



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 PM UTC

PDB ID : 9LUS / pdb_00009lus
Title : Structure of human G9a SET-domain in complex with FLAV27 inhibitor
Authors : Singh, R.K.; Dai, S.
Deposited on : 2025-02-10
Resolution : 2.70 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

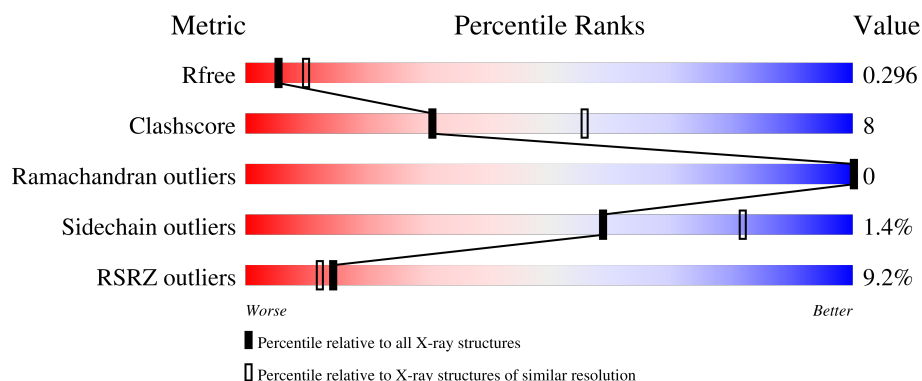
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	300	<div> <div>6%</div> <div>74%</div> <div>13%</div> <div>12%</div> </div>
1	B	300	<div> <div>10%</div> <div>66%</div> <div>22%</div> <div>11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4277 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 Histone-lysine N-methyltransferase EHMT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	2	0
			2077	1308	355	401	13			
1	B	267	Total	C	N	O	S	0	1	0
			2104	1317	365	407	15			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	894	MET	-	initiating methionine	UNP Q96KQ7
A	895	GLY	-	expression tag	UNP Q96KQ7
A	896	SER	-	expression tag	UNP Q96KQ7
A	897	SER	-	expression tag	UNP Q96KQ7
A	898	HIS	-	expression tag	UNP Q96KQ7
A	899	HIS	-	expression tag	UNP Q96KQ7
A	900	HIS	-	expression tag	UNP Q96KQ7
A	901	HIS	-	expression tag	UNP Q96KQ7
A	902	HIS	-	expression tag	UNP Q96KQ7
A	903	HIS	-	expression tag	UNP Q96KQ7
A	904	SER	-	expression tag	UNP Q96KQ7
A	905	SER	-	expression tag	UNP Q96KQ7
A	906	GLY	-	expression tag	UNP Q96KQ7
A	907	LEU	-	expression tag	UNP Q96KQ7
A	908	VAL	-	expression tag	UNP Q96KQ7
A	909	PRO	-	expression tag	UNP Q96KQ7
A	910	ARG	-	expression tag	UNP Q96KQ7
A	911	GLY	-	expression tag	UNP Q96KQ7
A	912	SER	-	expression tag	UNP Q96KQ7
B	894	MET	-	initiating methionine	UNP Q96KQ7
B	895	GLY	-	expression tag	UNP Q96KQ7
B	896	SER	-	expression tag	UNP Q96KQ7
B	897	SER	-	expression tag	UNP Q96KQ7
B	898	HIS	-	expression tag	UNP Q96KQ7
B	899	HIS	-	expression tag	UNP Q96KQ7

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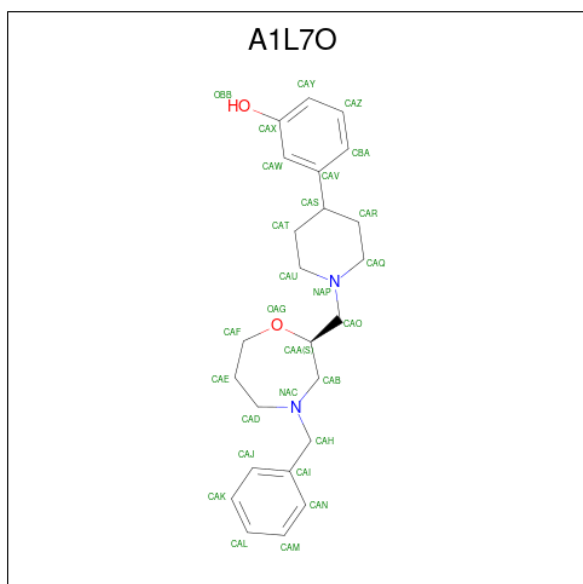
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Chain	Residue	Modelled	Actual	Comment	Reference
B	900	HIS	-	expression tag	UNP Q96KQ7
B	901	HIS	-	expression tag	UNP Q96KQ7
B	902	HIS	-	expression tag	UNP Q96KQ7
B	903	HIS	-	expression tag	UNP Q96KQ7
B	904	SER	-	expression tag	UNP Q96KQ7
B	905	SER	-	expression tag	UNP Q96KQ7
B	906	GLY	-	expression tag	UNP Q96KQ7
B	907	LEU	-	expression tag	UNP Q96KQ7
B	908	VAL	-	expression tag	UNP Q96KQ7
B	909	PRO	-	expression tag	UNP Q96KQ7
B	910	ARG	-	expression tag	UNP Q96KQ7
B	911	GLY	-	expression tag	UNP Q96KQ7
B	912	SER	-	expression tag	UNP Q96KQ7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is 3-[1-[[[(2 {S})-4-(phenylmethyl)-1,4-oxazepan-2-yl]methyl]piperidin-4-yl]phenol (CCD ID: A1L7O) (formula: C₂₄H₃₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	24	2	2		
3	B	1	Total	C	N	O	0	0
			28	24	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	15	Total	O	0	0
			15	15		

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.

- Chain A:
-
- | Amino Acid | Category | Percentage |
|------------|----------|------------|
| Met | Grey | 12% |
| Gly | Green | 74% |
| Ser | Green | 74% |
| Ser | Green | 74% |
| His | Green | 74% |
| His | Green | 74% |
| His | Green | 74% |
| His | Green | 74% |
| His | Green | 74% |
| His | Green | 74% |
| His | Green | 74% |
| Ser | Green | 74% |
| Ser | Green | 74% |
| Ser | Green | 74% |
| Gly | Green | 74% |
| Leu | Green | 74% |
| Val | Green | 74% |
| Pro | Green | 74% |
| Arg | Green | 74% |
| Gly | Green | 74% |
| Ser | Green | 74% |
| Asn | Green | 74% |
| Arg | Green | 74% |
| Ala | Green | 74% |
| Ile | Green | 74% |
| Arg | Green | 74% |
| Thr | Green | 74% |
| Glu | Green | 74% |
| Lys | Green | 74% |
| I921 | Red | 6% |
| I922 | Red | 6% |
| V926 | Red | 6% |
| C946 | Yellow | 13% |
| T959 | Yellow | 13% |
| N962 | Red | 6% |
| N963 | Red | 6% |
| I964 | Red | 6% |
| N967 | Yellow | 13% |
| H970 | Yellow | 13% |
| C974 | Red | 6% |
| D979 | Yellow | 13% |
| C980 | Yellow | 13% |
| N984 | Red | 6% |
| C985 | Red | 6% |
| L986 | Yellow | 13% |
| C987 | Red | 6% |
| S991 | Yellow | 13% |
| I992 | Yellow | 13% |
| R993 | Yellow | 13% |
| Y996 | Yellow | 13% |
| D997 | Yellow | 13% |
| F1006 | Red | 6% |
| N1007 | Red | 6% |
| K1008 | Red | 6% |
| E1016 | Red | 6% |
| C1017 | Red | 6% |
| N1018 | Red | 6% |
| C1019 | Red | 6% |
| C1020 | Red | 6% |
| C1021 | Red | 6% |
| C1027 | Red | 6% |
| K1028 | Red | 6% |
| N1029 | Red | 6% |
| R1030 | Red | 6% |
| V1031 | Red | 6% |
| R1039 | Red | 6% |
| L1040 | Red | 6% |
| Q1041 | Red | 6% |
| L1042 | Red | 6% |
| R1043 | Red | 6% |
| R1044 | Red | 6% |
| T1045 | Red | 6% |
| L1055 | Red | 6% |
| T1056 | Red | 6% |
| T1057 | Red | 6% |
| E1066 | Red | 6% |
| Y1067 | Red | 6% |
| V1068 | Red | 6% |
| D1090 | Red | 6% |
| Asn | Red | 6% |
| Lys | Red | 6% |
| Asp | Red | 6% |
| Gly | Red | 6% |
| E1095 | Red | 6% |
| A1101 | Red | 6% |
| Y1104 | Red | 6% |
| G1105 | Red | 6% |
| N1106 | Red | 6% |
| R1109 | Red | 6% |
| H1113 | Red | 6% |
| M1126 | Red | 6% |
| L1127 | Red | 6% |
| H1128 | Red | 6% |
| R1132 | Red | 6% |
| F1133 | Red | 6% |
| P1134 | Red | 6% |
| R1135 | Red | 6% |
| T1136 | Red | 6% |
| F1139 | Red | 6% |
| Y1154 | Red | 6% |
| G1155 | Red | 6% |
| D1156 | Red | 6% |
| C1170 | Red | 6% |
| E1173 | Red | 6% |
| E1180 | Red | 6% |
| L1189 | Red | 6% |
| Ala | Red | 6% |
| Arg | Red | 6% |
| Leu | Red | 6% |
| Asp | Red | 6% |

- Chain B:
-
- 10% 66% 22% 11%
- MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG ARG GLY SER ASN ARG ALA ILE ARG THR GLU LYS I921 I921 C937 P945 C946 T961 M962 N963 N967 L971 Q972 H973 C974 T975 C976 V977 D978 D979 C980 S981 S982 S983 N984 C985 L986 S987 G988 C989 L990 S991 I992 R993 C994 Q995 D996 G1000 R1001 L1002 L1003 Q1004 E1005 P1006 N1007 K1008 I1009 P1012 L1013 I1014 C1017 M1018 S1022 C1023 W1024 C1027 L1042 Y1043 M1048 G1051 V1052 R1053 Y1057 V1068 G1069 A1075 D1083 S1084 Y1085 L1086 D1090 M1091 LYS ASP G1094 E1095

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.15Å 55.83Å 67.17Å 89.35° 73.18° 67.04°	Depositor
Resolution (Å)	42.33 – 2.70 42.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (42.33-2.70) 94.4 (42.33-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.267 , 0.309 0.284 , 0.296	Depositor DCC
R_{free} test set	749 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4277	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.84% 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, A1L7O

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	0.59	0/2128	1.05	7/2888 (0.2%)
1	B	0.60	0/2150	1.07	4/2912 (0.1%)
All	All	0.60	0/4278	1.06	11/5800 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	980	CYS	N-CA-C	-12.38	94.42	111.87
1	A	1170	CYS	CB-CA-C	-7.53	98.35	110.84
1	B	984	ASN	N-CA-C	-6.87	103.30	113.61
1	A	1017	CYS	CB-CA-C	6.82	120.80	109.89
1	A	946	CYS	CB-CA-C	6.61	120.39	109.56
1	B	983	SER	N-CA-C	-5.47	102.34	113.29
1	B	1008	LYS	N-CA-C	-5.34	105.63	111.82
1	A	980	CYS	CB-CA-C	5.23	119.87	111.66
1	A	1028	LYS	N-CA-C	-5.07	107.25	112.93
1	A	1139	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	1156	ASP	N-CA-C	-5.01	106.43	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2077	0	1906	24	0
1	B	2104	0	1963	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	0	2	0
3	B	28	0	0	3	0
4	A	23	0	0	1	0
4	B	15	0	0	0	0
All	All	4277	0	3869	67	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 8.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:LYS:O	1:B:1176:LYS:HG3	1.92	0.68
1:B:937:CYS:HG	1:B:946:CYS:HG	0.72	0.67
1:B:977:VAL:HG12	1:B:977:VAL:O	1.97	0.64
1:B:1090:ASP:O	1:B:1091:ASN:C	2.42	0.62
1:B:978:ASP:O	1:B:979:ASP:C	2.44	0.61
1:A:984:ASN:O	1:A:985:CYS:C	2.44	0.61
1:B:1168:CYS:SG	1:B:1170:CYS:N	2.73	0.58
1:B:1188:ARG:O	1:B:1189:LEU:C	2.49	0.56
1:B:973:HIS:HB2	1:B:1021:CYS:HA	1.88	0.56
1:B:1083:ASP:HA	1:B:1086:LEU:HD12	1.88	0.55
1:B:1169:GLN:O	1:B:1170:CYS:C	2.49	0.55
1:A:1113:HIS:HB2	1:A:1154:TYR:CD1	2.42	0.55
1:B:1084:SER:HB3	3:B:1202:A1L7O:CAU	2.37	0.54
1:B:1068:VAL:HB	1:B:1106:ASN:CG	2.32	0.54
1:A:991:SER:O	1:A:993:ARG:N	2.36	0.53
1:A:1113:HIS:HB2	1:A:1154:TYR:CG	2.44	0.52
1:B:1085:TYR:CE2	3:B:1202:A1L7O:CAT	2.92	0.52
1:B:1118:ASN:O	1:B:1144:ILE:HD11	2.09	0.52
1:B:991:SER:HB3	1:B:1014:ILE:HA	1.92	0.52
1:B:1174:LYS:O	1:B:1175:CYS:C	2.54	0.51
1:B:1069:GLY:HA2	1:B:1104:TYR:O	2.10	0.51
1:A:1132:ARG:O	1:A:1134:PRO:HD3	2.11	0.51
1:B:1018:ASN:OD1	1:B:1021:CYS:SG	2.68	0.51
1:B:1118:ASN:HB3	1:B:1142:ARG:CZ	2.42	0.50
1:A:1043:TYR:CZ	1:A:1045:THR:HG22	2.47	0.50
1:B:1163:SER:HA	1:B:1166:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:CYS:SG	1:B:946:CYS:SG	2.71	0.48
3:A:1202:A1L7O:CAB	3:A:1202:A1L7O:CAJ	2.92	0.47
1:B:1113:HIS:CE1	1:B:1153:ASP:HA	2.49	0.47
1:A:991:SER:C	1:A:993:ARG:N	2.73	0.47
1:A:979:ASP:OD1	1:A:979:ASP:N	2.49	0.46
1:A:1041:GLN:HB2	1:A:1055:LEU:HD11	1.96	0.46
1:B:1042:LEU:HD12	1:B:1051:GLY:O	2.15	0.46
1:A:922:ILE:HB	1:A:946:CYS:SG	2.57	0.45
1:A:991:SER:C	1:A:993:ARG:H	2.20	0.45
1:B:1048:MET:HE2	1:B:1169:GLN:HB2	1.97	0.45
1:B:990:LEU:C	1:B:992:ILE:H	2.24	0.45
1:B:997:ASP:OD1	1:B:1000:GLY:N	2.49	0.45
1:A:1018:ASN:OD1	1:A:1020:ALA:HB3	2.17	0.45
1:A:1109:ARG:O	3:A:1202:A1L7O:CAT	2.64	0.44
1:B:1120:ILE:HG23	1:B:1141:SER:HB3	1.99	0.44
1:A:984:ASN:O	1:A:986:LEU:N	2.50	0.44
1:B:1179:ALA:O	1:B:1182:ILE:HB	2.18	0.44
1:A:1101:ALA:HA	1:A:1104:TYR:O	2.18	0.43
1:B:977:VAL:O	1:B:977:VAL:CG1	2.66	0.43
1:B:1043:TYR:CE1	1:B:1053:ARG:HB3	2.53	0.43
1:A:959:THR:O	1:B:967:ASN:CG	2.61	0.43
1:A:1045:THR:HB	4:A:1309:HOH:O	2.18	0.43
1:B:1085:TYR:CZ	3:B:1202:A1L7O:CAT	3.01	0.43
1:B:972:GLN:O	1:B:1018:ASN:ND2	2.51	0.43
1:B:983:SER:O	1:B:989:GLN:NE2	2.51	0.43
1:A:1016:GLU:HA	1:A:1029:ASN:ND2	2.33	0.43
1:B:985:CYS:C	1:B:987:CYS:H	2.26	0.42
1:B:985:CYS:C	1:B:987:CYS:N	2.77	0.42
1:A:1066:GLU:HG2	1:A:1136:ILE:O	2.18	0.42
1:B:971:LEU:HB3	1:B:1018:ASN:ND2	2.34	0.42
1:A:996:TYR:CD1	1:A:1031:VAL:HG21	2.55	0.42
1:B:979:ASP:HA	1:B:1027:CYS:HA	2.02	0.41
1:B:922:ILE:HB	1:B:946:CYS:SG	2.61	0.41
1:A:1068:VAL:HB	1:A:1106:ASN:CG	2.46	0.41
1:B:1006:PHE:CZ	1:B:1012:PRO:HD2	2.56	0.41
1:A:1126:MET:C	1:A:1128:HIS:H	2.29	0.41
1:B:1003:LEU:C	1:B:1005:GLU:N	2.79	0.41
1:A:967:ASN:HB3	1:A:970:HIS:ND1	2.37	0.40
1:A:997:ASP:OD1	1:A:997:ASP:C	2.63	0.40
1:B:1003:LEU:C	1:B:1005:GLU:H	2.29	0.40
1:B:1117:PRO:O	1:B:1142:ARG:NH1	2.54	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	263/300 (88%)	242 (92%)	21 (8%)	0	100	100
1	B	264/300 (88%)	240 (91%)	24 (9%)	0	100	100
All	All	527/600 (88%)	482 (92%)	45 (8%)	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	217/268 (81%)	214 (99%)	3 (1%)	59	82
1	B	225/268 (84%)	222 (99%)	3 (1%)	61	83
All	All	442/536 (82%)	436 (99%)	6 (1%)	59	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1068	VAL
1	A	1128	HIS
1	A	1180	GLU
1	B	1009	ILE
1	B	1013	LEU

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Mol	Chain	Res	Type
1	B	1024	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1029	ASN
1	A	1056	GLN
1	A	1177	HIS
1	B	984	ASN
1	B	1056	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	A1L7O	B	1202	-	31,31,31	2.27	1 (3%)	36,41,41	2.30	11 (30%)
3	A1L7O	A	1202	-	31,31,31	2.11	1 (3%)	36,41,41	3.03	12 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1L7O	B	1202	-	-	8/10/33/33	0/3/4/4
3	A1L7O	A	1202	-	-	7/10/33/33	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	A1L7O	CAH-NAC	-11.84	1.24	1.47
3	A	1202	A1L7O	CAH-NAC	-11.03	1.26	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	A1L7O	CAQ-CAR-CAS	-9.20	100.23	111.00
3	B	1202	A1L7O	CAD-NAC-CAB	7.94	124.22	111.71
3	A	1202	A1L7O	CAU-CAT-CAS	-6.58	103.30	111.00
3	A	1202	A1L7O	CAD-NAC-CAB	5.99	121.14	111.71
3	A	1202	A1L7O	CAT-CAS-CAV	5.93	126.72	112.67
3	B	1202	A1L7O	CAR-CAS-CAV	5.33	125.30	112.67
3	A	1202	A1L7O	CAH-NAC-CAB	5.02	121.11	111.86
3	A	1202	A1L7O	CAR-CAS-CAV	4.83	124.11	112.67
3	B	1202	A1L7O	CAH-NAC-CAD	4.49	118.40	111.09
3	A	1202	A1L7O	CAI-CAH-NAC	3.85	121.02	113.15
3	A	1202	A1L7O	CAH-NAC-CAD	3.68	117.07	111.09
3	B	1202	A1L7O	CAU-CAT-CAS	-3.58	106.81	111.00
3	A	1202	A1L7O	CAH-CAI-CAJ	3.37	126.95	120.75
3	A	1202	A1L7O	CAH-CAI-CAN	-3.30	114.66	120.75
3	A	1202	A1L7O	CAU-NAP-CAQ	3.26	115.87	108.84
3	B	1202	A1L7O	CAT-CAS-CAV	3.15	120.12	112.67
3	B	1202	A1L7O	CAQ-CAR-CAS	-2.79	107.73	111.00
3	B	1202	A1L7O	CAR-CAQ-NAP	2.38	114.92	111.08
3	A	1202	A1L7O	CAR-CAQ-NAP	2.29	114.77	111.08
3	B	1202	A1L7O	CAU-NAP-CAQ	2.26	113.71	108.84
3	B	1202	A1L7O	CAH-CAI-CAJ	2.24	124.87	120.75
3	B	1202	A1L7O	CAT-CAS-CAR	2.23	114.53	109.68
3	B	1202	A1L7O	CAH-CAI-CAN	-2.15	116.79	120.75

There are no chirality outliers.

All (15) torsion outliers are listed below:

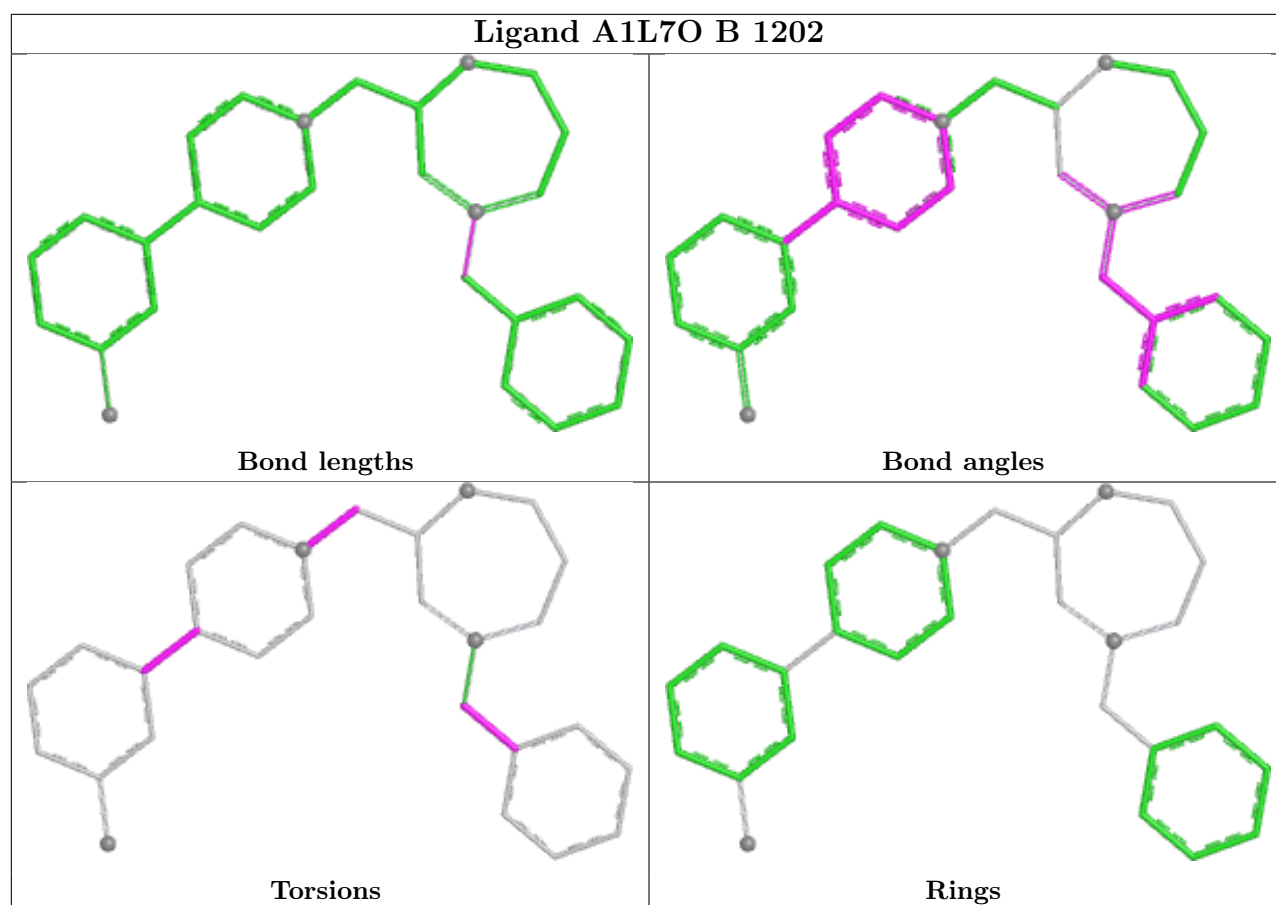
Mol	Chain	Res	Type	Atoms
3	A	1202	A1L7O	CAA-CAO-NAP-CAQ
3	A	1202	A1L7O	CAI-CAH-NAC-CAD
3	A	1202	A1L7O	CAI-CAH-NAC-CAB
3	B	1202	A1L7O	CAA-CAO-NAP-CAU
3	B	1202	A1L7O	CAT-CAS-CAV-CBA
3	B	1202	A1L7O	CAR-CAS-CAV-CAW
3	B	1202	A1L7O	CAT-CAS-CAV-CAW
3	B	1202	A1L7O	CAR-CAS-CAV-CBA
3	A	1202	A1L7O	CAR-CAS-CAV-CAW
3	A	1202	A1L7O	CAR-CAS-CAV-CBA
3	A	1202	A1L7O	CAT-CAS-CAV-CBA
3	A	1202	A1L7O	CAT-CAS-CAV-CAW
3	B	1202	A1L7O	NAC-CAH-CAI-CAJ
3	B	1202	A1L7O	NAC-CAH-CAI-CAN
3	B	1202	A1L7O	CAA-CAO-NAP-CAQ

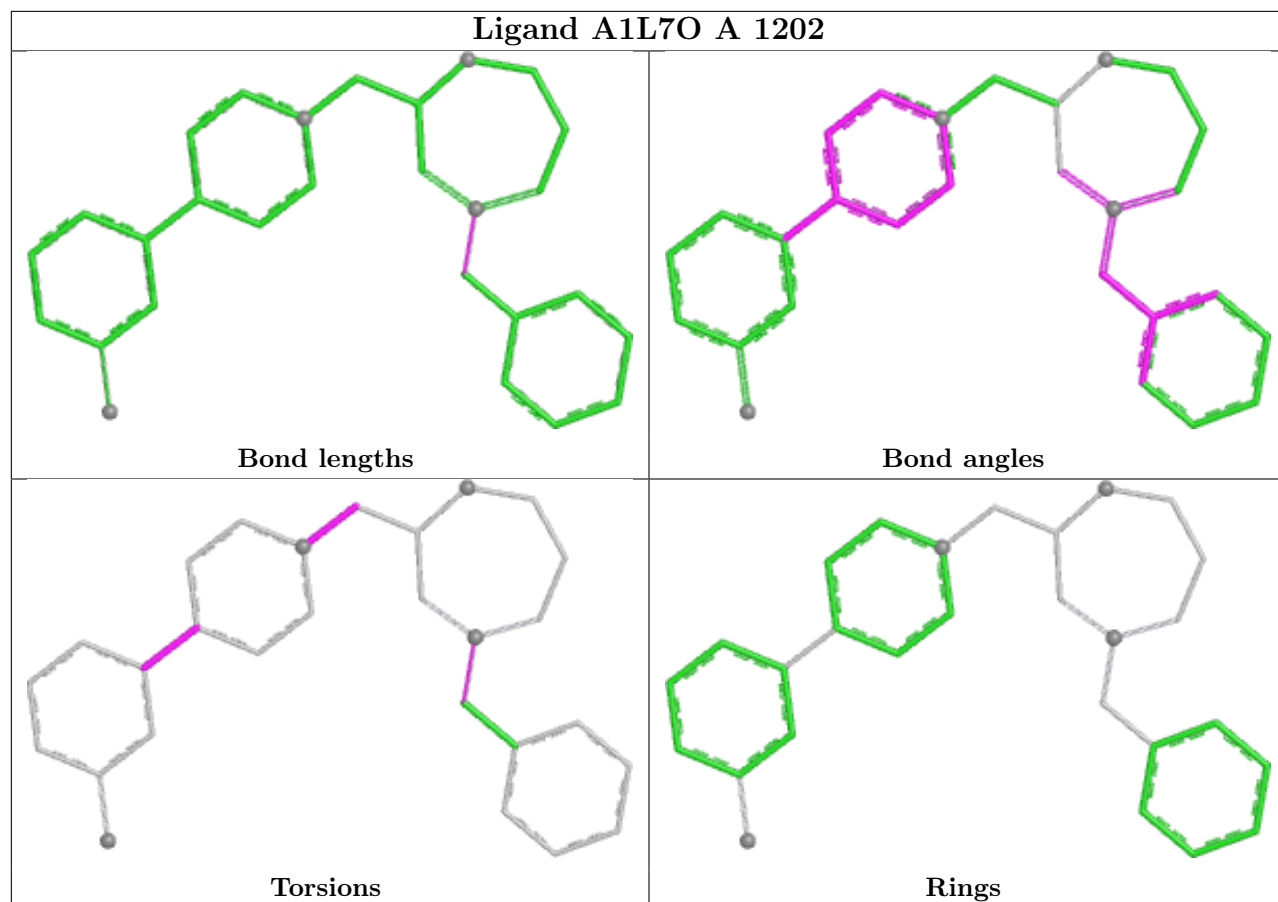
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1202	A1L7O	3	0
3	A	1202	A1L7O	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/300 (88%)	0.64	19 (7%) 21 18	26, 50, 99, 123	2 (0%)
1	B	267/300 (89%)	0.96	30 (11%) 10 8	30, 70, 97, 130	1 (0%)
All	All	532/600 (88%)	0.80	49 (9%) 14 12	26, 62, 99, 130	3 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	980	CYS	9.0
1	B	979	ASP	6.4
1	B	995	TRP	6.3
1	B	1002	LEU	5.4
1	B	1027	CYS	5.2
1	B	974	CYS	4.9
1	B	987	CYS	4.7
1	A	963	ASN	3.9
1	B	963	ASN	3.8
1	A	1173	GLU	3.5
1	A	964	ILE	3.4
1	B	1003	LEU	3.3
1	A	1027	CYS	3.3
1	B	1075	ALA	3.1
1	A	985	CYS	3.1
1	A	1039	ARG	3.1
1	A	980	CYS	3.0
1	B	985	CYS	3.0
1	A	962	MET	2.8
1	B	1108[A]	SER	2.8
1	B	988	GLY	2.8
1	B	1155	GLY	2.7
1	B	961	THR	2.7
1	B	1094	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1006	PHE	2.6
1	B	1170	CYS	2.6
1	A	926	VAL	2.5
1	A	1189	LEU	2.5
1	B	1023	CYS	2.5
1	B	1067	TYR	2.5
1	A	1021	CYS	2.4
1	B	982	SER	2.4
1	B	994	CYS	2.3
1	A	1180	GLU	2.3
1	A	1057	THR	2.3
1	B	1096	VAL	2.3
1	B	992	ILE	2.2
1	B	1122	VAL	2.2
1	B	1130	ASP	2.2
1	A	1017	CYS	2.2
1	A	1008	LYS	2.1
1	A	987	CYS	2.1
1	B	1017	CYS	2.1
1	B	996	TYR	2.1
1	B	978	ASP	2.1
1	A	974	CYS	2.1
1	B	945	PRO	2.0
1	A	922	ILE	2.0
1	B	976	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

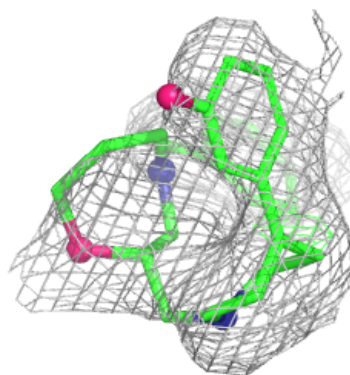
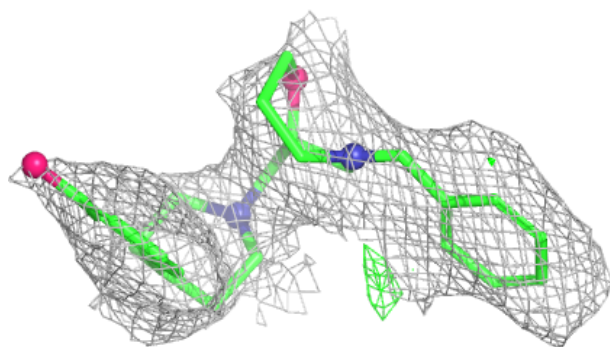
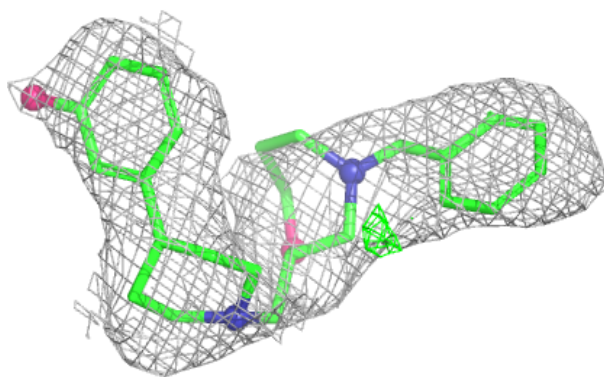
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1L7O	A	1202	28/28	0.80	0.16	55,61,75,76	0
3	A1L7O	B	1202	28/28	0.85	0.12	58,71,81,81	0
2	ZN	B	1201	1/1	0.97	0.04	58,58,58,58	0
2	ZN	A	1201	1/1	0.99	0.04	74,74,74,74	0

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

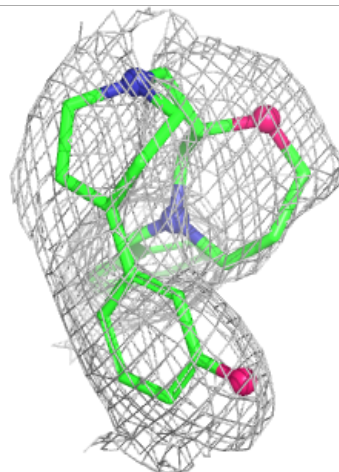
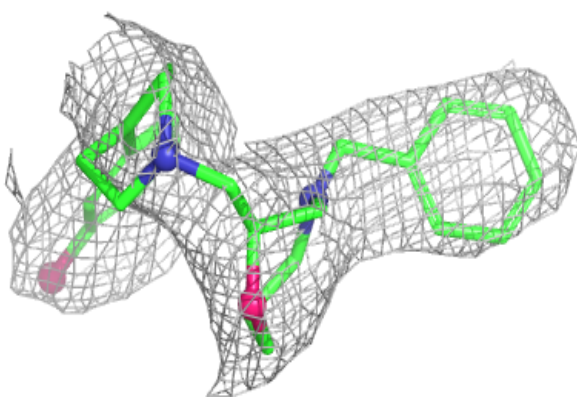
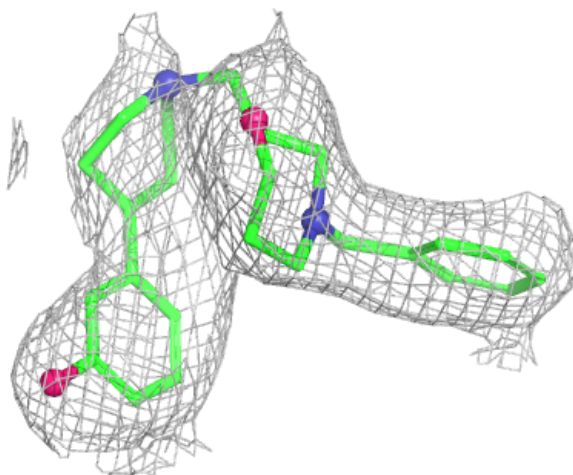
Electron density around A1L7O A 1202:

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 A1L7O B 1202:

$2mF_o-DF_c$ (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.