



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 02:44 PM EDT

PDB ID : 6W8W
Title : Crystal structure of mouse DNMT1 in complex with CCG DNA
Authors : Anteneh, H.; Song, J.
Deposited on : 2020-03-21
Resolution : 3.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

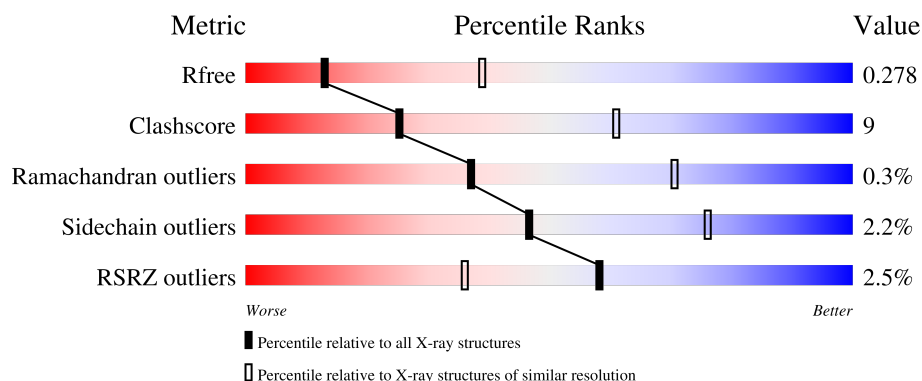
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	873	<div> <div>2%</div> <div>72%</div> <div>21%</div> <div>5%</div> </div>
1	B	873	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>5%</div> </div>
2	C	12	<div> <div>25%</div> <div>33%</div> <div>50%</div> <div>17%</div> </div>
2	E	12	<div> <div>17%</div> <div>33%</div> <div>58%</div> <div>8%</div> </div>
3	D	12	<div> <div>17%</div> <div>50%</div> <div>42%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	12	<p>17% 33% 58% 8%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13939 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	S	0	0	0
			6424	4078	1125	1182	39			
1	B	826	Total	C	N	O	S	0	0	0
			6433	4087	1122	1184	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	expression tag	UNP P13864
B	730	SER	-	expression tag	UNP P13864

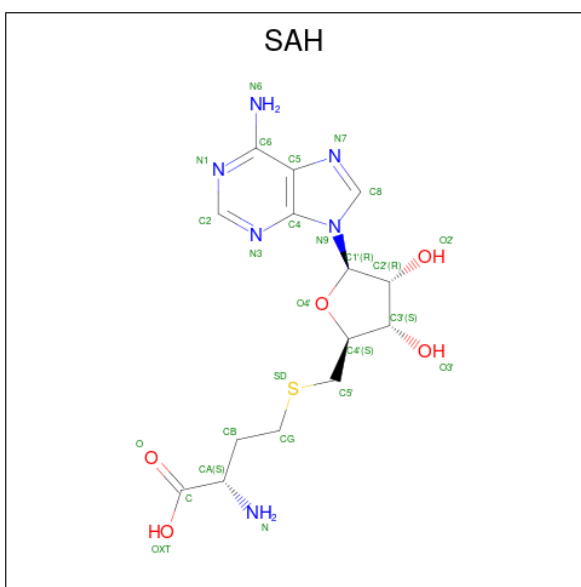
- Molecule 2 is a DNA chain called CCG DNA (5'-D(*AP*CP*TP*TP*AP*(5CM)P*GP*GP*AP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			248	119	50	68	11			
2	E	12	Total	C	N	O	P	0	0	0
			248	119	50	68	11			

- Molecule 3 is a DNA chain called CCG DNA (5'-D(*CP*CP*TP*TP*CP*(C49)P*GP*TP*AP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	F	N	O	P	0	0
			234	113	1	38	71	11		
3	F	12	Total	C	F	N	O	P	0	0
			234	113	1	38	71	11		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

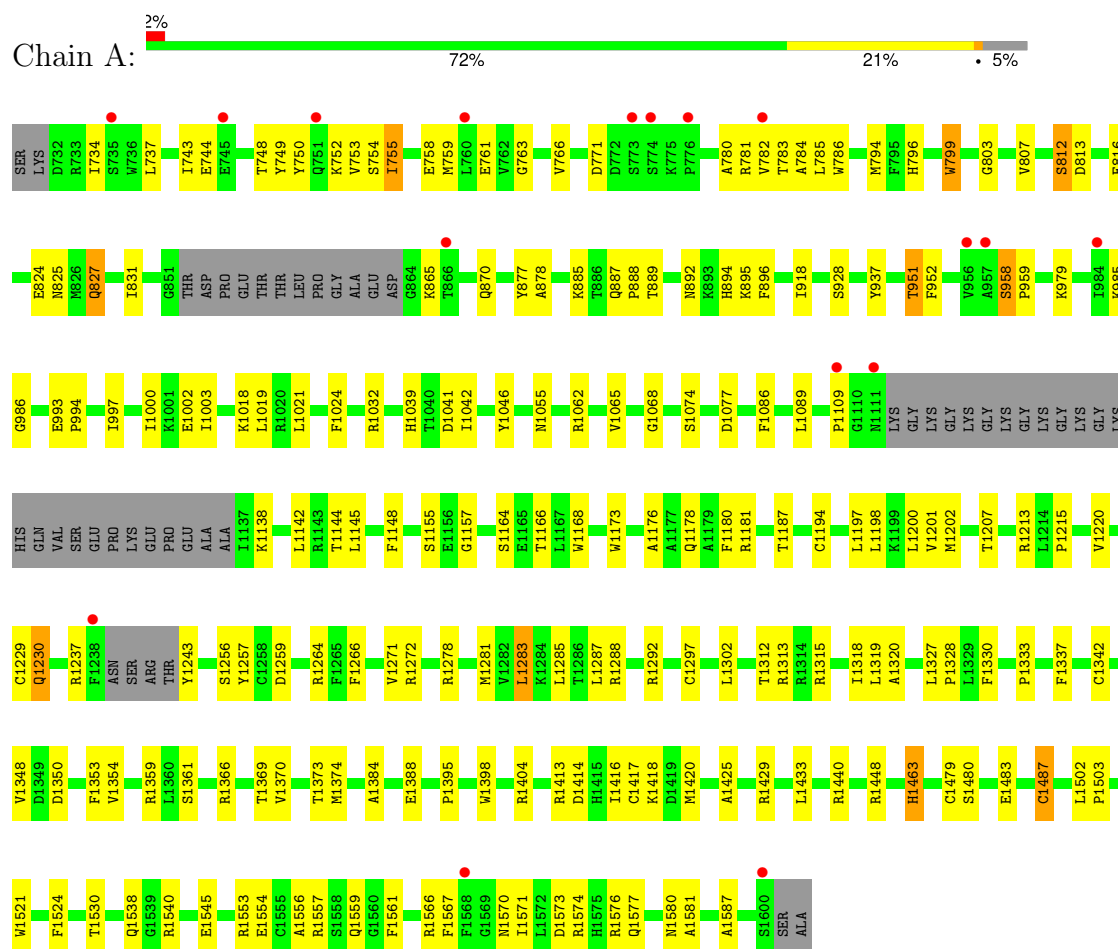
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	30	Total	O	0	0
			30	30		

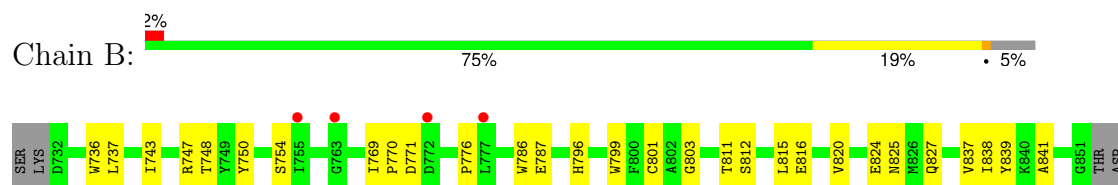
3 Residue-property plots

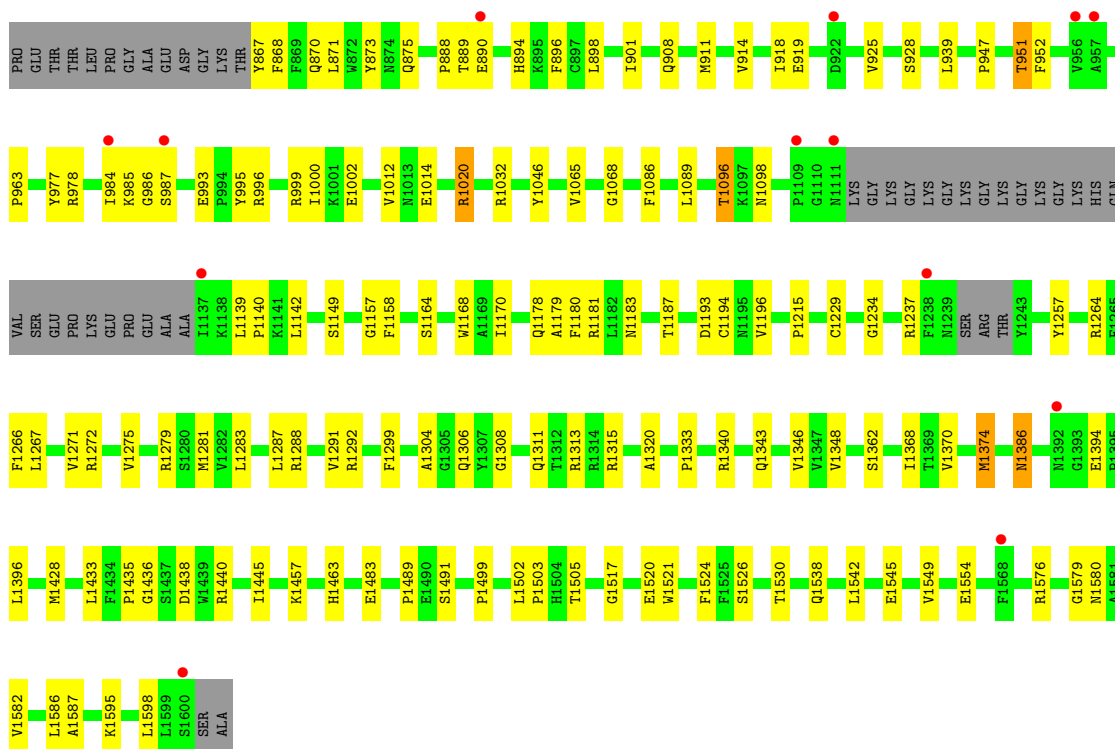
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA (cytosine-5)-methyltransferase 1

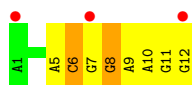


• Molecule 1: DNA (cytosine-5)-methyltransferase 1





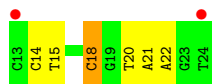
- Molecule 2: CCG DNA (5'-D(*AP*CP*TP*TP*AP*(5CM)P*GP*GP*AP*AP*GP*G)-3')



- Molecule 2: CCG DNA (5'-D(*AP*CP*TP*TP*AP*(5CM)P*GP*GP*AP*AP*GP*G)-3')



- Molecule 3: CCG DNA (5'-D(*CP*CP*TP*TP*CP*(C49)P*GP*TP*AP*AP*GP*T)-3')



- Molecule 3: CCG DNA (5'-D(*CP*CP*TP*TP*CP*(C49)P*GP*TP*AP*AP*GP*T)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.79Å 152.59Å 95.63Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	48.44 – 3.00 48.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.44-3.00) 98.2 (48.44-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.238 , 0.280 0.240 , 0.278	Depositor DCC
R_{free} test set	49375 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13939	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% 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: 5CM, ZN, SAH, C49

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	0.26	0/6595	0.46	0/8970
1	B	0.25	0/6607	0.44	0/8991
2	C	0.71	0/256	1.03	1/392 (0.3%)
2	E	0.70	0/256	1.07	0/392
3	D	0.64	0/236	0.97	0/360
3	F	0.70	0/236	1.03	0/360
All	All	0.31	0/14186	0.52	1/19465 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	DG	C1'-O4'-C4'	-5.35	104.75	110.10

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	6424	0	6044	120	0
1	B	6433	0	6041	107	0
2	C	248	0	138	12	0
2	E	248	0	138	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	234	0	134	7	0
3	F	234	0	134	9	0
4	A	26	0	19	3	0
4	B	26	0	19	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	32	0	0	5	0
6	B	30	0	0	1	0
All	All	13939	0	12667	248	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 (248) 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:1266:PHE:HB3	1:B:1320:ALA:HB3	1.61	0.82
1:A:918:ILE:HD11	1:A:928:SER:HB3	1.66	0.77
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.65	0.76
1:A:1556:ALA:HB1	1:A:1561:PHE:HB2	1.70	0.73
1:A:734:ILE:HG12	1:A:755:ILE:HD12	1.71	0.72
1:B:1433:LEU:HD23	1:B:1545:GLU:HA	1.73	0.71
1:B:1313:ARG:NH2	3:F:18:C49:O2	2.24	0.71
1:B:1435:PRO:HB3	1:B:1520:GLU:HG2	1.72	0.70
1:A:1285:LEU:HA	1:A:1288:ARG:HB3	1.72	0.70
1:A:1479:CYS:SG	6:A:1811:HOH:O	2.53	0.66
1:B:811:THR:HB	1:B:1288:ARG:HH11	1.59	0.66
1:B:1505:THR:HG21	2:E:6:5CM:H5'	1.76	0.65
1:A:1042:ILE:HG22	1:A:1366:ARG:HH21	1.61	0.65
1:A:1288:ARG:HE	1:A:1292:ARG:NH2	1.95	0.65
1:A:1487:CYS:SG	6:A:1820:HOH:O	2.55	0.64
2:C:7:DG:H2''	2:C:8:DG:C5'	2.28	0.64
2:C:10:DA:H2''	2:C:11:DG:O4'	1.97	0.63
1:B:1170:ILE:HG22	4:B:1701:SAH:H2	1.79	0.63
1:B:796:HIS:ND1	1:B:825:ASN:OD1	2.31	0.63
1:B:947:PRO:HA	1:B:996:ARG:HG3	1.81	0.63
1:A:1018:LYS:NZ	1:A:1055:ASN:OD1	2.32	0.62
1:A:1319:LEU:HD13	1:A:1328:PRO:HG2	1.82	0.62
1:A:796:HIS:ND1	1:A:825:ASN:OD1	2.33	0.61
1:A:1278:ARG:NH1	6:A:1802:HOH:O	2.24	0.61
3:D:20:DT:H2''	3:D:21:DA:C8	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1234:GLY:O	2:E:8:DG:N1	2.34	0.61
1:A:1313:ARG:NH2	3:D:18:C49:O2	2.33	0.61
1:B:870:GLN:HG3	1:B:871:LEU:HG	1.82	0.61
1:A:743:ILE:HG13	1:A:748:THR:HA	1.83	0.60
1:A:780:ALA:HB2	1:A:799:TRP:CD1	2.36	0.60
2:E:11:DG:H2'	2:E:12:DG:C8	2.36	0.60
1:A:1556:ALA:HA	1:A:1559:GLN:HB2	1.84	0.60
1:A:1178:GLN:OE1	1:A:1181:ARG:NH1	2.35	0.59
1:B:1580:ASN:HB3	3:F:18:C49:HM53	1.85	0.59
1:B:898:LEU:HD23	1:B:901:ILE:HD11	1.85	0.59
2:E:8:DG:H2''	2:E:9:DA:O4'	2.03	0.58
3:F:22:DA:H2''	3:F:23:DG:O4'	2.03	0.58
1:A:889:THR:H	1:A:892:ASN:HB2	1.68	0.58
1:A:1570:ASN:O	1:A:1574:ARG:HG2	2.04	0.57
1:A:1327:LEU:HD12	1:A:1328:PRO:HD2	1.87	0.57
1:B:799:TRP:HE1	1:B:824:GLU:HG2	1.70	0.57
2:C:9:DA:H2''	2:C:10:DA:O5'	2.04	0.57
1:A:1271:VAL:HA	1:A:1315:ARG:HD3	1.85	0.56
1:B:1445:ILE:HA	1:B:1457:LYS:HE2	1.87	0.56
1:A:1580:ASN:HB3	4:A:1701:SAH:SD	2.46	0.56
1:B:1168:TRP:CE2	1:B:1215:PRO:HB3	2.40	0.56
1:B:889:THR:HG22	1:B:890:GLU:H	1.70	0.56
1:B:743:ILE:HG13	1:B:748:THR:HA	1.89	0.55
1:B:1002:GLU:HG3	1:B:1020:ARG:HB3	1.88	0.55
1:A:766:VAL:HG11	1:A:831:ILE:HG12	1.88	0.55
1:A:993:GLU:HG2	1:A:994:PRO:HD2	1.88	0.54
1:B:1068:GLY:HA3	1:B:1089:LEU:HD23	1.88	0.54
1:A:1168:TRP:CZ3	1:A:1220:VAL:HG12	2.43	0.54
1:A:1567:PHE:HB3	1:A:1577:GLN:OE1	2.08	0.54
1:B:837:VAL:HG22	1:B:867:TYR:HB2	1.90	0.54
1:A:813:ASP:HB3	1:A:816:GLU:HB2	1.89	0.54
1:B:748:THR:O	1:B:748:THR:OG1	2.25	0.54
1:B:873:TYR:CE2	1:B:875:GLN:HG3	2.43	0.54
1:A:1148:PHE:HB3	4:A:1701:SAH:H5'2	1.89	0.53
1:A:783:THR:OG1	1:A:784:ALA:N	2.41	0.53
1:A:783:THR:OG1	1:A:796:HIS:HB3	2.08	0.53
1:A:1573:ASP:O	1:A:1577:GLN:HG3	2.07	0.53
1:B:1299:PHE:HE2	1:B:1346:VAL:HG11	1.73	0.53
1:B:1530:THR:HB	1:B:1576:ARG:HG3	1.91	0.53
1:B:1158:PHE:HZ	1:B:1267:LEU:HD13	1.74	0.53
1:B:1306:GLN:HB3	1:B:1333:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:THR:HG1	1:B:750:TYR:HE1	1.57	0.53
1:B:914:VAL:HG23	1:B:1014:GLU:HG2	1.90	0.53
1:A:1374:MET:HG2	1:A:1554:GLU:HG2	1.91	0.53
1:A:1413:ARG:CZ	1:A:1566:ARG:HH12	2.22	0.52
2:C:5:DA:H2''	2:C:6:5CM:H5'	1.92	0.52
2:C:7:DG:H2''	2:C:8:DG:H5''	1.91	0.52
1:A:1207:THR:HG22	1:A:1213:ARG:HA	1.91	0.52
3:F:20:DT:H2''	3:F:21:DA:C8	2.45	0.52
1:A:1229:CYS:CB	3:D:18:C49:F	2.47	0.51
1:A:1373:THR:O	1:A:1557:ARG:NH1	2.42	0.51
1:B:1499:PRO:HB2	1:B:1502:LEU:HG	1.91	0.51
1:B:1502:LEU:HB2	1:B:1503:PRO:HD3	1.93	0.51
1:A:750:TYR:N	1:A:785:LEU:O	2.43	0.51
1:A:1256:SER:HA	1:A:1259:ASP:HB3	1.93	0.51
1:B:827:GLN:N	1:B:827:GLN:OE1	2.43	0.51
1:B:1229:CYS:CB	3:F:18:C49:F	2.49	0.51
1:B:748:THR:O	1:B:786:TRP:HA	2.11	0.51
1:A:1068:GLY:HA3	1:A:1089:LEU:HD23	1.92	0.51
1:A:1142:LEU:HD21	1:A:1264:ARG:HH21	1.75	0.51
3:D:21:DA:H2''	3:D:22:DA:C8	2.45	0.51
1:B:1180:PHE:HE1	1:B:1187:THR:HG21	1.76	0.50
1:A:1333:PRO:HD2	1:A:1359:ARG:HB2	1.92	0.50
1:B:918:ILE:HD11	1:B:928:SER:HB3	1.93	0.50
1:A:1370:VAL:HG23	1:A:1524:PHE:HA	1.94	0.50
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.93	0.50
1:B:1139:LEU:HD22	1:B:1140:PRO:HD2	1.93	0.50
1:A:1243:TYR:HA	6:A:1802:HOH:O	2.12	0.50
1:B:1065:VAL:HG22	1:B:1086:PHE:HB2	1.94	0.50
1:B:737:LEU:HD11	1:B:754:SER:HB3	1.94	0.50
1:A:1433:LEU:HD12	1:A:1545:GLU:HA	1.94	0.50
1:A:894:HIS:CE1	1:A:895:LYS:HG3	2.47	0.49
1:A:1197:LEU:HD12	1:A:1200:LEU:HD12	1.94	0.49
1:B:1428:MET:SD	1:B:1542:LEU:HG	2.52	0.49
1:B:873:TYR:HE2	1:B:875:GLN:HG3	1.76	0.49
1:A:803:GLY:HA3	1:A:812:SER:OG	2.13	0.49
1:A:1003:ILE:HG12	1:A:1019:LEU:HD22	1.95	0.49
1:A:1281:MET:O	1:A:1285:LEU:HD12	2.12	0.49
1:B:803:GLY:HA3	1:B:812:SER:OG	2.13	0.49
1:B:870:GLN:NE2	1:B:1291:VAL:O	2.45	0.49
1:A:748:THR:O	1:A:786:TRP:HA	2.12	0.48
1:B:816:GLU:HB2	1:B:868:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1479:CYS:SG	1:A:1480:SER:N	2.86	0.48
1:B:1142:LEU:H	1:B:1164:SER:HA	1.78	0.48
1:B:1374:MET:HG2	1:B:1554:GLU:HG2	1.94	0.48
1:A:744:GLU:HG2	1:A:749:TYR:HE2	1.79	0.47
1:A:763:GLY:H	1:A:782:VAL:CG2	2.26	0.47
1:A:1288:ARG:HH21	1:A:1292:ARG:HH22	1.62	0.47
1:A:1530:THR:HB	1:A:1576:ARG:HG3	1.96	0.47
1:B:747:ARG:HD2	1:B:786:TRP:CG	2.48	0.47
1:B:1463:HIS:HB2	1:B:1483:GLU:HG2	1.96	0.47
1:B:908:GLN:HA	1:B:911:MET:HG2	1.96	0.47
1:B:1313:ARG:NH2	1:B:1579:GLY:O	2.43	0.47
1:A:1144:THR:OG1	1:A:1164:SER:HB2	2.13	0.47
1:A:1384:ALA:H	1:A:1417:CYS:HB3	1.79	0.47
1:A:1502:LEU:HB2	1:A:1503:PRO:HD3	1.96	0.47
1:B:748:THR:OG1	1:B:787:GLU:HB3	2.14	0.47
1:A:753:VAL:HG12	1:A:754:SER:N	2.29	0.47
1:A:1463:HIS:HB2	1:A:1483:GLU:HG2	1.95	0.47
1:B:839:TYR:CE2	1:B:841:ALA:HB2	2.50	0.47
1:B:888:PRO:HG3	1:B:896:PHE:CD2	2.50	0.47
1:B:1179:ALA:O	1:B:1183:ASN:ND2	2.48	0.47
1:B:1275:VAL:HG12	1:B:1283:LEU:HD13	1.97	0.47
2:E:2:DC:H2''	2:E:3:DT:H71	1.96	0.47
1:A:758:GLU:HG3	1:A:759:MET:H	1.80	0.47
1:B:1271:VAL:HA	1:B:1315:ARG:HD3	1.96	0.47
1:A:878:ALA:HB2	1:A:1353:PHE:CD1	2.50	0.47
1:A:816:GLU:OE2	1:A:870:GLN:NE2	2.48	0.46
1:B:1096:THR:H	1:B:1096:THR:HG1	1.55	0.46
3:F:23:DG:H2'	3:F:24:DT:C6	2.50	0.46
1:A:1418:LYS:HE3	1:A:1420:MET:HE1	1.98	0.46
1:B:786:TRP:HZ3	1:B:796:HIS:HB2	1.80	0.46
1:A:1384:ALA:HB3	1:A:1417:CYS:H	1.80	0.46
1:B:1032:ARG:HH12	1:B:1046:TYR:HE2	1.64	0.46
1:A:1337:PHE:HB3	1:A:1342:CYS:SG	2.55	0.45
1:B:815:LEU:HG	1:B:868:PHE:HE1	1.81	0.45
1:A:1180:PHE:HE1	1:A:1187:THR:HG21	1.80	0.45
1:A:752:LYS:HG2	1:A:761:GLU:HB3	1.98	0.45
1:A:1168:TRP:CE2	1:A:1215:PRO:HB3	2.50	0.45
1:B:1428:MET:CE	1:B:1549:VAL:HG23	2.46	0.45
2:C:11:DG:H2''	2:C:12:DG:H5'	1.97	0.45
3:F:24:DT:H4'	3:F:24:DT:OP1	2.17	0.45
1:A:877:TYR:HD1	1:A:1354:VAL:HG23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:LEU:O	1:B:1291:VAL:HG23	2.16	0.45
1:B:1370:VAL:HG23	1:B:1524:PHE:HA	1.98	0.45
1:A:812:SER:O	1:B:776:PRO:HG3	2.16	0.45
1:B:951:THR:HG22	1:B:952:PHE:H	1.81	0.45
1:B:1149:SER:HB2	1:B:1180:PHE:CE2	2.52	0.44
1:A:1155:SER:HB3	1:A:1166:THR:HG21	2.00	0.44
1:B:1237:ARG:HD3	2:E:7:DG:C8	2.53	0.44
1:B:1394:GLU:O	1:B:1396:LEU:HD12	2.17	0.44
1:A:794:MET:HA	1:A:827:GLN:HA	1.98	0.44
1:B:801:CYS:HB2	1:B:820:VAL:HG13	1.99	0.44
1:A:888:PRO:HG3	1:A:896:PHE:CD2	2.53	0.44
1:A:1041:ASP:HA	1:A:1398:TRP:HB2	1.99	0.44
1:A:1302:LEU:HD11	1:A:1330:PHE:HD2	1.82	0.44
1:B:1193:ASP:HB3	1:B:1196:VAL:HG23	2.00	0.44
2:E:11:DG:C6	2:E:12:DG:C6	3.06	0.44
2:E:7:DG:H2''	2:E:8:DG:H5''	1.99	0.44
1:A:1425:ALA:O	1:A:1429:ARG:HG3	2.18	0.44
1:A:1173:TRP:HE3	1:A:1176:ALA:HB2	1.83	0.44
1:B:743:ILE:HG13	1:B:747:ARG:O	2.18	0.44
1:A:813:ASP:HB3	1:A:816:GLU:CB	2.48	0.43
1:B:1386:ASN:O	1:B:1386:ASN:ND2	2.48	0.43
1:B:993:GLU:O	1:B:1362:SER:OG	2.30	0.43
2:C:9:DA:H4'	2:C:10:DA:OP1	2.17	0.43
1:A:986:GLY:HA2	1:A:1524:PHE:CZ	2.53	0.43
1:B:747:ARG:HD2	1:B:786:TRP:CD1	2.53	0.43
3:F:13:DC:H2''	3:F:14:DC:O5'	2.18	0.43
1:A:780:ALA:HA	1:A:799:TRP:HA	2.01	0.43
1:B:1595:LYS:HA	1:B:1598:LEU:HD12	2.01	0.43
1:A:951:THR:HG22	1:A:952:PHE:H	1.82	0.43
1:A:1388:GLU:HG2	1:A:1413:ARG:HG2	2.00	0.43
1:A:1416:ILE:HD12	1:A:1571:ILE:HG12	1.99	0.43
1:B:1194:CYS:O	1:B:1257:TYR:OH	2.23	0.43
1:A:1194:CYS:O	1:A:1257:TYR:OH	2.28	0.43
1:B:1142:LEU:HD21	1:B:1264:ARG:HH21	1.84	0.43
1:A:1283:LEU:HD12	1:A:1318:ILE:HD11	1.99	0.43
1:A:781:ARG:HG2	1:A:782:VAL:O	2.18	0.43
1:A:985:LYS:O	1:A:1540:ARG:NH2	2.52	0.43
1:B:918:ILE:HG22	1:B:919:GLU:N	2.34	0.43
1:A:786:TRP:HE1	1:A:794:MET:HE2	1.84	0.42
1:A:812:SER:OG	1:A:813:ASP:N	2.52	0.42
1:A:1237:ARG:HG2	2:C:7:DG:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:VAL:HG12	1:A:1315:ARG:CZ	2.49	0.42
1:B:1288:ARG:HH21	1:B:1292:ARG:NH1	2.17	0.42
1:A:1287:LEU:HD23	1:A:1297:CYS:HB2	2.01	0.42
1:B:999:ARG:NH2	6:B:1807:HOH:O	2.48	0.42
2:C:10:DA:H61	3:D:14:DC:N4	2.17	0.42
1:A:958:SER:N	1:A:959:PRO:CD	2.83	0.42
1:A:1395:PRO:HG3	1:A:1404:ARG:HD3	2.01	0.42
1:B:769:ILE:HA	1:B:770:PRO:HD3	1.92	0.42
1:B:985:LYS:H	1:B:985:LYS:HG2	1.71	0.42
1:A:865:LYS:HE2	1:B:867:TYR:OH	2.19	0.42
1:A:937:TYR:CE2	1:A:1062:ARG:HB2	2.54	0.42
1:B:986:GLY:HA2	1:B:1524:PHE:CE2	2.55	0.42
1:B:1178:GLN:OE1	1:B:1181:ARG:NH1	2.52	0.42
1:A:885:LYS:O	1:A:887:GLN:NE2	2.51	0.42
1:A:892:ASN:HB3	1:A:896:PHE:HD1	1.85	0.42
1:A:1065:VAL:HG22	1:A:1086:PHE:HB2	2.02	0.42
1:B:1311:GLN:HG3	1:B:1526:SER:O	2.20	0.42
1:B:1521:TRP:HE1	1:B:1545:GLU:HG3	1.84	0.42
1:B:977:TYR:OH	1:B:978:ARG:NH2	2.52	0.41
1:B:1489:PRO:C	1:B:1491:SER:H	2.22	0.41
1:A:1198:LEU:O	1:A:1202:MET:HG3	2.20	0.41
1:B:736:TRP:HZ2	1:B:787:GLU:HB2	1.85	0.41
1:B:1308:GLY:C	1:B:1368:ILE:HG13	2.41	0.41
2:C:10:DA:C6	2:C:11:DG:C6	3.08	0.41
1:A:766:VAL:HG13	1:A:831:ILE:HG23	2.02	0.41
1:A:1230:GLN:HG2	3:D:20:DT:OP1	2.20	0.41
1:A:1369:THR:OG1	1:A:1521:TRP:O	2.38	0.41
1:B:984:ILE:HG22	1:B:1436:GLY:HA3	2.02	0.41
1:B:1343:GLN:HE21	1:B:1343:GLN:HB2	1.69	0.41
1:B:995:TYR:CD1	1:B:1362:SER:HB3	2.55	0.41
1:B:1304:ALA:HA	1:B:1586:LEU:HD12	2.02	0.41
1:A:807:VAL:HG23	1:A:1348:VAL:HG21	2.03	0.41
1:A:1173:TRP:CE3	1:A:1176:ALA:HB2	2.56	0.41
1:A:1581:ALA:HA	4:A:1701:SAH:C	2.51	0.41
1:B:771:ASP:N	1:B:771:ASP:OD1	2.53	0.41
1:B:894:HIS:CD2	1:B:894:HIS:H	2.39	0.41
1:B:925:VAL:HG11	1:B:1012:VAL:HG12	2.02	0.41
1:B:838:ILE:HD12	1:B:839:TYR:H	1.86	0.41
1:B:984:ILE:HG13	1:B:987:SER:HB2	2.03	0.41
1:A:979:LYS:HD3	1:A:1440:ARG:HB2	2.01	0.41
1:A:1138:LYS:HA	6:A:1819:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:ASP:O	1:A:1553:ARG:N	2.54	0.41
1:B:1157:GLY:HA3	1:B:1587:ALA:HB3	2.02	0.41
1:A:1145:LEU:HD13	1:A:1168:TRP:HB2	2.03	0.41
3:F:23:DG:C2	3:F:24:DT:C2	3.09	0.41
1:A:748:THR:O	1:A:748:THR:OG1	2.39	0.41
2:C:9:DA:C2'	2:C:10:DA:C8	3.04	0.41
1:A:1074:SER:OG	1:A:1077:ASP:OD2	2.39	0.40
1:A:737:LEU:HB2	1:A:752:LYS:O	2.22	0.40
1:A:1032:ARG:HH21	1:A:1046:TYR:HE2	1.67	0.40
1:B:1438:ASP:HA	1:B:1517:GLY:HA2	2.04	0.40
1:B:1438:ASP:OD2	1:B:1440:ARG:NH2	2.46	0.40
1:A:997:ILE:O	1:A:1024:PHE:HB2	2.21	0.40
1:B:1142:LEU:N	1:B:1164:SER:HA	2.36	0.40
2:C:10:DA:H2	3:D:15:DT:H3	1.69	0.40
1:A:753:VAL:HG23	1:A:785:LEU:CD1	2.52	0.40
1:B:939:LEU:HD23	1:B:1000:ILE:HG22	2.04	0.40
1:B:1582:VAL:HG12	4:B:1701:SAH:O	2.22	0.40
1:A:1350:ASP:OD2	1:B:1279:ARG:HD2	2.22	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	820/873 (94%)	775 (94%)	41 (5%)	4 (0%)	25	61
1	B	818/873 (94%)	774 (95%)	43 (5%)	1 (0%)	48	81
All	All	1638/1746 (94%)	1549 (95%)	84 (5%)	5 (0%)	37	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1361	SER
1	A	1109	PRO
1	B	963	PRO
1	A	958	SER
1	A	1000	ILE

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	666/759 (88%)	647 (97%)	19 (3%)	37	70
1	B	669/759 (88%)	658 (98%)	11 (2%)	58	82
All	All	1335/1518 (88%)	1305 (98%)	30 (2%)	47	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	755	ILE
1	A	771	ASP
1	A	799	TRP
1	A	812	SER
1	A	824	GLU
1	A	827	GLN
1	A	951	THR
1	A	1002	GLU
1	A	1021	LEU
1	A	1039	HIS
1	A	1201	VAL
1	A	1230	GLN
1	A	1272	ARG
1	A	1283	LEU
1	A	1312	THR
1	A	1448	ARG
1	A	1463	HIS
1	A	1487	CYS
1	A	1538	GLN

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Mol	Chain	Res	Type
1	B	951	THR
1	B	1020	ARG
1	B	1096	THR
1	B	1098	ASN
1	B	1272	ARG
1	B	1281	MET
1	B	1340	ARG
1	B	1348	VAL
1	B	1374	MET
1	B	1386	ASN
1	B	1538	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5CM	E	6	3,2	18,21,22	4.23	9 (50%)	24,30,33	1.82	7 (29%)
2	5CM	C	6	3,2	18,21,22	4.23	10 (55%)	24,30,33	1.58	5 (20%)
3	C49	D	18	3,1	17,22,24	4.95	10 (58%)	17,33,38	2.15	5 (29%)
3	C49	F	18	3,1	17,22,24	4.95	9 (52%)	17,33,38	2.23	5 (29%)

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	5CM	E	6	3,2	-	2/7/21/22	0/2/2/2
2	5CM	C	6	3,2	-	2/7/21/22	0/2/2/2
3	C49	D	18	3,1	-	4/7/40/46	0/2/2/2
3	C49	F	18	3,1	-	4/7/40/46	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	18	C49	C2-N1	10.32	1.49	1.35
3	D	18	C49	C2-N1	10.19	1.49	1.35
3	F	18	C49	C3'-C4'	-9.03	1.29	1.53
3	D	18	C49	C3'-C4'	-8.85	1.29	1.53
2	E	6	5CM	C2'-C3'	-8.64	1.30	1.52
2	C	6	5CM	C2'-C3'	-8.64	1.30	1.52
3	D	18	C49	O4'-C4'	7.69	1.62	1.45
3	F	18	C49	O4'-C4'	7.64	1.62	1.45
2	E	6	5CM	C1'-N1	-7.32	1.29	1.48
2	C	6	5CM	C1'-N1	-7.10	1.30	1.48
2	E	6	5CM	O4'-C4'	-6.99	1.29	1.45
2	C	6	5CM	C6-C5	6.86	1.45	1.34
2	C	6	5CM	O4'-C4'	-6.85	1.29	1.45
2	E	6	5CM	C6-C5	6.85	1.45	1.34
3	D	18	C49	C2-N3	6.72	1.49	1.38
3	F	18	C49	C2-N3	6.61	1.49	1.38
2	C	6	5CM	O4'-C1'	6.50	1.56	1.42
2	E	6	5CM	O4'-C1'	6.28	1.56	1.42
3	D	18	C49	CM5-C5	6.22	1.64	1.51
3	F	18	C49	CM5-C5	6.20	1.64	1.51
3	F	18	C49	O4'-C1'	-5.19	1.30	1.42
3	D	18	C49	O4'-C1'	-5.17	1.30	1.42
3	D	18	C49	C6-N1	-4.76	1.41	1.46
3	F	18	C49	F-C5	-4.61	1.33	1.42
3	D	18	C49	F-C5	-4.52	1.34	1.42
3	F	18	C49	C6-N1	-4.41	1.42	1.46
2	E	6	5CM	C2-N3	4.18	1.44	1.36
2	C	6	5CM	C2-N3	4.02	1.44	1.36
2	C	6	5CM	C4-N3	3.83	1.40	1.34
2	E	6	5CM	C3'-C4'	3.59	1.62	1.53
2	E	6	5CM	C4-N3	3.53	1.39	1.34
2	C	6	5CM	C3'-C4'	3.21	1.61	1.53
3	D	18	C49	O3'-C3'	3.19	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	18	C49	O3'-C3'	3.06	1.49	1.43
2	C	6	5CM	C2-N1	2.32	1.44	1.40
2	E	6	5CM	C2-N1	2.28	1.44	1.40
2	C	6	5CM	C4-N4	2.09	1.39	1.34
3	D	18	C49	C4-N3	2.06	1.42	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	18	C49	F-C5-CM5	-5.93	98.36	106.49
3	D	18	C49	F-C5-CM5	-5.93	98.37	106.49
3	F	18	C49	N3-C2-N1	4.46	121.13	116.65
3	D	18	C49	N3-C2-N1	4.00	120.67	116.65
2	E	6	5CM	C5-C6-N1	-3.95	119.02	123.31
2	C	6	5CM	C5-C6-N1	-3.91	119.07	123.31
3	D	18	C49	O2-C2-N1	-3.40	119.02	123.10
2	C	6	5CM	C5-C4-N3	-3.35	118.32	121.75
3	F	18	C49	O2-C2-N1	-3.30	119.13	123.10
2	E	6	5CM	O4'-C1'-N1	3.19	113.52	107.86
2	E	6	5CM	C5-C4-N3	-3.15	118.53	121.75
2	E	6	5CM	O4'-C1'-C2'	-2.93	100.77	106.25
2	E	6	5CM	O2-C2-N3	-2.91	117.74	122.33
2	E	6	5CM	C4'-O4'-C1'	-2.74	103.01	109.51
2	C	6	5CM	O2-C2-N3	-2.67	118.12	122.33
3	D	18	C49	C2'-C1'-N1	-2.56	112.55	115.59
3	F	18	C49	C4'-O4'-C1'	-2.53	103.49	109.51
3	F	18	C49	O4'-C1'-N1	2.32	111.27	108.39
2	C	6	5CM	O4'-C1'-N1	2.31	111.97	107.86
2	E	6	5CM	C2'-C3'-C4'	2.24	107.35	102.80
2	C	6	5CM	C5A-C5-C6	-2.14	119.95	122.85
3	D	18	C49	C4'-O4'-C1'	-2.12	104.47	109.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	18	C49	O4'-C1'-N1-C6
3	F	18	C49	O4'-C1'-N1-C6
2	C	6	5CM	O4'-C4'-C5'-O5'
2	C	6	5CM	C3'-C4'-C5'-O5'
3	D	18	C49	C2'-C1'-N1-C6
3	F	18	C49	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	E	6	5CM	C3'-C4'-C5'-O5'
2	E	6	5CM	O4'-C4'-C5'-O5'
3	D	18	C49	C2'-C1'-N1-C2
3	F	18	C49	C2'-C1'-N1-C2
3	F	18	C49	O4'-C1'-N1-C2
3	D	18	C49	O4'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	6	5CM	1	0
2	C	6	5CM	1	0
3	D	18	C49	2	0
3	F	18	C49	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
4	SAH	A	1701	-	23,28,28	1.28	3 (13%)	22,40,40	1.95	4 (18%)
4	SAH	B	1701	-	23,28,28	1.28	3 (13%)	22,40,40	2.07	5 (22%)

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
4	SAH	A	1701	-	-	6/11/31/31	0/3/3/3
4	SAH	B	1701	-	-	4/11/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1701	SAH	C2-N3	4.16	1.38	1.32
4	A	1701	SAH	C2-N3	4.09	1.38	1.32
4	B	1701	SAH	C2-N1	2.60	1.38	1.33
4	A	1701	SAH	C2-N1	2.57	1.38	1.33
4	A	1701	SAH	OXT-C	-2.27	1.23	1.30
4	B	1701	SAH	OXT-C	-2.23	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	SAH	N3-C2-N1	-6.35	120.05	128.67
4	B	1701	SAH	N3-C2-N1	-6.32	120.09	128.67
4	B	1701	SAH	C4'-O4'-C1'	-3.53	106.69	109.92
4	A	1701	SAH	C5'-SD-CG	-3.34	92.34	102.26
4	B	1701	SAH	C5'-SD-CG	-3.21	92.74	102.26
4	B	1701	SAH	O4'-C1'-N9	3.05	112.80	108.75
4	A	1701	SAH	OXT-C-O	-2.96	117.37	124.08
4	B	1701	SAH	OXT-C-O	-2.83	117.67	124.08
4	A	1701	SAH	C4'-O4'-C1'	-2.43	107.70	109.92

There are no chirality outliers.

All (10) torsion outliers are listed below:

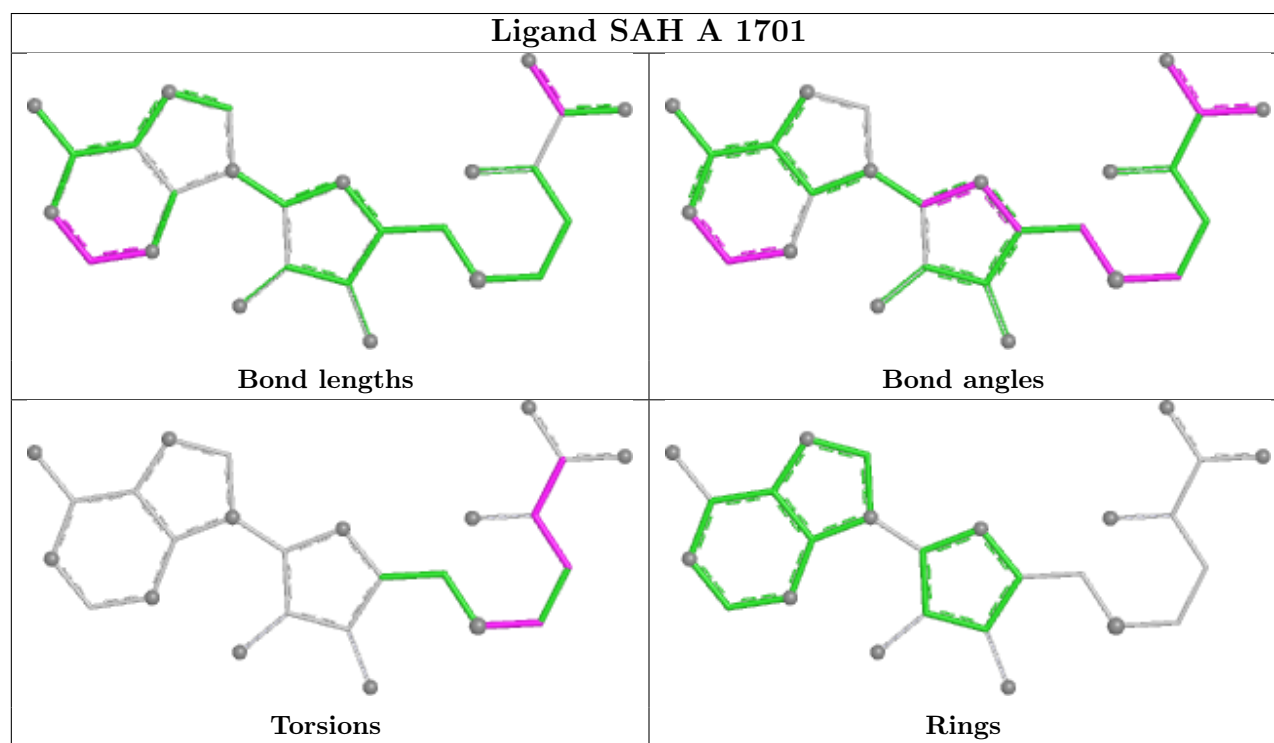
Mol	Chain	Res	Type	Atoms
4	A	1701	SAH	N-CA-CB-CG
4	A	1701	SAH	C-CA-CB-CG
4	B	1701	SAH	N-CA-CB-CG
4	B	1701	SAH	C-CA-CB-CG
4	A	1701	SAH	OXT-C-CA-CB
4	A	1701	SAH	O-C-CA-CB
4	A	1701	SAH	CB-CG-SD-C5'
4	A	1701	SAH	OXT-C-CA-N
4	B	1701	SAH	OXT-C-CA-CB
4	B	1701	SAH	CB-CG-SD-C5'

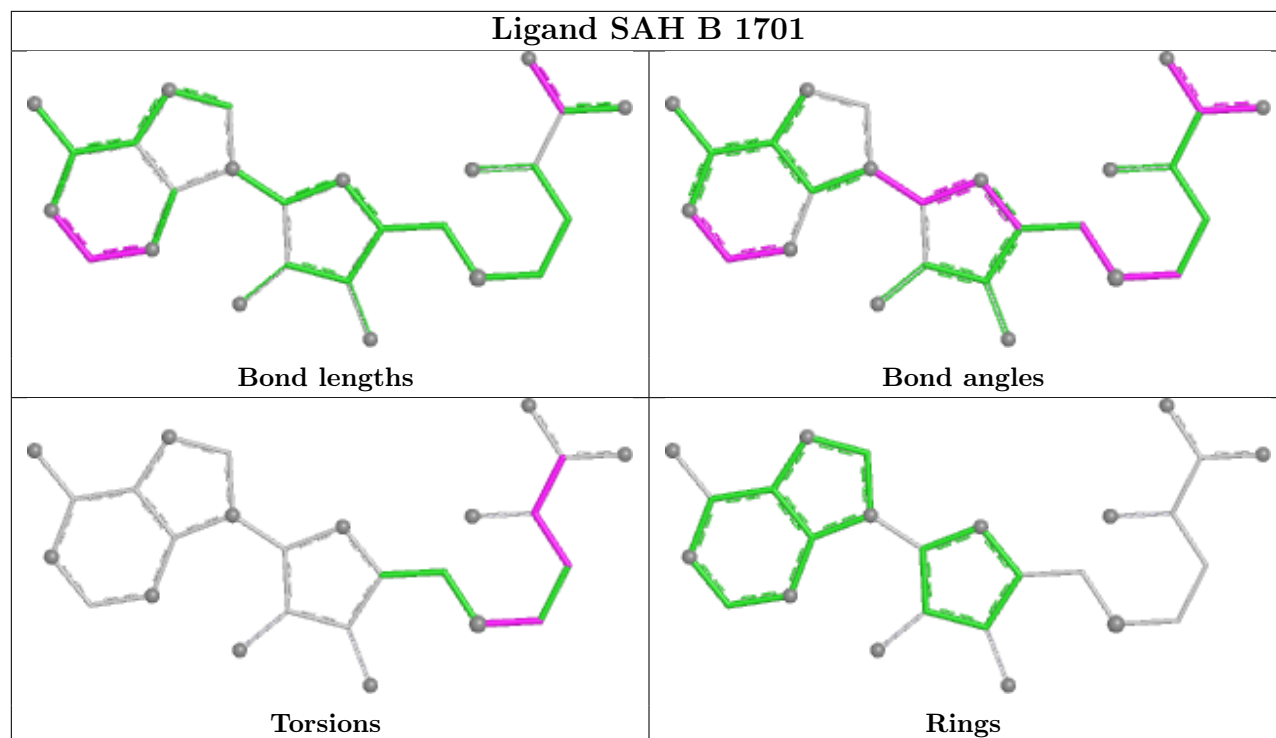
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1701	SAH	3	0
4	B	1701	SAH	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	828/873 (94%)	0.21	17 (2%)	63 41	39, 76, 150, 188	0
1	B	826/873 (94%)	0.19	17 (2%)	63 41	39, 76, 136, 197	2 (0%)
2	C	11/12 (91%)	1.35	3 (27%)	2 2	76, 110, 196, 196	0
2	E	11/12 (91%)	1.33	2 (18%)	4 3	79, 123, 205, 206	0
3	D	11/12 (91%)	1.23	2 (18%)	4 3	87, 117, 152, 163	0
3	F	11/12 (91%)	1.35	2 (18%)	4 3	98, 126, 184, 205	0
All	All	1698/1794 (94%)	0.23	43 (2%)	58 36	39, 77, 146, 206	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	13	DC	4.2
1	A	1238	PHE	4.1
1	A	866	THR	3.8
1	A	1111	ASN	3.6
3	D	13	DC	3.3
1	B	957	ALA	3.2
1	B	956	VAL	3.2
1	A	751	GLN	3.0
1	B	772	ASP	3.0
1	B	890	GLU	2.9
1	A	1600	SER	2.9
1	B	1238	PHE	2.9
1	A	776	PRO	2.9
1	B	1568	PHE	2.8
1	B	1600	SER	2.7
1	A	956	VAL	2.7
2	E	12	DG	2.7
1	B	1111	ASN	2.7
1	A	773	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	760	LEU	2.6
2	C	12	DG	2.6
1	A	1109	PRO	2.6
1	A	745	GLU	2.5
1	A	1568	PHE	2.5
1	A	782	VAL	2.5
1	B	777	LEU	2.4
1	B	1137	ILE	2.3
1	A	957	ALA	2.3
2	E	2	DC	2.2
1	A	984	ILE	2.2
3	D	24	DT	2.2
3	F	24	DT	2.2
1	B	763	GLY	2.1
1	B	922	ASP	2.1
2	C	7	DG	2.1
1	B	1109	PRO	2.1
1	B	984	ILE	2.1
2	C	1	DA	2.1
1	B	755	ILE	2.1
1	A	774	SER	2.1
1	A	735	SER	2.0
1	B	1392	ASN	2.0
1	B	987	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
3	C49	F	18	21/23	0.89	0.14	98,105,111,135	0
3	C49	D	18	21/23	0.90	0.12	83,90,105,124	0
2	5CM	E	6	20/21	0.92	0.14	73,85,90,92	0
2	5CM	C	6	20/21	0.93	0.13	74,81,88,91	0

6.3 Carbohydrates [i](#)

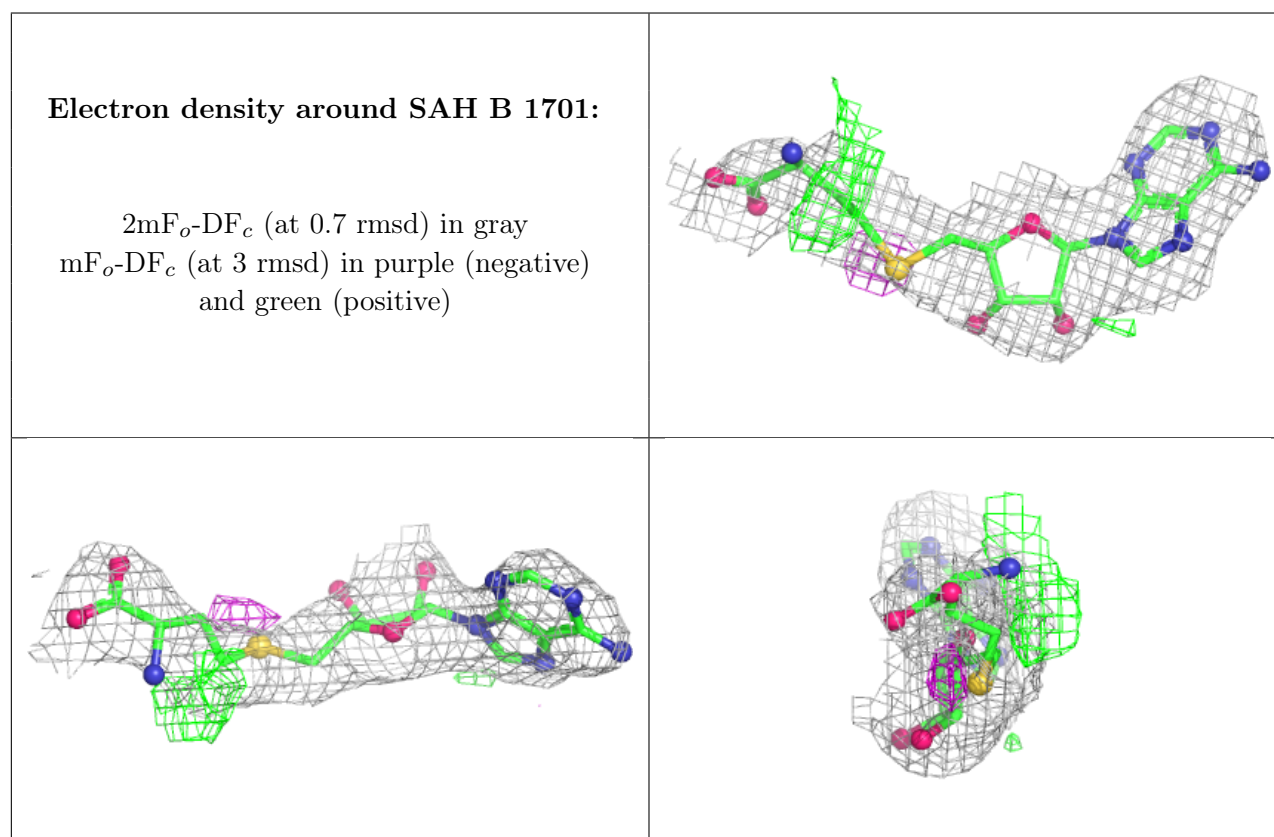
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

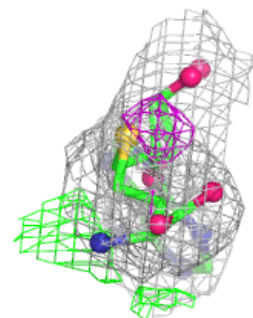
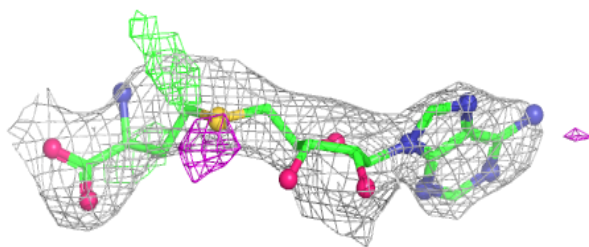
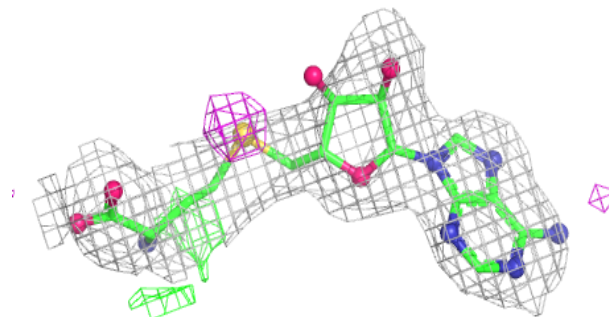
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SAH	B	1701	26/26	0.83	0.17	61,83,101,119	0
4	SAH	A	1701	26/26	0.84	0.15	55,79,100,107	0
5	ZN	A	1702	1/1	0.94	0.06	75,75,75,75	0
5	ZN	A	1703	1/1	0.94	0.08	124,124,124,124	0
5	ZN	B	1702	1/1	0.98	0.05	68,68,68,68	0
5	ZN	B	1703	1/1	0.98	0.04	104,104,104,104	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.



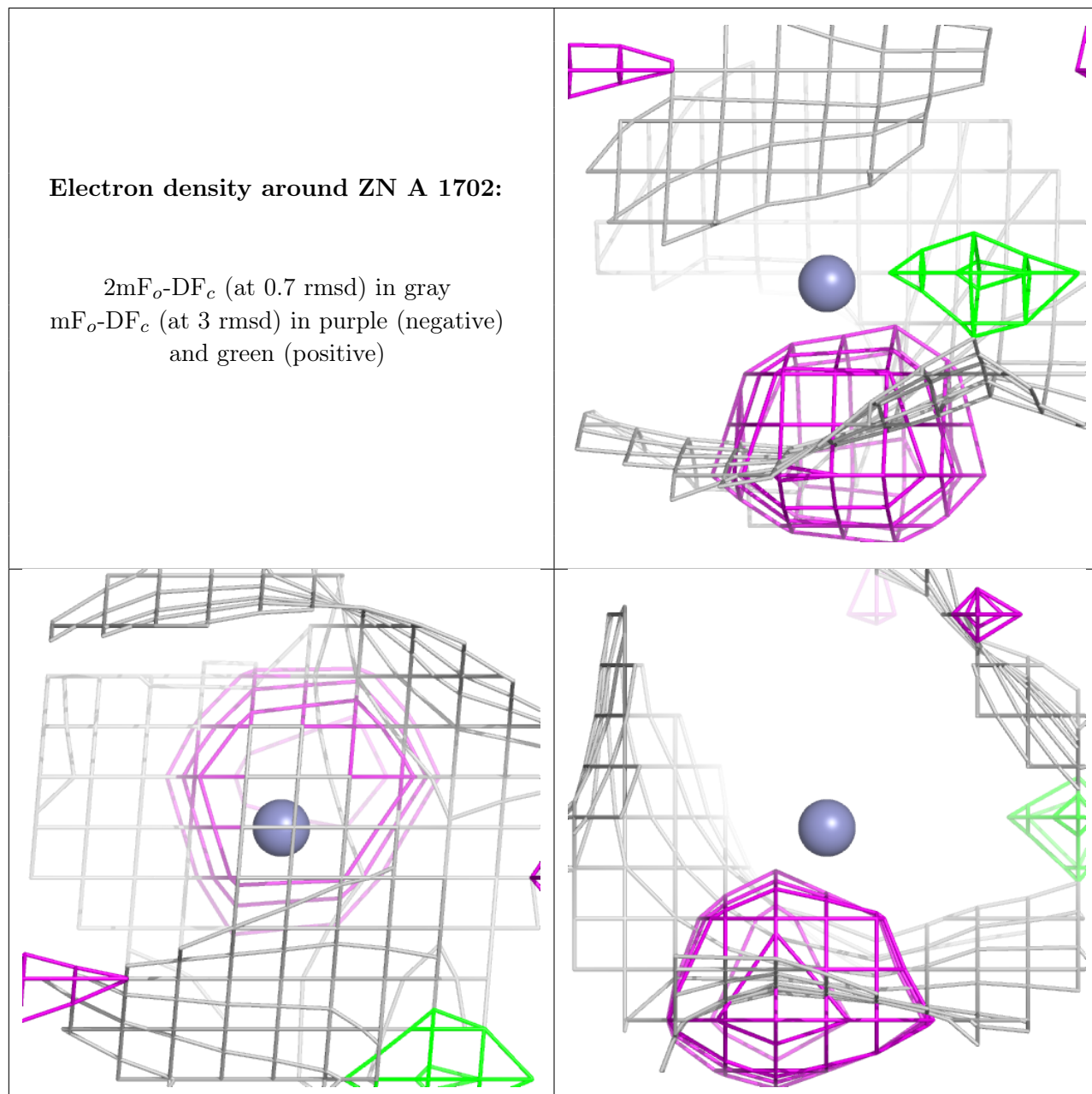
Electron density around SAH A 1701:

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



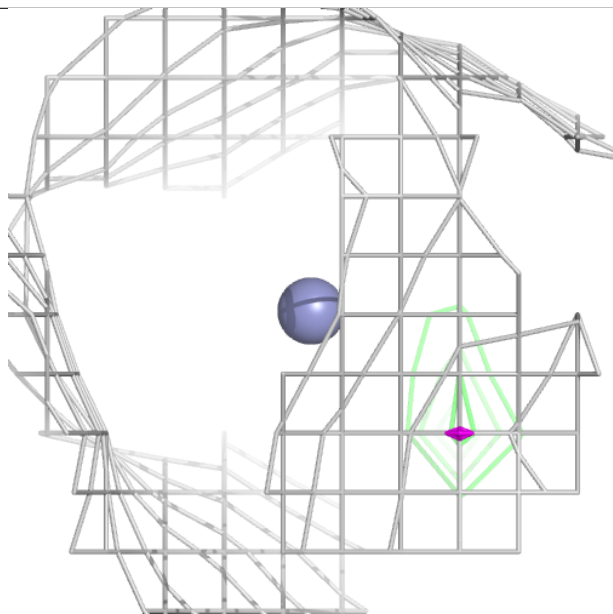
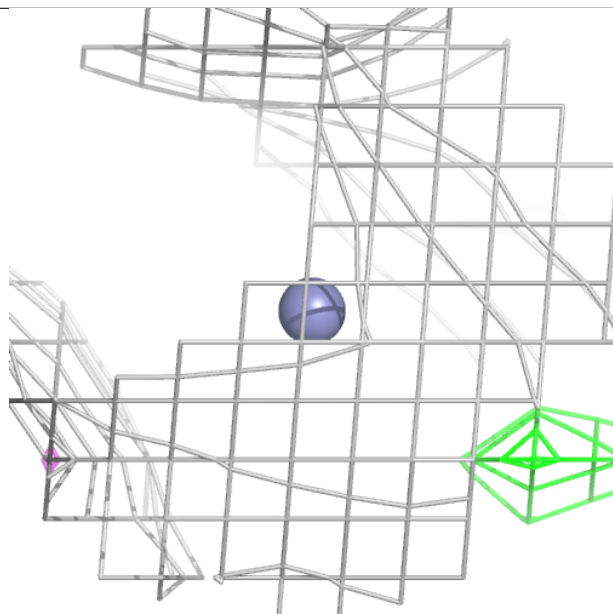
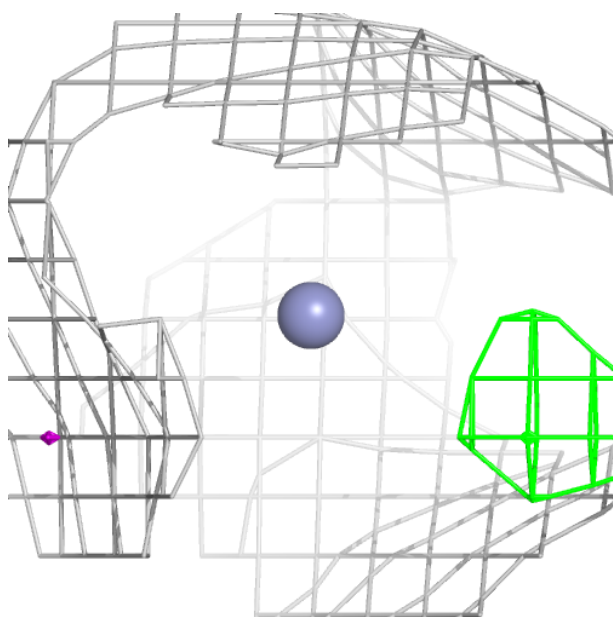
Electron density around ZN A 1702:

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



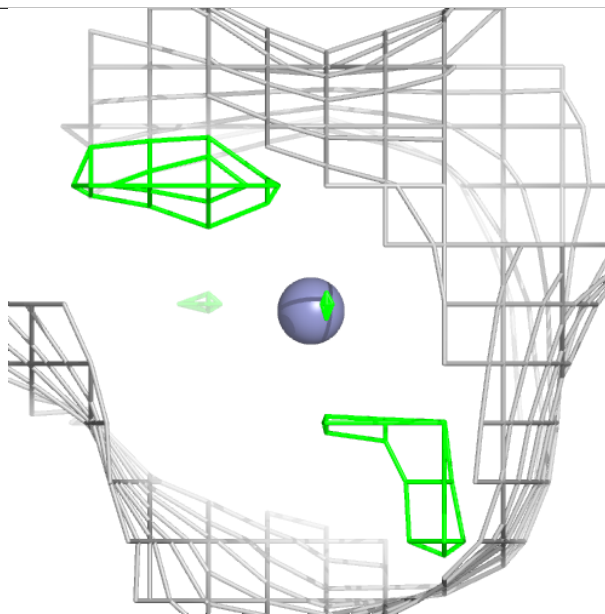
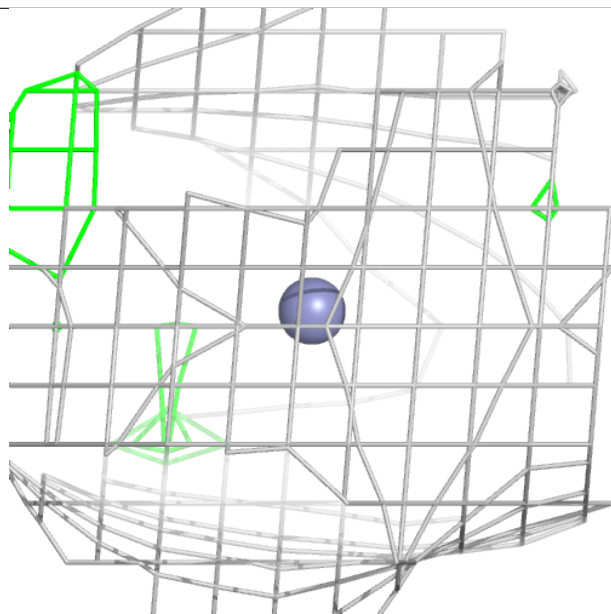
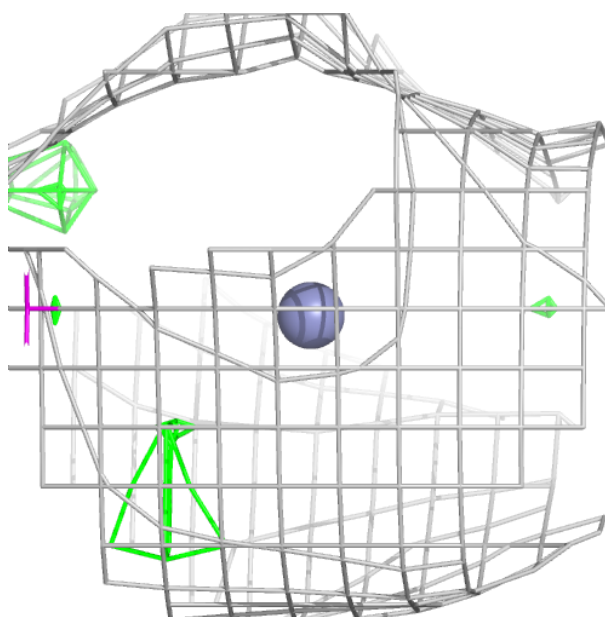
Electron density around ZN A 1703:

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



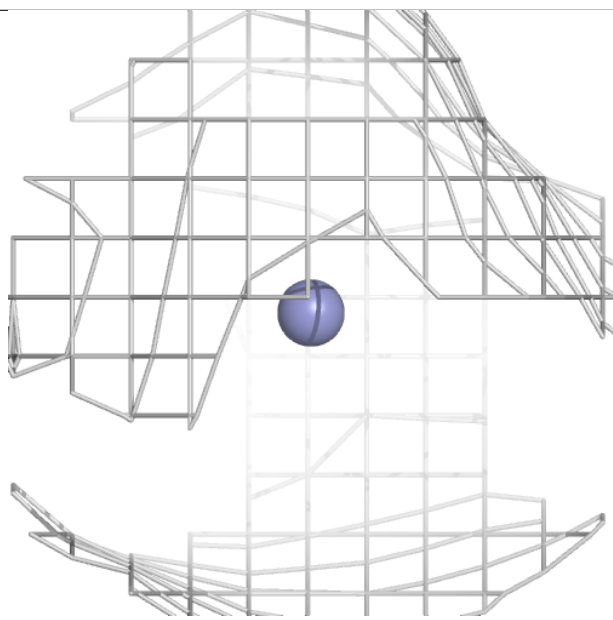
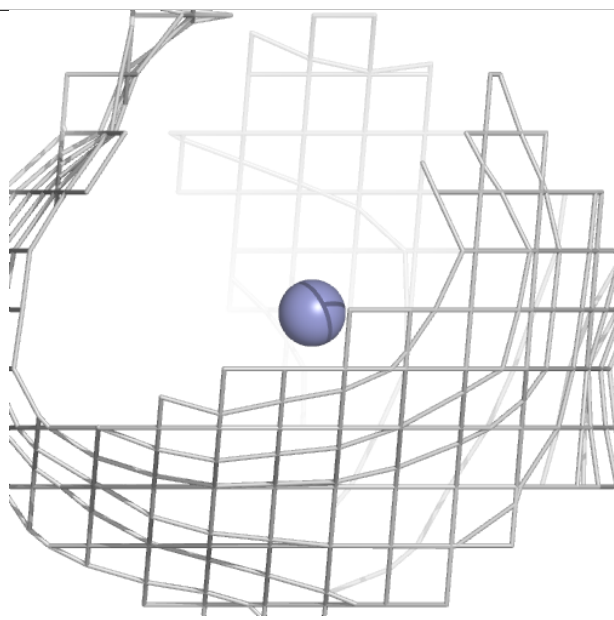
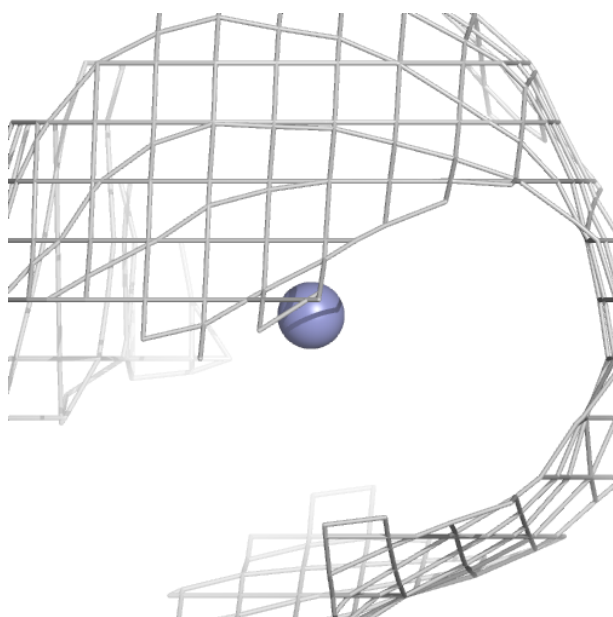
Electron density around ZN B 1702:

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



Electron density around ZN B 1703:

$2mF_o-DF_c$ (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.