



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:06 PM UTC

PDB ID : 3BUL / pdb_00003bul
Title : E. coli I690C/G743C MetH C-terminal fragment (649-1227)
Authors : Koutmos, M.; Patridge, K.A.; Ludwig, M.L.
Deposited on : 2008-01-03
Resolution : 2.30 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

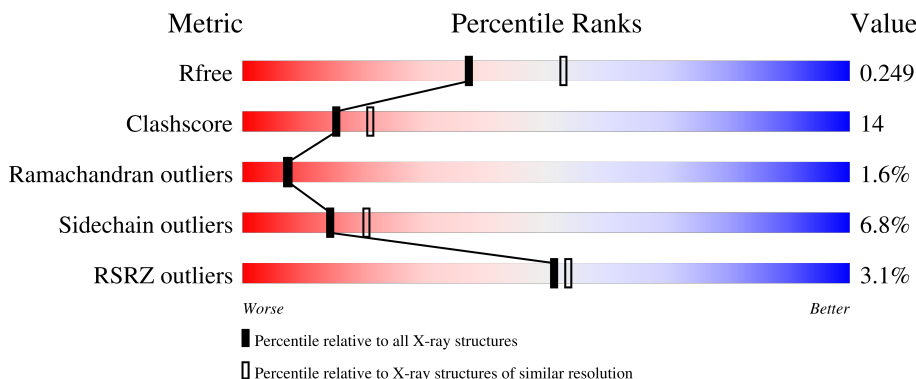
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

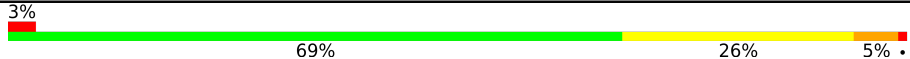
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	579	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B12	A	1301	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4726 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.

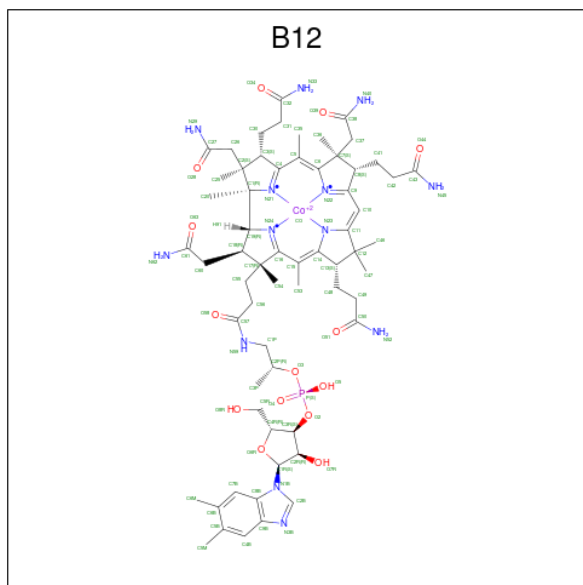
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4572	2890	789	874	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	690	CYS	ILE	engineered mutation	UNP P13009
A	743	CYS	GLY	engineered mutation	UNP P13009

- Molecule 2 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

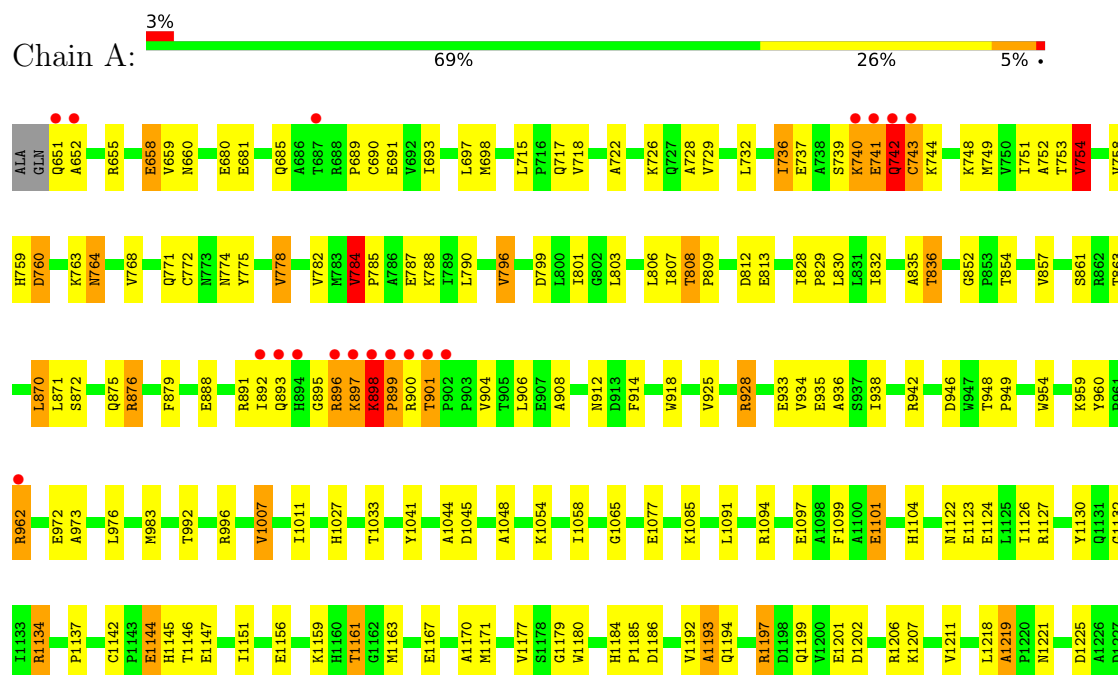
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Methionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.53Å 106.53Å 137.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.07 – 2.30 42.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.07-2.30) 100.0 (42.07-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.247 0.197 , 0.249	Depositor DCC
R_{free} test set	1773 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B12

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.40	18/4671 (0.4%)	1.32	31/6336 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	778	VAL	CA-CB	7.92	1.63	1.53
1	A	1101	GLU	N-CA	7.43	1.55	1.46
1	A	1151	ILE	CA-CB	7.42	1.63	1.54
1	A	1104	HIS	C-O	-6.62	1.16	1.24
1	A	948	THR	C-O	-6.59	1.18	1.24
1	A	787	GLU	CG-CD	6.44	1.68	1.52
1	A	1048	ALA	N-CA	6.30	1.53	1.45
1	A	784	VAL	CA-CB	6.28	1.61	1.54
1	A	1132	GLY	N-CA	5.99	1.50	1.45
1	A	1099	PHE	C-O	-5.96	1.17	1.24
1	A	1185	PRO	C-O	-5.53	1.17	1.24
1	A	718	VAL	CA-CB	-5.47	1.47	1.54
1	A	754	VAL	CA-CB	-5.46	1.48	1.54
1	A	925	VAL	CA-CB	5.44	1.60	1.54
1	A	728	ALA	CA-CB	-5.28	1.45	1.53
1	A	715	LEU	N-CA	-5.11	1.41	1.46
1	A	936	ALA	CA-CB	-5.10	1.45	1.53
1	A	933	GLU	N-CA	-5.09	1.39	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	784	VAL	CB-CA-C	10.17	122.47	110.78
1	A	852	GLY	N-CA-C	-8.48	101.67	112.10
1	A	778	VAL	CB-CA-C	8.46	122.53	111.53
1	A	801	ILE	CA-C-N	-7.33	115.96	121.61
1	A	801	ILE	C-N-CA	-7.33	115.96	121.61
1	A	784	VAL	N-CA-C	7.04	115.65	107.77
1	A	1065	GLY	N-CA-C	-6.47	106.63	114.66
1	A	1101	GLU	CB-CA-C	-6.32	100.96	110.88
1	A	1134	ARG	CA-C-N	6.29	126.24	119.76
1	A	1134	ARG	C-N-CA	6.29	126.24	119.76
1	A	784	VAL	CA-C-O	6.28	123.78	119.20
1	A	1219	ALA	CA-C-N	-6.26	113.36	119.87
1	A	1219	ALA	C-N-CA	-6.26	113.36	119.87
1	A	1094	ARG	N-CA-C	-6.01	104.73	111.28
1	A	1130	TYR	N-CA-C	-5.99	99.85	108.60
1	A	1077	GLU	N-CA-C	-5.81	104.94	111.28
1	A	1161	THR	CB-CA-C	-5.79	99.78	109.27
1	A	742	GLN	N-CA-C	5.75	117.20	110.41
1	A	960	TYR	C-N-CD	-5.71	108.04	120.60
1	A	973	ALA	N-CA-C	-5.68	105.16	111.36
1	A	796	VAL	N-CA-C	-5.46	108.18	113.53
1	A	760	ASP	N-CA-C	5.45	119.71	112.30
1	A	1041	TYR	N-CA-C	5.33	118.02	110.50
1	A	1177	VAL	N-CA-C	-5.25	100.67	108.45
1	A	992	THR	CA-C-N	-5.21	114.67	122.39
1	A	992	THR	C-N-CA	-5.21	114.67	122.39
1	A	901	THR	CA-C-N	-5.15	115.07	120.38
1	A	901	THR	C-N-CA	-5.15	115.07	120.38
1	A	1170	ALA	N-CA-C	-5.14	103.89	110.53
1	A	960	TYR	CA-C-N	5.04	139.10	127.00
1	A	960	TYR	C-N-CA	5.04	139.10	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	742	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4572	0	4482	108	0
2	A	91	0	86	22	0
3	A	63	0	0	4	0
All	All	4726	0	4568	125	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 14.

All (125) 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:A:1097:GLU:HB2	3:A:1314:HOH:O	1.29	1.25
2:A:1301:B12:H362	2:A:1301:B12:H351	1.48	0.96
1:A:1011:ILE:HD11	1:A:1044:ALA:HA	1.48	0.94
1:A:749:MET:CE	1:A:751:ILE:HD12	1.98	0.93
1:A:938:ILE:O	1:A:942:ARG:HG3	1.79	0.83
1:A:693:ILE:HD12	1:A:729:VAL:HG22	1.64	0.78
1:A:741:GLU:O	1:A:742:GLN:HG2	1.83	0.77
1:A:726:LYS:NZ	1:A:771:GLN:HE22	1.83	0.77
1:A:808:THR:N	1:A:836:THR:HG21	2.00	0.77
2:A:1301:B12:H601	2:A:1301:B12:H262	1.68	0.76
1:A:749:MET:HE1	1:A:751:ILE:HD12	1.70	0.71
1:A:693:ILE:HD11	1:A:732:LEU:HD12	1.71	0.71
1:A:906:LEU:HD22	1:A:1199:GLN:HA	1.72	0.71
1:A:752:ALA:HB1	1:A:784:VAL:HG13	1.73	0.70
1:A:896:ARG:O	1:A:898:LYS:N	2.27	0.68
1:A:1097:GLU:CB	3:A:1314:HOH:O	2.05	0.68
1:A:1197:ARG:NH1	1:A:1201:GLU:OE2	2.28	0.67
1:A:759:HIS:ND1	2:A:1301:B12:N52	2.42	0.67
1:A:748:LYS:HD3	1:A:796:VAL:HG12	1.77	0.66
1:A:748:LYS:HD3	1:A:796:VAL:CG1	2.27	0.65
2:A:1301:B12:O51	2:A:1301:B12:N59	2.25	0.65
1:A:758:VAL:HG11	1:A:1171:MET:O	1.97	0.65
2:A:1301:B12:H203	2:A:1301:B12:H301	1.79	0.64
1:A:807:ILE:HA	2:A:1301:B12:H331	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ARG:HH11	1:A:928:ARG:HG3	1.64	0.61
1:A:759:HIS:CE1	2:A:1301:B12:N52	2.69	0.61
2:A:1301:B12:H8	2:A:1301:B12:N40	2.15	0.61
1:A:904:VAL:HG12	1:A:908:ALA:HB3	1.83	0.60
1:A:698:MET:HE2	1:A:774:ASN:HB2	1.84	0.60
1:A:1122:ASN:O	1:A:1126:ILE:HG12	2.02	0.60
2:A:1301:B12:H351	2:A:1301:B12:C36	2.26	0.59
1:A:726:LYS:HZ3	1:A:771:GLN:HE22	1.51	0.59
1:A:1145:HIS:HE1	2:A:1301:B12:H332	1.49	0.59
2:A:1301:B12:H353	2:A:1301:B12:H302	1.83	0.59
2:A:1301:B12:H8	2:A:1301:B12:H401	1.69	0.58
1:A:693:ILE:HD13	1:A:697:LEU:CD2	2.34	0.58
1:A:752:ALA:HB1	1:A:784:VAL:CG1	2.33	0.58
1:A:807:ILE:C	1:A:836:THR:HG21	2.30	0.56
1:A:806:LEU:HD12	1:A:835:ALA:HB3	1.87	0.56
1:A:959:LYS:HD3	1:A:962:ARG:HH22	1.70	0.56
1:A:1027:HIS:CD2	1:A:1207:LYS:HD3	2.42	0.55
1:A:897:LYS:O	1:A:898:LYS:O	2.24	0.54
2:A:1301:B12:H362	2:A:1301:B12:C35	2.31	0.54
2:A:1301:B12:O28	2:A:1301:B12:H3	2.07	0.54
1:A:760:ASP:HB2	1:A:763:LYS:HE2	1.90	0.54
1:A:891:ARG:NH2	3:A:1349:HOH:O	2.41	0.54
1:A:870:LEU:HD13	1:A:879:PHE:CD1	2.44	0.53
1:A:681:GLU:O	1:A:685:GLN:HG2	2.08	0.53
1:A:934:VAL:HG12	1:A:935:GLU:N	2.22	0.52
1:A:928:ARG:HG3	1:A:928:ARG:NH1	2.25	0.52
1:A:693:ILE:CD1	1:A:732:LEU:HD12	2.40	0.52
1:A:954:TRP:CD1	1:A:976:LEU:HD21	2.46	0.51
1:A:1144:GLU:OE1	1:A:1146:THR:HG23	2.10	0.51
1:A:764:ASN:OD1	1:A:1085:LYS:HE3	2.11	0.51
1:A:1197:ARG:NH2	3:A:1358:HOH:O	2.42	0.51
1:A:1145:HIS:CE1	2:A:1301:B12:H332	2.28	0.51
1:A:717:GLN:OE1	1:A:972:GLU:HG3	2.11	0.50
1:A:1202:ASP:O	1:A:1206:ARG:HG3	2.13	0.49
1:A:693:ILE:CD1	1:A:729:VAL:HG22	2.41	0.49
1:A:1184:HIS:HD2	1:A:1186:ASP:H	1.60	0.48
1:A:808:THR:HG22	1:A:809:PRO:HD3	1.95	0.48
1:A:1156:GLU:OE1	1:A:1159:LYS:HE2	2.13	0.48
1:A:983:MET:SD	1:A:1091:LEU:HD12	2.54	0.48
1:A:748:LYS:CD	1:A:796:VAL:HG12	2.42	0.48
1:A:693:ILE:HD13	1:A:697:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLN:O	1:A:876:ARG:C	2.56	0.48
2:A:1301:B12:C15	2:A:1301:B12:H492	2.36	0.47
1:A:659:VAL:HG13	1:A:660:ASN:N	2.29	0.47
1:A:900:ARG:HH12	1:A:1194:GLN:HE21	1.62	0.47
1:A:764:ASN:O	1:A:768:VAL:HG23	2.14	0.47
2:A:1301:B12:H2B	2:A:1301:B12:O2	2.13	0.47
1:A:1101:GLU:CD	1:A:1134:ARG:HH22	2.22	0.47
1:A:857:VAL:HG11	1:A:863:THR:HA	1.97	0.46
1:A:784:VAL:HA	1:A:785:PRO:HD3	1.69	0.46
1:A:832:ILE:HD12	1:A:854:THR:HG23	1.97	0.46
1:A:1134:ARG:HA	1:A:1180:TRP:O	2.15	0.46
1:A:655:ARG:HA	1:A:655:ARG:HD2	1.60	0.46
2:A:1301:B12:H473	2:A:1301:B12:H482	1.45	0.46
1:A:690:CYS:SG	1:A:736:ILE:HG12	2.56	0.45
1:A:888:GLU:OE2	1:A:891:ARG:NH1	2.47	0.45
1:A:799:ASP:O	1:A:829:PRO:HD2	2.17	0.45
1:A:737:GLU:C	1:A:739:SER:H	2.25	0.45
1:A:740:LYS:O	1:A:741:GLU:O	2.35	0.45
1:A:749:MET:HE3	1:A:751:ILE:HD12	1.91	0.45
1:A:775:TYR:HE2	1:A:871:LEU:HD12	1.81	0.45
2:A:1301:B12:H552	2:A:1301:B12:H531	1.97	0.45
1:A:689:PRO:HB2	1:A:736:ILE:HG13	1.97	0.45
1:A:870:LEU:HD13	1:A:879:PHE:CE1	2.52	0.45
1:A:1027:HIS:HD2	1:A:1147:GLU:OE2	2.00	0.45
1:A:1184:HIS:CD2	1:A:1186:ASP:H	2.35	0.45
1:A:680:GLU:OE1	1:A:680:GLU:HA	2.17	0.44
1:A:658:GLU:H	1:A:658:GLU:HG3	1.52	0.44
1:A:803:LEU:CD1	1:A:830:LEU:HD11	2.48	0.44
1:A:898:LYS:O	1:A:900:ARG:N	2.50	0.44
2:A:1301:B12:C42	2:A:1301:B12:C10	2.95	0.44
1:A:872:SER:O	1:A:876:ARG:HB2	2.17	0.44
1:A:722:ALA:HB2	1:A:772:CYS:SG	2.58	0.44
1:A:799:ASP:O	1:A:828:ILE:HB	2.18	0.44
1:A:1194:GLN:HA	1:A:1221:ASN:O	2.17	0.44
1:A:726:LYS:NZ	1:A:771:GLN:NE2	2.61	0.43
1:A:1218:LEU:O	1:A:1219:ALA:C	2.61	0.43
1:A:754:VAL:CG1	1:A:813:GLU:HB3	2.49	0.43
1:A:1007:VAL:O	1:A:1007:VAL:HG23	2.17	0.43
1:A:754:VAL:HG13	1:A:813:GLU:HB3	2.00	0.43
2:A:1301:B12:O51	2:A:1301:B12:H561	2.18	0.43
1:A:1201:GLU:HG2	1:A:1211:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:VAL:O	1:A:1193:ALA:HB3	2.19	0.43
1:A:914:PHE:HB3	1:A:1045:ASP:HB3	2.01	0.42
1:A:1123:GLU:OE1	1:A:1127:ARG:NE	2.43	0.42
1:A:1007:VAL:O	1:A:1007:VAL:CG2	2.66	0.42
1:A:693:ILE:HA	1:A:697:LEU:HB2	2.02	0.42
1:A:1201:GLU:HG2	1:A:1211:VAL:CG2	2.50	0.42
1:A:1011:ILE:HD11	1:A:1044:ALA:CA	2.35	0.42
1:A:946:ASP:O	1:A:949:PRO:HD2	2.19	0.41
1:A:1137:PRO:HD3	1:A:1179:GLY:HA2	2.02	0.41
1:A:934:VAL:CG1	1:A:935:GLU:N	2.82	0.41
1:A:891:ARG:O	1:A:895:GLY:HA3	2.21	0.41
1:A:900:ARG:NH1	1:A:1194:GLN:HE21	2.18	0.41
2:A:1301:B12:C10	2:A:1301:B12:H421	2.51	0.41
1:A:898:LYS:O	1:A:899:PRO:C	2.63	0.40
1:A:912:ASN:O	1:A:912:ASN:CG	2.64	0.40
1:A:753:THR:HB	1:A:782:VAL:HA	2.01	0.40
1:A:918:TRP:O	1:A:1054:LYS:HE3	2.21	0.40
1:A:1161:THR:OG1	1:A:1163:MET:HG3	2.22	0.40
1:A:784:VAL:HG23	1:A:788:LYS:HB3	2.03	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	575/579 (99%)	546 (95%)	20 (4%)	9 (2%)	7 7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	740	LYS
1	A	741	GLU

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Mol	Chain	Res	Type
1	A	897	LYS
1	A	898	LYS
1	A	899	PRO
1	A	652	ALA
1	A	893	GLN
1	A	1193	ALA
1	A	743	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/484 (100%)	450 (93%)	33 (7%)	14	20

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	658	GLU
1	A	691	GLU
1	A	736	ILE
1	A	743	CYS
1	A	744	LYS
1	A	754	VAL
1	A	764	ASN
1	A	778	VAL
1	A	784	VAL
1	A	790	LEU
1	A	808	THR
1	A	812	ASP
1	A	836	THR
1	A	861	SER
1	A	870	LEU
1	A	876	ARG
1	A	892	ILE
1	A	896	ARG

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Mol	Chain	Res	Type
1	A	898	LYS
1	A	901	THR
1	A	928	ARG
1	A	962	ARG
1	A	996	ARG
1	A	1007	VAL
1	A	1033	THR
1	A	1058	ILE
1	A	1124	GLU
1	A	1142	CYS
1	A	1144	GLU
1	A	1167	GLU
1	A	1197	ARG
1	A	1225	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	ASN
1	A	684	GLN
1	A	742	GLN
1	A	746	ASN
1	A	771	GLN
1	A	841	HIS
1	A	858	GLN
1	A	893	GLN
1	A	1021	HIS
1	A	1027	HIS
1	A	1079	GLN
1	A	1122	ASN
1	A	1129	ASN
1	A	1145	HIS
1	A	1184	HIS
1	A	1194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	A	1301	-	94,101,101	1.62	13 (13%)	149,166,166	2.37	48 (32%)

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	A	1301	-	-	20/56/223/223	0/3/11/11

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C19-N24	-7.20	1.40	1.49
2	A	1301	B12	C8B-C9B	5.94	1.50	1.40
2	A	1301	B12	C14-N23	4.62	1.41	1.35
2	A	1301	B12	C6B-C5B	3.97	1.50	1.40
2	A	1301	B12	C2B-N3B	3.52	1.38	1.31
2	A	1301	B12	C1-C2	-2.58	1.52	1.58
2	A	1301	B12	C47-C12	-2.52	1.49	1.54
2	A	1301	B12	C14-C15	2.44	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C16-C15	-2.31	1.38	1.44
2	A	1301	B12	C1-C19	-2.24	1.50	1.55
2	A	1301	B12	C1R-N1B	2.24	1.52	1.46
2	A	1301	B12	C12-C11	-2.04	1.48	1.52
2	A	1301	B12	C12-C13	2.01	1.61	1.55

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C1-C19-C18	7.81	134.57	121.90
2	A	1301	B12	C13-C12-C11	-6.93	93.22	100.97
2	A	1301	B12	C20-C1-N21	-6.63	99.30	110.26
2	A	1301	B12	C12-C11-C10	-6.39	115.16	123.40
2	A	1301	B12	C18-C19-N24	6.11	111.51	102.33
2	A	1301	B12	C19-C1-N21	5.51	107.81	102.14
2	A	1301	B12	C20-C1-C19	-5.20	104.34	109.35
2	A	1301	B12	C12-C11-N23	4.80	118.44	111.83
2	A	1301	B12	C47-C12-C11	4.59	126.50	110.08
2	A	1301	B12	C30-C3-C4	-4.53	99.02	109.66
2	A	1301	B12	C15-C14-N23	-4.45	120.90	126.26
2	A	1301	B12	C1P-N59-C57	-4.16	113.76	122.69
2	A	1301	B12	C9B-C8B-N1B	4.11	107.12	105.30
2	A	1301	B12	C25-C2-C1	-4.08	107.66	113.75
2	A	1301	B12	C2-C1-N21	4.02	107.37	101.78
2	A	1301	B12	C18-C60-C61	-3.98	103.93	114.04
2	A	1301	B12	C19-N24-C16	3.95	111.61	107.29
2	A	1301	B12	C1-C19-N24	3.95	110.64	106.25
2	A	1301	B12	C26-C2-C1	3.88	115.99	110.00
2	A	1301	B12	C18-C17-C16	3.87	105.35	100.69
2	A	1301	B12	C46-C12-C13	-3.57	98.25	112.74
2	A	1301	B12	C13-C14-C15	3.38	129.46	124.32
2	A	1301	B12	C47-C12-C13	-3.35	99.17	112.74
2	A	1301	B12	C37-C38-N40	-3.17	106.68	116.49
2	A	1301	B12	C12-C13-C14	3.15	107.43	102.26
2	A	1301	B12	C2-C1-C19	3.12	123.46	118.61
2	A	1301	B12	C8B-C9B-N3B	-3.05	106.70	110.00
2	A	1301	B12	O34-C32-C31	-3.03	111.90	121.04
2	A	1301	B12	C60-C18-C19	3.02	122.45	114.59
2	A	1301	B12	C47-C12-C46	2.98	114.34	109.41
2	A	1301	B12	O3-C2P-C3P	-2.91	97.64	108.70
2	A	1301	B12	O58-C57-N59	-2.89	117.37	123.03
2	A	1301	B12	O2-P-O4	-2.87	100.64	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C7B-C8B-C9B	-2.86	119.04	122.47
2	A	1301	B12	O5-P-O2	2.83	118.22	106.70
2	A	1301	B12	C17-C16-C15	2.70	130.53	126.26
2	A	1301	B12	P-O3-C2P	2.66	130.18	121.10
2	A	1301	B12	C10-C9-N22	-2.55	122.83	125.74
2	A	1301	B12	O44-C43-N45	-2.44	116.01	122.53
2	A	1301	B12	O7R-C2R-C3R	-2.34	104.63	111.19
2	A	1301	B12	O2-C3R-C2R	-2.19	103.83	111.68
2	A	1301	B12	O63-C61-C60	2.18	125.43	120.87
2	A	1301	B12	O39-C38-N40	2.18	128.35	122.53
2	A	1301	B12	C48-C49-C50	2.18	119.94	112.55
2	A	1301	B12	O3-C2P-C1P	-2.14	102.70	106.94
2	A	1301	B12	C15-C16-N24	-2.07	119.48	122.42
2	A	1301	B12	C31-C32-N33	2.06	123.09	116.49
2	A	1301	B12	C55-C17-C16	-2.04	112.61	116.59

There are no chirality outliers.

All (20) torsion outliers are listed below:

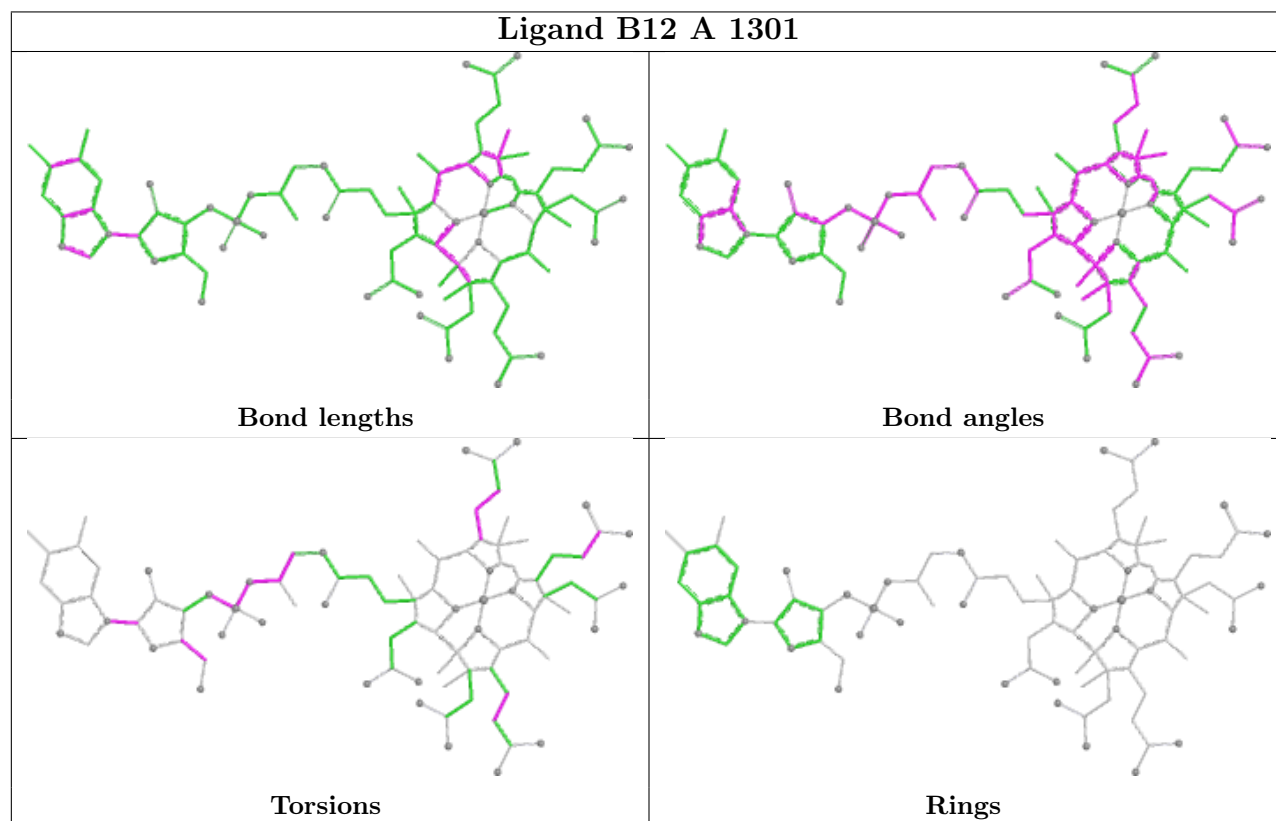
Mol	Chain	Res	Type	Atoms
2	A	1301	B12	C3-C30-C31-C32
2	A	1301	B12	C14-C13-C48-C49
2	A	1301	B12	N59-C1P-C2P-O3
2	A	1301	B12	C1P-C2P-O3-P
2	A	1301	B12	C3P-C2P-O3-P
2	A	1301	B12	C2P-O3-P-O5
2	A	1301	B12	C2P-O3-P-O2
2	A	1301	B12	C3R-O2-P-O3
2	A	1301	B12	O6R-C4R-C5R-O8R
2	A	1301	B12	C3R-C4R-C5R-O8R
2	A	1301	B12	N59-C1P-C2P-C3P
2	A	1301	B12	C13-C48-C49-C50
2	A	1301	B12	C2R-C1R-N1B-C8B
2	A	1301	B12	O6R-C1R-N1B-C8B
2	A	1301	B12	C12-C13-C48-C49
2	A	1301	B12	C41-C42-C43-N45
2	A	1301	B12	C2R-C1R-N1B-C2B
2	A	1301	B12	C2P-O3-P-O4
2	A	1301	B12	C3R-O2-P-O5
2	A	1301	B12	C41-C42-C43-O44

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	B12	22	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	577/579 (99%)	-0.16	18 (3%) 51 53	18, 36, 69, 105	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	LYS	5.0
1	A	899	PRO	4.8
1	A	894	HIS	3.8
1	A	651	GLN	3.6
1	A	898	LYS	3.2
1	A	740	LYS	3.2
1	A	900	ARG	3.0
1	A	892	ILE	2.7
1	A	962	ARG	2.7
1	A	896	ARG	2.5
1	A	652	ALA	2.4
1	A	901	THR	2.4
1	A	741	GLU	2.3
1	A	742	GLN	2.3
1	A	902	PRO	2.3
1	A	687	THR	2.2
1	A	743	CYS	2.1
1	A	893	GLN	2.1

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](#)

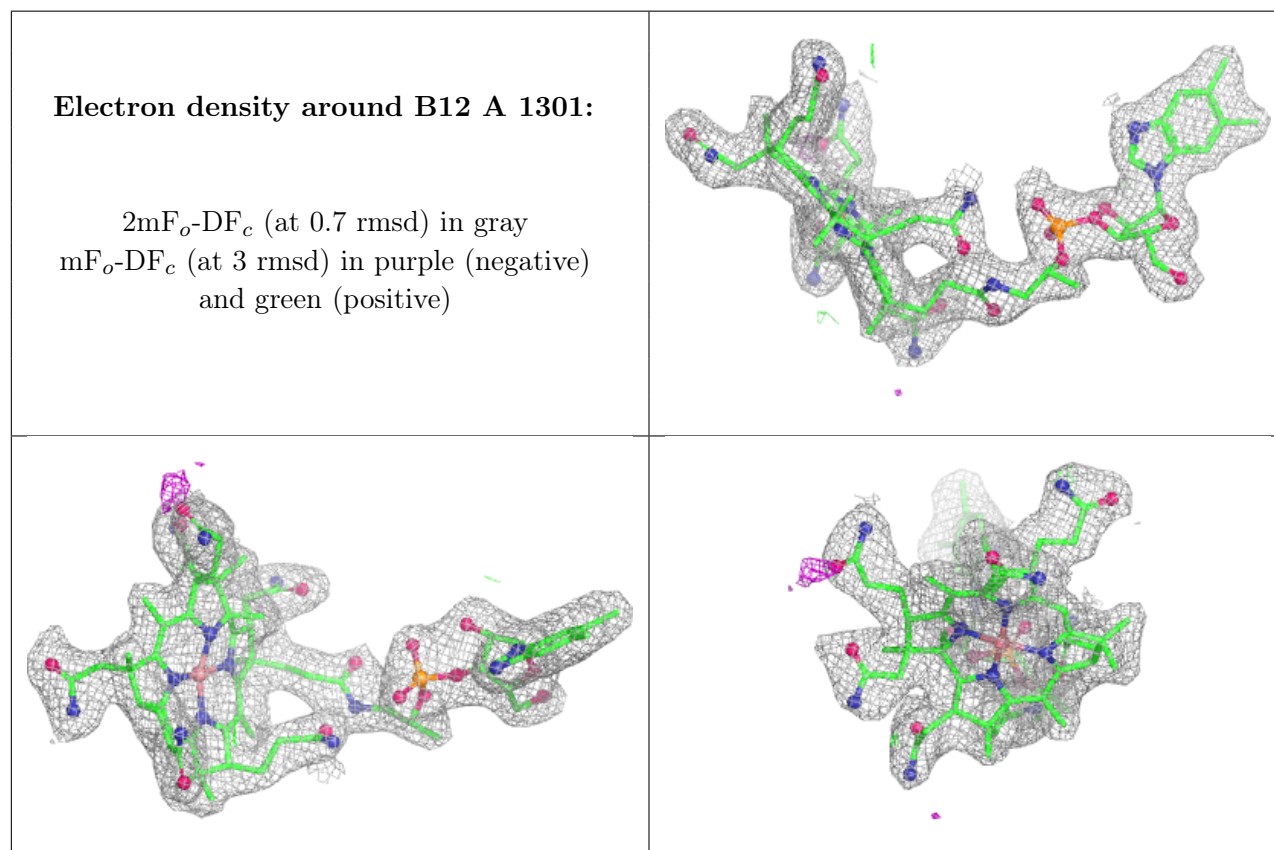
There are no oligosaccharides in this entry.

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	A	1301	91/91	0.98	0.06	14,32,44,52	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.