



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2021 – 10:04 PM EST

PDB ID : 7LW4
Title : Structure of SARS-CoV-2 nsp16/nsp10 complex in presence of S-adenosyl-L-homocysteine (SAH)
Authors : Gupta, Y.K.; Viswanathan, T.; Misra, A.; Qi, S.
Deposited on : 2021-02-27
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
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) : 2.23.2

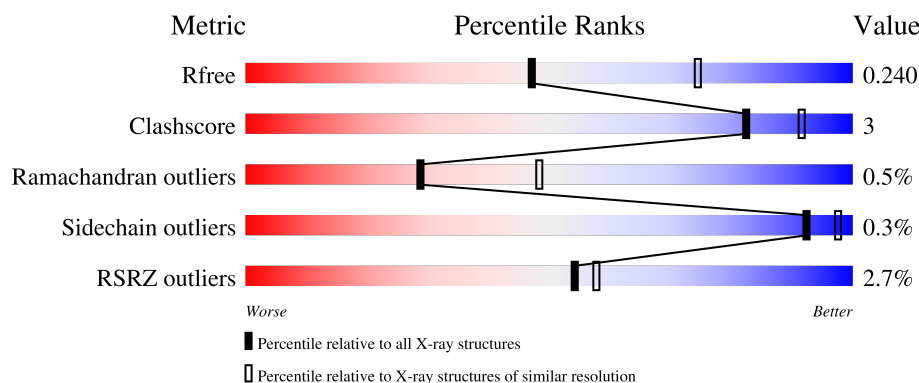
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	298	<div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
2	B	139	<div> <div>6%</div> <div>72%</div> <div>9%</div> <div>.</div> <div>18%</div> </div>

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
4	ACT	A	310	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6489 atoms, of which 3105 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 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	H	N	O	S	0	0	0
			4546	1466	2247	386	431	16			

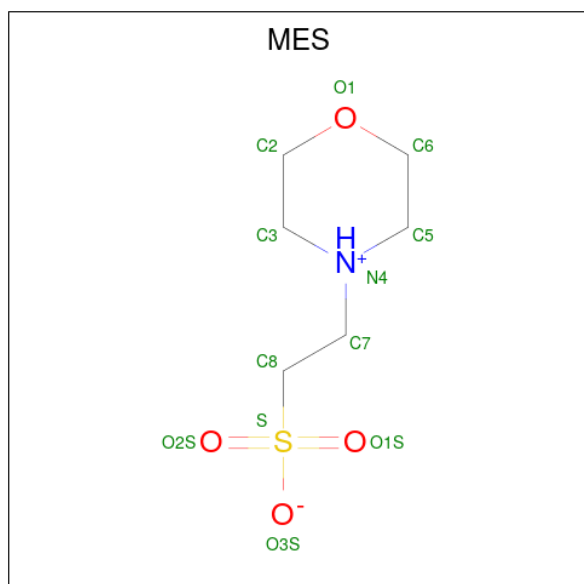
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	LYS	ASN	conflict	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	114	Total	C	H	N	O	S	0	0	0
			1621	519	789	140	158	15			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



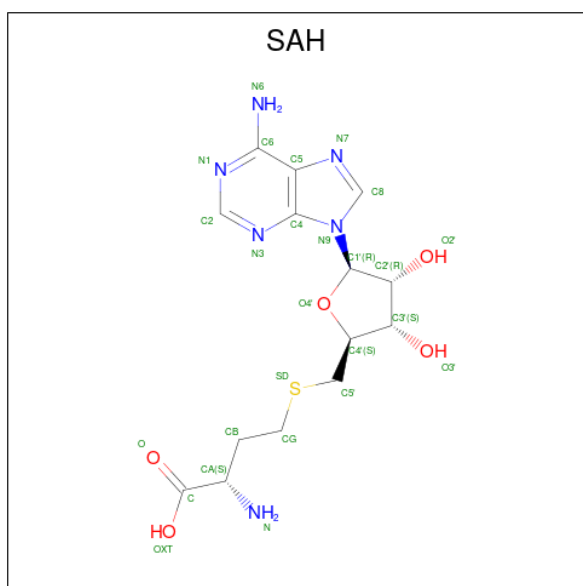
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O		
			7	2	3	2	0	0
4	A	1	Total	C	H	O		
			7	2	3	2	0	0
4	A	1	Total	C	H	O		
			7	2	3	2	0	0
4	A	1	Total	C	H	O		
			7	2	3	2	0	0
4	A	1	Total	C	H	O		
			7	2	3	2	0	0
4	A	1	Total	C	H	O		
			5	2	1	2	0	0
4	A	1	Total	C	H	O		
			7	2	3	2	0	0
4	A	1	Total	C	O			
			4	2	2		0	0
4	B	1	Total	C	O			
			4	2	2		0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			45	14	19	6	5	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Zn	0	0
			2	2		

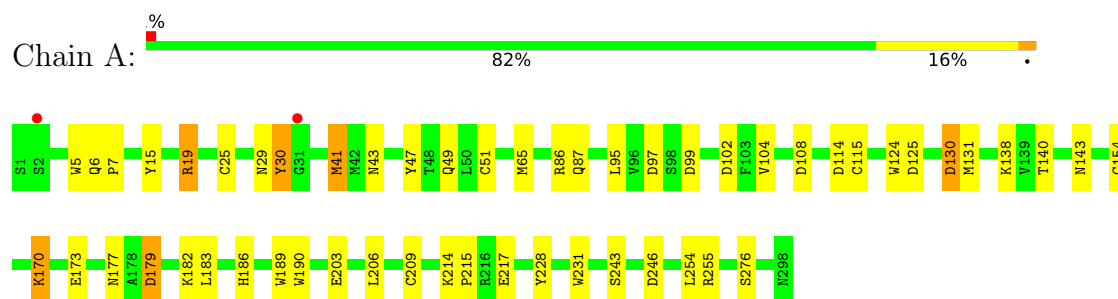
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	140	Total	O	0	0
			140	140		
8	B	25	Total	O	0	0
			25	25		

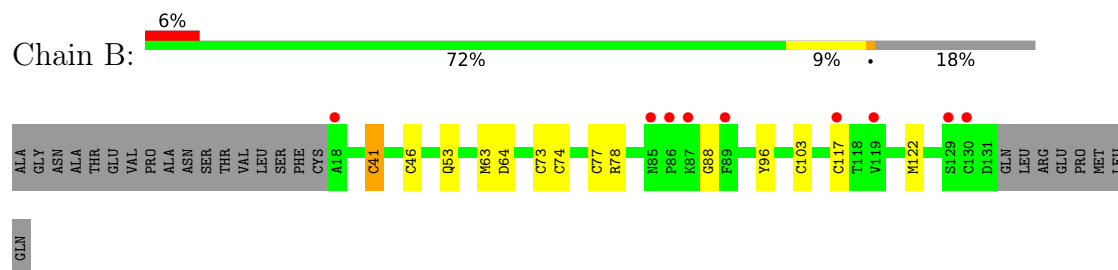
3 Residue-property plots [i](#)

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: 2'-O-methyltransferase



- Molecule 2: Non-structural protein 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.59Å 184.59Å 56.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 2.50 29.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.75-2.50) 99.9 (29.75-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.204 , 0.240 0.204 , 0.240	Depositor DCC
R_{free} test set	1966 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 96.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6489	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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, SAH, EDO, MES, ACT

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	1.67	34/2349 (1.4%)	1.27	17/3195 (0.5%)
2	B	1.36	9/851 (1.1%)	1.06	4/1155 (0.3%)
All	All	1.59	43/3200 (1.3%)	1.21	21/4350 (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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	CYS	CB-SG	11.55	2.01	1.82
2	B	73	CYS	CB-SG	9.84	1.99	1.82
1	A	51	CYS	CB-SG	9.11	1.97	1.82
1	A	209	CYS	CB-SG	8.90	1.97	1.82
1	A	154	CYS	CB-SG	8.72	1.97	1.82
2	B	74	CYS	CB-SG	8.37	1.96	1.82
1	A	25	CYS	CB-SG	8.35	1.96	1.82
1	A	173	GLU	CG-CD	7.69	1.63	1.51
1	A	114	ASP	CB-CG	7.30	1.67	1.51
2	B	46	CYS	CB-SG	7.08	1.94	1.82
1	A	231	TRP	CB-CG	7.07	1.62	1.50
1	A	173	GLU	CB-CG	6.93	1.65	1.52
2	B	117	CYS	CB-SG	6.76	1.93	1.82
2	B	77	CYS	CB-SG	6.65	1.93	1.82
1	A	125	ASP	CB-CG	6.55	1.65	1.51
1	A	190	TRP	CB-CG	6.55	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	TRP	CE3-CZ3	6.53	1.49	1.38
1	A	47	TYR	CB-CG	6.46	1.61	1.51
2	B	64	ASP	CB-CG	6.37	1.65	1.51
1	A	115	CYS	CB-SG	6.30	1.93	1.82
2	B	103	CYS	CB-SG	6.28	1.93	1.82
1	A	41	MET	CG-SD	6.14	1.97	1.81
1	A	203	GLU	CG-CD	5.96	1.60	1.51
1	A	130	ASP	CB-CG	5.92	1.64	1.51
1	A	43	ASN	CB-CG	5.78	1.64	1.51
1	A	131	MET	CG-SD	5.68	1.96	1.81
1	A	47	TYR	CD2-CE2	5.66	1.47	1.39
1	A	124	TRP	CA-CB	5.64	1.66	1.53
1	A	47	TYR	CD1-CE1	5.57	1.47	1.39
1	A	243	SER	CB-OG	5.56	1.49	1.42
1	A	189	TRP	CB-CG	5.41	1.59	1.50
1	A	87	GLN	CG-CD	5.36	1.63	1.51
2	B	96	TYR	CA-CB	5.35	1.65	1.53
1	A	41	MET	CB-CG	5.34	1.68	1.51
1	A	49	GLN	CG-CD	5.31	1.63	1.51
1	A	97	ASP	CB-CG	5.24	1.62	1.51
1	A	99	ASP	CB-CG	5.15	1.62	1.51
1	A	177	ASN	CB-CG	5.12	1.62	1.51
1	A	143	ASN	CB-CG	5.06	1.62	1.51
1	A	15	TYR	CB-CG	5.04	1.59	1.51
1	A	228	TYR	CB-CG	5.04	1.59	1.51
1	A	108	ASP	CB-CG	5.02	1.62	1.51
1	A	5	TRP	CB-CG	5.00	1.59	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ARG	CG-CD-NE	-12.85	84.82	111.80
1	A	179	ASP	CB-CG-OD2	-9.19	110.03	118.30
2	B	78	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	102	ASP	CB-CG-OD1	7.44	125.00	118.30
1	A	246	ASP	CB-CG-OD1	7.42	124.98	118.30
2	B	64	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	41	MET	CA-CB-CG	6.81	124.88	113.30
1	A	206	LEU	CA-CB-CG	6.71	130.73	115.30
1	A	255	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	19	ARG	CD-NE-CZ	6.24	132.33	123.60
1	A	173	GLU	OE1-CD-OE2	-5.99	116.12	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	104	VAL	CG1-CB-CG2	-5.71	101.76	110.90
2	B	78	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	19	ARG	CA-CB-CG	-5.44	101.44	113.40
1	A	65	MET	CG-SD-CE	5.42	108.86	100.20
1	A	86	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	B	63	MET	CB-CG-SD	5.32	128.37	112.40
1	A	114	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	170	LYS	CD-CE-NZ	-5.16	99.83	111.70
1	A	95	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	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	2299	2247	2251	14	0
2	B	832	789	789	2	0
3	A	12	13	13	0	0
4	A	32	19	24	6	0
4	B	4	0	3	0	0
5	A	12	18	18	1	0
6	A	26	19	19	0	0
7	B	2	0	0	0	0
8	A	140	0	0	2	0
8	B	25	0	0	0	0
All	All	3384	3105	3117	16	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 3.

All (16) 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)
2:B:41:CYS:SG	2:B:41:CYS:CB	2.01	1.47
1:A:186:HIS:NE2	4:A:310:ACT:H3	1.97	0.80
1:A:276:SER:O	8:A:401:HOH:O	2.07	0.71
1:A:29:ASN:O	1:A:30:TYR:CB	2.38	0.70
1:A:186:HIS:NE2	4:A:310:ACT:CH3	2.65	0.60
1:A:215:PRO:HB3	4:A:310:ACT:CH3	2.42	0.50
1:A:215:PRO:HB3	4:A:310:ACT:H3	1.94	0.49
1:A:214:LYS:HB2	1:A:215:PRO:HD2	1.96	0.47
1:A:217:GLU:OE2	5:A:307:EDO:O1	2.27	0.47
1:A:6:GLN:HB3	1:A:7:PRO:HD2	1.99	0.44
1:A:130:ASP:OD2	1:A:170:LYS:HD3	2.18	0.44
1:A:182:LYS:NZ	4:A:310:ACT:OXT	2.35	0.43
1:A:41:MET:HG2	4:A:313:ACT:H2	2.00	0.43
1:A:254:LEU:HD23	8:A:527:HOH:O	2.18	0.42
1:A:138:LYS:HG2	1:A:140:THR:H	1.85	0.42
2:B:53:GLN:HG2	2:B:122:MET:CE	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	296/298 (99%)	283 (96%)	12 (4%)	1 (0%)	41	61
2	B	112/139 (81%)	103 (92%)	8 (7%)	1 (1%)	17	31
All	All	408/437 (93%)	386 (95%)	20 (5%)	2 (0%)	29	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
2	B	88	GLY

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	248/258 (96%)	247 (100%)	1 (0%)	91	97
2	B	90/113 (80%)	90 (100%)	0	100	100
All	All	338/371 (91%)	337 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ASP

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	43	ASN
1	A	218	GLN
1	A	286	ASN
2	B	53	GLN
2	B	98	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

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
4	ACT	A	306	-	1,3,3	4.82	1 (100%)	0,3,3	-	-
5	EDO	A	304	-	3,3,3	0.22	0	2,2,2	0.43	0
4	ACT	A	309	-	1,3,3	4.57	1 (100%)	0,3,3	-	-
5	EDO	A	305	-	3,3,3	0.14	0	2,2,2	0.48	0
5	EDO	A	307	-	3,3,3	0.11	0	2,2,2	0.39	0
4	ACT	A	308	-	1,3,3	4.92	1 (100%)	0,3,3	-	-
6	SAH	A	312	-	21,28,28	1.14	2 (9%)	20,40,40	1.58	5 (25%)
4	ACT	A	302	-	1,3,3	5.63	1 (100%)	0,3,3	-	-
4	ACT	A	303	-	1,3,3	6.74	1 (100%)	0,3,3	-	-
4	ACT	A	313	-	1,3,3	4.50	1 (100%)	0,3,3	-	-
4	ACT	B	203	-	1,3,3	6.17	1 (100%)	0,3,3	-	-
4	ACT	A	310	-	1,3,3	2.92	1 (100%)	0,3,3	-	-
3	MES	A	301	-	12,12,12	1.24	1 (8%)	14,16,16	0.78	0
4	ACT	A	311	-	1,3,3	5.01	1 (100%)	0,3,3	-	-

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
5	EDO	A	304	-	-	1/1/1/1	-
5	EDO	A	305	-	-	1/1/1/1	-
5	EDO	A	307	-	-	0/1/1/1	-
6	SAH	A	312	-	-	0/7/31/31	0/3/3/3
3	MES	A	301	-	-	0/6/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	ACT	CH3-C	6.74	1.57	1.48
4	B	203	ACT	CH3-C	6.17	1.56	1.48
4	A	302	ACT	CH3-C	5.63	1.55	1.48
4	A	311	ACT	CH3-C	5.01	1.55	1.48
4	A	308	ACT	CH3-C	4.92	1.55	1.48
4	A	306	ACT	CH3-C	4.82	1.54	1.48
4	A	309	ACT	CH3-C	4.57	1.54	1.48
4	A	313	ACT	CH3-C	4.50	1.54	1.48
3	A	301	MES	C8-S	3.13	1.82	1.77
4	A	310	ACT	CH3-C	2.92	1.52	1.48
6	A	312	SAH	C5'-SD	2.82	1.92	1.80
6	A	312	SAH	O4'-C1'	2.09	1.44	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	312	SAH	O4'-C4'-C5'	4.04	119.24	108.83
6	A	312	SAH	C4'-C5'-SD	2.83	123.96	113.78
6	A	312	SAH	O4'-C1'-C2'	-2.48	103.30	106.93
6	A	312	SAH	C5-C6-N6	2.22	123.73	120.35
6	A	312	SAH	CB-CG-SD	2.03	117.87	113.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305	EDO	O1-C1-C2-O2
5	A	304	EDO	O1-C1-C2-O2

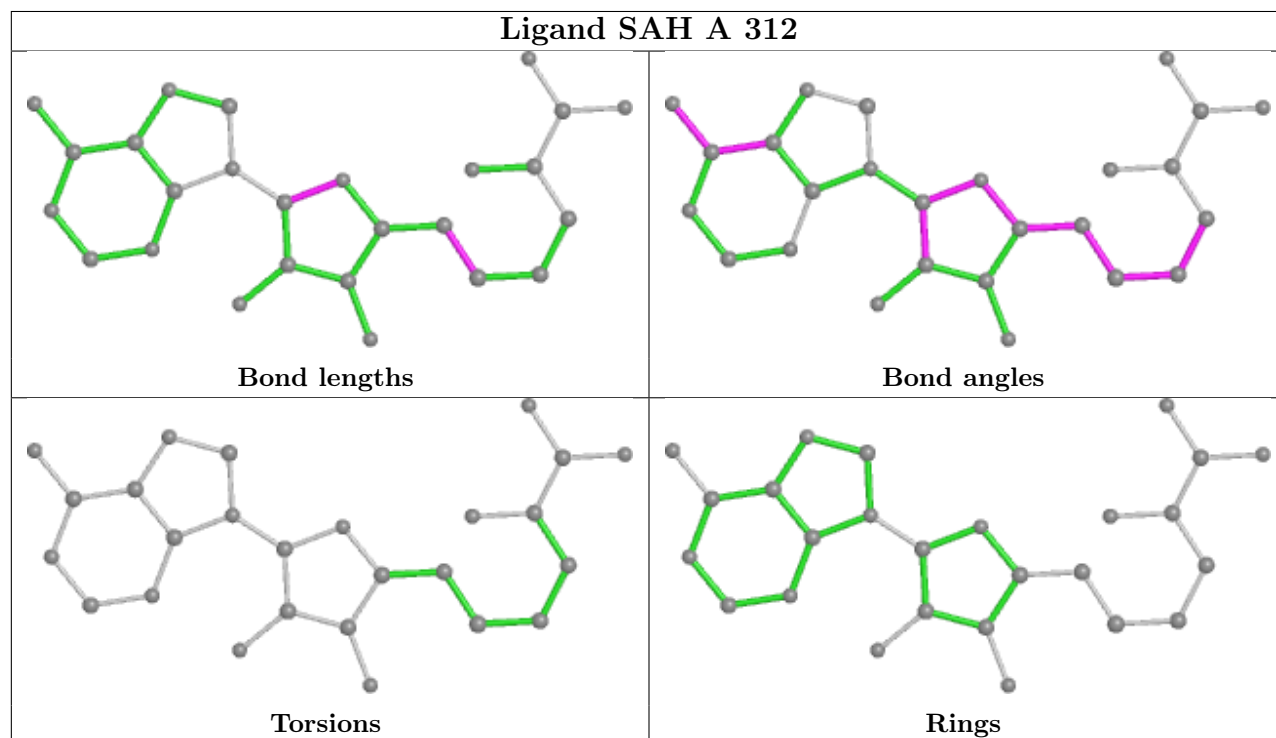
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	307	EDO	1	0
4	A	313	ACT	1	0
4	A	310	ACT	5	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	298/298 (100%)	-0.40	2 (0%) 87 89	32, 46, 101, 126	0
2	B	114/139 (82%)	0.10	9 (7%) 12 12	36, 67, 118, 172	0
All	All	412/437 (94%)	-0.26	11 (2%) 54 58	32, 51, 110, 172	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	86	PRO	4.2
2	B	130	CYS	3.6
2	B	119	VAL	3.0
1	A	31	GLY	2.8
2	B	87	LYS	2.6
2	B	18	ALA	2.5
2	B	117	CYS	2.5
2	B	85	ASN	2.4
2	B	89	PHE	2.3
1	A	2	SER	2.3
2	B	129	SER	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

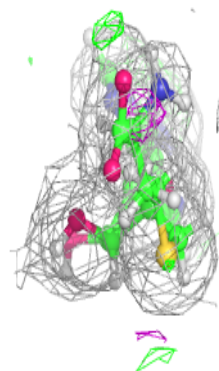
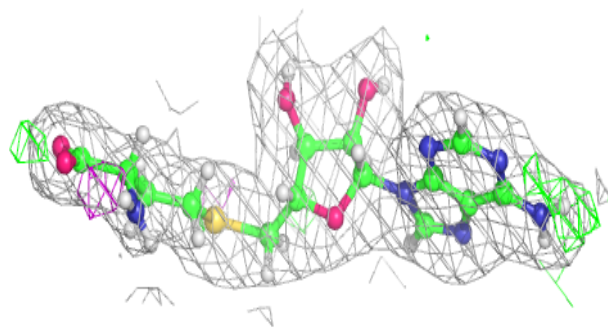
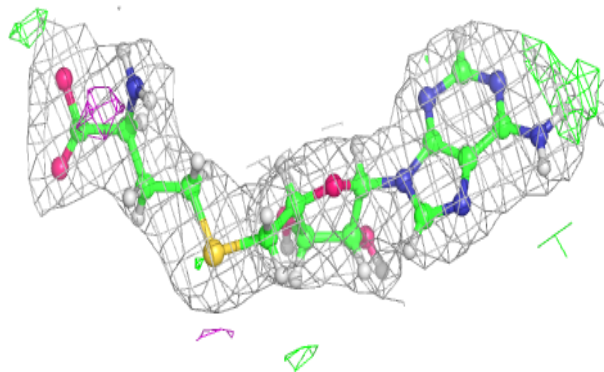
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	305	4/4	0.69	0.23	72,87,93,107	0
4	ACT	A	313	4/4	0.74	0.20	76,85,102,127	0
4	ACT	A	302	4/4	0.84	0.22	54,62,65,70	0
4	ACT	A	310	4/4	0.84	0.66	98,107,116,118	0
4	ACT	A	303	4/4	0.87	0.15	59,70,71,77	0
4	ACT	B	203	4/4	0.88	0.18	55,56,57,58	0
5	EDO	A	307	4/4	0.89	0.13	59,75,87,95	0
4	ACT	A	311	4/4	0.90	0.14	65,77,78,86	0
5	EDO	A	304	4/4	0.90	0.36	55,66,76,80	0
4	ACT	A	308	4/4	0.91	0.15	62,78,100,100	0
3	MES	A	301	12/12	0.93	0.11	47,60,72,76	0
4	ACT	A	306	4/4	0.94	0.20	69,72,83,83	0
6	SAH	A	312	26/26	0.95	0.09	34,41,50,51	0
4	ACT	A	309	4/4	0.97	0.18	70,80,84,84	0
7	ZN	B	202	1/1	0.97	0.07	92,92,92,92	0
7	ZN	B	201	1/1	0.98	0.04	52,52,52,52	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.

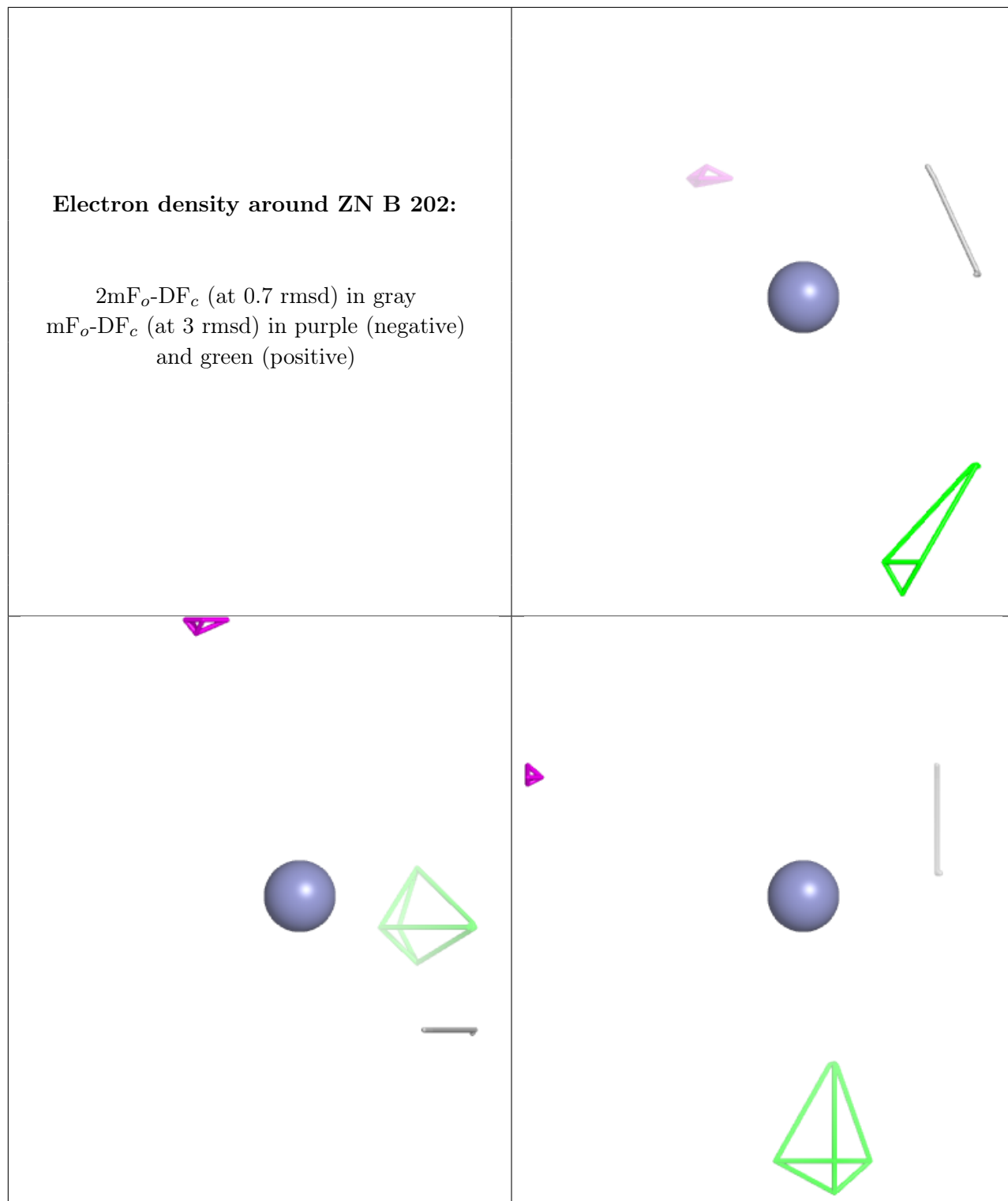
Electron density around SAH A 312:

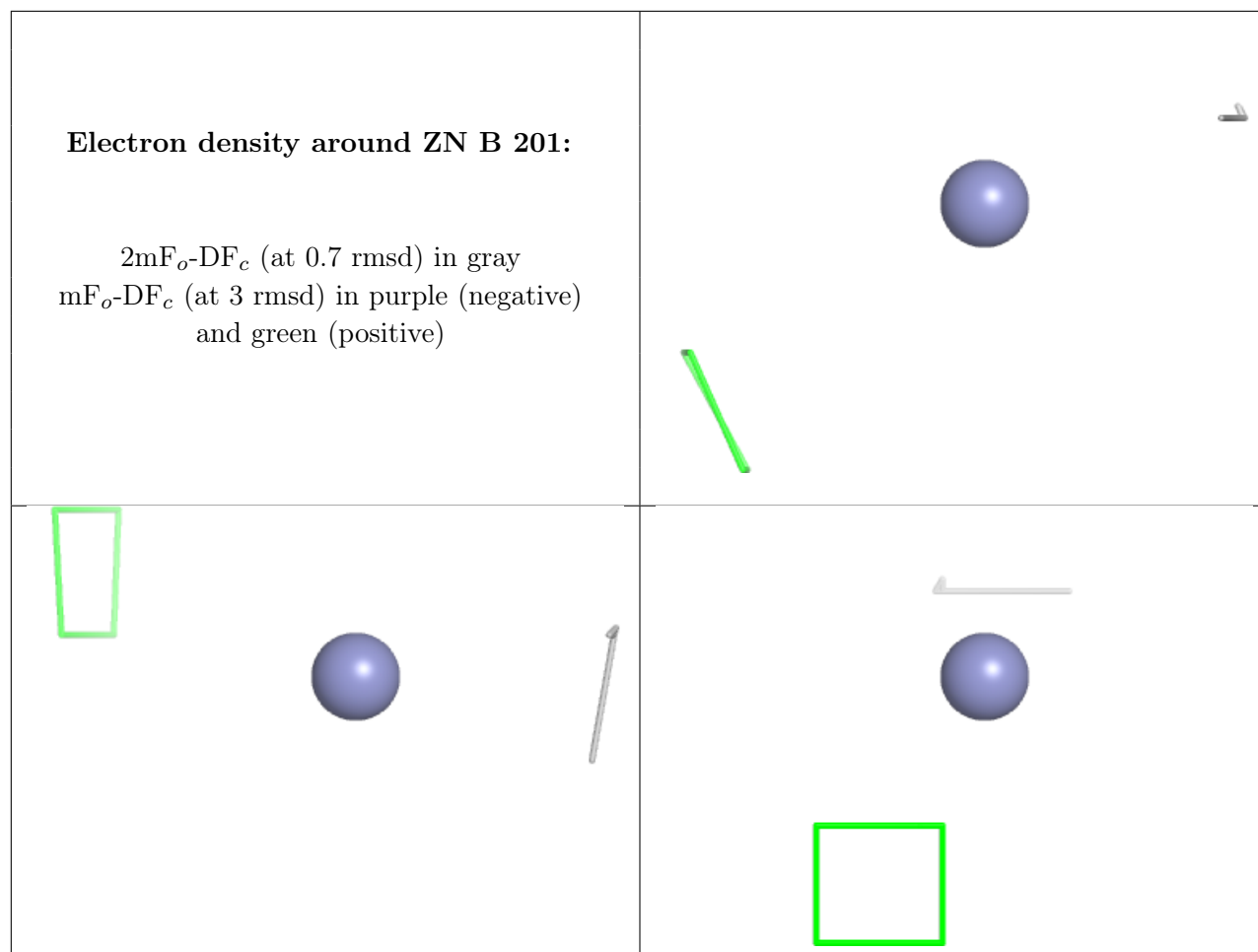
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 202:

$2mF_o - DF_c$ (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.