



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 07:30 PM EDT

PDB ID : 4DA4 / pdb_00004da4
Title : Structure of mouse DNMT1 (731-1602) bound to hemimethylated CpG DNA
Authors : Song, J.; Patel, D.J.
Deposited on : 2012-01-12
Resolution : 2.60 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)
Xtrriage (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

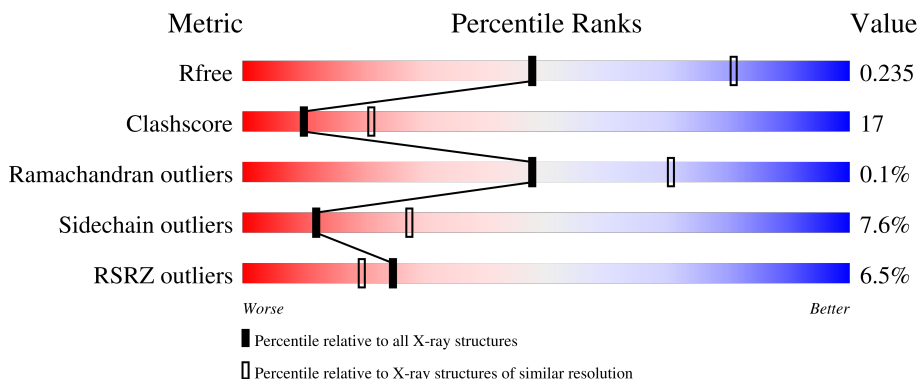
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	
1	B	873	
2	C	12	
2	E	12	
3	D	12	

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Mol	Chain	Length	Quality of chain
3	F	12	

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	SAH	B	1701	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15059 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
			Total	C	N	O	S			
1	A	834	6585	4179	1158	1207	41	0	0	0
1	B	832	6567	4170	1150	1206	41	0	0	0

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

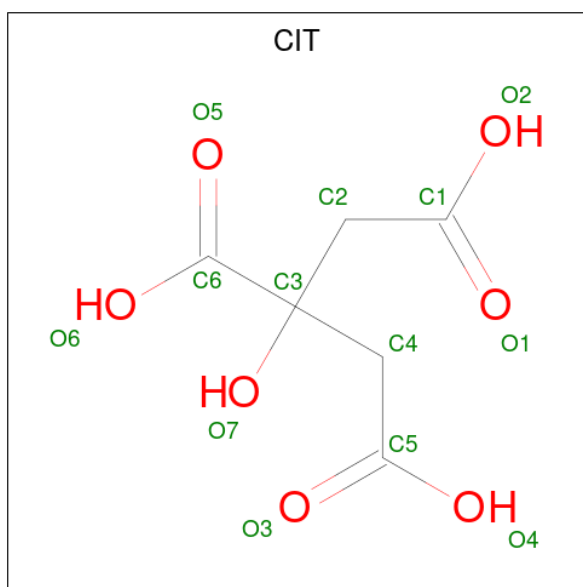
- Molecule 2 is a DNA chain called DNA_UPPER_STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	12	244	116	47	70	11	0	0	0
2	E	12	244	116	47	70	11	0	0	0

- Molecule 3 is a DNA chain called DNA_LOWER_STRAND.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
3	D	12	245	116	1	47	70	11	0	0	0
3	F	12	245	116	1	47	70	11	0	0	0

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			13	6 7		

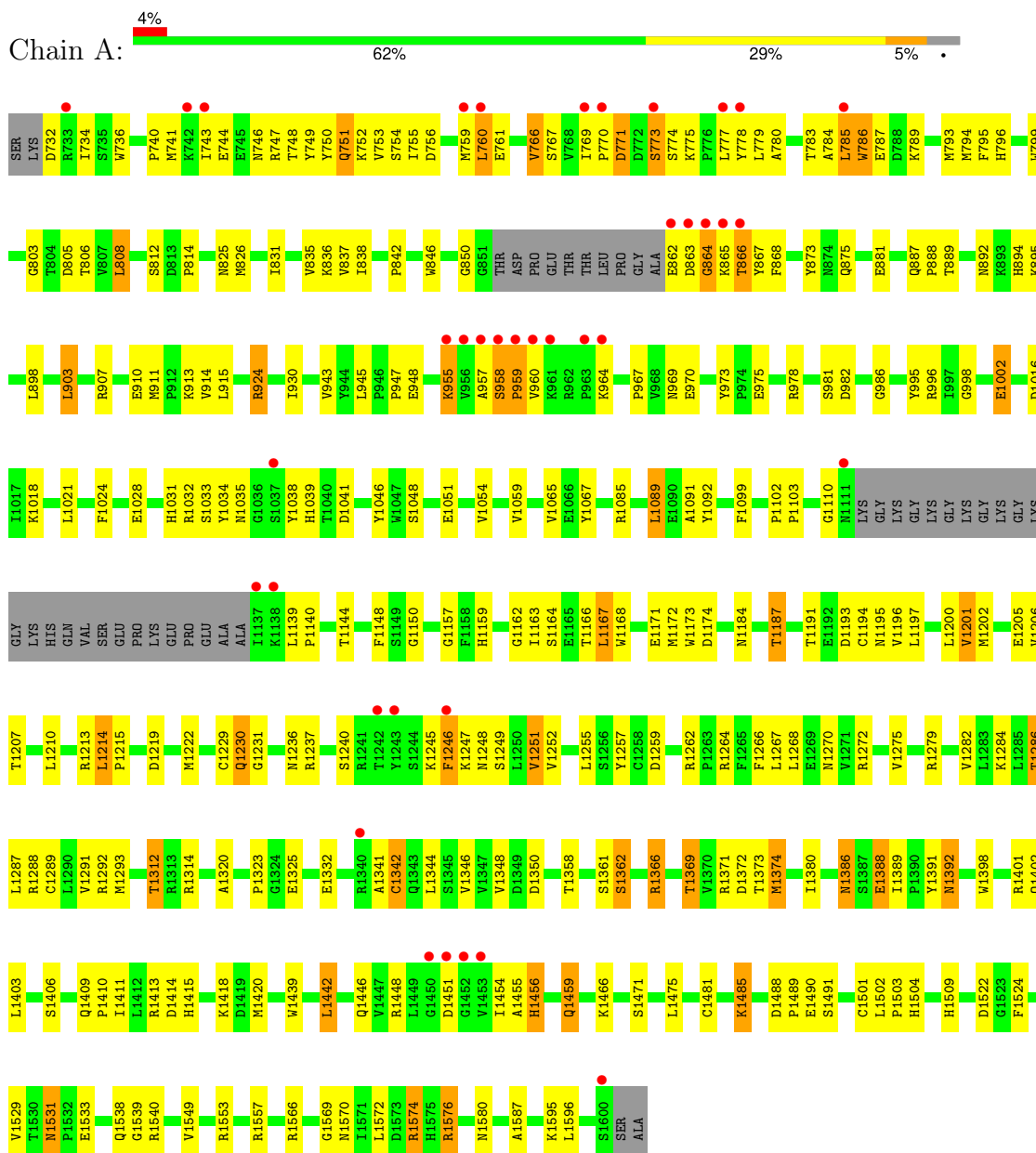
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	417	Total	O	0	0
			417	417		
7	B	388	Total	O	0	0
			388	388		
7	C	11	Total	O	0	0
			11	11		
7	D	18	Total	O	0	0
			18	18		
7	E	10	Total	O	0	0
			10	10		
7	F	16	Total	O	0	0
			16	16		

3 Residue-property plots [i](#)

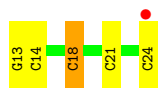
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

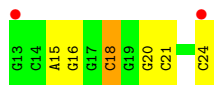


- Molecule 1: DNA (cytosine-5)-methyltransferase 1

● Molecule 3: DNA_LOWER_STRAND



● Molecule 3: DNA_LOWER_STRAND



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.68Å 152.04Å 96.05Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	39.47 – 2.60 39.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.47-2.60) 94.0 (39.47-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.196 , 0.246 0.187 , 0.235	Depositor DCC
R_{free} test set	3884 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtrriage
Anisotropy	0.480	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15059	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: C49, 5CM, CIT, SAH, ZN

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	0.41	0/6760	0.88	21/9172 (0.2%)
1	B	0.41	0/6742	0.86	20/9151 (0.2%)
2	C	0.23	0/250	0.87	1/382 (0.3%)
2	E	0.22	0/250	0.76	0/382
3	D	0.22	0/250	0.81	0/382
3	F	0.36	0/250	0.92	0/382
All	All	0.40	0/14502	0.87	42/19851 (0.2%)

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	3

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	785	LEU	N-CA-C	7.49	122.13	112.92
1	A	774	SER	N-CA-C	-7.14	104.57	113.28
1	B	1374	MET	N-CA-C	6.22	121.63	113.30
1	A	1539	GLY	CA-C-N	-6.03	113.85	122.77
1	A	1539	GLY	C-N-CA	-6.03	113.85	122.77
1	B	1491	SER	N-CA-C	-5.96	105.50	112.89
1	B	1391	TYR	N-CA-C	-5.91	101.16	109.96
1	B	1167	LEU	N-CA-C	-5.90	100.67	110.17
1	B	786	TRP	N-CA-C	5.75	117.71	110.24
1	A	786	TRP	N-CA-C	5.63	117.56	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	785	LEU	N-CA-C	5.59	119.80	112.92
1	A	1167	LEU	N-CA-C	-5.57	101.20	110.17
1	A	1491	SER	N-CA-C	-5.56	106.45	113.18
1	B	775	LYS	CA-C-N	5.55	125.07	119.19
1	B	775	LYS	C-N-CA	5.55	125.07	119.19
1	A	1374	MET	N-CA-C	5.51	120.69	113.30
1	A	1531	ASN	CA-C-N	-5.49	113.61	119.98
1	A	1531	ASN	C-N-CA	-5.49	113.61	119.98
1	A	1509	HIS	N-CA-C	5.46	119.93	112.88
2	C	3	DG	N9-C1'-C2'	5.43	121.65	113.50
1	A	973	TYR	CA-C-N	5.34	124.85	119.19
1	A	973	TYR	C-N-CA	5.34	124.85	119.19
1	B	813	ASP	CA-C-N	5.32	124.99	119.56
1	B	813	ASP	C-N-CA	5.32	124.99	119.56
1	B	1451	ASP	CB-CA-C	-5.31	110.47	116.63
1	A	1451	ASP	CB-CA-C	-5.30	110.45	116.54
1	A	1342	CYS	N-CA-C	5.29	119.43	112.92
1	A	960	VAL	N-CA-C	5.23	116.16	109.30
1	B	1391	TYR	CA-C-N	-5.17	115.11	122.77
1	B	1391	TYR	C-N-CA	-5.17	115.11	122.77
1	B	1411	ILE	N-CA-C	5.17	115.30	107.80
1	A	1409	GLN	CA-C-N	5.14	124.76	119.56
1	A	1409	GLN	C-N-CA	5.14	124.76	119.56
1	A	1110	GLY	N-CA-C	-5.14	106.66	115.08
1	B	1342	CYS	N-CA-C	5.08	119.17	112.92
1	A	958	SER	N-CA-C	5.07	120.56	113.57
1	A	1391	TYR	N-CA-C	-5.05	102.81	110.24
1	B	769	ILE	CA-C-N	5.05	125.50	120.14
1	B	769	ILE	C-N-CA	5.05	125.50	120.14
1	B	1509	HIS	N-CA-C	5.03	119.11	112.92
1	B	1539	GLY	CA-C-N	-5.03	115.33	122.77
1	B	1539	GLY	C-N-CA	-5.03	115.33	122.77

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	773	SER	Peptide
1	A	864	GLY	Peptide
1	A	958	SER	Peptide

5.2 Too-close contacts [i](#)

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	6585	0	6319	239	0
1	B	6567	0	6293	207	0
2	C	244	0	137	11	0
2	E	244	0	137	18	0
3	D	245	0	136	8	0
3	F	245	0	136	13	0
4	A	26	0	19	5	0
4	B	26	0	19	10	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	B	13	0	5	1	0
7	A	417	0	0	43	0
7	B	388	0	0	38	0
7	C	11	0	0	2	0
7	D	18	0	0	1	0
7	E	10	0	0	5	0
7	F	16	0	0	3	0
All	All	15059	0	13201	472	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 17.

All (472) 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:1229:CYS:SG	3:F:18:C49:C6	2.15	1.33
1:A:1229:CYS:SG	3:D:18:C49:C6	2.23	1.26
1:B:924:ARG:HG3	1:B:924:ARG:HH11	1.08	1.08
1:A:1392:ASN:N	7:A:1940:HOH:O	1.93	0.99
1:A:846:TRP:O	7:A:2134:HOH:O	1.81	0.98
4:B:1701:SAH:H8	7:B:2153:HOH:O	1.65	0.95
1:B:881:GLU:OE2	7:B:1935:HOH:O	1.88	0.92
2:E:2:DA:H2	3:F:24:DC:H41	1.15	0.90
1:A:770:PRO:HB2	1:A:773:SER:HB3	1.51	0.90
1:B:1371:ARG:NH2	1:B:1522:ASP:OD1	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:TYR:CD2	1:B:786:TRP:HB3	2.10	0.87
1:B:1174:ASP:OD2	7:B:1849:HOH:O	1.91	0.87
1:B:924:ARG:HG3	1:B:924:ARG:NH1	1.87	0.87
1:B:1369:THR:HG22	1:B:1372:ASP:H	1.40	0.86
1:A:1553:ARG:NH2	7:A:1865:HOH:O	2.06	0.86
1:A:975:GLU:OE1	1:A:978:ARG:HD2	1.75	0.86
1:B:900:CYS:SG	7:B:1999:HOH:O	2.36	0.84
2:E:1:DG:H1'	7:E:109:HOH:O	1.77	0.84
2:E:6:5CM:P	7:E:110:HOH:O	2.34	0.84
2:C:3:DG:N3	7:C:105:HOH:O	2.09	0.84
2:E:5:DC:O3'	7:E:110:HOH:O	1.96	0.83
1:B:975:GLU:OE1	1:B:978:ARG:HD2	1.78	0.82
1:A:1174:ASP:OD2	7:A:1957:HOH:O	1.98	0.82
1:B:750:TYR:O	1:B:785:LEU:HB2	1.80	0.81
1:A:924:ARG:HG3	1:A:924:ARG:HH11	1.45	0.81
1:A:1369:THR:HG22	1:A:1372:ASP:H	1.44	0.80
1:B:1206:VAL:HG12	1:B:1207:THR:HG23	1.60	0.80
1:A:1252:VAL:HG23	7:A:2087:HOH:O	1.80	0.80
1:A:1206:VAL:HG12	1:A:1207:THR:HG23	1.63	0.80
2:E:1:DG:N3	7:E:109:HOH:O	2.14	0.79
1:A:1150:GLY:HA3	4:A:1701:SAH:HB1	1.62	0.79
1:A:751:GLN:CD	1:A:751:GLN:H	1.90	0.79
1:A:1184:ASN:HB3	1:A:1187:THR:CG2	2.13	0.78
1:B:1392:ASN:N	7:B:1955:HOH:O	2.13	0.78
1:A:773:SER:HB2	1:A:775:LYS:O	1.86	0.76
1:B:1489:PRO:O	1:B:1490:GLU:HB2	1.85	0.76
1:A:749:TYR:CD2	1:A:786:TRP:HB3	2.21	0.75
1:B:1184:ASN:HB3	1:B:1187:THR:CG2	2.16	0.75
1:B:1449:LEU:HD11	7:B:2136:HOH:O	1.87	0.74
1:B:924:ARG:HH11	1:B:924:ARG:CG	1.94	0.74
1:A:1163:ILE:HD12	1:A:1222:MET:HE1	1.69	0.74
1:B:1391:TYR:O	7:B:2140:HOH:O	2.05	0.73
1:A:805:ASP:OD2	7:A:1929:HOH:O	2.07	0.73
1:B:1168:TRP:N	7:B:2138:HOH:O	2.05	0.72
1:B:1352:LYS:O	7:B:1835:HOH:O	2.06	0.72
1:B:1439:TRP:HA	1:B:1442:LEU:HD22	1.71	0.72
2:C:1:DG:H1'	7:C:111:HOH:O	1.89	0.72
1:A:864:GLY:HA3	1:B:866:THR:HA	1.72	0.72
1:B:747:ARG:HG2	1:B:786:TRP:CD1	2.24	0.72
1:A:766:VAL:HG13	1:A:831:ILE:HG23	1.72	0.72
1:A:1039:HIS:O	1:A:1401:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:TRP:CZ2	1:B:787:GLU:HB2	2.24	0.71
2:E:11:DG:H2'	2:E:12:DC:C6	2.26	0.71
1:A:1255:LEU:HD11	1:A:1286:THR:HB	1.71	0.71
1:A:1264:ARG:HD2	1:A:1325:GLU:OE1	1.91	0.71
1:A:1489:PRO:O	1:A:1490:GLU:HB2	1.89	0.71
1:A:1184:ASN:HB3	1:A:1187:THR:HG23	1.71	0.70
1:A:1032:ARG:NH2	1:A:1046:TYR:OH	2.24	0.70
1:A:924:ARG:NH1	7:A:2048:HOH:O	2.22	0.70
1:A:924:ARG:HG3	1:A:924:ARG:NH1	2.06	0.70
1:A:743:ILE:HG23	1:A:748:THR:HG22	1.73	0.70
1:A:734:ILE:HG13	1:A:755:ILE:HG12	1.73	0.69
1:B:891:ASP:OD1	1:B:891:ASP:N	2.26	0.69
1:A:924:ARG:HH11	1:A:924:ARG:CG	2.06	0.69
1:B:924:ARG:NH2	7:B:1937:HOH:O	2.10	0.68
1:A:732:ASP:N	1:A:756:ASP:OD1	2.25	0.68
1:B:1553:ARG:NH2	7:B:1891:HOH:O	2.21	0.68
1:B:924:ARG:NE	7:B:1937:HOH:O	2.21	0.68
1:B:1229:CYS:SG	3:F:18:C49:C5	2.81	0.68
3:F:15:DA:OP1	7:F:111:HOH:O	2.12	0.68
1:A:1371:ARG:NH1	7:A:2175:HOH:O	2.26	0.68
1:B:1166:THR:O	1:B:1187:THR:HB	1.94	0.68
2:E:10:DT:H2''	2:E:11:DG:OP1	1.94	0.67
1:A:1580:ASN:O	7:A:1834:HOH:O	2.10	0.67
1:A:967:PRO:O	7:A:2005:HOH:O	2.13	0.66
1:B:1366:ARG:NH1	7:B:2058:HOH:O	2.21	0.66
1:B:1350:ASP:OD2	7:B:2159:HOH:O	2.13	0.66
1:B:955:LYS:H	1:B:955:LYS:HD2	1.61	0.65
1:B:751:GLN:O	1:B:752:LYS:HG3	1.97	0.65
1:B:1148:PHE:O	4:B:1701:SAH:HG2	1.97	0.65
1:B:1266:PHE:HB3	1:B:1320:ALA:HB3	1.78	0.65
1:A:1456:HIS:O	7:A:2174:HOH:O	2.15	0.64
2:C:2:DA:H2	3:D:24:DC:H41	1.45	0.64
1:B:1111:ASN:HA	7:B:1961:HOH:O	1.95	0.64
1:B:1028:GLU:OE1	7:B:2036:HOH:O	2.15	0.64
1:A:1229:CYS:SG	3:D:18:C49:N1	2.70	0.64
1:B:947:PRO:HA	1:B:996:ARG:HG2	1.78	0.64
3:D:13:DG:H2''	3:D:14:DC:O5'	1.97	0.64
3:F:16:DG:H5'	3:F:16:DG:H8	1.62	0.64
1:A:1279:ARG:NH1	1:B:1350:ASP:HB2	2.12	0.64
1:A:1369:THR:CG2	1:A:1372:ASP:H	2.11	0.64
1:B:902:ARG:NH1	7:B:1994:HOH:O	2.20	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1369:THR:HG21	7:A:2083:HOH:O	1.97	0.63
1:A:1168:TRP:N	7:A:1844:HOH:O	2.19	0.63
1:A:1229:CYS:SG	3:D:18:C49:C5	2.87	0.62
1:B:955:LYS:H	1:B:955:LYS:CD	2.12	0.62
1:A:1246:PHE:C	1:A:1246:PHE:HD1	2.06	0.62
1:B:1501:CYS:HB2	2:E:5:DC:H3'	1.81	0.62
1:B:1041:ASP:OD1	1:B:1401:ARG:NH1	2.33	0.62
1:B:1376:ASP:HB3	1:B:1400:GLN:OE1	1.98	0.62
1:A:864:GLY:O	1:A:865:LYS:HB3	1.99	0.62
1:A:1272:ARG:O	1:A:1275:VAL:HG22	2.00	0.62
1:A:986:GLY:HA2	1:A:1524:PHE:CZ	2.35	0.62
1:A:1439:TRP:HA	1:A:1442:LEU:HD22	1.80	0.62
2:C:2:DA:H2	3:D:24:DC:N4	1.97	0.61
1:B:943:VAL:HG12	1:B:945:LEU:HD22	1.81	0.61
1:B:1332:GLU:OE2	1:B:1358:THR:N	2.32	0.61
1:A:1246:PHE:C	1:A:1246:PHE:CD1	2.79	0.61
1:B:1448:ARG:HA	1:B:1454:ILE:HD13	1.81	0.61
1:A:1350:ASP:HB2	1:B:1279:ARG:NH1	2.15	0.61
3:F:16:DG:H5'	3:F:16:DG:C8	2.36	0.61
1:A:1259:ASP:O	1:A:1262:ARG:HG2	2.00	0.60
1:A:1595:LYS:NZ	7:A:2017:HOH:O	2.33	0.60
1:B:1369:THR:CG2	1:B:1372:ASP:H	2.14	0.60
1:A:957:ALA:C	1:A:959:PRO:HD2	2.26	0.60
1:A:881:GLU:OE2	7:A:2101:HOH:O	2.16	0.60
1:A:955:LYS:H	1:A:955:LYS:HD2	1.67	0.60
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.83	0.60
1:B:1501:CYS:CB	2:E:5:DC:H3'	2.31	0.60
1:A:1028:GLU:HA	1:A:1033:SER:O	2.01	0.60
1:B:916:GLU:HB3	7:B:2085:HOH:O	2.01	0.59
1:B:1168:TRP:CH2	1:B:1219:ASP:HB3	2.37	0.59
2:E:1:DG:H8	2:E:1:DG:HO5'	1.48	0.59
1:B:1200:LEU:HD22	1:B:1205:GLU:HG3	1.83	0.59
1:A:1171:GLU:OE2	4:A:1701:SAH:H4'	2.03	0.59
1:B:1247:LYS:NZ	7:B:2153:HOH:O	2.23	0.59
1:A:750:TYR:O	1:A:785:LEU:HB2	2.03	0.58
1:B:1282:VAL:O	1:B:1286:THR:HG23	2.03	0.58
1:A:1414:ASP:OD2	7:A:2138:HOH:O	2.16	0.58
1:A:1041:ASP:OD1	1:A:1401:ARG:NH1	2.36	0.58
1:A:1248:ASN:OD1	7:A:2026:HOH:O	2.16	0.58
1:A:1418:LYS:HB2	1:A:1420:MET:HE3	1.85	0.58
1:A:1418:LYS:HE3	1:A:1420:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:TYR:CE2	1:A:1102:PRO:HG3	2.38	0.58
1:A:1262:ARG:O	7:A:2135:HOH:O	2.17	0.58
1:B:1167:LEU:HA	7:B:2138:HOH:O	2.04	0.57
1:B:1272:ARG:O	1:B:1275:VAL:HG22	2.04	0.57
1:A:943:VAL:HG13	1:A:945:LEU:CD2	2.34	0.57
1:A:998:GLY:HA3	1:A:1021:LEU:HD13	1.87	0.57
1:A:1166:THR:O	1:A:1187:THR:HB	2.05	0.57
1:A:1193:ASP:OD2	1:A:1195:ASN:HB2	2.05	0.57
1:B:1167:LEU:CA	7:B:2138:HOH:O	2.53	0.57
1:B:1264:ARG:HD2	1:B:1325:GLU:OE1	2.04	0.57
1:B:1018:LYS:NZ	1:B:1055:ASN:OD1	2.34	0.57
2:E:3:DG:H2'	2:E:4:DG:C8	2.39	0.57
1:B:745:GLU:H	1:B:745:GLU:CD	2.12	0.57
1:A:864:GLY:HA3	1:B:866:THR:HG22	1.86	0.56
1:B:1574:ARG:NH1	6:B:1704:CIT:O3	2.37	0.56
1:A:1171:GLU:O	1:A:1191:THR:HA	2.04	0.56
1:B:1340:ARG:H	1:B:1340:ARG:HD2	1.70	0.56
1:A:1289:CYS:SG	1:A:1293:MET:HE3	2.45	0.56
1:A:986:GLY:HA2	1:A:1524:PHE:CE2	2.41	0.56
1:A:783:THR:OG1	1:A:796:HIS:HB3	2.04	0.56
1:A:770:PRO:HB3	1:A:778:TYR:CE2	2.41	0.56
1:B:1229:CYS:SG	3:F:18:C49:N1	2.78	0.56
1:B:1303:GLN:HE22	1:B:1312:THR:HG22	1.72	0.55
1:A:1031:HIS:ND1	1:A:1092:TYR:OH	2.32	0.55
1:B:1489:PRO:O	1:B:1490:GLU:CB	2.55	0.55
1:A:736:TRP:CZ2	1:A:787:GLU:HB2	2.42	0.55
1:A:1332:GLU:OE2	1:A:1358:THR:N	2.38	0.55
1:A:1388:GLU:HG2	1:A:1411:ILE:HG21	1.88	0.55
1:B:1033:SER:OG	1:B:1034:TYR:N	2.36	0.55
2:C:9:DC:H2'	2:C:10:DT:C6	2.41	0.55
1:A:784:ALA:O	1:A:795:PHE:HA	2.07	0.55
1:A:1248:ASN:ND2	7:A:2026:HOH:O	2.38	0.55
1:B:894:HIS:CD2	1:B:895:LYS:H	2.25	0.55
4:B:1701:SAH:HG1	7:B:2009:HOH:O	2.05	0.55
2:C:2:DA:H4'	2:C:3:DG:OP1	2.07	0.55
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.87	0.55
1:B:744:GLU:HG3	1:B:749:TYR:HE1	1.70	0.55
1:B:1150:GLY:HA3	4:B:1701:SAH:HB1	1.89	0.54
1:B:1230:GLN:O	1:B:1236:ASN:ND2	2.38	0.54
1:A:748:THR:HG23	1:A:789:LYS:NZ	2.22	0.54
1:A:771:ASP:OD1	7:A:2094:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:CYS:O	1:A:1344:LEU:HG	2.08	0.54
1:B:1184:ASN:HB3	1:B:1187:THR:HG23	1.89	0.54
1:A:1282:VAL:O	1:A:1286:THR:HG23	2.08	0.54
1:B:1398:TRP:O	1:B:1402:GLN:HG2	2.08	0.54
2:E:10:DT:H2'	2:E:11:DG:C8	2.42	0.54
4:B:1701:SAH:SD	3:F:18:C49:CM5	2.95	0.54
1:A:1262:ARG:HG3	7:A:2134:HOH:O	2.08	0.54
1:B:795:PHE:CE2	1:B:826:MET:HB3	2.43	0.54
1:B:1139:LEU:HD22	1:B:1140:PRO:HD2	1.88	0.54
1:B:1312:THR:HG23	1:B:1341:ALA:HB1	1.89	0.54
1:A:1201:VAL:HG12	1:A:1214:LEU:HG	1.90	0.53
1:B:1255:LEU:HD11	1:B:1286:THR:HB	1.90	0.53
1:A:947:PRO:HA	1:A:996:ARG:HG2	1.91	0.53
1:B:745:GLU:CG	1:B:746:ASN:H	2.21	0.53
1:A:1366:ARG:NE	7:A:1897:HOH:O	1.99	0.53
1:A:850:GLY:C	7:A:1967:HOH:O	2.52	0.53
1:A:981:SER:O	1:A:982:ASP:HB2	2.07	0.53
1:A:1570:ASN:O	1:A:1574:ARG:HG2	2.09	0.53
1:B:749:TYR:CE2	1:B:786:TRP:HB3	2.43	0.53
1:A:1139:LEU:HD22	1:A:1140:PRO:HD2	1.91	0.53
1:A:1312:THR:HG23	1:A:1341:ALA:HB1	1.90	0.53
1:A:1350:ASP:HB2	1:B:1279:ARG:HH11	1.73	0.53
1:B:1171:GLU:O	1:B:1191:THR:HA	2.08	0.53
1:A:1369:THR:HG23	1:A:1371:ARG:N	2.24	0.53
1:B:840:LYS:NZ	7:B:2158:HOH:O	2.32	0.53
1:B:1171:GLU:OE2	4:B:1701:SAH:H4'	2.09	0.53
1:B:1504:HIS:ND1	7:E:110:HOH:O	2.14	0.53
1:A:779:LEU:HD22	1:A:835:VAL:HG21	1.91	0.53
1:A:1502:LEU:HB2	1:A:1503:PRO:HD3	1.89	0.53
1:B:1299:PHE:HE1	1:B:1346:VAL:HG11	1.74	0.53
1:A:734:ILE:HA	1:A:754:SER:O	2.09	0.53
1:A:1249:SER:HA	7:A:2087:HOH:O	2.08	0.53
1:B:1501:CYS:O	1:B:1504:HIS:HB3	2.09	0.53
1:A:1193:ASP:HB3	1:A:1196:VAL:HG23	1.91	0.52
1:B:734:ILE:N	1:B:734:ILE:HD12	2.24	0.52
1:B:1157:GLY:HA3	1:B:1587:ALA:HB3	1.91	0.52
1:B:1388:GLU:HG2	1:B:1411:ILE:HG21	1.91	0.52
1:A:796:HIS:ND1	1:A:825:ASN:OD1	2.43	0.52
1:B:943:VAL:HG12	1:B:945:LEU:CD2	2.39	0.52
1:A:770:PRO:CB	1:A:773:SER:HB3	2.30	0.52
1:A:1448:ARG:HA	1:A:1454:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1201:VAL:HG12	1:B:1214:LEU:HG	1.92	0.52
2:E:2:DA:C2	3:F:24:DC:N4	2.64	0.52
1:B:1230:GLN:HG2	3:F:20:DG:OP1	2.09	0.52
1:B:784:ALA:O	1:B:795:PHE:HA	2.10	0.51
1:B:803:GLY:HA3	1:B:812:SER:OG	2.10	0.51
1:B:1342:CYS:O	1:B:1344:LEU:HG	2.10	0.51
1:B:766:VAL:HG13	1:B:831:ILE:HG23	1.93	0.51
1:A:1501:CYS:O	1:A:1504:HIS:HB3	2.10	0.51
1:A:1033:SER:OG	1:A:1034:TYR:N	2.43	0.51
1:A:1246:PHE:HD1	1:A:1246:PHE:O	1.92	0.51
1:A:1459:GLN:HG2	7:A:2170:HOH:O	2.10	0.51
1:B:1246:PHE:CD1	1:B:1246:PHE:C	2.87	0.51
1:A:957:ALA:C	1:A:959:PRO:CD	2.84	0.51
1:B:734:ILE:HG13	1:B:755:ILE:HG23	1.93	0.51
1:B:1144:THR:OG1	1:B:1164:SER:HB2	2.10	0.51
3:F:21:DC:OP2	7:F:110:HOH:O	2.18	0.51
1:B:744:GLU:CG	1:B:749:TYR:HE1	2.23	0.50
1:B:1110:GLY:O	7:B:1961:HOH:O	2.19	0.50
1:B:745:GLU:CD	1:B:746:ASN:H	2.19	0.50
1:B:897:CYS:O	1:B:901:ILE:HG13	2.12	0.50
2:E:8:DC:H4'	2:E:9:DC:OP2	2.12	0.50
1:B:1401:ARG:NH1	7:B:1830:HOH:O	2.17	0.50
1:A:1489:PRO:O	1:A:1490:GLU:CB	2.59	0.50
1:B:955:LYS:H	1:B:955:LYS:CE	2.24	0.50
1:A:1035:ASN:HA	1:A:1038:TYR:CZ	2.46	0.49
1:B:782:VAL:HG22	1:B:795:PHE:CD1	2.47	0.49
1:A:749:TYR:HA	1:A:786:TRP:HA	1.95	0.49
1:A:1144:THR:OG1	1:A:1164:SER:HB2	2.13	0.49
1:A:1200:LEU:HD22	1:A:1205:GLU:HG3	1.93	0.49
1:A:1373:THR:HG23	1:A:1557:ARG:HB3	1.94	0.49
1:A:766:VAL:CG1	1:A:831:ILE:HG23	2.42	0.49
1:A:1173:TRP:CZ3	1:A:1576:ARG:HG2	2.48	0.49
1:A:1418:LYS:HE3	1:A:1420:MET:HE1	1.95	0.49
1:B:1401:ARG:NE	7:B:1990:HOH:O	2.04	0.49
1:B:1502:LEU:HB2	1:B:1503:PRO:HD3	1.95	0.49
1:A:747:ARG:HG2	1:A:786:TRP:CD1	2.46	0.49
1:A:1371:ARG:NH2	1:A:1522:ASP:OD1	2.44	0.49
1:B:1455:ALA:N	7:B:2136:HOH:O	2.45	0.49
1:A:1413:ARG:O	1:A:1553:ARG:HD2	2.13	0.49
1:A:1206:VAL:HG12	1:A:1207:THR:CG2	2.38	0.48
1:A:736:TRP:CZ2	1:A:793:MET:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:HIS:HB2	7:A:1945:HOH:O	2.11	0.48
1:A:1167:LEU:CA	7:A:1844:HOH:O	2.61	0.48
1:A:1168:TRP:CH2	1:A:1219:ASP:HB3	2.48	0.48
1:A:748:THR:HG23	1:A:789:LYS:HZ3	1.77	0.48
1:A:924:ARG:HG3	7:A:2048:HOH:O	2.13	0.48
1:A:766:VAL:HG11	1:A:831:ILE:HG12	1.95	0.48
1:A:1501:CYS:O	7:A:1813:HOH:O	2.20	0.48
1:A:760:LEU:HD23	1:A:761:GLU:H	1.77	0.48
1:A:1162:GLY:HA2	7:A:1912:HOH:O	2.13	0.48
1:A:1531:ASN:O	1:A:1533:GLU:HG3	2.12	0.48
1:B:839:TYR:CE1	1:B:841:ALA:HB2	2.48	0.48
1:A:1386:ASN:HB3	1:A:1389:ILE:CG2	2.44	0.48
1:B:1369:THR:HG23	1:B:1371:ARG:N	2.29	0.48
1:B:888:PRO:HB2	1:B:893:LYS:HD2	1.95	0.48
1:B:1074:SER:OG	1:B:1077:ASP:OD1	2.32	0.48
1:B:1268:LEU:C	1:B:1268:LEU:HD23	2.39	0.48
1:A:744:GLU:HG3	1:A:749:TYR:HE1	1.79	0.47
1:A:1267:LEU:C	1:A:1267:LEU:HD23	2.39	0.47
1:B:894:HIS:CD2	1:B:895:LYS:HG2	2.48	0.47
1:B:1028:GLU:HA	1:B:1033:SER:O	2.14	0.47
1:B:1496:THR:HG23	1:B:1498:ILE:O	2.14	0.47
1:A:1488:ASP:OD2	1:A:1489:PRO:O	2.32	0.47
1:B:1240:SER:O	1:B:1245:LYS:HE3	2.14	0.47
1:B:1312:THR:CG2	1:B:1341:ALA:HB1	2.44	0.47
1:A:806:THR:HG22	1:A:873:TYR:CE2	2.50	0.47
1:B:1191:THR:HG21	7:B:1849:HOH:O	2.14	0.47
1:A:744:GLU:N	1:A:747:ARG:O	2.47	0.47
1:A:1240:SER:O	1:A:1245:LYS:HE3	2.15	0.47
1:A:836:LYS:HD2	1:A:866:THR:HG22	1.95	0.47
1:B:879:ARG:NH1	1:B:1329:LEU:HD23	2.30	0.47
1:B:1171:GLU:OE1	4:B:1701:SAH:H1'	2.15	0.47
1:B:1516:TYR:OH	7:B:1827:HOH:O	2.21	0.47
1:A:752:LYS:CD	1:A:759:MET:HE2	2.45	0.47
1:A:1248:ASN:CG	7:A:2026:HOH:O	2.57	0.47
1:A:1448:ARG:HG2	1:A:1454:ILE:HD11	1.96	0.47
1:B:1163:ILE:HD12	1:B:1222:MET:HE1	1.96	0.47
1:A:1418:LYS:HE3	1:A:1420:MET:HE3	1.96	0.47
1:B:745:GLU:CG	1:B:746:ASN:N	2.78	0.47
1:B:894:HIS:NE2	1:B:895:LYS:HG2	2.30	0.47
1:B:958:SER:N	1:B:959:PRO:HD3	2.28	0.47
1:A:767:SER:OG	1:A:777:LEU:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:GLN:HG2	7:A:1974:HOH:O	2.15	0.46
1:B:1500:TRP:O	1:B:1503:PRO:HD2	2.15	0.46
1:A:808:LEU:O	1:A:1284:LYS:HD2	2.15	0.46
1:A:873:TYR:CE2	1:A:875:GLN:HA	2.51	0.46
1:B:769:ILE:HA	1:B:770:PRO:HD3	1.74	0.46
1:B:1246:PHE:HD1	1:B:1246:PHE:O	1.98	0.46
1:A:806:THR:HG22	1:A:873:TYR:CD2	2.50	0.46
1:A:1024:PHE:CZ	1:A:1065:VAL:HG11	2.50	0.46
1:A:1369:THR:HG22	1:A:1372:ASP:CG	2.41	0.46
1:B:741:MET:SD	1:B:751:GLN:HB3	2.55	0.46
1:B:915:LEU:HD12	1:B:915:LEU:HA	1.74	0.46
1:A:736:TRP:CE2	1:A:787:GLU:HB2	2.51	0.46
1:A:751:GLN:HG2	1:A:752:LYS:CE	2.46	0.46
1:A:1237:ARG:NH2	2:C:6:5CM:H1'	2.31	0.46
1:B:1149:SER:C	4:B:1701:SAH:HB1	2.40	0.46
1:B:1246:PHE:C	1:B:1246:PHE:HD1	2.23	0.46
1:B:1540:ARG:NH1	7:B:1868:HOH:O	2.46	0.46
1:A:746:ASN:HA	1:A:789:LYS:HG2	1.97	0.46
1:A:771:ASP:OD2	1:A:771:ASP:N	2.48	0.46
1:A:1168:TRP:CE2	1:A:1215:PRO:HB3	2.50	0.46
1:A:1418:LYS:CB	1:A:1420:MET:HE3	2.46	0.46
1:A:1018:LYS:HE2	7:A:2173:HOH:O	2.15	0.46
1:A:1380:ILE:HD13	1:A:1415:HIS:O	2.15	0.46
1:B:972:LEU:HD23	1:B:973:TYR:CE2	2.51	0.46
1:B:1413:ARG:O	1:B:1553:ARG:HD2	2.15	0.46
1:A:1089:LEU:HD12	1:A:1089:LEU:HA	1.73	0.46
1:A:1167:LEU:HA	7:A:1844:HOH:O	2.16	0.46
1:A:1540:ARG:NH1	7:A:1869:HOH:O	2.36	0.46
1:B:1565:TYR:HB3	7:B:1891:HOH:O	2.15	0.46
1:A:907:ARG:HA	1:A:910:GLU:HG2	1.98	0.46
1:A:1446:GLN:HA	1:A:1455:ALA:O	2.15	0.46
1:A:1574:ARG:HG2	1:A:1574:ARG:H	1.62	0.46
1:B:1282:VAL:O	1:B:1286:THR:CG2	2.64	0.46
1:B:1395:PRO:HG3	1:B:1404:ARG:HD3	1.97	0.46
1:A:1566:ARG:HD3	7:A:1958:HOH:O	2.16	0.45
1:B:1466:LYS:HB2	1:B:1466:LYS:HE2	1.65	0.45
1:A:1236:ASN:O	2:C:7:DG:N2	2.49	0.45
1:B:782:VAL:HG22	1:B:795:PHE:HD1	1.81	0.45
1:B:1317:ILE:HB	1:B:1330:PHE:HE1	1.80	0.45
1:A:751:GLN:H	1:A:751:GLN:NE2	2.15	0.45
1:A:862:GLU:N	7:A:2123:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1488:ASP:O	1:B:1491:SER:HB2	2.16	0.45
1:B:1018:LYS:C	1:B:1019:LEU:HD12	2.42	0.45
1:A:1448:ARG:HG2	1:A:1454:ILE:CD1	2.47	0.45
1:B:1236:ASN:O	1:B:1239:ASN:ND2	2.44	0.45
1:B:1362:SER:O	7:B:2137:HOH:O	2.21	0.45
1:B:1532:PRO:HG3	1:B:1575:HIS:CE1	2.51	0.45
1:B:745:GLU:CD	1:B:745:GLU:N	2.75	0.45
1:B:1228:PRO:HG2	1:B:1250:LEU:HD12	1.99	0.45
1:B:840:LYS:HE2	1:B:868:PHE:CE2	2.52	0.45
2:E:1:DG:H8	2:E:1:DG:O5'	1.98	0.45
1:A:970:GLU:HG3	1:A:1471:SER:OG	2.17	0.45
1:B:1173:TRP:CZ3	1:B:1576:ARG:HG2	2.52	0.45
1:A:778:TYR:HB3	1:A:799:TRP:CZ3	2.52	0.45
1:A:943:VAL:HG22	1:A:1059:VAL:HG13	1.98	0.45
1:B:928:SER:OG	7:B:2085:HOH:O	2.20	0.45
1:A:752:LYS:HD3	1:A:759:MET:HE2	1.98	0.44
1:A:786:TRP:CE2	1:A:794:MET:HB2	2.53	0.44
1:A:1481:CYS:HA	1:A:1485:LYS:O	2.16	0.44
1:B:744:GLU:HG3	1:B:749:TYR:CE1	2.50	0.44
1:B:964:LYS:C	1:B:966:ASP:N	2.74	0.44
1:B:1064:THR:HG22	1:B:1078:TYR:OH	2.17	0.44
1:A:838:ILE:O	1:A:868:PHE:HA	2.18	0.44
1:A:1288:ARG:CZ	1:A:1292:ARG:HH22	2.31	0.44
1:A:1529:VAL:HG22	7:A:2110:HOH:O	2.17	0.44
1:B:981:SER:HB2	7:B:2006:HOH:O	2.18	0.44
1:A:914:VAL:HA	1:A:930:ILE:HG22	2.00	0.44
1:B:914:VAL:HG23	1:B:1017:ILE:HD11	1.98	0.44
1:B:1039:HIS:O	1:B:1401:ARG:NH2	2.50	0.44
1:B:1281:MET:O	1:B:1285:LEU:HG	2.16	0.44
1:A:969:ASN:OD1	1:A:969:ASN:C	2.60	0.44
1:A:1173:TRP:CH2	1:A:1576:ARG:HG2	2.52	0.44
1:B:745:GLU:HG2	1:B:746:ASN:H	1.83	0.44
1:B:747:ARG:HD3	1:B:749:TYR:OH	2.16	0.44
1:B:802:ALA:HA	1:B:817:LEU:HD23	2.00	0.44
1:B:969:ASN:C	1:B:969:ASN:OD1	2.60	0.44
1:B:1168:TRP:CE2	1:B:1215:PRO:HB3	2.53	0.44
1:A:1002:GLU:HG2	7:A:2023:HOH:O	2.17	0.44
1:A:1401:ARG:NH1	7:A:2133:HOH:O	2.28	0.44
1:A:1016:ASP:C	7:A:2173:HOH:O	2.61	0.44
1:A:1144:THR:O	1:A:1167:LEU:O	2.35	0.44
1:B:964:LYS:O	1:B:966:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1306:GLN:HB3	1:B:1333:PRO:HB3	2.00	0.44
1:B:1412:LEU:HD11	1:B:1553:ARG:HG2	1.98	0.44
1:B:1165:GLU:HA	7:B:1874:HOH:O	2.18	0.43
1:B:1431:ILE:HD13	1:B:1442:LEU:HD13	1.98	0.43
1:A:741:MET:HE2	1:A:750:TYR:C	2.43	0.43
1:A:746:ASN:C	1:A:789:LYS:HG2	2.42	0.43
1:A:894:HIS:CE1	1:A:895:LYS:HG2	2.54	0.43
1:B:734:ILE:HG23	1:B:755:ILE:HG12	2.00	0.43
1:B:1445:ILE:HA	1:B:1457:LYS:HE2	2.00	0.43
2:E:2:DA:H1'	2:E:3:DG:C8	2.53	0.43
1:B:755:ILE:O	1:B:758:GLU:HB2	2.17	0.43
1:B:1371:ARG:O	1:B:1375:SER:HB3	2.18	0.43
1:A:740:PRO:HB3	1:A:750:TYR:CE2	2.53	0.43
1:A:787:GLU:HG3	1:A:793:MET:HG2	2.01	0.43
1:A:814:PRO:HD3	1:B:776:PRO:CG	2.49	0.43
1:B:745:GLU:HG2	1:B:746:ASN:N	2.34	0.43
1:B:828:LEU:HD12	1:B:828:LEU:N	2.33	0.43
1:A:769:ILE:HD13	1:A:777:LEU:HD12	2.00	0.43
1:A:995:TYR:CE1	1:A:1362:SER:HB3	2.53	0.43
1:A:1148:PHE:O	4:A:1701:SAH:HG2	2.18	0.43
1:B:1543:HIS:CG	1:B:1544:PRO:HD2	2.53	0.43
3:F:24:DC:O2	3:F:24:DC:C2'	2.67	0.43
1:A:769:ILE:HA	1:A:770:PRO:HD3	1.80	0.43
1:A:780:ALA:HB2	1:A:799:TRP:CE3	2.53	0.43
1:A:943:VAL:CG2	1:A:1059:VAL:HG13	2.49	0.43
1:B:955:LYS:HD2	1:B:955:LYS:N	2.31	0.43
1:B:1386:ASN:HB3	1:B:1389:ILE:CG2	2.49	0.43
2:E:4:DG:H2''	2:E:5:DC:O5'	2.19	0.43
1:A:1287:LEU:O	1:A:1291:VAL:HG23	2.19	0.42
1:A:743:ILE:CG2	1:A:748:THR:HG22	2.46	0.42
1:A:789:LYS:HA	1:A:789:LYS:HD3	1.62	0.42
1:A:957:ALA:O	1:A:959:PRO:HD2	2.18	0.42
1:A:1035:ASN:HA	1:A:1038:TYR:CE1	2.54	0.42
1:B:813:ASP:OD1	1:B:813:ASP:C	2.62	0.42
2:E:2:DA:H4'	2:E:3:DG:OP1	2.18	0.42
1:B:1000:ILE:HA	1:B:1021:LEU:HD23	2.02	0.42
1:B:1312:THR:HG21	7:F:106:HOH:O	2.19	0.42
1:B:1414:ASP:OD1	7:B:2037:HOH:O	2.21	0.42
1:A:1230:GLN:OE1	1:A:1247:LYS:HE3	2.19	0.42
1:B:801:CYS:SG	1:B:805:ASP:HB2	2.60	0.42
1:B:838:ILE:HD11	1:B:866:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:PRO:HG3	1:A:1323:PRO:HB3	2.01	0.42
1:A:1410:PRO:HG2	1:A:1411:ILE:HG12	2.02	0.42
1:B:1184:ASN:ND2	7:B:2109:HOH:O	2.24	0.42
3:D:21:DC:OP2	7:D:104:HOH:O	2.22	0.42
1:A:814:PRO:HD3	1:B:776:PRO:HG3	2.02	0.42
1:A:887:GLN:HA	1:A:888:PRO:HD3	1.85	0.42
1:A:1085:ARG:NE	7:A:2031:HOH:O	2.40	0.42
1:A:1197:LEU:O	1:A:1201:VAL:HG13	2.19	0.42
1:A:1369:THR:CG2	1:A:1371:ARG:HB3	2.49	0.42
1:B:940:GLY:O	1:B:999:ARG:HD3	2.19	0.42
2:C:1:DG:N2	3:D:24:DC:N4	2.68	0.42
1:B:943:VAL:HG13	1:B:1059:VAL:HG13	2.02	0.41
1:B:1369:THR:HG23	1:B:1371:ARG:H	1.84	0.41
1:A:826:MET:HE3	1:A:826:MET:HB2	1.99	0.41
1:A:889:THR:H	1:A:892:ASN:HB2	1.85	0.41
1:A:1102:PRO:HA	1:A:1103:PRO:HD2	1.87	0.41
1:A:1569:GLY:O	1:A:1574:ARG:HD3	2.21	0.41
1:B:1150:GLY:CA	4:B:1701:SAH:HB1	2.50	0.41
1:A:808:LEU:HB3	1:A:812:SER:HB2	2.03	0.41
1:B:945:LEU:HD11	1:B:1054:VAL:HG11	2.02	0.41
1:A:1091:ALA:O	1:A:1099:PHE:HA	2.21	0.41
1:A:1389:ILE:O	1:A:1389:ILE:HG13	2.20	0.41
1:B:1145:LEU:HD13	1:B:1168:TRP:HB3	2.02	0.41
1:A:753:VAL:HG22	1:A:754:SER:N	2.35	0.41
1:A:911:MET:CG	1:A:913:LYS:HE3	2.50	0.41
1:A:1172:MET:HG3	4:A:1701:SAH:C2	2.50	0.41
1:A:1268:LEU:HD23	1:A:1268:LEU:C	2.45	0.41
1:A:751:GLN:CD	1:A:751:GLN:N	2.62	0.41
1:A:1172:MET:HB2	4:A:1701:SAH:C4	2.50	0.41
1:A:1194:CYS:O	1:A:1257:TYR:OH	2.37	0.41
1:B:983:TYR:CE2	3:F:15:DA:H3'	2.55	0.41
1:A:1021:LEU:O	1:A:1051:GLU:HA	2.21	0.41
1:A:1504:HIS:CE1	2:C:6:5CM:OP1	2.74	0.41
1:A:1504:HIS:HE1	2:C:6:5CM:OP1	2.04	0.41
1:B:737:LEU:HD21	1:B:754:SER:HB2	2.03	0.41
1:B:950:PHE:CD2	1:B:950:PHE:C	2.99	0.41
1:A:803:GLY:HA3	1:A:812:SER:OG	2.21	0.41
1:A:903:LEU:O	1:A:907:ARG:HG2	2.21	0.40
1:B:813:ASP:HA	1:B:814:PRO:HD2	1.92	0.40
1:B:870:GLN:N	7:B:1960:HOH:O	2.41	0.40
1:B:1089:LEU:HD12	1:B:1089:LEU:HA	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ARG:HG3	1:A:747:ARG:HH11	1.87	0.40
1:A:1231:GLY:C	7:A:2026:HOH:O	2.64	0.40
1:B:873:TYR:CE2	1:B:875:GLN:HA	2.56	0.40
1:B:1172:MET:HB2	4:B:1701:SAH:C4	2.51	0.40
1:A:1248:ASN:O	1:A:1251:VAL:HG13	2.22	0.40
1:A:837:VAL:HG22	1:A:867:TYR:HB2	2.02	0.40
1:A:1398:TRP:O	1:A:1402:GLN:HG2	2.22	0.40
1:B:741:MET:O	1:B:742:LYS:C	2.65	0.40
1:B:1228:PRO:HB3	1:B:1247:LYS:HD3	2.03	0.40
1:A:863:ASP:O	1:A:864:GLY:C	2.65	0.40
1:B:766:VAL:CG1	1:B:767:SER:N	2.83	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	828/873 (95%)	800 (97%)	27 (3%)	1 (0%)	48 70
1	B	826/873 (95%)	796 (96%)	30 (4%)	0	100 100
All	All	1654/1746 (95%)	1596 (96%)	57 (3%)	1 (0%)	48 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	959	PRO

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	701/759 (92%)	647 (92%)	54 (8%)	12	27
1	B	699/759 (92%)	647 (93%)	52 (7%)	13	29
All	All	1400/1518 (92%)	1294 (92%)	106 (8%)	12	27

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	751	GLN
1	A	760	LEU
1	A	766	VAL
1	A	771	ASP
1	A	808	LEU
1	A	866	THR
1	A	898	LEU
1	A	903	LEU
1	A	915	LEU
1	A	924	ARG
1	A	948	GLU
1	A	955	LYS
1	A	964	LYS
1	A	1002	GLU
1	A	1048	SER
1	A	1054	VAL
1	A	1089	LEU
1	A	1187	THR
1	A	1201	VAL
1	A	1202	MET
1	A	1210	LEU
1	A	1213	ARG
1	A	1214	LEU
1	A	1230	GLN
1	A	1246	PHE
1	A	1251	VAL
1	A	1270	ASN
1	A	1286	THR
1	A	1312	THR
1	A	1314	ARG
1	A	1346	VAL
1	A	1348	VAL
1	A	1361	SER

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Mol	Chain	Res	Type
1	A	1362	SER
1	A	1366	ARG
1	A	1369	THR
1	A	1374	MET
1	A	1386	ASN
1	A	1388	GLU
1	A	1392	ASN
1	A	1403	LEU
1	A	1406	SER
1	A	1442	LEU
1	A	1456	HIS
1	A	1459	GLN
1	A	1466	LYS
1	A	1475	LEU
1	A	1485	LYS
1	A	1538	GLN
1	A	1549	VAL
1	A	1572	LEU
1	A	1574	ARG
1	A	1576	ARG
1	A	1596	LEU
1	B	745	GLU
1	B	758	GLU
1	B	760	LEU
1	B	762	VAL
1	B	771	ASP
1	B	788	ASP
1	B	808	LEU
1	B	891	ASP
1	B	898	LEU
1	B	903	LEU
1	B	915	LEU
1	B	924	ARG
1	B	943	VAL
1	B	948	GLU
1	B	955	LYS
1	B	999	ARG
1	B	1035	ASN
1	B	1048	SER
1	B	1054	VAL
1	B	1076	GLN
1	B	1089	LEU

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Mol	Chain	Res	Type
1	B	1104	ASN
1	B	1172	MET
1	B	1187	THR
1	B	1192	GLU
1	B	1201	VAL
1	B	1214	LEU
1	B	1230	GLN
1	B	1251	VAL
1	B	1270	ASN
1	B	1273	ASN
1	B	1286	THR
1	B	1312	THR
1	B	1314	ARG
1	B	1340	ARG
1	B	1346	VAL
1	B	1348	VAL
1	B	1369	THR
1	B	1371	ARG
1	B	1374	MET
1	B	1386	ASN
1	B	1388	GLU
1	B	1403	LEU
1	B	1442	LEU
1	B	1466	LYS
1	B	1475	LEU
1	B	1485	LYS
1	B	1538	GLN
1	B	1572	LEU
1	B	1574	ARG
1	B	1596	LEU
1	B	1599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	751	GLN
1	A	790	ASN
1	A	908	GLN
1	A	1104	ASN
1	A	1446	GLN
1	A	1459	GLN
1	A	1467	ASN

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Mol	Chain	Res	Type
1	B	790	ASN
1	B	1004	HIS
1	B	1159	HIS
1	B	1386	ASN
1	B	1459	GLN
1	B	1580	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
3	C49	D	18	3	17,22,24	3.58	9 (52%)	17,33,38	1.74	5 (29%)
2	5CM	C	6	3,2	18,21,22	2.71	4 (22%)	24,30,33	1.64	2 (8%)
3	C49	F	18	3	17,22,24	3.49	8 (47%)	17,33,38	1.66	4 (23%)
2	5CM	E	6	3,2	18,21,22	3.02	8 (44%)	24,30,33	1.82	4 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C49	D	18	3	-	4/7/40/46	0/2/2/2
2	5CM	C	6	3,2	-	0/7/21/22	0/2/2/2
3	C49	F	18	3	-	4/7/40/46	0/2/2/2
2	5CM	E	6	3,2	-	2/7/21/22	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	18	C49	C2-N1	8.18	1.47	1.35
2	C	6	5CM	C5-C4	-7.93	1.38	1.44
3	F	18	C49	C2-N1	7.80	1.46	1.35
3	D	18	C49	C4-N4	7.32	1.43	1.27
3	F	18	C49	C4-N4	7.20	1.42	1.27
2	E	6	5CM	C5-C4	-6.93	1.38	1.44
2	C	6	5CM	C4-N4	5.47	1.48	1.34
2	E	6	5CM	C4-N4	5.36	1.47	1.34
3	D	18	C49	C2'-C3'	-4.88	1.40	1.52
3	F	18	C49	C2'-C3'	-4.85	1.40	1.52
2	E	6	5CM	C2'-C3'	-4.80	1.40	1.52
3	F	18	C49	F-C5	4.56	1.50	1.42
3	D	18	C49	F-C5	4.54	1.50	1.42
3	D	18	C49	C2-N3	4.12	1.45	1.38
3	F	18	C49	C2-N3	4.12	1.45	1.38
2	E	6	5CM	O5'-C5'	-3.98	1.32	1.44
2	E	6	5CM	C2-N1	-3.69	1.32	1.40
2	C	6	5CM	C6-C5	3.63	1.40	1.34
2	E	6	5CM	C6-C5	3.37	1.40	1.34
3	F	18	C49	O4'-C4'	-2.76	1.38	1.45
3	D	18	C49	O4'-C4'	-2.74	1.38	1.45
2	E	6	5CM	O4'-C4'	-2.55	1.39	1.45
3	F	18	C49	C4-N3	2.49	1.43	1.36
3	D	18	C49	C4-N3	2.47	1.43	1.36
3	D	18	C49	C6-N1	-2.34	1.44	1.46
2	C	6	5CM	O3'-C3'	-2.22	1.38	1.43
2	E	6	5CM	C3'-C4'	-2.19	1.47	1.53
3	F	18	C49	C6-N1	-2.15	1.44	1.46
3	D	18	C49	C6-C5	-2.09	1.49	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	5CM	O4'-C1'-N1	5.29	117.25	107.86
2	C	6	5CM	C5-C6-N1	-4.74	118.16	123.31
2	E	6	5CM	C5-C6-N1	-4.73	118.17	123.31
2	C	6	5CM	O3'-C3'-C4'	-4.48	93.09	110.07
3	F	18	C49	N3-C2-N1	3.67	120.34	116.65
3	D	18	C49	F-C5-CM5	-3.06	102.29	106.49
3	D	18	C49	N3-C2-N1	3.00	119.66	116.65
3	D	18	C49	CM5-C5-C4	-2.77	104.83	109.11
3	D	18	C49	C2'-C1'-N1	-2.73	112.34	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	18	C49	CM5-C5-C4	-2.59	105.10	109.11
3	F	18	C49	F-C5-CM5	-2.51	103.05	106.49
3	D	18	C49	O4'-C1'-N1	2.45	111.42	108.39
2	E	6	5CM	C5A-C5-C6	-2.17	119.92	122.85
2	E	6	5CM	C4'-O4'-C1'	-2.06	104.61	109.51
3	F	18	C49	O2-C2-N1	-2.05	120.63	123.10

There are no chirality outliers.

All (10) 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	E	6	5CM	O4'-C4'-C5'-O5'
3	F	18	C49	C2'-C1'-N1-C6
3	F	18	C49	C2'-C1'-N1-C2
3	D	18	C49	C2'-C1'-N1-C6
3	D	18	C49	O4'-C1'-N1-C2
3	D	18	C49	C2'-C1'-N1-C2
2	E	6	5CM	C3'-C4'-C5'-O5'
3	F	18	C49	O4'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	18	C49	3	0
2	C	6	5CM	3	0
3	F	18	C49	4	0
2	E	6	5CM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	-	27,28,28	1.14	4 (14%)	36,40,40	2.08	10 (27%)
6	CIT	B	1704	-	12,12,12	1.10	0	17,17,17	1.46	2 (11%)
4	SAH	B	1701	-	27,28,28	1.13	4 (14%)	36,40,40	1.92	9 (25%)

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	-	-	6/15/31/31	0/3/3/3
6	CIT	B	1704	-	-	4/16/16/16	-
4	SAH	B	1701	-	-	8/15/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1701	SAH	C2-N1	2.83	1.39	1.33
4	A	1701	SAH	C2-N3	2.83	1.39	1.33
4	B	1701	SAH	C2-N3	2.79	1.38	1.33
4	A	1701	SAH	C2-N1	2.77	1.38	1.33
4	B	1701	SAH	C8-N7	2.22	1.35	1.31
4	A	1701	SAH	C8-N7	2.21	1.35	1.31
4	A	1701	SAH	OXT-C	-2.11	1.23	1.30
4	B	1701	SAH	OXT-C	-2.09	1.24	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	SAH	N3-C2-N1	-5.39	120.42	128.58
4	B	1701	SAH	N3-C2-N1	-5.26	120.62	128.58
4	A	1701	SAH	C5-C4-N3	-4.73	120.20	126.72
4	B	1701	SAH	C5-C4-N3	-4.27	120.84	126.72
6	B	1704	CIT	O6-C6-C3	3.90	120.62	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	SAH	N9-C8-N7	-3.77	108.59	113.94
4	B	1701	SAH	N9-C8-N7	-3.69	108.70	113.94
4	A	1701	SAH	C5-N7-C8	3.46	108.89	103.45
4	A	1701	SAH	C2-N3-C4	3.41	120.17	111.83
4	B	1701	SAH	C5-N7-C8	3.29	108.63	103.45
4	A	1701	SAH	N3-C4-N9	3.17	132.56	127.17
4	B	1701	SAH	C2-N3-C4	3.15	119.53	111.83
4	A	1701	SAH	O4'-C1'-N9	3.10	114.04	108.09
4	B	1701	SAH	C5'-SD-CG	-2.95	93.52	102.26
4	B	1701	SAH	N3-C4-N9	2.76	131.87	127.17
4	A	1701	SAH	C5'-SD-CG	-2.69	94.28	102.26
4	A	1701	SAH	OXT-C-O	-2.43	118.56	124.08
4	B	1701	SAH	C4-C5-N7	-2.42	107.81	110.58
4	A	1701	SAH	C4-C5-N7	-2.32	107.94	110.58
4	B	1701	SAH	OXT-C-O	-2.22	119.04	124.08
6	B	1704	CIT	O4-C5-O3	-2.07	118.00	123.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

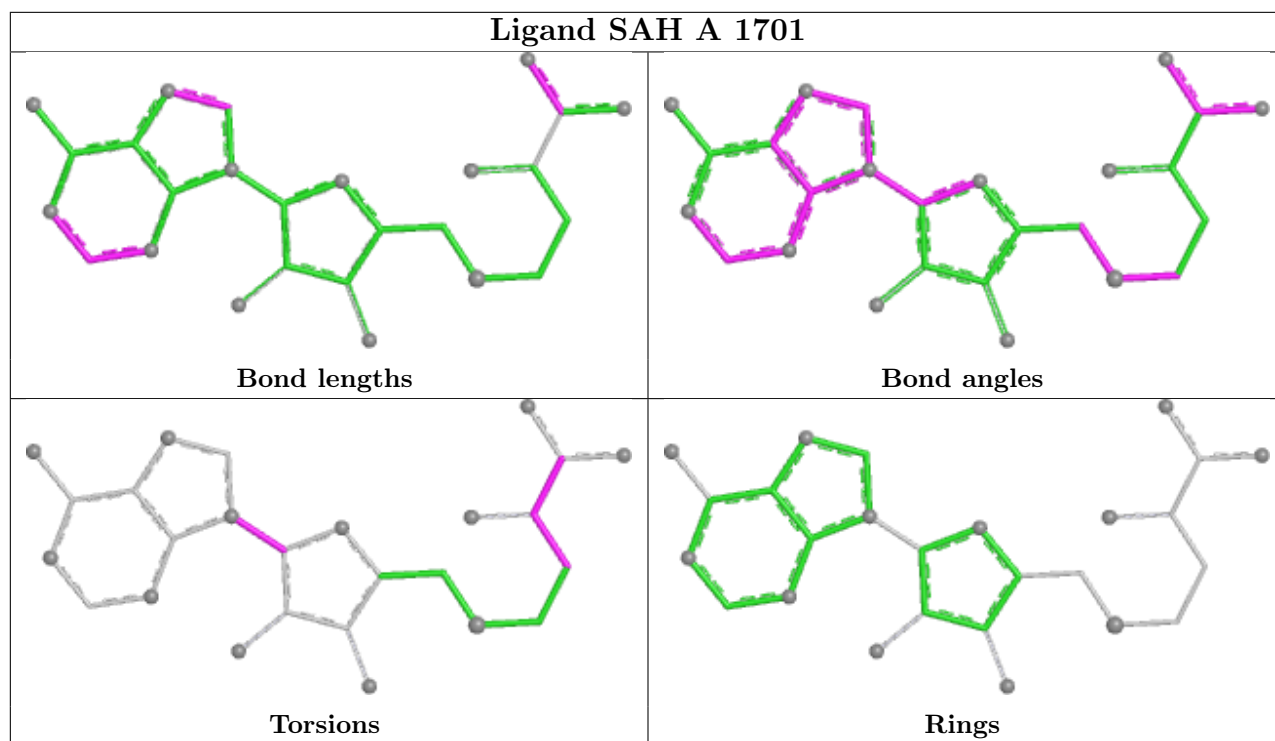
Mol	Chain	Res	Type	Atoms
4	B	1701	SAH	N-CA-CB-CG
4	B	1701	SAH	C2'-C1'-N9-C8
4	B	1701	SAH	C-CA-CB-CG
4	A	1701	SAH	C2'-C1'-N9-C8
4	A	1701	SAH	N-CA-CB-CG
4	A	1701	SAH	OXT-C-CA-CB
4	A	1701	SAH	O-C-CA-CB
4	B	1701	SAH	C2'-C1'-N9-C4
6	B	1704	CIT	C4-C3-C6-O5
6	B	1704	CIT	C4-C3-C6-O6
4	B	1701	SAH	CB-CG-SD-C5'
6	B	1704	CIT	C2-C3-C6-O5
6	B	1704	CIT	C2-C3-C6-O6
4	A	1701	SAH	O4'-C1'-N9-C8
4	B	1701	SAH	OXT-C-CA-CB
4	B	1701	SAH	O-C-CA-CB
4	B	1701	SAH	O4'-C1'-N9-C8
4	A	1701	SAH	C2'-C1'-N9-C4

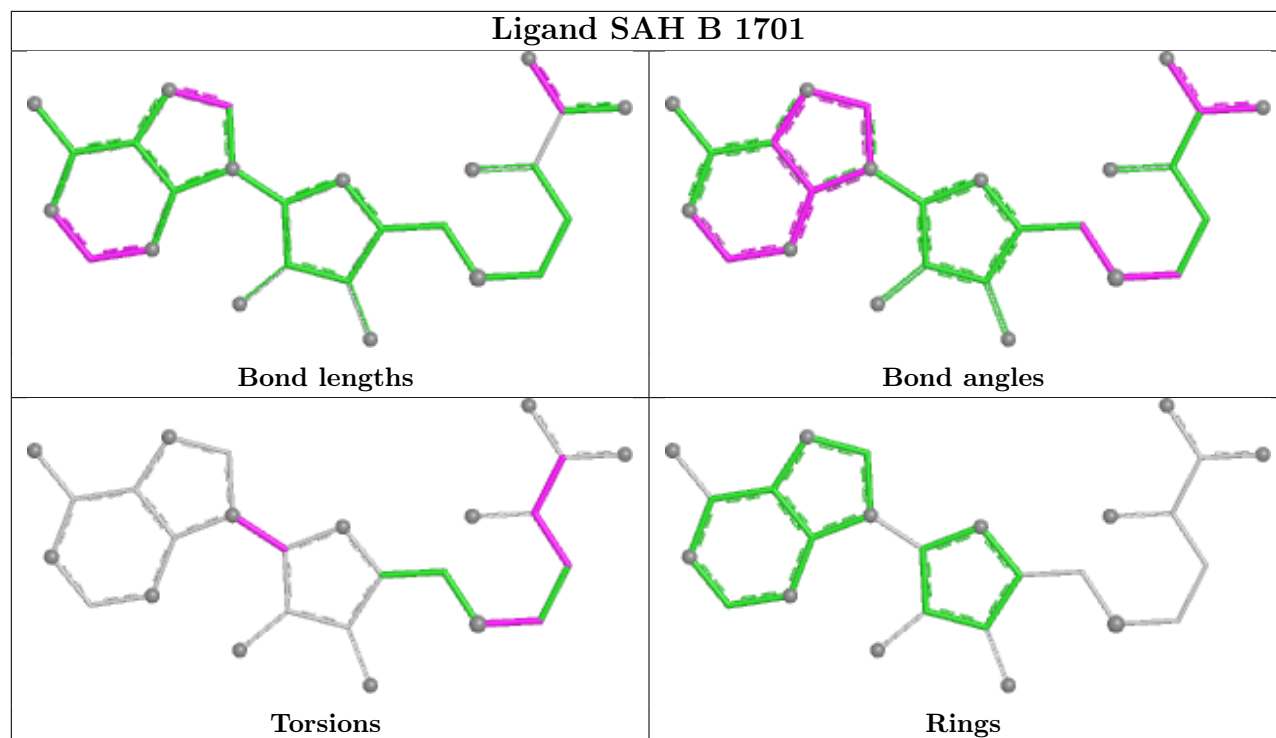
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1701	SAH	5	0
6	B	1704	CIT	1	0
4	B	1701	SAH	10	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	834/873 (95%)	-0.01	38 (4%) 37 32	16, 35, 87, 159	8 (0%)
1	B	832/873 (95%)	0.07	65 (7%) 19 15	16, 35, 99, 168	7 (0%)
2	C	11/12 (91%)	1.35	2 (18%) 3 3	33, 62, 98, 124	0
2	E	11/12 (91%)	1.45	4 (36%) 1 0	34, 67, 94, 112	0
3	D	11/12 (91%)	0.28	1 (9%) 15 11	32, 52, 83, 84	0
3	F	11/12 (91%)	0.62	2 (18%) 3 3	32, 53, 88, 91	0
All	All	1710/1794 (95%)	0.05	112 (6%) 25 19	16, 35, 94, 168	15 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1246	PHE	5.6
1	A	863	ASP	4.3
1	B	768	VAL	4.2
1	A	956	VAL	4.2
1	A	1137	ILE	4.0
1	B	959	PRO	4.0
1	B	1600	SER	3.9
1	B	866	THR	3.8
1	B	775	LYS	3.7
1	B	770	PRO	3.7
1	B	1246	PHE	3.6
2	C	8	DC	3.6
1	A	1243	TYR	3.6
1	A	960	VAL	3.6
1	B	1111	ASN	3.5
1	B	1451	ASP	3.5
1	B	743	ILE	3.5
1	B	742	LYS	3.5
1	B	732	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	966	ASP	3.5
1	A	957	ALA	3.5
2	E	8	DC	3.4
1	A	1451	ASP	3.4
1	B	957	ALA	3.3
1	B	831	ILE	3.3
1	B	1137	ILE	3.3
1	A	959	PRO	3.3
1	B	865	LYS	3.3
1	B	1453	VAL	3.1
1	B	748	THR	3.1
1	A	1450	GLY	3.1
1	B	835	VAL	3.1
1	B	960	VAL	3.1
1	A	963	PRO	3.1
1	B	963	PRO	3.1
1	B	1243	TYR	3.1
1	B	785	LEU	3.1
1	B	962	ARG	3.1
1	A	1600	SER	3.1
1	B	776	PRO	3.0
1	B	774	SER	3.0
1	B	769	ILE	3.0
1	B	836	LYS	3.0
1	B	964	LYS	3.0
3	F	24	DC	2.8
1	B	755	ILE	2.8
1	B	1245	LYS	2.8
1	B	757	GLU	2.8
1	B	777	LEU	2.7
1	A	866	THR	2.7
1	B	889	THR	2.7
1	B	961	LYS	2.7
1	A	864	GLY	2.7
1	A	743	ILE	2.6
1	A	770	PRO	2.6
1	A	1242	THR	2.6
1	A	785	LEU	2.6
1	B	795	PHE	2.6
1	B	793	MET	2.6
1	B	830	TYR	2.6
1	B	965	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1453	VAL	2.6
1	A	958	SER	2.6
1	A	1452	GLY	2.6
3	F	13	DG	2.6
1	B	1037	SER	2.5
1	A	955	LYS	2.5
1	B	753	VAL	2.5
1	B	783	THR	2.5
2	E	12	DC	2.5
1	B	956	VAL	2.5
1	A	961	LYS	2.5
1	B	738	GLY	2.5
1	A	773	SER	2.4
1	B	736	TRP	2.4
1	B	890	GLU	2.4
1	A	1138	LYS	2.3
1	B	765	CYS	2.3
1	B	773	SER	2.3
1	A	759	MET	2.3
1	B	750	TYR	2.3
3	D	24	DC	2.2
1	B	1454	ILE	2.2
1	B	967	PRO	2.2
1	A	1037	SER	2.2
1	B	788	ASP	2.2
1	B	1452	GLY	2.2
1	A	964	LYS	2.2
1	A	769	ILE	2.2
1	A	733	ARG	2.2
1	B	864	GLY	2.2
2	E	11	DG	2.1
1	B	1138	LYS	2.1
1	A	742	LYS	2.1
1	B	838	ILE	2.1
1	B	958	SER	2.1
1	B	1361	SER	2.1
1	A	778	TYR	2.1
1	B	735	SER	2.1
1	B	744	GLU	2.1
2	E	9	DC	2.1
1	A	760	LEU	2.1
1	A	1111	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	772	ASP	2.0
1	A	862	GLU	2.0
1	B	833	SER	2.0
1	A	777	LEU	2.0
1	B	737	LEU	2.0
1	A	1340	ARG	2.0
1	A	865	LYS	2.0
1	B	786	TRP	2.0
2	C	7	DG	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(Å ²)	Q<0.9
2	5CM	E	6	20/21	0.96	0.08	22,32,36,45	0
3	C49	D	18	21/23	0.97	0.07	24,28,31,34	0
2	5CM	C	6	20/21	0.97	0.07	23,30,39,40	0
3	C49	F	18	21/23	0.97	0.06	23,27,29,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

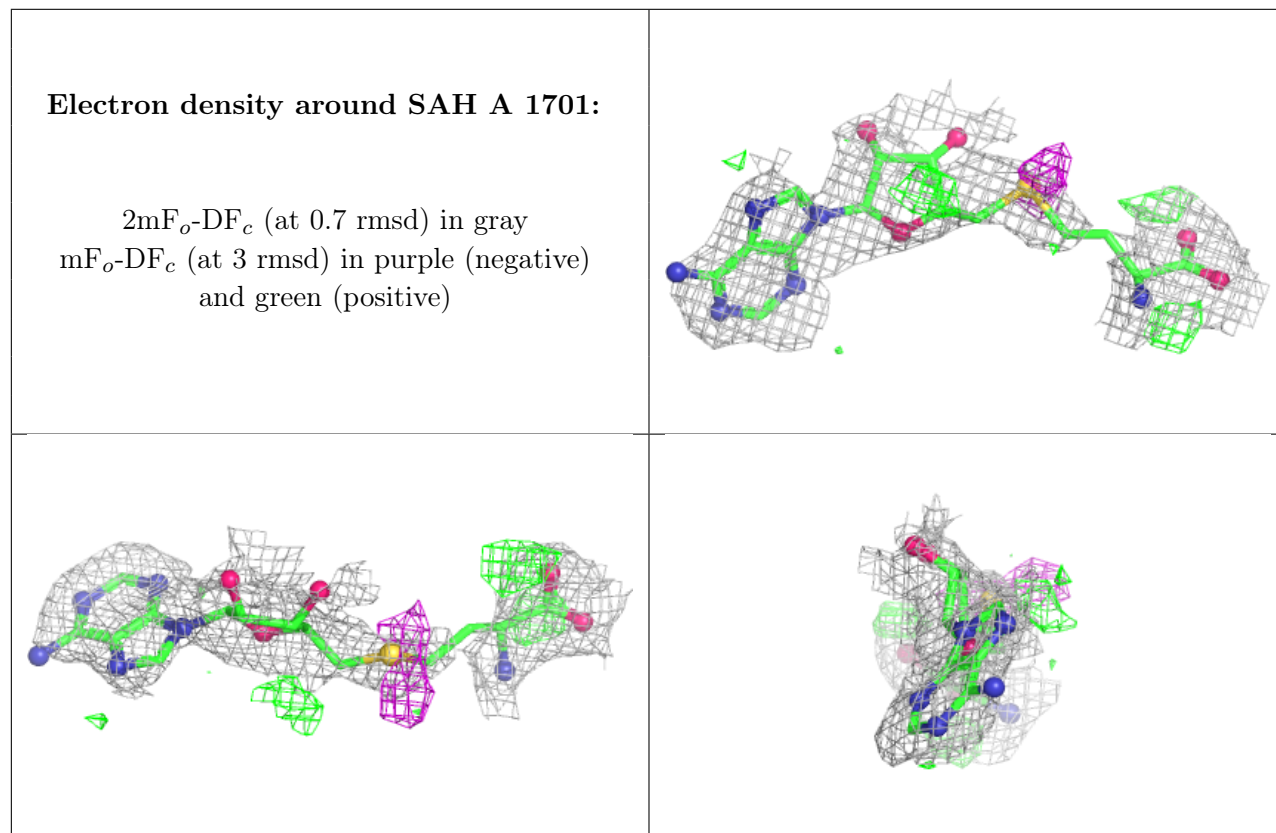
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CIT	B	1704	13/13	0.76	0.16	36,39,48,49	0
4	SAH	A	1701	26/26	0.81	0.18	18,36,41,42	26
4	SAH	B	1701	26/26	0.85	0.17	20,35,41,42	26
5	ZN	A	1703	1/1	0.99	0.02	43,43,43,43	0
5	ZN	B	1702	1/1	0.99	0.02	36,36,36,36	0

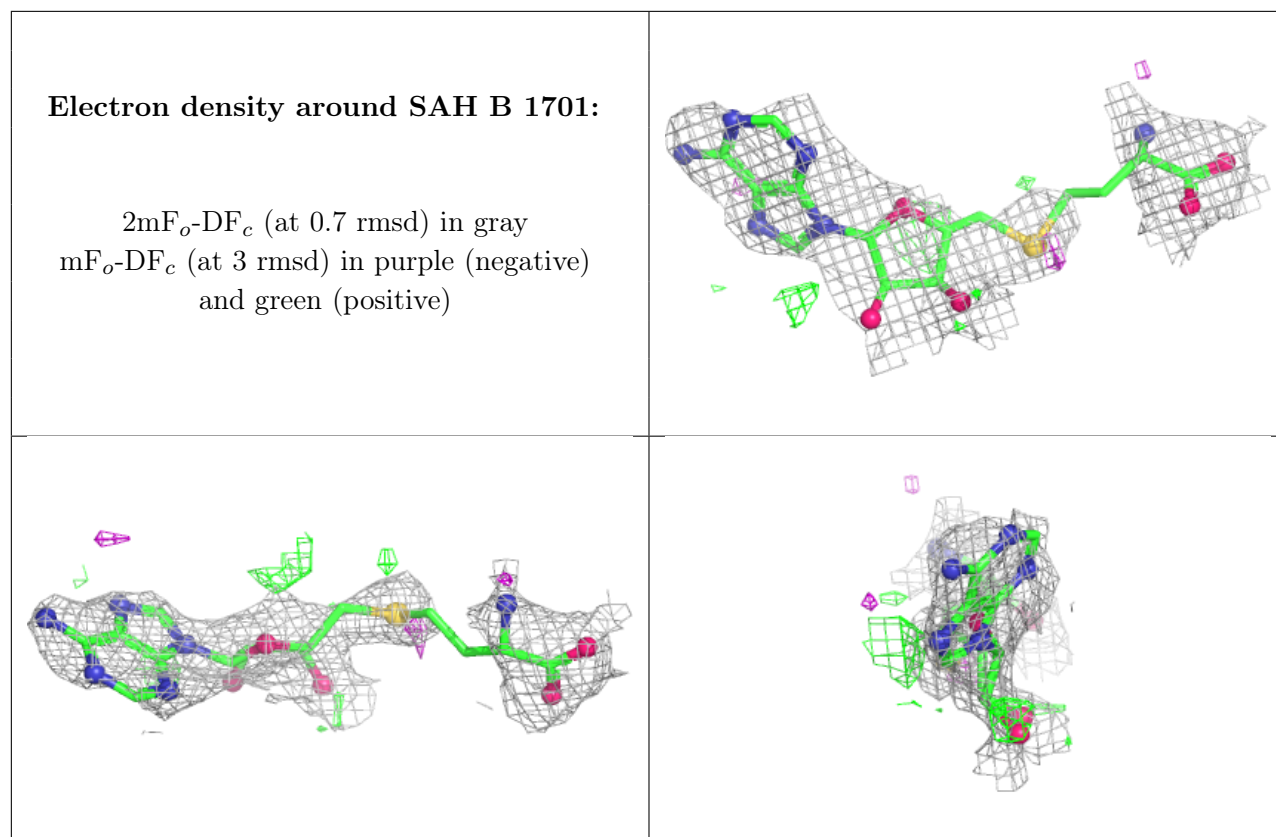
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	B	1703	1/1	0.99	0.03	48,48,48,48	0
5	ZN	A	1702	1/1	0.99	0.01	30,30,30,30	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.