



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:17 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 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/ValidationPDFNotes.html>

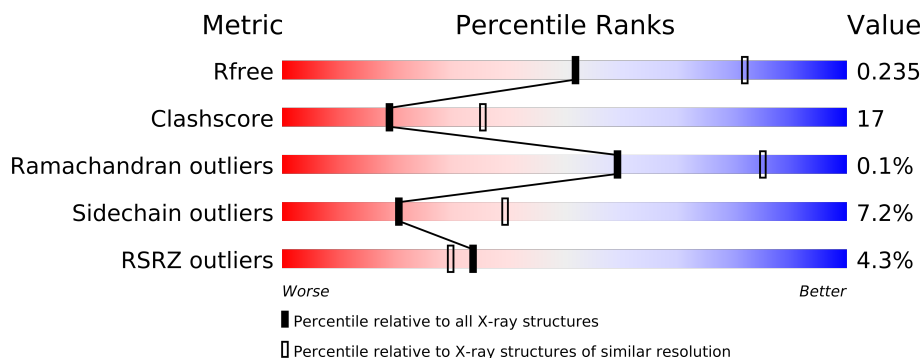
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	873	
1	B	873	
2	C	12	
2	E	12	
3	D	12	
3	F	12	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15059 atoms, of which 0 are hydrogen and 0 are deuterium.

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)-methyltransferase1.

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

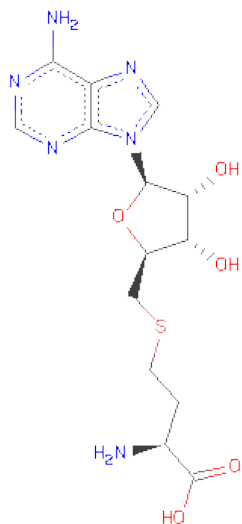
- Molecule 2 is a DNA chain called DNA_UPPER_STRAND.

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
			245	116	1	47	70	11		
3	F	12	Total	C	F	N	O	P	0	0
			245	116	1	47	70	11		

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

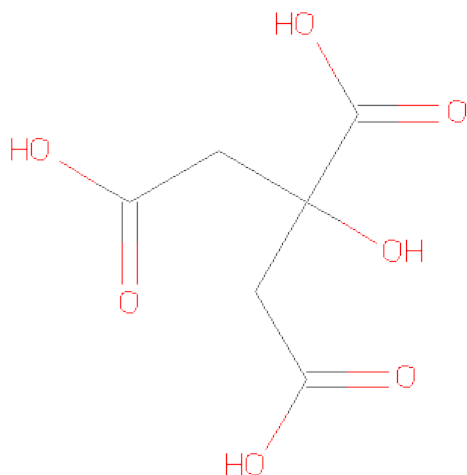


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

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

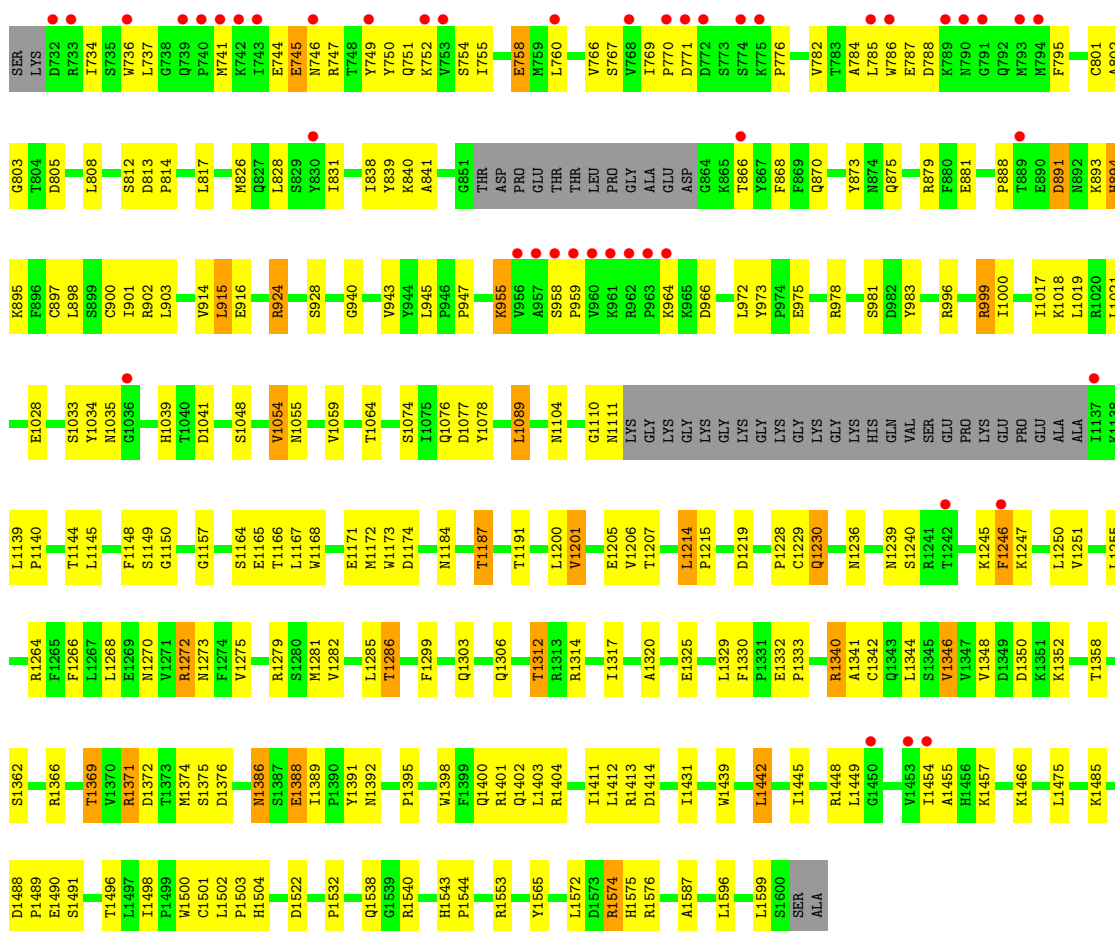
- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



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		



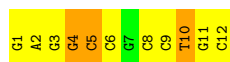
- Molecule 2: DNA_UPPER_STRAND

Chain C:



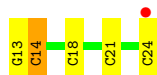
- Molecule 2: DNA_UPPER_STRAND

Chain E:



- Molecule 3: DNA_LOWER_STRAND

Chain D:



- Molecule 3: DNA_LOWER_STRAND

Chain F:



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 0.189 , 0.235	Depositor DCC
R_{free} test set	3741 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77098 reflections	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.

5 Model quality i

5.1 Standard geometry i

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
3	D	1	0
3	F	1	0
All	All	2	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	18	C49	C1'
3	F	18	C49	C1'

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	10	0	0	5	0
7	F	16	0	0	3	0
All	All	15059	0	13201	452	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (452) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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
2:E:1:DG:H1'	7:E:109:HOH:O	1.77	0.84
1:B:900:CYS:SG	7:B:1999:HOH:O	2.36	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:B:1392:ASN:N	7:B:1955:HOH:O	2.13	0.78
1:A:1184:ASN:HB3	1:A:1187:THR:CG2	2.13	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:1168:TRP:N	7:B:2138:HOH:O	2.05	0.72
2:C:1:DG:H1'	7:C:111:HOH:O	1.89	0.72
1:B:1439:TRP:HA	1:B:1442:LEU:HD22	1.71	0.72
1:B:1352:LYS:O	7:B:1835:HOH:O	2.06	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:B:736:TRP:CZ2	1:B:787:GLU:HB2	2.24	0.71
1:A:1039:HIS:O	1:A:1401:ARG:NH2	2.23	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:1489:PRO:O	1:A:1490:GLU:HB2	1.89	0.71
1:A:1264:ARG:HD2	1:A:1325:GLU:OE1	1.91	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:B:1553:ARG:NH2	7:B:1891:HOH:O	2.21	0.68
1:A:732:ASP:N	1:A:756:ASP:OD1	2.25	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
2:C:1:DG:HO5'	2:C:1:DG:H8	1.46	0.64
1:A:1369:THR:CG2	1:A:1372:ASP:H	2.11	0.64
1:A:1279:ARG:NH1	1:B:1350:ASP:HB2	2.12	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:1376:ASP:HB3	1:B:1400:GLN:OE1	1.98	0.62
1:B:1041:ASP:OD1	1:B:1401:ARG:NH1	2.33	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: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
3:F:16:DG:C8	3:F:16:DG:H5'	2.36	0.61
1:A:1350:ASP:HB2	1:B:1279:ARG:NH1	2.15	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:B:1501:CYS:CB	2:E:5:DC:H3'	2.31	0.60
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.83	0.60
1:A:955:LYS:HD2	1:A:955:LYS:H	1.67	0.60
1:A:881:GLU:OE2	7:A:2101:HOH:O	2.16	0.60
1:A:1028:GLU:HA	1:A:1033:SER:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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: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:1262:ARG:O	7:A:2135:HOH:O	2.17	0.58
1:A:1246:PHE:HD1	1:A:1246:PHE:C	2.06	0.58
1:A:1418:LYS:HB2	1:A:1420:MET:HE3	1.86	0.57
1:B:1167:LEU:HA	7:B:2138:HOH:O	2.04	0.57
1:B:1033:SER:OG	1:B:1034:TYR:N	2.36	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:B:1167:LEU:CA	7:B:2138:HOH:O	2.53	0.57
1:A:1193:ASP:OD2	1:A:1195:ASN:HB2	2.05	0.57
1:A:998:GLY:HA3	1:A:1021:LEU:HD13	1.87	0.57
1:A:943:VAL:HG13	1:A:945:LEU:CD2	2.34	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:864:GLY:HA3	1:B:866:THR:HG22	1.86	0.56
1:A:1246:PHE:CD1	1:A:1246:PHE:C	2.79	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: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:957:ALA:C	1:A:959:PRO:HD2	2.26	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:B:1489:PRO:O	1:B:1490:GLU:CB	2.55	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
1:A:1332:GLU:OE2	1:A:1358:THR:N	2.38	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:C:2:DA:H4'	2:C:3:DG:OP1	2.07	0.55
1:B:894:HIS:CD2	1:B:895:LYS:H	2.25	0.55
1:B:744:GLU:HG3	1:B:749:TYR:HE1	1.70	0.55
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.87	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:B:1184:ASN:HB3	1:B:1187:THR:HG23	1.89	0.54
1:A:1342:CYS:O	1:A:1344:LEU:HG	2.08	0.54
1:A:1282:VAL:O	1:A:1286:THR:HG23	2.08	0.54
2:E:10:DT:H2'	2:E:11:DG:C8	2.42	0.54
1:B:1398:TRP:O	1:B:1402:GLN:HG2	2.08	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: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:B:1139:LEU:HD22	1:B:1140:PRO:HD2	1.88	0.54
1:B:1255:LEU:HD11	1:B:1286:THR:HB	1.90	0.53
1:A:1201:VAL:HG12	1:A:1214:LEU:HG	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:981:SER:O	1:A:982:ASP:HB2	2.07	0.53
1:A:1366:ARG:NE	7:A:1897:HOH:O	1.99	0.53
1:B:749:TYR:CE2	1:B:786:TRP:HB3	2.43	0.53
1:A:1570:ASN:O	1:A:1574:ARG:HG2	2.09	0.53
1:B:1171:GLU:O	1:B:1191:THR:HA	2.08	0.53
1:A:1350:ASP:HB2	1:B:1279:ARG:HH11	1.73	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: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: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:1299:PHE:HE1	1:B:1346:VAL:HG11	1.74	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:1501:CYS:O	1:B:1504:HIS:HB3	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:1193:ASP:HB3	1:A:1196:VAL:HG23	1.91	0.52
1:B:745:GLU:CD	1:B:745:GLU:H	2.12	0.52
1:B:734:ILE:HD12	1:B:734:ILE:N	2.24	0.52
1:B:1388:GLU:HG2	1:B:1411:ILE:HG21	1.91	0.52
1:B:1157:GLY:HA3	1:B:1587:ALA:HB3	1.91	0.52
1:B:943:VAL:HG12	1:B:945:LEU:CD2	2.39	0.52
1:A:796:HIS:ND1	1:A:825:ASN:OD1	2.43	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:784:ALA:O	1:B:795:PHE:HA	2.10	0.51
1:B:1342:CYS:O	1:B:1344:LEU:HG	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: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
2:E:8:DC:H4'	2:E:9:DC:OP2	2.12	0.50
1:B:897:CYS:O	1:B:901:ILE:HG13	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: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:B:1401:ARG:NE	7:B:1990:HOH:O	2.04	0.49
1:A:1173:TRP:CZ3	1:A:1576:ARG:HG2	2.48	0.49
1:B:1502:LEU:HB2	1:B:1503:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:1206:VAL:HG12	1:A:1207:THR:CG2	2.38	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:1159:HIS:HB2	7:A:1945:HOH:O	2.11	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:1595:LYS:NZ	7:A:2017:HOH:O	2.33	0.48
1:A:1501:CYS:O	7:A:1813:HOH:O	2.20	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:1162:GLY:HA2	7:A:1912:HOH:O	2.13	0.48
1:B:1369:THR:HG23	1:B:1371:ARG:N	2.29	0.48
1:A:1386:ASN:HB3	1:A:1389:ILE:CG2	2.44	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:894:HIS:CD2	1:B:895:LYS:HG2	2.48	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:1312:THR:CG2	1:B:1341:ALA:HB1	2.44	0.47
1:B:1240:SER:O	1:B:1245:LYS:HE3	2.14	0.47
1:B:1191:THR:HG21	7:B:1849:HOH:O	2.14	0.47
1:A:806:THR:HG22	1:A:873:TYR:CE2	2.50	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:B:1171:GLU:OE1	4:B:1701:SAH:H1'	2.15	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: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:894:HIS:NE2	1:B:895:LYS:HG2	2.30	0.47
1:B:745:GLU:CG	1:B:746:ASN:N	2.78	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
1:B:1500:TRP:O	1:B:1503:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1230:GLN:HG2	7:A:1974:HOH:O	2.15	0.46
1:A:873:TYR:CE2	1:A:875:GLN:HA	2.51	0.46
1:A:808:LEU:O	1:A:1284:LYS:HD2	2.15	0.46
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:B:741:MET:SD	1:B:751:GLN:HB3	2.55	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:915:LEU:HA	1:B:915:LEU:HD12	1.74	0.46
1:A:1024:PHE:CZ	1:A:1065:VAL:HG11	2.50	0.46
1:A:751:GLN:HG2	1:A:752:LYS:CE	2.46	0.46
1:A:957:ALA:C	1:A:959:PRO:CD	2.84	0.46
1:A:736:TRP:CE2	1:A:787:GLU:HB2	2.51	0.46
1:A:1237:ARG:NH2	2:C:6:5CM:H1'	2.31	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: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:B:1413:ARG:O	1:B:1553:ARG:HD2	2.15	0.46
1:A:1380:ILE:HD13	1:A:1415:HIS:O	2.15	0.46
1:A:1018:LYS:HE2	7:A:2173:HOH:O	2.15	0.46
1:B:972:LEU:HD23	1:B:973:TYR:CE2	2.51	0.46
1:A:1167:LEU:HA	7:A:1844:HOH:O	2.16	0.46
1:A:1089:LEU:HD12	1:A:1089:LEU:HA	1.73	0.46
1:B:1565:TYR:HB3	7:B:1891:HOH:O	2.15	0.46
1:A:1540:ARG:NH1	7:A:1869:HOH:O	2.36	0.46
1:B:1282:VAL:O	1:B:1286:THR:CG2	2.64	0.46
1:A:1418:LYS:CB	1:A:1420:MET:HE3	2.46	0.46
1:A:1574:ARG:HG2	1:A:1574:ARG:H	1.62	0.46
1:A:1446:GLN:HA	1:A:1455:ALA:O	2.15	0.46
1:A:907:ARG:HA	1:A:910:GLU:HG2	1.98	0.46
1:B:1395:PRO:HG3	1:B:1404:ARG:HD3	1.97	0.46
1:B:745:GLU:CD	1:B:746:ASN:H	2.19	0.45
1:A:1566:ARG:HD3	7:A:1958:HOH:O	2.16	0.45
1:B:1466:LYS:HE2	1:B:1466:LYS:HB2	1.65	0.45
1:B:782:VAL:HG22	1:B:795:PHE:HD1	1.81	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: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:B:1236:ASN:O	1:B:1239:ASN:ND2	2.44	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1448:ARG:HG2	1:A:1454:ILE:CD1	2.47	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:1228:PRO:HG2	1:B:1250:LEU:HD12	1.99	0.45
2:E:1:DG:H8	2:E:1:DG:O5'	1.98	0.45
1:B:840:LYS:HE2	1:B:868:PHE:CE2	2.52	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:B:928:SER:OG	7:B:2085:HOH:O	2.20	0.45
1:A:943:VAL:HG22	1:A:1059:VAL:HG13	1.98	0.45
1:A:786:TRP:CE2	1:A:794:MET:HB2	2.53	0.44
1:B:744:GLU:HG3	1:B:749:TYR:CE1	2.50	0.44
1:B:1064:THR:HG22	1:B:1078:TYR:OH	2.17	0.44
1:A:1481:CYS:HA	1:A:1485:LYS:O	2.16	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:B:981:SER:HB2	7:B:2006:HOH:O	2.18	0.44
1:A:1529:VAL:HG22	7:A:2110:HOH:O	2.17	0.44
1:B:1039:HIS:O	1:B:1401:ARG:NH2	2.50	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:1281:MET:O	1:B:1285:LEU:HG	2.16	0.44
1:B:747:ARG:HD3	1:B:749:TYR:OH	2.16	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:A:1173:TRP:CH2	1:A:1576:ARG:HG2	2.52	0.44
1:B:802:ALA:HA	1:B:817:LEU:HD23	2.00	0.44
1:A:1401:ARG:NH1	7:A:2133:HOH:O	2.28	0.44
1:A:1002:GLU:HG2	7:A:2023:HOH:O	2.17	0.44
1:B:1412:LEU:HD11	1:B:1553:ARG:HG2	1.98	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: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
2:E:2:DA:H1'	2:E:3:DG:C8	2.53	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
1:A:894:HIS:CE1	1:A:895:LYS:HG2	2.54	0.43
1:B:1371:ARG:O	1:B:1375:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:755:ILE:O	1:B:758:GLU:HB2	2.17	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: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:814:PRO:HD3	1:B:776:PRO:CG	2.49	0.43
1:A:769:ILE:HD13	1:A:777:LEU:HD12	2.00	0.43
1:A:1148:PHE:O	4:A:1701:SAH:HG2	2.18	0.43
1:A:995:TYR:CE1	1:A:1362:SER:HB3	2.53	0.43
3:F:24:DC:O2	3:F:24:DC:C2'	2.67	0.43
1:B:1543:HIS:CG	1:B:1544:PRO:HD2	2.53	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
2:E:4:DG:H2''	2:E:5:DC:O5'	2.19	0.43
1:B:955:LYS:N	1:B:955:LYS:HD2	2.31	0.43
1:B:1386:ASN:HB3	1:B:1389:ILE:CG2	2.49	0.43
1:A:1287:LEU:O	1:A:1291:VAL:HG23	2.19	0.42
1:B:1149:SER:C	4:B:1701:SAH:HB1	2.40	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
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:1312:THR:HG21	7:F:106:HOH:O	2.19	0.42
1:B:1000:ILE:HA	1:B:1021:LEU:HD23	2.02	0.42
1:B:1414:ASP:OD1	7:B:2037:HOH:O	2.21	0.42
1:B:838:ILE:HD11	1:B:866:THR:OG1	2.19	0.42
1:A:748:THR:HG23	1:A:789:LYS:HZ3	1.84	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:1184:ASN:ND2	7:B:2109:HOH:O	2.24	0.42
1:A:1410:PRO:HG2	1:A:1411:ILE:HG12	2.02	0.42
3:D:21:DC:OP2	7:D:104:HOH:O	2.22	0.42
1:A:842:PRO:HG3	1:A:1323:PRO:HB3	2.01	0.42
1:A:814:PRO:HD3	1:B:776:PRO:HG3	2.02	0.42
2:C:1:DG:N2	3:D:24:DC:N4	2.68	0.42
1:A:1369:THR:CG2	1:A:1371:ARG:HB3	2.49	0.42
1:A:1197:LEU:O	1:A:1201:VAL:HG13	2.19	0.42
1:A:1085:ARG:NE	7:A:2031:HOH:O	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:940:GLY:O	1:B:999:ARG:HD3	2.19	0.42
1:A:887:GLN:HA	1:A:888:PRO:HD3	1.85	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:B:1150:GLY:CA	4:B:1701:SAH:HB1	2.50	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:945:LEU:HD11	1:B:1054:VAL:HG11	2.02	0.41
1:A:808:LEU:HB3	1:A:812:SER:HB2	2.03	0.41
1:B:1145:LEU:HD13	1:B:1168:TRP:HB3	2.02	0.41
1:A:1389:ILE:O	1:A:1389:ILE:HG13	2.20	0.41
1:A:1091:ALA:O	1:A:1099:PHE:HA	2.21	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:B:766:VAL:CG1	1:B:767:SER:N	2.83	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:A:803:GLY:HA3	1:A:812:SER:OG	2.21	0.41
1:B:1018:LYS:C	1:B:1019:LEU:HD12	2.42	0.40
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:A:969:ASN:OD1	1:A:969:ASN:C	2.60	0.40
1:B:1089:LEU:HA	1:B:1089:LEU:HD12	1.70	0.40
1:B:870:GLN:N	7:B:1960:HOH:O	2.41	0.40
1:B:1172:MET:HB2	4:B:1701:SAH:C4	2.51	0.40
1:A:747:ARG:HG3	1:A:747:ARG:HH11	1.87	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: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
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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	828/873 (95%)	800 (97%)	27 (3%)	1 (0%)	59	85
1	B	826/873 (95%)	796 (96%)	30 (4%)	0	100	100
All	All	1654/1746 (95%)	1596 (96%)	57 (3%)	1 (0%)	59	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	959	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	701/759 (92%)	649 (93%)	52 (7%)	20	38
1	B	699/759 (92%)	650 (93%)	49 (7%)	21	41
All	All	1400/1518 (92%)	1299 (93%)	101 (7%)	21	39

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

Mol	Chain	Res	Type
1	A	751	GLN
1	A	758	GLU
1	A	759	MET
1	A	760	LEU
1	A	770	PRO
1	A	771	ASP
1	A	788	ASP
1	A	808	LEU

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Mol	Chain	Res	Type
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
1	A	1459	GLN
1	A	1466	LYS
1	A	1475	LEU
1	A	1485	LYS
1	A	1538	GLN
1	A	1572	LEU

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Mol	Chain	Res	Type
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
1	B	1348	VAL
1	B	1369	THR
1	B	1371	ARG
1	B	1374	MET
1	B	1386	ASN
1	B	1388	GLU

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Mol	Chain	Res	Type
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 chains 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	19,21,22	2.34	4 (21%)	24,30,33	2.38	5 (20%)
3	C49	D	18	3	19,22,24	5.72	9 (47%)	22,33,38	1.82	4 (18%)
2	5CM	E	6	3,2	19,21,22	2.79	6 (31%)	24,30,33	2.13	4 (16%)
3	C49	F	18	3	19,22,24	5.76	9 (47%)	22,33,38	1.77	4 (18%)

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	-	0/5/21/22	0/2/2/2
3	C49	D	18	3	1/1/8/10	0/8/40/46	0/2/2/2
2	5CM	E	6	3,2	-	1/5/21/22	0/2/2/2
3	C49	F	18	3	1/1/8/10	0/8/40/46	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	18	C49	C6-N1	19.15	1.44	1.36
3	D	18	C49	C6-N1	18.70	1.44	1.36
3	D	18	C49	P-O1P	10.88	1.59	1.46
3	F	18	C49	P-O1P	10.61	1.58	1.46
3	D	18	C49	C4-N4	7.41	1.43	1.27
3	F	18	C49	C4-N4	7.29	1.42	1.27
2	C	6	5CM	P-OP1	7.23	1.54	1.46
2	E	6	5CM	P-OP1	6.92	1.54	1.46
2	E	6	5CM	C2-N1	-5.37	1.32	1.38
2	C	6	5CM	C4-N4	5.32	1.48	1.34
2	E	6	5CM	C4-N4	5.21	1.47	1.34
3	D	18	C49	C2'-C3'	-4.46	1.40	1.52
3	F	18	C49	C2'-C3'	-4.44	1.40	1.52
2	E	6	5CM	C2'-C3'	-4.39	1.40	1.52
3	D	18	C49	C2-N1	4.30	1.47	1.34
3	F	18	C49	F-C5	4.23	1.50	1.42
3	D	18	C49	F-C5	4.21	1.50	1.42
3	F	18	C49	C2-N1	4.12	1.46	1.34
3	D	18	C49	C2-N3	3.84	1.45	1.38
3	F	18	C49	C2-N3	3.84	1.45	1.38
3	F	18	C49	C4-N3	2.95	1.43	1.35
3	D	18	C49	C4-N3	2.92	1.43	1.35
3	F	18	C49	O4'-C4'	-2.64	1.38	1.45
3	D	18	C49	O4'-C4'	-2.62	1.38	1.45
2	E	6	5CM	O4'-C4'	-2.43	1.39	1.45
2	C	6	5CM	C5-C4	-2.17	1.38	1.41
2	E	6	5CM	C5A-C5	2.06	1.55	1.51
2	C	6	5CM	O3'-C3'	-2.05	1.38	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	C2-N3-C4	6.17	121.00	115.41
2	E	6	5CM	C6-N1-C2	5.76	121.45	118.62
3	F	18	C49	N3-C4-N4	5.68	121.23	111.48
2	C	6	5CM	C6-N1-C2	5.30	121.23	118.62
3	D	18	C49	N3-C4-N4	5.12	120.28	111.48
2	E	6	5CM	O4'-C1'-N1	5.09	117.25	107.68
2	C	6	5CM	P-O5'-C5'	-4.26	106.55	123.19
2	C	6	5CM	O3'-C3'-C4'	-4.15	93.09	110.14
2	E	6	5CM	C2-N3-C4	4.03	119.06	115.41
3	D	18	C49	C2'-C1'-N1	-3.78	112.34	115.74
2	C	6	5CM	C5-C6-N1	-3.52	118.16	121.59
2	E	6	5CM	C5-C6-N1	-3.51	118.17	121.59
3	D	18	C49	O4'-C1'-N1	3.13	111.42	108.06
3	F	18	C49	C2'-C1'-N1	-2.61	113.39	115.74
3	F	18	C49	C1'-N1-C2	-2.33	114.69	117.78
3	D	18	C49	F-C5-CM5	-2.17	102.29	105.89
3	F	18	C49	N3-C2-N1	2.08	120.34	116.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	18	C49	C1'
3	F	18	C49	C1'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	5CM	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	28,28,28	1.01	2 (7%)	40,40,40	2.38	11 (27%)
4	SAH	B	1701	-	28,28,28	1.00	2 (7%)	40,40,40	2.11	8 (20%)
6	CIT	B	1704	-	12,12,12	0.97	0	17,17,17	1.69	2 (11%)

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	-	-	0/15/31/31	0/1/3/3
4	SAH	B	1701	-	-	0/15/31/31	0/1/3/3
6	CIT	B	1704	-	-	0/16/16/16	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-N3	3.43	1.39	1.32
4	B	1701	SAH	C2-N3	3.40	1.38	1.32
4	B	1701	SAH	C2-N1	2.57	1.39	1.33
4	A	1701	SAH	C2-N1	2.51	1.38	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	SAH	N3-C2-N1	-9.91	120.42	128.71
4	B	1701	SAH	N3-C2-N1	-9.68	120.62	128.71
4	A	1701	SAH	O4'-C1'-N9	6.02	114.04	108.44
6	B	1704	CIT	O6-C6-C3	5.31	120.62	112.89
4	A	1701	SAH	N3-C4-N9	3.95	132.56	125.43
4	B	1701	SAH	N3-C4-N9	3.56	131.87	125.43
4	B	1701	SAH	C5'-SD-CG	-2.98	93.52	102.42
4	A	1701	SAH	C5'-SD-CG	-2.73	94.28	102.42
4	A	1701	SAH	CG-CB-CA	2.71	117.75	113.22
4	A	1701	SAH	C5-C4-N3	-2.53	120.20	125.70
4	A	1701	SAH	OXT-C-O	-2.44	118.56	124.07
4	A	1701	SAH	C3'-C2'-C1'	2.42	104.70	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1701	SAH	CG-CB-CA	2.37	117.20	113.22
4	B	1701	SAH	O4'-C1'-N9	2.28	110.56	108.44
4	B	1701	SAH	C5-C4-N3	-2.23	120.84	125.70
4	B	1701	SAH	OXT-C-O	-2.23	119.04	124.07
4	A	1701	SAH	C2-N3-C4	2.16	120.17	114.01
4	A	1701	SAH	C-CA-N	2.11	112.85	109.36
6	B	1704	CIT	O4-C5-O3	-2.08	118.00	123.30
4	A	1701	SAH	N7-C8-N9	-2.04	108.59	114.36
4	B	1701	SAH	N7-C8-N9	-2.00	108.70	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å²)	Q<0.9
1	A	834/873 (95%)	-0.17	26 (3%)	47	43	16, 35, 87, 159	8 (0%)
1	B	832/873 (95%)	0.01	45 (5%)	25	21	16, 35, 99, 168	7 (0%)
2	C	12/12 (100%)	0.08	1 (8%)	11	8	32, 62, 98, 124	0
2	E	12/12 (100%)	-0.11	0	100	100	33, 67, 94, 112	0
3	D	12/12 (100%)	-0.25	1 (8%)	11	8	29, 52, 83, 84	0
3	F	12/12 (100%)	0.08	1 (8%)	11	8	28, 53, 88, 91	0
All	All	1714/1794 (95%)	-0.08	74 (4%)	34	30	16, 35, 94, 168	15 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	959	PRO	12.0
1	B	960	VAL	10.5
1	B	963	PRO	7.4
1	A	959	PRO	7.0
1	A	960	VAL	6.3
1	B	961	LYS	6.0
1	B	732	ASP	5.6
1	B	956	VAL	5.3
1	B	958	SER	5.3
1	B	770	PRO	4.5
1	A	962	ARG	4.4
1	A	1451	ASP	4.4
1	A	958	SER	4.2
1	B	772	ASP	4.2
1	A	1242	THR	3.8
1	A	956	VAL	3.8
1	A	1452	GLY	3.8
1	B	957	ALA	3.7
1	A	961	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	830	TYR	3.7
1	A	863	ASP	3.6
1	B	785	LEU	3.6
1	B	1137	ILE	3.5
1	A	957	ALA	3.4
1	B	962	ARG	3.4
1	B	739	GLN	3.3
1	B	736	TRP	3.1
1	B	786	TRP	3.1
1	A	732	ASP	3.0
1	A	1137	ILE	3.0
1	B	768	VAL	3.0
1	B	964	LYS	3.0
1	B	1246	PHE	3.0
1	B	789	LYS	3.0
1	B	1242	THR	2.9
1	A	1246	PHE	2.8
1	A	759	MET	2.8
1	A	741	MET	2.8
1	B	771	ASP	2.7
1	B	775	LYS	2.7
1	A	1600	SER	2.7
1	A	862	GLU	2.7
1	A	1243	TYR	2.7
1	B	793	MET	2.6
1	B	746	ASN	2.6
1	B	791	GLY	2.6
1	B	1450	GLY	2.6
3	D	24	DC	2.6
1	B	752	LYS	2.6
1	A	760	LEU	2.5
3	F	24	DC	2.5
1	A	785	LEU	2.5
1	A	1245	LYS	2.5
1	B	790	ASN	2.5
1	B	749	TYR	2.5
1	B	794	MET	2.4
1	B	774	SER	2.4
1	B	740	PRO	2.4
1	B	743	ILE	2.4
1	B	760	LEU	2.4
1	A	739	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	733	ARG	2.3
1	A	1096	THR	2.3
1	B	742	LYS	2.3
1	A	889	THR	2.3
1	B	889	THR	2.3
1	B	753	VAL	2.2
1	A	751	GLN	2.1
1	B	1454	ILE	2.1
1	B	741	MET	2.1
2	C	8	DC	2.1
1	B	866	THR	2.0
1	B	1453	VAL	2.0
1	B	1036	GLY	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	5CM	E	6	20/21	0.13	-0.13	22,32,36,45	0
2	5CM	C	6	20/21	0.13	-0.38	23,30,39,40	0
3	C49	D	18	21/23	0.12	-0.86	24,28,31,34	0
3	C49	F	18	21/23	0.12	-1.01	23,27,29,33	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SAH	B	1701	26/26	0.28	3.11	20,35,41,42	26
4	SAH	A	1701	26/26	0.27	1.89	18,36,41,42	26
6	CIT	B	1704	13/13	0.22	0.85	36,39,48,49	0
5	ZN	B	1703	1/1	0.08	-1.11	48,48,48,48	0
5	ZN	A	1703	1/1	0.08	-1.54	43,43,43,43	0
5	ZN	B	1702	1/1	0.08	-1.55	36,36,36,36	0
5	ZN	A	1702	1/1	0.09	-7.27	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.