



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 02:14 PM EDT

PDB ID : 9CBQ / pdb_00009cbq
Title : Methionine synthase from *Thermus thermophilus* HB8, Folate demethylation state (Fol-on)
Authors : Yamada, K.; Mendoza, J.; Koutmos, M.
Deposited on : 2024-06-19
Resolution : 2.87 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

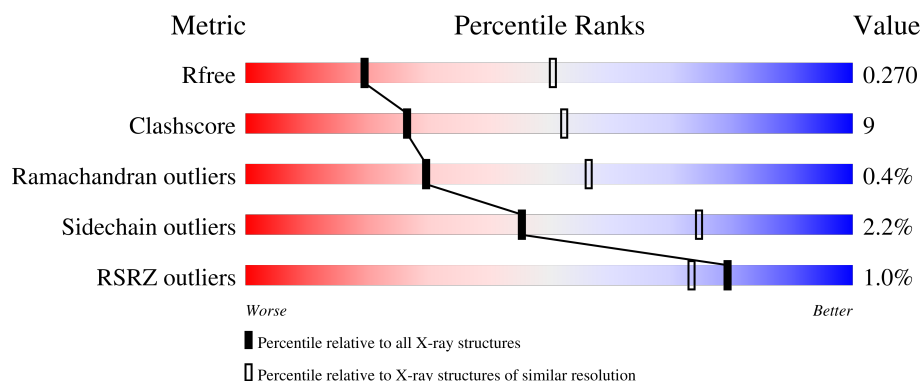
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

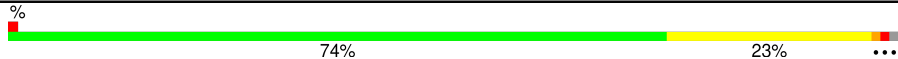
The reported resolution of this entry is 2.87 Å.

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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	511	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4115 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.

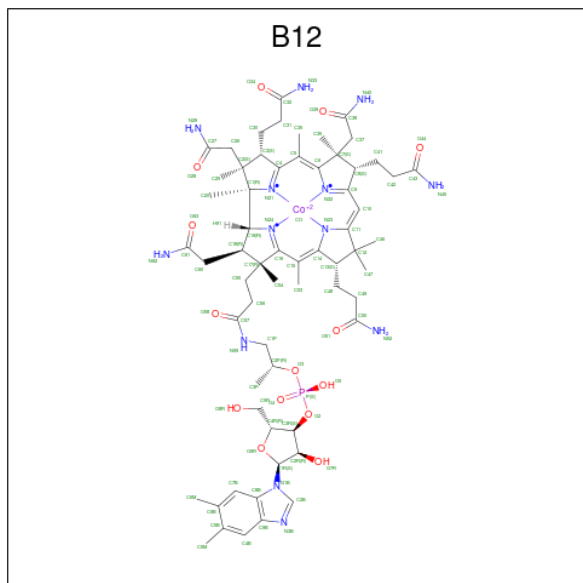
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	504	3941	2512	688	726	15	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	GLY	ASP	engineered mutation	UNP Q5SKM5

- Molecule 2 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



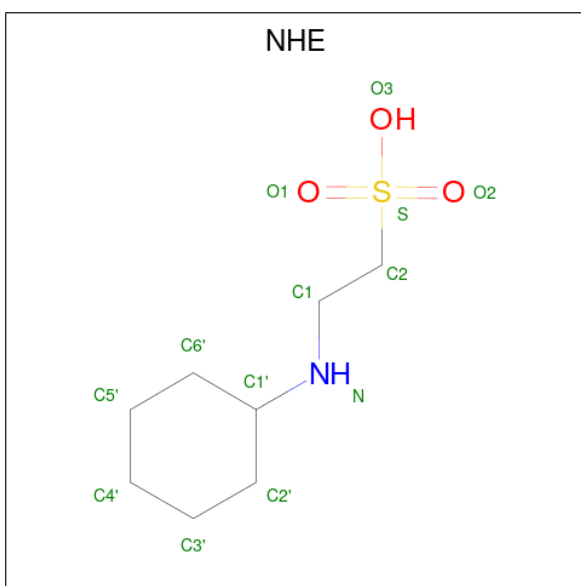
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Co	N	O P		
2	A	1	91	62	1	13	14 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

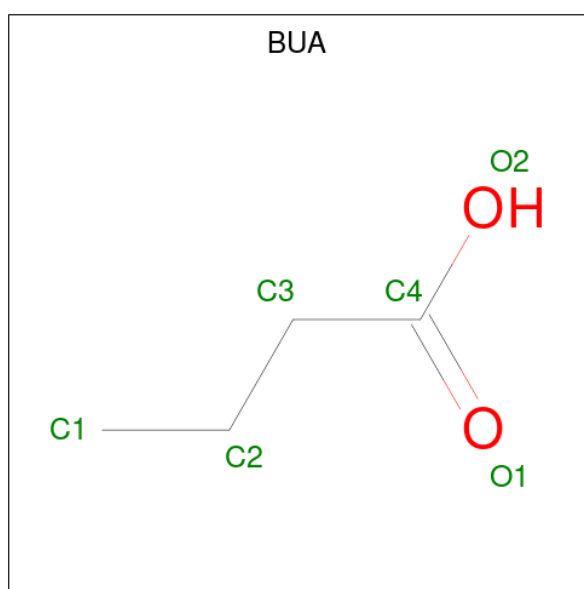
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is butanoic acid (CCD ID: BUA) (formula: C₄H₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

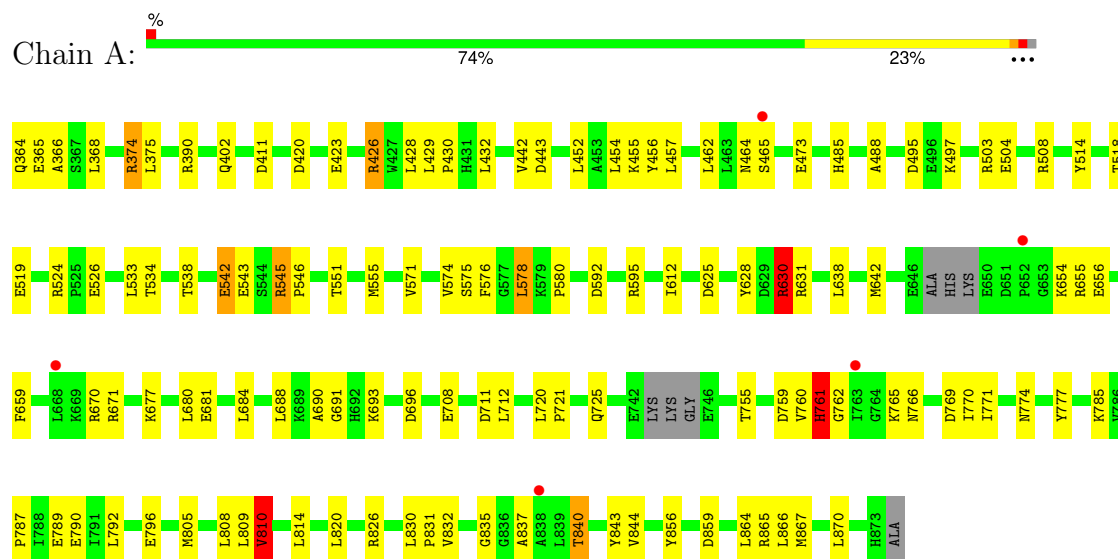
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	28	Total	O	0	0
			28	28		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.16Å 95.16Å 274.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.77 – 2.87 52.77 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.77-2.87) 99.8 (52.77-2.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.217 , 0.276 0.214 , 0.270	Depositor DCC
R_{free} test set	903 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	100.5	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 105.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: ZN, CL, GOL, SO4, B12, BUA, NHE

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	0.78	0/4005	1.29	22/5405 (0.4%)

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	10

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	630	ARG	NE-CZ-NH2	12.47	130.43	119.20
1	A	761[A]	HIS	N-CA-C	-8.07	98.63	110.42
1	A	761[B]	HIS	N-CA-C	-8.07	98.63	110.42
1	A	711	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	769	ASP	CA-CB-CG	6.83	119.44	112.60
1	A	534	THR	OG1-CB-CG2	-6.13	97.04	109.30
1	A	551	THR	OG1-CB-CG2	-5.78	97.73	109.30
1	A	508	ARG	CD-NE-CZ	5.61	132.26	124.40
1	A	504	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	497	LYS	CG-CD-CE	5.53	124.01	111.30
1	A	810	VAL	N-CA-C	-5.41	105.10	111.00
1	A	495	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	826	ARG	NH1-CZ-NH2	5.38	126.30	119.30
1	A	542	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	630	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	859	ASP	CA-CB-CG	5.24	117.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	543	GLU	N-CA-CB	5.16	117.80	110.06
1	A	508	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	814	LEU	N-CA-CB	5.07	117.36	110.01
1	A	630	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
1	A	840	THR	CA-CB-CG2	5.01	119.02	110.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	ARG	Sidechain
1	A	390	ARG	Sidechain
1	A	426	ARG	Sidechain
1	A	465	SER	Peptide
1	A	524	ARG	Sidechain
1	A	545	ARG	Sidechain
1	A	630	ARG	Sidechain
1	A	631	ARG	Sidechain
1	A	761[B]	HIS	Mainchain
1	A	865	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	3941	0	4044	71	0
2	A	91	0	88	10	0
3	A	15	0	0	1	0
4	A	26	0	34	2	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	6	0	6	0	0
8	A	6	0	8	0	0
9	A	28	0	0	4	0
All	All	4115	0	4180	77	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 9.

All (77) 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:428:LEU:HG	1:A:432:LEU:HD11	1.39	1.00
1:A:428:LEU:CG	1:A:432:LEU:HD11	2.09	0.82
1:A:428:LEU:HG	1:A:432:LEU:CD1	2.14	0.76
2:A:901:B12:H362	2:A:901:B12:H351	1.70	0.73
1:A:374:ARG:HB2	1:A:402:GLN:OE1	1.92	0.69
1:A:428:LEU:CD1	1:A:432:LEU:HD11	2.26	0.65
1:A:759:ASP:OD2	1:A:761[B]:HIS:HB2	1.99	0.63
1:A:638:LEU:O	1:A:642:MET:HG3	2.00	0.62
1:A:680:LEU:HB2	9:A:1026:HOH:O	1.99	0.60
1:A:759:ASP:OD2	1:A:761[A]:HIS:HB2	2.01	0.60
1:A:808:LEU:HD13	1:A:837:ALA:HB3	1.84	0.59
1:A:809:LEU:HD21	2:A:901:B12:H411	1.84	0.59
1:A:760:VAL:O	1:A:761[B]:HIS:C	2.39	0.58
1:A:625:ASP:HA	1:A:630:ARG:HG3	1.85	0.58
1:A:777:TYR:CE2	1:A:867:MET:HG3	2.40	0.57
1:A:538:THR:HG21	1:A:575:SER:HA	1.87	0.56
1:A:755:THR:HG21	1:A:761[A]:HIS:O	2.06	0.54
1:A:429:LEU:HB2	1:A:430:PRO:HD3	1.88	0.54
1:A:426:ARG:HG2	1:A:456:TYR:HE2	1.74	0.53
2:A:901:B12:H552	2:A:901:B12:H531	1.91	0.53
1:A:375:LEU:HD22	1:A:375:LEU:N	2.25	0.51
1:A:688:LEU:C	1:A:690:ALA:N	2.67	0.51
1:A:820:LEU:HD21	1:A:832:VAL:HG11	1.92	0.51
1:A:514:TYR:O	1:A:518:THR:HG22	2.08	0.51
1:A:503:ARG:HD2	9:A:1014:HOH:O	2.12	0.50
1:A:592:ASP:OD1	1:A:595:ARG:NH1	2.44	0.50
1:A:840:THR:HG23	1:A:843:TYR:H	1.76	0.50
1:A:428:LEU:O	1:A:429:LEU:C	2.55	0.49
1:A:655:ARG:HH12	1:A:659:PHE:HB2	1.76	0.49
1:A:844:VAL:HG21	1:A:856:TYR:HB2	1.94	0.49
1:A:680:LEU:O	1:A:684:LEU:HG	2.13	0.49
1:A:457:LEU:CD2	9:A:1004:HOH:O	2.60	0.49
1:A:787:PRO:HG2	1:A:790:GLU:HG2	1.95	0.49
1:A:365:GLU:O	1:A:366:ALA:HB3	2.14	0.48
1:A:761[A]:HIS:CG	1:A:808:LEU:HB2	2.48	0.48
1:A:830:LEU:HD12	1:A:831:PRO:HD2	1.95	0.48
1:A:720:LEU:N	1:A:721:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HG	1:A:681:GLU:H	1.79	0.46
1:A:770:ILE:O	1:A:774:ASN:ND2	2.48	0.46
1:A:368:LEU:HD21	1:A:595:ARG:HG3	1.98	0.46
1:A:688:LEU:O	1:A:691:GLY:N	2.42	0.46
1:A:725:GLN:HB2	9:A:1006:HOH:O	2.16	0.45
1:A:519:GLU:HB2	3:A:908:SO4:O1	2.16	0.45
2:A:901:B12:H531	2:A:901:B12:H543	1.99	0.44
1:A:428:LEU:O	1:A:432:LEU:HD12	2.17	0.44
1:A:677:LYS:O	1:A:680:LEU:HD23	2.17	0.44
1:A:792:LEU:O	1:A:796:GLU:HG2	2.17	0.44
1:A:721:PRO:O	1:A:725:GLN:HG2	2.18	0.44
1:A:810:VAL:H	2:A:901:B12:H331	1.65	0.44
1:A:835:GLY:HA3	2:A:901:B12:C6B	2.48	0.44
1:A:580:PRO:HD2	4:A:907:NHE:HC11	2.00	0.43
2:A:901:B12:H2B	2:A:901:B12:O2	2.18	0.43
1:A:462:LEU:HG	1:A:488:ALA:HB3	2.01	0.43
1:A:411:ASP:OD1	1:A:443:ASP:HB2	2.19	0.42
1:A:538:THR:OG1	1:A:576:PHE:O	2.35	0.42
1:A:542:GLU:HA	1:A:545:ARG:HG3	2.01	0.42
1:A:545:ARG:HB2	1:A:546:PRO:HD3	2.01	0.42
1:A:765:LYS:HG3	1:A:766:ASN:N	2.33	0.42
1:A:420:ASP:O	1:A:423:GLU:HG2	2.19	0.42
1:A:538:THR:HB	1:A:578:LEU:HD13	2.00	0.42
1:A:592:ASP:HB2	1:A:612:ILE:HD11	2.01	0.42
1:A:555:MET:HE3	1:A:555:MET:HB2	1.91	0.42
1:A:571:VAL:O	1:A:574:VAL:HG12	2.19	0.42
1:A:771:ILE:HG22	1:A:864:LEU:HD12	2.02	0.41
2:A:901:B12:H411	2:A:901:B12:H363	1.66	0.41
1:A:443:ASP:HA	1:A:464:ASN:HB3	2.02	0.41
1:A:452:LEU:O	1:A:455:LYS:HG2	2.20	0.41
1:A:708:GLU:O	1:A:712:LEU:HG	2.20	0.41
1:A:755:THR:HG21	1:A:761[B]:HIS:O	2.20	0.41
1:A:454:LEU:HD13	1:A:485:HIS:ND1	2.36	0.41
1:A:693:LYS:HB2	1:A:696:ASP:OD1	2.21	0.41
1:A:809:LEU:CD2	2:A:901:B12:H363	2.51	0.41
1:A:866:LEU:O	1:A:870:LEU:HG	2.21	0.40
1:A:654:LYS:O	1:A:655:ARG:C	2.62	0.40
2:A:901:B12:H261	2:A:901:B12:H91	1.73	0.40
1:A:628:TYR:CD2	4:A:903:NHE:HC12	2.57	0.40
1:A:670:ARG:O	1:A:671:ARG:C	2.63	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	499/511 (98%)	474 (95%)	23 (5%)	2 (0%)	30	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	762	GLY
1	A	533	LEU

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	411/414 (99%)	402 (98%)	9 (2%)	45	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	442	VAL
1	A	473	GLU
1	A	578	LEU
1	A	656	GLU
1	A	785	LYS
1	A	789	GLU
1	A	805	MET
1	A	810	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	B12	A	901	1	94,101,101	0.64	2 (2%)	149,166,166	0.89	8 (5%)
3	SO4	A	906	-	4,4,4	0.31	0	6,6,6	0.20	0
7	BUA	A	909	-	5,5,5	1.00	0	5,5,5	1.60	2 (40%)
3	SO4	A	908	-	4,4,4	0.75	0	6,6,6	0.58	0
4	NHE	A	907	-	13,13,13	1.97	3 (23%)	16,17,17	2.69	4 (25%)
8	GOL	A	910	-	5,5,5	0.30	0	5,5,5	0.69	0
4	NHE	A	903	-	13,13,13	1.82	3 (23%)	16,17,17	2.10	8 (50%)
3	SO4	A	902	-	4,4,4	0.27	0	6,6,6	0.25	0

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	901	1	-	22/56/223/223	0/3/11/11
7	BUA	A	909	-	-	0/3/3/3	-
4	NHE	A	907	-	-	6/7/15/15	0/1/1/1
8	GOL	A	910	-	-	4/4/4/4	-
4	NHE	A	903	-	-	4/7/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	907	NHE	C2-S	5.11	1.84	1.77
4	A	903	NHE	C2-S	4.39	1.83	1.77
2	A	901	B12	C16-C15	-2.85	1.36	1.44
4	A	903	NHE	O1-S	2.82	1.53	1.45
4	A	907	NHE	O2-S	2.70	1.52	1.45
4	A	903	NHE	O2-S	2.40	1.51	1.45
4	A	907	NHE	O1-S	2.38	1.51	1.45
2	A	901	B12	CO-N22	-2.10	1.86	1.96

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	907	NHE	O3-S-C2	5.90	117.55	106.00
4	A	907	NHE	C6'-C1'-C2'	5.43	120.17	110.80
4	A	907	NHE	C3'-C2'-C1'	-4.50	103.02	111.09
4	A	903	NHE	O2-S-O1	-4.33	99.75	113.82
4	A	903	NHE	O2-S-C2	3.47	111.97	106.73
4	A	907	NHE	C4'-C5'-C6'	3.39	118.39	111.42
4	A	903	NHE	O1-S-C2	3.06	111.35	106.73
2	A	901	B12	C19-C1-N21	2.93	105.16	102.14
2	A	901	B12	C19-N24-C16	2.78	110.33	107.29
4	A	903	NHE	C4'-C5'-C6'	2.74	117.04	111.42
7	A	909	BUA	O1-C4-C3	-2.70	114.52	123.09
2	A	901	B12	C9-N22-C6	2.62	108.43	105.28
2	A	901	B12	C37-C7-C6	2.52	114.90	107.11
4	A	903	NHE	C3'-C2'-C1'	2.37	115.34	111.09
2	A	901	B12	C48-C13-C14	2.26	114.12	108.51
7	A	909	BUA	O2-C4-C3	2.25	121.09	114.00
4	A	903	NHE	C4'-C3'-C2'	2.20	115.94	111.42
4	A	903	NHE	C2-C1-N	2.13	117.48	111.40
2	A	901	B12	C9B-C8B-N1B	2.05	106.21	105.30
2	A	901	B12	C2-C1-N21	2.04	104.62	101.78
2	A	901	B12	C2-C1-C19	-2.04	115.44	118.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	NHE	O3-S-O1	2.02	116.44	111.40

There are no chirality outliers.

All (36) torsion outliers are listed below:

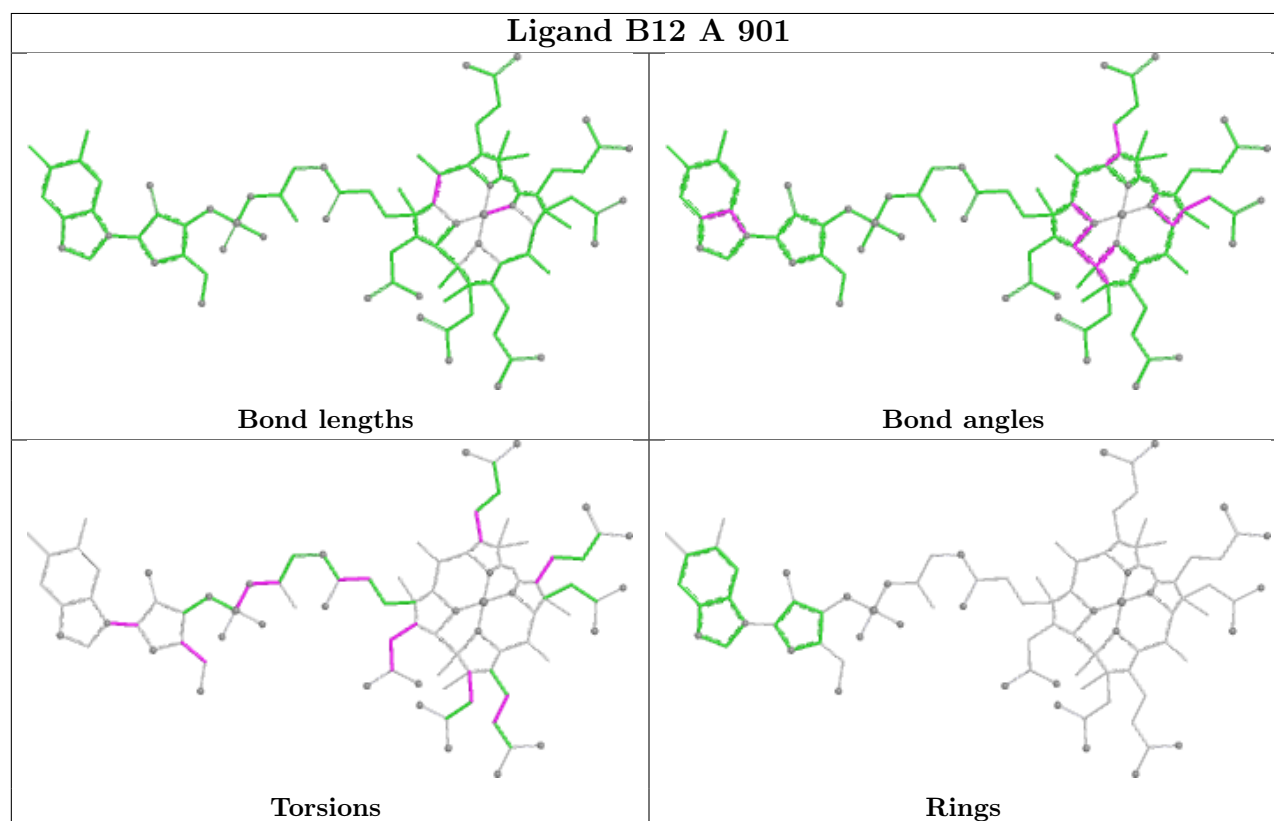
Mol	Chain	Res	Type	Atoms
2	A	901	B12	C1-C2-C26-C27
2	A	901	B12	C25-C2-C26-C27
2	A	901	B12	C3-C2-C26-C27
2	A	901	B12	C42-C41-C8-C9
2	A	901	B12	C14-C13-C48-C49
2	A	901	B12	C18-C60-C61-O63
2	A	901	B12	C18-C60-C61-N62
2	A	901	B12	C1P-C2P-O3-P
2	A	901	B12	C3P-C2P-O3-P
2	A	901	B12	C2P-O3-P-O2
4	A	907	NHE	C1-C2-S-O1
4	A	907	NHE	C1-C2-S-O2
4	A	907	NHE	C1-C2-S-O3
8	A	910	GOL	C1-C2-C3-O3
2	A	901	B12	C3R-C4R-C5R-O8R
2	A	901	B12	O6R-C4R-C5R-O8R
2	A	901	B12	C42-C41-C8-C7
4	A	903	NHE	C1-C2-S-O3
8	A	910	GOL	O1-C1-C2-C3
2	A	901	B12	C2R-C1R-N1B-C8B
2	A	901	B12	O6R-C1R-N1B-C8B
8	A	910	GOL	O1-C1-C2-O2
4	A	907	NHE	C2-C1-N-C1'
8	A	910	GOL	O2-C2-C3-O3
4	A	907	NHE	C6'-C1'-N-C1
4	A	903	NHE	C2-C1-N-C1'
4	A	903	NHE	C1-C2-S-O1
4	A	903	NHE	C1-C2-S-O2
4	A	907	NHE	N-C1-C2-S
2	A	901	B12	C3-C30-C31-C32
2	A	901	B12	C17-C18-C60-C61
2	A	901	B12	C19-C18-C60-C61
2	A	901	B12	C2P-O3-P-O4
2	A	901	B12	C2P-O3-P-O5
2	A	901	B12	C55-C56-C57-O58
2	A	901	B12	C55-C56-C57-N59

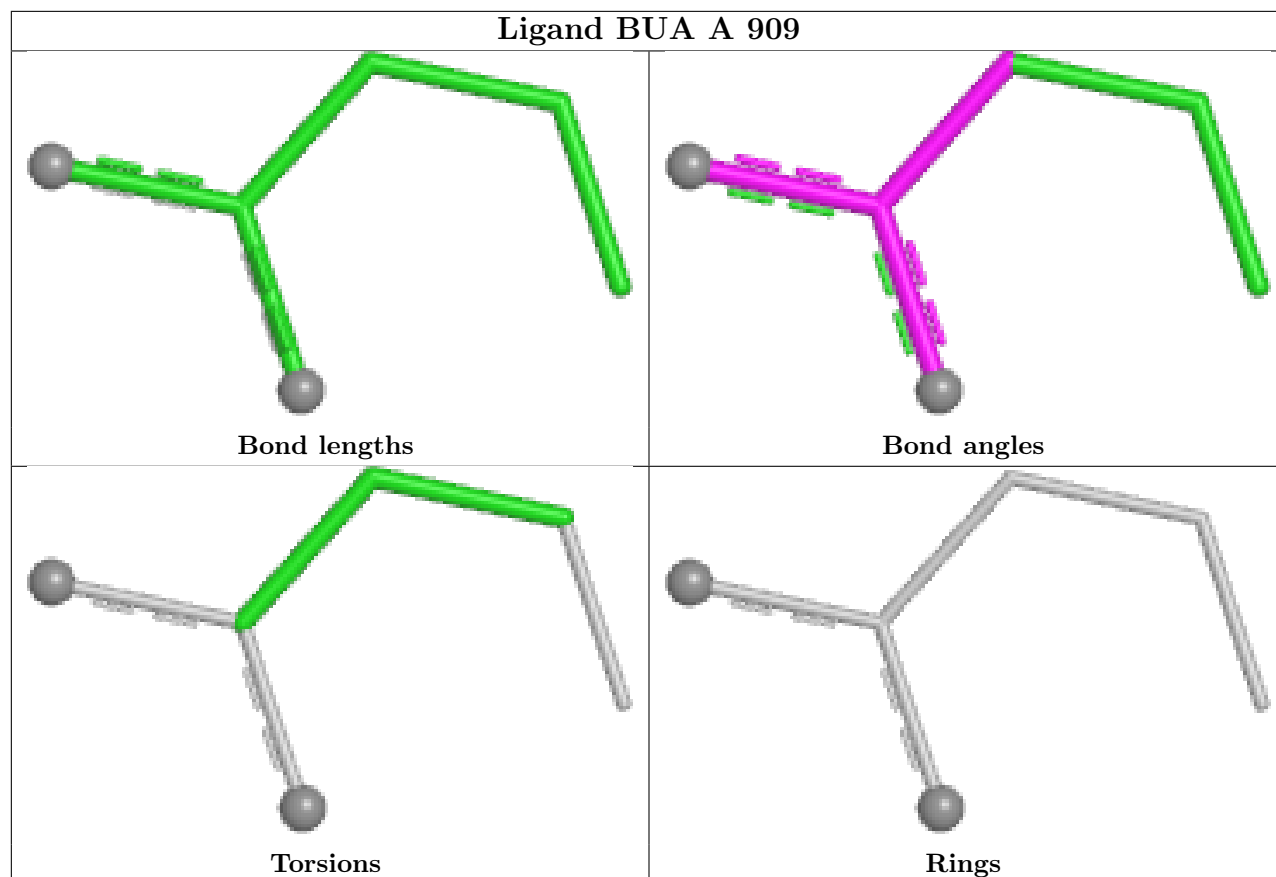
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	B12	10	0
3	A	908	SO4	1	0
4	A	907	NHE	1	0
4	A	903	NHE	1	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	504/511 (98%)	-0.16	5 (0%) 79 73	56, 123, 206, 273	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	763	ILE	3.7
1	A	838	ALA	3.1
1	A	668	LEU	2.7
1	A	652	PRO	2.2
1	A	465	SER	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(Å ²)	Q<0.9
4	NHE	A	907	13/13	0.52	0.16	122,169,216,237	0
4	NHE	A	903	13/13	0.79	0.15	102,168,220,243	0

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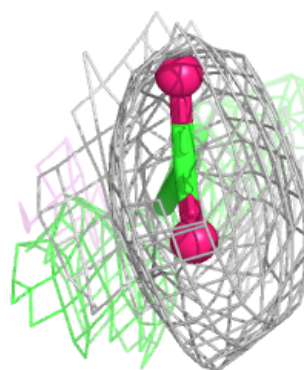
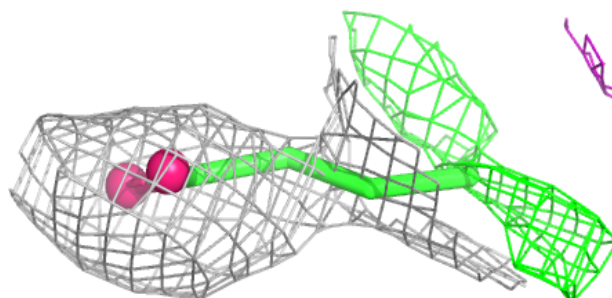
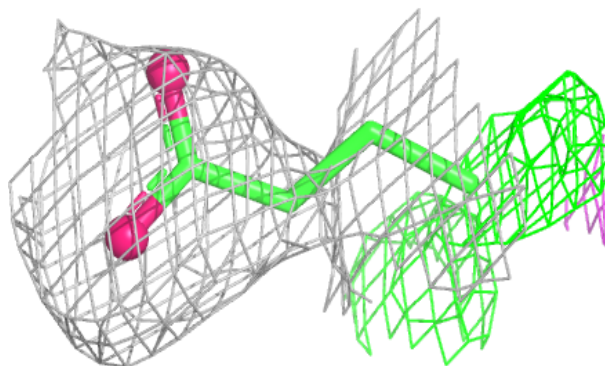
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	902	5/5	0.84	0.08	156,165,198,198	0
8	GOL	A	910	6/6	0.86	0.09	99,119,157,159	0
3	SO4	A	908	5/5	0.89	0.13	65,78,113,139	5
3	SO4	A	906	5/5	0.89	0.05	148,163,170,203	0
7	BUA	A	909	6/6	0.92	0.12	94,99,123,125	0
6	ZN	A	905	1/1	0.92	0.06	161,161,161,161	0
2	B12	A	901	91/91	0.95	0.10	80,101,128,144	0
5	CL	A	904	1/1	0.99	0.04	88,88,88,88	1

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.

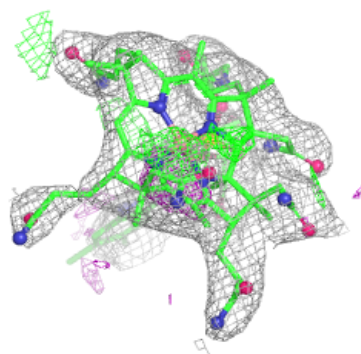
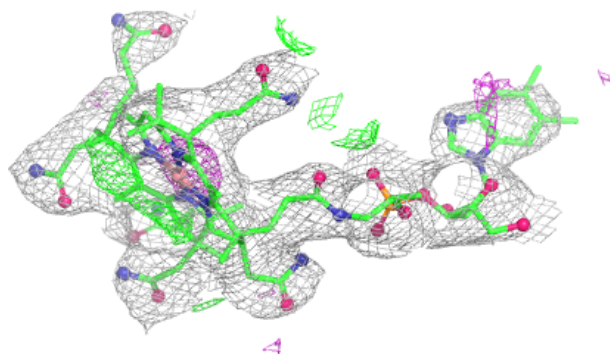
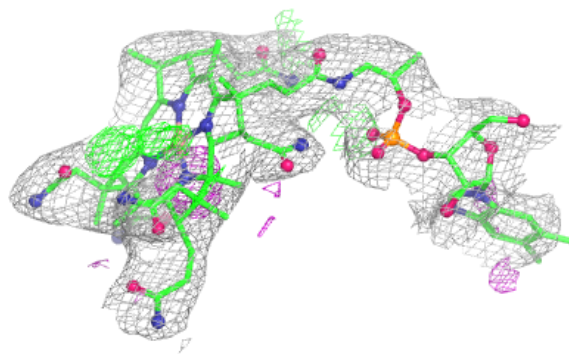
Electron density around BUA A 909:

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 901:

$2mF_o-DF_c$ (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.