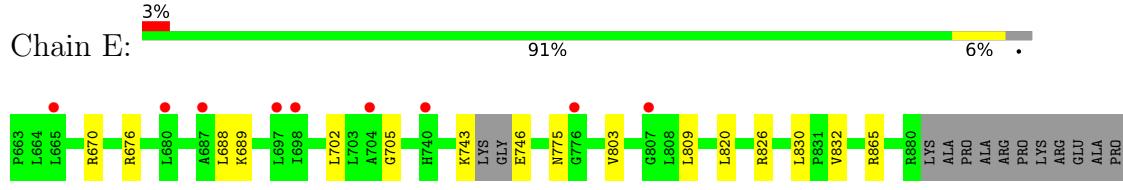




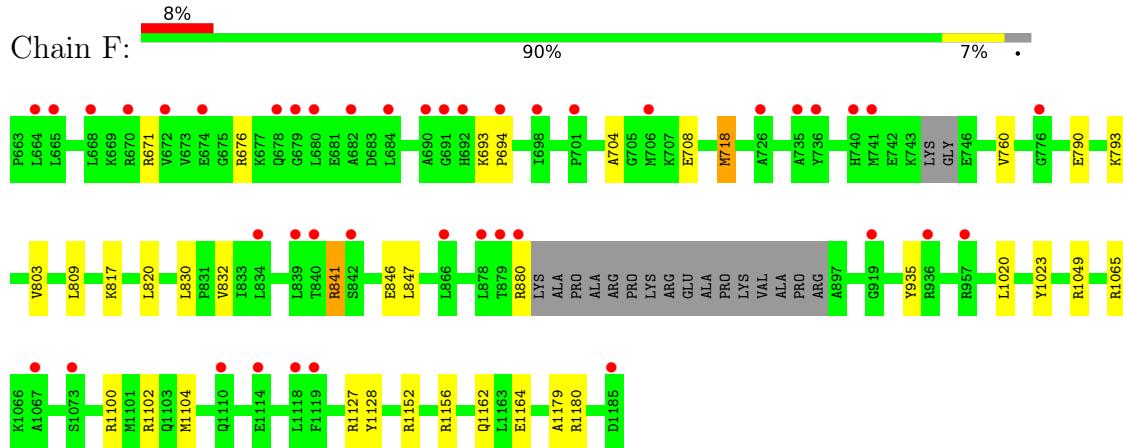
- Molecule 1: Methionine synthase



- Molecule 1: Methionine synthase



- Molecule 1: Methionine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.13 Å 95.84 Å 238.75 Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	49.30 – 3.15 49.25 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.30-3.15) 98.7 (49.25-3.15)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.70 (at 3.12 Å)	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 (5.09%)	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 , 68.8	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 i

5.1 Standard geometry i

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	0.66	5/4107 (0.1%)	1.00	11/5548 (0.2%)
1	B	0.57	1/4099 (0.0%)	0.97	10/5537 (0.2%)
1	C	0.66	5/4107 (0.1%)	0.99	4/5548 (0.1%)
1	D	0.57	0/4099	0.96	2/5537 (0.0%)
1	E	0.64	3/4107 (0.1%)	0.98	3/5548 (0.1%)
1	F	0.55	0/4088	0.96	8/5523 (0.1%)
All	All	0.61	14/24607 (0.1%)	0.98	38/33241 (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	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1095	GLU	CD-OE2	8.50	1.34	1.25
1	A	1095	GLU	CD-OE2	8.27	1.34	1.25
1	E	1095	GLU	CD-OE2	7.57	1.33	1.25
1	A	993	GLU	CD-OE1	7.27	1.33	1.25
1	C	869	GLU	CD-OE2	6.33	1.32	1.25
1	C	1061	GLU	CD-OE2	6.05	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	993	GLU	CD-OE1	5.33	1.31	1.25
1	E	1061	GLU	CD-OE2	5.29	1.31	1.25
1	B	902	GLU	CD-OE2	5.28	1.31	1.25
1	E	917	GLU	CD-OE1	5.27	1.31	1.25
1	C	917	GLU	CD-OE2	5.21	1.31	1.25
1	A	960	GLU	CD-OE1	5.10	1.31	1.25
1	A	1003	GLU	CD-OE2	5.04	1.31	1.25
1	A	992	GLU	CD-OE2	5.00	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1027	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	B	1025	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	1158	THR	OG1-CB-CG2	-7.33	93.13	110.00
1	B	1027	ARG	CG-CD-NE	7.24	127.01	111.80
1	A	1146	ARG	CG-CD-NE	6.70	125.87	111.80
1	E	1152	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	826	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	1152	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	F	1152	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	F	1049	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	E	1100	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	1100	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	935	TYR	CB-CG-CD1	5.97	124.58	121.00
1	B	1065	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	F	841	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	F	718	MET	CG-SD-CE	5.83	109.52	100.20
1	B	1100	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	1127	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	1152	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	F	935	TYR	CB-CG-CD1	5.70	124.42	121.00
1	C	1065	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	F	1065	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	1027	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	A	826	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	943	ARG	CG-CD-NE	5.39	123.12	111.80
1	C	1025	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	898	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	B	1127	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	935	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	E	1152	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1027	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	B	667	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	1100	ARG	CG-CD-NE	5.19	122.69	111.80
1	C	1150	PHE	CB-CG-CD1	5.17	124.42	120.80
1	D	1045	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	730	MET	CB-CG-SD	5.14	127.82	112.40
1	F	671	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	957	ARG	NE-CZ-NH1	5.03	122.81	120.30

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
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

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Mol	Chain	Res	Type	Group
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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4012	0	4013	13	0
1	B	4005	0	4005	9	0
1	C	4012	0	4013	12	0
1	D	4005	0	4005	11	0
1	E	4012	0	4013	14	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	94	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 (94) 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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	406 (100%)	2 (0%)	88 95
1	B	407/419 (97%)	404 (99%)	3 (1%)	84 93
1	C	408/419 (97%)	407 (100%)	1 (0%)	93 98
1	D	407/419 (97%)	405 (100%)	2 (0%)	88 95
1	E	408/419 (97%)	407 (100%)	1 (0%)	93 98
1	F	406/419 (97%)	405 (100%)	1 (0%)	93 98
All	All	2444/2514 (97%)	2434 (100%)	10 (0%)	91 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1105	TRP
1	A	1146	ARG
1	B	814	LEU
1	B	1003	GLU
1	B	1105	TRP
1	C	936	ARG
1	D	746	GLU
1	D	830	LEU
1	E	775	ASN
1	F	718	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1162	GLN
1	B	1110	GLN
1	B	1162	GLN
1	C	1160	ASN
1	C	1162	GLN
1	D	725	GLN
1	E	699	ASN

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Mol	Chain	Res	Type
1	F	692	HIS
1	F	1160	ASN
1	F	1162	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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	B	1201	-	90,101,101	1.12	7 (7%)	137,166,166	1.57	26 (18%)
2	B12	D	1201	-	90,101,101	1.11	6 (6%)	137,166,166	1.69	36 (26%)
2	B12	C	1201	-	90,101,101	1.12	7 (7%)	137,166,166	1.65	33 (24%)
2	B12	A	1201	-	90,101,101	1.05	7 (7%)	137,166,166	1.79	32 (23%)
2	B12	F	1201	-	90,101,101	1.16	8 (8%)	137,166,166	1.47	27 (19%)
2	B12	E	1201	-	90,101,101	1.14	8 (8%)	137,166,166	1.61	26 (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
2	B12	B	1201	-	-	21/52/223/223	0/3/11/11
2	B12	D	1201	-	-	18/52/223/223	0/3/11/11
2	B12	C	1201	-	-	22/52/223/223	0/3/11/11
2	B12	A	1201	-	-	21/52/223/223	0/3/11/11
2	B12	F	1201	-	-	22/52/223/223	0/3/11/11
2	B12	E	1201	-	-	23/52/223/223	0/3/11/11

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	B12	C20-C1	3.43	1.60	1.53
2	C	1201	B12	O51-C50	3.33	1.33	1.24
2	D	1201	B12	C19-N24	-3.31	1.42	1.48
2	F	1201	B12	C19-N24	-3.26	1.42	1.48
2	E	1201	B12	C19-N24	-3.24	1.42	1.48
2	B	1201	B12	C19-N24	-3.15	1.42	1.48
2	E	1201	B12	C18-C19	-3.11	1.47	1.53
2	F	1201	B12	C18-C19	-3.05	1.47	1.53
2	F	1201	B12	C6B-C5B	3.05	1.48	1.40
2	C	1201	B12	C19-N24	-3.00	1.43	1.48
2	A	1201	B12	O44-C43	2.93	1.32	1.24
2	A	1201	B12	C19-N24	-2.83	1.43	1.48
2	D	1201	B12	C6B-C5B	2.76	1.47	1.40
2	C	1201	B12	C37-C38	2.57	1.60	1.51
2	B	1201	B12	C6B-C5B	2.54	1.47	1.40
2	A	1201	B12	C6B-C5B	2.54	1.47	1.40
2	E	1201	B12	C53-C15	-2.51	1.45	1.50
2	F	1201	B12	C54-C17	2.49	1.58	1.54
2	F	1201	B12	C35-C5	-2.47	1.45	1.50
2	D	1201	B12	C18-C19	-2.44	1.48	1.53
2	C	1201	B12	C6B-C5B	2.44	1.47	1.40
2	D	1201	B12	C46-C12	2.31	1.59	1.54
2	F	1201	B12	C36-C7	2.31	1.58	1.54
2	F	1201	B12	C46-C12	2.28	1.58	1.54
2	E	1201	B12	O34-C32	2.26	1.30	1.24
2	E	1201	B12	C31-C32	2.26	1.60	1.51
2	B	1201	B12	C47-C12	2.22	1.58	1.54
2	E	1201	B12	C35-C5	-2.22	1.46	1.50
2	C	1201	B12	P-O4	-2.20	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1201	B12	C26-C2	2.19	1.60	1.55
2	A	1201	B12	O7R-C2R	-2.18	1.37	1.43
2	B	1201	B12	C18-C19	-2.18	1.49	1.53
2	B	1201	B12	O6R-C1R	2.18	1.44	1.41
2	A	1201	B12	C18-C19	-2.17	1.49	1.53
2	F	1201	B12	O28-C27	2.16	1.30	1.24
2	B	1201	B12	C26-C2	2.15	1.60	1.55
2	E	1201	B12	C6B-C5B	2.14	1.46	1.40
2	C	1201	B12	C18-C19	-2.11	1.49	1.53
2	C	1201	B12	O6R-C1R	2.11	1.44	1.41
2	D	1201	B12	C54-C17	2.11	1.58	1.54
2	A	1201	B12	C2R-C3R	-2.07	1.48	1.52
2	B	1201	B12	C60-C61	2.05	1.57	1.51
2	A	1201	B12	C43-N45	2.00	1.39	1.32

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	B12	C41-C8-C9	-7.30	98.32	111.19
2	E	1201	B12	O34-C32-N33	-5.67	107.03	122.50
2	B	1201	B12	O58-C57-C56	-5.55	111.87	122.02
2	C	1201	B12	C35-C5-C6	-5.00	114.47	122.43
2	A	1201	B12	O58-C57-C56	-4.99	112.88	122.02
2	E	1201	B12	C41-C8-C9	-4.92	102.53	111.19
2	D	1201	B12	C12-C13-C14	-4.72	94.36	102.26
2	D	1201	B12	O63-C61-C60	-4.60	111.17	120.87
2	A	1201	B12	C60-C61-N62	4.38	126.76	116.21
2	E	1201	B12	O58-C57-C56	-4.38	114.01	122.02
2	A	1201	B12	O34-C32-N33	-4.25	110.90	122.50
2	C	1201	B12	O58-C57-C56	-4.09	114.53	122.02
2	E	1201	B12	C7B-C8B-C9B	4.03	124.53	120.54
2	C	1201	B12	C2-C3-C4	3.95	106.12	101.63
2	A	1201	B12	C2-C3-C4	3.94	106.11	101.63
2	C	1201	B12	C2P-C1P-N59	-3.89	107.20	112.93
2	A	1201	B12	C55-C17-C16	3.88	124.32	116.65
2	B	1201	B12	C41-C8-C9	-3.87	104.37	111.19
2	D	1201	B12	C55-C17-C16	3.80	124.16	116.65
2	A	1201	B12	C7B-C8B-C9B	3.75	124.25	120.54
2	D	1201	B12	C20-C1-C2	3.73	119.52	113.28
2	B	1201	B12	O63-C61-N62	-3.66	112.52	122.50
2	B	1201	B12	O58-C57-N59	3.61	129.84	123.01
2	A	1201	B12	C47-C12-C46	-3.53	103.38	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	B12	C7B-C8B-C9B	3.52	124.03	120.54
2	D	1201	B12	C7B-C8B-C9B	3.51	124.02	120.54
2	D	1201	B12	O51-C50-C49	-3.49	110.81	121.07
2	A	1201	B12	C15-C14-N23	-3.47	122.02	126.26
2	D	1201	B12	C13-C14-C15	-3.46	119.04	124.32
2	A	1201	B12	C5B-C4B-C9B	-3.40	116.41	121.22
2	E	1201	B12	O34-C32-C31	3.39	131.02	121.07
2	E	1201	B12	C30-C3-C4	3.38	117.49	109.63
2	E	1201	B12	C55-C17-C16	3.38	123.32	116.65
2	B	1201	B12	C60-C61-N62	3.35	124.28	116.21
2	B	1201	B12	C54-C17-C16	-3.30	95.28	112.40
2	C	1201	B12	O58-C57-N59	3.28	129.21	123.01
2	C	1201	B12	C13-C12-C11	-3.27	97.26	100.97
2	A	1201	B12	C2P-C1P-N59	-3.26	108.12	112.93
2	D	1201	B12	O34-C32-N33	-3.26	113.59	122.50
2	D	1201	B12	C36-C7-C37	3.25	116.16	110.80
2	F	1201	B12	C54-C17-C16	-3.23	95.65	112.40
2	C	1201	B12	C5-C6-N22	-3.23	118.95	123.88
2	F	1201	B12	C55-C17-C16	3.22	123.01	116.65
2	D	1201	B12	C60-C61-N62	3.21	123.94	116.21
2	C	1201	B12	C54-C17-C18	-3.17	108.29	112.98
2	B	1201	B12	O34-C32-N33	-3.17	113.84	122.50
2	B	1201	B12	C18-C19-N24	3.15	107.10	102.31
2	F	1201	B12	C60-C61-N62	3.14	123.78	116.21
2	A	1201	B12	C35-C5-C6	-3.12	117.46	122.43
2	E	1201	B12	C47-C12-C46	-3.12	104.08	109.35
2	E	1201	B12	C19-C1-N21	-3.11	98.98	102.16
2	F	1201	B12	C7B-C8B-C9B	3.08	123.59	120.54
2	B	1201	B12	C31-C32-N33	3.07	126.05	116.51
2	C	1201	B12	O63-C61-N62	-3.06	114.16	122.50
2	D	1201	B12	C2-C3-C4	3.05	105.10	101.63
2	E	1201	B12	C5B-C4B-C9B	-3.04	116.92	121.22
2	C	1201	B12	C60-C61-N62	3.03	123.51	116.21
2	E	1201	B12	C2P-C1P-N59	-2.99	108.52	112.93
2	B	1201	B12	C49-C50-N52	2.97	125.77	116.51
2	A	1201	B12	C3-C4-N21	-2.96	108.25	111.97
2	E	1201	B12	C54-C17-C16	-2.93	97.17	112.40
2	F	1201	B12	O58-C57-C56	-2.93	116.65	122.02
2	E	1201	B12	C60-C61-N62	2.93	123.26	116.21
2	F	1201	B12	C13-C12-C11	-2.89	97.70	100.97
2	A	1201	B12	O58-C57-N59	2.86	128.42	123.01
2	F	1201	B12	C18-C19-N24	2.85	106.65	102.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1201	B12	C12-C13-C14	-2.84	97.51	102.26
2	E	1201	B12	C12-C11-C10	2.83	127.06	123.37
2	A	1201	B12	C10-C11-N23	-2.83	119.58	124.43
2	A	1201	B12	C31-C32-N33	2.83	125.31	116.51
2	D	1201	B12	C36-C7-C8	2.82	117.29	112.08
2	A	1201	B12	C12-C11-C10	2.81	127.03	123.37
2	D	1201	B12	C20-C1-N21	-2.81	105.66	110.27
2	A	1201	B12	C36-C7-C37	2.80	115.42	110.80
2	F	1201	B12	C53-C15-C16	2.79	125.19	120.38
2	C	1201	B12	C55-C17-C16	2.79	122.16	116.65
2	C	1201	B12	C5B-C4B-C9B	-2.78	117.28	121.22
2	D	1201	B12	C49-C50-N52	2.78	125.16	116.51
2	D	1201	B12	C1P-N59-C57	-2.78	116.64	122.69
2	F	1201	B12	O34-C32-N33	-2.76	114.98	122.50
2	B	1201	B12	C16-C15-C14	-2.74	117.09	121.25
2	A	1201	B12	C54-C17-C16	-2.74	98.16	112.40
2	C	1201	B12	O7R-C2R-C3R	2.71	118.86	111.17
2	B	1201	B12	C2P-C1P-N59	-2.67	109.00	112.93
2	F	1201	B12	C31-C32-N33	2.67	124.81	116.51
2	C	1201	B12	O28-C27-C26	2.65	130.38	121.99
2	C	1201	B12	C20-C1-C19	-2.63	106.82	109.36
2	D	1201	B12	C4B-C9B-C8B	-2.63	118.41	121.10
2	D	1201	B12	C17-C16-N24	-2.62	107.12	111.15
2	F	1201	B12	O58-C57-N59	2.61	127.94	123.01
2	B	1201	B12	C5B-C4B-C9B	-2.60	117.53	121.22
2	B	1201	B12	C36-C7-C37	2.60	115.08	110.80
2	F	1201	B12	O7R-C2R-C3R	2.59	118.53	111.17
2	C	1201	B12	C47-C12-C11	2.58	119.36	110.08
2	E	1201	B12	C35-C5-C6	-2.58	118.32	122.43
2	E	1201	B12	C10-C11-N23	-2.58	120.02	124.43
2	F	1201	B12	C5B-C4B-C9B	-2.57	117.58	121.22
2	A	1201	B12	O7R-C2R-C3R	2.57	118.47	111.17
2	F	1201	B12	C12-C11-C10	2.57	126.71	123.37
2	F	1201	B12	C20-C1-C2	2.57	117.57	113.28
2	D	1201	B12	C1-C19-N24	-2.57	103.35	106.24
2	E	1201	B12	O58-C57-N59	2.56	127.84	123.01
2	E	1201	B12	C36-C7-C37	2.53	114.98	110.80
2	A	1201	B12	C19-C1-N21	-2.51	99.59	102.16
2	B	1201	B12	C55-C17-C16	2.50	121.58	116.65
2	C	1201	B12	C19-C1-N21	-2.49	99.61	102.16
2	D	1201	B12	C4B-C5B-C6B	2.49	124.10	119.91
2	C	1201	B12	C2R-C3R-C4R	2.48	107.61	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	B12	C47-C12-C11	2.47	118.98	110.08
2	F	1201	B12	C16-C15-C14	-2.47	117.50	121.25
2	D	1201	B12	C20-C1-C19	2.46	111.73	109.36
2	B	1201	B12	C55-C56-C57	2.45	116.58	111.23
2	D	1201	B12	C3-C4-N21	-2.45	108.90	111.97
2	C	1201	B12	O34-C32-N33	-2.44	115.84	122.50
2	F	1201	B12	C36-C7-C37	2.43	114.81	110.80
2	B	1201	B12	O7R-C2R-C3R	2.43	118.06	111.17
2	C	1201	B12	C3-C4-N21	-2.42	108.94	111.97
2	D	1201	B12	C31-C32-N33	2.41	124.00	116.51
2	C	1201	B12	C47-C12-C46	-2.41	105.28	109.35
2	F	1201	B12	C49-C50-N52	2.40	123.98	116.51
2	C	1201	B12	C48-C49-C50	-2.39	104.50	112.59
2	A	1201	B12	O2-C3R-C2R	2.38	120.32	111.68
2	A	1201	B12	C10-C9-N22	2.38	128.46	125.73
2	B	1201	B12	C7B-C8B-C9B	2.37	122.88	120.54
2	A	1201	B12	O5-P-O4	2.35	123.84	112.24
2	B	1201	B12	C13-C12-C11	-2.34	98.32	100.97
2	D	1201	B12	C55-C56-C57	2.32	116.31	111.23
2	C	1201	B12	C12-C13-C14	-2.32	98.38	102.26
2	D	1201	B12	C5B-C4B-C9B	-2.32	117.94	121.22
2	D	1201	B12	C6M-C6B-C5B	2.31	125.48	120.74
2	B	1201	B12	O51-C50-N52	-2.30	116.21	122.50
2	D	1201	B12	O6R-C4R-C5R	2.30	114.19	109.21
2	E	1201	B12	C12-C13-C14	-2.30	98.42	102.26
2	D	1201	B12	C7B-C6B-C5B	-2.28	116.08	119.91
2	D	1201	B12	C54-C17-C16	-2.27	100.61	112.40
2	F	1201	B12	C8-C9-C10	-2.27	118.42	123.32
2	C	1201	B12	O28-C27-N29	-2.27	116.31	122.50
2	A	1201	B12	C47-C12-C11	2.25	118.16	110.08
2	A	1201	B12	O63-C61-N62	-2.24	116.39	122.50
2	D	1201	B12	C5M-C5B-C6B	-2.24	116.15	120.74
2	C	1201	B12	C7-C8-C9	-2.23	98.05	100.90
2	B	1201	B12	C12-C13-C14	-2.23	98.53	102.26
2	C	1201	B12	C31-C32-N33	2.23	123.44	116.51
2	C	1201	B12	C10-C9-N22	2.22	128.28	125.73
2	D	1201	B12	C37-C7-C8	-2.20	102.49	108.39
2	E	1201	B12	C20-C1-N21	2.20	113.88	110.27
2	F	1201	B12	C6M-C6B-C5B	2.20	125.24	120.74
2	B	1201	B12	C20-C1-C2	2.20	116.95	113.28
2	D	1201	B12	C12-C11-C10	-2.19	120.52	123.37
2	C	1201	B12	C55-C56-C57	2.19	116.01	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	B12	C5M-C5B-C6B	-2.17	116.28	120.74
2	F	1201	B12	C2-C3-C4	2.17	104.09	101.63
2	D	1201	B12	C47-C12-C11	2.17	117.87	110.08
2	F	1201	B12	C3-C4-C5	2.16	127.45	123.81
2	D	1201	B12	C30-C3-C2	2.16	123.67	119.09
2	E	1201	B12	O63-C61-N62	-2.14	116.65	122.50
2	D	1201	B12	O2-C3R-C2R	2.14	119.45	111.68
2	E	1201	B12	C47-C12-C11	2.12	117.72	110.08
2	A	1201	B12	C18-C19-N24	2.11	105.52	102.31
2	E	1201	B12	O51-C50-N52	-2.09	116.78	122.50
2	A	1201	B12	C25-C2-C1	2.09	116.93	113.78
2	F	1201	B12	C10-C11-N23	-2.08	120.87	124.43
2	A	1201	B12	C4B-C5B-C6B	2.07	123.40	119.91
2	A	1201	B12	C3-C4-C5	2.06	127.29	123.81
2	C	1201	B12	C60-C18-C19	2.06	120.00	114.62
2	D	1201	B12	O8R-C5R-C4R	-2.06	104.23	111.29
2	A	1201	B12	C1-C2-C3	-2.06	98.97	101.60
2	F	1201	B12	C35-C5-C4	-2.05	112.61	116.79
2	F	1201	B12	C20-C1-N21	-2.05	106.91	110.27
2	A	1201	B12	O6R-C4R-C5R	2.04	113.62	109.21
2	C	1201	B12	C54-C17-C16	-2.03	101.86	112.40
2	E	1201	B12	O2-C3R-C2R	2.03	119.04	111.68
2	C	1201	B12	C30-C3-C4	2.03	114.35	109.63
2	B	1201	B12	C3-C4-N21	-2.02	109.43	111.97
2	C	1201	B12	O5-P-O4	2.02	122.22	112.24
2	D	1201	B12	C19-C1-N21	-2.02	100.10	102.16
2	F	1201	B12	C2P-C1P-N59	-2.02	109.96	112.93
2	E	1201	B12	C4B-C9B-C8B	-2.02	119.04	121.10
2	E	1201	B12	O6R-C4R-C5R	2.01	113.56	109.21
2	B	1201	B12	O2-C3R-C2R	2.00	118.93	111.68

There are no chirality outliers.

All (127) 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	C12-C13-C48-C49
2	A	1201	B12	C18-C60-C61-O63
2	A	1201	B12	C18-C60-C61-N62
2	B	1201	B12	C18-C60-C61-O63

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Mol	Chain	Res	Type	Atoms
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	C12-C13-C48-C49
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	C8-C41-C42-C43
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	A	1201	B12	C13-C48-C49-C50
2	C	1201	B12	C8-C41-C42-C43
2	E	1201	B12	C12-C13-C48-C49
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	C8-C41-C42-C43
2	B	1201	B12	C8-C41-C42-C43
2	C	1201	B12	C2-C3-C30-C31
2	D	1201	B12	C3-C2-C26-C27
2	F	1201	B12	C48-C49-C50-N52
2	B	1201	B12	C7-C37-C38-N40
2	E	1201	B12	C7-C37-C38-N40
2	E	1201	B12	C38-C37-C7-C36
2	E	1201	B12	C38-C37-C7-C8
2	F	1201	B12	C48-C49-C50-O51
2	E	1201	B12	C14-C13-C48-C49
2	B	1201	B12	C13-C48-C49-C50
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

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Mol	Chain	Res	Type	Atoms
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	A	1201	B12	C42-C41-C8-C9
2	C	1201	B12	C30-C31-C32-N33
2	B	1201	B12	C2P-O3-P-O2
2	F	1201	B12	C2P-O3-P-O2
2	F	1201	B12	C13-C48-C49-C50
2	F	1201	B12	C3-C2-C26-C27
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	F	1201	B12	C8-C41-C42-C43
2	A	1201	B12	C2P-O3-P-O2
2	D	1201	B12	C7-C37-C38-O39
2	D	1201	B12	C48-C49-C50-O51
2	C	1201	B12	C13-C48-C49-C50
2	E	1201	B12	C3P-C2P-O3-P
2	C	1201	B12	C2P-O3-P-O2
2	E	1201	B12	C2P-O3-P-O2
2	A	1201	B12	C48-C49-C50-O51
2	F	1201	B12	C7-C37-C38-O39
2	E	1201	B12	C42-C41-C8-C9
2	E	1201	B12	C48-C49-C50-N52
2	B	1201	B12	C3-C30-C31-C32
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	A	1201	B12	C48-C49-C50-N52
2	E	1201	B12	C30-C31-C32-O34
2	C	1201	B12	N59-C1P-C2P-C3P
2	D	1201	B12	C25-C2-C26-C27
2	D	1201	B12	C17-C55-C56-C57
2	C	1201	B12	C19-C18-C60-C61
2	D	1201	B12	C19-C18-C60-C61
2	E	1201	B12	C1P-C2P-O3-P
2	D	1201	B12	C2P-O3-P-O2
2	D	1201	B12	C38-C37-C7-C8
2	F	1201	B12	C38-C37-C7-C36

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

There are no ring outliers.

6 monomers are involved in 27 short contacts:

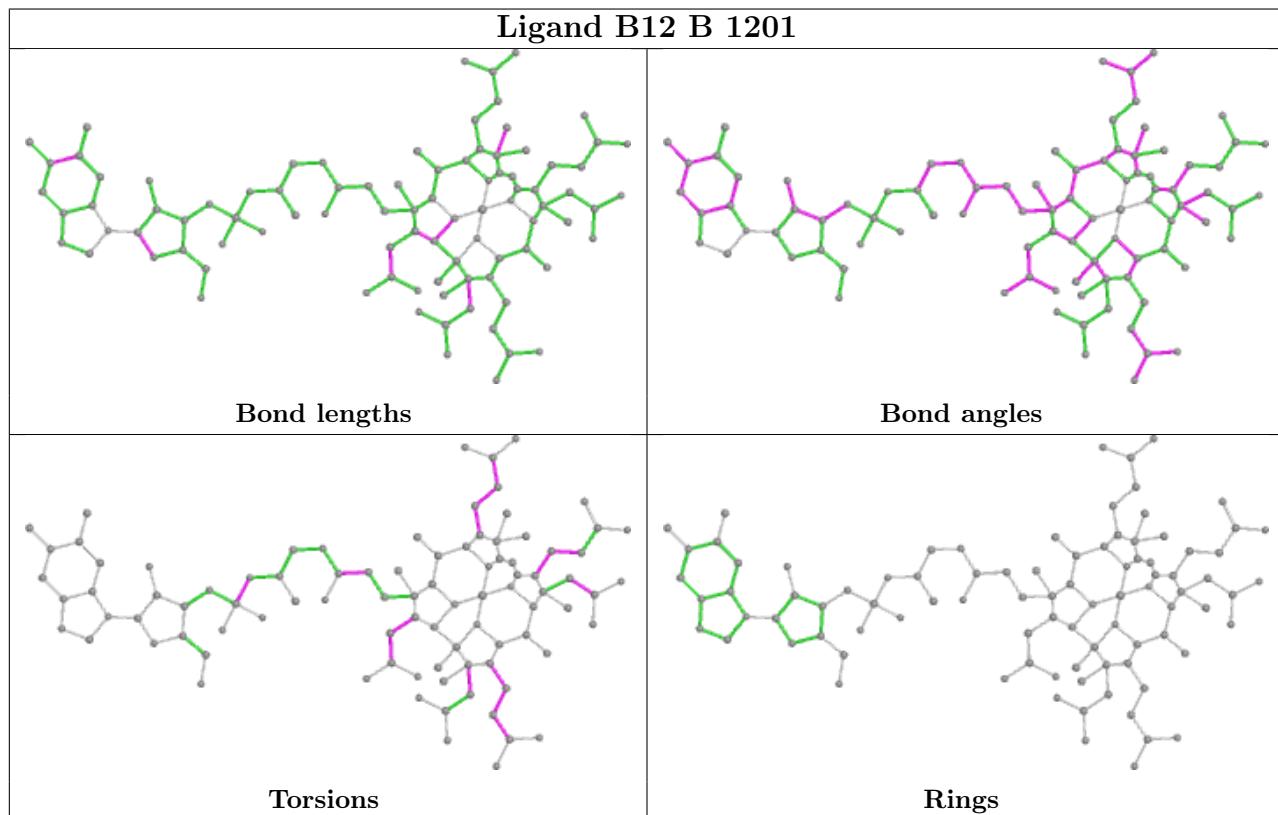
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	B12	2	0

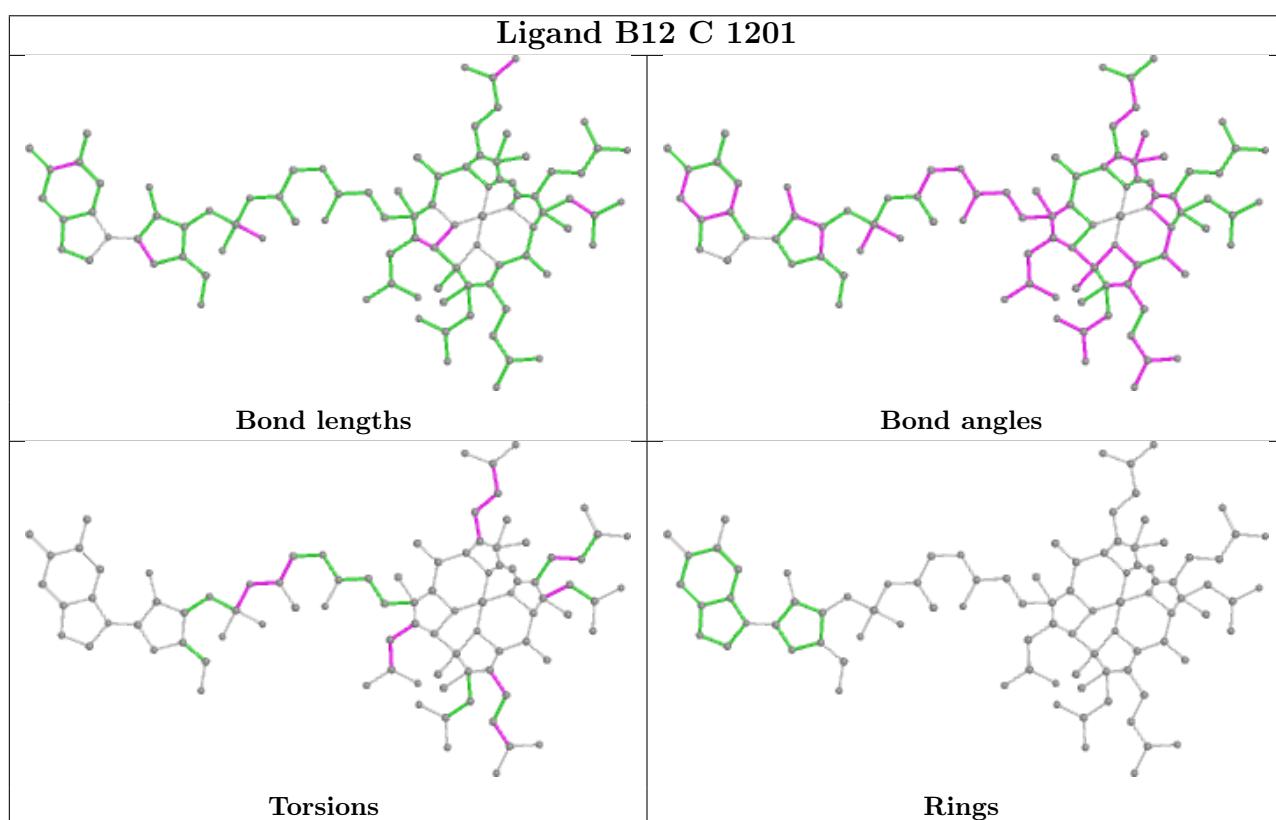
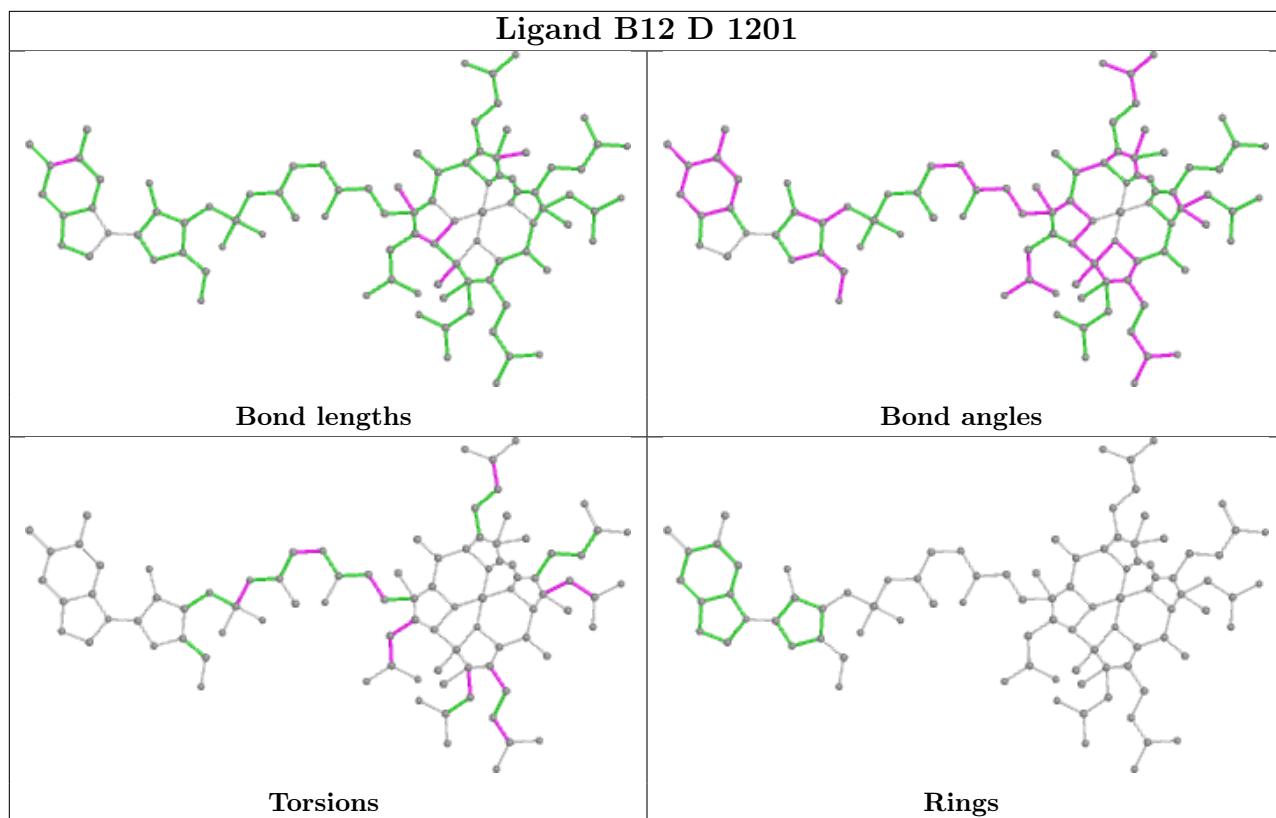
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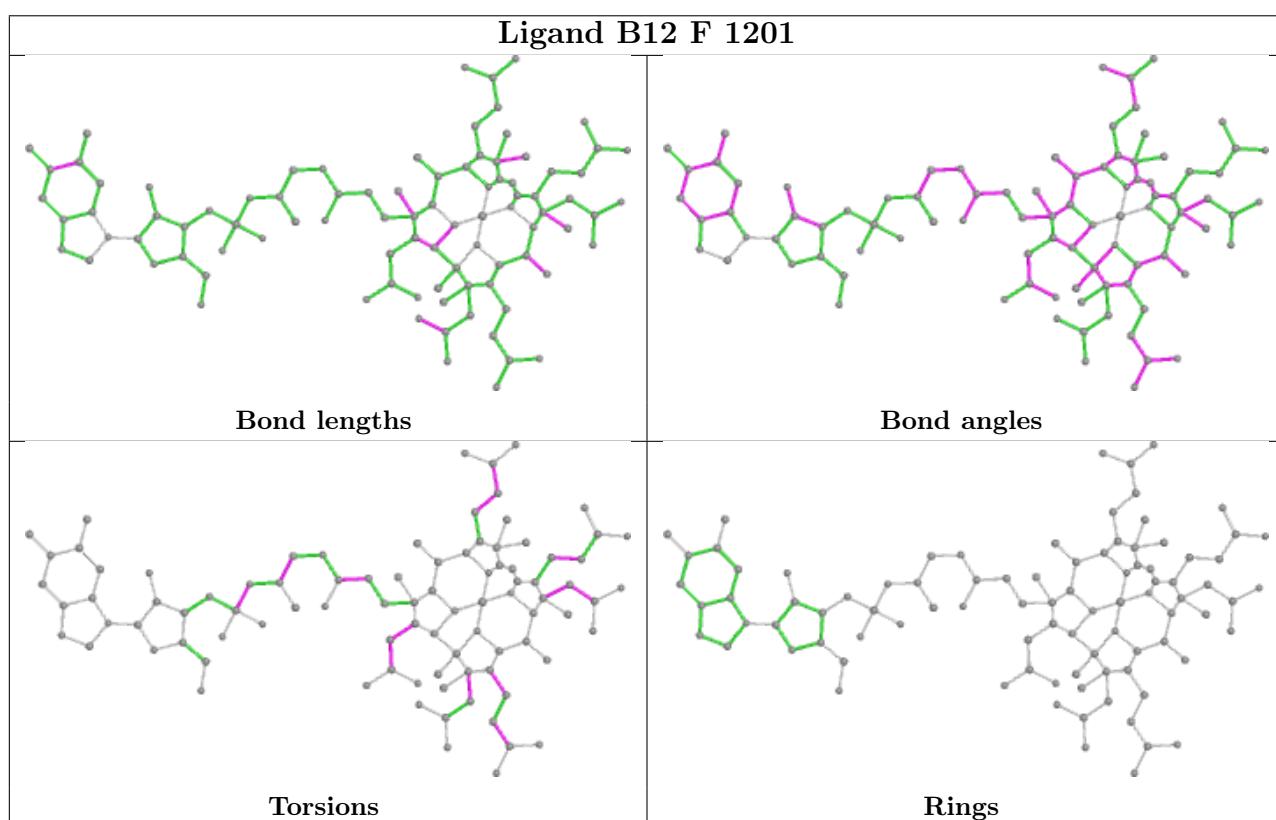
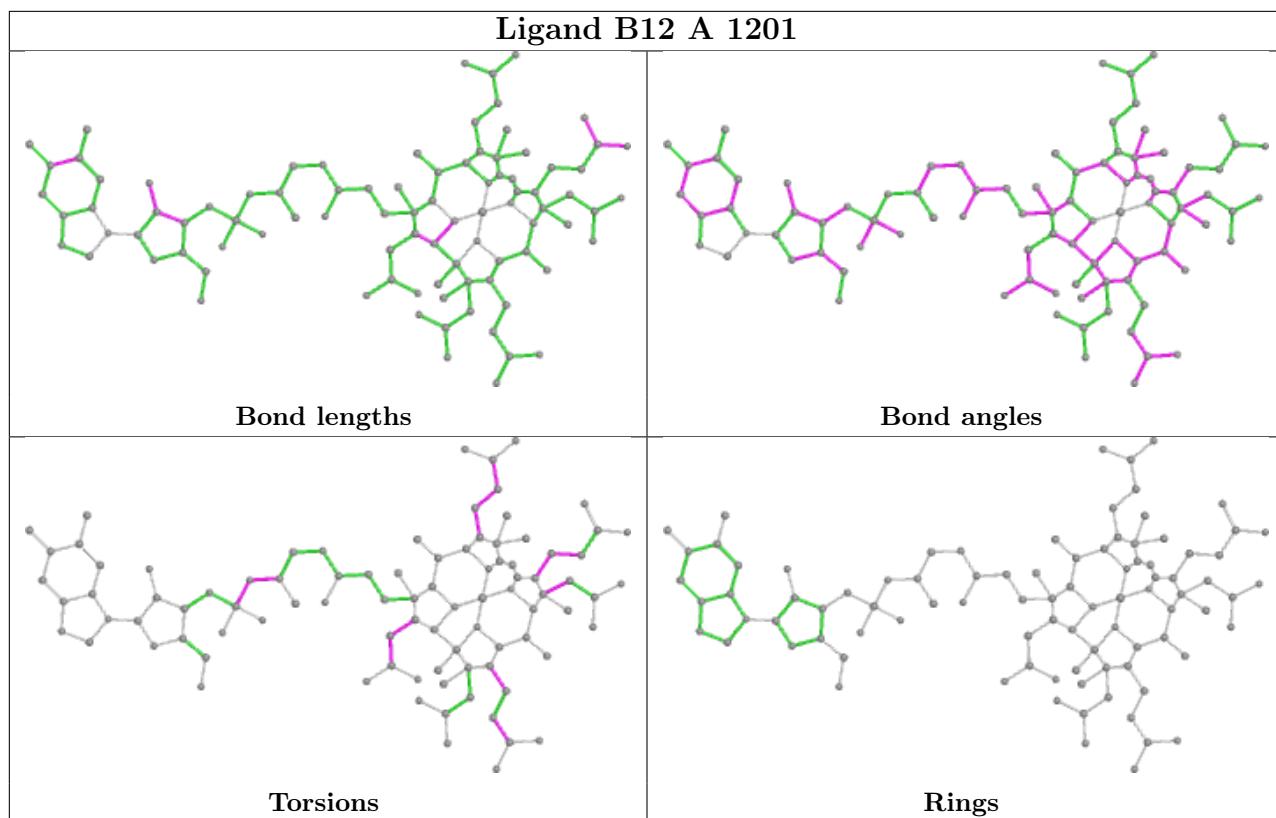
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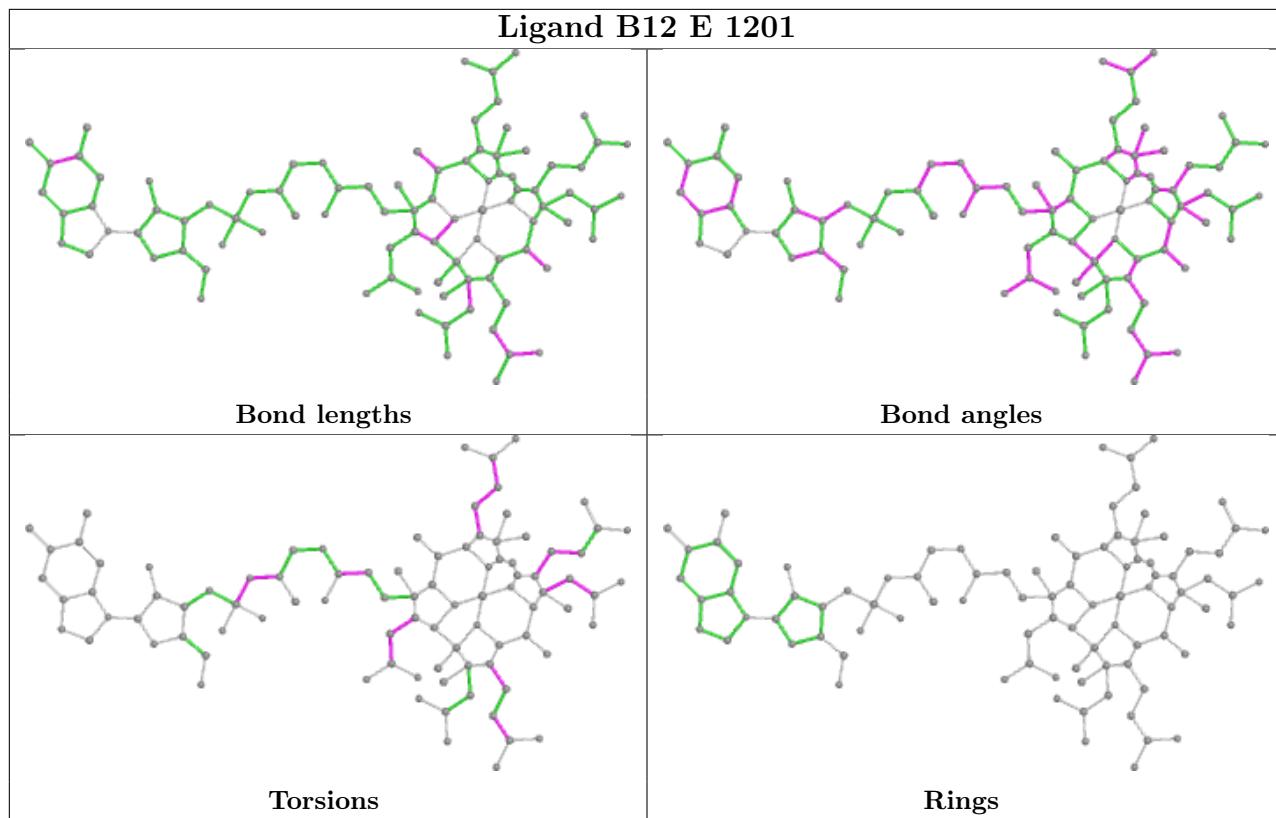
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1201	B12	5	0
2	C	1201	B12	7	0
2	A	1201	B12	6	0
2	F	1201	B12	3	0
2	E	1201	B12	4	0

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	507/523 (96%)	0.25	34 (6%) 17 9	30, 65, 160, 219	0
1	B	506/523 (96%)	0.56	52 (10%) 6 3	49, 86, 163, 226	0
1	C	507/523 (96%)	0.21	31 (6%) 21 11	30, 65, 151, 220	0
1	D	506/523 (96%)	0.40	34 (6%) 17 9	45, 86, 147, 211	0
1	E	507/523 (96%)	0.13	17 (3%) 45 28	30, 63, 133, 176	0
1	F	505/523 (96%)	0.60	42 (8%) 11 6	46, 86, 156, 271	0
All	All	3038/3138 (96%)	0.36	210 (6%) 16 9	30, 77, 154, 271	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	879	THR	37.0
1	F	880	ARG	8.1
1	D	896	ARG	7.8
1	D	1185	ASP	7.8
1	A	665	LEU	7.4
1	F	680	LEU	7.3
1	B	739	PRO	7.0
1	F	1185	ASP	6.8
1	B	684	LEU	5.6
1	B	688	LEU	5.5
1	A	1185	ASP	5.4
1	A	895	PRO	5.2
1	A	668	LEU	5.2
1	C	668	LEU	5.0
1	F	665	LEU	5.0
1	A	684	LEU	4.8
1	B	1185	ASP	4.7
1	C	688	LEU	4.6
1	A	736	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	668	LEU	4.5
1	F	684	LEU	4.4
1	E	1111	ASP	4.2
1	B	737	LEU	4.2
1	D	1111	ASP	4.2
1	C	692	HIS	4.1
1	C	1185	ASP	4.1
1	A	740	HIS	4.1
1	B	1122	GLY	4.0
1	B	680	LEU	4.0
1	B	692	HIS	4.0
1	F	674	GLU	3.9
1	D	688	LEU	3.9
1	D	776	GLY	3.9
1	F	679	GLY	3.9
1	F	664	LEU	3.8
1	F	678	GLN	3.8
1	B	690	ALA	3.8
1	F	1118	LEU	3.7
1	B	740	HIS	3.7
1	B	738	GLU	3.6
1	F	690	ALA	3.6
1	A	680	LEU	3.6
1	A	678	GLN	3.5
1	A	688	LEU	3.5
1	D	665	LEU	3.5
1	B	944	LYS	3.5
1	C	679	GLY	3.5
1	F	740	HIS	3.5
1	F	741	MET	3.5
1	C	706	MET	3.5
1	B	665	LEU	3.5
1	C	740	HIS	3.4
1	B	710	GLY	3.4
1	A	943	ARG	3.4
1	C	691	GLY	3.4
1	F	670	ARG	3.4
1	A	664	LEU	3.4
1	C	680	LEU	3.4
1	C	684	LEU	3.3
1	B	741	MET	3.3
1	B	694	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	897	ALA	3.3
1	B	782	LEU	3.3
1	F	691	GLY	3.2
1	B	734	VAL	3.2
1	C	739	PRO	3.2
1	A	679	GLY	3.2
1	B	736	TYR	3.2
1	D	801	HIS	3.2
1	B	668	LEU	3.2
1	A	663	PRO	3.2
1	B	1120	GLN	3.2
1	D	777	TYR	3.1
1	D	865	ARG	3.1
1	B	702	LEU	3.1
1	F	834	LEU	3.1
1	E	687	ALA	3.0
1	B	957	ARG	3.0
1	C	689	LYS	3.0
1	D	691	GLY	3.0
1	A	1119	PHE	3.0
1	B	691	GLY	3.0
1	B	687	ALA	3.0
1	D	740	HIS	2.9
1	A	742	GLU	2.9
1	D	965	ARG	2.9
1	A	735	ALA	2.9
1	F	866	LEU	2.9
1	A	1120	GLN	2.8
1	C	1115	ILE	2.8
1	C	736	TYR	2.8
1	D	898	ARG	2.8
1	C	742	GLU	2.8
1	C	741	MET	2.8
1	B	682	ALA	2.8
1	F	1114	GLU	2.8
1	A	1118	LEU	2.8
1	B	942	SER	2.7
1	A	692	HIS	2.7
1	A	697	LEU	2.7
1	B	778	ARG	2.7
1	B	730	MET	2.7
1	F	842	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	777	TYR	2.7
1	D	828	TYR	2.7
1	E	740	HIS	2.7
1	F	698	ILE	2.7
1	E	698	ILE	2.7
1	A	698	ILE	2.7
1	D	698	ILE	2.7
1	A	1114	GLU	2.6
1	F	706	MET	2.6
1	C	690	ALA	2.6
1	C	952	GLN	2.6
1	C	682	ALA	2.6
1	D	742	GLU	2.6
1	C	964	GLN	2.6
1	B	698	ILE	2.6
1	D	752	VAL	2.6
1	C	730	MET	2.6
1	D	864	LEU	2.6
1	F	736	TYR	2.6
1	D	863	GLY	2.5
1	E	1185	ASP	2.5
1	C	957	ARG	2.5
1	C	687	ALA	2.5
1	F	692	HIS	2.5
1	E	665	LEU	2.5
1	A	865	ARG	2.5
1	E	704	ALA	2.5
1	D	870	LEU	2.5
1	A	952	GLN	2.5
1	F	1073	SER	2.5
1	B	701	PRO	2.5
1	F	1110	GLN	2.5
1	C	678	GLN	2.5
1	E	1119	PHE	2.5
1	B	1173	VAL	2.4
1	F	694	PRO	2.4
1	C	665	LEU	2.4
1	D	664	LEU	2.4
1	B	689	LYS	2.4
1	A	1111	ASP	2.4
1	C	737	LEU	2.4
1	D	1118	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	735	ALA	2.4
1	A	701	PRO	2.4
1	B	901	GLY	2.4
1	C	1118	LEU	2.4
1	A	687	ALA	2.4
1	D	951	TRP	2.4
1	B	1018	LEU	2.4
1	E	1112	ALA	2.4
1	F	936	ARG	2.4
1	F	878	LEU	2.4
1	B	834	LEU	2.4
1	B	872	GLY	2.3
1	D	1120	GLN	2.3
1	F	776	GLY	2.3
1	D	743	LYS	2.3
1	F	726	ALA	2.3
1	E	944	LYS	2.3
1	D	1160	ASN	2.3
1	D	943	ARG	2.3
1	D	753	LEU	2.3
1	B	1118	LEU	2.3
1	C	681	GLU	2.2
1	F	957	ARG	2.2
1	E	943	ARG	2.2
1	D	1117	LYS	2.2
1	E	952	GLN	2.2
1	E	807	GLY	2.2
1	B	1068	GLN	2.2
1	B	873	HIS	2.2
1	E	776	GLY	2.2
1	B	1111	ASP	2.2
1	F	1067	ALA	2.2
1	F	1119	PHE	2.2
1	B	1115	ILE	2.2
1	B	958	GLU	2.2
1	A	957	ARG	2.2
1	E	680	LEU	2.2
1	F	839	LEU	2.2
1	B	700	GLY	2.2
1	A	718	MET	2.1
1	C	776	GLY	2.1
1	A	758	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	919	GLY	2.1
1	F	672	VAL	2.1
1	B	735	ALA	2.1
1	A	834	LEU	2.1
1	C	753	LEU	2.1
1	D	737	LEU	2.1
1	D	952	GLN	2.1
1	F	701	PRO	2.1
1	B	696	ASP	2.1
1	B	697	LEU	2.1
1	A	951	TRP	2.1
1	B	732	ARG	2.1
1	E	896	ARG	2.1
1	B	727	ALA	2.1
1	B	798	HIS	2.1
1	B	863	GLY	2.0
1	F	840	THR	2.0
1	D	697	LEU	2.0
1	A	942	SER	2.0
1	F	682	ALA	2.0
1	D	710	GLY	2.0
1	B	706	MET	2.0
1	E	697	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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

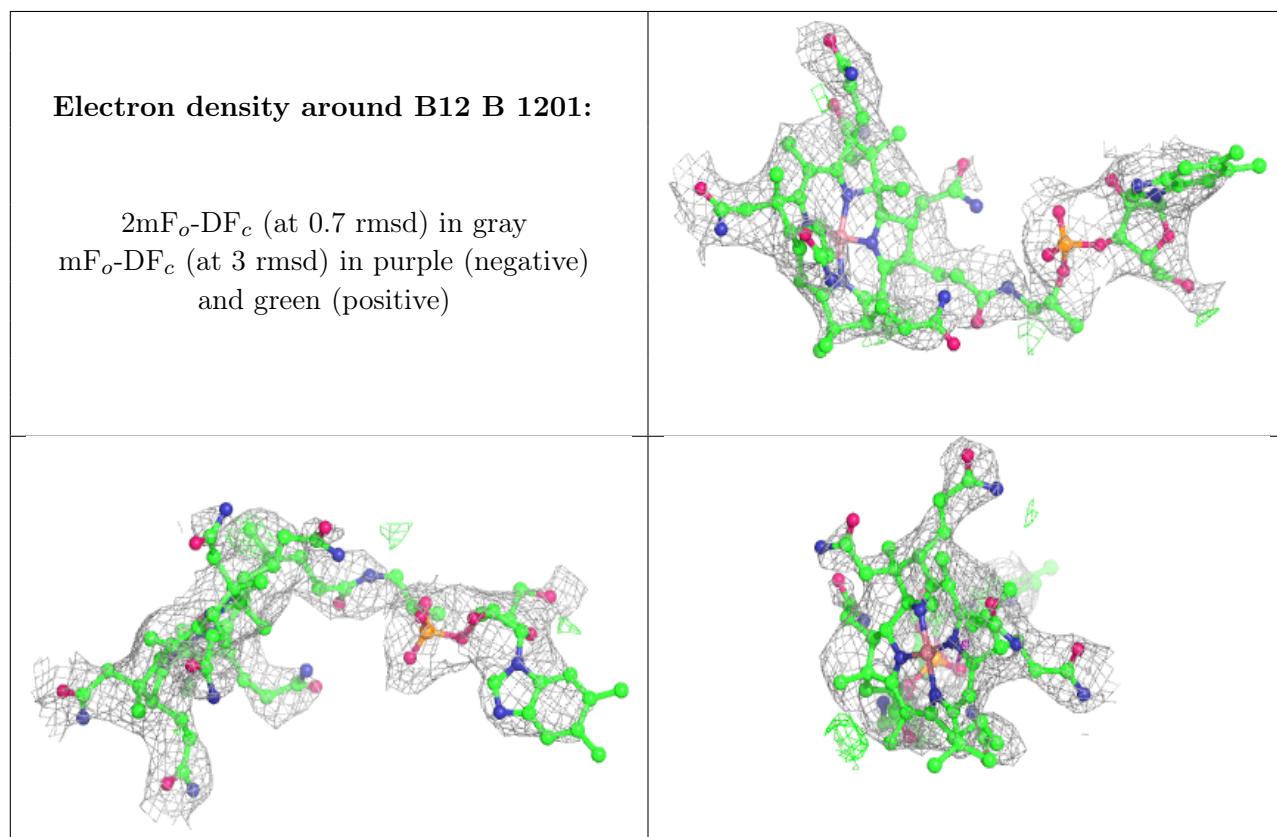
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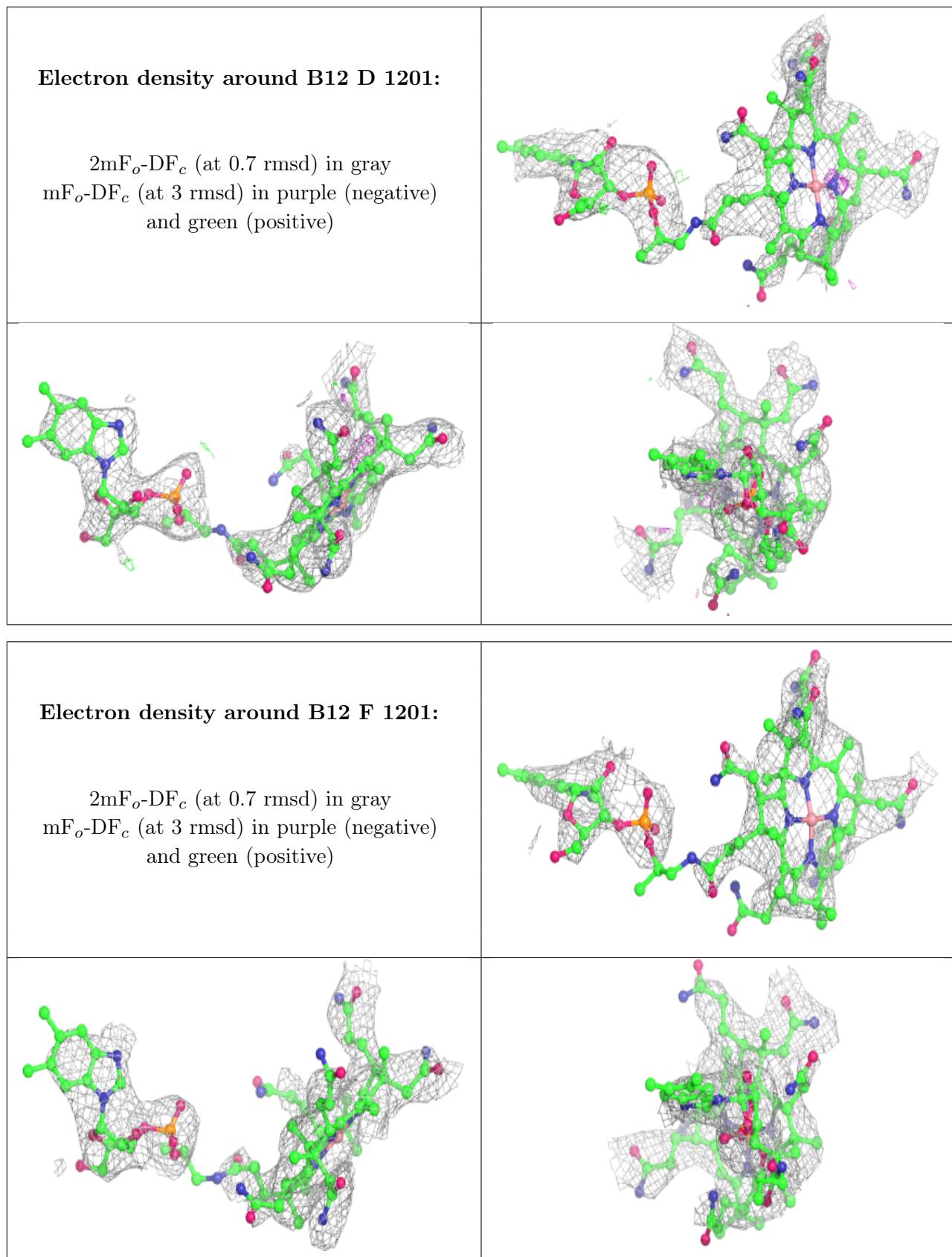
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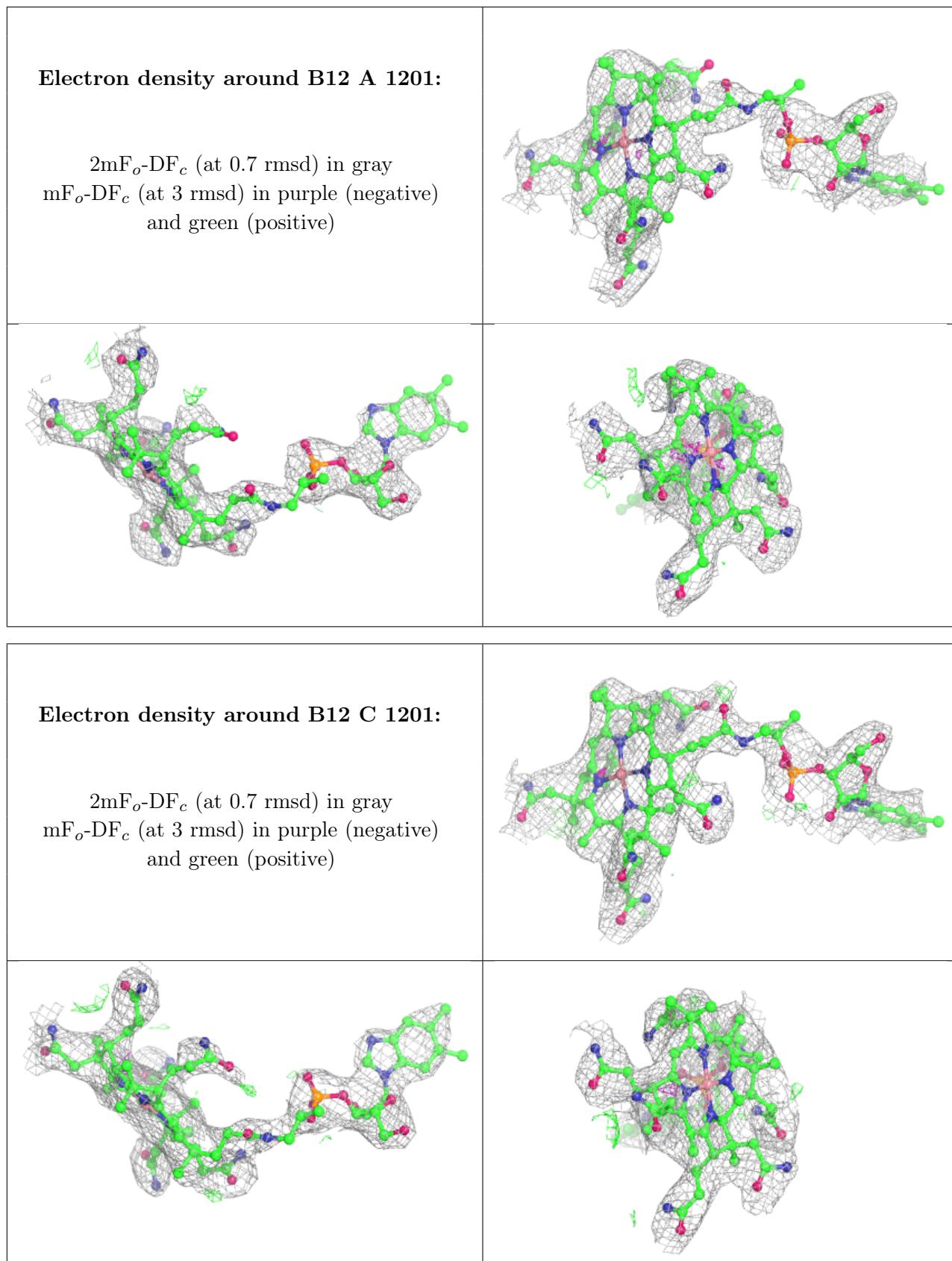
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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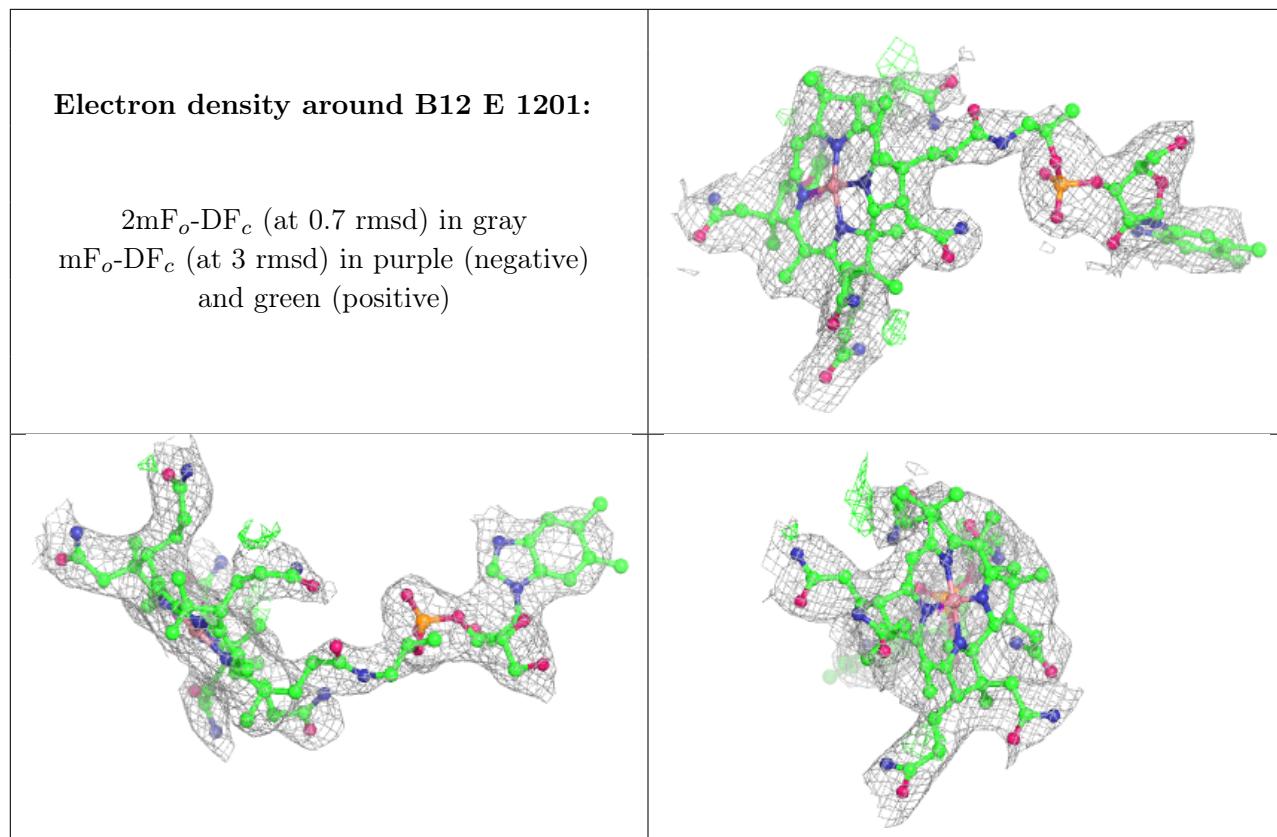
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B12	B	1201	91/91	0.92	0.27	56,80,101,115	0
2	B12	D	1201	91/91	0.92	0.29	53,78,104,119	0
2	B12	F	1201	91/91	0.93	0.30	49,83,119,134	0
2	B12	A	1201	91/91	0.95	0.25	34,54,86,103	0
2	B12	C	1201	91/91	0.95	0.22	41,56,79,94	0
2	B12	E	1201	91/91	0.96	0.24	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.









6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.