



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:53 PM GMT

PDB ID : 4U7T  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

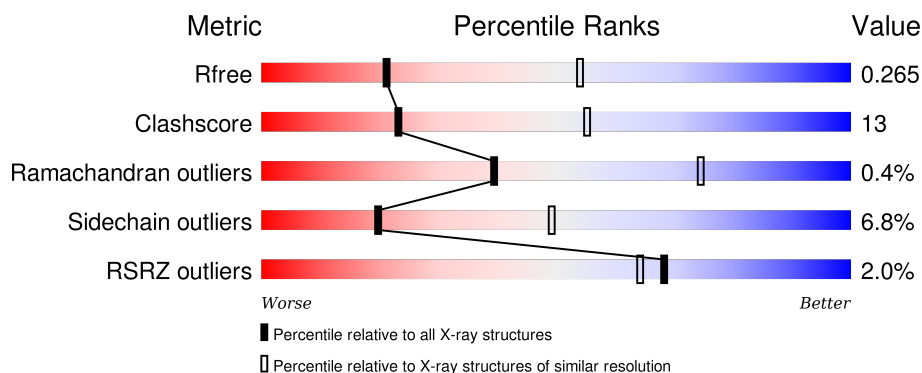
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	<div> <div>0%</div> <div> <div>66%</div> <div>26%</div> <div>6%</div> </div> </div>
1	C	445	<div> <div>2%</div> <div> <div>65%</div> <div>28%</div> <div>6%</div> </div> </div>
2	B	209	<div> <div>2%</div> <div> <div>57%</div> <div>30%</div> <div>11%</div> </div> </div>
2	D	209	<div> <div>3%</div> <div> <div>53%</div> <div>32%</div> <div>6%</div> <div>9%</div> </div> </div>
3	F	12	<div> <div>67%</div> <div>17%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	12	

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	ZN	A	1001	-	-	-	X
4	ZN	C	1001	-	-	-	X

## 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

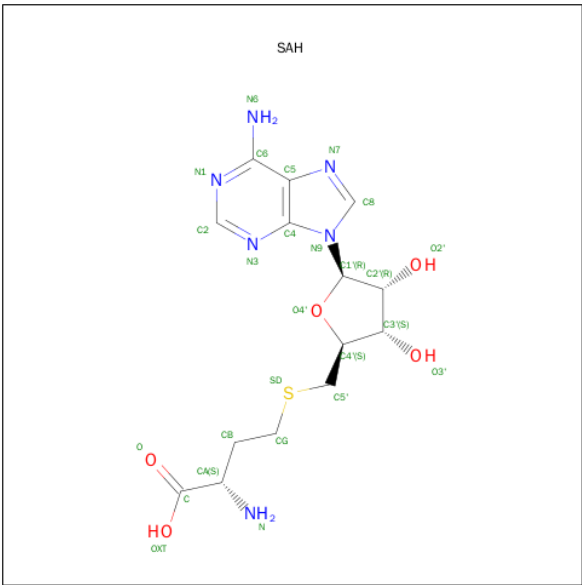
- Molecule 3 is a protein called peptide from Histone H3.3.

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 (three-letter code: 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 (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



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		

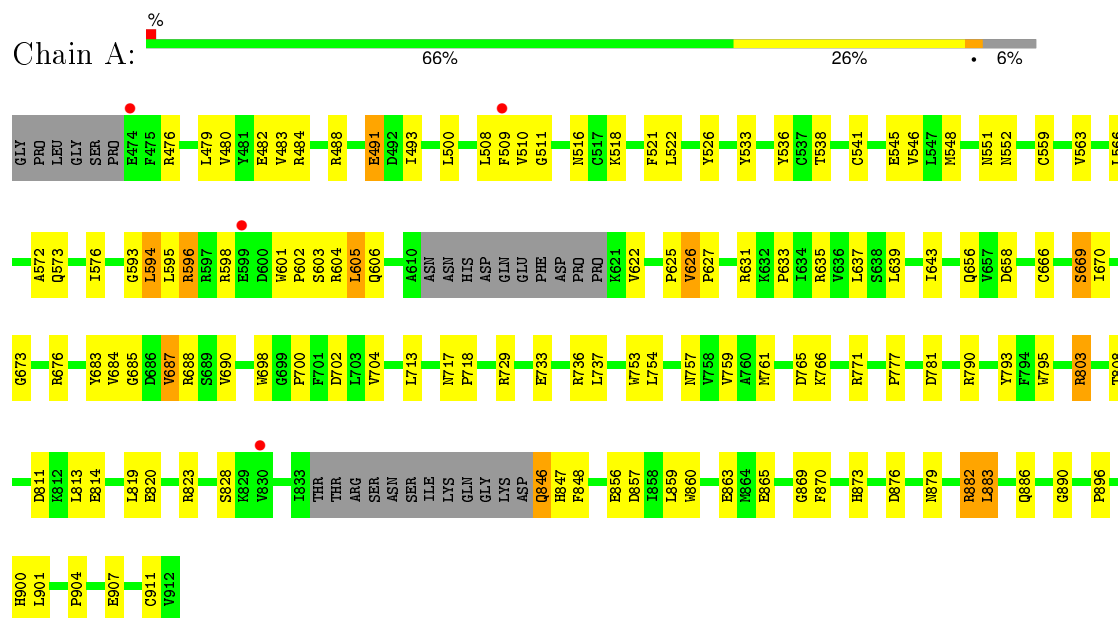
- Molecule 6 is water.

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		

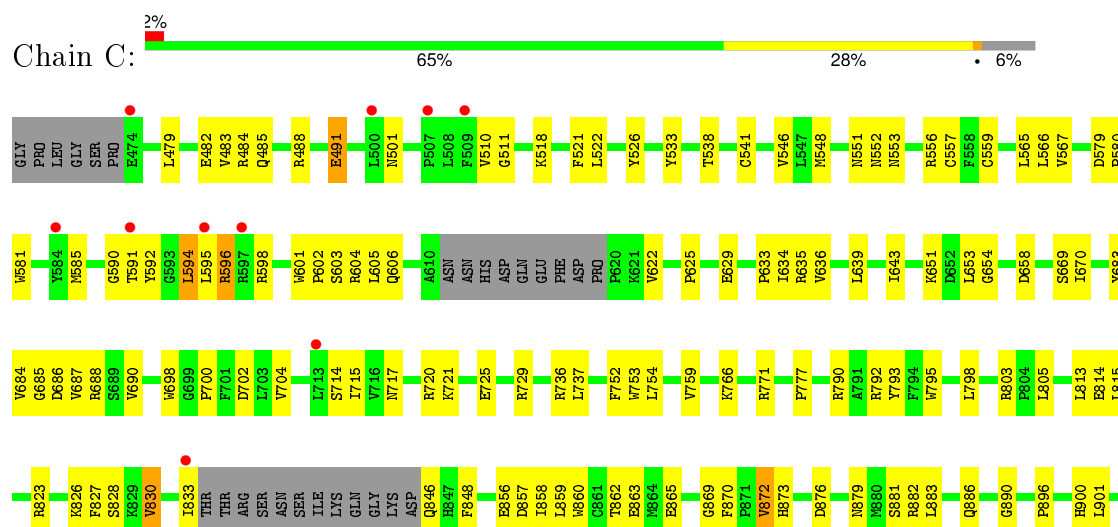
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

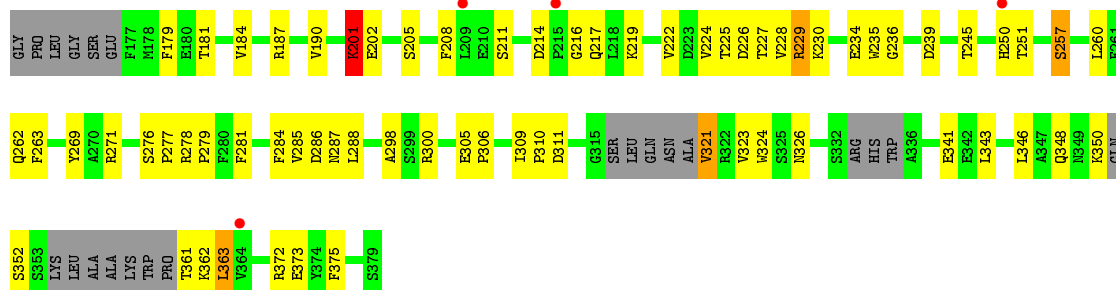


#### • Molecule 1: DNA (cytosine-5)-methyltransferase 3A

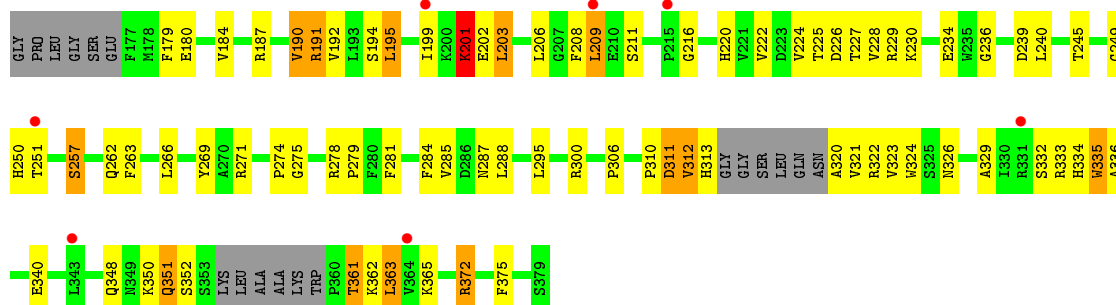




- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



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



- Molecule 3: peptide from Histone H3.3



- Molecule 3: peptide from Histone H3.3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.7 (40.21-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.223 , 0.261 0.231 , 0.265	Depositor DCC
$R_{free}$ test set	2669 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.5	EDS
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 52419 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/3426	0.68	0/4625
1	C	0.53	0/3434	0.69	0/4636
2	B	0.48	0/1584	0.70	0/2149
2	D	0.47	0/1629	0.70	2/2215 (0.1%)
3	F	0.31	0/78	0.53	0/101
3	G	0.39	0/78	0.53	0/101
All	All	0.51	0/10229	0.69	2/13827 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	372	ARG	NE-CZ-NH1	-5.99	117.30	120.30
2	D	372	ARG	CG-CD-NE	-5.12	101.05	111.80

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	94	0
2	B	1540	0	1516	45	1
2	D	1579	0	1558	51	1
3	F	79	0	91	2	0
3	G	79	0	91	2	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	266	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 13.

All (266) 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
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
1:A:602:PRO:HB3	1:A:625:PRO:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:761:MET:HE2	1:A:765:ASP:HB3	1.75	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
2:D:202:GLU:O	2:D:206:LEU:HD23	1.96	0.65
1:C:606:GLN:HG2	1:C:622:VAL:HG11	1.77	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
1:C:598:ARG:HD3	1:C:604:ARG:NH1	2.14	0.62
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.35	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: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:823:ARG:NH1	1:C:857:ASP:OD2	2.31	0.60
1:C:684:VAL:HG12	1:C:685:GLY:H	1.67	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: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: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:B:229:ARG:HB2	2:B:269:TYR:CD1	2.41	0.56
2:D:199:ILE:O	2:D:203:LEU:HB2	2.05	0.56
2:B:234:GLU:C	2:B:236:GLY:H	2.09	0.56
2:B:208:PHE:CZ	2:B:372:ARG:HG3	2.41	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:ASN:O	1:C:720:ARG:HG3	2.06	0.55
2:B:224:VAL:O	2:B:227:THR:N	2.25	0.55
1:A:546:VAL:HA	1:A:559:CYS:HA	1.88	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:826:LYS:HZ3	1:C:846:GLN:HG3	1.73	0.54
1:C:484:ARG:NH2	1:C:565:LEU:O	2.37	0.54
2:D:234:GLU:C	2:D:236:GLY:H	2.10	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:865:GLU:OE1	1:C:873:HIS:N	2.28	0.53
1:C:579:ASP:HB3	1:C:580:PRO:HD3	1.90	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
2:D:192:VAL:HG22	2:D:240:LEU:HB3	1.91	0.53
2:B:363:LEU:HD12	2:B:363:LEU:H	1.74	0.53
1:A:813:LEU:O	1:A:814:GLU:HB2	2.07	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
1:C:882:ARG:O	1:C:886:GLN:HG2	2.09	0.52
2:B:281:PHE:HA	2:B:326:ASN:HD21	1.73	0.52
1:C:484:ARG:NH2	1:C:594:LEU:HD21	2.24	0.52
1:A:687:VAL:HG22	5:A:1004:SAH:N1	2.25	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
1:C:526:TYR:CD2	1:C:904:PRO:HB3	2.45	0.51
2:B:201:LYS:NZ	2:B:205:SER:HB2	2.25	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:713:LEU:HD13	1:A:761:MET:HE3	1.94	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:823:ARG:NH1	1:A:863:GLU:OE1	2.45	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
1:A:551:ASN:OD1	1:A:552:ASN:N	2.45	0.49
2:B:179:PHE:CE2	2:B:279:PRO:HA	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
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:670:ILE:HG23	1:C:683:TYR:CE1	2.47	0.49
1:A:545:GLU:HG3	3:F:5:GLN:OE1	2.12	0.49
1:A:790:ARG:NH2	1:A:890:GLY:O	2.44	0.49
1:C:686:ASP:OD2	1:C:688:ARG:NH2	2.45	0.49
1:C:556:ARG:HD2	1:C:585:MET:HG3	1.95	0.49
2:B:202:GLU:HB3	2:B:362:LYS:HD3	1.95	0.49
1:A:759:VAL:HG23	1:A:793:TYR:CZ	2.48	0.49
2:D:249:GLY:N	2:D:350:LYS:HZ1	2.09	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:882:ARG:HH11	1:A:882:ARG:H	1.61	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:C:482:GLU:HA	1:C:485:GLN:HB2	1.96	0.47
1:A:643:ILE:HD11	1:A:870:PHE:CZ	2.49	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:715:ILE:O	1:C:720:ARG:NH1	2.47	0.47
1:C:526:TYR:CE2	1:C:904:PRO:HB3	2.50	0.46
1:A:666:CYS:SG	1:A:669:SER:OG	2.72	0.46
1:A:883:LEU:HA	1:A:883:LEU:HD12	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:C:862:THR:OG1	1:C:872:VAL:HG23	2.16	0.46
1:A:670:ILE:HG23	1:A:683:TYR:CD1	2.50	0.46
1:A:626:VAL:HG22	1:A:631:ARG:HG2	1.96	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
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:D:288:LEU:HD23	2:D:288:LEU:HA	1.77	0.45
2:B:260:LEU:HD21	2:B:298:ALA:HA	1.99	0.45
1:C:860:TRP:O	1:C:863:GLU:N	2.50	0.45
2:B:184:VAL:HA	2:B:187:ARG:NE	2.32	0.45
1:A:704:VAL:O	1:A:753:TRP:HA	2.16	0.45
2:B:201:LYS:O	2:B:362:LYS:NZ	2.47	0.45
1:C:546:VAL:HA	1:C:559:CYS:HA	1.97	0.45
1:A:823:ARG:HD3	1:A:863:GLU:OE2	2.17	0.45
1:A:713:LEU:HD12	1:A:757:ASN:ND2	2.32	0.45
2:B:276:SER:HA	2:B:277:PRO:HD3	1.78	0.45
2:D:351:GLN:O	2:D:352:SER:OG	2.27	0.45
2:D:274:PRO:HA	2:D:275:GLY:HA2	1.72	0.45
1:C:518:LYS:O	1:C:522:LEU:HG	2.15	0.45
1:C:601:TRP:N	1:C:602:PRO:HD2	2.32	0.45
1:A:673:GLY:HA3	1:A:683:TYR:OH	2.17	0.45
1:A:598:ARG:HH11	1:A:604:ARG:HH12	1.64	0.44
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:736:ARG:HH12	2:B:300:ARG:HH11	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:THR:O	2:B:363:LEU:HD12	2.18	0.44
1:C:815:LEU:HD11	1:C:859:LEU:HD21	1.99	0.44
1:C:643:ILE:HD11	1:C:870:PHE:CZ	2.51	0.44
1:A:656:GLN:NE2	1:A:911:CYS:O	2.39	0.44
1:C:533:TYR:CD2	1:C:548:MET:HB3	2.52	0.44
1:C:590:GLY:C	1:C:596:ARG:HD3	2.38	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:C:736:ARG:HH12	2:D:300:ARG:HH11	1.66	0.44
1:A:733:GLU:CD	2:B:300:ARG:HH12	2.21	0.44
1:A:533:TYR:CE2	1:A:548:MET:HB3	2.53	0.44
2:D:192:VAL:HG21	2:D:203:LEU:HD21	1.99	0.44
2:B:219:LYS:HE2	2:B:235:TRP:CD2	2.52	0.44
1:A:491:GLU:HG2	1:A:491:GLU:H	1.38	0.44
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:526:TYR:CD2	1:A:904:PRO:HG3	2.53	0.43
1:A:860:TRP:O	1:A:863:GLU:N	2.51	0.43
2:D:190:VAL:HG13	2:D:192:VAL:HG23	2.00	0.43
1:A:814:GLU:HA	1:A:828:SER:O	2.18	0.43
1:A:482:GLU:HB3	1:A:488:ARG:HG3	2.00	0.43
1:C:729:ARG:NH2	2:D:257:SER:OG	2.51	0.43
1:A:879:ASN:CG	1:C:882:ARG:HD2	2.38	0.43
2:B:201:LYS:HZ3	2:B:205:SER:HB2	1.84	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
2:B:309:ILE:HD11	2:B:321:VAL:HG12	1.99	0.43
2:B:260:LEU:CD2	2:B:298:ALA:HA	2.49	0.43
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.79	0.43
2:B:350:LYS:HD2	2:B:350:LYS:HA	1.80	0.43
2:D:312:VAL:HG23	2:D:313:HIS:H	1.84	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
2:D:195:LEU:HA	2:D:195:LEU:HD12	1.72	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
2:D:184:VAL:HA	2:D:187:ARG:NE	2.34	0.42
1:C:736:ARG:NH1	2:D:300:ARG:NH1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:ARG:NH1	2:D:300:ARG:HH11	2.18	0.42
1:A:637:LEU:HG	1:A:639:LEU:CD1	2.49	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: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
1:C:548:MET:HE1	3:G:4:LYS:HB3	2.02	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
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:805:LEU:HD23	1:C:805:LEU:HA	1.90	0.41
1:C:766:LYS:HD2	1:C:793:TYR:CE2	2.56	0.41
2:D:372:ARG:HE	2:D:372:ARG:HB3	1.47	0.41
1:C:552:ASN:O	1:C:553:ASN:HB2	2.21	0.41
1:C:684:VAL:HG11	1:C:698:TRP:HH2	1.85	0.41
1:A:781:ASP:HA	1:A:790:ARG:O	2.20	0.41
1:A:536:TYR:OH	3:F:9:LYS:HG2	2.20	0.41
1:C:759:VAL:HG23	1:C:793:TYR:CZ	2.55	0.41
1:C:491:GLU:H	1:C:491:GLU:HG2	1.37	0.41
1:A:808:THR:HG22	1:A:811:ASP:OD2	2.21	0.41
2:D:311:ASP:HB2	2:D:312:VAL:H	1.65	0.41
1:A:777:PRO:HD3	1:A:795:TRP:NE1	2.36	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
2:D:234:GLU:C	2:D:236:GLY:N	2.74	0.41
1:A:717:ASN:HA	1:A:718:PRO:HD3	1.90	0.41
2:D:240:LEU:HA	2:D:281:PHE:O	2.20	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:A:493:ILE:HD13	1:A:500:LEU:HD13	2.03	0.41
1:C:752:PHE:HB3	1:C:798:LEU:HD23	2.03	0.41
2:B:309:ILE:HA	2:B:310:PRO:HD3	1.80	0.40
2:D:201:LYS:HB2	2:D:362:LYS:NZ	2.36	0.40
1:C:827:PHE:CZ	1:C:846:GLN:HB2	2.57	0.40
1:A:533:TYR:CD2	1:A:548:MET:HB3	2.56	0.40
2:B:305:GLU:HG3	2:B:306:PRO:HD2	2.02	0.40
2:D:249:GLY:N	2:D:350:LYS:NZ	2.70	0.40
1:A:626:VAL:HA	1:A:627:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:869:GLY:HA3	1:A:896:PRO:HD3	2.04	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%)	17	51
2	D	185/209 (88%)	162 (88%)	20 (11%)	3 (2%)	12	40
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%)	39	74

All (5) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	346 (95%)	19 (5%)	29	64
1	C	366/390 (94%)	350 (96%)	16 (4%)	35	70
2	B	173/189 (92%)	156 (90%)	17 (10%)	10	30
2	D	177/189 (94%)	154 (87%)	23 (13%)	5	15
3	F	8/9 (89%)	8 (100%)	0	100	100
3	G	8/9 (89%)	8 (100%)	0	100	100
All	All	1097/1176 (93%)	1022 (93%)	75 (7%)	20	49

All (75) 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	594	LEU
1	A	595	LEU
1	A	596	ARG
1	A	603	SER
1	A	605	LEU
1	A	626	VAL
1	A	669	SER
1	A	676	ARG
1	A	687	VAL
1	A	803	ARG
1	A	819	LEU
1	A	846	GLN

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Mol	Chain	Res	Type
1	A	882	ARG
1	A	883	LEU
1	A	886	GLN
1	A	907	GLU
2	B	201	LYS
2	B	211	SER
2	B	214	ASP
2	B	217	GLN
2	B	222	VAL
2	B	229	ARG
2	B	250	HIS
2	B	251	THR
2	B	257	SER
2	B	271	ARG
2	B	278	ARG
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	594	LEU
1	C	595	LEU
1	C	596	ARG
1	C	603	SER
1	C	605	LEU
1	C	629	GLU
1	C	669	SER
1	C	714	SER
1	C	771	ARG
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

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Mol	Chain	Res	Type
2	D	209	LEU
2	D	211	SER
2	D	222	VAL
2	D	250	HIS
2	D	251	THR
2	D	257	SER
2	D	271	ARG
2	D	278	ARG
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	846	GLN
1	A	879	ASN
1	C	879	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 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	-	20,28,28	1.18	2 (10%)	19,40,40	2.85	5 (26%)
5	SAH	C	1004	-	20,28,28	1.13	2 (10%)	19,40,40	3.06	3 (15%)

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	-	-	0/7/31/31	0/3/3/3
5	SAH	C	1004	-	-	0/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1004	SAH	C2-N1	2.63	1.38	1.33
5	A	1004	SAH	C2-N1	2.66	1.38	1.33
5	C	1004	SAH	C2-N3	3.24	1.37	1.32
5	A	1004	SAH	C2-N3	3.54	1.38	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1004	SAH	N3-C2-N1	-11.80	119.86	128.89
5	A	1004	SAH	N3-C2-N1	-10.77	120.64	128.89
5	C	1004	SAH	CB-CG-SD	-2.73	108.31	113.57
5	A	1004	SAH	CB-CG-SD	-2.42	108.90	113.57
5	A	1004	SAH	C4-C5-N7	-2.02	107.62	109.48
5	A	1004	SAH	C4'-C5'-SD	2.22	120.38	113.53
5	C	1004	SAH	O4'-C1'-N9	2.82	113.99	108.10
5	A	1004	SAH	O4'-C1'-N9	3.31	115.04	108.10

There are no chirality outliers.

There are no torsion outliers.

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	417/445 (93%)	0.17	4 (0%) 84 82	43, 72, 132, 162	0
1	C	418/445 (93%)	0.16	10 (2%) 62 57	44, 73, 133, 179	0
2	B	187/209 (89%)	0.17	4 (2%) 67 62	51, 82, 155, 182	0
2	D	191/209 (91%)	0.20	7 (3%) 45 38	52, 85, 155, 174	0
3	F	10/12 (83%)	0.05	0 100 100	97, 106, 117, 133	0
3	G	10/12 (83%)	-0.20	0 100 100	96, 104, 117, 127	0
All	All	1233/1332 (92%)	0.17	25 (2%) 68 64	43, 77, 140, 182	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	215	PRO	3.1
2	D	209	LEU	2.9
2	D	364	VAL	2.7
1	C	591	THR	2.7
1	A	599	GLU	2.6
2	D	331	ARG	2.6
1	C	507	PRO	2.6
1	C	584	TYR	2.5
1	C	713	LEU	2.4
1	A	474	GLU	2.4
1	C	509	PHE	2.4
1	A	830	VAL	2.4
2	D	343	LEU	2.3
1	C	833	ILE	2.3
2	B	250	HIS	2.3
1	C	597	ARG	2.3
2	B	215	PRO	2.2
1	A	509	PHE	2.2
2	B	209	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	199	ILE	2.1
1	C	500	LEU	2.1
2	D	251	THR	2.1
2	B	364	VAL	2.1
1	C	474	GLU	2.0
1	C	595	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ZN	C	1001	1/1	0.99	0.22	4.83	79,79,79,79	0
4	ZN	A	1001	1/1	0.99	0.23	2.32	80,80,80,80	0
4	ZN	A	1002	1/1	0.97	0.22	0.52	108,108,108,108	0
4	ZN	C	1002	1/1	0.99	0.22	0.50	103,103,103,103	0
4	ZN	C	1003	1/1	0.99	0.21	0.31	95,95,95,95	0
4	ZN	A	1003	1/1	0.99	0.21	-0.02	99,99,99,99	0
5	SAH	A	1004	26/26	0.96	0.19	-0.38	44,55,65,77	0
5	SAH	C	1004	26/26	0.96	0.18	-0.55	46,55,64,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.