



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:43 am BST

PDB ID : 6JW5
Title : RVD Q* recognizes 5hmC through water-mediated H bonds
Authors : Liu, L.; Yi, C.
Deposited on : 2019-04-18
Resolution : 2.99 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
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

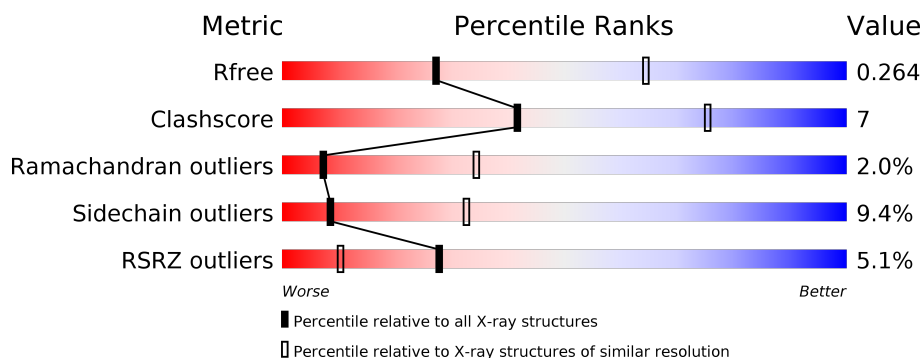
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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









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

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

Mol	Chain	Length	Quality of chain
1	A	498	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>...</div> </div> </div>
1	B	498	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>...</div> </div> </div>
1	E	498	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>...</div> </div> </div>
1	H	498	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>...</div> </div> </div>
2	C	17	<div> <div></div> <div> <div>53%</div> <div>47%</div> </div> </div>
2	F	17	<div> <div>6%</div> <div> <div>47%</div> <div>53%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	17	 59% 41%
2	K	17	 6% 47% 53%
3	D	17	 88% 12%
3	G	17	 6% 65% 35%
3	J	17	 82% 18%
3	L	17	 12% 76% 24%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17094 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 TAL effector.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			
1	B	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			
1	E	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			
1	H	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	C	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	F	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	K	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	D	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	G	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

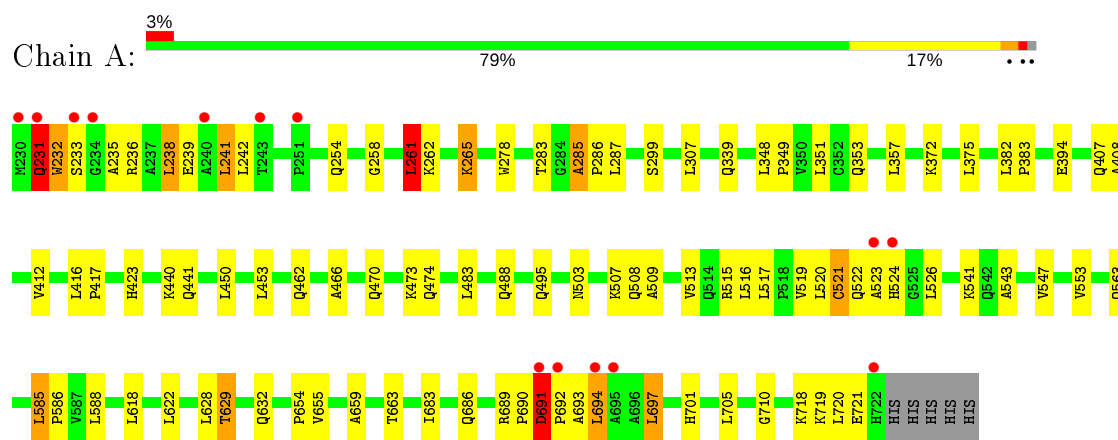
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	I	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		

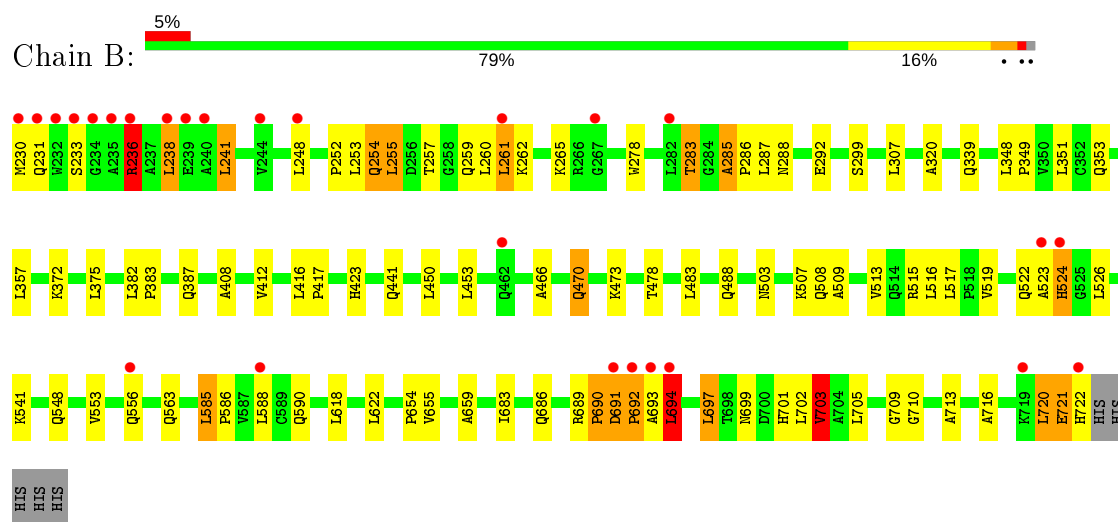
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

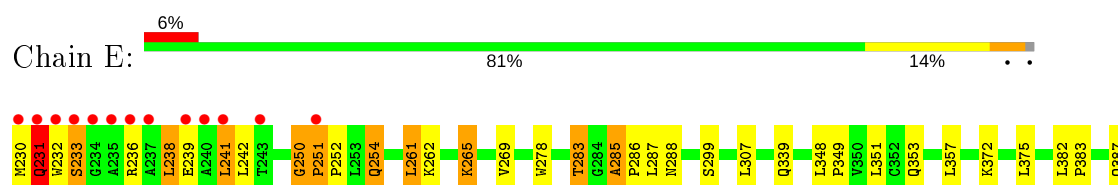
• Molecule 1: TAL effector

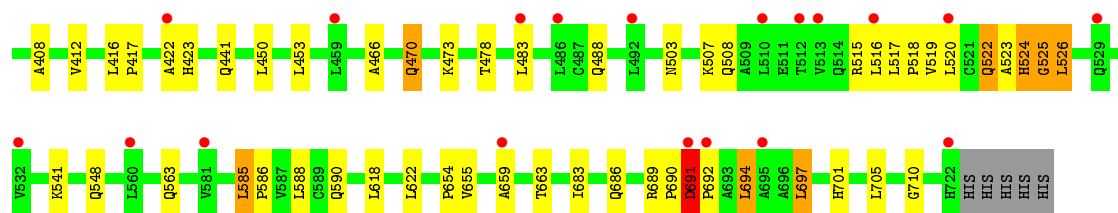


• Molecule 1: TAL effector

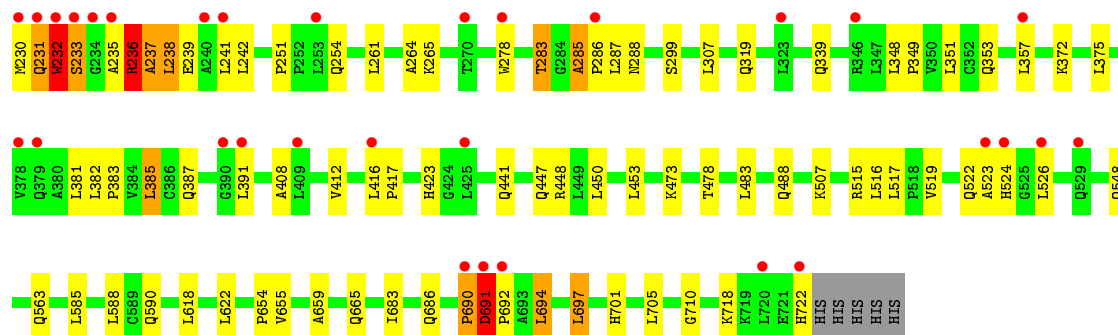
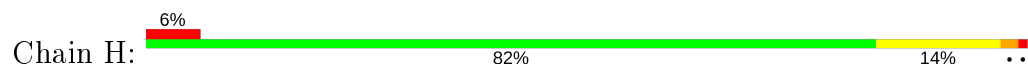


• Molecule 1: TAL effector

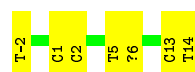




● Molecule 1: TAL effector



● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



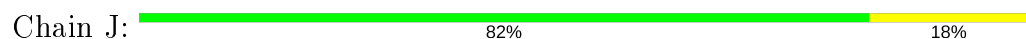
● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



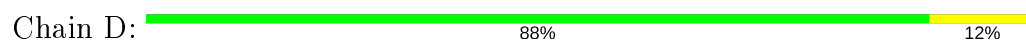
● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



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



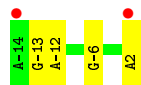
- Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.42Å 93.78Å 168.16Å 90.00° 102.73° 90.00°	Depositor
Resolution (Å)	164.03 – 2.99 47.23 – 2.99	Depositor EDS
% Data completeness (in resolution range)	84.3 (164.03-2.99) 84.4 (47.23-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.244 , 0.267 0.240 , 0.264	Depositor DCC
R_{free} test set	2485 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17094	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5HC

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	0.54	0/3632	0.74	3/4961 (0.1%)
1	B	0.55	0/3632	0.73	4/4961 (0.1%)
1	E	0.52	0/3632	0.70	2/4961 (0.0%)
1	H	0.50	0/3632	0.69	4/4961 (0.1%)
2	C	0.71	0/349	0.90	0/533
2	F	0.78	2/349 (0.6%)	0.89	0/533
2	I	0.74	0/349	0.91	0/533
2	K	0.74	1/349 (0.3%)	0.90	0/533
3	D	0.54	0/402	0.79	0/620
3	G	0.59	1/402 (0.2%)	0.85	1/620 (0.2%)
3	J	0.55	0/402	0.82	0/620
3	L	0.52	0/402	0.86	1/620 (0.2%)
All	All	0.55	4/17532 (0.0%)	0.75	15/24456 (0.1%)

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	B	0	1
1	E	0	3
1	H	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	10	DT	O3'-P	-6.63	1.53	1.61
2	F	10	DT	O3'-P	-6.43	1.53	1.61
2	F	9	DG	O3'-P	-6.03	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	-6	DG	O3'-P	-5.14	1.54	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	694	LEU	CA-CB-CG	8.27	134.33	115.30
1	H	694	LEU	CA-CB-CG	7.32	132.12	115.30
1	E	694	LEU	CA-CB-CG	7.21	131.89	115.30
1	A	261	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	261	LEU	CB-CG-CD1	6.95	122.82	111.00
1	B	703	VAL	N-CA-CB	6.81	126.48	111.50
1	B	703	VAL	N-CA-C	-6.51	93.42	111.00
1	H	385	LEU	CA-CB-CG	6.38	129.97	115.30
1	H	236	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	231	GLN	CB-CA-C	5.78	121.95	110.40
3	L	-6	DG	C1'-O4'-C4'	-5.38	104.72	110.10
1	B	236	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	522	GLN	N-CA-C	-5.17	97.03	111.00
3	G	-6	DG	C1'-O4'-C4'	-5.15	104.95	110.10
1	H	251	PRO	C-N-CD	5.04	138.97	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	MET	Peptide
1	E	250	GLY	Peptide
1	E	251	PRO	Peptide
1	E	525	GLY	Peptide
1	H	232	TRP	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	3580	0	3725	56	10
1	B	3580	0	3725	62	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3580	0	3725	48	17
1	H	3580	0	3725	35	5
2	C	337	0	195	4	1
2	F	337	0	195	6	0
2	I	337	0	195	6	0
2	K	337	0	195	17	0
3	D	355	0	189	1	0
3	G	355	0	189	5	10
3	J	355	0	189	1	8
3	L	355	0	189	7	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
All	All	17094	0	16436	233	33

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 7.

All (233) 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:K:-2:DT:O4	3:L:2:DA:N1	1.70	1.23
2:K:-2:DT:O4	3:L:2:DA:C6	1.95	1.17
2:K:-2:DT:C4	3:L:2:DA:N1	2.17	1.13
2:K:13:DC:H2''	2:K:14:DT:H5'	1.46	0.97
1:A:258:GLY:O	1:A:261:LEU:HD12	1.63	0.97
1:A:233:SER:OG	2:I:-2:DT:O5'	1.60	0.92
1:B:255:LEU:HD23	1:B:259:GLN:HB2	1.55	0.86
1:A:629:THR:HG22	1:A:632:GLN:OE1	1.77	0.84
1:A:238:LEU:HA	1:A:241:LEU:HD23	1.60	0.84
2:K:13:DC:C2'	2:K:14:DT:H5'	2.07	0.83
1:B:255:LEU:CD2	1:B:259:GLN:HB2	2.10	0.82
1:A:285:ALA:HB1	1:A:286:PRO:HD2	1.63	0.80
1:E:285:ALA:HB1	1:E:286:PRO:HD2	1.65	0.79
1:E:231:GLN:O	1:E:232:TRP:HD1	1.66	0.78
1:H:285:ALA:HB1	1:H:286:PRO:HD2	1.64	0.78
1:E:518:PRO:O	1:E:522:GLN:CB	2.31	0.77
1:B:285:ALA:HB1	1:B:286:PRO:HD2	1.67	0.77
1:B:702:LEU:O	1:B:703:VAL:HG23	1.86	0.75
1:A:692:PRO:HD2	1:A:718:LYS:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:PRO:O	1:B:722:HIS:CD2	2.40	0.74
1:E:231:GLN:O	1:E:232:TRP:CD1	2.41	0.73
1:E:525:GLY:CA	1:E:526:LEU:HD13	2.18	0.73
1:H:236:ARG:O	1:H:237:ALA:O	2.06	0.72
1:B:691:ASP:HB3	1:B:692:PRO:CD	2.20	0.71
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.20	0.71
1:E:285:ALA:HB1	1:E:286:PRO:CD	2.21	0.71
1:B:236:ARG:NE	1:B:236:ARG:HA	2.05	0.71
1:A:520:LEU:O	1:A:521:CYS:CB	2.38	0.70
1:H:285:ALA:HB1	1:H:286:PRO:CD	2.21	0.70
1:A:233:SER:CB	2:I:-2:DT:O5'	2.38	0.70
1:E:518:PRO:O	1:E:522:GLN:HB3	1.91	0.70
1:B:691:ASP:C	1:B:693:ALA:H	1.94	0.69
1:A:258:GLY:O	1:A:261:LEU:CD1	2.41	0.69
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.23	0.69
1:B:692:PRO:O	1:B:722:HIS:CG	2.47	0.67
1:B:694:LEU:HD13	1:B:722:HIS:CE1	2.29	0.67
1:A:520:LEU:O	1:A:521:CYS:HB2	1.95	0.67
3:L:-13:DG:H5'	3:L:-13:DG:C8	2.30	0.66
1:A:233:SER:HG	2:I:-2:DT:HO5'	0.89	0.66
2:K:13:DC:C5	2:K:14:DT:C5	2.84	0.66
1:B:694:LEU:H	1:B:722:HIS:CE1	2.14	0.65
1:B:716:ALA:O	1:B:720:LEU:HG	1.98	0.64
1:E:238:LEU:HD22	1:E:242:LEU:HG	1.80	0.64
1:B:721:GLU:HG2	1:B:722:HIS:N	2.14	0.63
1:A:235:ALA:O	1:A:236:ARG:HB2	1.99	0.63
1:A:663:THR:HG21	1:B:320:ALA:HB1	1.83	0.61
1:E:520:LEU:O	1:E:524:HIS:O	2.20	0.60
1:B:255:LEU:CD2	1:B:259:GLN:CB	2.79	0.59
1:A:509:ALA:O	1:A:513:VAL:HG13	2.03	0.59
2:K:-2:DT:C4	3:L:2:DA:C2	2.89	0.59
1:B:691:ASP:C	1:B:693:ALA:N	2.57	0.58
1:B:509:ALA:O	1:B:513:VAL:HG13	2.03	0.58
1:A:691:ASP:HB3	1:A:692:PRO:HD2	1.86	0.58
1:B:691:ASP:HB3	1:B:692:PRO:HD2	1.84	0.58
1:E:262:LYS:HE3	3:G:-5:DA:OP1	2.03	0.58
2:K:13:DC:C1'	2:K:14:DT:H5'	2.33	0.57
1:B:694:LEU:HD13	1:B:722:HIS:HE1	1.69	0.57
2:K:13:DC:H1'	2:K:14:DT:H5'	1.86	0.57
1:E:238:LEU:HD23	1:E:241:LEU:HD23	1.87	0.56
1:E:518:PRO:O	1:E:522:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD22	1:A:242:LEU:HG	1.87	0.56
1:E:691:ASP:HB3	1:E:692:PRO:HD2	1.87	0.56
2:K:-2:DT:O2	2:K:-1:DG:O4'	2.24	0.56
1:B:701:HIS:CE1	1:E:701:HIS:CE1	2.95	0.55
1:B:339:GLN:HB3	1:B:372:LYS:HD3	1.87	0.55
1:H:238:LEU:CD2	1:H:242:LEU:HG	2.36	0.55
1:A:407:GLN:HB3	1:A:440:LYS:HD3	1.87	0.55
1:A:231:GLN:O	1:A:231:GLN:HG2	2.07	0.54
1:H:339:GLN:HB3	1:H:372:LYS:HD3	1.89	0.54
1:A:718:LYS:O	1:A:720:LEU:N	2.41	0.54
1:E:339:GLN:HB3	1:E:372:LYS:HD3	1.89	0.54
1:A:339:GLN:HB3	1:A:372:LYS:HD3	1.88	0.54
1:H:382:LEU:N	1:H:383:PRO:HD2	2.23	0.54
1:A:261:LEU:HD13	1:A:262:LYS:N	2.23	0.54
1:A:517:LEU:O	1:A:520:LEU:O	2.25	0.54
1:A:382:LEU:N	1:A:383:PRO:HD2	2.23	0.53
1:A:522:GLN:O	1:A:523:ALA:HB3	2.08	0.53
1:E:519:VAL:O	1:E:523:ALA:HB3	2.08	0.53
1:H:522:GLN:O	1:H:523:ALA:HB3	2.08	0.53
1:A:694:LEU:O	1:A:694:LEU:HD13	2.09	0.53
1:E:422:ALA:HB2	1:H:319:GLN:HB3	1.90	0.53
1:B:522:GLN:O	1:B:523:ALA:HB3	2.09	0.53
2:K:13:DC:H5	2:K:14:DT:C5	2.27	0.53
1:A:474:GLN:HB3	1:A:507:LYS:HD2	1.90	0.53
1:B:699:ASN:O	1:B:702:LEU:O	2.27	0.52
2:K:13:DC:H1'	2:K:14:DT:C5'	2.38	0.52
1:A:261:LEU:CD2	1:A:265:LYS:HD3	2.40	0.52
1:H:691:ASP:HB3	1:H:692:PRO:HD2	1.91	0.52
1:E:518:PRO:O	1:E:522:GLN:N	2.41	0.52
1:B:694:LEU:H	1:B:722:HIS:HE1	1.56	0.51
1:A:441:GLN:HB3	1:A:473:LYS:HD2	1.93	0.51
1:B:382:LEU:N	1:B:383:PRO:HD2	2.26	0.51
1:B:441:GLN:HB3	1:B:473:LYS:HD2	1.93	0.50
1:H:441:GLN:HB3	1:H:473:LYS:HD2	1.93	0.50
1:B:709:GLY:O	1:B:713:ALA:HB3	2.11	0.50
1:E:516:LEU:HA	1:E:519:VAL:CG1	2.42	0.50
1:H:285:ALA:CB	1:H:286:PRO:CD	2.90	0.50
1:A:285:ALA:CB	1:A:286:PRO:CD	2.90	0.49
1:B:416:LEU:N	1:B:417:PRO:CD	2.75	0.49
1:B:236:ARG:NE	1:B:236:ARG:CA	2.75	0.49
1:A:394:GLU:N	1:A:394:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HD21	1:B:259:GLN:CB	2.41	0.49
1:B:515:ARG:O	1:B:517:LEU:N	2.43	0.49
1:H:516:LEU:HA	1:H:519:VAL:CG1	2.43	0.49
1:H:237:ALA:O	1:H:239:GLU:N	2.36	0.49
1:A:423:HIS:HB3	1:A:450:LEU:HD23	1.94	0.49
1:B:238:LEU:O	1:B:241:LEU:HB3	2.13	0.49
1:E:285:ALA:CB	1:E:286:PRO:CD	2.90	0.49
1:E:382:LEU:N	1:E:383:PRO:HD2	2.27	0.49
1:E:515:ARG:HB3	1:E:516:LEU:HD12	1.94	0.49
1:B:423:HIS:HB3	1:B:450:LEU:HD23	1.95	0.48
1:E:441:GLN:HB3	1:E:473:LYS:HD2	1.93	0.48
1:H:236:ARG:O	1:H:237:ALA:C	2.51	0.48
1:B:236:ARG:HE	1:B:236:ARG:HA	1.78	0.48
1:B:515:ARG:NH2	1:B:516:LEU:CD1	2.76	0.48
1:E:515:ARG:O	1:E:517:LEU:N	2.45	0.48
1:B:285:ALA:CB	1:B:286:PRO:CD	2.92	0.48
1:A:515:ARG:O	1:A:517:LEU:N	2.43	0.48
1:A:516:LEU:HA	1:A:519:VAL:CG1	2.43	0.48
1:B:255:LEU:HD21	1:B:259:GLN:HB3	1.95	0.48
1:E:423:HIS:HB3	1:E:450:LEU:HD23	1.95	0.48
1:E:265:LYS:NZ	3:G:-4:DA:OP2	2.33	0.48
2:K:-2:DT:H71	3:L:2:DA:H61	1.77	0.48
1:B:516:LEU:HA	1:B:519:VAL:CG1	2.44	0.48
1:B:716:ALA:O	1:B:720:LEU:CG	2.62	0.48
1:E:233:SER:HB2	2:F:-2:DT:O5'	2.14	0.47
1:A:416:LEU:N	1:A:417:PRO:CD	2.78	0.47
1:A:718:LYS:C	1:A:720:LEU:H	2.17	0.47
1:E:525:GLY:C	1:E:526:LEU:HD13	2.35	0.47
1:A:285:ALA:CB	1:A:286:PRO:HD2	2.40	0.47
1:B:702:LEU:O	1:B:703:VAL:CG2	2.61	0.47
1:E:525:GLY:HA3	1:E:526:LEU:HD13	1.95	0.47
3:L:-13:DG:H2''	3:L:-12:DA:OP2	2.15	0.47
2:I:1:DC:H2''	2:I:2:DC:O5'	2.15	0.46
1:B:248:LEU:O	1:B:253:LEU:O	2.33	0.46
1:B:348:LEU:N	1:B:349:PRO:CD	2.78	0.46
3:G:-14:DA:N7	3:G:-13:DG:N1	2.64	0.46
1:H:232:TRP:CE3	1:H:233:SER:HA	2.50	0.46
1:H:348:LEU:N	1:H:349:PRO:CD	2.79	0.46
1:A:470:GLN:HB2	1:A:503:ASN:N	2.31	0.46
1:H:381:LEU:HB3	1:H:385:LEU:HD12	1.98	0.46
1:B:285:ALA:CB	1:B:286:PRO:HD2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:718:LYS:HB3	1:H:722:HIS:CE1	2.51	0.46
1:A:520:LEU:O	1:A:521:CYS:SG	2.74	0.46
2:K:1:DC:H2"	2:K:2:DC:O5'	2.16	0.46
1:B:697:LEU:HD23	1:B:701:HIS:CD2	2.51	0.46
1:A:348:LEU:N	1:A:349:PRO:CD	2.79	0.46
2:I:5:DT:H2"	2:I:6:5HC:O5'	2.17	0.45
1:A:232:TRP:HD1	1:A:232:TRP:H	1.64	0.45
2:K:-2:DT:H1'	2:K:-1:DG:O5'	2.15	0.45
1:H:351:LEU:HB3	1:H:357:LEU:HD12	1.98	0.45
2:K:5:DT:H2"	2:K:6:5HC:O5'	2.16	0.45
1:E:470:GLN:HB2	1:E:503:ASN:N	2.32	0.45
1:B:238:LEU:CD2	1:B:241:LEU:HD22	2.46	0.45
1:E:526:LEU:N	1:E:526:LEU:HD13	2.31	0.45
1:H:423:HIS:HB3	1:H:450:LEU:HD23	1.98	0.45
1:H:230:MET:O	1:H:231:GLN:HG3	2.17	0.45
1:H:385:LEU:HD23	1:H:391:LEU:HD12	1.98	0.45
1:B:690:PRO:O	1:B:691:ASP:O	2.34	0.45
1:E:691:ASP:HB3	1:E:692:PRO:CD	2.47	0.45
2:F:5:DT:H2"	2:F:6:5HC:O5'	2.17	0.45
2:C:1:DC:H2"	2:C:2:DC:O5'	2.17	0.44
1:B:508:GLN:HB3	1:B:541:LYS:HD3	2.00	0.44
1:B:697:LEU:HD23	1:B:701:HIS:HD2	1.83	0.44
2:F:1:DC:H2"	2:F:2:DC:O5'	2.17	0.44
1:E:348:LEU:N	1:E:349:PRO:CD	2.81	0.44
1:A:655:VAL:O	1:A:659:ALA:HB3	2.18	0.44
1:H:416:LEU:N	1:H:417:PRO:CD	2.80	0.44
1:A:720:LEU:O	1:A:721:GLU:HG3	2.18	0.43
1:A:232:TRP:N	1:A:232:TRP:CD1	2.87	0.43
1:A:408:ALA:O	1:A:412:VAL:HG23	2.18	0.43
1:B:408:ALA:O	1:B:412:VAL:HG23	2.18	0.43
2:C:5:DT:H2"	2:C:6:5HC:O5'	2.18	0.43
1:E:416:LEU:N	1:E:417:PRO:CD	2.82	0.43
1:A:261:LEU:HD22	1:A:265:LYS:HD3	2.00	0.43
1:B:238:LEU:HD23	1:B:241:LEU:HD22	1.99	0.43
1:B:466:ALA:O	1:B:470:GLN:HG2	2.17	0.43
1:B:351:LEU:HB3	1:B:357:LEU:HD12	2.00	0.43
1:B:478:THR:OG1	1:B:507:LYS:HG3	2.19	0.43
2:C:13:DC:C5	2:C:14:DT:C4	3.07	0.43
1:A:697:LEU:HD23	1:A:701:HIS:CD2	2.54	0.43
1:E:508:GLN:HB3	1:E:541:LYS:HD3	2.01	0.43
1:B:470:GLN:HB2	1:B:503:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:-2:DT:H2''	2:C:-1:DG:OP2	2.18	0.43
1:E:241:LEU:HD11	1:E:269:VAL:HB	2.01	0.43
1:A:466:ALA:O	1:A:470:GLN:HG2	2.18	0.43
1:B:515:ARG:NH2	1:B:516:LEU:HD11	2.33	0.43
1:E:478:THR:OG1	1:E:507:LYS:HG3	2.19	0.43
2:F:14:DT:C4	3:G:-14:DA:N6	2.87	0.43
1:H:655:VAL:O	1:H:659:ALA:HB3	2.19	0.43
1:B:655:VAL:O	1:B:659:ALA:HB3	2.19	0.43
1:E:351:LEU:HB3	1:E:357:LEU:HD12	2.00	0.43
1:E:466:ALA:O	1:E:470:GLN:HG2	2.19	0.43
1:E:655:VAL:O	1:E:659:ALA:HB3	2.19	0.43
1:E:697:LEU:HD23	1:E:701:HIS:CD2	2.54	0.43
1:A:629:THR:CG2	1:A:632:GLN:OE1	2.57	0.42
1:H:478:THR:OG1	1:H:507:LYS:HG3	2.19	0.42
2:F:13:DC:H1'	2:F:14:DT:O4'	2.19	0.42
1:H:408:ALA:O	1:H:412:VAL:HG23	2.19	0.42
1:H:447:GLN:OE1	1:H:448:ARG:N	2.52	0.42
3:D:-13:DG:H2''	3:D:-12:DA:OP2	2.18	0.42
1:H:515:ARG:O	1:H:517:LEU:N	2.47	0.42
1:H:691:ASP:HB3	1:H:692:PRO:CD	2.49	0.42
1:H:692:PRO:HG2	1:H:722:HIS:NE2	2.34	0.42
1:H:697:LEU:HD23	1:H:701:HIS:CD2	2.54	0.42
1:E:408:ALA:O	1:E:412:VAL:HG23	2.19	0.42
1:A:508:GLN:HB3	1:A:541:LYS:HD3	2.02	0.42
1:H:285:ALA:CB	1:H:286:PRO:HD2	2.41	0.42
1:A:351:LEU:HB3	1:A:357:LEU:HD12	2.00	0.41
1:B:261:LEU:HG	1:B:262:LYS:N	2.35	0.41
1:H:697:LEU:HD23	1:H:701:HIS:HD2	1.85	0.41
3:J:-13:DG:H2''	3:J:-12:DA:OP2	2.20	0.41
1:A:693:ALA:CB	1:A:721:GLU:OE2	2.68	0.41
1:H:690:PRO:O	1:H:691:ASP:O	2.38	0.41
1:E:515:ARG:CB	1:E:516:LEU:HD12	2.50	0.41
1:A:543:ALA:O	1:A:547:VAL:HG23	2.20	0.41
1:H:283:THR:O	1:H:288:ASN:HA	2.20	0.41
1:B:255:LEU:HD22	1:B:260:LEU:HG	2.01	0.41
3:G:-14:DA:C8	3:G:-13:DG:C2	3.09	0.41
1:E:230:MET:HA	1:E:238:LEU:HD12	2.03	0.41
1:E:697:LEU:HD23	1:E:701:HIS:HD2	1.85	0.41
2:I:13:DC:C5	2:I:14:DT:O4	2.74	0.41
1:A:697:LEU:HD23	1:A:701:HIS:HD2	1.86	0.41
1:E:261:LEU:HG	1:E:262:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:O	1:E:288:ASN:HA	2.20	0.40
1:A:629:THR:HG23	1:A:632:GLN:HG3	2.02	0.40
2:F:14:DT:H2'	2:F:14:DT:O2	2.20	0.40
2:K:-2:DT:C2	2:K:-1:DG:C4	3.10	0.40
1:A:585:LEU:HB3	1:A:586:PRO:CD	2.52	0.40
1:B:283:THR:O	1:B:288:ASN:HA	2.22	0.40
1:B:585:LEU:HB3	1:B:586:PRO:CD	2.51	0.40
1:E:585:LEU:HB3	1:E:586:PRO:CD	2.51	0.40
1:B:523:ALA:O	1:B:524:HIS:HB2	2.22	0.40

All (33) 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)
1:A:236:ARG:CZ	3:G:-3:DG:OP2[2_445]	0.57	1.63
1:A:236:ARG:NH2	3:G:-3:DG:OP2[2_445]	0.85	1.35
1:B:236:ARG:NH2	1:H:264:ALA:O[2_556]	1.23	0.97
1:E:251:PRO:CA	1:E:524:HIS:NE2[2_455]	1.39	0.81
3:J:-3:DG:OP1	1:E:236:ARG:NH1[2_445]	1.39	0.81
1:A:236:ARG:NH1	3:G:-3:DG:P[2_445]	1.47	0.73
1:A:236:ARG:CZ	3:G:-3:DG:P[2_445]	1.50	0.70
1:A:236:ARG:NE	3:G:-3:DG:OP2[2_445]	1.50	0.70
1:A:236:ARG:NH2	3:G:-3:DG:P[2_445]	1.51	0.69
1:A:236:ARG:NH1	3:G:-3:DG:OP1[2_445]	1.52	0.68
1:E:251:PRO:CA	1:E:524:HIS:CD2[2_455]	1.56	0.64
1:E:250:GLY:C	1:E:524:HIS:CE1[2_455]	1.56	0.64
1:E:250:GLY:O	1:E:524:HIS:CE1[2_455]	1.58	0.62
1:B:236:ARG:CZ	1:H:264:ALA:O[2_556]	1.59	0.61
3:J:-3:DG:OP2	1:E:236:ARG:CZ[2_445]	1.63	0.57
3:J:-3:DG:OP2	1:E:236:ARG:NH2[2_445]	1.66	0.54
1:E:251:PRO:N	1:E:524:HIS:NE2[2_455]	1.72	0.48
1:B:236:ARG:NH2	1:H:264:ALA:C[2_556]	1.73	0.47
3:J:-3:DG:P	1:E:236:ARG:NH2[2_445]	1.77	0.43
1:B:236:ARG:NH1	1:H:264:ALA:O[2_556]	1.82	0.38
1:A:236:ARG:NH1	3:G:-3:DG:OP2[2_445]	1.85	0.35
1:E:254:GLN:OE1	1:E:524:HIS:ND1[2_455]	1.87	0.33
3:J:-3:DG:P	1:E:236:ARG:NH1[2_445]	1.90	0.30
1:E:250:GLY:C	1:E:524:HIS:NE2[2_455]	1.96	0.24
3:J:-3:DG:P	1:E:236:ARG:CZ[2_445]	1.97	0.23
1:E:250:GLY:O	1:E:524:HIS:NE2[2_455]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:-3:DG:O5'	1:E:236:ARG:NH2[2_445]	1.99	0.21
3:J:-3:DG:OP1	1:E:236:ARG:CZ[2_445]	2.03	0.17
1:A:236:ARG:NH2	3:G:-3:DG:O5'[2_445]	2.03	0.17
1:E:251:PRO:N	1:E:524:HIS:CE1[2_455]	2.12	0.08
1:B:556:GLN:OE1	2:C:-2:DT:O4[2_556]	2.13	0.07
1:A:236:ARG:NH1	3:G:-4:DA:O3'[2_445]	2.13	0.07
1:B:524:HIS:N	1:H:231:GLN:OE1[1_565]	2.19	0.01

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	491/498 (99%)	445 (91%)	38 (8%)	8 (2%)	9	40
1	B	491/498 (99%)	447 (91%)	32 (6%)	12 (2%)	6	29
1	E	491/498 (99%)	453 (92%)	30 (6%)	8 (2%)	9	40
1	H	491/498 (99%)	446 (91%)	34 (7%)	11 (2%)	6	31
All	All	1964/1992 (99%)	1791 (91%)	134 (7%)	39 (2%)	7	34

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ALA
1	B	285	ALA
1	B	691	ASP
1	B	703	VAL
1	E	233	SER
1	E	252	PRO
1	E	285	ALA
1	H	231	GLN
1	H	233	SER
1	H	237	ALA

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Mol	Chain	Res	Type
1	H	285	ALA
1	A	524	HIS
1	A	710	GLY
1	B	233	SER
1	B	236	ARG
1	B	254	GLN
1	B	710	GLY
1	E	710	GLY
1	H	710	GLY
1	A	521	CYS
1	A	690	PRO
1	B	252	PRO
1	E	231	GLN
1	E	690	PRO
1	H	238	LEU
1	H	690	PRO
1	A	691	ASP
1	B	524	HIS
1	E	691	ASP
1	H	524	HIS
1	H	691	ASP
1	A	719	LYS
1	B	690	PRO
1	H	235	ALA
1	B	692	PRO
1	E	654	PRO
1	H	654	PRO
1	A	654	PRO
1	B	654	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/384 (98%)	342 (90%)	36 (10%)	8	32
1	B	378/384 (98%)	340 (90%)	38 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	378/384 (98%)	342 (90%)	36 (10%)	8	32
1	H	378/384 (98%)	346 (92%)	32 (8%)	10	38
All	All	1512/1536 (98%)	1370 (91%)	142 (9%)	8	32

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	232	TRP
1	A	238	LEU
1	A	239	GLU
1	A	241	LEU
1	A	254	GLN
1	A	261	LEU
1	A	265	LYS
1	A	278	TRP
1	A	283	THR
1	A	287	LEU
1	A	299	SER
1	A	307	LEU
1	A	353	GLN
1	A	375	LEU
1	A	453	LEU
1	A	462	GLN
1	A	483	LEU
1	A	488	GLN
1	A	495	GLN
1	A	526	LEU
1	A	553	VAL
1	A	563	GLN
1	A	585	LEU
1	A	588	LEU
1	A	618	LEU
1	A	622	LEU
1	A	628	LEU
1	A	629	THR
1	A	683	ILE
1	A	686	GLN
1	A	689	ARG
1	A	691	ASP
1	A	694	LEU

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	705	LEU
1	B	231	GLN
1	B	238	LEU
1	B	241	LEU
1	B	254	GLN
1	B	255	LEU
1	B	257	THR
1	B	261	LEU
1	B	265	LYS
1	B	278	TRP
1	B	283	THR
1	B	287	LEU
1	B	292	GLU
1	B	299	SER
1	B	307	LEU
1	B	353	GLN
1	B	375	LEU
1	B	387	GLN
1	B	453	LEU
1	B	470	GLN
1	B	483	LEU
1	B	488	GLN
1	B	526	LEU
1	B	548	GLN
1	B	553	VAL
1	B	563	GLN
1	B	585	LEU
1	B	588	LEU
1	B	590	GLN
1	B	618	LEU
1	B	622	LEU
1	B	683	ILE
1	B	686	GLN
1	B	689	ARG
1	B	694	LEU
1	B	697	LEU
1	B	705	LEU
1	B	720	LEU
1	B	721	GLU
1	E	231	GLN
1	E	238	LEU

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Mol	Chain	Res	Type
1	E	239	GLU
1	E	241	LEU
1	E	254	GLN
1	E	261	LEU
1	E	265	LYS
1	E	278	TRP
1	E	283	THR
1	E	287	LEU
1	E	299	SER
1	E	307	LEU
1	E	353	GLN
1	E	375	LEU
1	E	387	GLN
1	E	453	LEU
1	E	470	GLN
1	E	483	LEU
1	E	488	GLN
1	E	524	HIS
1	E	526	LEU
1	E	548	GLN
1	E	563	GLN
1	E	585	LEU
1	E	588	LEU
1	E	590	GLN
1	E	618	LEU
1	E	622	LEU
1	E	663	THR
1	E	683	ILE
1	E	686	GLN
1	E	689	ARG
1	E	691	ASP
1	E	694	LEU
1	E	697	LEU
1	E	705	LEU
1	H	232	TRP
1	H	236	ARG
1	H	241	LEU
1	H	254	GLN
1	H	261	LEU
1	H	265	LYS
1	H	278	TRP
1	H	283	THR

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Mol	Chain	Res	Type
1	H	287	LEU
1	H	299	SER
1	H	307	LEU
1	H	353	GLN
1	H	375	LEU
1	H	387	GLN
1	H	453	LEU
1	H	483	LEU
1	H	488	GLN
1	H	526	LEU
1	H	548	GLN
1	H	563	GLN
1	H	585	LEU
1	H	588	LEU
1	H	590	GLN
1	H	618	LEU
1	H	622	LEU
1	H	665	GLN
1	H	683	ILE
1	H	686	GLN
1	H	691	ASP
1	H	694	LEU
1	H	697	LEU
1	H	705	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	GLN
1	A	488	GLN
1	A	686	GLN
1	A	699	ASN
1	A	701	HIS
1	B	254	GLN
1	B	590	GLN
1	B	686	GLN
1	B	699	ASN
1	B	701	HIS
1	B	722	HIS
1	E	428	GLN
1	E	590	GLN
1	E	686	GLN

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Mol	Chain	Res	Type
1	E	699	ASN
1	E	701	HIS
1	H	428	GLN
1	H	590	GLN
1	H	686	GLN
1	H	699	ASN
1	H	701	HIS
1	H	722	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	5HC	F	6	3,2	16,22,23	1.14	2 (12%)	20,31,34	1.20	2 (10%)
2	5HC	C	6	3,2	16,22,23	1.04	1 (6%)	20,31,34	1.32	2 (10%)
2	5HC	I	6	3,2	16,22,23	1.15	1 (6%)	20,31,34	1.50	4 (20%)
2	5HC	K	6	3,2	16,22,23	1.13	1 (6%)	20,31,34	1.64	5 (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
2	5HC	F	6	3,2	-	1/6/23/24	0/2/2/2
2	5HC	C	6	3,2	-	0/6/23/24	0/2/2/2
2	5HC	I	6	3,2	-	0/6/23/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5HC	K	6	3,2	-	1/6/23/24	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	5HC	C5-C4	2.76	1.47	1.42
2	K	6	5HC	C5-C4	2.64	1.47	1.42
2	F	6	5HC	C5-C4	2.52	1.47	1.42
2	F	6	5HC	C2-N3	-2.26	1.33	1.38
2	C	6	5HC	O5'-C5'	-2.10	1.39	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5HC	C2-N3-C4	4.17	121.05	116.02
2	I	6	5HC	C2-N3-C4	4.12	120.99	116.02
2	K	6	5HC	C2-N3-C4	3.81	120.61	116.02
2	K	6	5HC	C2'-C3'-C4'	2.88	108.76	102.76
2	I	6	5HC	O5-C5M-C5	-2.75	104.12	111.87
2	I	6	5HC	N4-C4-N3	2.63	120.75	117.03
2	K	6	5HC	N4-C4-N3	2.46	120.50	117.03
2	K	6	5HC	O5-C5M-C5	-2.43	105.00	111.87
2	F	6	5HC	C2-N3-C4	2.41	118.92	116.02
2	F	6	5HC	O5-C5M-C5	-2.34	105.26	111.87
2	I	6	5HC	C5-C4-N3	-2.11	117.92	121.24
2	K	6	5HC	O4'-C1'-C2'	2.07	110.15	106.25
2	C	6	5HC	O5-C5M-C5	-2.01	106.20	111.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	6	5HC	O4'-C4'-C5'-O5'
2	F	6	5HC	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	6	5HC	1	0
2	C	6	5HC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	6	5HC	1	0
2	K	6	5HC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	493/498 (98%)	0.13	14 (2%)	53	25	21, 48, 82, 122	0
1	B	493/498 (98%)	0.30	26 (5%)	26	10	22, 47, 97, 161	0
1	E	493/498 (98%)	0.42	32 (6%)	18	5	30, 61, 103, 131	0
1	H	493/498 (98%)	0.46	31 (6%)	20	6	28, 62, 104, 147	0
2	C	16/17 (94%)	-0.25	0	100	100	24, 32, 85, 89	0
2	F	16/17 (94%)	0.08	1 (6%)	20	6	24, 38, 105, 114	0
2	I	16/17 (94%)	-0.32	0	100	100	20, 29, 67, 85	0
2	K	16/17 (94%)	-0.12	1 (6%)	20	6	26, 42, 112, 117	0
3	D	17/17 (100%)	-0.52	0	100	100	25, 43, 77, 87	0
3	G	17/17 (100%)	-0.17	1 (5%)	22	7	23, 42, 98, 111	0
3	J	17/17 (100%)	-0.51	0	100	100	27, 37, 76, 83	0
3	L	17/17 (100%)	0.01	2 (11%)	4	1	32, 53, 111, 118	0
All	All	2104/2128 (98%)	0.29	108 (5%)	28	10	20, 54, 100, 161	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	16.7
1	H	233	SER	12.4
1	B	233	SER	10.8
1	B	722	HIS	10.5
1	E	232	TRP	9.6
1	H	234	GLY	9.5
1	A	230	MET	7.9
1	H	232	TRP	7.7
1	A	722	HIS	7.6
1	B	235	ALA	7.4
1	E	233	SER	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	232	TRP	7.1
1	B	692	PRO	6.3
1	E	237	ALA	6.1
1	B	524	HIS	6.1
1	E	235	ALA	5.4
1	H	524	HIS	4.9
1	B	282	LEU	4.9
1	A	233	SER	4.8
1	A	243	THR	4.7
1	B	523	ALA	4.6
1	E	239	GLU	4.5
1	A	231	GLN	4.4
1	A	234	GLY	4.4
1	B	231	GLN	4.4
1	B	236	ARG	4.4
1	H	391	LEU	4.4
3	L	2	DA	4.3
1	E	529	GLN	4.3
1	B	694	LEU	4.3
1	E	230	MET	4.2
1	B	239	GLU	4.2
1	H	390	GLY	4.1
1	E	695	ALA	4.1
1	E	234	GLY	4.0
1	E	231	GLN	4.0
1	B	691	ASP	3.9
1	E	243	THR	3.8
1	E	240	ALA	3.6
3	L	-14	DA	3.6
1	E	520	LEU	3.5
1	A	692	PRO	3.5
1	E	692	PRO	3.5
1	H	722	HIS	3.4
1	E	560	LEU	3.4
1	H	253	LEU	3.3
1	A	695	ALA	3.3
1	E	241	LEU	3.3
1	E	492	LEU	3.2
1	H	523	ALA	3.1
1	B	244	VAL	3.1
1	E	486	LEU	3.1
1	H	240	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	3.1
1	A	691	ASP	3.0
1	H	357	LEU	3.0
1	B	261	LEU	3.0
1	B	693	ALA	3.0
1	E	722	HIS	3.0
1	H	378	VAL	3.0
1	B	556	GLN	2.9
3	G	2	DA	2.9
1	H	425	LEU	2.9
1	E	251	PRO	2.9
1	B	230	MET	2.8
1	E	512	THR	2.7
1	A	251	PRO	2.7
1	A	240	ALA	2.6
1	E	513	VAL	2.6
2	K	14	DT	2.5
1	E	483	LEU	2.5
1	E	691	ASP	2.4
1	H	235	ALA	2.4
1	A	694	LEU	2.4
1	B	248	LEU	2.4
1	H	278	TRP	2.4
1	E	422	ALA	2.4
1	H	346	ARG	2.4
2	F	-2	DT	2.4
1	H	529	GLN	2.3
1	B	240	ALA	2.3
1	H	690	PRO	2.3
1	H	230	MET	2.3
1	E	236	ARG	2.3
1	E	459	LEU	2.3
1	H	323	LEU	2.3
1	H	692	PRO	2.3
1	H	231	GLN	2.2
1	B	462	GLN	2.2
1	B	719	LYS	2.2
1	H	379	GLN	2.2
1	E	532	VAL	2.2
1	E	581	VAL	2.2
1	H	526	LEU	2.2
1	H	270	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	409	LEU	2.1
1	H	241	LEU	2.1
1	H	286	PRO	2.1
1	E	659	ALA	2.1
1	B	267	GLY	2.1
1	B	588	LEU	2.1
1	E	516	LEU	2.1
1	H	691	ASP	2.1
1	H	416	LEU	2.0
1	A	524	HIS	2.0
1	B	238	LEU	2.0
1	E	510	LEU	2.0
1	H	720	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	5HC	K	6	21/22	0.97	0.14	27,31,38,41	0
2	5HC	I	6	21/22	0.98	0.15	17,20,24,26	0
2	5HC	F	6	21/22	0.98	0.15	22,27,37,40	0
2	5HC	C	6	21/22	0.99	0.16	22,25,30,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.