



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:16 PM UTC

PDB ID : 4U7T / pdb_00004u7t
Title : Crystal structure of DNMT3A-DNMT3L in complex with histone H3
Authors : Guo, X.; Wang, L.; Yin, X.; Li, J.; Xiao, J.; He, S.; Wang, J.; Xu, Y.
Deposited on : 2014-07-31
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

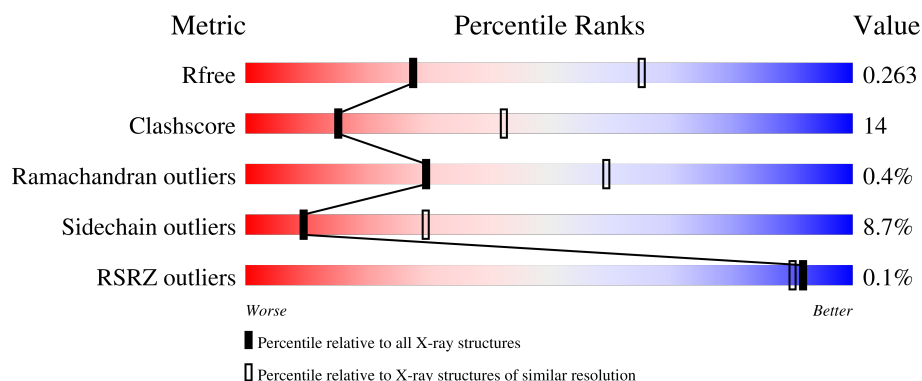
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	
1	C	445	
2	B	209	
2	D	209	
3	F	12	

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Mol	Chain	Length	Quality of chain
3	G	12	 58% 25% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10047 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 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3347	2125	592	595	35			
1	C	418	Total	C	N	O	S	0	0	0
			3354	2130	593	596	35			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	468	GLY	-	expression tag	UNP Q9Y6K1
A	469	PRO	-	expression tag	UNP Q9Y6K1
A	470	LEU	-	expression tag	UNP Q9Y6K1
A	471	GLY	-	expression tag	UNP Q9Y6K1
A	472	SER	-	expression tag	UNP Q9Y6K1
A	473	PRO	-	expression tag	UNP Q9Y6K1
A	474	GLU	-	expression tag	UNP Q9Y6K1
A	475	PHE	-	expression tag	UNP Q9Y6K1
C	468	GLY	-	expression tag	UNP Q9Y6K1
C	469	PRO	-	expression tag	UNP Q9Y6K1
C	470	LEU	-	expression tag	UNP Q9Y6K1
C	471	GLY	-	expression tag	UNP Q9Y6K1
C	472	SER	-	expression tag	UNP Q9Y6K1
C	473	PRO	-	expression tag	UNP Q9Y6K1
C	474	GLU	-	expression tag	UNP Q9Y6K1
C	475	PHE	-	expression tag	UNP Q9Y6K1

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	0	1	0
			1540	1003	257	275	5			
2	D	191	Total	C	N	O	S	0	0	0
			1579	1030	267	277	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP Q9UJW3
B	172	PRO	-	expression tag	UNP Q9UJW3
B	173	LEU	-	expression tag	UNP Q9UJW3
B	174	GLY	-	expression tag	UNP Q9UJW3
B	175	SER	-	expression tag	UNP Q9UJW3
B	176	GLU	-	expression tag	UNP Q9UJW3
B	177	PHE	-	expression tag	UNP Q9UJW3
D	171	GLY	-	expression tag	UNP Q9UJW3
D	172	PRO	-	expression tag	UNP Q9UJW3
D	173	LEU	-	expression tag	UNP Q9UJW3
D	174	GLY	-	expression tag	UNP Q9UJW3
D	175	SER	-	expression tag	UNP Q9UJW3
D	176	GLU	-	expression tag	UNP Q9UJW3
D	177	PHE	-	expression tag	UNP Q9UJW3

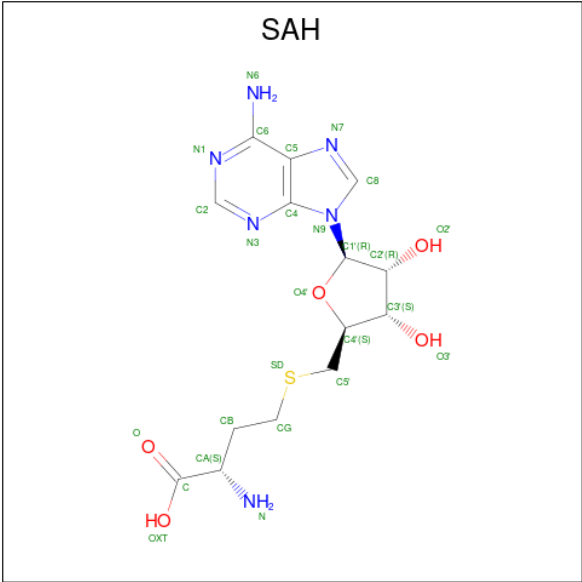
- Molecule 3 is a protein called peptide from Histone H3.3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	10	Total	C	N	O	0	0	0
			79	46	19	14			
3	G	10	Total	C	N	O	0	0	0
			79	46	19	14			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		
4	C	3	Total	Zn	0	0
			3	3		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

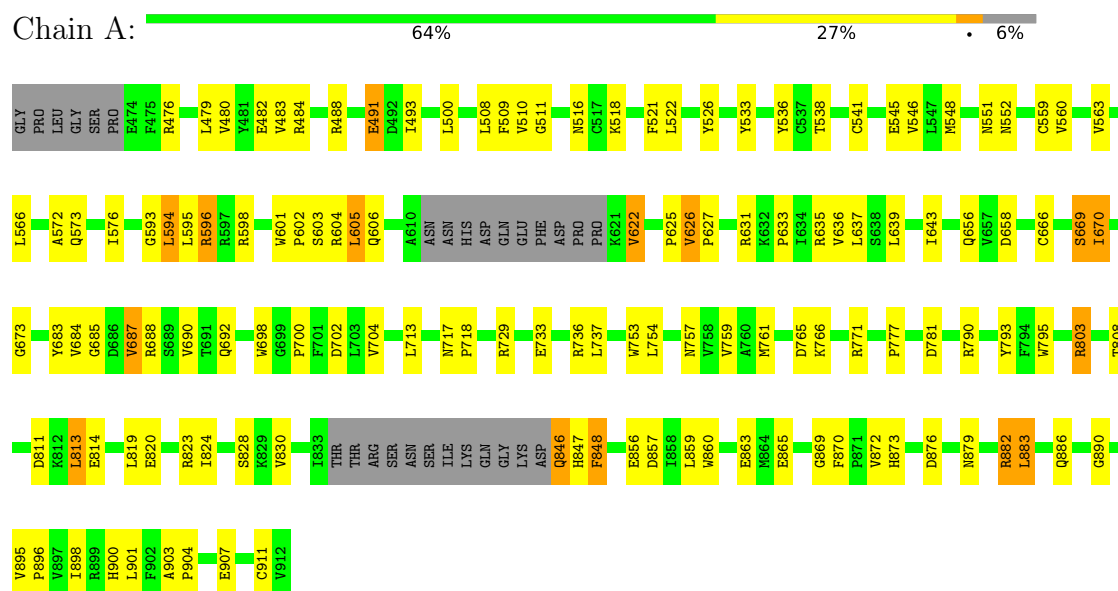
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		

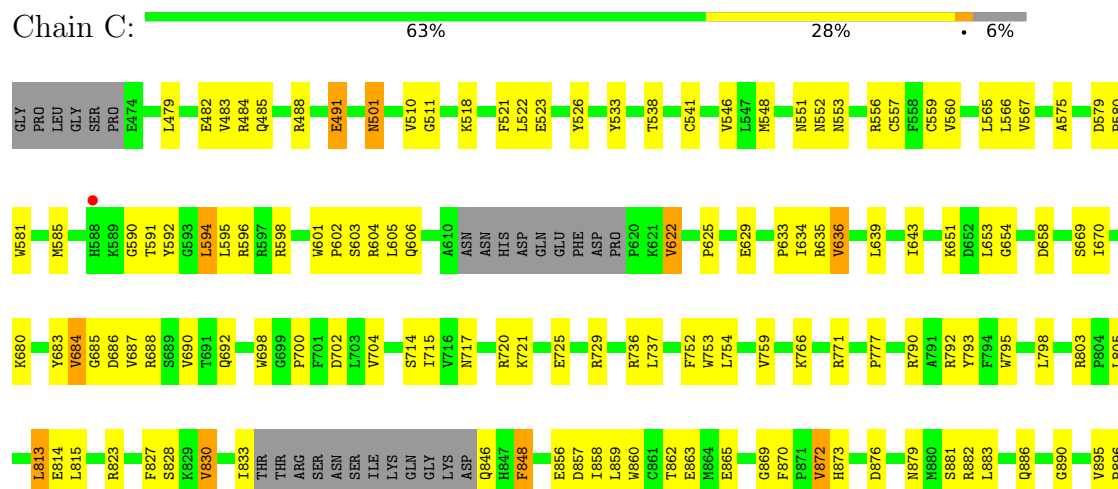
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA (cytosine-5)-methyltransferase 3A



• Molecule 1: DNA (cytosine-5)-methyltransferase 3A





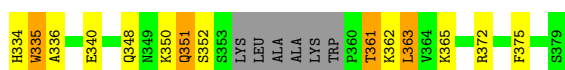
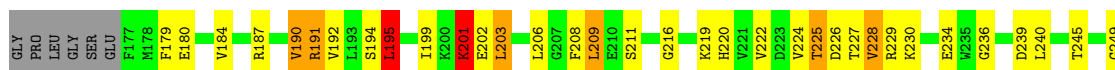
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain B: 56% 27% 6% 11%



- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain D: 51% 33% 7% 9%



- Molecule 3: peptide from Histone H3.3

Chain F: 58% 25% 17%



- Molecule 3: peptide from Histone H3.3

Chain G: 58% 25% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	183.82Å 183.82Å 123.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.21 – 2.90 40.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.21-2.90) 99.8 (40.21-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.223 , 0.261 0.226 , 0.263	Depositor DCC
R_{free} test set	2669 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10047	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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	0.66	2/3426 (0.1%)	1.02	7/4625 (0.2%)
1	C	0.66	3/3434 (0.1%)	1.02	9/4636 (0.2%)
2	B	0.55	0/1584	1.06	7/2149 (0.3%)
2	D	0.55	0/1629	1.06	10/2215 (0.5%)
3	F	0.32	0/78	0.79	0/101
3	G	0.47	0/78	0.75	0/101
All	All	0.63	5/10229 (0.0%)	1.03	33/13827 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	895	VAL	CA-CB	9.00	1.60	1.53
1	A	895	VAL	CA-CB	7.59	1.59	1.53
1	C	684	VAL	CA-CB	-5.55	1.47	1.54
1	A	898	ILE	CA-CB	-5.40	1.47	1.54
1	C	898	ILE	CA-CB	-5.06	1.48	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	903	ALA	CA-C-N	-9.06	110.25	120.04
1	C	903	ALA	C-N-CA	-9.06	110.25	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	903	ALA	CA-C-N	-8.57	110.96	119.87
1	A	903	ALA	C-N-CA	-8.57	110.96	119.87
2	B	312	VAL	N-CA-C	8.26	119.80	107.75
2	B	362	LYS	N-CA-C	7.06	120.61	109.39
2	D	309	ILE	CA-C-N	7.06	128.66	119.84
2	D	309	ILE	C-N-CA	7.06	128.66	119.84
1	A	848	PHE	CA-C-N	7.05	128.65	119.84
1	A	848	PHE	C-N-CA	7.05	128.65	119.84
1	C	636	VAL	N-CA-C	6.72	117.80	108.12
1	A	636	VAL	N-CA-C	6.62	117.65	108.12
2	B	195	LEU	CA-C-N	-5.94	113.03	122.17
2	B	195	LEU	C-N-CA	-5.94	113.03	122.17
2	D	327	ILE	CA-C-N	5.89	125.85	119.78
2	D	327	ILE	C-N-CA	5.89	125.85	119.78
1	C	848	PHE	CA-C-N	5.78	126.54	120.12
1	C	848	PHE	C-N-CA	5.78	126.54	120.12
2	D	276	SER	CA-C-N	5.77	125.87	119.87
2	D	276	SER	C-N-CA	5.77	125.87	119.87
2	B	202	GLU	N-CA-C	-5.63	98.81	110.80
2	D	195	LEU	CA-C-N	-5.47	113.75	122.17
2	D	195	LEU	C-N-CA	-5.47	113.75	122.17
1	C	680	LYS	N-CA-C	5.44	117.97	111.71
1	A	895	VAL	CA-C-N	-5.33	114.17	119.56
1	A	895	VAL	C-N-CA	-5.33	114.17	119.56
2	D	273	LYS	CA-C-N	-5.20	113.95	120.51
2	D	273	LYS	C-N-CA	-5.20	113.95	120.51
2	B	276	SER	CA-C-N	5.09	125.16	119.87
2	B	276	SER	C-N-CA	5.09	125.16	119.87
1	C	895	VAL	CA-C-N	-5.04	114.47	119.56
1	C	895	VAL	C-N-CA	-5.04	114.47	119.56
1	C	523	GLU	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	201	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3347	0	3278	94	0
1	C	3354	0	3286	95	0
2	B	1540	0	1516	47	1
2	D	1579	0	1558	52	1
3	F	79	0	91	2	0
3	G	79	0	91	3	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	26	0	19	1	0
5	C	26	0	19	0	0
6	A	6	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
All	All	10047	0	9858	270	1

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 14.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:ARG:HH21	1:C:700:PRO:HB2	1.33	0.91
1:A:635:ARG:HH21	1:A:700:PRO:HB2	1.39	0.85
2:D:245:THR:O	2:D:287:ASN:ND2	2.17	0.78
1:A:882:ARG:HE	1:C:881:SER:HA	1.49	0.76
1:C:803:ARG:NH2	1:C:900:HIS:O	2.21	0.74
1:A:823:ARG:NH2	1:A:857:ASP:OD2	2.20	0.74
2:D:249:GLY:N	2:D:350:LYS:HZ1	1.85	0.73
1:C:715:ILE:HA	1:C:720:ARG:HD3	1.71	0.73
2:D:191:ARG:HH11	2:D:191:ARG:HB3	1.53	0.73
1:A:606:GLN:HG2	1:A:622:VAL:HG11	1.68	0.72
2:B:245:THR:O	2:B:287:ASN:ND2	2.23	0.72
1:A:593:GLY:O	1:A:596:ARG:NH1	2.23	0.72
2:B:350:LYS:O	2:B:352:SER:N	2.24	0.70
1:C:754:LEU:HD11	1:C:901:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:HE2	1:A:765:ASP:HB3	1.73	0.69
1:A:602:PRO:HB3	1:A:625:PRO:HD2	1.74	0.68
2:D:202:GLU:HB3	2:D:362:LYS:HD3	1.76	0.67
2:D:195:LEU:HD21	2:D:266:LEU:HD12	1.77	0.67
1:A:803:ARG:NH2	1:A:900:HIS:O	2.27	0.67
1:A:754:LEU:HD11	1:A:901:LEU:HD13	1.77	0.66
1:A:848:PHE:HB2	1:A:856:GLU:HG2	1.78	0.66
1:C:602:PRO:HB3	1:C:625:PRO:HD2	1.78	0.65
1:C:606:GLN:HG2	1:C:622:VAL:HG11	1.77	0.65
2:D:202:GLU:O	2:D:206:LEU:HD23	1.96	0.65
2:B:228:VAL:HG12	2:B:230:LYS:H	1.61	0.64
1:A:484:ARG:HH21	1:A:594:LEU:HD11	1.63	0.64
1:A:873:HIS:ND1	1:C:876:ASP:OD2	2.22	0.63
1:C:690:VAL:O	1:C:736:ARG:NH2	2.32	0.62
1:C:639:LEU:HD22	1:C:687:VAL:HG23	1.81	0.62
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.35	0.62
1:C:598:ARG:HD3	1:C:604:ARG:NH1	2.14	0.62
1:C:653:LEU:O	1:C:906:LYS:HE2	2.00	0.61
1:A:598:ARG:HD3	1:A:604:ARG:NH1	2.15	0.61
2:B:234:GLU:C	2:B:236:GLY:H	2.09	0.61
2:D:228:VAL:HG12	2:D:230:LYS:H	1.66	0.61
1:A:736:ARG:HH21	1:A:737:LEU:HD21	1.65	0.60
2:B:181:THR:HG23	2:B:373:GLU:HG3	1.83	0.60
1:C:684:VAL:HG12	1:C:685:GLY:H	1.67	0.60
1:C:823:ARG:NH1	1:C:857:ASP:OD2	2.31	0.60
1:A:879:ASN:ND2	1:C:882:ARG:HD2	2.16	0.60
2:D:281:PHE:HA	2:D:326:ASN:HD21	1.67	0.60
2:B:219:LYS:HE2	2:B:235:TRP:CE2	2.37	0.59
1:C:736:ARG:HH21	1:C:737:LEU:HD21	1.67	0.59
1:A:684:VAL:HG12	1:A:685:GLY:H	1.67	0.59
2:D:310:PRO:HA	2:D:320:ALA:N	2.18	0.59
2:D:234:GLU:C	2:D:236:GLY:H	2.10	0.58
2:D:192:VAL:HG11	2:D:199:ILE:HD11	1.86	0.58
1:A:690:VAL:O	1:A:736:ARG:NH2	2.37	0.58
1:C:790:ARG:NH2	1:C:890:GLY:O	2.36	0.57
1:C:591:THR:HG23	1:C:596:ARG:CZ	2.35	0.57
2:B:229:ARG:HB2	2:B:269:TYR:CD1	2.41	0.56
2:B:287:ASN:HA	2:B:321:VAL:HG22	1.85	0.56
1:C:598:ARG:O	1:C:601:TRP:HD1	1.89	0.56
2:D:199:ILE:O	2:D:203:LEU:HB2	2.05	0.56
2:B:208:PHE:CZ	2:B:372:ARG:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:LEU:HD21	2:B:343:LEU:HD22	1.87	0.56
1:A:476:ARG:O	1:A:480:VAL:HG23	2.06	0.56
1:C:717:ASN:O	1:C:720:ARG:HG3	2.06	0.55
1:A:546:VAL:HA	1:A:559:CYS:HA	1.88	0.55
2:B:224:VAL:O	2:B:227:THR:N	2.25	0.55
1:A:876:ASP:OD2	1:C:873:HIS:ND1	2.25	0.55
1:C:848:PHE:HB2	1:C:856:GLU:HG2	1.89	0.55
1:C:479:LEU:O	1:C:483:VAL:HG23	2.07	0.55
1:C:484:ARG:NH2	1:C:565:LEU:O	2.37	0.54
1:A:511:GLY:H	1:A:598:ARG:HH21	1.54	0.54
1:A:633:PRO:HB2	1:A:658:ASP:HB2	1.90	0.54
1:A:820:GLU:O	1:A:823:ARG:HG3	2.08	0.54
1:C:511:GLY:H	1:C:598:ARG:HH21	1.56	0.54
2:D:179:PHE:CE2	2:D:279:PRO:HA	2.42	0.54
1:C:579:ASP:HB3	1:C:580:PRO:HD3	1.90	0.53
1:C:865:GLU:OE1	1:C:873:HIS:N	2.28	0.53
2:D:306:PRO:HB3	2:D:324:TRP:CE2	2.42	0.53
1:A:736:ARG:NH1	2:B:300:ARG:HG2	2.24	0.53
2:D:361:THR:O	2:D:363:LEU:N	2.36	0.53
1:A:598:ARG:O	1:A:601:TRP:HD1	1.92	0.53
1:A:736:ARG:NH1	2:B:300:ARG:HH11	2.06	0.53
1:A:813:LEU:O	1:A:814:GLU:HB2	2.07	0.53
2:B:363:LEU:HD12	2:B:363:LEU:H	1.74	0.53
2:D:192:VAL:HG22	2:D:240:LEU:HB3	1.91	0.53
1:A:846:GLN:HG3	1:A:847:HIS:ND1	2.24	0.53
1:C:633:PRO:HB2	1:C:658:ASP:HB2	1.89	0.52
2:D:322:ARG:NH2	2:D:340:GLU:OE2	2.42	0.52
2:B:281:PHE:HA	2:B:326:ASN:HD21	1.73	0.52
1:C:882:ARG:O	1:C:886:GLN:HG2	2.09	0.52
1:A:687:VAL:HG22	5:A:1004:SAH:N1	2.25	0.52
1:C:484:ARG:NH2	1:C:594:LEU:HD21	2.24	0.52
1:A:509:PHE:O	1:A:598:ARG:NE	2.32	0.52
1:A:566:LEU:HA	1:A:594:LEU:HD12	1.90	0.52
1:A:729:ARG:NH2	2:B:257:SER:OG	2.42	0.52
1:C:813:LEU:O	1:C:814:GLU:HB2	2.09	0.52
1:A:484:ARG:NH2	1:A:594:LEU:HD11	2.26	0.51
2:B:190:VAL:HG12	2:B:375:PHE:CG	2.45	0.51
2:B:201:LYS:NZ	2:B:205:SER:HB2	2.25	0.51
1:C:526:TYR:CD2	1:C:904:PRO:HB3	2.45	0.51
1:A:508:LEU:HD21	1:A:605:LEU:HD22	1.92	0.51
2:B:285:VAL:HG22	2:B:323:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ASN:ND2	1:C:858:ILE:HD11	2.25	0.51
1:A:510:VAL:HG21	1:A:596:ARG:HD3	1.93	0.50
1:A:766:LYS:HD2	1:A:793:TYR:CE2	2.46	0.50
1:C:814:GLU:HA	1:C:828:SER:O	2.11	0.50
1:A:688:ARG:O	2:B:300:ARG:HD2	2.11	0.50
1:C:823:ARG:NH2	1:C:863:GLU:OE1	2.41	0.50
1:A:601:TRP:CG	1:A:602:PRO:HD3	2.46	0.50
1:A:479:LEU:O	1:A:483:VAL:HG23	2.11	0.50
1:A:551:ASN:OD1	1:A:552:ASN:N	2.45	0.49
1:A:823:ARG:NH1	1:A:863:GLU:OE1	2.45	0.49
2:B:179:PHE:CE2	2:B:279:PRO:HA	2.47	0.49
2:B:208:PHE:CE1	2:B:372:ARG:HG3	2.46	0.49
2:D:208:PHE:CZ	2:D:372:ARG:HG3	2.47	0.49
2:D:285:VAL:HG22	2:D:323:VAL:HG22	1.94	0.49
1:C:777:PRO:HD3	1:C:795:TRP:NE1	2.28	0.49
1:A:545:GLU:HG3	3:F:5:GLN:OE1	2.12	0.49
2:B:239:ASP:HB3	2:B:375:PHE:CZ	2.48	0.49
2:B:263:PHE:CE2	2:B:284:PHE:HB2	2.47	0.49
1:C:590:GLY:C	1:C:596:ARG:HD3	2.38	0.49
1:C:670:ILE:HG23	1:C:683:TYR:CE1	2.47	0.49
1:A:790:ARG:NH2	1:A:890:GLY:O	2.44	0.49
1:C:556:ARG:HD2	1:C:585:MET:HG3	1.95	0.49
1:C:686:ASP:OD2	1:C:688:ARG:NH2	2.45	0.49
1:A:733:GLU:CD	2:B:300:ARG:HH12	2.21	0.49
1:A:759:VAL:HG23	1:A:793:TYR:CZ	2.48	0.49
2:B:202:GLU:HB3	2:B:362:LYS:HD3	1.95	0.49
1:C:566:LEU:O	1:C:594:LEU:HG	2.12	0.48
1:C:567:VAL:HA	1:C:592:TYR:O	2.13	0.48
1:A:521:PHE:HA	1:A:541:CYS:SG	2.53	0.48
1:C:521:PHE:HA	1:C:541:CYS:SG	2.53	0.48
1:A:879:ASN:CG	1:C:882:ARG:HD2	2.38	0.48
1:A:882:ARG:H	1:A:882:ARG:HH11	1.61	0.48
1:C:548:MET:HE3	3:G:2:ARG:HB3	1.94	0.48
1:C:510:VAL:HA	1:C:598:ARG:NH2	2.28	0.48
1:C:815:LEU:HD13	1:C:830:VAL:HG12	1.96	0.48
2:D:263:PHE:CE2	2:D:284:PHE:HB2	2.49	0.48
1:A:518:LYS:O	1:A:522:LEU:HG	2.14	0.48
2:D:203:LEU:HD23	2:D:209:LEU:HD11	1.96	0.48
1:C:482:GLU:OE1	1:C:488:ARG:HD2	2.14	0.47
1:A:643:ILE:HD11	1:A:870:PHE:CZ	2.49	0.47
1:C:482:GLU:HA	1:C:485:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:VAL:HB	1:A:572:ALA:HB2	1.95	0.47
1:A:573:GLN:HA	1:A:576:ILE:HD12	1.95	0.47
1:A:846:GLN:HE21	1:A:847:HIS:CE1	2.32	0.47
2:D:229:ARG:HB2	2:D:269:TYR:CD1	2.49	0.47
1:A:606:GLN:CG	1:A:622:VAL:HG11	2.40	0.47
1:C:827:PHE:HZ	1:C:846:GLN:HB2	1.80	0.47
2:B:201:LYS:O	2:B:362:LYS:NZ	2.47	0.47
1:C:715:ILE:O	1:C:720:ARG:NH1	2.47	0.47
1:A:666:CYS:SG	1:A:669:SER:OG	2.72	0.46
1:C:526:TYR:CE2	1:C:904:PRO:HB3	2.50	0.46
1:A:883:LEU:HD12	1:A:883:LEU:HA	1.80	0.46
1:C:869:GLY:HA3	1:C:896:PRO:HD3	1.97	0.46
1:A:684:VAL:HG12	1:A:685:GLY:N	2.30	0.46
1:C:551:ASN:OD1	1:C:552:ASN:N	2.49	0.46
1:A:626:VAL:HG22	1:A:631:ARG:HG2	1.96	0.46
1:A:670:ILE:HG23	1:A:683:TYR:CD1	2.50	0.46
1:C:862:THR:OG1	1:C:872:VAL:HG23	2.16	0.46
2:D:329:ALA:HB1	2:D:332:SER:HB2	1.97	0.46
1:C:813:LEU:H	1:C:813:LEU:HG	1.58	0.46
1:C:684:VAL:HG12	1:C:685:GLY:N	2.30	0.46
1:A:882:ARG:HH21	1:C:882:ARG:H	1.64	0.45
1:C:670:ILE:HG23	1:C:683:TYR:CD1	2.51	0.45
1:C:792:ARG:HH22	1:C:833:ILE:HB	1.81	0.45
2:D:234:GLU:C	2:D:236:GLY:N	2.74	0.45
1:C:606:GLN:CG	1:C:622:VAL:HG11	2.46	0.45
1:A:865:GLU:OE1	1:A:873:HIS:N	2.30	0.45
2:B:260:LEU:HD21	2:B:298:ALA:HA	1.99	0.45
2:D:288:LEU:HD23	2:D:288:LEU:HA	1.77	0.45
1:A:704:VAL:O	1:A:753:TRP:HA	2.16	0.45
2:B:184:VAL:HA	2:B:187:ARG:NE	2.32	0.45
1:C:860:TRP:O	1:C:863:GLU:N	2.50	0.45
1:C:546:VAL:HA	1:C:559:CYS:HA	1.97	0.45
1:A:713:LEU:HD12	1:A:757:ASN:ND2	2.32	0.45
1:A:823:ARG:HD3	1:A:863:GLU:OE2	2.17	0.45
2:B:276:SER:HA	2:B:277:PRO:HD3	1.78	0.45
1:C:518:LYS:O	1:C:522:LEU:HG	2.15	0.45
2:D:274:PRO:HA	2:D:275:GLY:HA2	1.72	0.45
2:D:351:GLN:O	2:D:352:SER:OG	2.27	0.45
1:A:673:GLY:HA3	1:A:683:TYR:OH	2.17	0.45
1:C:601:TRP:N	1:C:602:PRO:HD2	2.32	0.45
1:A:598:ARG:HH11	1:A:604:ARG:HH12	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:SER:O	2:D:220:HIS:HA	2.17	0.44
1:A:635:ARG:HD3	1:A:702:ASP:OD2	2.17	0.44
1:A:656:GLN:NE2	1:A:911:CYS:O	2.39	0.44
1:A:736:ARG:HH12	2:B:300:ARG:HH11	1.64	0.44
2:B:224:VAL:O	2:B:225:THR:C	2.60	0.44
2:B:361:THR:O	2:B:363:LEU:HD12	2.18	0.44
1:C:643:ILE:HD11	1:C:870:PHE:CZ	2.51	0.44
1:C:815:LEU:HD11	1:C:859:LEU:HD21	1.99	0.44
1:C:533:TYR:CD2	1:C:548:MET:HB3	2.52	0.44
2:B:224:VAL:O	2:B:226:ASP:N	2.50	0.44
1:C:484:ARG:HH21	1:C:594:LEU:HD21	1.82	0.44
1:A:533:TYR:CE2	1:A:548:MET:HB3	2.53	0.44
1:C:736:ARG:HH12	2:D:300:ARG:HH11	1.66	0.44
1:A:491:GLU:H	1:A:491:GLU:HG2	1.38	0.44
1:A:823:ARG:HH11	1:A:863:GLU:CD	2.26	0.44
2:B:219:LYS:HE2	2:B:235:TRP:CD2	2.52	0.44
2:D:192:VAL:HG21	2:D:203:LEU:HD21	1.99	0.44
1:A:526:TYR:CD2	1:A:904:PRO:HG3	2.53	0.43
2:B:245:THR:OG1	2:B:286:ASP:HA	2.18	0.43
1:C:598:ARG:HH11	1:C:604:ARG:HH12	1.66	0.43
2:D:239:ASP:HB3	2:D:375:PHE:CZ	2.53	0.43
1:A:482:GLU:HB3	1:A:488:ARG:HG3	2.00	0.43
1:A:814:GLU:HA	1:A:828:SER:O	2.18	0.43
1:A:860:TRP:O	1:A:863:GLU:N	2.51	0.43
1:C:729:ARG:NH2	2:D:257:SER:OG	2.51	0.43
2:D:190:VAL:HG13	2:D:192:VAL:HG23	2.00	0.43
1:A:666:CYS:O	1:A:670:ILE:HG12	2.18	0.43
1:A:670:ILE:HG23	1:A:683:TYR:CE1	2.53	0.43
1:C:581:TRP:CB	3:G:1:ALA:HB2	2.48	0.43
2:D:229:ARG:HA	2:D:269:TYR:CD2	2.53	0.43
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.79	0.43
2:B:260:LEU:CD2	2:B:298:ALA:HA	2.49	0.43
2:B:309:ILE:HD11	2:B:321:VAL:HG12	1.99	0.43
2:B:350:LYS:HA	2:B:350:LYS:HD2	1.80	0.43
2:D:224:VAL:O	2:D:225:THR:C	2.62	0.43
2:D:312:VAL:HG23	2:D:313:HIS:H	1.84	0.43
2:B:234:GLU:C	2:B:236:GLY:N	2.74	0.43
2:D:224:VAL:HG21	2:D:262:GLN:HB3	1.99	0.43
2:D:335:TRP:HB2	2:D:336:ALA:H	1.71	0.42
1:C:591:THR:HG23	1:C:596:ARG:NE	2.35	0.42
1:C:872:VAL:HG22	1:C:873:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:VAL:HA	2:D:187:ARG:NE	2.34	0.42
2:D:195:LEU:HD12	2:D:195:LEU:HA	1.72	0.42
1:A:637:LEU:HG	1:A:639:LEU:CD1	2.49	0.42
1:C:736:ARG:NH1	2:D:300:ARG:NH1	2.67	0.42
1:C:736:ARG:NH1	2:D:300:ARG:HH11	2.18	0.42
2:D:295:LEU:HA	2:D:295:LEU:HD23	1.81	0.42
1:C:704:VAL:O	1:C:753:TRP:HA	2.19	0.42
1:A:510:VAL:HA	1:A:598:ARG:NH2	2.34	0.42
1:C:501:ASN:HD22	1:C:501:ASN:C	2.26	0.42
1:A:639:LEU:HD21	1:A:737:LEU:HD12	2.02	0.42
1:C:546:VAL:HB	1:C:557:CYS:HB3	2.01	0.42
2:D:224:VAL:O	2:D:227:THR:N	2.31	0.42
1:C:634:ILE:HG23	1:C:636:VAL:HG23	2.01	0.42
1:C:635:ARG:HD3	1:C:702:ASP:OD2	2.19	0.42
1:C:575:ALA:O	3:G:1:ALA:N	2.51	0.41
2:D:206:LEU:HD21	2:D:365:LYS:HG3	2.02	0.41
1:A:771:ARG:NH1	2:B:226:ASP:OD1	2.53	0.41
1:C:766:LYS:HD2	1:C:793:TYR:CE2	2.56	0.41
1:C:805:LEU:HA	1:C:805:LEU:HD23	1.90	0.41
1:C:552:ASN:O	1:C:553:ASN:HB2	2.21	0.41
2:D:249:GLY:H	2:D:350:LYS:HZ1	1.65	0.41
2:D:372:ARG:HE	2:D:372:ARG:HB3	1.47	0.41
1:A:536:TYR:OH	3:F:9:LYS:HG2	2.20	0.41
1:A:781:ASP:HA	1:A:790:ARG:O	2.20	0.41
1:C:684:VAL:HG11	1:C:698:TRP:HH2	1.85	0.41
1:A:808:THR:HG22	1:A:811:ASP:OD2	2.21	0.41
1:C:491:GLU:H	1:C:491:GLU:HG2	1.37	0.41
1:C:759:VAL:HG23	1:C:793:TYR:CZ	2.55	0.41
1:A:777:PRO:HD3	1:A:795:TRP:NE1	2.36	0.41
2:B:201:LYS:HZ3	2:B:205:SER:HB2	1.85	0.41
2:D:311:ASP:HB2	2:D:312:VAL:H	1.65	0.41
1:C:721:LYS:HB3	1:C:725:GLU:HB2	2.01	0.41
1:A:684:VAL:HG11	1:A:698:TRP:HH2	1.85	0.41
1:A:717:ASN:HA	1:A:718:PRO:HD3	1.90	0.41
1:A:493:ILE:HD13	1:A:500:LEU:HD13	2.03	0.41
2:B:224:VAL:HG21	2:B:262:GLN:HB3	2.03	0.41
1:C:533:TYR:CE2	1:C:548:MET:HB3	2.56	0.41
1:C:752:PHE:HB3	1:C:798:LEU:HD23	2.03	0.41
2:D:240:LEU:HA	2:D:281:PHE:O	2.20	0.41
1:A:533:TYR:CD2	1:A:548:MET:HB3	2.56	0.40
2:B:309:ILE:HA	2:B:310:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:827:PHE:CZ	1:C:846:GLN:HB2	2.57	0.40
2:D:201:LYS:HB2	2:D:362:LYS:NZ	2.36	0.40
1:A:626:VAL:HA	1:A:627:PRO:HD3	1.96	0.40
2:B:305:GLU:HG3	2:B:306:PRO:HD2	2.02	0.40
1:C:827:PHE:HZ	1:C:846:GLN:N	2.19	0.40
2:D:179:PHE:CD2	2:D:279:PRO:HA	2.56	0.40
2:D:224:VAL:O	2:D:226:ASP:N	2.55	0.40
1:A:869:GLY:HA3	1:A:896:PRO:HD3	2.04	0.40
2:B:309:ILE:H	2:B:309:ILE:HG13	1.77	0.40
1:C:651:LYS:O	1:C:654:GLY:N	2.41	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:LYS:NZ	2:D:180:GLU:OE1[2_664]	2.14	0.06

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	411/445 (92%)	380 (92%)	31 (8%)	0	100	100
1	C	412/445 (93%)	381 (92%)	31 (8%)	0	100	100
2	B	178/209 (85%)	156 (88%)	20 (11%)	2 (1%)	11	36
2	D	185/209 (88%)	162 (88%)	20 (11%)	3 (2%)	7	27
3	F	8/12 (67%)	8 (100%)	0	0	100	100
3	G	8/12 (67%)	8 (100%)	0	0	100	100
All	All	1202/1332 (90%)	1095 (91%)	102 (8%)	5 (0%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	225	THR
2	D	201	LYS
2	D	225	THR
2	B	216	GLY
2	D	216	GLY

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	365/390 (94%)	339 (93%)	26 (7%)	13	40
1	C	366/390 (94%)	347 (95%)	19 (5%)	21	52
2	B	173/189 (92%)	151 (87%)	22 (13%)	4	14
2	D	177/189 (94%)	151 (85%)	26 (15%)	3	10
3	F	8/9 (89%)	7 (88%)	1 (12%)	4	15
3	G	8/9 (89%)	7 (88%)	1 (12%)	4	15
All	All	1097/1176 (93%)	1002 (91%)	95 (9%)	9	30

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	GLU
1	A	516	ASN
1	A	538	THR
1	A	560	VAL
1	A	594	LEU
1	A	595	LEU
1	A	596	ARG
1	A	603	SER
1	A	605	LEU
1	A	622	VAL
1	A	626	VAL
1	A	669	SER
1	A	670	ILE
1	A	687	VAL

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Mol	Chain	Res	Type
1	A	692	GLN
1	A	803	ARG
1	A	813	LEU
1	A	819	LEU
1	A	824	ILE
1	A	830	VAL
1	A	846	GLN
1	A	872	VAL
1	A	882	ARG
1	A	883	LEU
1	A	886	GLN
1	A	907	GLU
2	B	195	LEU
2	B	201	LYS
2	B	203	LEU
2	B	211	SER
2	B	214	ASP
2	B	217	GLN
2	B	219	LYS
2	B	222	VAL
2	B	229	ARG
2	B	245	THR
2	B	251	THR
2	B	257	SER
2	B	271	ARG
2	B	278	ARG
2	B	288	LEU
2	B	309	ILE
2	B	311	ASP
2	B	321	VAL
2	B	341	GLU
2	B	346	LEU
2	B	348	GLN
2	B	363	LEU
1	C	491	GLU
1	C	501	ASN
1	C	538	THR
1	C	560	VAL
1	C	594	LEU
1	C	595	LEU
1	C	603	SER
1	C	605	LEU

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Mol	Chain	Res	Type
1	C	622	VAL
1	C	629	GLU
1	C	669	SER
1	C	692	GLN
1	C	714	SER
1	C	771	ARG
1	C	813	LEU
1	C	830	VAL
1	C	872	VAL
1	C	879	ASN
1	C	883	LEU
2	D	190	VAL
2	D	191	ARG
2	D	195	LEU
2	D	201	LYS
2	D	203	LEU
2	D	209	LEU
2	D	211	SER
2	D	219	LYS
2	D	222	VAL
2	D	228	VAL
2	D	250	HIS
2	D	251	THR
2	D	257	SER
2	D	271	ARG
2	D	278	ARG
2	D	309	ILE
2	D	311	ASP
2	D	312	VAL
2	D	321	VAL
2	D	333	ARG
2	D	334	HIS
2	D	335	TRP
2	D	348	GLN
2	D	351	GLN
2	D	361	THR
2	D	363	LEU
3	F	3	THR
3	G	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	802	ASN
1	A	846	GLN
1	A	879	ASN
1	C	606	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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
5	SAH	A	1004	-	27,28,28	1.15	4 (14%)	36,40,40	2.01	10 (27%)
5	SAH	C	1004	-	27,28,28	1.07	3 (11%)	36,40,40	1.95	9 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAH	A	1004	-	-	7/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAH	C	1004	-	-	6/15/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1004	SAH	C2-N1	2.82	1.38	1.33
5	C	1004	SAH	C2-N1	2.79	1.38	1.33
5	A	1004	SAH	C2-N3	2.54	1.38	1.33
5	C	1004	SAH	C2-N3	2.25	1.37	1.33
5	C	1004	SAH	C8-N7	2.20	1.35	1.31
5	A	1004	SAH	C8-N7	2.17	1.35	1.31
5	A	1004	SAH	C5-N7	-2.04	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1004	SAH	N3-C2-N1	-5.76	119.86	128.58
5	A	1004	SAH	N3-C2-N1	-5.24	120.64	128.58
5	A	1004	SAH	C5-C4-N3	-4.50	120.52	126.72
5	C	1004	SAH	C5-C4-N3	-3.97	121.24	126.72
5	A	1004	SAH	O4'-C1'-N9	3.62	115.04	108.09
5	A	1004	SAH	N9-C8-N7	-3.45	109.04	113.94
5	A	1004	SAH	C5-N7-C8	3.39	108.78	103.45
5	C	1004	SAH	N9-C8-N7	-3.28	109.29	113.94
5	C	1004	SAH	C2-N3-C4	3.22	119.70	111.83
5	A	1004	SAH	C2-N3-C4	3.15	119.53	111.83
5	C	1004	SAH	O4'-C1'-N9	3.07	113.99	108.09
5	C	1004	SAH	C5-N7-C8	2.82	107.89	103.45
5	A	1004	SAH	N3-C4-N9	2.69	131.74	127.17
5	A	1004	SAH	C4-C5-N7	-2.59	107.62	110.58
5	C	1004	SAH	N3-C4-N9	2.51	131.43	127.17
5	C	1004	SAH	CB-CG-SD	-2.30	108.31	113.45
5	A	1004	SAH	C6-C5-C4	2.26	120.26	117.18
5	A	1004	SAH	CB-CG-SD	-2.04	108.90	113.45
5	C	1004	SAH	C2'-C3'-C4'	2.03	106.54	102.61

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1004	SAH	N-CA-CB-CG

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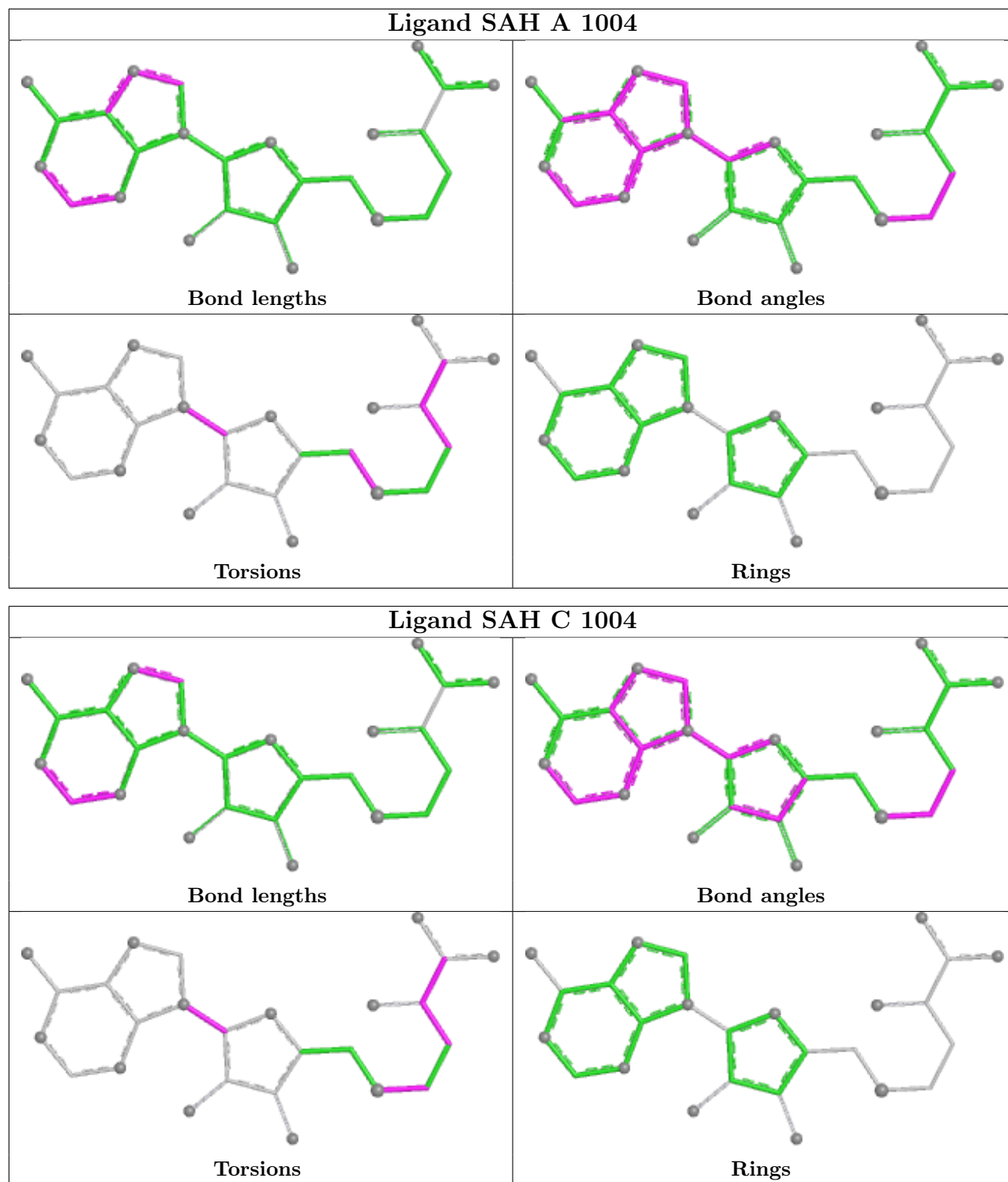
Mol	Chain	Res	Type	Atoms
5	A	1004	SAH	C-CA-CB-CG
5	C	1004	SAH	N-CA-CB-CG
5	A	1004	SAH	C2'-C1'-N9-C8
5	C	1004	SAH	C2'-C1'-N9-C8
5	A	1004	SAH	C4'-C5'-SD-CG
5	C	1004	SAH	O4'-C1'-N9-C8
5	A	1004	SAH	O4'-C1'-N9-C8
5	C	1004	SAH	CB-CG-SD-C5'
5	A	1004	SAH	O-C-CA-CB
5	C	1004	SAH	OXT-C-CA-CB
5	C	1004	SAH	C2'-C1'-N9-C4
5	A	1004	SAH	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1004	SAH	1	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	417/445 (93%)	-1.16	0 100 100	43, 72, 132, 162	0
1	C	418/445 (93%)	-1.16	1 (0%) 91 89	44, 73, 133, 179	0
2	B	187/209 (89%)	-1.06	0 100 100	46, 81, 155, 182	1 (0%)
2	D	191/209 (91%)	-1.02	0 100 100	52, 85, 155, 174	0
3	F	10/12 (83%)	-0.83	0 100 100	97, 106, 117, 133	0
3	G	10/12 (83%)	-0.80	0 100 100	96, 104, 117, 127	0
All	All	1233/1332 (92%)	-1.12	1 (0%) 92 90	43, 77, 140, 182	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	588	HIS	2.4

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](#)

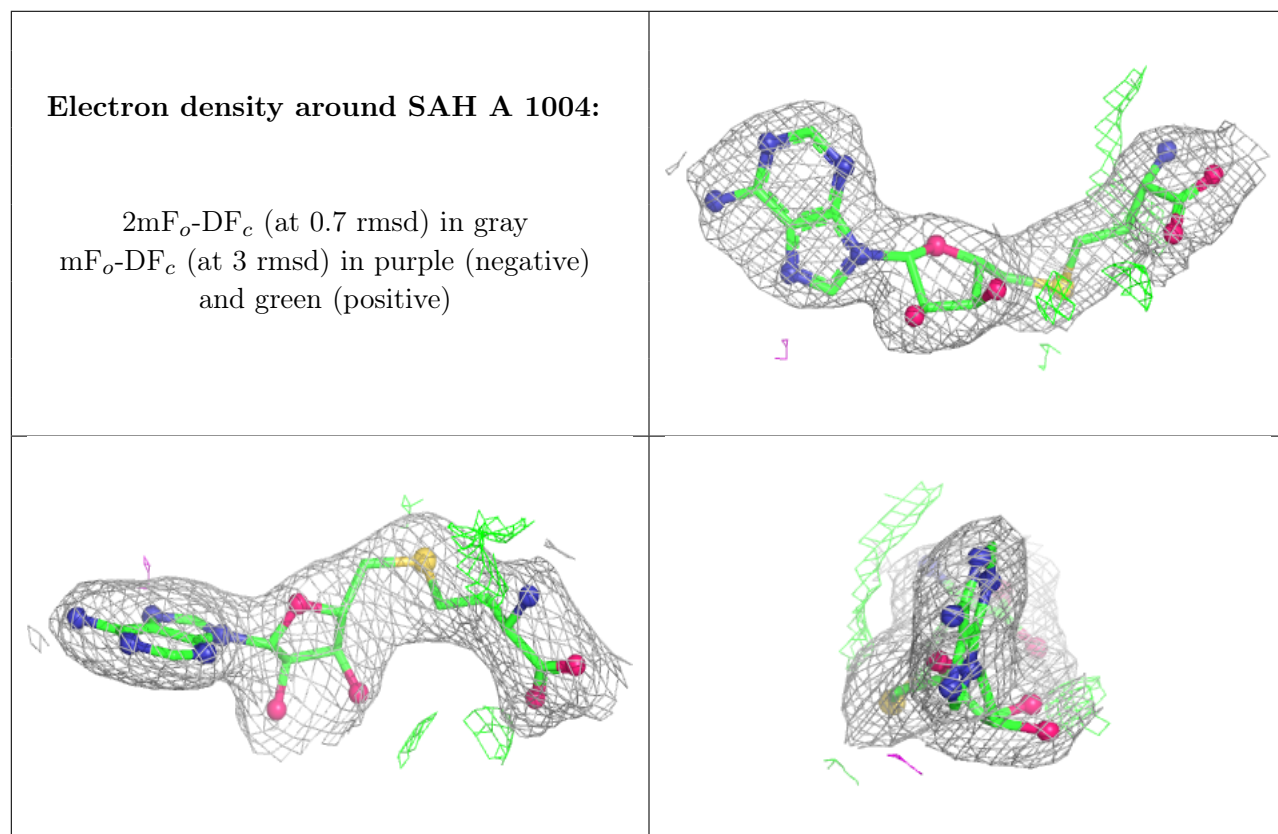
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

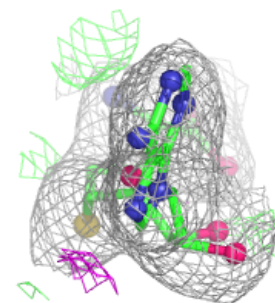
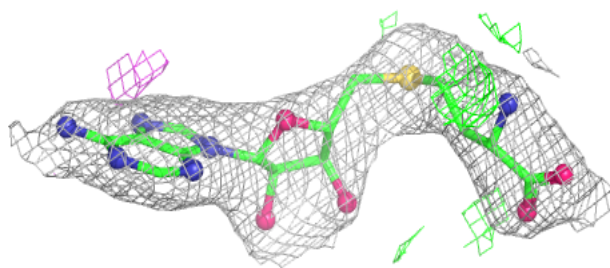
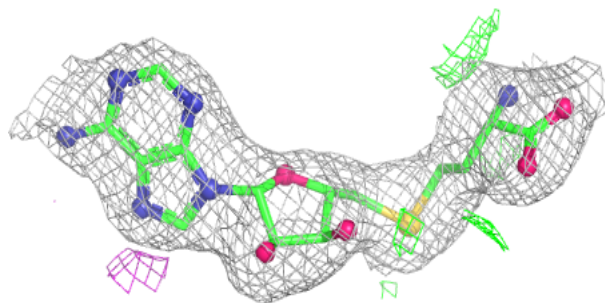
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SAH	A	1004	26/26	0.99	0.04	44,55,65,77	0
5	SAH	C	1004	26/26	0.99	0.05	46,55,64,75	0
4	ZN	A	1003	1/1	1.00	0.02	99,99,99,99	0
4	ZN	C	1001	1/1	1.00	0.01	79,79,79,79	0
4	ZN	C	1002	1/1	1.00	0.01	103,103,103,103	0
4	ZN	C	1003	1/1	1.00	0.01	95,95,95,95	0
4	ZN	A	1001	1/1	1.00	0.01	80,80,80,80	0
4	ZN	A	1002	1/1	1.00	0.01	108,108,108,108	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.



Electron density around SAH C 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.