



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:07 am BST

PDB ID : 3PTA
Title : Crystal structure of human DNMT1(646-1600) in complex with DNA
Authors : Song, J.; Patel, D.J.
Deposited on : 2010-12-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

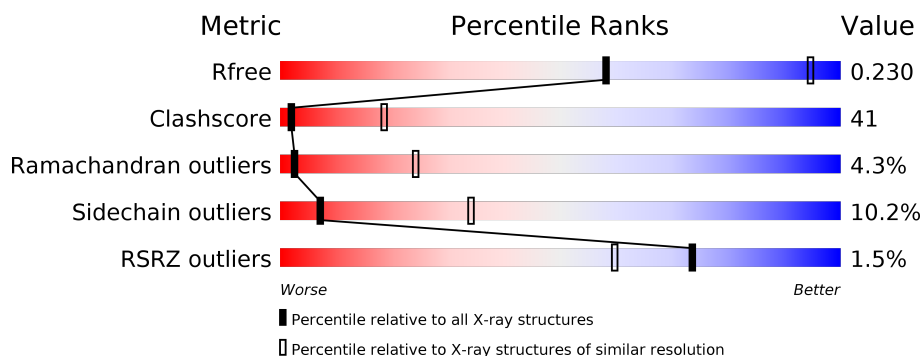
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	956	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 44%, green 42%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 44% 42% 9% 5% </div> </div>
2	B	19	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 89%, green 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 5% 89% 5% </div> </div>
3	C	19	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 21%, yellow 74%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 21% 74% 5% </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	1601	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7989 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	904	Total	C	N	O	S	0	0	0
			7186	4527	1282	1322	55			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	SER	-	EXPRESSION TAG	UNP P26358

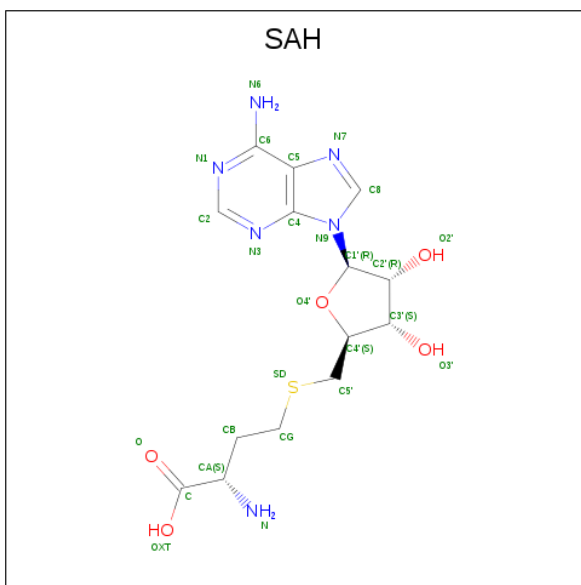
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*CP*CP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	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	C	19	Total	C	N	O	P	0	0	0
			390	184	77	111	18			

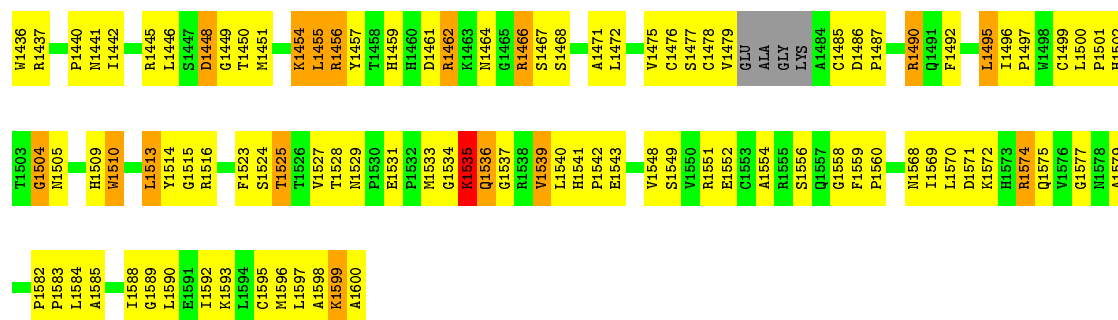
- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



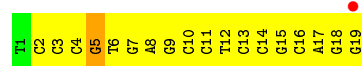
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

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



- Molecule 2: DNA (5'-D(*TP*CP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*CP*CP*GP*CP*AP*GP*G)-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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.80 Å 87.90 Å 113.90 Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 29.45 – 3.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 97.8 (29.45-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.55 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.291 0.244 , 0.230	Depositor DCC
R_{free} test set	984 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	124.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7989	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/7360	0.51	0/9941
2	B	0.48	0/428	0.83	1/658 (0.2%)
3	C	0.40	0/438	0.79	0/675
All	All	0.31	0/8226	0.56	1/11274 (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	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	DG	N9-C1'-C2'	5.05	122.20	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1405	TYR	Sidechain
3	C	21	DC	Sidechain

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	7186	0	7049	588	0
2	B	383	0	214	28	0
3	C	390	0	213	20	0
4	A	26	0	19	5	0
5	A	4	0	0	0	0
All	All	7989	0	7495	634	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 41.

All (634) 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)
2:B:2:DC:C2'	2:B:3:DC:H5''	1.77	1.15
1:A:685:ALA:HB2	2:B:13:DC:H5'	1.31	1.09
2:B:15:DG:H2''	2:B:16:DC:H5'	1.28	1.09
1:A:1020:LYS:O	1:A:1020:LYS:HE3	1.53	1.08
1:A:1454:LYS:HE2	1:A:1454:LYS:HA	1.37	1.07
1:A:1020:LYS:HE2	1:A:1020:LYS:N	1.71	1.05
2:B:2:DC:H2''	2:B:3:DC:C5'	1.86	1.05
1:A:1003:LYS:HD2	1:A:1008:ARG:HA	1.38	1.04
1:A:1015:LYS:HD3	1:A:1016:ILE:N	1.73	1.03
1:A:1020:LYS:CD	1:A:1047:GLU:HB2	1.90	0.99
1:A:919:SER:HB2	1:A:1003:LYS:HG2	1.42	0.99
1:A:1020:LYS:HD3	1:A:1047:GLU:HB2	1.45	0.95
1:A:966:GLU:HG2	1:A:1468:SER:HB2	1.46	0.95
1:A:1441:ASN:C	1:A:1454:LYS:HD2	1.88	0.94
1:A:724:LYS:HE2	1:A:726:GLN:HG2	1.51	0.93
1:A:1160:ILE:HD11	1:A:1593:LYS:HB3	1.48	0.93
2:B:2:DC:H2''	2:B:3:DC:H5''	0.93	0.92
1:A:1210:ARG:H	1:A:1210:ARG:HE	0.93	0.89
1:A:1487:PRO:O	1:A:1490:ARG:HD2	1.73	0.89
1:A:655:VAL:HG13	1:A:1533:MET:HB2	1.52	0.88
1:A:655:VAL:HG21	1:A:1534:GLY:HA2	1.54	0.88
1:A:1016:ILE:HD11	1:A:1053:PHE:HD2	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:LYS:HE3	1:A:997:LYS:HA	1.56	0.87
1:A:1020:LYS:HE2	1:A:1020:LYS:H	1.34	0.87
1:A:1210:ARG:H	1:A:1210:ARG:NE	1.72	0.86
1:A:1207:ARG:HH21	1:A:1209:GLN:HG2	1.41	0.86
1:A:903:ARG:HH11	1:A:906:GLU:HG3	1.41	0.86
1:A:931:ILE:HD11	1:A:1059:ARG:HH11	1.42	0.84
1:A:728:LYS:HG2	1:A:731:ILE:HD11	1.58	0.84
1:A:1379:ASN:HD22	1:A:1380:GLY:N	1.76	0.83
1:A:1000:PHE:CZ	1:A:1015:LYS:HD2	2.13	0.83
1:A:722:LYS:O	1:A:768:ASP:HB2	1.78	0.82
1:A:734:VAL:HB	1:A:749:LYS:HG3	1.61	0.81
1:A:724:LYS:HE2	1:A:726:GLN:CG	2.10	0.81
1:A:1015:LYS:HE3	1:A:1050:VAL:HG22	1.62	0.81
1:A:928:LYS:O	1:A:931:ILE:HG22	1.79	0.80
1:A:720:GLN:HG3	1:A:721:GLY:H	1.45	0.80
1:A:1476:CYS:O	1:A:1479:VAL:HG23	1.82	0.80
1:A:1590:LEU:O	1:A:1593:LYS:HG2	1.82	0.80
1:A:1015:LYS:CE	1:A:1050:VAL:HG22	2.12	0.79
2:B:17:DA:H2''	2:B:18:DG:O5'	1.80	0.79
1:A:668:LYS:HG2	1:A:669:ALA:H	1.47	0.79
1:A:1585:ALA:O	1:A:1588:ILE:HG22	1.82	0.79
1:A:1209:GLN:HA	1:A:1210:ARG:HH11	1.46	0.79
1:A:965:ASP:OD2	1:A:968:LEU:HB2	1.83	0.79
1:A:748:LYS:HA	1:A:748:LYS:NZ	1.97	0.78
1:A:1020:LYS:HD2	1:A:1047:GLU:HB2	1.65	0.78
1:A:1418:SER:HB3	1:A:1421:VAL:HG23	1.65	0.78
1:A:1233:ASN:ND2	1:A:1234:ARG:H	1.82	0.78
1:A:1442:ILE:O	1:A:1454:LYS:HE3	1.84	0.78
1:A:919:SER:HA	1:A:1003:LYS:HD3	1.65	0.78
1:A:1462:ARG:HE	1:A:1462:ARG:HA	1.47	0.77
3:C:21:DC:H2''	3:C:22:DT:O5'	1.83	0.77
3:C:33:DA:H2''	3:C:34:DC:O5'	1.84	0.77
1:A:1160:ILE:HD11	1:A:1593:LYS:CB	2.15	0.77
1:A:961:LYS:N	1:A:961:LYS:HZ3	1.83	0.76
1:A:1154:GLY:HA3	1:A:1585:ALA:HB3	1.68	0.76
1:A:722:LYS:NZ	1:A:722:LYS:HA	1.99	0.76
1:A:743:LYS:H	1:A:743:LYS:HD3	1.50	0.76
1:A:1456:ARG:HE	1:A:1456:ARG:HA	1.49	0.76
1:A:1065:GLY:O	1:A:1068:LEU:HD22	1.84	0.76
1:A:724:LYS:CG	1:A:766:ILE:HB	2.16	0.75
1:A:833:LYS:HA	1:A:833:LYS:NZ	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:LYS:HE2	1:A:1242:LYS:HA	1.68	0.75
1:A:668:LYS:HD3	1:A:668:LYS:H	1.50	0.75
1:A:1016:ILE:HD11	1:A:1053:PHE:CD2	2.21	0.75
1:A:724:LYS:HE3	1:A:766:ILE:HB	1.67	0.75
1:A:943:PRO:HG2	1:A:944:GLU:OE2	1.86	0.75
2:B:15:DG:H2''	2:B:16:DC:C5'	2.12	0.75
1:A:1015:LYS:C	1:A:1015:LYS:HD3	2.06	0.75
1:A:1088:ALA:HB3	1:A:1097:GLU:HG3	1.68	0.75
1:A:1454:LYS:HD3	1:A:1455:LEU:H	1.50	0.74
1:A:1527:VAL:HG21	1:A:1535:LYS:NZ	2.02	0.74
1:A:1454:LYS:CE	1:A:1454:LYS:HA	2.10	0.74
1:A:1527:VAL:HG22	1:A:1528:THR:H	1.50	0.74
1:A:1500:LEU:HB2	1:A:1501:PRO:HD3	1.68	0.74
1:A:1308:GLN:HE21	1:A:1310:ARG:HB2	1.52	0.74
1:A:905:LYS:HA	1:A:905:LYS:HE2	1.70	0.74
1:A:701:ASP:HA	1:A:1270:ASN:HD22	1.54	0.73
1:A:1244:LYS:HE2	1:A:1244:LYS:HA	1.70	0.73
1:A:884:PRO:HB2	1:A:889:LYS:HZ2	1.53	0.73
1:A:1558:GLY:HA3	1:A:1583:PRO:CD	2.18	0.73
1:A:1015:LYS:CG	1:A:1050:VAL:HG13	2.19	0.72
1:A:1020:LYS:CE	1:A:1020:LYS:N	2.48	0.72
1:A:1289:ARG:HH11	1:A:1289:ARG:HG2	1.53	0.72
2:B:7:DG:H2''	2:B:8:DA:C8	2.25	0.72
1:A:919:SER:HA	1:A:1003:LYS:CD	2.20	0.72
1:A:1187:PHE:HB3	1:A:1189:GLU:OE2	1.89	0.71
1:A:655:VAL:HG11	1:A:1531:GLU:HB3	1.72	0.71
1:A:1441:ASN:CA	1:A:1454:LYS:HD2	2.19	0.71
1:A:746:TYR:CD1	1:A:783:TRP:HB3	2.25	0.71
1:A:1461:ASP:HA	1:A:1479:VAL:HG11	1.72	0.71
1:A:1031:THR:HG23	1:A:1032:PRO:HD3	1.74	0.70
3:C:20:DC:H2'	3:C:21:DC:C5	2.27	0.70
1:A:1068:LEU:HD11	1:A:1072:VAL:HA	1.74	0.70
1:A:1558:GLY:HA3	1:A:1583:PRO:HD3	1.73	0.69
1:A:884:PRO:HB2	1:A:889:LYS:NZ	2.08	0.69
1:A:1015:LYS:CD	1:A:1016:ILE:N	2.54	0.69
1:A:1406:GLN:HB3	1:A:1408:ILE:HG12	1.74	0.69
1:A:738:VAL:O	1:A:739:LYS:HG2	1.93	0.69
1:A:1011:GLU:HG3	1:A:1012:THR:N	2.08	0.69
1:A:769:ASP:OD2	1:A:771:SER:HB3	1.94	0.68
1:A:1585:ALA:HA	1:A:1588:ILE:HG22	1.73	0.68
3:C:25:DG:H1'	3:C:26:DG:H5'	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:DC:H2'	3:C:21:DC:C6	2.28	0.68
1:A:1011:GLU:O	1:A:1012:THR:HG22	1.93	0.67
1:A:1210:ARG:N	1:A:1210:ARG:HE	1.78	0.67
1:A:919:SER:CB	1:A:1003:LYS:HG2	2.19	0.67
2:B:13:DC:H2''	2:B:14:DC:C5	2.29	0.67
1:A:966:GLU:HG2	1:A:1468:SER:CB	2.24	0.67
1:A:1490:ARG:HD3	1:A:1490:ARG:O	1.95	0.67
1:A:1020:LYS:NZ	1:A:1047:GLU:O	2.26	0.66
1:A:1235:PHE:HD2	1:A:1239:THR:HG23	1.60	0.66
1:A:1300:GLN:HE22	1:A:1309:THR:HA	1.60	0.66
1:A:1000:PHE:CE2	1:A:1015:LYS:HD2	2.30	0.66
1:A:1378:ARG:H	1:A:1378:ARG:HD2	1.60	0.66
1:A:931:ILE:HG21	1:A:933:TYR:OH	1.95	0.66
1:A:1490:ARG:HG2	1:A:1492:PHE:CZ	2.29	0.66
1:A:1003:LYS:HG3	1:A:1007:GLY:O	1.96	0.66
1:A:1423:ALA:O	1:A:1426:ARG:HG3	1.96	0.66
1:A:884:PRO:HG3	1:A:892:PHE:CD2	2.31	0.66
1:A:1224:PRO:HD2	1:A:1265:LEU:CD1	2.26	0.65
1:A:1015:LYS:HE3	1:A:1050:VAL:CG2	2.26	0.65
2:B:15:DG:C2'	2:B:16:DC:H5'	2.17	0.65
1:A:1016:ILE:HG22	1:A:1018:VAL:HG23	1.78	0.65
1:A:1139:LEU:HD21	1:A:1261:ARG:HH21	1.60	0.65
1:A:1005:SER:O	1:A:1006:ASN:HB2	1.96	0.65
1:A:1139:LEU:HD21	1:A:1261:ARG:NH2	2.11	0.65
1:A:722:LYS:HZ3	1:A:722:LYS:HA	1.61	0.65
1:A:1328:PRO:HG3	1:A:1588:ILE:HA	1.78	0.65
1:A:724:LYS:HG2	1:A:766:ILE:HB	1.76	0.65
1:A:1015:LYS:HD3	1:A:1016:ILE:CA	2.25	0.65
1:A:1136:LEU:H	1:A:1136:LEU:HD13	1.62	0.65
2:B:4:DC:OP1	2:B:4:DC:H4'	1.95	0.65
1:A:1141:THR:OG1	1:A:1161:SER:HB2	1.96	0.65
1:A:1327:PHE:H	1:A:1353:ASN:HD21	1.44	0.64
1:A:724:LYS:HG3	1:A:766:ILE:O	1.96	0.64
1:A:1024:PRO:HG2	1:A:1025:GLU:OE1	1.97	0.64
1:A:1000:PHE:HE2	1:A:1015:LYS:HZ2	1.44	0.64
1:A:1236:ASN:HD21	1:A:1238:ARG:HB3	1.61	0.64
1:A:728:LYS:CG	1:A:731:ILE:HD11	2.28	0.64
1:A:909:ARG:HH21	1:A:1011:GLU:HB2	1.63	0.64
1:A:1068:LEU:CD1	1:A:1072:VAL:HA	2.28	0.64
1:A:655:VAL:HG13	1:A:1533:MET:CB	2.25	0.64
1:A:1073:GLN:HE21	1:A:1074:VAL:CG2	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:LYS:NZ	1:A:1595:CYS:HA	2.13	0.63
1:A:1571:ASP:O	1:A:1575:GLN:HG3	1.99	0.63
1:A:1052:ASP:OD2	1:A:1054:LYS:HG2	1.99	0.63
1:A:1073:GLN:HE21	1:A:1074:VAL:HG22	1.63	0.62
3:C:22:DT:H2''	3:C:23:DG:OP2	1.98	0.62
1:A:1053:PHE:O	1:A:1056:VAL:HG13	1.99	0.62
1:A:1087:GLU:HA	1:A:1099:PRO:HD3	1.81	0.62
1:A:1527:VAL:HG21	1:A:1535:LYS:HZ3	1.63	0.62
1:A:1015:LYS:HG2	1:A:1050:VAL:HG13	1.79	0.62
1:A:1235:PHE:CD2	1:A:1239:THR:HG23	2.35	0.62
1:A:798:CYS:HB2	1:A:817:VAL:HG21	1.80	0.62
1:A:1020:LYS:CE	1:A:1047:GLU:O	2.48	0.62
1:A:1080:PRO:HG2	1:A:1081:ASN:H	1.63	0.62
1:A:1020:LYS:HZ2	1:A:1047:GLU:H	1.45	0.61
1:A:941:LEU:HD23	1:A:1056:VAL:HA	1.79	0.61
1:A:1020:LYS:CE	1:A:1020:LYS:O	2.41	0.61
1:A:1308:GLN:NE2	1:A:1310:ARG:HB2	2.15	0.61
1:A:662:PRO:HD3	1:A:1492:PHE:CD2	2.36	0.61
1:A:1015:LYS:NZ	1:A:1017:ARG:HB2	2.15	0.61
1:A:1136:LEU:N	1:A:1136:LEU:HD13	2.15	0.61
1:A:1485:CYS:O	1:A:1487:PRO:HD3	2.01	0.61
1:A:717:LYS:O	1:A:718:MET:HB3	2.01	0.61
1:A:1551:ARG:HE	1:A:1551:ARG:HA	1.65	0.61
1:A:885:THR:O	1:A:889:LYS:HB2	1.99	0.61
1:A:923:TYR:HE2	1:A:1001:CYS:HG	1.49	0.61
1:A:724:LYS:CE	1:A:766:ILE:HB	2.29	0.61
1:A:743:LYS:HD3	1:A:743:LYS:N	2.15	0.60
1:A:739:LYS:NZ	1:A:739:LYS:HB3	2.15	0.60
1:A:767:PRO:HG3	1:A:775:TYR:CE2	2.36	0.60
1:A:1020:LYS:HZ2	1:A:1047:GLU:N	1.99	0.60
1:A:730:ARG:HD2	1:A:731:ILE:N	2.16	0.60
1:A:774:LEU:HD12	1:A:774:LEU:O	2.01	0.60
1:A:1499:CYS:O	1:A:1502:HIS:HB3	2.01	0.60
1:A:724:LYS:HG2	1:A:766:ILE:CG2	2.31	0.60
1:A:824:GLN:O	1:A:827:TYR:HD1	1.85	0.60
3:C:21:DC:H2'	3:C:22:DT:C6	2.37	0.60
1:A:1379:ASN:HD21	1:A:1417:MET:H	1.50	0.60
1:A:1386:ILE:HG12	1:A:1387:SER:N	2.17	0.60
1:A:775:TYR:C	1:A:776:LEU:HD12	2.22	0.60
1:A:931:ILE:HD11	1:A:1059:ARG:NH1	2.14	0.60
1:A:1233:ASN:HD22	1:A:1234:ARG:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:ARG:HD3	1:A:1269:ARG:C	2.23	0.59
1:A:1190:ASP:HB3	1:A:1193:ILE:HG13	1.83	0.59
1:A:969:TYR:HE1	1:A:1440:PRO:HG3	1.66	0.59
1:A:1585:ALA:C	1:A:1588:ILE:HG22	2.22	0.59
1:A:1020:LYS:HD3	1:A:1047:GLU:CB	2.25	0.59
1:A:1236:ASN:ND2	1:A:1238:ARG:HB3	2.17	0.59
1:A:1006:ASN:C	1:A:1008:ARG:HH21	2.06	0.59
1:A:903:ARG:NH1	1:A:906:GLU:HG3	2.13	0.59
1:A:1068:LEU:HG	1:A:1070:GLU:O	2.01	0.59
1:A:1585:ALA:CA	1:A:1588:ILE:HG22	2.32	0.59
1:A:1599:LYS:O	1:A:1600:ALA:HB3	2.02	0.59
1:A:1136:LEU:HD12	1:A:1597:LEU:HD11	1.84	0.58
1:A:1527:VAL:HG13	1:A:1529:ASN:H	1.67	0.58
1:A:668:LYS:HG2	1:A:669:ALA:N	2.18	0.58
1:A:1585:ALA:HA	1:A:1588:ILE:CG2	2.34	0.58
1:A:1264:LEU:HD13	1:A:1316:LEU:HD23	1.85	0.58
1:A:655:VAL:CG2	1:A:1534:GLY:HA2	2.32	0.58
1:A:1005:SER:O	1:A:1006:ASN:CB	2.51	0.58
1:A:1153:GLU:O	1:A:1157:GLN:HG3	2.03	0.58
1:A:1252:LEU:HD13	1:A:1286:CYS:SG	2.44	0.58
1:A:1428:ILE:HG22	1:A:1516:ARG:HD2	1.86	0.58
1:A:1527:VAL:HG22	1:A:1528:THR:N	2.16	0.58
1:A:734:VAL:HG11	1:A:749:LYS:HD2	1.84	0.58
1:A:652:ARG:HH22	1:A:689:ARG:HB3	1.68	0.58
1:A:1189:GLU:OE1	1:A:1190:ASP:O	2.22	0.58
1:A:1461:ASP:HA	1:A:1479:VAL:CG1	2.34	0.58
1:A:1169:MET:HB2	4:A:1601:SAH:C2	2.34	0.58
1:A:903:ARG:HH11	1:A:906:GLU:CG	2.16	0.58
1:A:1068:LEU:HD11	1:A:1072:VAL:CA	2.33	0.58
1:A:1287:LEU:O	1:A:1292:TYR:HB2	2.04	0.58
1:A:940:TYR:OH	1:A:1081:ASN:HB3	2.04	0.57
1:A:1327:PHE:H	1:A:1353:ASN:ND2	2.02	0.57
1:A:1154:GLY:HA3	1:A:1585:ALA:CB	2.35	0.57
1:A:974:ARG:HG2	1:A:1509:HIS:ND1	2.19	0.57
1:A:1323:LYS:HZ3	1:A:1595:CYS:HA	1.69	0.57
1:A:899:LEU:O	1:A:899:LEU:HD23	2.04	0.57
1:A:670:CYS:HB2	1:A:686:CYS:HA	1.87	0.57
1:A:780:THR:HB	1:A:892:PHE:O	2.05	0.57
2:B:16:DC:H2"	2:B:17:DA:C8	2.40	0.57
1:A:1388:TYR:CE1	1:A:1409:LEU:HD13	2.40	0.57
1:A:655:VAL:CG1	1:A:1531:GLU:HB3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:LYS:NZ	1:A:1047:GLU:N	2.53	0.56
1:A:1467:SER:HB3	1:A:1471:ALA:HB3	1.85	0.56
1:A:1549:SER:OG	1:A:1552:GLU:HG3	2.05	0.56
1:A:723:LYS:HD3	1:A:723:LYS:N	2.20	0.56
1:A:1289:ARG:HH12	1:A:1290:MET:HG3	1.69	0.56
1:A:1195:LEU:HB2	1:A:1254:TYR:CE2	2.40	0.56
1:A:1136:LEU:CD1	1:A:1597:LEU:HD11	2.35	0.56
1:A:891:LYS:O	1:A:891:LYS:HD2	2.05	0.56
1:A:968:LEU:O	1:A:970:PRO:HD3	2.05	0.56
1:A:724:LYS:C	1:A:724:LYS:HD2	2.26	0.56
1:A:1441:ASN:C	1:A:1454:LYS:CD	2.70	0.56
1:A:833:LYS:HZ3	1:A:833:LYS:HA	1.71	0.56
1:A:1015:LYS:HE2	1:A:1016:ILE:O	2.05	0.56
1:A:1030:SER:C	1:A:1032:PRO:HD2	2.25	0.56
1:A:1528:THR:HB	1:A:1574:ARG:HG3	1.86	0.56
1:A:1396:PHE:CZ	1:A:1400:LEU:HD11	2.41	0.56
1:A:728:LYS:HD2	1:A:728:LYS:O	2.05	0.56
1:A:1145:PHE:CE2	1:A:1224:PRO:HG3	2.41	0.56
2:B:6:DT:H2''	2:B:7:DG:O5'	2.06	0.56
1:A:652:ARG:NH2	1:A:689:ARG:HB3	2.21	0.56
2:B:12:DT:H2''	2:B:13:DC:O5'	2.05	0.55
1:A:1441:ASN:CG	1:A:1454:LYS:HD2	2.26	0.55
1:A:903:ARG:HA	1:A:903:ARG:HE	1.71	0.55
1:A:1328:PRO:CG	1:A:1588:ILE:HA	2.36	0.55
1:A:919:SER:HA	1:A:1003:LYS:HZ2	1.70	0.55
3:C:30:DC:H2''	3:C:31:DT:OP2	2.06	0.55
2:B:18:DG:H4'	2:B:19:DG:OP1	2.06	0.55
1:A:1306:VAL:HG13	1:A:1556:SER:O	2.06	0.55
1:A:668:LYS:HD3	1:A:668:LYS:N	2.18	0.55
1:A:1015:LYS:CE	1:A:1050:VAL:HG13	2.36	0.55
1:A:1289:ARG:HH12	1:A:1290:MET:CG	2.20	0.55
1:A:910:VAL:HG21	1:A:923:TYR:CD2	2.41	0.55
1:A:1135:LYS:HD3	1:A:1135:LYS:N	2.22	0.55
1:A:772:LYS:NZ	1:A:772:LYS:HB3	2.21	0.55
1:A:931:ILE:HG12	1:A:1059:ARG:HB2	1.89	0.55
1:A:1315:ILE:N	1:A:1315:ILE:HD12	2.22	0.55
1:A:1311:ARG:NH1	1:A:1340:GLN:HB2	2.22	0.55
1:A:724:LYS:CE	1:A:726:GLN:HG2	2.33	0.55
1:A:1378:ARG:N	1:A:1378:ARG:HD2	2.23	0.54
1:A:1160:ILE:CD1	1:A:1593:LYS:HB3	2.30	0.54
1:A:655:VAL:HG21	1:A:1534:GLY:CA	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:LEU:CD2	1:A:1261:ARG:HH21	2.18	0.54
1:A:1582:PRO:HB2	1:A:1583:PRO:HD3	1.90	0.54
1:A:748:LYS:HA	1:A:748:LYS:HZ1	1.69	0.54
1:A:1168:GLU:O	1:A:1188:THR:HA	2.06	0.54
1:A:1513:LEU:HD12	1:A:1533:MET:HA	1.90	0.54
3:C:34:DC:H2''	3:C:35:DG:C8	2.42	0.54
1:A:1011:GLU:CG	1:A:1012:THR:N	2.70	0.54
1:A:1289:ARG:CG	1:A:1289:ARG:HH11	2.20	0.54
3:C:20:DC:C2'	3:C:21:DC:C6	2.90	0.54
1:A:1265:LEU:HB3	1:A:1315:ILE:HB	1.90	0.54
1:A:748:LYS:HA	1:A:748:LYS:HZ2	1.71	0.54
1:A:1020:LYS:NZ	1:A:1045:SER:O	2.40	0.54
1:A:1031:THR:HG23	1:A:1032:PRO:CD	2.38	0.54
1:A:1187:PHE:CB	1:A:1189:GLU:OE2	2.55	0.54
3:C:22:DT:H3'	3:C:22:DT:OP2	2.08	0.54
1:A:1515:GLY:O	1:A:1540:LEU:HB2	2.06	0.54
1:A:909:ARG:CZ	1:A:909:ARG:HA	2.38	0.54
1:A:1196:LYS:NZ	1:A:1196:LYS:HB3	2.23	0.53
1:A:966:GLU:CG	1:A:1468:SER:HB2	2.30	0.53
1:A:1477:SER:OG	1:A:1486:ASP:HB2	2.08	0.53
1:A:1163:THR:HG21	1:A:1177:PHE:HZ	1.73	0.53
1:A:724:LYS:HG2	1:A:766:ILE:CB	2.38	0.53
1:A:1142:LEU:HD13	1:A:1165:TRP:HB2	1.90	0.53
3:C:21:DC:H2'	3:C:22:DT:C5	2.43	0.53
1:A:1015:LYS:HE2	1:A:1016:ILE:C	2.29	0.53
1:A:1145:PHE:O	4:A:1601:SAH:HB1	2.08	0.53
1:A:1398:ARG:NH1	1:A:1398:ARG:HB2	2.24	0.53
1:A:668:LYS:CD	1:A:668:LYS:H	2.22	0.53
1:A:724:LYS:HZ2	1:A:766:ILE:H	1.56	0.53
1:A:968:LEU:C	1:A:970:PRO:HD3	2.29	0.53
1:A:1156:HIS:CE1	1:A:1163:THR:H	2.27	0.53
1:A:1379:ASN:HD22	1:A:1379:ASN:C	2.07	0.52
1:A:1436:TRP:CD2	1:A:1500:LEU:HD13	2.44	0.52
1:A:1534:GLY:O	1:A:1535:LYS:C	2.47	0.52
1:A:1079:GLY:HA3	1:A:1082:ARG:NE	2.25	0.52
1:A:753:ASP:O	1:A:754:ALA:HB3	2.09	0.52
1:A:1285:ARG:HA	1:A:1288:VAL:HG12	1.91	0.52
1:A:1398:ARG:HH11	1:A:1398:ARG:HB2	1.75	0.52
1:A:1143:ASP:OD2	1:A:1146:SER:HA	2.09	0.52
1:A:1207:ARG:O	1:A:1207:ARG:HD2	2.10	0.52
1:A:1309:THR:HG23	1:A:1338:ALA:HB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:PHE:HA	1:A:1274:PHE:CD2	2.45	0.52
1:A:776:LEU:HD12	1:A:776:LEU:N	2.25	0.52
1:A:1233:ASN:ND2	1:A:1234:ARG:N	2.53	0.52
1:A:1293:GLN:O	1:A:1317:ALA:HA	2.10	0.52
1:A:1395:TRP:HA	1:A:1398:ARG:NH1	2.25	0.52
1:A:655:VAL:HG22	1:A:1533:MET:O	2.10	0.52
1:A:1264:LEU:HD13	1:A:1316:LEU:CD2	2.39	0.51
1:A:1446:LEU:C	1:A:1448:ASP:H	2.13	0.51
1:A:909:ARG:NH1	1:A:910:VAL:H	2.07	0.51
1:A:919:SER:HA	1:A:1003:LYS:NZ	2.24	0.51
1:A:1448:ASP:C	1:A:1450:THR:H	2.13	0.51
1:A:1456:ARG:NE	1:A:1456:ARG:HA	2.22	0.51
1:A:1441:ASN:OD1	1:A:1454:LYS:HD3	2.10	0.51
1:A:1015:LYS:C	1:A:1015:LYS:CD	2.78	0.51
1:A:1207:ARG:NH2	1:A:1209:GLN:HG2	2.16	0.51
1:A:1272:VAL:HA	1:A:1280:LEU:HD22	1.93	0.51
1:A:1475:VAL:CG1	1:A:1502:HIS:HA	2.40	0.51
1:A:893:CYS:SG	1:A:895:SER:HB3	2.51	0.51
1:A:1247:LEU:HD13	4:A:1601:SAH:HN61	1.75	0.51
1:A:702:ASP:O	1:A:703:GLU:C	2.49	0.51
1:A:734:VAL:HB	1:A:749:LYS:CG	2.37	0.51
1:A:910:VAL:HG22	1:A:911:LEU:N	2.26	0.51
1:A:1445:ARG:HA	1:A:1451:MET:HG2	1.92	0.51
1:A:1472:LEU:N	1:A:1472:LEU:HD12	2.25	0.51
1:A:1539:VAL:HG22	1:A:1548:VAL:HG22	1.93	0.51
1:A:1405:TYR:HB3	1:A:1406:GLN:OE1	2.11	0.51
1:A:1524:SER:HB2	1:A:1536:GLN:CD	2.31	0.51
1:A:685:ALA:CB	2:B:13:DC:H5'	2.22	0.51
1:A:651:ARG:HH11	1:A:697:LYS:HA	1.74	0.50
1:A:923:TYR:HE2	1:A:1001:CYS:SG	2.34	0.50
1:A:1015:LYS:HE3	1:A:1050:VAL:HG13	1.93	0.50
1:A:1234:ARG:HB2	1:A:1234:ARG:NH1	2.27	0.50
1:A:1541:HIS:ND1	1:A:1542:PRO:HD2	2.26	0.50
1:A:931:ILE:HG21	1:A:933:TYR:CZ	2.47	0.50
1:A:997:LYS:CE	1:A:997:LYS:HA	2.38	0.50
1:A:1189:GLU:OE1	1:A:1194:LEU:HD13	2.12	0.50
2:B:4:DC:H2'	2:B:5:DG:C8	2.47	0.50
1:A:1329:GLU:OE1	1:A:1354:ILE:HG23	2.11	0.50
1:A:1478:CYS:O	1:A:1479:VAL:C	2.50	0.50
1:A:708:ASN:HA	1:A:1340:GLN:HE22	1.77	0.50
1:A:922:LEU:HD12	1:A:1000:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:DC:C3'	2:B:3:DC:H5''	2.36	0.50
1:A:1004:LYS:O	1:A:1005:SER:C	2.50	0.50
1:A:1041:LEU:O	1:A:1042:LEU:HD12	2.11	0.50
1:A:701:ASP:HB3	1:A:1268:VAL:HB	1.93	0.50
1:A:652:ARG:NH1	1:A:689:ARG:HH11	2.10	0.50
1:A:738:VAL:CG2	1:A:746:TYR:HB2	2.42	0.50
1:A:801:THR:HA	1:A:806:GLY:O	2.12	0.49
1:A:1379:ASN:C	1:A:1379:ASN:ND2	2.65	0.49
1:A:1379:ASN:ND2	1:A:1380:GLY:N	2.55	0.49
1:A:1490:ARG:HG2	1:A:1492:PHE:CE1	2.46	0.49
1:A:651:ARG:NE	1:A:697:LYS:HG2	2.26	0.49
1:A:836:TYR:CD2	1:A:836:TYR:C	2.84	0.49
1:A:759:VAL:O	1:A:759:VAL:HG13	2.11	0.49
1:A:943:PRO:HA	1:A:992:ARG:NH1	2.27	0.49
1:A:1461:ASP:HB3	1:A:1464:ASN:HB2	1.95	0.49
1:A:652:ARG:HH12	1:A:689:ARG:HH11	1.58	0.49
1:A:1008:ARG:H	1:A:1009:PRO:HD2	1.77	0.49
1:A:1279:VAL:O	1:A:1283:THR:HG23	2.13	0.49
1:A:1236:ASN:OD1	1:A:1239:THR:HG22	2.13	0.49
1:A:1308:GLN:HE22	1:A:1310:ARG:HD2	1.77	0.49
3:C:29:DG:H2''	3:C:30:DC:C5	2.48	0.49
1:A:994:GLY:HA3	1:A:1018:VAL:CG1	2.43	0.49
1:A:1445:ARG:NH1	1:A:1445:ARG:HB3	2.28	0.48
1:A:1524:SER:O	1:A:1525:THR:C	2.51	0.48
2:B:2:DC:C2'	2:B:3:DC:C5'	2.68	0.48
1:A:709:ILE:N	1:A:710:PRO:CD	2.76	0.48
1:A:1231:GLY:O	1:A:1232:MET:HG2	2.13	0.48
1:A:1327:PHE:N	1:A:1353:ASN:HD21	2.11	0.48
1:A:1000:PHE:CZ	1:A:1015:LYS:CD	2.90	0.48
1:A:1415:LYS:HE3	1:A:1570:LEU:HD21	1.94	0.48
1:A:1442:ILE:N	1:A:1454:LYS:HE3	2.29	0.48
1:A:1307:ALA:HB2	1:A:1365:ILE:HG22	1.96	0.48
1:A:1008:ARG:HB2	1:A:1009:PRO:HD3	1.95	0.48
1:A:1475:VAL:HG11	1:A:1502:HIS:N	2.29	0.48
1:A:1599:LYS:O	1:A:1600:ALA:CB	2.61	0.48
1:A:1285:ARG:O	1:A:1288:VAL:HG12	2.13	0.48
1:A:1301:ALA:HB3	1:A:1310:ARG:HB3	1.95	0.48
1:A:1461:ASP:CA	1:A:1479:VAL:HG11	2.42	0.48
1:A:791:MET:SD	1:A:824:GLN:HA	2.53	0.48
1:A:1000:PHE:CE2	1:A:1015:LYS:NZ	2.80	0.47
1:A:1479:VAL:HG12	1:A:1479:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:LYS:HG3	1:A:1029:LYS:O	2.14	0.47
1:A:1171:ASP:HB3	1:A:1172:PRO:HD3	1.96	0.47
1:A:1466:ARG:HD2	1:A:1467:SER:O	2.13	0.47
1:A:881:LYS:HD3	1:A:881:LYS:C	2.35	0.47
1:A:888:ASN:ND2	1:A:892:PHE:HD1	2.12	0.47
1:A:1523:PHE:HD2	1:A:1523:PHE:H	1.63	0.47
1:A:1537:GLY:O	1:A:1539:VAL:N	2.48	0.47
1:A:720:GLN:HG3	1:A:721:GLY:N	2.21	0.47
1:A:1145:PHE:HE2	1:A:1224:PRO:HG3	1.80	0.47
1:A:1023:ARG:O	1:A:1026:ASN:HB2	2.15	0.47
1:A:1312:ARG:HG2	1:A:1312:ARG:HH11	1.80	0.47
1:A:1593:LYS:O	1:A:1597:LEU:HD13	2.14	0.47
1:A:971:GLU:HG3	1:A:974:ARG:HD2	1.97	0.47
1:A:1314:ILE:C	1:A:1315:ILE:HD12	2.36	0.47
1:A:1405:TYR:O	1:A:1407:PRO:HD3	2.15	0.47
3:C:28:DG:H2''	3:C:29:DG:H8	1.80	0.47
1:A:1467:SER:CB	1:A:1471:ALA:HB3	2.45	0.47
1:A:1510:TRP:HB3	1:A:1513:LEU:HG	1.95	0.47
1:A:746:TYR:HD1	1:A:783:TRP:HB3	1.73	0.47
2:B:13:DC:H2''	2:B:14:DC:C6	2.50	0.47
1:A:1459:HIS:O	1:A:1472:LEU:HB3	2.14	0.47
1:A:757:LEU:C	1:A:757:LEU:HD13	2.35	0.46
1:A:1021:PHE:HB3	1:A:1042:LEU:HD23	1.97	0.46
1:A:902:MET:O	1:A:906:GLU:HG2	2.14	0.46
1:A:909:ARG:HB3	1:A:909:ARG:HH11	1.81	0.46
1:A:1406:GLN:C	1:A:1408:ILE:H	2.19	0.46
1:A:1457:TYR:O	1:A:1472:LEU:HB2	2.15	0.46
1:A:824:GLN:O	1:A:826:SER:N	2.48	0.46
1:A:934:ARG:O	1:A:996:ILE:HD12	2.14	0.46
1:A:1003:LYS:CG	1:A:1007:GLY:O	2.63	0.46
1:A:971:GLU:HG2	1:A:1436:TRP:CZ3	2.50	0.46
1:A:962:GLU:HB2	1:A:963:PRO:HD2	1.97	0.46
2:B:9:DG:H2''	2:B:10:DC:OP2	2.16	0.46
1:A:1392:PRO:HG3	1:A:1401:ARG:HD3	1.98	0.46
1:A:965:ASP:OD2	1:A:968:LEU:CB	2.60	0.46
2:B:4:DC:H2''	2:B:5:DG:O5'	2.16	0.46
1:A:1258:TYR:O	1:A:1259:ARG:C	2.54	0.46
1:A:759:VAL:O	1:A:759:VAL:CG1	2.63	0.46
1:A:931:ILE:CG2	1:A:933:TYR:CZ	2.98	0.46
1:A:1053:PHE:C	1:A:1055:ALA:H	2.18	0.46
1:A:1475:VAL:HG11	1:A:1502:HIS:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:CYS:HB3	1:A:689:ARG:CD	2.46	0.46
1:A:1308:GLN:NE2	1:A:1310:ARG:HD2	2.30	0.46
3:C:28:DG:H2''	3:C:29:DG:C8	2.51	0.46
1:A:909:ARG:NH2	1:A:1011:GLU:HB2	2.31	0.46
1:A:1068:LEU:HD13	1:A:1072:VAL:HG22	1.97	0.46
1:A:1240:TYR:O	1:A:1243:PHE:HB3	2.16	0.46
1:A:1462:ARG:NE	1:A:1462:ARG:HA	2.25	0.46
1:A:729:ASN:HD22	1:A:729:ASN:N	2.12	0.46
1:A:796:TRP:CD1	1:A:820:CYS:HA	2.50	0.46
1:A:988:PRO:HD3	1:A:1336:PRO:HD3	1.98	0.46
3:C:36:DG:H2''	3:C:37:DG:O5'	2.15	0.46
1:A:1068:LEU:HD11	1:A:1072:VAL:N	2.31	0.45
1:A:686:CYS:HB3	1:A:689:ARG:HD3	1.97	0.45
1:A:871:GLN:HG2	1:A:872:ASP:N	2.31	0.45
1:A:913:GLN:O	1:A:914:LEU:HD23	2.16	0.45
1:A:1015:LYS:HG3	1:A:1050:VAL:HG13	1.97	0.45
1:A:1435:ASP:HA	1:A:1515:GLY:HA2	1.99	0.45
1:A:1472:LEU:H	1:A:1472:LEU:HD12	1.81	0.45
1:A:651:ARG:HE	1:A:697:LYS:CA	2.28	0.45
1:A:871:GLN:OE1	1:A:871:GLN:N	2.48	0.45
1:A:910:VAL:HG21	1:A:923:TYR:CG	2.51	0.45
1:A:1551:ARG:HA	1:A:1551:ARG:NE	2.32	0.45
1:A:1445:ARG:HG3	1:A:1449:GLY:O	2.17	0.45
1:A:1441:ASN:OD1	1:A:1454:LYS:CD	2.65	0.45
2:B:4:DC:H1'	2:B:5:DG:H5'	1.98	0.45
1:A:1500:LEU:CB	1:A:1501:PRO:HD3	2.44	0.45
1:A:919:SER:CA	1:A:1003:LYS:HD3	2.42	0.44
1:A:1163:THR:O	1:A:1184:SER:HB3	2.17	0.44
1:A:1187:PHE:O	1:A:1189:GLU:OE2	2.35	0.44
1:A:1386:ILE:HG12	1:A:1387:SER:H	1.82	0.44
1:A:740:THR:O	1:A:740:THR:HG23	2.17	0.44
1:A:751:CYS:HA	1:A:755:GLU:O	2.17	0.44
1:A:913:GLN:HA	1:A:923:TYR:HA	1.98	0.44
1:A:1410:ARG:O	1:A:1551:ARG:HD2	2.17	0.44
1:A:1145:PHE:HE1	4:A:1601:SAH:N6	2.14	0.44
1:A:833:LYS:HZ2	1:A:833:LYS:HA	1.77	0.44
3:C:29:DG:H1'	3:C:30:DC:C6	2.53	0.44
1:A:1020:LYS:HD2	1:A:1045:SER:OG	2.17	0.44
1:A:1302:GLY:HA2	1:A:1306:VAL:O	2.17	0.44
1:A:700:ASP:OD2	1:A:1268:VAL:HG21	2.17	0.44
2:B:4:DC:H2''	2:B:5:DG:C5'	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:ILE:HG21	1:A:1516:ARG:HG3	1.99	0.44
1:A:692:PRO:C	1:A:694:MET:H	2.21	0.44
1:A:706:ASP:OD2	1:A:707:ASP:N	2.50	0.44
1:A:723:LYS:HB2	1:A:823:MET:HE1	2.00	0.44
1:A:937:ASP:O	1:A:996:ILE:HG13	2.17	0.44
1:A:716:LYS:O	1:A:718:MET:N	2.51	0.44
1:A:715:PRO:O	1:A:716:LYS:HG2	2.17	0.44
1:A:1020:LYS:HD3	1:A:1047:GLU:C	2.38	0.44
1:A:792:PHE:CE2	1:A:823:MET:HB2	2.53	0.44
1:A:1287:LEU:HA	1:A:1290:MET:HE3	1.99	0.44
1:A:1369:ASP:O	1:A:1397:GLN:HG3	2.18	0.44
1:A:1148:CYS:HB3	1:A:1575:GLN:HB3	1.99	0.44
1:A:1031:THR:N	1:A:1032:PRO:HD2	2.33	0.44
1:A:1136:LEU:O	1:A:1136:LEU:HD22	2.17	0.44
1:A:1160:ILE:HG13	1:A:1596:MET:CE	2.48	0.44
1:A:1229:PHE:C	1:A:1231:GLY:H	2.21	0.44
1:A:1306:VAL:HG12	1:A:1308:GLN:HB3	2.00	0.44
1:A:995:ARG:NH2	1:A:995:ARG:HG2	2.33	0.44
1:A:664:CYS:SG	1:A:665:GLY:N	2.86	0.43
1:A:909:ARG:HB3	1:A:909:ARG:NH1	2.32	0.43
1:A:962:GLU:H	1:A:962:GLU:CD	2.21	0.43
1:A:1454:LYS:HD3	1:A:1455:LEU:N	2.25	0.43
1:A:995:ARG:HG2	1:A:995:ARG:HH21	1.83	0.43
1:A:1289:ARG:CZ	1:A:1289:ARG:HB3	2.49	0.43
1:A:1312:ARG:HG2	1:A:1312:ARG:NH1	2.33	0.43
1:A:718:MET:O	1:A:718:MET:HG3	2.18	0.43
1:A:813:GLU:HG2	1:A:815:PHE:CZ	2.53	0.43
1:A:1071:CYS:HB3	1:A:1074:VAL:HG23	2.00	0.43
1:A:1213:GLN:HB2	1:A:1216:ASP:OD2	2.19	0.43
1:A:1490:ARG:CG	1:A:1492:PHE:CZ	3.01	0.43
1:A:931:ILE:HG23	1:A:933:TYR:CE2	2.53	0.43
1:A:972:HIS:HA	1:A:1437:ARG:O	2.19	0.43
1:A:1068:LEU:CD1	1:A:1072:VAL:HG22	2.49	0.43
1:A:1428:ILE:HD13	1:A:1514:TYR:O	2.18	0.43
1:A:1379:ASN:HD22	1:A:1380:GLY:H	1.63	0.43
1:A:828:ILE:HG22	1:A:829:HIS:N	2.33	0.43
1:A:700:ASP:O	1:A:701:ASP:CG	2.57	0.43
1:A:1008:ARG:HB2	1:A:1009:PRO:CD	2.49	0.43
1:A:1190:ASP:OD2	1:A:1191:CYS:N	2.51	0.43
1:A:1395:TRP:O	1:A:1399:GLN:HG2	2.19	0.43
1:A:1441:ASN:CG	1:A:1454:LYS:CD	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:PRO:O	1:A:711:GLU:C	2.57	0.43
1:A:873:TYR:CD2	1:A:873:TYR:N	2.87	0.43
2:B:4:DC:C2'	2:B:5:DG:C8	3.01	0.43
1:A:1227:GLN:O	1:A:1229:PHE:N	2.51	0.43
1:A:1015:LYS:HE3	1:A:1050:VAL:CG1	2.49	0.43
1:A:1504:GLY:HA2	1:A:1510:TRP:CD1	2.54	0.43
1:A:1527:VAL:HG21	1:A:1535:LYS:HZ1	1.83	0.43
1:A:949:ASN:HD21	1:A:1047:GLU:CD	2.22	0.43
1:A:1004:LYS:HD3	1:A:1004:LYS:C	2.39	0.42
1:A:1015:LYS:HZ1	1:A:1017:ARG:HB2	1.84	0.42
1:A:1374:LEU:CD1	1:A:1552:GLU:HG2	2.48	0.42
1:A:1475:VAL:HG11	1:A:1502:HIS:HA	2.01	0.42
1:A:1414:CYS:C	1:A:1569:ILE:HD11	2.38	0.42
1:A:835:ILE:HG13	1:A:864:PHE:CB	2.49	0.42
1:A:1020:LYS:CE	1:A:1020:LYS:CA	2.97	0.42
1:A:1024:PRO:C	1:A:1026:ASN:H	2.22	0.42
1:A:1329:GLU:OE1	1:A:1329:GLU:HA	2.19	0.42
1:A:1015:LYS:HZ1	1:A:1017:ARG:CB	2.32	0.42
1:A:1377:VAL:HG21	1:A:1412:HIS:CD2	2.54	0.42
1:A:1399:GLN:NE2	1:A:1399:GLN:HA	2.34	0.42
1:A:1430:LEU:HD22	1:A:1543:GLU:HA	2.00	0.42
1:A:889:LYS:NZ	1:A:889:LYS:HB2	2.33	0.42
1:A:928:LYS:O	1:A:931:ILE:CG2	2.61	0.42
2:B:15:DG:C2'	2:B:16:DC:C5'	2.87	0.42
1:A:1021:PHE:CB	1:A:1042:LEU:HD23	2.50	0.42
1:A:1559:PHE:HA	1:A:1560:PRO:HD3	1.91	0.42
1:A:1003:LYS:HE2	1:A:1007:GLY:O	2.20	0.42
1:A:1305:GLY:N	1:A:1332:HIS:HD2	2.18	0.42
3:C:22:DT:H1'	3:C:23:DG:C8	2.54	0.42
1:A:715:PRO:HG2	1:A:872:ASP:OD1	2.19	0.42
3:C:21:DC:OP1	3:C:21:DC:H4'	2.19	0.42
1:A:1261:ARG:HD2	1:A:1322:GLU:OE1	2.20	0.42
1:A:724:LYS:HE3	1:A:766:ILE:CB	2.44	0.42
1:A:1217:VAL:HB	1:A:1258:TYR:HD2	1.84	0.42
1:A:1500:LEU:O	1:A:1504:GLY:N	2.47	0.42
1:A:1516:ARG:NH2	1:A:1543:GLU:O	2.53	0.42
1:A:1569:ILE:HG23	1:A:1570:LEU:N	2.34	0.42
1:A:651:ARG:HE	1:A:697:LYS:CB	2.33	0.42
1:A:872:ASP:C	1:A:873:TYR:HD2	2.23	0.42
1:A:879:PRO:HA	1:A:880:PRO:HD3	1.87	0.42
2:B:10:DC:H1'	2:B:11:DC:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:PHE:N	1:A:890:PHE:CD1	2.88	0.42
1:A:961:LYS:N	1:A:961:LYS:HD2	2.35	0.42
1:A:1225:PRO:HG2	1:A:1247:LEU:HD12	2.02	0.42
1:A:1289:ARG:CG	1:A:1289:ARG:NH1	2.78	0.42
1:A:1551:ARG:HH21	1:A:1554:ALA:CB	2.33	0.42
1:A:1568:ASN:O	1:A:1572:LYS:HG3	2.19	0.42
1:A:1589:GLY:O	1:A:1592:ILE:HB	2.20	0.42
1:A:675:LYS:O	1:A:675:LYS:HG2	2.20	0.42
1:A:738:VAL:HG23	1:A:739:LYS:N	2.35	0.42
1:A:1015:LYS:NZ	1:A:1017:ARG:CA	2.83	0.41
1:A:1395:TRP:HA	1:A:1398:ARG:HH12	1.83	0.41
1:A:1015:LYS:CG	1:A:1016:ILE:N	2.83	0.41
1:A:1020:LYS:NZ	1:A:1045:SER:C	2.74	0.41
1:A:1068:LEU:O	1:A:1068:LEU:HD23	2.20	0.41
1:A:1305:GLY:N	1:A:1332:HIS:CD2	2.88	0.41
1:A:1528:THR:HA	1:A:1577:GLY:HA3	2.02	0.41
1:A:1225:PRO:HG3	4:A:1601:SAH:C8	2.49	0.41
1:A:974:ARG:HH11	1:A:1505:ASN:N	2.18	0.41
1:A:1220:LEU:HD23	1:A:1263:PHE:HD2	1.85	0.41
1:A:1428:ILE:HD12	1:A:1540:LEU:HD23	2.02	0.41
1:A:738:VAL:HG22	1:A:746:TYR:C	2.41	0.41
1:A:843:TRP:C	1:A:845:MET:H	2.23	0.41
1:A:843:TRP:O	1:A:845:MET:N	2.51	0.41
1:A:1235:PHE:CE2	1:A:1240:TYR:HA	2.56	0.41
2:B:14:DC:H2"	2:B:15:DG:C8	2.55	0.41
1:A:1269:ARG:HD3	1:A:1269:ARG:O	2.21	0.41
1:A:1039:ILE:HD12	1:A:1362:PHE:CD1	2.55	0.41
1:A:1386:ILE:CG1	1:A:1387:SER:N	2.83	0.41
1:A:1428:ILE:HA	1:A:1429:PRO:HD3	1.95	0.41
1:A:757:LEU:HD12	1:A:782:LEU:HD11	2.01	0.41
1:A:1195:LEU:HD22	1:A:1254:TYR:CD2	2.56	0.41
1:A:1574:ARG:HB2	1:A:1574:ARG:HH11	1.86	0.41
1:A:1598:ALA:O	1:A:1600:ALA:N	2.53	0.41
1:A:776:LEU:HD22	1:A:814:LEU:HD11	2.03	0.41
1:A:1455:LEU:HD12	1:A:1496:ILE:HB	2.03	0.41
1:A:698:GLU:OE1	1:A:699:ALA:N	2.53	0.41
1:A:750:VAL:HG22	1:A:751:CYS:N	2.34	0.41
1:A:1015:LYS:HZ1	1:A:1017:ARG:CA	2.33	0.41
1:A:686:CYS:HB3	1:A:689:ARG:HG3	2.03	0.41
1:A:706:ASP:C	1:A:706:ASP:OD2	2.58	0.41
1:A:933:TYR:HE1	1:A:1059:ARG:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:THR:HG23	1:A:947:THR:O	2.20	0.41
1:A:1020:LYS:HE2	1:A:1047:GLU:O	2.20	0.41
1:A:1098:ASP:HA	1:A:1099:PRO:HD3	1.98	0.41
1:A:1289:ARG:NH1	1:A:1290:MET:HG3	2.34	0.41
1:A:651:ARG:HD2	1:A:651:ARG:C	2.41	0.41
1:A:690:ARG:HG3	1:A:690:ARG:O	2.21	0.41
1:A:700:ASP:OD1	1:A:700:ASP:N	2.54	0.41
1:A:700:ASP:HB2	1:A:701:ASP:H	1.73	0.41
1:A:752:ILE:CD1	1:A:828:ILE:HD12	2.51	0.41
1:A:888:ASN:HD21	1:A:892:PHE:HD1	1.69	0.41
3:C:21:DC:C2'	3:C:22:DT:C6	3.04	0.41
1:A:1188:THR:O	1:A:1188:THR:HG23	2.21	0.41
1:A:1495:LEU:O	1:A:1497:PRO:HD3	2.21	0.41
1:A:1144:VAL:O	1:A:1145:PHE:HB2	2.21	0.41
1:A:974:ARG:HG2	1:A:1509:HIS:CG	2.56	0.41
1:A:1593:LYS:HA	1:A:1596:MET:HE2	2.02	0.41
1:A:722:LYS:HZ2	1:A:722:LYS:HA	1.84	0.41
1:A:724:LYS:NZ	1:A:766:ILE:H	2.19	0.41
1:A:1003:LYS:HE2	1:A:1008:ARG:CZ	2.51	0.40
1:A:1015:LYS:NZ	1:A:1017:ARG:CB	2.83	0.40
1:A:1015:LYS:CE	1:A:1016:ILE:C	2.89	0.40
1:A:1388:TYR:HE1	1:A:1409:LEU:HD13	1.86	0.40
1:A:965:ASP:HB3	1:A:968:LEU:HB3	2.03	0.40
1:A:1030:SER:OG	1:A:1031:THR:N	2.54	0.40
1:A:1178:ARG:HG2	1:A:1186:VAL:CG2	2.51	0.40
1:A:1325:PRO:HA	1:A:1595:CYS:SG	2.62	0.40
1:A:651:ARG:CZ	1:A:697:LYS:HG2	2.52	0.40
1:A:919:SER:HA	1:A:1003:LYS:CE	2.51	0.40
1:A:1021:PHE:CG	1:A:1042:LEU:HD23	2.57	0.40
1:A:1142:LEU:HD12	1:A:1165:TRP:O	2.22	0.40
1:A:1333:VAL:HG23	1:A:1364:THR:HB	2.04	0.40
1:A:1406:GLN:HA	1:A:1407:PRO:HD3	1.82	0.40
1:A:1539:VAL:O	1:A:1548:VAL:HG13	2.21	0.40
1:A:1015:LYS:HZ3	1:A:1017:ARG:HB2	1.86	0.40
1:A:1236:ASN:H	1:A:1239:THR:CG2	2.35	0.40
1:A:1423:ALA:HB2	1:A:1446:LEU:HD22	2.02	0.40
1:A:876:PHE:O	1:A:1293:GLN:HA	2.22	0.40
1:A:948:PHE:C	1:A:950:ILE:H	2.24	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	892/956 (93%)	729 (82%)	125 (14%)	38 (4%)	2	24

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	CYS
1	A	715	PRO
1	A	717	LYS
1	A	825	LEU
1	A	844	ALA
1	A	1579	ALA
1	A	656	CYS
1	A	703	GLU
1	A	742	GLY
1	A	806	GLY
1	A	1006	ASN
1	A	1080	PRO
1	A	1228	GLY
1	A	1229	PHE
1	A	1504	GLY
1	A	1525	THR
1	A	1599	LYS
1	A	690	ARG
1	A	847	GLY
1	A	848	GLY
1	A	888	ASN
1	A	929	ASN
1	A	965	ASP
1	A	1301	ALA
1	A	1510	TRP
1	A	951	LYS
1	A	970	PRO
1	A	1201	GLY

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Mol	Chain	Res	Type
1	A	1270	ASN
1	A	1535	LYS
1	A	741	ASP
1	A	1232	MET
1	A	767	PRO
1	A	1005	SER
1	A	1407	PRO
1	A	1002	PRO
1	A	1008	ARG
1	A	1351	VAL

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	782/824 (95%)	702 (90%)	80 (10%)	7 34

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	663	GLU
1	A	668	LYS
1	A	687	GLN
1	A	698	GLU
1	A	700	ASP
1	A	704	GLU
1	A	722	LYS
1	A	724	LYS
1	A	728	LYS
1	A	743	LYS
1	A	748	LYS
1	A	753	ASP
1	A	792	PHE
1	A	833	LYS
1	A	836	TYR
1	A	850	ASP

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Mol	Chain	Res	Type
1	A	866	GLN
1	A	881	LYS
1	A	889	LYS
1	A	891	LYS
1	A	909	ARG
1	A	922	LEU
1	A	937	ASP
1	A	949	ASN
1	A	961	LYS
1	A	962	GLU
1	A	964	VAL
1	A	974	ARG
1	A	995	ARG
1	A	996	ILE
1	A	997	LYS
1	A	1003	LYS
1	A	1010	ASN
1	A	1012	THR
1	A	1020	LYS
1	A	1031	THR
1	A	1038	ASP
1	A	1056	VAL
1	A	1059	ARG
1	A	1062	VAL
1	A	1067	ASP
1	A	1068	LEU
1	A	1135	LYS
1	A	1136	LEU
1	A	1144	VAL
1	A	1160	ILE
1	A	1189	GLU
1	A	1210	ARG
1	A	1226	CYS
1	A	1233	ASN
1	A	1235	PHE
1	A	1242	LYS
1	A	1276	ARG
1	A	1279	VAL
1	A	1292	TYR
1	A	1323	LYS
1	A	1344	VAL
1	A	1357	LEU

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Mol	Chain	Res	Type
1	A	1363	ARG
1	A	1369	ASP
1	A	1378	ARG
1	A	1379	ASN
1	A	1389	ASN
1	A	1391	GLU
1	A	1404	GLN
1	A	1426	ARG
1	A	1448	ASP
1	A	1454	LYS
1	A	1455	LEU
1	A	1456	ARG
1	A	1462	ARG
1	A	1466	ARG
1	A	1490	ARG
1	A	1495	LEU
1	A	1513	LEU
1	A	1535	LYS
1	A	1536	GLN
1	A	1539	VAL
1	A	1574	ARG
1	A	1584	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	729	ASN
1	A	793	HIS
1	A	824	GLN
1	A	866	GLN
1	A	949	ASN
1	A	1010	ASN
1	A	1026	ASN
1	A	1057	GLN
1	A	1073	GLN
1	A	1090	ASN
1	A	1156	HIS
1	A	1181	ASN
1	A	1213	GLN
1	A	1233	ASN
1	A	1236	ASN
1	A	1300	GLN

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Mol	Chain	Res	Type
1	A	1308	GLN
1	A	1379	ASN
1	A	1399	GLN
1	A	1412	HIS
1	A	1507	HIS
1	A	1573	HIS
1	A	1578	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	1601	-	21,28,28	1.20	2 (9%)	20,40,40	1.83	4 (20%)

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	1601	-	-	0/7/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1601	SAH	O4'-C1'	3.79	1.46	1.41
4	A	1601	SAH	C8-N7	-2.50	1.30	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1601	SAH	N3-C2-N1	-4.43	121.75	128.68
4	A	1601	SAH	CB-CG-SD	-3.52	105.42	113.31
4	A	1601	SAH	C3'-C2'-C1'	3.34	106.01	100.98
4	A	1601	SAH	C4'-C5'-SD	-2.42	105.10	113.78

There are no chirality outliers.

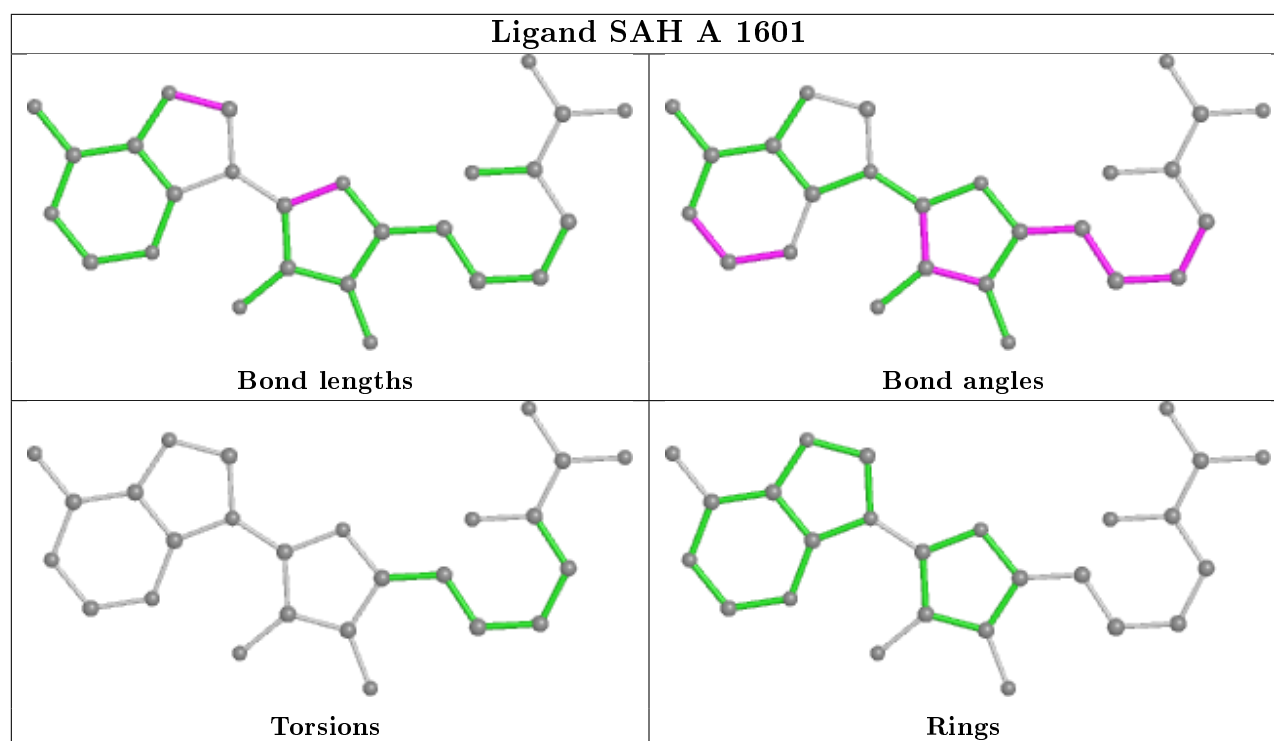
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1601	SAH	5	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	904/956 (94%)	-0.16	13 (1%) 75 61	45, 126, 167, 189	0
2	B	19/19 (100%)	0.03	1 (5%) 26 16	129, 173, 197, 200	1 (5%)
3	C	19/19 (100%)	-0.27	0 100 100	164, 175, 200, 200	0
All	All	942/994 (94%)	-0.16	14 (1%) 73 60	45, 128, 173, 200	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	984	ASN	4.6
1	A	706	ASP	3.6
1	A	1222	GLY	3.6
2	B	19	DG	3.3
1	A	1405	TYR	2.6
1	A	849	MET	2.4
1	A	1406	GLN	2.4
1	A	700	ASP	2.3
1	A	690	ARG	2.3
1	A	704	GLU	2.2
1	A	688	GLU	2.1
1	A	1223	GLY	2.1
1	A	720	GLN	2.1
1	A	742	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

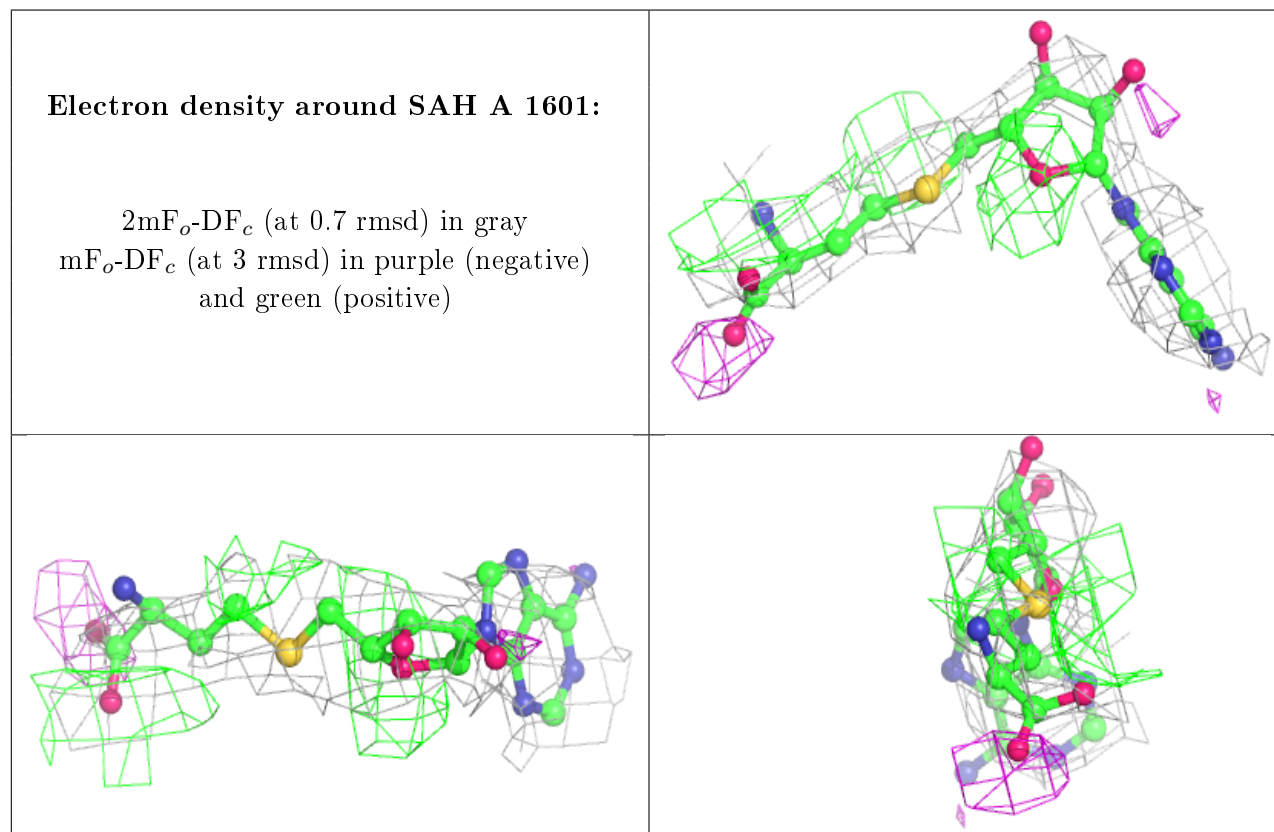
There are no carbohydrates in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SAH	A	1601	26/26	0.72	0.43	128,128,128,128	0
5	ZN	A	5	1/1	0.81	0.08	128,128,128,128	1
5	ZN	A	1	1/1	0.92	0.04	128,128,128,128	1
5	ZN	A	3	1/1	0.95	0.10	128,128,128,128	0
5	ZN	A	2	1/1	0.96	0.06	128,128,128,128	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

There are no such residues in this entry.