



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:23 pm BST

PDB ID : 3PT6
Title : Crystal structure of mouse DNMT1(650-1602) in complex with DNA
Authors : Song, J.; Patel, D.J.
Deposited on : 2010-12-02
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

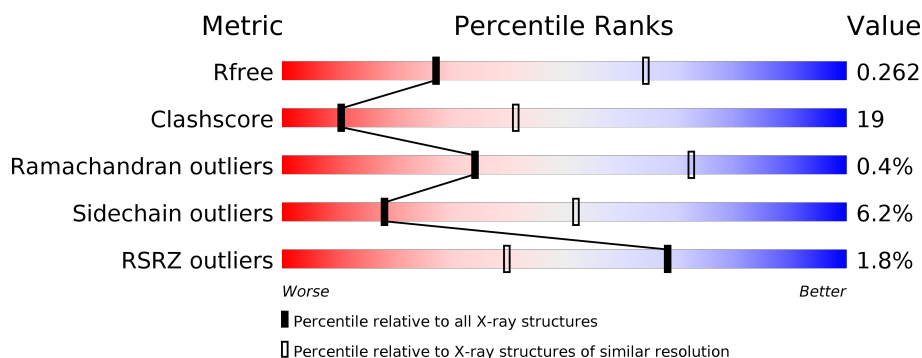
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	954	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>• •</div> </div> </div>
1	B	954	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• •</div> </div> </div>
2	C	19	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>26%</div> <div>26%</div> </div> </div>
2	D	19	<div> <div>11%</div> <div> <div></div> <div>32%</div> <div>58%</div> <div>11%</div> </div> </div>
3	I	19	<div> <div>5%</div> <div> <div></div> <div>21%</div> <div>58%</div> <div>21%</div> </div> </div>
3	J	19	<div> <div>5%</div> <div> <div></div> <div>21%</div> <div>68%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15593 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	914	Total	C	N	O	S	0	0	0
			6970	4404	1238	1278	50			
1	B	915	Total	C	N	O	S	0	0	0
			6993	4417	1248	1278	50			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	649	SER	-	EXPRESSION TAG	UNP P13864
B	649	SER	-	EXPRESSION TAG	UNP P13864

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			383	182	70	113	18			
2	D	19	Total	C	N	O	P	0	0	0
			383	182	70	113	18			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*CP*GP*GP*AP*GP*GP*CP*TP*CP*AP*CP*GP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	19	Total	C	N	O	P	0	0	0
			390	184	77	111	18			
3	J	19	Total	C	N	O	P	0	0	0
			390	184	77	111	18			

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



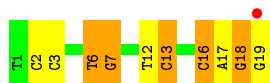
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	Zn	0	0
			4	4		
5	A	4	Total	Zn	0	0
			4	4		

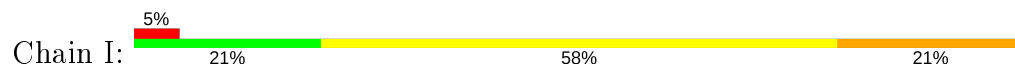
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	13	Total	O	0	0
			13	13		

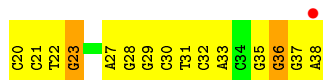




- Molecule 3: DNA (5'-D(*CP*CP*TP*GP*CP*GP*GP*AP*GP*GP*CP*TP*CP*AP*CP*GP*GP*GP*A)-3')



- Molecule 3: DNA (5'-D(*CP*CP*TP*GP*CP*GP*GP*AP*GP*GP*CP*TP*CP*AP*CP*GP*GP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.19Å 213.51Å 86.27Å 90.00° 99.64° 90.00°	Depositor
Resolution (Å)	29.82 – 3.00 29.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.82-3.00) 96.4 (29.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.211 , 0.266 0.207 , 0.262	Depositor DCC
R_{free} test set	1993 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15593	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAH

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	0/7146	0.48	0/9707
1	B	0.32	0/7172	0.48	0/9745
2	C	0.56	0/428	1.25	6/658 (0.9%)
2	D	0.60	0/428	1.21	3/658 (0.5%)
3	I	0.58	0/438	1.26	7/675 (1.0%)
3	J	0.56	0/438	1.27	4/675 (0.6%)
All	All	0.36	0/16050	0.62	20/22118 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	DG	O4'-C1'-N9	7.94	113.56	108.00
3	I	36	DG	O4'-C1'-N9	7.83	113.48	108.00
3	J	36	DG	O4'-C4'-C3'	-7.68	101.39	106.00
2	C	18	DG	O4'-C1'-N9	7.49	113.24	108.00
3	I	36	DG	C4'-C3'-C2'	-7.47	96.38	103.10
3	I	31	DT	O4'-C4'-C3'	-6.53	101.89	104.50
3	J	36	DG	C4'-C3'-C2'	-6.34	97.40	103.10
2	D	16	DC	C1'-O4'-C4'	-5.75	104.35	110.10
2	C	13	DC	C4'-C3'-C2'	-5.73	97.94	103.10
2	C	7	DG	O4'-C1'-N9	5.65	111.95	108.00
2	C	16	DC	O4'-C1'-N1	5.51	111.86	108.00
3	J	23	DG	O4'-C1'-N9	5.50	111.85	108.00
3	I	31	DT	N3-C4-O4	5.49	123.20	119.90
3	I	28	DG	O4'-C1'-N9	5.33	111.73	108.00
2	D	5	DG	O4'-C1'-N9	5.24	111.67	108.00
3	J	23	DG	C1'-O4'-C4'	-5.24	104.86	110.10
3	I	36	DG	O4'-C1'-C2'	-5.23	101.72	105.90
2	C	13	DC	C3'-C2'-C1'	-5.22	96.23	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	DT	N3-C4-O4	5.16	122.99	119.90
3	I	22	DT	N3-C4-O4	5.02	122.91	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6970	0	6453	228	0
1	B	6993	0	6474	256	0
2	C	383	0	214	11	0
2	D	383	0	214	17	0
3	I	390	0	213	30	0
3	J	390	0	213	18	0
4	A	26	0	19	4	0
4	B	26	0	19	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	11	0	0	0	0
6	B	13	0	0	0	0
All	All	15593	0	13819	546	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 19.

All (546) 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)
3:I:21:DC:H2''	3:I:22:DT:O5'	1.62	0.96
1:A:1303:GLN:HE21	1:A:1305:GLY:H	0.99	0.93
1:B:1303:GLN:HE21	1:B:1305:GLY:H	1.16	0.91
3:J:20:DC:H2''	3:J:21:DC:O5'	1.71	0.90
1:A:1315:ARG:HH11	1:A:1315:ARG:HG2	1.36	0.90
1:B:889:THR:HG22	1:B:891:ASP:H	1.34	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1266:PHE:HB3	1:B:1320:ALA:HB3	1.55	0.88
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.54	0.88
1:A:670:CYS:HB2	1:A:673:CYS:H	1.40	0.87
2:C:12:DT:H2''	2:C:13:DC:H5'	1.57	0.84
1:B:845:ASN:O	1:B:849:GLU:HG2	1.78	0.83
1:A:1282:VAL:O	1:A:1286:THR:HG23	1.79	0.81
1:A:938:ARG:O	1:A:1000:ILE:HD11	1.82	0.80
1:B:889:THR:HB	1:B:892:ASN:ND2	1.96	0.80
1:B:1560:GLY:HA3	1:B:1585:PRO:CD	2.13	0.79
1:A:746:ASN:HB3	1:A:789:LYS:HE2	1.65	0.79
1:A:729:GLN:HA	1:A:729:GLN:HE21	1.46	0.79
1:A:1035:ASN:HD22	1:A:1035:ASN:H	1.31	0.79
1:A:702:ALA:HA	1:A:1230:GLN:HE21	1.48	0.79
3:I:36:DG:H2''	3:I:37:DG:C8	2.19	0.77
1:B:1431:ILE:HD13	1:B:1516:TYR:O	1.84	0.77
1:A:1035:ASN:ND2	1:A:1035:ASN:H	1.81	0.77
1:A:1330:PHE:H	1:A:1356:ASN:HD21	1.31	0.76
1:A:769:ILE:HD11	1:A:832:HIS:HB2	1.68	0.76
2:C:18:DG:H2''	2:C:19:DG:OP2	1.86	0.75
1:B:1512:TRP:HB3	1:B:1515:LEU:HD22	1.69	0.74
2:D:19:DG:H5'	2:D:19:DG:H8	1.52	0.74
1:A:1107:ARG:HG2	1:A:1108:SER:N	2.01	0.74
1:B:979:LYS:HG2	1:B:1440:ARG:NH1	2.03	0.74
1:A:1332:GLU:HG3	1:A:1359:ARG:HG3	1.69	0.74
1:B:995:TYR:CE1	1:B:1362:SER:HB3	2.23	0.74
1:A:1560:GLY:HA3	1:A:1585:PRO:CD	2.18	0.74
1:B:1239:ASN:H	1:B:1242:THR:HG22	1.51	0.73
1:B:656:CYS:SG	1:B:659:CYS:HB3	2.29	0.73
1:B:1272:ARG:HD2	1:B:1314:ARG:CZ	2.19	0.72
1:A:906:LEU:O	1:A:910:GLU:HG2	1.88	0.72
1:B:654:ARG:HD2	1:B:655:ARG:O	1.89	0.72
1:B:741:MET:SD	1:B:751:GLN:HB2	2.30	0.72
1:B:727:LYS:HE2	1:B:769:ILE:HG21	1.71	0.72
1:A:1303:GLN:HE21	1:A:1305:GLY:N	1.83	0.71
1:A:1303:GLN:NE2	1:A:1305:GLY:H	1.82	0.71
1:B:1023:LYS:HD2	1:B:1050:GLU:HB2	1.71	0.71
3:I:30:DC:H2''	3:I:31:DT:OP2	1.90	0.71
2:C:16:DC:H2''	2:C:17:DA:C8	2.25	0.70
1:A:1315:ARG:NH1	1:A:1315:ARG:HG2	2.05	0.69
1:B:754:SER:HA	1:B:758:GLU:O	1.91	0.69
1:A:694:CYS:O	1:A:697:LEU:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:CYS:O	1:B:663:GLN:HG3	1.93	0.69
1:A:1065:VAL:HG22	1:A:1086:PHE:HB2	1.73	0.69
1:B:894:HIS:NE2	1:B:895:LYS:HD2	2.08	0.69
1:A:803:GLY:HA3	1:A:812:SER:OG	1.93	0.68
1:A:1311:GLN:NE2	1:A:1313:ARG:HD2	2.09	0.68
1:B:689:CYS:HB3	1:B:692:ARG:HG3	1.76	0.68
1:B:659:CYS:SG	1:B:661:VAL:HG12	2.34	0.68
1:A:749:TYR:CD1	1:A:786:TRP:HB3	2.29	0.67
1:B:980:TYR:HE2	1:B:1511:HIS:CD2	2.13	0.67
1:B:839:TYR:CE1	1:B:841:ALA:HB2	2.30	0.67
1:A:1560:GLY:HA3	1:A:1585:PRO:HD3	1.76	0.67
1:A:702:ALA:HA	1:A:1230:GLN:NE2	2.08	0.67
1:A:975:GLU:HG3	1:A:978:ARG:HD2	1.76	0.67
1:B:924:ARG:HH11	1:B:1005:CYS:C	1.97	0.66
1:B:924:ARG:HH11	1:B:1006:GLY:N	1.94	0.66
1:B:1293:MET:HE2	1:B:1295:TYR:CE1	2.30	0.66
1:A:670:CYS:HB2	1:A:673:CYS:HB2	1.78	0.66
1:A:975:GLU:HG2	1:A:1439:TRP:CZ3	2.31	0.66
1:A:710:ASP:CG	1:A:711:ASP:H	1.99	0.66
1:B:755:ILE:O	1:B:758:GLU:HG2	1.96	0.65
1:B:889:THR:HB	1:B:892:ASN:HD21	1.59	0.65
1:A:1184:ASN:HB2	1:A:1187:THR:CG2	2.27	0.65
1:B:788:ASP:HB3	1:B:790:ASN:OD1	1.96	0.65
1:B:803:GLY:HA3	1:B:812:SER:OG	1.96	0.65
3:J:32:DC:H2"	3:J:33:DA:OP2	1.97	0.65
1:A:1238:PHE:CE2	1:A:1278:ARG:HG3	2.32	0.64
1:A:668:GLY:HA2	1:A:673:CYS:HB3	1.80	0.64
1:B:1318:ILE:HD12	1:B:1318:ILE:C	2.18	0.64
1:B:1031:HIS:HD1	1:B:1092:TYR:HH	1.45	0.64
1:A:779:LEU:HD23	1:A:835:VAL:HG21	1.79	0.64
1:A:1311:GLN:HE22	1:A:1313:ARG:HH11	1.46	0.63
1:B:1188:THR:HG22	1:B:1212:GLN:HE21	1.63	0.63
1:B:1408:TYR:CZ	1:B:1410:PRO:HG3	2.33	0.63
2:D:3:DC:H2"	2:D:4:DC:OP2	1.97	0.63
1:B:669:LYS:HA	1:B:674:LYS:HE2	1.81	0.63
1:A:678:LYS:HG3	1:A:679:PHE:HD2	1.64	0.63
3:I:24:DC:H2"	3:I:25:DG:H5"	1.79	0.63
2:D:3:DC:H42	3:J:36:DG:H1	1.44	0.63
1:B:1431:ILE:HD11	1:B:1516:TYR:HB3	1.80	0.63
1:B:703:ASP:H	1:B:1230:GLN:HG2	1.64	0.63
1:B:1233:SER:HB2	1:B:1277:TYR:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:ASP:HB2	1:A:1515:LEU:O	1.99	0.62
1:B:1576:ARG:HB2	1:B:1576:ARG:NH1	2.14	0.62
1:B:979:LYS:HG2	1:B:1440:ARG:HH11	1.64	0.62
1:B:1170:ILE:HD13	1:B:1197:LEU:HD23	1.82	0.62
1:A:1166:THR:O	1:A:1187:THR:HB	2.00	0.62
1:B:1303:GLN:HE22	1:B:1313:ARG:H	1.47	0.62
1:B:806:THR:HG22	1:B:873:TYR:CE2	2.35	0.62
1:B:1144:THR:OG1	1:B:1164:SER:HB2	2.00	0.61
1:B:1560:GLY:HA3	1:B:1585:PRO:HD3	1.82	0.61
2:D:6:DT:H2'	2:D:7:DG:C8	2.36	0.61
1:A:1433:LEU:HD22	1:A:1545:GLU:HA	1.83	0.61
1:A:665:PRO:HG3	1:A:1492:ARG:NH1	2.16	0.61
2:C:17:DA:H2''	2:C:18:DG:H5'	1.81	0.61
1:A:1000:ILE:HA	1:A:1021:LEU:HD23	1.82	0.61
1:B:914:VAL:HG12	1:B:1014:GLU:HG2	1.82	0.61
1:B:655:ARG:HH22	1:B:692:ARG:HB3	1.65	0.61
1:A:1526:SER:OG	1:A:1540:ARG:NH1	2.33	0.61
2:D:18:DG:H2''	2:D:19:DG:H5'	1.83	0.61
1:B:1293:MET:HE2	1:B:1295:TYR:HE1	1.66	0.60
1:A:990:ASP:HB3	1:A:1339:PRO:HD2	1.84	0.60
1:B:1480:SER:HB2	1:B:1486:ALA:O	2.00	0.60
1:A:915:LEU:HD21	1:A:931:THR:HB	1.83	0.60
2:C:12:DT:C2'	2:C:13:DC:H5'	2.31	0.60
1:B:1439:TRP:CD2	1:B:1502:LEU:HD23	2.36	0.60
1:B:980:TYR:HE2	1:B:1511:HIS:NE2	1.98	0.60
1:A:661:VAL:HG21	1:A:695:PRO:CD	2.31	0.60
3:I:20:DC:C2'	3:I:21:DC:H5'	2.31	0.60
1:A:839:TYR:CE1	1:A:841:ALA:HB2	2.36	0.60
1:B:1008:LYS:HB2	1:B:1013:ASN:HB2	1.83	0.60
1:B:806:THR:HG22	1:B:873:TYR:CD2	2.37	0.60
3:I:28:DG:H2''	3:I:29:DG:C8	2.37	0.60
2:D:2:DC:H42	3:J:37:DG:H1	1.50	0.59
1:A:769:ILE:HD11	1:A:832:HIS:CB	2.31	0.59
1:B:1272:ARG:HD2	1:B:1314:ARG:NH1	2.17	0.59
1:A:725:LYS:CB	1:A:771:ASP:HB2	2.33	0.59
1:A:772:ASP:OD1	1:A:774:SER:N	2.34	0.59
1:A:1332:GLU:CG	1:A:1359:ARG:HG3	2.33	0.59
1:B:906:LEU:O	1:B:910:GLU:HG2	2.03	0.59
1:B:1157:GLY:HA3	1:B:1587:ALA:HB3	1.85	0.59
1:B:661:VAL:HG11	1:B:695:PRO:HD3	1.83	0.59
1:A:1200:LEU:HD23	1:A:1205:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:TYR:CE2	1:A:1331:PRO:HB2	2.38	0.58
1:B:924:ARG:NH1	1:B:1006:GLY:N	2.51	0.58
1:B:1180:PHE:HE2	1:B:1187:THR:HG21	1.68	0.58
2:C:17:DA:H2''	2:C:18:DG:C5'	2.34	0.58
1:B:737:LEU:HD11	1:B:754:SER:HB3	1.84	0.58
1:B:777:LEU:HD13	1:B:777:LEU:H	1.68	0.58
1:A:1470:SER:HB3	1:A:1474:ALA:H	1.68	0.58
1:A:825:ASN:O	1:A:826:MET:HG3	2.04	0.58
1:B:1526:SER:O	1:B:1527:THR:C	2.41	0.58
3:I:36:DG:H2''	3:I:37:DG:N7	2.18	0.58
1:A:1403:LEU:HD23	1:A:1557:ARG:HD3	1.84	0.58
1:A:1168:TRP:CD1	1:A:1215:PRO:HG3	2.40	0.57
1:B:1024:PHE:CE2	1:B:1065:VAL:HG21	2.39	0.57
3:I:21:DC:C2'	3:I:22:DT:O5'	2.43	0.57
3:I:31:DT:H5'	3:I:31:DT:C6	2.40	0.57
1:B:798:HIS:CE1	1:B:899:SER:HB2	2.40	0.57
2:D:19:DG:H5'	2:D:19:DG:C8	2.37	0.57
2:D:19:DG:H1	3:J:20:DC:N4	2.01	0.57
1:A:655:ARG:HG2	1:A:656:CYS:O	2.04	0.57
3:I:32:DC:H2''	3:I:33:DA:C8	2.40	0.57
1:A:1193:ASP:OD1	1:A:1195:ASN:HB2	2.03	0.57
1:A:690:LEU:HA	1:A:693:ARG:HH11	1.69	0.57
1:A:721:LEU:HD22	1:A:799:TRP:CE3	2.40	0.57
1:A:788:ASP:HB3	1:A:790:ASN:OD1	2.04	0.57
1:B:1192:GLU:HG3	1:B:1193:ASP:H	1.69	0.57
1:B:1516:TYR:HE2	1:B:1535:MET:HE2	1.69	0.57
1:B:1584:PRO:HB2	1:B:1585:PRO:HD3	1.85	0.56
1:A:1239:ASN:OD1	1:A:1242:THR:HB	2.05	0.56
1:B:1060:GLN:OE1	1:B:1060:GLN:HA	2.06	0.56
1:B:1232:PHE:CE1	1:B:1249:SER:HB2	2.39	0.56
1:B:751:GLN:HG2	1:B:751:GLN:O	2.06	0.56
1:A:1332:GLU:OE2	1:A:1358:THR:HB	2.05	0.56
1:B:1184:ASN:HB3	1:B:1187:THR:HG22	1.88	0.56
1:B:1431:ILE:CD1	1:B:1516:TYR:HB3	2.35	0.56
1:B:1369:THR:O	1:B:1373:THR:HG23	2.04	0.56
1:B:1438:ASP:OD2	1:B:1440:ARG:HG3	2.05	0.56
2:D:1:DT:H2''	2:D:2:DC:H5''	1.88	0.56
1:A:1239:ASN:H	1:A:1242:THR:HG22	1.71	0.56
1:A:741:MET:HE3	1:A:894:HIS:HB2	1.88	0.56
1:B:1166:THR:O	1:B:1187:THR:HB	2.05	0.56
1:B:1303:GLN:HE21	1:B:1305:GLY:N	1.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:LEU:CD1	1:B:777:LEU:H	2.19	0.56
3:I:28:DG:H2'	3:I:29:DG:H8	1.69	0.56
1:B:1188:THR:HG22	1:B:1212:GLN:NE2	2.19	0.55
1:B:1398:TRP:O	1:B:1402:GLN:HG2	2.06	0.55
1:B:1413:ARG:O	1:B:1553:ARG:HD2	2.07	0.55
1:A:662:CYS:SG	1:A:694:CYS:HB2	2.46	0.55
1:B:1333:PRO:HD2	1:B:1359:ARG:HB2	1.88	0.55
1:B:1391:TYR:CE1	1:B:1412:LEU:HD13	2.42	0.55
1:A:727:LYS:HB3	1:A:769:ILE:HB	1.87	0.55
1:B:1500:TRP:O	1:B:1503:PRO:HD2	2.07	0.55
1:B:719:LYS:HB2	1:B:722:HIS:CB	2.36	0.55
1:B:1065:VAL:HG12	1:B:1086:PHE:HB2	1.89	0.55
1:B:1044:MET:HG3	1:B:1087:TYR:CE1	2.42	0.55
1:A:924:ARG:HD3	1:A:1006:GLY:HA2	1.89	0.55
1:A:1170:ILE:CD1	1:A:1197:LEU:HD23	2.37	0.54
1:A:1336:VAL:O	1:A:1367:THR:HB	2.07	0.54
1:A:832:HIS:HD2	1:A:833:SER:CB	2.21	0.54
1:A:1067:TYR:CE2	1:A:1102:PRO:HG2	2.42	0.54
1:B:1233:SER:HB2	1:B:1277:TYR:CE2	2.43	0.54
1:A:1001:LYS:HG2	1:A:1002:GLU:HG3	1.89	0.54
1:A:1481:CYS:HA	1:A:1485:LYS:O	2.08	0.54
1:B:932:LYS:HB2	1:B:1056:PHE:CE1	2.42	0.54
1:A:729:GLN:HA	1:A:729:GLN:NE2	2.18	0.54
1:B:1002:GLU:HB2	1:B:1020:ARG:HB3	1.89	0.54
1:B:1044:MET:HG3	1:B:1087:TYR:CZ	2.43	0.54
1:B:980:TYR:CE2	1:B:1511:HIS:CD2	2.95	0.54
1:A:728:LYS:HB2	1:A:830:TYR:CE2	2.43	0.54
1:B:994:PRO:HB2	1:B:1026:ARG:CZ	2.38	0.53
1:B:661:VAL:HG11	1:B:694:CYS:HA	1.90	0.53
3:I:25:DG:H5'	3:I:25:DG:H8	1.74	0.53
1:B:1543:HIS:CG	1:B:1544:PRO:HD2	2.43	0.53
1:A:1264:ARG:HD2	1:A:1325:GLU:OE1	2.09	0.53
2:D:8:DA:H2'	1:B:1241:ARG:HH12	1.74	0.53
1:A:1200:LEU:CD2	1:A:1205:GLU:HG3	2.39	0.53
1:A:1458:LEU:HD12	1:A:1493:GLN:OE1	2.09	0.53
1:A:920:GLU:O	1:A:921:VAL:HG23	2.08	0.53
1:B:1093:ASN:OD1	1:B:1096:THR:HG23	2.08	0.53
2:D:3:DC:N4	3:J:36:DG:H1	2.06	0.53
1:A:1101:ASP:HB2	1:A:1102:PRO:HD2	1.90	0.53
1:B:1306:GLN:HB3	1:B:1333:PRO:HB3	1.90	0.53
1:A:1067:TYR:HE2	1:A:1102:PRO:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1559:GLN:OE1	1:A:1583:PRO:HG3	2.09	0.53
1:A:1171:GLU:OE2	4:A:1603:SAH:H1'	2.08	0.53
1:A:734:ILE:HG23	1:A:755:ILE:HG12	1.90	0.53
1:B:1348:VAL:HG13	1:B:1353:PHE:CE2	2.43	0.53
1:A:878:ALA:HB2	1:A:1353:PHE:CD1	2.43	0.52
1:B:1034:TYR:O	1:B:1036:GLY:N	2.41	0.52
1:B:777:LEU:O	1:B:777:LEU:HD22	2.09	0.52
1:B:1315:ARG:HH11	1:B:1315:ARG:HG2	1.74	0.52
1:A:737:LEU:HD11	1:A:754:SER:HB3	1.91	0.52
1:B:1293:MET:CE	1:B:1295:TYR:HE1	2.23	0.52
1:B:1348:VAL:HG13	1:B:1353:PHE:HE2	1.74	0.52
1:A:1184:ASN:HB2	1:A:1187:THR:HG22	1.90	0.52
1:A:710:ASP:CG	1:A:711:ASP:N	2.63	0.52
1:B:1002:GLU:CD	1:B:1020:ARG:HD2	2.29	0.52
1:B:986:GLY:HA2	1:B:1524:PHE:CE2	2.44	0.52
1:A:832:HIS:CD2	1:A:833:SER:N	2.78	0.52
3:J:30:DC:H2'	3:J:31:DT:H72	1.90	0.52
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.90	0.52
1:A:1172:MET:HB2	4:A:1603:SAH:C2	2.40	0.52
1:A:1287:LEU:O	1:A:1291:VAL:HG12	2.08	0.52
3:I:25:DG:H2''	3:I:26:DG:O4'	2.10	0.52
1:A:795:PHE:HD2	1:A:828:LEU:HD23	1.75	0.52
1:B:980:TYR:HE2	1:B:1511:HIS:HE2	1.56	0.52
1:B:1263:PRO:HD2	1:B:1295:TYR:OH	2.11	0.51
1:B:655:ARG:HH12	1:B:692:ARG:NH1	2.08	0.51
2:C:6:DT:H3	3:I:33:DA:H61	1.57	0.51
3:J:35:DG:H2''	3:J:36:DG:C5'	2.40	0.51
1:B:832:HIS:HD2	1:B:833:SER:CB	2.23	0.51
1:A:1156:GLU:O	1:A:1160:GLN:HG3	2.10	0.51
1:B:1311:GLN:OE1	1:B:1313:ARG:HD2	2.09	0.51
1:B:938:ARG:O	1:B:1000:ILE:HD11	2.11	0.51
1:B:741:MET:HE1	1:B:894:HIS:HB2	1.92	0.51
1:A:808:LEU:HD21	1:A:1291:VAL:HG11	1.92	0.51
1:B:656:CYS:O	1:B:662:CYS:SG	2.69	0.51
3:I:20:DC:H2''	3:I:21:DC:H5'	1.93	0.51
1:B:1262:ARG:N	1:B:1263:PRO:HD3	2.27	0.50
1:B:1389:ILE:HD11	1:B:1412:LEU:HD23	1.92	0.50
2:D:7:DG:H4'	2:D:8:DA:OP1	2.10	0.50
1:B:799:TRP:HE1	1:B:824:GLU:HG2	1.75	0.50
1:A:655:ARG:HH12	1:A:692:ARG:NH1	2.09	0.50
2:D:15:DG:OP1	1:B:653:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:GLY:HA3	1:A:1089:LEU:HD23	1.93	0.50
1:A:1277:TYR:O	1:A:1282:VAL:HG23	2.11	0.50
1:A:1429:ARG:HG3	1:A:1547:HIS:CD2	2.47	0.50
1:A:1391:TYR:CE1	1:A:1412:LEU:HD13	2.46	0.50
1:B:914:VAL:HG21	1:B:927:CYS:SG	2.52	0.50
2:D:16:DC:H2"	2:D:17:DA:C8	2.47	0.50
1:A:1149:SER:O	4:A:1603:SAH:HA	2.11	0.49
1:A:1184:ASN:CB	1:A:1187:THR:HG22	2.42	0.49
1:A:1470:SER:HB2	1:A:1474:ALA:HB3	1.94	0.49
1:B:1282:VAL:O	1:B:1286:THR:HG23	2.12	0.49
1:B:1464:ASP:OD2	1:B:1467:ASN:HB2	2.12	0.49
1:A:1103:PRO:HB2	1:A:1105:HIS:CD2	2.47	0.49
1:A:723:GLN:HE22	1:A:775:LYS:NZ	2.10	0.49
1:B:1236:ASN:O	1:B:1278:ARG:HD3	2.12	0.49
1:B:693:ARG:O	1:B:695:PRO:HD3	2.12	0.49
1:B:1234:GLY:O	1:B:1278:ARG:N	2.42	0.49
1:B:1290:LEU:O	1:B:1295:TYR:HB2	2.12	0.49
1:B:807:VAL:HG22	1:B:1353:PHE:CZ	2.48	0.49
1:A:1267:LEU:HD21	1:A:1317:ILE:HG23	1.93	0.49
1:A:1172:MET:HB2	4:A:1603:SAH:N1	2.28	0.49
1:A:700:LYS:H	1:A:700:LYS:CE	2.25	0.49
1:A:799:TRP:HE1	1:A:824:GLU:HG2	1.77	0.49
1:A:953:ASN:HB2	1:A:1050:GLU:OE1	2.13	0.49
1:B:1574:ARG:O	1:B:1578:VAL:HG23	2.12	0.49
1:B:719:LYS:HB2	1:B:722:HIS:HB2	1.95	0.49
1:B:741:MET:HE2	1:B:750:TYR:O	2.13	0.49
1:A:1311:GLN:NE2	1:A:1313:ARG:HH11	2.11	0.49
1:A:1311:GLN:HE22	1:A:1313:ARG:HD2	1.77	0.49
1:A:1373:THR:HG22	1:A:1374:MET:HB3	1.95	0.49
1:B:719:LYS:HB2	1:B:722:HIS:HB3	1.94	0.49
1:B:1313:ARG:HG3	1:B:1527:THR:HG23	1.95	0.49
1:A:668:GLY:CA	1:A:673:CYS:HB3	2.42	0.49
3:J:27:DA:H5'	3:J:27:DA:C8	2.47	0.48
1:B:1145:LEU:HD12	1:B:1146:ASP:N	2.27	0.48
1:B:886:THR:HG22	1:B:887:GLN:H	1.78	0.48
2:D:19:DG:H1	3:J:20:DC:H42	1.61	0.48
1:A:1272:ARG:HD3	1:A:1272:ARG:C	2.33	0.48
1:B:1000:ILE:HG22	1:B:1021:LEU:CD2	2.44	0.48
1:A:659:CYS:SG	1:A:661:VAL:HB	2.53	0.48
1:A:721:LEU:HD22	1:A:799:TRP:CD2	2.49	0.48
1:A:938:ARG:C	1:A:1000:ILE:HD11	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:ASP:O	1:A:895:LYS:HE2	2.14	0.48
1:B:690:LEU:HA	1:B:693:ARG:NH1	2.29	0.48
1:B:661:VAL:CG1	1:B:694:CYS:HA	2.44	0.48
3:I:31:DT:H2"	3:I:32:DC:C5	2.49	0.48
1:A:1502:LEU:HB2	1:A:1503:PRO:HD3	1.96	0.48
1:B:741:MET:HE1	1:B:894:HIS:CB	2.42	0.48
1:A:1107:ARG:HD3	1:A:1109:PRO:HA	1.95	0.48
1:A:1500:TRP:O	1:A:1503:PRO:HD2	2.14	0.48
1:A:1516:TYR:HE2	1:A:1535:MET:CE	2.26	0.48
1:A:1551:SER:OG	1:A:1554:GLU:HG3	2.13	0.48
1:B:1403:LEU:HD12	1:B:1557:ARG:HD3	1.95	0.48
1:B:886:THR:HG22	1:B:887:GLN:N	2.28	0.48
3:I:27:DA:H2"	3:I:28:DG:C8	2.48	0.48
1:A:1526:SER:O	1:A:1527:THR:C	2.52	0.48
1:A:700:LYS:HZ2	3:I:29:DG:P	2.37	0.48
1:B:909:LYS:O	1:B:933:ASN:HA	2.14	0.48
3:I:31:DT:H2"	3:I:32:DC:C6	2.49	0.48
1:B:1024:PHE:CZ	1:B:1065:VAL:HG21	2.48	0.47
1:B:1034:TYR:C	1:B:1036:GLY:H	2.17	0.47
1:A:660:GLU:O	1:A:664:GLN:HG3	2.15	0.47
1:B:1516:TYR:CE2	1:B:1535:MET:HE2	2.49	0.47
3:I:24:DC:H2"	3:I:25:DG:C8	2.49	0.47
1:A:670:CYS:HB2	1:A:673:CYS:N	2.20	0.47
1:A:806:THR:HG22	1:A:873:TYR:CD2	2.49	0.47
1:B:1188:THR:CG2	1:B:1212:GLN:HE21	2.27	0.47
1:B:1409:GLN:C	1:B:1409:GLN:OE1	2.53	0.47
1:B:832:HIS:C	1:B:832:HIS:CD2	2.87	0.47
1:A:1543:HIS:CG	1:A:1544:PRO:HD2	2.49	0.47
1:B:1008:LYS:CB	1:B:1013:ASN:HB2	2.45	0.47
1:A:700:LYS:H	1:A:700:LYS:HE2	1.79	0.47
1:B:984:ILE:HG22	1:B:987:SER:CB	2.45	0.47
1:A:997:ILE:O	1:A:1024:PHE:HB2	2.15	0.47
1:A:1330:PHE:H	1:A:1356:ASN:ND2	2.07	0.47
1:A:1543:HIS:ND1	1:A:1544:PRO:HD2	2.30	0.47
3:J:35:DG:H2"	3:J:36:DG:H5'	1.96	0.47
1:B:1268:LEU:HD23	1:B:1268:LEU:C	2.36	0.47
1:A:975:GLU:HG3	1:A:978:ARG:CD	2.43	0.46
1:B:777:LEU:HD13	1:B:777:LEU:N	2.29	0.46
1:A:1180:PHE:HE2	1:A:1187:THR:HG21	1.79	0.46
1:B:1408:TYR:CE1	1:B:1410:PRO:HG3	2.51	0.46
1:A:1238:PHE:HD2	1:A:1242:THR:CG2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LYS:HD3	1:A:759:MET:HE3	1.96	0.46
1:A:1311:GLN:NE2	1:A:1528:THR:H	2.12	0.46
1:A:1373:THR:O	1:A:1557:ARG:HD2	2.15	0.46
1:A:742:LYS:HG3	1:A:743:ILE:N	2.30	0.46
1:B:1230:GLN:HB2	1:B:1230:GLN:HE21	1.54	0.46
3:J:20:DC:H2'	3:J:21:DC:C5	2.50	0.46
1:B:1192:GLU:HG3	1:B:1193:ASP:N	2.30	0.46
2:C:6:DT:H2'	2:C:7:DG:C4	2.50	0.46
3:I:27:DA:H4'	3:I:28:DG:OP1	2.14	0.46
3:J:22:DT:H2''	3:J:23:DG:C8	2.51	0.46
3:J:29:DG:H5''	1:B:654:ARG:NE	2.31	0.46
1:A:1355:SER:OG	1:A:1357:ILE:HG13	2.15	0.46
1:B:1228:PRO:HG2	1:B:1250:LEU:HD12	1.97	0.46
1:B:1315:ARG:NH1	1:B:1315:ARG:HG2	2.31	0.46
1:B:1467:ASN:ND2	1:B:1507:ASN:HD21	2.14	0.46
1:A:656:CYS:O	1:A:662:CYS:SG	2.74	0.46
1:A:795:PHE:CE1	1:A:797:ALA:HB2	2.51	0.46
1:B:1023:LYS:HD2	1:B:1050:GLU:CB	2.41	0.46
1:A:689:CYS:HB3	1:A:692:ARG:HD3	1.98	0.46
1:A:655:ARG:HH12	1:A:692:ARG:HH11	1.63	0.46
1:A:728:LYS:HE2	1:A:829:SER:OG	2.16	0.46
1:B:1184:ASN:HB3	1:B:1187:THR:CG2	2.45	0.46
1:A:742:LYS:HD3	1:A:894:HIS:CE1	2.51	0.46
3:J:27:DA:H1'	3:J:28:DG:H5''	1.97	0.46
1:A:1335:HIS:CE1	1:A:1368:ILE:HD11	2.51	0.45
1:A:769:ILE:HD11	1:A:832:HIS:CG	2.51	0.45
1:A:839:TYR:HB2	1:A:869:PHE:CE2	2.51	0.45
1:B:670:CYS:CB	1:B:673:CYS:H	2.29	0.45
1:B:778:TYR:HB3	1:B:799:TRP:CZ3	2.50	0.45
1:B:937:TYR:CD2	1:B:937:TYR:N	2.84	0.45
1:A:1251:VAL:O	1:A:1255:LEU:HG	2.16	0.45
1:A:1418:LYS:HD2	1:A:1532:PRO:HD2	1.98	0.45
1:B:1559:GLN:OE1	1:B:1583:PRO:HG3	2.16	0.45
3:J:35:DG:H1'	3:J:36:DG:H5''	1.98	0.45
1:A:1302:LEU:O	1:A:1314:ARG:HA	2.17	0.45
1:B:1446:GLN:HE21	1:B:1456:HIS:CD2	2.35	0.45
3:I:27:DA:H1'	3:I:28:DG:C8	2.51	0.45
2:D:8:DA:O5'	1:B:1241:ARG:NH1	2.47	0.45
3:I:25:DG:H5'	3:I:25:DG:C8	2.52	0.45
1:B:1377:LEU:HA	1:B:1378:PRO:HD3	1.85	0.45
1:A:1090:GLU:HA	1:A:1102:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1429:ARG:HG3	1:B:1547:HIS:CD2	2.51	0.45
1:B:1439:TRP:CG	1:B:1502:LEU:HD23	2.52	0.45
3:I:29:DG:H2"	3:I:30:DC:C6	2.52	0.45
1:B:1557:ARG:O	1:B:1559:GLN:O	2.35	0.45
1:A:1431:ILE:HG22	1:A:1437:SER:HB3	1.98	0.45
1:A:1047:TRP:CD1	1:A:1047:TRP:C	2.90	0.45
1:A:726:LYS:HD3	1:A:826:MET:HE1	1.99	0.45
1:B:902:ARG:O	1:B:906:LEU:HD23	2.17	0.45
1:B:945:LEU:HD11	1:B:1021:LEU:HD11	1.98	0.45
3:I:31:DT:H5'	3:I:31:DT:H6	1.82	0.45
1:B:995:TYR:HE1	1:B:1362:SER:HB3	1.77	0.45
1:B:932:LYS:HB2	1:B:1056:PHE:CZ	2.52	0.45
1:A:769:ILE:HD11	1:A:832:HIS:ND1	2.32	0.44
1:A:775:LYS:HA	1:A:776:PRO:HD3	1.85	0.44
1:A:842:PRO:HG2	1:A:1323:PRO:HB3	1.99	0.44
3:J:20:DC:H2'	3:J:21:DC:C6	2.52	0.44
1:B:722:HIS:O	1:B:723:GLN:C	2.54	0.44
2:C:2:DC:H2"	2:C:3:DC:O4'	2.18	0.44
1:A:1067:TYR:CE1	1:A:1069:GLU:HB2	2.52	0.44
1:A:1442:LEU:HA	1:A:1443:PRO:HD3	1.81	0.44
1:A:824:GLU:HG3	1:A:826:MET:HE3	1.99	0.44
1:A:909:LYS:O	1:A:933:ASN:HA	2.16	0.44
1:B:1207:THR:OG1	1:B:1211:GLY:HA2	2.18	0.44
1:B:1168:TRP:CD1	1:B:1215:PRO:HG3	2.52	0.44
1:A:1258:CYS:SG	1:A:1266:PHE:CD2	3.08	0.44
1:B:1224:CYS:HA	1:B:1267:LEU:O	2.17	0.44
1:B:1239:ASN:H	1:B:1242:THR:CG2	2.28	0.44
1:B:1380:ILE:HD13	1:B:1415:HIS:CD2	2.52	0.44
1:B:1440:ARG:HH21	1:B:1513:ALA:CB	2.30	0.44
1:B:721:LEU:HD22	1:B:799:TRP:CE3	2.53	0.44
1:B:786:TRP:CE2	1:B:794:MET:HB2	2.53	0.44
1:B:872:TRP:C	1:B:872:TRP:CD1	2.91	0.44
1:A:693:ARG:O	1:A:695:PRO:HD3	2.17	0.44
1:B:1148:PHE:CE2	1:B:1227:PRO:HB3	2.52	0.44
1:B:1303:GLN:NE2	1:B:1313:ARG:H	2.16	0.44
1:A:1408:TYR:CZ	1:A:1410:PRO:HG3	2.52	0.44
1:B:1108:SER:CB	1:B:1109:PRO:HD2	2.48	0.44
1:B:1481:CYS:HA	1:B:1485:LYS:O	2.17	0.44
1:B:721:LEU:HD23	1:B:778:TYR:CG	2.53	0.44
1:B:972:LEU:C	1:B:974:PRO:HD3	2.38	0.44
1:A:1090:GLU:C	1:A:1102:PRO:HD3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1412:LEU:HD11	1:B:1553:ARG:HG2	2.00	0.44
1:A:661:VAL:HG11	1:A:694:CYS:HA	2.00	0.44
1:B:819:LEU:HB3	1:B:872:TRP:CE3	2.53	0.44
1:B:1293:MET:HE2	1:B:1295:TYR:CD1	2.52	0.43
1:B:1395:PRO:HB2	1:B:1401:ARG:CG	2.48	0.43
1:A:1512:TRP:HB3	1:A:1515:LEU:HD13	2.00	0.43
1:A:655:ARG:NH1	1:A:692:ARG:NH1	2.66	0.43
1:A:1270:ASN:HB3	1:A:1274:PHE:HB2	2.00	0.43
1:A:1000:ILE:HG22	1:A:1021:LEU:CD2	2.48	0.43
1:A:1383:GLY:O	1:A:1384:ALA:C	2.55	0.43
1:B:702:ALA:HA	1:B:1230:GLN:CD	2.38	0.43
1:B:1432:PRO:O	1:B:1518:ARG:HD2	2.19	0.43
1:A:672:ALA:O	1:A:676:MET:HG3	2.18	0.43
1:B:1356:ASN:ND2	1:B:1356:ASN:H	2.16	0.43
1:B:727:LYS:HE2	1:B:769:ILE:CG2	2.46	0.43
1:B:1560:GLY:HA3	1:B:1585:PRO:CG	2.47	0.43
1:B:716:PRO:O	1:B:717:SER:C	2.57	0.43
1:B:972:LEU:HD23	1:B:973:TYR:HE2	1.83	0.43
2:D:8:DA:H2'	1:B:1241:ARG:NH1	2.34	0.43
1:B:841:ALA:HB1	1:B:842:PRO:HD2	2.01	0.43
3:I:32:DC:H2''	3:I:33:DA:O5'	2.18	0.43
1:A:661:VAL:HG21	1:A:695:PRO:HD2	1.99	0.43
1:A:838:ILE:O	1:A:868:PHE:HA	2.19	0.43
1:B:1309:VAL:CG1	1:B:1311:GLN:HB3	2.49	0.43
1:A:1376:ASP:HB3	1:A:1400:GLN:OE1	2.18	0.42
1:A:832:HIS:HD2	1:A:833:SER:N	2.16	0.42
1:B:918:ILE:HD11	1:B:928:SER:HB3	1.99	0.42
1:A:1305:GLY:HA2	1:A:1309:VAL:O	2.19	0.42
1:A:1395:PRO:HG3	1:A:1404:ARG:HD3	2.01	0.42
1:B:1529:VAL:HG22	1:B:1531:ASN:H	1.84	0.42
1:B:728:LYS:HB2	1:B:830:TYR:CE2	2.54	0.42
1:B:915:LEU:HD12	1:B:929:SER:OG	2.18	0.42
3:J:37:DG:H2''	3:J:38:DA:C8	2.54	0.42
1:A:972:LEU:HD23	1:A:973:TYR:CE2	2.53	0.42
1:A:974:PRO:O	1:A:977:TYR:HD2	2.03	0.42
1:B:1000:ILE:HA	1:B:1021:LEU:HD23	2.01	0.42
1:B:969:ASN:OD1	1:B:972:LEU:N	2.46	0.42
1:B:986:GLY:O	1:B:1523:GLY:HA3	2.19	0.42
1:B:677:VAL:HA	1:B:681:GLY:O	2.19	0.42
1:A:1002:GLU:HB2	1:A:1020:ARG:HB3	2.01	0.42
1:A:1184:ASN:CB	1:A:1187:THR:CG2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:LEU:HA	1:A:808:LEU:HD12	1.75	0.42
1:B:975:GLU:HG3	1:B:978:ARG:HE	1.84	0.42
2:C:18:DG:C2'	2:C:19:DG:OP2	2.62	0.42
3:I:21:DC:H6	3:I:21:DC:OP2	2.01	0.42
1:A:1044:MET:HG3	1:A:1087:TYR:CE1	2.54	0.42
1:A:1047:TRP:CD1	1:A:1048:SER:N	2.87	0.42
1:A:795:PHE:CD2	1:A:828:LEU:HD23	2.53	0.42
1:B:1184:ASN:CB	1:B:1187:THR:HG22	2.48	0.42
1:A:1216:GLN:O	1:A:1217:LYS:C	2.58	0.42
1:A:1309:VAL:HG13	1:A:1558:SER:O	2.19	0.42
1:A:807:VAL:HG13	1:A:1353:PHE:CZ	2.55	0.42
1:B:1174:ASP:O	1:B:1178:GLN:HG2	2.19	0.42
1:B:1310:ALA:HB3	1:B:1373:THR:HG21	2.01	0.42
3:I:27:DA:H2"	3:I:28:DG:H8	1.83	0.42
1:A:1035:ASN:N	1:A:1035:ASN:ND2	2.58	0.42
1:A:1584:PRO:HB2	1:A:1585:PRO:HD3	2.02	0.42
1:B:1238:PHE:HD2	1:B:1242:THR:CG2	2.33	0.42
1:A:700:LYS:C	1:A:702:ALA:H	2.24	0.42
1:B:655:ARG:NH1	1:B:692:ARG:NH1	2.68	0.42
1:A:1167:LEU:HB2	1:A:1168:TRP:CE3	2.55	0.41
1:B:751:GLN:O	1:B:761:GLU:HG3	2.20	0.41
1:A:1315:ARG:NH1	1:A:1315:ARG:CG	2.78	0.41
1:A:1437:SER:HA	1:A:1441:ASP:OD2	2.21	0.41
1:B:1001:LYS:HD3	1:B:1020:ARG:HG2	2.02	0.41
1:B:1039:HIS:O	1:B:1401:ARG:NH2	2.52	0.41
1:B:1067:TYR:CE1	1:B:1069:GLU:HB2	2.56	0.41
1:B:1217:LYS:HE3	1:B:1260:TYR:CE2	2.54	0.41
1:B:1270:ASN:O	1:B:1315:ARG:HB3	2.20	0.41
1:B:784:ALA:HB2	1:B:895:LYS:HA	2.01	0.41
2:C:6:DT:H3	3:I:33:DA:N6	2.18	0.41
1:A:1019:LEU:O	1:A:1053:VAL:HA	2.20	0.41
1:A:664:GLN:HA	1:A:665:PRO:HD3	1.79	0.41
1:B:1170:ILE:CD1	1:B:1197:LEU:HD23	2.49	0.41
1:A:1026:ARG:O	1:A:1029:ASN:HB2	2.20	0.41
1:A:754:SER:HA	1:A:758:GLU:O	2.20	0.41
1:A:938:ARG:O	1:A:941:ASP:HB2	2.21	0.41
1:B:1023:LYS:HG3	1:B:1050:GLU:O	2.20	0.41
1:B:1034:TYR:C	1:B:1036:GLY:N	2.74	0.41
1:B:1047:TRP:O	1:B:1092:TYR:N	2.38	0.41
1:B:1101:ASP:HA	1:B:1102:PRO:HD3	1.84	0.41
1:B:1327:LEU:HA	1:B:1328:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:ARG:HB2	1:B:698:ALA:C	2.40	0.41
1:B:722:HIS:C	1:B:722:HIS:CD2	2.93	0.41
1:B:736:TRP:CE3	1:B:753:VAL:HG23	2.56	0.41
1:B:938:ARG:C	1:B:1000:ILE:HD11	2.41	0.41
1:B:1001:LYS:HB2	1:B:1022:TYR:CE2	2.55	0.41
1:B:1440:ARG:HH21	1:B:1513:ALA:HB2	1.85	0.41
1:A:1227:PRO:HA	1:A:1228:PRO:HD3	1.94	0.41
1:A:1239:ASN:H	1:A:1242:THR:CG2	2.31	0.41
1:A:1535:MET:HB2	1:A:1535:MET:HE3	1.82	0.41
1:B:1541:VAL:HG13	1:B:1541:VAL:O	2.21	0.41
1:B:949:ALA:O	1:B:950:PHE:HB3	2.20	0.41
1:A:1418:LYS:HB2	1:A:1420:MET:CE	2.51	0.41
1:A:1373:THR:HG23	1:A:1557:ARG:HB3	2.02	0.41
1:B:1480:SER:O	1:B:1483:GLU:HB2	2.20	0.41
1:B:1576:ARG:HB2	1:B:1576:ARG:CZ	2.51	0.41
1:B:838:ILE:O	1:B:868:PHE:HA	2.21	0.41
1:B:783:THR:HB	1:B:896:PHE:O	2.20	0.41
1:A:1167:LEU:HB2	1:A:1168:TRP:CZ3	2.55	0.41
1:A:1296:GLN:O	1:A:1320:ALA:HA	2.20	0.41
1:A:685:SER:O	1:A:686:LYS:HB2	2.20	0.41
1:B:1590:ILE:O	1:B:1593:GLU:HB2	2.21	0.41
1:B:736:TRP:HA	1:B:753:VAL:HG23	2.03	0.41
1:A:1424:VAL:O	1:A:1428:MET:HG3	2.21	0.41
1:B:1345:SER:CB	1:B:1352:LYS:HE2	2.50	0.41
1:B:1442:LEU:HA	1:B:1443:PRO:HD3	1.80	0.41
1:A:700:LYS:HZ3	3:I:29:DG:H5'	1.86	0.41
1:B:702:ALA:HA	1:B:1230:GLN:OE1	2.21	0.41
1:B:1464:ASP:OD2	1:B:1467:ASN:ND2	2.54	0.41
1:B:664:GLN:O	1:B:692:ARG:CD	2.69	0.41
1:A:1026:ARG:O	1:A:1027:PRO:C	2.59	0.40
1:A:1067:TYR:HD2	1:A:1088:PHE:CE1	2.40	0.40
1:A:871:LEU:HD12	1:A:1291:VAL:HG23	2.02	0.40
1:A:1510:ASN:CG	1:A:1510:ASN:O	2.60	0.40
1:A:1531:ASN:HA	1:A:1532:PRO:HD3	1.87	0.40
1:B:1290:LEU:HD11	1:B:1318:ILE:HD11	2.02	0.40
1:B:979:LYS:HE2	1:B:1440:ARG:NH1	2.36	0.40
1:A:1529:VAL:HG22	1:A:1530:THR:N	2.36	0.40
1:B:1395:PRO:HB2	1:B:1401:ARG:HG2	2.03	0.40
1:B:653:ARG:HH11	1:B:697:LEU:HG	1.86	0.40
1:A:1395:PRO:HB2	1:A:1401:ARG:HG3	2.02	0.40
1:A:659:CYS:HB3	1:A:696:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:THR:HG22	1:A:873:TYR:CE2	2.56	0.40
1:B:1303:GLN:HE22	1:B:1312:THR:HA	1.86	0.40
1:B:1336:VAL:O	1:B:1367:THR:HB	2.21	0.40
1:A:1338:ALA:HA	1:A:1339:PRO:HD3	1.81	0.40
1:A:1312:THR:HG23	1:A:1341:ALA:HB1	2.03	0.40
1:A:1516:TYR:HE2	1:A:1535:MET:HE3	1.86	0.40
1:B:1200:LEU:O	1:B:1205:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	908/954 (95%)	825 (91%)	83 (9%)	0	100	100
1	B	909/954 (95%)	834 (92%)	67 (7%)	8 (1%)	17	55
All	All	1817/1908 (95%)	1659 (91%)	150 (8%)	8 (0%)	34	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	963	PRO
1	B	1035	ASN
1	B	1232	PHE
1	B	1271	VAL
1	B	1432	PRO
1	B	697	LEU
1	B	712	VAL
1	B	995	TYR

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	696/828 (84%)	661 (95%)	35 (5%)	24	60
1	B	698/828 (84%)	647 (93%)	51 (7%)	14	44
All	All	1394/1656 (84%)	1308 (94%)	86 (6%)	18	52

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	700	LYS
1	A	723	GLN
1	A	729	GLN
1	A	734	ILE
1	A	769	ILE
1	A	807	VAL
1	A	808	LEU
1	A	891	ASP
1	A	906	LEU
1	A	915	LEU
1	A	943	VAL
1	A	948	GLU
1	A	975	GLU
1	A	1033	SER
1	A	1035	ASN
1	A	1107	ARG
1	A	1201	VAL
1	A	1229	CYS
1	A	1238	PHE
1	A	1240	SER
1	A	1242	THR
1	A	1251	VAL
1	A	1267	LEU
1	A	1270	ASN
1	A	1309	VAL
1	A	1315	ARG
1	A	1346	VAL

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Mol	Chain	Res	Type
1	A	1358	THR
1	A	1362	SER
1	A	1366	ARG
1	A	1385	SER
1	A	1387	SER
1	A	1403	LEU
1	A	1409	GLN
1	A	1496	THR
1	B	654	ARG
1	B	659	CYS
1	B	677	VAL
1	B	709	ASP
1	B	710	ASP
1	B	714	GLU
1	B	723	GLN
1	B	729	GLN
1	B	753	VAL
1	B	758	GLU
1	B	759	MET
1	B	777	LEU
1	B	808	LEU
1	B	825	ASN
1	B	914	VAL
1	B	931	THR
1	B	937	TYR
1	B	942	SER
1	B	975	GLU
1	B	984	ILE
1	B	985	LYS
1	B	1028	GLU
1	B	1032	ARG
1	B	1055	ASN
1	B	1070	ASP
1	B	1096	THR
1	B	1163	ILE
1	B	1164	SER
1	B	1188	THR
1	B	1214	LEU
1	B	1230	GLN
1	B	1242	THR
1	B	1267	LEU
1	B	1269	GLU

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Mol	Chain	Res	Type
1	B	1270	ASN
1	B	1309	VAL
1	B	1311	GLN
1	B	1312	THR
1	B	1318	ILE
1	B	1346	VAL
1	B	1348	VAL
1	B	1350	ASP
1	B	1366	ARG
1	B	1386	ASN
1	B	1392	ASN
1	B	1409	GLN
1	B	1421	SER
1	B	1433	LEU
1	B	1440	ARG
1	B	1527	THR
1	B	1541	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	723	GLN
1	A	729	GLN
1	A	832	HIS
1	A	870	GLN
1	A	1004	HIS
1	A	1035	ASN
1	A	1039	HIS
1	A	1105	HIS
1	A	1159	HIS
1	A	1184	ASN
1	A	1216	GLN
1	A	1303	GLN
1	A	1311	GLN
1	A	1356	ASN
1	A	1402	GLN
1	A	1509	HIS
1	B	722	HIS
1	B	729	GLN
1	B	832	HIS
1	B	870	GLN
1	B	887	GLN

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Mol	Chain	Res	Type
1	B	892	ASN
1	B	953	ASN
1	B	1004	HIS
1	B	1013	ASN
1	B	1055	ASN
1	B	1080	GLN
1	B	1159	HIS
1	B	1212	GLN
1	B	1216	GLN
1	B	1230	GLN
1	B	1270	ASN
1	B	1303	GLN
1	B	1343	GLN
1	B	1456	HIS
1	B	1467	ASN
1	B	1511	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SAH	A	1603	-	21,28,28	1.23	2 (9%)	20,40,40	1.64	2 (10%)
4	SAH	B	1603	-	21,28,28	1.23	2 (9%)	20,40,40	1.63	2 (10%)

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	1603	-	-	2/7/31/31	0/3/3/3
4	SAH	B	1603	-	-	2/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1603	SAH	C2-N3	4.30	1.39	1.32
4	B	1603	SAH	C2-N3	4.29	1.39	1.32
4	B	1603	SAH	C2-N1	2.67	1.38	1.33
4	A	1603	SAH	C2-N1	2.61	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1603	SAH	N3-C2-N1	-5.44	120.17	128.68
4	B	1603	SAH	N3-C2-N1	-5.37	120.28	128.68
4	B	1603	SAH	C5'-SD-CG	-3.40	92.08	102.27
4	A	1603	SAH	C5'-SD-CG	-3.15	92.82	102.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

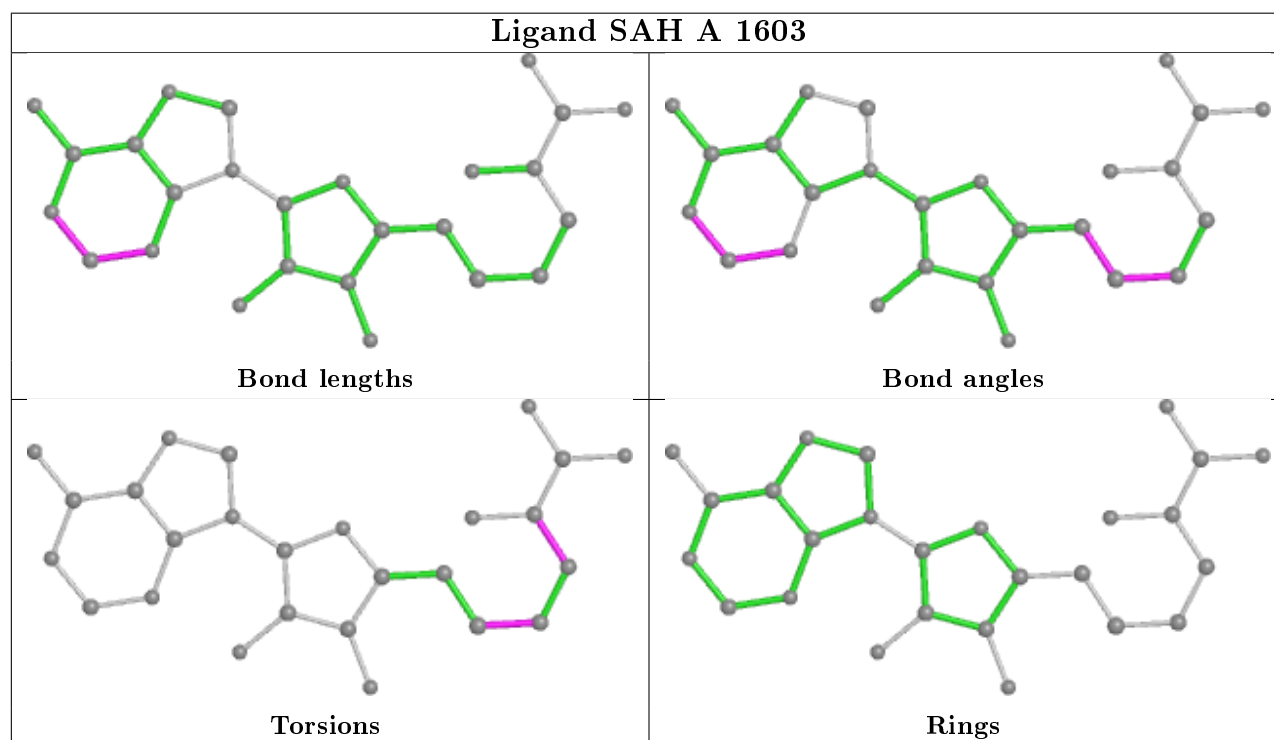
Mol	Chain	Res	Type	Atoms
4	B	1603	SAH	N-CA-CB-CG
4	B	1603	SAH	C-CA-CB-CG
4	A	1603	SAH	N-CA-CB-CG
4	A	1603	SAH	CB-CG-SD-C5'

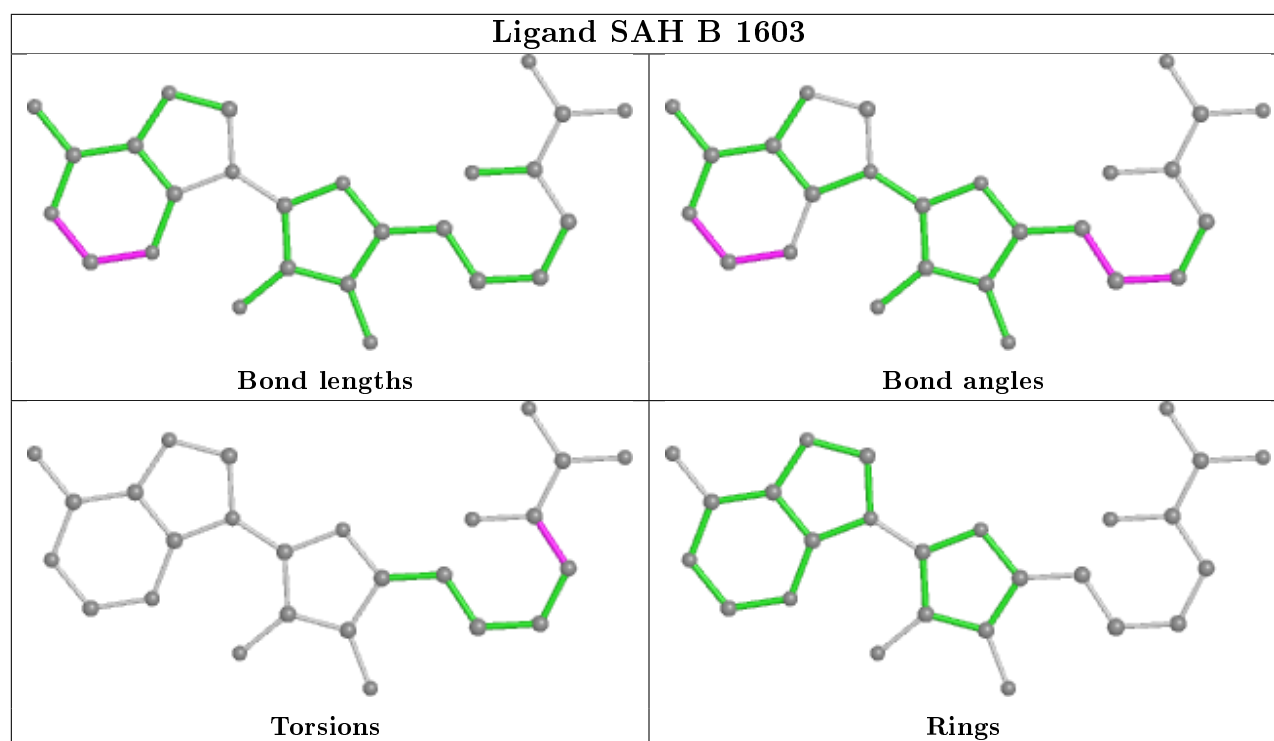
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1603	SAH	4	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	914/954 (95%)	-0.45	17 (1%) 66 37	29, 53, 98, 122	0
1	B	915/954 (95%)	-0.39	13 (1%) 75 49	31, 61, 100, 117	0
2	C	19/19 (100%)	0.36	1 (5%) 26 10	66, 93, 108, 114	0
2	D	19/19 (100%)	0.60	2 (10%) 6 2	74, 93, 111, 112	0
3	I	19/19 (100%)	0.32	1 (5%) 26 10	84, 99, 115, 115	0
3	J	19/19 (100%)	0.29	1 (5%) 26 10	89, 94, 113, 117	0
All	All	1905/1984 (96%)	-0.39	35 (1%) 68 40	29, 58, 102, 122	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	DT	4.7
1	A	1450	GLY	3.8
1	A	680	GLY	3.7
2	C	19	DG	3.6
1	B	1241	ARG	3.5
1	B	989	LEU	3.5
3	J	38	DA	3.5
1	A	1111	ASN	3.3
1	B	982	ASP	3.2
1	A	960	VAL	3.1
1	A	1241	ARG	3.1
1	A	702	ALA	3.1
1	A	1240	SER	2.9
1	A	1110	GLY	2.9
2	D	4	DC	2.9
1	A	1109	PRO	2.8
1	A	1115	GLY	2.8
1	B	650	ALA	2.8
1	B	984	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1451	ASP	2.7
1	B	1240	SER	2.7
1	A	986	GLY	2.6
1	A	1113	GLY	2.5
1	B	1111	ASN	2.5
1	B	961	LYS	2.4
1	B	983	TYR	2.3
1	B	723	GLN	2.3
1	A	700	LYS	2.2
1	A	963	PRO	2.2
1	B	960	VAL	2.2
1	B	863	ASP	2.1
1	B	1112	LYS	2.1
1	A	959	PRO	2.1
1	A	1112	LYS	2.1
3	I	31	DT	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

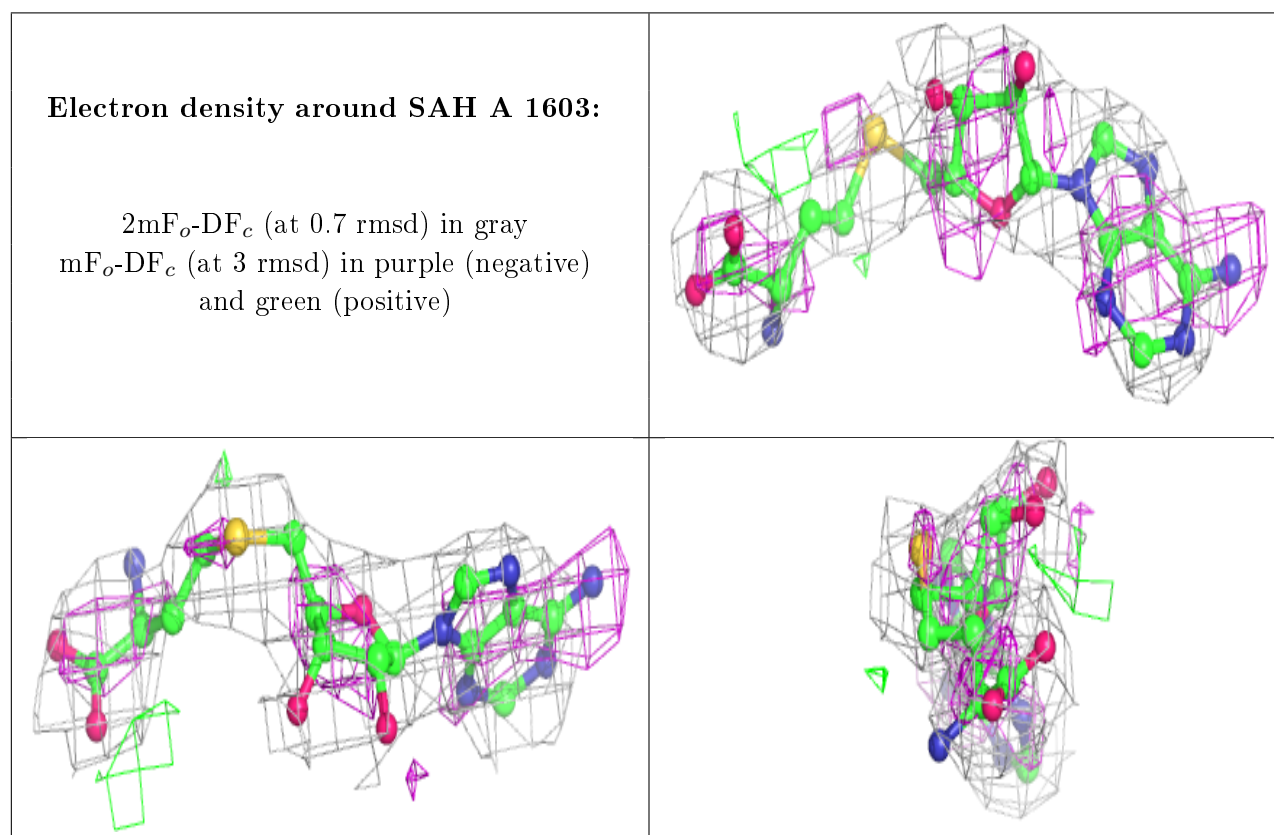
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	B	4	1/1	0.62	0.08	128,128,128,128	0
5	ZN	A	4	1/1	0.89	0.07	117,117,117,117	0
5	ZN	B	2	1/1	0.92	0.03	99,99,99,99	0
4	SAH	A	1603	26/26	0.92	0.24	38,52,56,67	0
4	SAH	B	1603	26/26	0.92	0.25	43,60,67,69	0
5	ZN	B	3	1/1	0.97	0.04	91,91,91,91	0
5	ZN	B	1	1/1	0.97	0.04	91,91,91,91	0

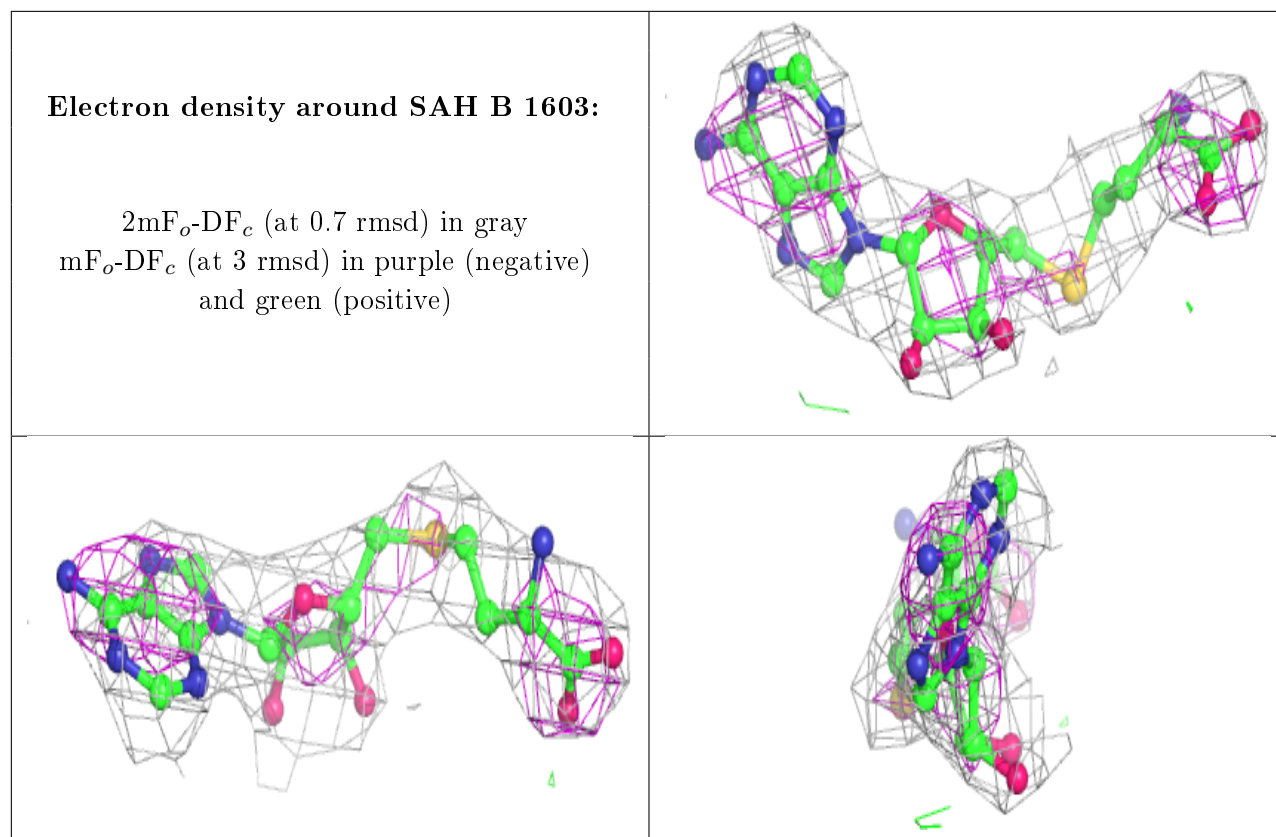
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	A	3	1/1	0.98	0.05	65,65,65,65	0
5	ZN	A	2	1/1	0.98	0.04	92,92,92,92	0
5	ZN	A	1	1/1	0.99	0.04	71,71,71,71	0

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.