



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:01 am GMT

PDB ID : 4DA4
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

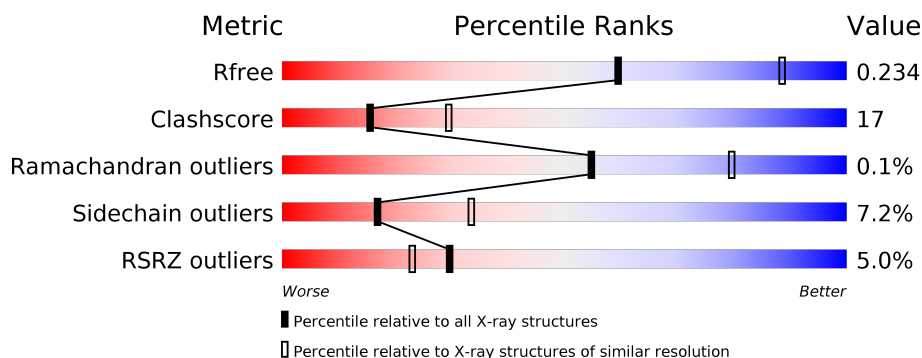
1 Overall quality at a glance

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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>3%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>• •</div> </div> </div>
1	B	873	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• 5%</div> </div> </div>
2	C	12	<div> <div>8%</div> <div> <div></div> <div>42%</div> <div>50%</div> <div>8%</div> </div> </div>
2	E	12	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>25%</div> </div> </div>
3	D	12	<div> <div>8%</div> <div> <div></div> <div>58%</div> <div>33%</div> <div>8%</div> </div> </div>
3	F	12	<div> <div>17%</div> <div> <div></div> <div>42%</div> <div>58%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SAH	A	1701	-	-	-	X
4	SAH	B	1701	-	-	X	X

2 Entry composition

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
1	A	834	Total	C	N	O	S	0	0	0
			6585	4179	1158	1207	41			
1	B	832	Total	C	N	O	S	0	0	0
			6567	4170	1150	1206	41			

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

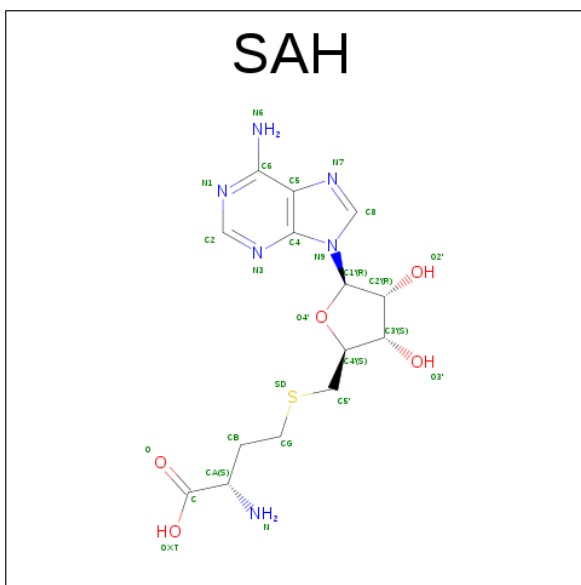
- Molecule 2 is a DNA chain called DNA_UPPER_STRAND.

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

- Molecule 3 is a DNA chain called DNA_LOWER_STRAND.

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

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).

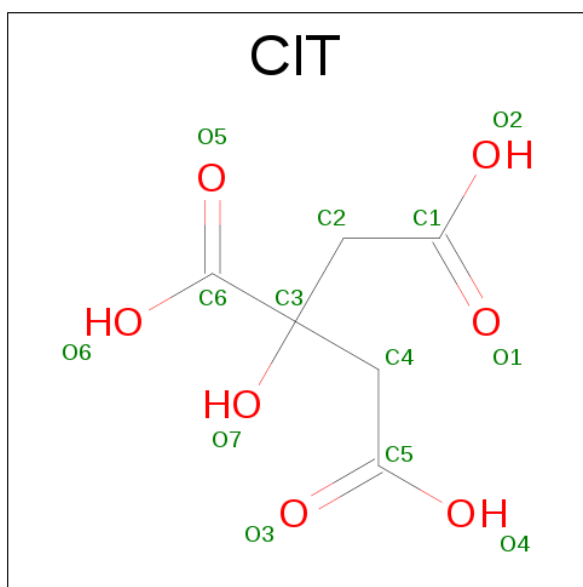


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
4	B	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

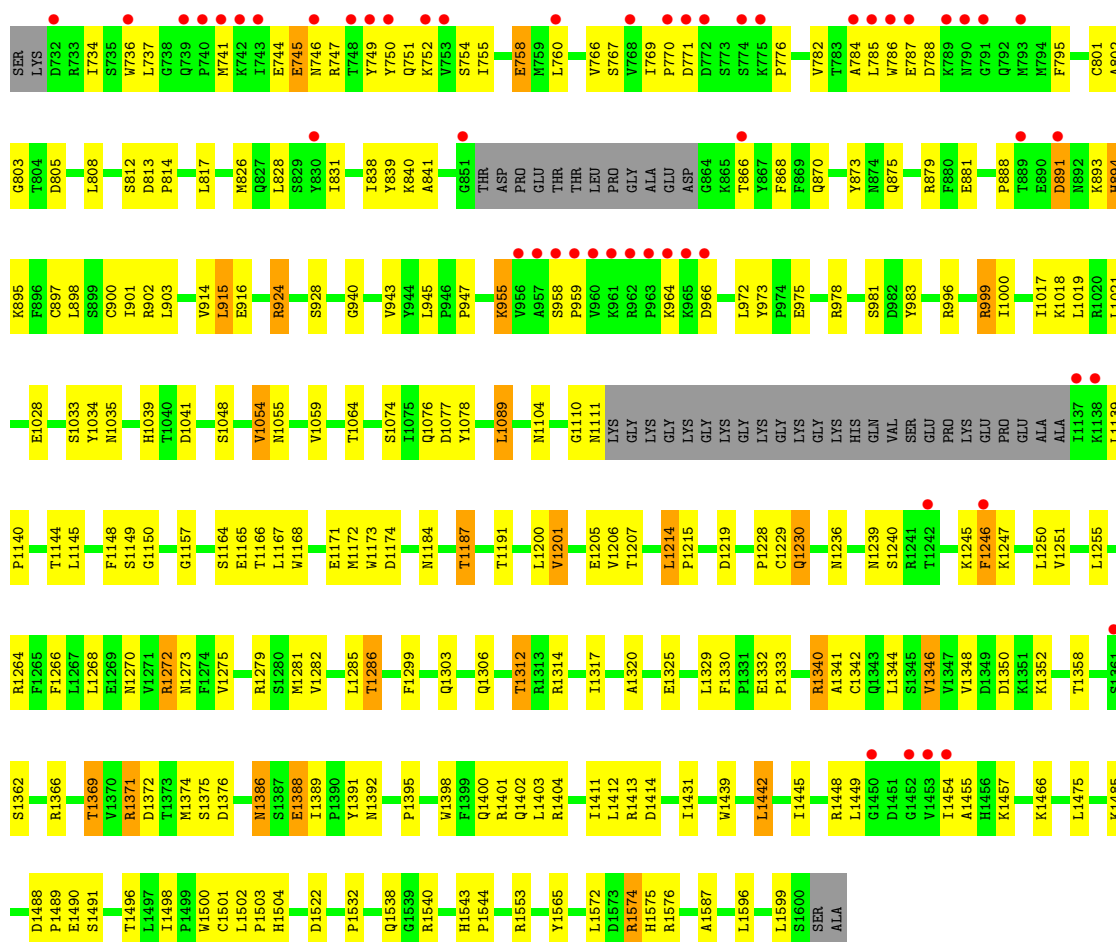
- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $\text{C}_6\text{H}_8\text{O}_7$).



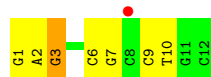
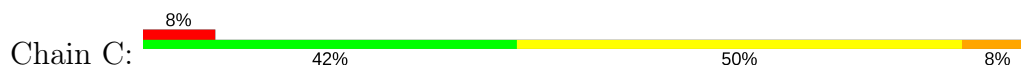
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is water.

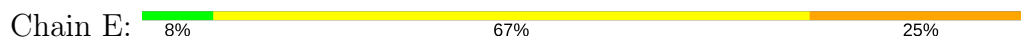
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	417	Total	O	0	0
			417	417		
7	B	388	Total	O	0	0
			388	388		
7	C	11	Total	O	0	0
			11	11		
7	D	18	Total	O	0	0
			18	18		
7	E	10	Total	O	0	0
			10	10		
7	F	16	Total	O	0	0
			16	16		



• Molecule 2: DNA_UPPER_STRAND



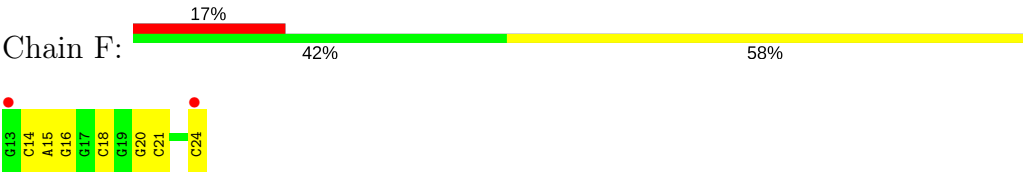
• Molecule 2: DNA_UPPER_STRAND



• 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 48.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.47-2.60) 94.0 (48.47-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.196 , 0.246 0.183 , 0.234	Depositor DCC
R_{free} test set	3883 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, CIT

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	0.33	0/6760	0.55	0/9172
1	B	0.32	0/6742	0.55	0/9151
2	C	0.64	0/250	1.20	1/382 (0.3%)
2	E	0.63	0/250	1.30	6/382 (1.6%)
3	D	0.60	0/250	1.24	1/382 (0.3%)
3	F	0.77	0/250	1.31	1/382 (0.3%)
All	All	0.36	0/14502	0.63	9/19851 (0.0%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	DC	O4'-C4'-C3'	-10.90	99.46	106.00
3	D	14	DC	O4'-C1'-N1	7.29	113.10	108.00
2	E	5	DC	O4'-C1'-N1	6.79	112.75	108.00
3	F	14	DC	O4'-C1'-N1	6.75	112.73	108.00
2	E	10	DT	N3-C4-O4	6.11	123.57	119.90
2	E	10	DT	C5-C4-O4	-5.92	120.76	124.90
2	E	5	DC	C1'-O4'-C4'	-5.89	104.21	110.10
2	C	3	DG	C1'-O4'-C4'	-5.71	104.39	110.10
2	E	4	DG	O4'-C1'-N9	-5.52	104.13	108.00

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

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	225	0
1	B	6567	0	6293	200	0
2	C	244	0	137	12	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	41	0
7	B	388	0	0	37	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	452	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 (452) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NH1	1:B:924:ARG:HG3	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: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:A:751:GLN:H	1:A:751:GLN:CD	1.90	0.74
1:B:924:ARG:HH11	1:B:924:ARG:CG	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1247:LYS:NZ	7:B:2153:HOH:O	2.23	0.70
1:A:924:ARG:NH1	7:A:2048:HOH:O	2.22	0.70
1:A:924:ARG:NH1	1:A:924:ARG:HG3	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:N	1:B:891:ASP:OD1	2.26	0.69
1:A:924:ARG:CG	1:A:924:ARG:HH11	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:HD2	1:B:955:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1229:CYS:SG	3:D:18:C49:N1	2.70	0.64
3:F:16:DG:H5'	3:F:16:DG:H8	1.62	0.64
2:C:1:DG:HO5'	2:C:1:DG:H8	1.46	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
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: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:1272:ARG:O	1:A:1275:VAL:HG22	2.00	0.62
1:A:864:GLY:O	1:A:865:LYS:HB3	1.99	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:1332:GLU:OE2	1:B:1358:THR:N	2.32	0.61
1:B:943:VAL:HG12	1:B:945:LEU:HD22	1.81	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:C8	3:F:16:DG:H5'	2.36	0.61
1:A:1259:ASP:O	1:A:1262:ARG:HG2	2.00	0.60
1:B:1369:THR:CG2	1:B:1372:ASP:H	2.14	0.60
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.83	0.60
1:A:881:GLU:OE2	7:A:2101:HOH:O	2.16	0.60
1:A:955:LYS:HD2	1:A:955:LYS:H	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:ASP:OD2	7:A:2138:HOH:O	2.16	0.58
1:A:1248:ASN:OD1	7:A:2026:HOH:O	2.16	0.58
1:A:1041:ASP:OD1	1:A:1401:ARG:NH1	2.36	0.58
1:A:1418:LYS:HE3	1:A:1420:MET:CE	2.34	0.58
1:A:1067:TYR:CE2	1:A:1102:PRO:HG3	2.38	0.58
1:A:1418:LYS:HE3	1:A:1420:MET:HE1	1.86	0.58
1:A:1246:PHE:HD1	1:A:1246:PHE:C	2.06	0.58
1:A:1262:ARG:O	7:A:2135:HOH:O	2.17	0.58
1:A:1418:LYS:HB2	1:A:1420:MET:HE3	1.86	0.57
1:B:1033:SER:OG	1:B:1034:TYR:N	2.36	0.57
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: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: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: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:A:1246:PHE:C	1:A:1246:PHE:CD1	2.79	0.56
1:B:1574:ARG:NH1	6:B:1704:CIT:O3	2.37	0.56
1:A:864:GLY:HA3	1:B:866:THR:HG22	1.86	0.56
1:A:1171:GLU:O	1:A:1191:THR:HA	2.04	0.56
1:B:1340:ARG:HD2	1:B:1340:ARG:H	1.70	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:957:ALA:C	1:A:959:PRO:HD2	2.26	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:B:1489:PRO:O	1:B:1490:GLU:CB	2.55	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:A:736:TRP:CZ2	1:A:787:GLU:HB2	2.42	0.55
2:C:9:DC:H2'	2:C:10:DT:C6	2.41	0.55
1:A:1248:ASN:ND2	7:A:2026:HOH:O	2.38	0.55
1:A:784:ALA:O	1:A:795:PHE:HA	2.07	0.55
4:B:1701:SAH:HG1	7:B:2009:HOH:O	2.05	0.55
1:B:894:HIS:CD2	1:B:895:LYS:H	2.25	0.55
2:C:2:DA:H4'	2:C:3:DG:OP1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:795:PHE:CE2	1:B:826:MET:HB3	2.43	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:981:SER:O	1:A:982:ASP:HB2	2.07	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: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: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:B:840:LYS:NZ	7:B:2158:HOH:O	2.32	0.53
1:A:1502:LEU:HB2	1:A:1503:PRO:HD3	1.89	0.53
1:A:779:LEU:HD22	1:A:835:VAL:HG21	1.91	0.53
1:B:1299:PHE:HE1	1:B:1346:VAL:HG11	1.74	0.53
1:A:1249:SER:HA	7:A:2087:HOH:O	2.08	0.53
1:A:734:ILE:HA	1:A:754:SER:O	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:ILE:N	1:B:734:ILE:HD12	2.24	0.52
1:B:745:GLU:CD	1:B:745:GLU:H	2.12	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
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:1342:CYS:O	1:B:1344:LEU:HG	2.10	0.51
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: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:1144:THR:OG1	1:B:1164:SER:HB2	2.10	0.51
1:B:734:ILE:HG13	1:B:755:ILE:HG23	1.93	0.51
3:F:21:DC:OP2	7:F:110:HOH:O	2.18	0.51
1:B:1110:GLY:O	7:B:1961:HOH:O	2.19	0.50
1:B:744:GLU:CG	1:B:749:TYR:HE1	2.23	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:CE	1:B:955:LYS:H	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: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:749:TYR:HA	1:A:786:TRP:HA	1.95	0.49
1:A:1373:THR:HG23	1:A:1557:ARG:HB3	1.94	0.49
1:A:1173:TRP:CZ3	1:A:1576:ARG:HG2	2.48	0.49
1:A:766:VAL:CG1	1:A:831:ILE:HG23	2.42	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:1371:ARG:NH2	1:A:1522:ASP:OD1	2.44	0.49
1:A:747:ARG:HG2	1:A:786:TRP:CD1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:VAL:HG12	1:A:1207:THR:CG2	2.38	0.48
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:736:TRP:CZ2	1:A:793:MET:HG2	2.48	0.48
1:A:850:GLY:C	7:A:1967:HOH:O	2.52	0.48
1:A:924:ARG:HG3	7:A:2048:HOH:O	2.13	0.48
1:A:1595:LYS:NZ	7:A:2017:HOH:O	2.33	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: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:A:760:LEU:HD23	1:A:761:GLU:H	1.77	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:A:744:GLU:HG3	1:A:749:TYR:HE1	1.79	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:B:894:HIS:CD2	1:B:895:LYS:HG2	2.48	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:1240:SER:O	1:A:1245:LYS:HE3	2.15	0.47
1:A:744:GLU:N	1:A:747:ARG:O	2.47	0.47
1:A:1259:ASP:HB2	1:A:1293:MET:HE1	1.96	0.47
1:A:836:LYS:HD2	1:A:866:THR:HG22	1.95	0.47
1:B:1171:GLU:OE1	4:B:1701:SAH:H1'	2.15	0.47
1:B:879:ARG:NH1	1:B:1329:LEU:HD23	2.30	0.47
1:A:1448:ARG:HG2	1:A:1454:ILE:HD11	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:1230:GLN:HG2	7:A:1974:HOH:O	2.15	0.46
1:A:767:SER:OG	1:A:777:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1246:PHE:O	1:B:1246:PHE:HD1	1.98	0.46
1:B:769:ILE:HA	1:B:770:PRO:HD3	1.74	0.46
1:A:1024:PHE:CZ	1:A:1065:VAL:HG11	2.50	0.46
1:A:806:THR:HG22	1:A:873:TYR:CD2	2.50	0.46
1:B:1246:PHE:CD1	1:B:1246:PHE:C	2.87	0.46
1:B:741:MET:SD	1:B:751:GLN:HB3	2.55	0.46
1:B:915:LEU:HA	1:B:915:LEU:HD12	1.74	0.46
1:A:751:GLN:HG2	1:A:752:LYS:CE	2.46	0.46
1:A:736:TRP:CE2	1:A:787:GLU:HB2	2.51	0.46
1:A:957:ALA:C	1:A:959:PRO:CD	2.84	0.46
1:B:1540:ARG:NH1	7:B:1868:HOH:O	2.46	0.46
1:A:1237:ARG:NH2	2:C:6:5CM:H1'	2.31	0.46
1:A:1168:TRP:CE2	1:A:1215:PRO:HB3	2.50	0.46
1:A:771:ASP:OD2	1:A:771:ASP:N	2.48	0.46
1:A:746:ASN:HA	1:A:789:LYS:HG2	1.97	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:1413:ARG:O	1:B:1553:ARG:HD2	2.15	0.46
1:B:972:LEU:HD23	1:B:973:TYR:CE2	2.51	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:1418:LYS:CB	1:A:1420:MET:HE3	2.46	0.46
1:A:1446:GLN:HA	1:A:1455:ALA:O	2.15	0.46
1:A:1574:ARG:H	1:A:1574:ARG:HG2	1.62	0.46
1:A:907:ARG:HA	1:A:910:GLU:HG2	1.98	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:B:745:GLU:CD	1:B:746:ASN:H	2.19	0.45
1:A:1236:ASN:O	2:C:7:DG:N2	2.49	0.45
1:B:1317:ILE:HB	1:B:1330:PHE:HE1	1.80	0.45
1:B:782:VAL:HG22	1:B:795:PHE:HD1	1.81	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
1:B:1488:ASP:O	1:B:1491:SER:HB2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1532:PRO:HG3	1:B:1575:HIS:CE1	2.51	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: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:1064:THR:HG22	1:B:1078:TYR:OH	2.17	0.44
1:B:744:GLU:HG3	1:B:749:TYR:CE1	2.50	0.44
1:A:1288:ARG:CZ	1:A:1292:ARG:HH22	2.31	0.44
1:A:838:ILE:O	1:A:868:PHE:HA	2.18	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:1173:TRP:CH2	1:A:1576:ARG:HG2	2.52	0.44
1:B:1168:TRP:CE2	1:B:1215:PRO:HB3	2.53	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: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:1144:THR:O	1:A:1167:LEU:O	2.35	0.44
1:B:1268:LEU:HD23	1:B:1268:LEU:C	2.39	0.44
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:964:LYS:O	1:B:966:ASP:N	2.51	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:894:HIS:CE1	1:A:895:LYS:HG2	2.54	0.43
1:B:1445:ILE:HA	1:B:1457:LYS:HE2	2.00	0.43
1:B:734:ILE:HG23	1:B:755:ILE:HG12	2.00	0.43
2:E:2:DA:H1'	2:E:3:DG:C8	2.53	0.43
1:B:1371:ARG:O	1:B:1375:SER:HB3	2.18	0.43
1:B:755:ILE:O	1:B:758:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:828:LEU:HD12	2.33	0.43
1:A:1148:PHE:O	4:A:1701:SAH:HG2	2.18	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: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:1267:LEU:C	1:A:1267:LEU:HD23	2.39	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:1386:ASN:HB3	1:B:1389:ILE:CG2	2.49	0.43
1:B:955:LYS:N	1:B:955:LYS:HD2	2.31	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:1035:ASN:HA	1:A:1038:TYR:CE1	2.54	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:B:1149:SER:C	4:B:1701:SAH:HB1	2.40	0.42
2:E:2:DA:H4'	2:E:3:DG:OP1	2.18	0.42
1:A:1248:ASN:CG	7:A:2026:HOH:O	2.57	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:A:748:THR:HG23	1:A:789:LYS:HZ3	1.84	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
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: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:A:887:GLN:HA	1:A:888:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1369:THR:HG23	1:B:1371:ARG:H	1.84	0.41
1:B:943:VAL:HG13	1:B:1059:VAL:HG13	2.02	0.41
1:A:1102:PRO:HA	1:A:1103:PRO:HD2	1.87	0.41
1:A:889:THR:H	1:A:892:ASN:HB2	1.85	0.41
1:A:1369:THR:HG22	1:A:1372:ASP:CG	2.41	0.41
1:B:1246:PHE:C	1:B:1246:PHE:HD1	2.23	0.41
1:A:1569:GLY:O	1:A:1574:ARG:HD3	2.21	0.41
1:B:1074:SER:OG	1:B:1077:ASP:OD1	2.32	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:1172:MET:HG3	4:A:1701:SAH:C2	2.50	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:HB2	4:A:1701:SAH:C4	2.50	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:766:VAL:CG1	1:B:767:SER:N	2.83	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:A:969:ASN:OD1	1:A:969:ASN:C	2.60	0.40
1:B:1018:LYS:C	1:B:1019:LEU:HD12	2.42	0.40
1:B:1089:LEU:HA	1:B:1089:LEU:HD12	1.70	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:A:747:ARG:HG3	1:A:747:ARG:HH11	1.87	0.40
1:B:1172:MET:HB2	4:B:1701:SAH:C4	2.51	0.40
1:B:873:TYR:CE2	1:B:875:GLN:HA	2.56	0.40
1:A:1248:ASN:O	1:A:1251:VAL:HG13	2.22	0.40
1:A:1398:TRP:O	1:A:1402:GLN:HG2	2.22	0.40
1:A:837:VAL:HG22	1:A:867:TYR:HB2	2.02	0.40
1:B:1228:PRO:HB3	1:B:1247:LYS:HD3	2.03	0.40
1:B:745:GLU:CD	1:B:745:GLU:N	2.75	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%)	55	79
1	B	826/873 (95%)	796 (96%)	30 (4%)	0	100	100
All	All	1654/1746 (95%)	1596 (96%)	57 (3%)	1 (0%)	55	79

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%)	649 (93%)	52 (7%)	16	32
1	B	699/759 (92%)	650 (93%)	49 (7%)	18	35
All	All	1400/1518 (92%)	1299 (93%)	101 (7%)	17	33

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	751	GLN
1	A	758	GLU

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Mol	Chain	Res	Type
1	A	759	MET
1	A	760	LEU
1	A	770	PRO
1	A	771	ASP
1	A	788	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	1089	LEU
1	A	1168	TRP
1	A	1187	THR
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	1272	ARG
1	A	1286	THR
1	A	1314	ARG
1	A	1348	VAL
1	A	1361	SER
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	1448	ARG
1	A	1456	HIS

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Mol	Chain	Res	Type
1	A	1459	GLN
1	A	1466	LYS
1	A	1475	LEU
1	A	1485	LYS
1	A	1538	GLN
1	A	1572	LEU
1	A	1574	ARG
1	A	1596	LEU
1	B	745	GLU
1	B	758	GLU
1	B	760	LEU
1	B	771	ASP
1	B	788	ASP
1	B	808	LEU
1	B	891	ASP
1	B	894	HIS
1	B	898	LEU
1	B	903	LEU
1	B	915	LEU
1	B	924	ARG
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
1	B	1104	ASN
1	B	1187	THR
1	B	1201	VAL
1	B	1214	LEU
1	B	1230	GLN
1	B	1246	PHE
1	B	1251	VAL
1	B	1270	ASN
1	B	1272	ARG
1	B	1273	ASN
1	B	1286	THR
1	B	1312	THR
1	B	1314	ARG
1	B	1340	ARG
1	B	1346	VAL

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Mol	Chain	Res	Type
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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1463	HIS

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	C	6	3,2	14,21,22	2.21	6 (42%)	18,30,33	1.79	2 (11%)
3	C49	D	18	3	15,22,24	3.39	8 (53%)	17,33,38	2.48	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5CM	E	6	3,2	14,21,22	3.25	6 (42%)	18,30,33	1.99	3 (16%)
3	C49	F	18	3	15,22,24	3.31	8 (53%)	17,33,38	3.02	3 (17%)

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

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	5CM	O5'-C5'	-8.68	1.32	1.44
3	D	18	C49	C2'-C3'	-4.67	1.40	1.52
3	F	18	C49	C2'-C3'	-4.65	1.40	1.52
2	E	6	5CM	C2'-C3'	-4.60	1.40	1.52
2	C	6	5CM	O5'-C5'	-3.48	1.39	1.44
3	D	18	C49	O5'-C5'	-3.29	1.40	1.44
3	F	18	C49	O5'-C5'	-3.27	1.40	1.44
3	F	18	C49	O4'-C4'	-2.72	1.38	1.45
3	D	18	C49	O4'-C4'	-2.70	1.38	1.45
2	C	6	5CM	C2-N3	-2.68	1.32	1.38
2	E	6	5CM	O4'-C4'	-2.51	1.39	1.45
3	D	18	C49	C6-N1	-2.22	1.44	1.46
2	C	6	5CM	O3'-C3'	-2.13	1.38	1.43
2	C	6	5CM	C5-C4	-2.09	1.38	1.41
2	E	6	5CM	C3'-C4'	-2.09	1.47	1.53
3	F	18	C49	C6-N1	-2.04	1.44	1.46
3	D	18	C49	C4-N3	2.06	1.43	1.36
3	F	18	C49	C4-N3	2.08	1.43	1.36
2	C	6	5CM	C5A-C5	2.16	1.55	1.51
2	E	6	5CM	C5A-C5	2.24	1.55	1.51
3	F	18	C49	C2-N3	3.96	1.45	1.38
3	D	18	C49	C2-N3	3.97	1.45	1.38
2	E	6	5CM	C4-N4	5.21	1.47	1.34
2	C	6	5CM	C4-N4	5.32	1.48	1.34
3	F	18	C49	C4-N4	6.28	1.42	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	18	C49	C4-N4	6.39	1.43	1.27
3	F	18	C49	C2-N1	7.32	1.46	1.35
3	D	18	C49	C2-N1	7.68	1.47	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	O3'-C3'-C4'	-4.31	93.09	110.13
2	C	6	5CM	C5-C6-N1	-3.68	118.16	122.15
2	E	6	5CM	C5-C6-N1	-3.67	118.17	122.15
3	D	18	C49	C2'-C1'-N1	-2.67	112.34	115.61
3	F	18	C49	C1'-N1-C2	-2.29	114.69	117.89
3	D	18	C49	O4'-C1'-N1	2.36	111.42	108.41
3	D	18	C49	N3-C2-N1	2.94	119.66	116.73
2	E	6	5CM	O5'-C5'-C4'	3.22	120.33	109.01
3	F	18	C49	N3-C2-N1	3.62	120.34	116.73
2	E	6	5CM	O4'-C1'-N1	5.62	117.25	107.78
3	D	18	C49	F-C5-C6	8.45	115.20	107.02
3	F	18	C49	F-C5-C6	11.00	117.67	107.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	20,28,28	1.21	2 (10%)	20,40,40	2.45	2 (10%)
4	SAH	B	1701	-	20,28,28	1.20	2 (10%)	20,40,40	2.41	2 (10%)
6	CIT	B	1704	-	3,12,12	1.21	0	3,17,17	1.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAH	A	1701	-	-	0/7/31/31	0/3/3/3
4	SAH	B	1701	-	-	0/7/31/31	0/3/3/3
6	CIT	B	1704	-	-	0/6/16/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1701	SAH	C2-N1	2.64	1.38	1.33
4	B	1701	SAH	C2-N1	2.70	1.39	1.33
4	B	1701	SAH	C2-N3	4.03	1.38	1.32
4	A	1701	SAH	C2-N3	4.07	1.39	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	SAH	N3-C2-N1	-9.69	120.42	128.86
4	B	1701	SAH	N3-C2-N1	-9.46	120.62	128.86
4	B	1701	SAH	C5'-SD-CG	-2.90	93.52	102.29
4	A	1701	SAH	C5'-SD-CG	-2.64	94.28	102.29

There are no chirality outliers.

There are no torsion outliers.

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
4	B	1701	SAH	10	0
6	B	1704	CIT	1	0

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%)	-0.13	28 (3%)	46	38	16, 35, 87, 159	8 (0%)
1	B	832/873 (95%)	0.05	53 (6%)	20	15	16, 35, 99, 168	7 (0%)
2	C	11/12 (91%)	0.32	1 (9%)	10	6	33, 62, 98, 124	0
2	E	11/12 (91%)	0.09	0	100	100	34, 67, 94, 112	0
3	D	11/12 (91%)	0.03	1 (9%)	10	6	32, 52, 83, 84	0
3	F	11/12 (91%)	0.41	2 (18%)	1	1	32, 53, 88, 91	0
All	All	1710/1794 (95%)	-0.03	85 (4%)	30	23	16, 35, 94, 168	15 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	959	PRO	12.0
1	B	960	VAL	10.1
1	B	963	PRO	7.7
1	A	959	PRO	7.2
1	A	960	VAL	6.7
1	B	732	ASP	5.9
1	B	961	LYS	5.7
1	A	962	ARG	5.5
1	B	958	SER	5.4
1	B	956	VAL	5.0
1	A	1242	THR	4.8
1	A	961	LYS	4.6
1	A	863	ASP	4.1
1	B	770	PRO	4.0
1	A	1452	GLY	3.9
3	F	24	DC	3.9
1	A	958	SER	3.9
1	B	739	GLN	3.8
1	B	786	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	772	ASP	3.6
1	A	1451	ASP	3.6
1	A	732	ASP	3.5
3	D	24	DC	3.5
1	B	830	TYR	3.4
1	B	768	VAL	3.4
1	A	1137	ILE	3.3
1	B	789	LYS	3.2
1	A	957	ALA	3.2
1	A	741	MET	3.1
1	B	741	MET	3.1
1	B	957	ALA	3.1
1	A	956	VAL	3.1
1	B	866	THR	3.0
1	A	862	GLU	3.0
1	B	791	GLY	3.0
1	B	1137	ILE	2.9
1	A	889	THR	2.9
1	B	1242	THR	2.8
1	B	790	ASN	2.8
1	B	785	LEU	2.8
1	A	1096	THR	2.8
1	B	740	PRO	2.8
1	A	963	PRO	2.7
1	B	962	ARG	2.7
1	A	1600	SER	2.7
1	B	964	LYS	2.7
1	B	889	THR	2.6
2	C	8	DC	2.6
1	B	746	ASN	2.6
1	B	743	ILE	2.6
1	B	774	SER	2.6
1	B	1450	GLY	2.6
1	B	742	LYS	2.5
1	A	964	LYS	2.5
1	B	752	LYS	2.5
1	B	965	LYS	2.5
1	B	784	ALA	2.5
1	A	1246	PHE	2.5
1	B	750	TYR	2.5
1	B	736	TRP	2.5
1	B	749	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1246	PHE	2.5
1	B	771	ASP	2.4
1	B	1452	GLY	2.4
1	A	751	GLN	2.4
3	F	13	DG	2.3
1	B	787	GLU	2.3
1	B	793	MET	2.2
1	B	1361	SER	2.2
1	A	866	THR	2.2
1	B	748	THR	2.2
1	B	1453	VAL	2.2
1	A	785	LEU	2.2
1	A	756	ASP	2.2
1	A	1243	TYR	2.2
1	A	888	PRO	2.2
1	B	760	LEU	2.2
1	B	775	LYS	2.1
1	B	891	ASP	2.1
1	B	753	VAL	2.1
1	B	851	GLY	2.1
1	A	739	GLN	2.1
1	B	1454	ILE	2.1
1	B	966	ASP	2.1
1	B	1138	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	5CM	C	6	20/21	0.97	0.14	-	23,30,39,40	0
2	5CM	E	6	20/21	0.97	0.13	-	22,32,36,45	0
3	C49	D	18	21/23	0.98	0.14	-	24,28,31,34	0
3	C49	F	18	21/23	0.98	0.14	-	23,27,29,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	SAH	B	1701	26/26	0.82	0.30	3.33	20,35,41,42	26
4	SAH	A	1701	26/26	0.82	0.28	2.26	18,36,41,42	26
6	CIT	B	1704	13/13	0.87	0.24	0.45	36,39,48,49	0
5	ZN	A	1703	1/1	0.98	0.07	-2.80	43,43,43,43	0
5	ZN	B	1703	1/1	0.97	0.08	-	48,48,48,48	0
5	ZN	B	1702	1/1	0.99	0.09	-	36,36,36,36	0
5	ZN	A	1702	1/1	1.00	0.10	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.