Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 09:08 PM JST

PDB ID	:	6JW2
Title	:	Universal RVD R* accommodates 5hmC via water-mediated interactions
Authors	:	Liu, L.; Yi, C.
Deposited on	:	2019-04-18
Resolution	:	3.03 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:

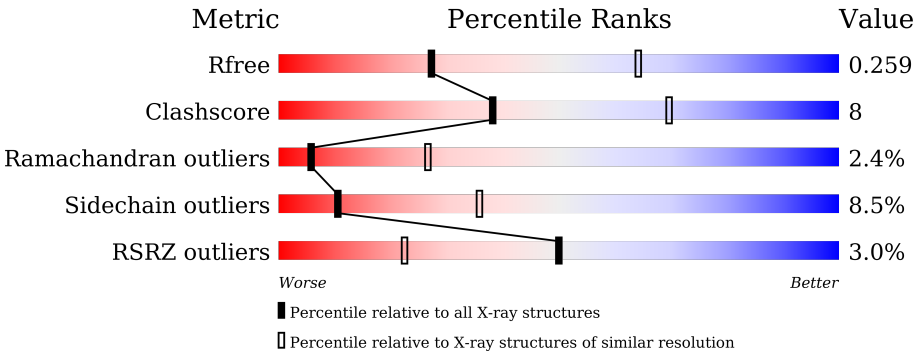
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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 <=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	2% 82% 15% ••
1	B	498	4% 77% 17% 5% ••
1	E	498	3% 81% 15% •••
1	H	498	3% 79% 16% • ••
2	C	17	59% 41%
2	F	17	12% 53% 47%

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Mol	Chain	Length	Quality of chain
2	I	17	65% 29% 6%
2	K	17	12% 53% 41% 6%
3	D	17	82% 18%
3	G	17	6% 94% 6%
3	J	17	82% 18%
3	L	17	6% 88% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17098 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
			3582	2238	669	663	12			
1	B	493	Total	C	N	O	S	0	0	0
			3582	2238	669	663	12			
1	E	493	Total	C	N	O	S	0	0	0
			3582	2238	669	663	12			
1	H	493	Total	C	N	O	S	0	0	0
			3582	2238	669	663	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.

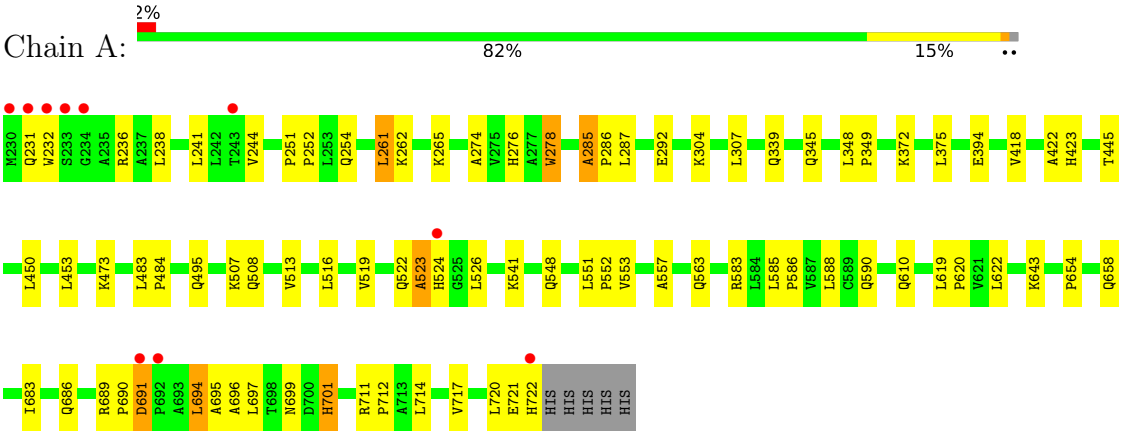
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		

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.

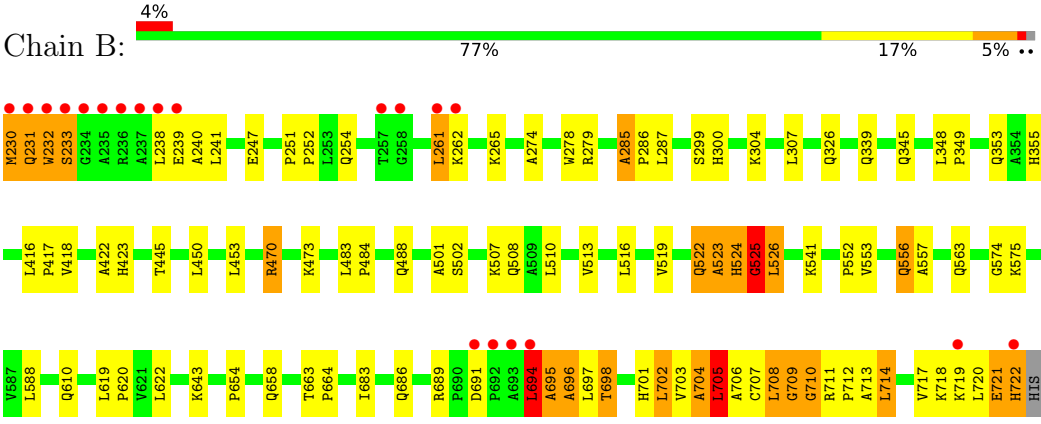
• Molecule 1: TAL effector

Chain A:



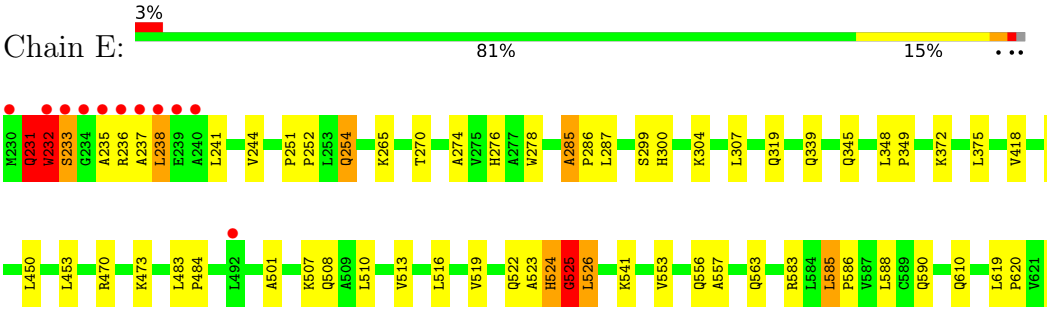
• Molecule 1: TAL effector

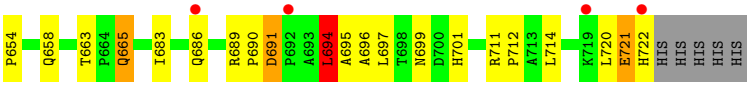
Chain B:



• Molecule 1: TAL effector

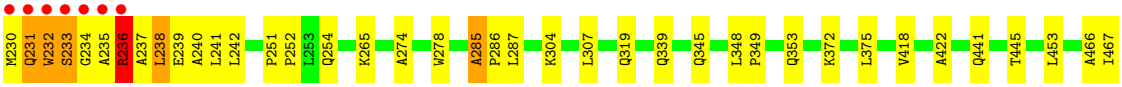
Chain E:

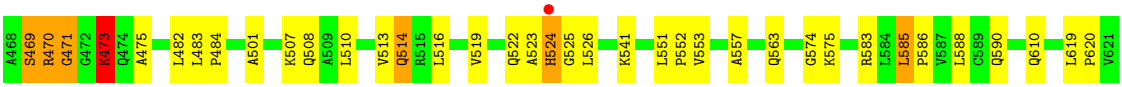


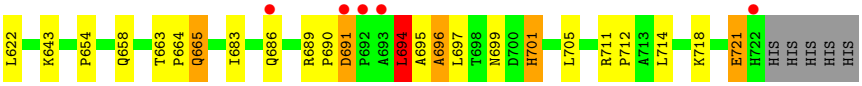


• Molecule 1: TAL effector

Chain H:

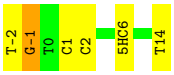






• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP *CP*T)-3')

Chain I:

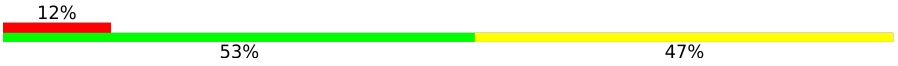


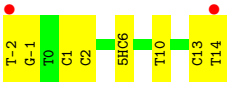
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP *CP*T)-3')

Chain C:

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

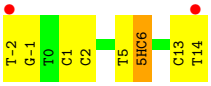
Chain F:





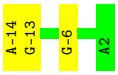
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP *CP*T)-3')

Chain K:



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

Chain J:

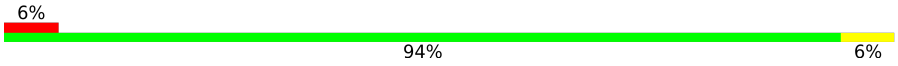


• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain D:

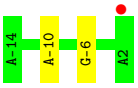
• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain G:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.52Å 93.78Å 167.75Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	163.67 – 3.03 40.68 – 3.03	Depositor EDS
% Data completeness (in resolution range)	85.0 (163.67-3.03) 85.0 (40.68-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.237 , 0.261 0.234 , 0.259	Depositor DCC
R_{free} test set	2416 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17098	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/3634	0.69	1/4963 (0.0%)
1	B	0.54	0/3634	0.76	3/4963 (0.1%)
1	E	0.53	1/3634 (0.0%)	0.71	2/4963 (0.0%)
1	H	0.49	1/3634 (0.0%)	0.69	4/4963 (0.1%)
2	C	0.74	0/349	0.89	0/533
2	F	0.73	1/349 (0.3%)	0.93	0/533
2	I	0.80	1/349 (0.3%)	0.97	0/533
2	K	0.68	0/349	0.90	0/533
3	D	0.60	0/402	0.89	0/620
3	G	0.64	1/402 (0.2%)	0.82	1/620 (0.2%)
3	J	0.60	1/402 (0.2%)	0.81	0/620
3	L	0.54	0/402	0.82	1/620 (0.2%)
All	All	0.55	6/17540 (0.0%)	0.75	12/24464 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	6
1	E	0	2
1	H	0	2
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	232	TRP	CB-CG	-5.99	1.39	1.50
3	G	-6	DG	O3'-P	-5.78	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	-6	DG	O3'-P	-5.50	1.54	1.61
2	F	10	DT	O3'-P	-5.38	1.54	1.61
2	I	-1	DG	O3'-P	-5.11	1.55	1.61
1	H	232	TRP	CB-CG	-5.06	1.41	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	694	LEU	CA-CB-CG	6.93	131.25	115.30
1	E	231	GLN	N-CA-C	6.43	128.35	111.00
1	H	233	SER	N-CA-CB	-6.23	101.16	110.50
1	H	694	LEU	CA-CB-CG	5.99	129.06	115.30
3	L	-6	DG	C1'-O4'-C4'	-5.96	104.14	110.10
1	A	694	LEU	CA-CB-CG	5.93	128.94	115.30
1	B	523	ALA	N-CA-C	-5.73	95.52	111.00
1	B	694	LEU	CA-CB-CG	5.70	128.41	115.30
3	G	-6	DG	C1'-O4'-C4'	-5.41	104.69	110.10
1	H	471	GLY	N-CA-C	-5.12	100.30	113.10
1	H	469	SER	N-CA-C	-5.07	97.31	111.00
1	B	705	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	PRO	Peptide
1	A	523	ALA	Peptide
1	B	230	MET	Peptide
1	B	251	PRO	Peptide
1	B	522	GLN	Peptide
1	B	525	GLY	Peptide
1	B	705	LEU	Peptide
1	B	719	LYS	Peptide
1	E	251	PRO	Peptide
1	E	525	GLY	Peptide
1	H	232	TRP	Peptide
1	H	251	PRO	Peptide

5.2 Too-close contacts (i)

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	3582	0	3730	34	1
1	B	3582	0	3730	83	3
1	E	3582	0	3730	54	4
1	H	3582	0	3730	55	3
2	C	337	0	195	6	0
2	F	337	0	195	9	0
2	I	337	0	195	5	0
2	K	337	0	195	11	0
3	D	355	0	189	2	0
3	G	355	0	189	0	0
3	J	355	0	189	4	0
3	L	355	0	189	1	0
4	C	1	0	0	0	0
4	I	1	0	0	0	0
All	All	17098	0	16456	252	7

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 8.

All (252) 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:5:DT:H2"	2:K:6:5HC:H5"	1.54	0.88
1:B:708:LEU:CD1	1:E:720:LEU:HD13	2.04	0.87
1:B:717:VAL:O	1:B:720:LEU:O	1.93	0.85
1:B:709:GLY:O	1:B:711:ARG:N	2.09	0.85
1:H:231:GLN:C	1:H:233:SER:OG	2.15	0.85
1:B:705:LEU:HB2	1:B:710:GLY:CA	2.05	0.85
1:B:708:LEU:HG	1:B:708:LEU:O	1.79	0.82
1:B:285:ALA:HB1	1:B:286:PRO:HD2	1.63	0.81
1:H:285:ALA:HB1	1:H:286:PRO:HD2	1.61	0.80
1:E:285:ALA:HB1	1:E:286:PRO:HD2	1.63	0.80
1:A:285:ALA:HB1	1:A:286:PRO:HD2	1.62	0.80
1:B:697:LEU:HD22	1:B:701:HIS:ND1	1.96	0.80
2:F:13:DC:C5	2:F:14:DT:C6	2.70	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:-14:DA:H2"	3:D:-13:DG:OP2	1.83	0.77
1:B:698:THR:HG23	1:B:701:HIS:CB	2.15	0.77
1:H:470:ARG:NH1	3:L:-10:DA:OP2	2.17	0.76
1:E:695:ALA:O	1:E:697:LEU:N	2.20	0.74
1:H:238:LEU:O	1:H:241:LEU:HB3	1.88	0.72
1:E:441:GLN:HB3	1:E:473:LYS:HD3	1.72	0.71
2:K:13:DC:H2"	2:K:14:DT:C5'	2.20	0.71
2:F:13:DC:H2"	2:F:14:DT:C5'	2.21	0.70
1:E:522:GLN:C	1:E:524:HIS:N	2.39	0.70
1:B:708:LEU:HD11	1:E:720:LEU:HD13	1.72	0.69
1:E:422:ALA:HB2	1:H:319:GLN:HB3	1.72	0.69
1:B:710:GLY:O	1:B:711:ARG:C	2.25	0.69
1:H:235:ALA:C	1:H:236:ARG:HD2	2.13	0.69
1:H:469:SER:O	1:H:470:ARG:HB2	1.93	0.69
1:B:698:THR:HG23	1:B:701:HIS:HB3	1.75	0.68
1:B:708:LEU:HD13	1:E:720:LEU:HD13	1.75	0.68
1:B:230:MET:CB	1:B:231:GLN:HG2	2.23	0.68
1:B:708:LEU:C	1:B:710:GLY:H	1.97	0.68
1:B:698:THR:HG23	1:B:701:HIS:HB2	1.77	0.67
1:A:261:LEU:HG	1:A:262:LYS:N	2.11	0.65
1:H:285:ALA:HB1	1:H:286:PRO:CD	2.26	0.65
1:B:470:ARG:NH2	1:B:502:SER:O	2.30	0.65
1:E:285:ALA:HB1	1:E:286:PRO:CD	2.27	0.65
1:H:471:GLY:O	1:H:475:ALA:HB3	1.96	0.65
1:B:720:LEU:O	1:B:721:GLU:HB3	1.96	0.64
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.27	0.64
1:H:466:ALA:O	1:H:469:SER:O	2.15	0.64
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.26	0.64
1:B:705:LEU:HD12	1:B:714:LEU:HD11	1.81	0.63
1:B:708:LEU:O	1:B:710:GLY:N	2.32	0.63
1:B:708:LEU:C	1:B:710:GLY:N	2.49	0.62
1:H:694:LEU:O	1:H:696:ALA:N	2.31	0.62
3:J:-14:DA:N3	3:J:-14:DA:H2'	2.13	0.62
1:B:522:GLN:C	1:B:524:HIS:N	2.44	0.61
2:I:14:DT:C5	3:J:-14:DA:N6	2.68	0.61
1:A:508:GLN:HB3	1:A:541:LYS:HD3	1.83	0.61
1:B:708:LEU:HD13	1:E:720:LEU:HB3	1.81	0.61
1:B:508:GLN:HB3	1:B:541:LYS:HD3	1.82	0.60
1:E:508:GLN:HB3	1:E:541:LYS:HD3	1.83	0.60
1:E:238:LEU:CD2	1:E:241:LEU:HD23	2.33	0.59
1:B:703:VAL:CA	1:B:705:LEU:HD13	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:LEU:HB2	1:B:710:GLY:HA2	1.85	0.59
1:H:508:GLN:HB3	1:H:541:LYS:HD3	1.83	0.59
1:H:663:THR:OG1	1:H:665:GLN:OE1	2.18	0.59
1:B:339:GLN:HB3	1:B:372:LYS:HD3	1.85	0.59
1:E:339:GLN:HB3	1:E:372:LYS:HD3	1.84	0.59
1:H:231:GLN:O	1:H:233:SER:OG	2.18	0.59
1:B:705:LEU:HB2	1:B:710:GLY:HA3	1.84	0.58
2:I:-2:DT:H4'	2:I:-1:DG:O5'	2.03	0.58
1:H:339:GLN:HB3	1:H:372:LYS:HD3	1.85	0.58
1:E:522:GLN:O	1:E:523:ALA:C	2.41	0.58
1:B:701:HIS:O	1:B:703:VAL:N	2.33	0.57
1:E:663:THR:OG1	1:E:665:GLN:OE1	2.18	0.57
1:E:422:ALA:CB	1:H:319:GLN:HB3	2.34	0.57
1:E:523:ALA:O	1:E:525:GLY:N	2.37	0.57
1:B:705:LEU:CB	1:B:710:GLY:HA2	2.35	0.56
1:B:710:GLY:O	1:B:713:ALA:N	2.38	0.56
1:A:339:GLN:HB3	1:A:372:LYS:HD3	1.86	0.56
1:B:522:GLN:O	1:B:523:ALA:C	2.44	0.56
3:J:-14:DA:H4'	3:J:-13:DG:OP1	2.05	0.56
1:A:394:GLU:N	1:A:394:GLU:OE1	2.37	0.56
1:A:238:LEU:CD2	1:A:241:LEU:HD23	2.36	0.56
1:A:292:GLU:CD	1:A:292:GLU:H	2.09	0.55
1:A:553:VAL:O	1:A:557:ALA:HB3	2.06	0.55
1:B:524:HIS:O	1:B:525:GLY:C	2.44	0.55
1:B:525:GLY:C	1:B:526:LEU:HD13	2.26	0.55
1:B:553:VAL:O	1:B:557:ALA:HB3	2.06	0.55
1:E:519:VAL:HA	1:E:522:GLN:HB3	1.89	0.55
1:H:697:LEU:HD23	1:H:701:HIS:HD2	1.72	0.55
2:K:5:DT:H2"	2:K:6:5HC:C5'	2.33	0.55
2:K:13:DC:H2"	2:K:14:DT:O5'	2.06	0.55
2:F:13:DC:C5	2:F:14:DT:C5	2.96	0.54
1:B:523:ALA:O	1:B:525:GLY:N	2.40	0.54
1:B:708:LEU:HD13	1:E:720:LEU:CD1	2.38	0.54
1:B:695:ALA:O	1:B:697:LEU:N	2.41	0.54
1:H:231:GLN:C	1:H:233:SER:HG	2.04	0.54
1:H:237:ALA:O	1:H:239:GLU:N	2.41	0.54
1:H:553:VAL:O	1:H:557:ALA:HB3	2.07	0.54
1:B:708:LEU:O	1:B:709:GLY:C	2.45	0.54
1:E:525:GLY:C	1:E:526:LEU:HD13	2.28	0.54
2:F:13:DC:H2"	2:F:14:DT:O5'	2.08	0.54
1:H:441:GLN:HB3	1:H:473:LYS:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:DC:N4	2:C:14:DT:O4	2.42	0.53
1:E:231:GLN:O	1:E:232:TRP:CD1	2.62	0.53
1:E:238:LEU:HD21	1:E:241:LEU:HD23	1.90	0.53
1:E:553:VAL:O	1:E:557:ALA:HB3	2.08	0.53
1:A:292:GLU:N	1:A:292:GLU:OE2	2.42	0.52
1:A:697:LEU:HD23	1:A:701:HIS:HD2	1.72	0.52
1:A:689:ARG:O	1:A:691:ASP:N	2.43	0.52
1:E:232:TRP:O	1:E:233:SER:HB2	2.09	0.52
1:A:238:LEU:HD21	1:A:241:LEU:HD23	1.91	0.52
1:B:708:LEU:HD13	1:E:720:LEU:CB	2.39	0.52
1:B:232:TRP:O	1:B:233:SER:OG	2.21	0.51
1:E:516:LEU:HA	1:E:519:VAL:CG1	2.40	0.51
1:B:720:LEU:O	1:B:721:GLU:CB	2.58	0.51
1:E:689:ARG:O	1:E:691:ASP:N	2.44	0.51
1:H:516:LEU:HA	1:H:519:VAL:CG1	2.40	0.51
1:A:516:LEU:HA	1:A:519:VAL:CG1	2.41	0.51
1:B:704:ALA:O	1:B:705:LEU:HB3	2.10	0.50
1:B:694:LEU:O	1:B:696:ALA:N	2.45	0.50
1:B:703:VAL:HA	1:B:705:LEU:HD13	1.93	0.50
1:B:516:LEU:HA	1:B:519:VAL:CG1	2.41	0.50
1:E:516:LEU:HA	1:E:519:VAL:HG12	1.94	0.50
1:E:610:GLN:HB3	1:E:643:LYS:HD3	1.94	0.49
1:E:619:LEU:HB3	1:E:620:PRO:HD3	1.93	0.49
1:H:619:LEU:HB3	1:H:620:PRO:HD3	1.94	0.49
1:B:519:VAL:HG22	1:B:519:VAL:O	2.13	0.49
1:H:516:LEU:HA	1:H:519:VAL:HG12	1.94	0.49
1:A:244:VAL:HG13	1:A:276:HIS:HB2	1.94	0.49
1:B:619:LEU:HB3	1:B:620:PRO:HD3	1.94	0.49
1:E:524:HIS:O	1:E:525:GLY:C	2.51	0.49
1:H:689:ARG:O	1:H:691:ASP:N	2.46	0.49
2:K:-2:DT:H1'	2:K:-1:DG:C8	2.47	0.49
2:C:13:DC:H2"	2:C:14:DT:O5'	2.12	0.49
1:E:231:GLN:O	1:E:232:TRP:HD1	1.96	0.49
2:C:13:DC:C4	2:C:14:DT:C4	3.02	0.48
1:A:516:LEU:HA	1:A:519:VAL:HG12	1.96	0.48
2:K:13:DC:H2"	2:K:14:DT:C4'	2.44	0.48
1:A:619:LEU:HB3	1:A:620:PRO:HD3	1.95	0.48
1:B:705:LEU:HA	1:B:708:LEU:H	1.79	0.48
1:B:705:LEU:C	1:B:707:CYS:N	2.65	0.48
1:H:239:GLU:O	1:H:241:LEU:N	2.46	0.48
1:A:610:GLN:HB3	1:A:643:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:LEU:CD1	1:E:720:LEU:HB3	2.43	0.47
1:B:516:LEU:HA	1:B:519:VAL:HG12	1.96	0.47
2:I:-2:DT:H1'	2:I:-1:DG:C8	2.49	0.47
1:B:585:LEU:HB3	1:B:586:PRO:CD	2.44	0.47
1:E:519:VAL:HG22	1:E:519:VAL:O	2.14	0.47
2:F:13:DC:H2"	2:F:14:DT:C4'	2.44	0.47
1:H:239:GLU:O	1:H:242:LEU:N	2.47	0.47
2:K:13:DC:C5	2:K:14:DT:C6	3.02	0.47
1:B:703:VAL:C	1:B:705:LEU:HD13	2.35	0.47
1:E:231:GLN:C	1:E:232:TRP:HD1	2.17	0.47
1:A:585:LEU:HB3	1:A:586:PRO:CD	2.44	0.47
1:B:705:LEU:HD22	1:B:706:ALA:N	2.30	0.47
1:E:231:GLN:O	1:E:232:TRP:HB2	2.15	0.47
1:E:585:LEU:HB3	1:E:586:PRO:CD	2.45	0.47
1:B:445:THR:OG1	1:B:473:LYS:HG3	2.15	0.47
1:H:483:LEU:N	1:H:484:PRO:HD2	2.30	0.47
1:H:519:VAL:O	1:H:519:VAL:HG22	2.15	0.47
1:H:610:GLN:HB3	1:H:643:LYS:HD3	1.97	0.47
1:H:585:LEU:HB3	1:H:586:PRO:CD	2.45	0.46
1:E:483:LEU:N	1:E:484:PRO:HD2	2.31	0.46
1:A:699:ASN:N	1:A:699:ASN:HD22	2.13	0.46
1:B:610:GLN:HB3	1:B:643:LYS:HD3	1.96	0.46
1:A:519:VAL:O	1:A:519:VAL:HG22	2.15	0.46
1:E:235:ALA:O	1:E:237:ALA:N	2.48	0.46
1:H:235:ALA:O	1:H:236:ARG:HB2	2.16	0.46
1:A:445:THR:OG1	1:A:473:LYS:HG3	2.15	0.45
2:C:-2:DT:H4'	2:C:-1:DG:O5'	2.17	0.45
1:H:231:GLN:CA	1:H:233:SER:OG	2.64	0.45
1:H:418:VAL:O	1:H:422:ALA:HB3	2.16	0.45
1:H:699:ASN:N	1:H:699:ASN:HD22	2.15	0.45
1:E:418:VAL:O	1:E:422:ALA:HB3	2.17	0.45
1:H:467:ILE:O	1:H:471:GLY:O	2.35	0.45
1:A:418:VAL:O	1:A:422:ALA:HB3	2.16	0.45
1:H:239:GLU:C	1:H:241:LEU:N	2.68	0.45
1:B:552:PRO:O	1:B:556:GLN:OE1	2.34	0.44
1:B:697:LEU:HD23	1:B:697:LEU:HA	1.76	0.44
2:I:14:DT:OP1	2:I:14:DT:O4'	2.35	0.44
2:K:-2:DT:H4'	2:K:-1:DG:O5'	2.18	0.44
1:A:717:VAL:O	1:A:720:LEU:N	2.47	0.44
1:B:704:ALA:N	1:B:705:LEU:HD13	2.31	0.44
2:K:1:DC:H2"	2:K:2:DC:O5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:ALA:HB2	1:H:304:LYS:HG3	2.00	0.44
1:A:244:VAL:CG1	1:A:276:HIS:HB2	2.47	0.44
1:B:519:VAL:HA	1:B:522:GLN:HB3	2.00	0.44
1:E:232:TRP:O	1:E:233:SER:CB	2.65	0.44
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.99	0.44
1:H:237:ALA:O	1:H:238:LEU:C	2.57	0.44
1:B:418:VAL:O	1:B:422:ALA:HB3	2.17	0.43
1:A:348:LEU:N	1:A:349:PRO:CD	2.81	0.43
1:H:285:ALA:CB	1:H:286:PRO:CD	2.96	0.43
1:H:524:HIS:O	1:H:525:GLY:C	2.56	0.43
1:B:423:HIS:HB3	1:B:450:LEU:HD23	2.01	0.43
1:B:416:LEU:N	1:B:417:PRO:CD	2.82	0.43
2:F:1:DC:H2"	2:F:2:DC:O5'	2.19	0.43
1:A:522:GLN:O	1:A:523:ALA:HB3	2.18	0.43
2:I:1:DC:H2"	2:I:2:DC:O5'	2.18	0.43
1:H:348:LEU:N	1:H:349:PRO:CD	2.82	0.43
1:A:483:LEU:N	1:A:484:PRO:HD2	2.34	0.43
1:B:703:VAL:HA	1:B:705:LEU:CD1	2.48	0.43
1:B:701:HIS:C	1:B:703:VAL:H	2.20	0.43
1:E:711:ARG:HB3	1:E:712:PRO:HD3	2.01	0.43
2:K:5:DT:C2'	2:K:6:5HC:H5"	2.38	0.43
1:A:274:ALA:HB2	1:A:304:LYS:HG3	2.00	0.42
3:D:-13:DG:H2"	3:D:-12:DA:OP2	2.19	0.42
1:E:274:ALA:HB2	1:E:304:LYS:HG3	2.00	0.42
1:H:235:ALA:O	1:H:236:ARG:HD2	2.18	0.42
1:H:522:GLN:O	1:H:523:ALA:HB3	2.18	0.42
1:E:348:LEU:N	1:E:349:PRO:CD	2.82	0.42
1:E:525:GLY:HA3	1:E:526:LEU:HD22	2.02	0.42
1:E:694:LEU:O	1:E:695:ALA:C	2.57	0.42
1:B:261:LEU:HG	1:B:262:LYS:N	2.34	0.42
1:B:483:LEU:N	1:B:484:PRO:HD2	2.35	0.42
2:C:1:DC:H2"	2:C:2:DC:O5'	2.18	0.42
1:H:711:ARG:HB3	1:H:712:PRO:HD3	2.01	0.42
1:E:423:HIS:HB3	1:E:450:LEU:HD23	2.02	0.42
1:E:299:SER:O	1:E:300:HIS:CG	2.73	0.42
1:A:274:ALA:O	1:A:278:TRP:CD1	2.73	0.42
1:A:551:LEU:N	1:A:552:PRO:HD2	2.34	0.42
1:B:247:GLU:HB3	1:B:279:ARG:HH12	1.84	0.41
1:E:699:ASN:N	1:E:699:ASN:HD22	2.18	0.41
1:H:663:THR:O	1:H:664:PRO:C	2.58	0.41
1:B:348:LEU:N	1:B:349:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:HIS:C	2:F:14:DT:H2"	2.40	0.41
1:E:285:ALA:CB	1:E:286:PRO:CD	2.97	0.41
1:B:663:THR:O	1:B:664:PRO:C	2.58	0.41
1:E:501:ALA:HB2	1:E:510:LEU:HD11	2.02	0.41
1:H:445:THR:OG1	1:H:473:LYS:HG2	2.20	0.41
2:K:13:DC:C2'	2:K:14:DT:C5'	2.96	0.41
1:B:709:GLY:O	1:B:710:GLY:C	2.58	0.41
1:B:711:ARG:HB3	1:B:712:PRO:HD3	2.02	0.41
1:H:231:GLN:N	1:H:233:SER:OG	2.54	0.41
1:A:423:HIS:HB3	1:A:450:LEU:HD23	2.02	0.41
1:H:551:LEU:N	1:H:552:PRO:HD2	2.36	0.41
1:A:711:ARG:HB3	1:A:712:PRO:HD3	2.03	0.41
1:B:501:ALA:HB2	1:B:510:LEU:HD11	2.03	0.41
1:E:721:GLU:C	1:E:721:GLU:CD	2.79	0.41
2:F:13:DC:C6	2:F:14:DT:C6	3.08	0.41
1:H:721:GLU:C	1:H:721:GLU:CD	2.79	0.41
1:A:695:ALA:O	1:A:697:LEU:N	2.53	0.41
1:B:239:GLU:C	1:B:241:LEU:N	2.74	0.41
2:C:13:DC:H2"	2:C:14:DT:C5'	2.50	0.41
1:H:501:ALA:HB2	1:H:510:LEU:HD11	2.03	0.41
1:B:232:TRP:O	1:B:233:SER:CB	2.68	0.41
1:E:231:GLN:C	1:E:232:TRP:CD1	2.93	0.41
2:F:-2:DT:H2"	2:F:-1:DG:O5'	2.21	0.41
1:B:721:GLU:C	1:B:721:GLU:CD	2.79	0.40
1:H:238:LEU:C	1:H:238:LEU:HD23	2.42	0.40
1:H:482:LEU:HD22	1:H:514:GLN:HE21	1.87	0.40
1:B:299:SER:O	1:B:300:HIS:CG	2.75	0.40
1:B:705:LEU:HB2	1:B:710:GLY:N	2.34	0.40
1:E:244:VAL:CG1	1:E:276:HIS:HB2	2.51	0.40
1:H:574:GLY:O	1:H:575:LYS:C	2.59	0.40
1:H:705:LEU:HD12	1:H:705:LEU:HA	1.98	0.40
3:J:-14:DA:N3	3:J:-14:DA:C2'	2.84	0.40
1:B:574:GLY:O	1:B:575:LYS:C	2.59	0.40
1:B:720:LEU:HD12	1:B:721:GLU:N	2.36	0.40

All (7) 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:231:GLN:O	1:E:231:GLN:C[2_746]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:NE2	1:H:234:GLY:O[2_655]	2.02	0.18
1:E:254:GLN:OE1	1:E:524:HIS:CG[2_756]	2.05	0.15
1:E:254:GLN:OE1	1:E:524:HIS:N[2_756]	2.06	0.14
1:B:524:HIS:NE2	1:H:230:MET:O[1_565]	2.10	0.10
1:E:254:GLN:OE1	1:E:524:HIS:CD2[2_756]	2.10	0.10
1:B:231:GLN:CD	1:H:234:GLY:O[2_655]	2.18	0.02

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%)	444 (90%)	39 (8%)	8 (2%)	9	37
1	B	491/498 (99%)	442 (90%)	33 (7%)	16 (3%)	4	19
1	E	491/498 (99%)	447 (91%)	33 (7%)	11 (2%)	6	28
1	H	491/498 (99%)	442 (90%)	36 (7%)	13 (3%)	5	24
All	All	1964/1992 (99%)	1775 (90%)	141 (7%)	48 (2%)	6	26

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	PRO
1	A	285	ALA
1	A	524	HIS
1	B	240	ALA
1	B	252	PRO
1	B	285	ALA
1	B	524	HIS
1	B	696	ALA
1	B	702	LEU
1	B	705	LEU
1	B	721	GLU

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Mol	Chain	Res	Type
1	E	232	TRP
1	E	233	SER
1	E	236	ARG
1	E	252	PRO
1	E	285	ALA
1	E	524	HIS
1	H	238	LEU
1	H	285	ALA
1	H	524	HIS
1	H	695	ALA
1	A	721	GLU
1	B	233	SER
1	B	695	ALA
1	B	710	GLY
1	E	696	ALA
1	H	236	ARG
1	H	240	ALA
1	H	252	PRO
1	H	470	ARG
1	H	696	ALA
1	A	236	ARG
1	A	690	PRO
1	A	696	ALA
1	H	473	LYS
1	E	525	GLY
1	E	690	PRO
1	E	721	GLU
1	H	690	PRO
1	H	721	GLU
1	B	525	GLY
1	B	704	ALA
1	B	709	GLY
1	A	654	PRO
1	B	654	PRO
1	B	691	ASP
1	E	654	PRO
1	H	654	PRO

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	378/384 (98%)	350 (93%)	28 (7%)	13 42
1	B	378/384 (98%)	340 (90%)	38 (10%)	7 27
1	E	378/384 (98%)	346 (92%)	32 (8%)	10 36
1	H	378/384 (98%)	347 (92%)	31 (8%)	11 37
All	All	1512/1536 (98%)	1383 (92%)	129 (8%)	10 36

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	TRP
1	A	254	GLN
1	A	261	LEU
1	A	265	LYS
1	A	278	TRP
1	A	287	LEU
1	A	307	LEU
1	A	345	GLN
1	A	375	LEU
1	A	453	LEU
1	A	495	GLN
1	A	507	LYS
1	A	513	VAL
1	A	526	LEU
1	A	548	GLN
1	A	563	GLN
1	A	583	ARG
1	A	588	LEU
1	A	590	GLN
1	A	622	LEU
1	A	658	GLN
1	A	683	ILE
1	A	686	GLN
1	A	691	ASP
1	A	694	LEU
1	A	701	HIS
1	A	714	LEU
1	A	722	HIS

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Mol	Chain	Res	Type
1	B	231	GLN
1	B	232	TRP
1	B	238	LEU
1	B	254	GLN
1	B	261	LEU
1	B	265	LYS
1	B	278	TRP
1	B	287	LEU
1	B	307	LEU
1	B	326	GLN
1	B	345	GLN
1	B	353	GLN
1	B	355	HIS
1	B	375	LEU
1	B	453	LEU
1	B	470	ARG
1	B	488	GLN
1	B	507	LYS
1	B	513	VAL
1	B	526	LEU
1	B	556	GLN
1	B	563	GLN
1	B	583	ARG
1	B	585	LEU
1	B	588	LEU
1	B	622	LEU
1	B	658	GLN
1	B	683	ILE
1	B	686	GLN
1	B	689	ARG
1	B	694	LEU
1	B	698	THR
1	B	702	LEU
1	B	705	LEU
1	B	708	LEU
1	B	714	LEU
1	B	718	LYS
1	B	722	HIS
1	E	231	GLN
1	E	238	LEU
1	E	254	GLN
1	E	265	LYS

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Mol	Chain	Res	Type
1	E	270	THR
1	E	278	TRP
1	E	287	LEU
1	E	307	LEU
1	E	319	GLN
1	E	345	GLN
1	E	375	LEU
1	E	453	LEU
1	E	470	ARG
1	E	507	LYS
1	E	513	VAL
1	E	526	LEU
1	E	556	GLN
1	E	563	GLN
1	E	583	ARG
1	E	585	LEU
1	E	588	LEU
1	E	590	GLN
1	E	622	LEU
1	E	658	GLN
1	E	665	GLN
1	E	683	ILE
1	E	686	GLN
1	E	691	ASP
1	E	694	LEU
1	E	701	HIS
1	E	714	LEU
1	E	722	HIS
1	H	231	GLN
1	H	236	ARG
1	H	254	GLN
1	H	265	LYS
1	H	278	TRP
1	H	287	LEU
1	H	307	LEU
1	H	345	GLN
1	H	353	GLN
1	H	375	LEU
1	H	453	LEU
1	H	473	LYS
1	H	507	LYS
1	H	513	VAL

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Mol	Chain	Res	Type
1	H	514	GLN
1	H	526	LEU
1	H	563	GLN
1	H	583	ARG
1	H	585	LEU
1	H	588	LEU
1	H	590	GLN
1	H	622	LEU
1	H	658	GLN
1	H	665	GLN
1	H	683	ILE
1	H	686	GLN
1	H	691	ASP
1	H	694	LEU
1	H	701	HIS
1	H	714	LEU
1	H	718	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	300	HIS
1	A	548	GLN
1	A	699	ASN
1	A	701	HIS
1	B	254	GLN
1	B	300	HIS
1	B	699	ASN
1	E	254	GLN
1	E	300	HIS
1	E	436	ASN
1	E	605	ASN
1	E	699	ASN
1	E	701	HIS
1	H	231	GLN
1	H	254	GLN
1	H	300	HIS
1	H	514	GLN
1	H	605	ASN
1	H	699	ASN
1	H	701	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2,3	18,22,23	1.24	1 (5%)	23,31,34	1.61	6 (26%)
2	5HC	K	6	2,3	18,22,23	1.38	2 (11%)	23,31,34	1.86	7 (30%)
2	5HC	I	6	2,3	18,22,23	1.07	1 (5%)	23,31,34	0.95	0
2	5HC	C	6	2,3	18,22,23	1.00	1 (5%)	23,31,34	1.07	1 (4%)

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	2,3	-	1/9/23/24	0/2/2/2
2	5HC	K	6	2,3	-	2/9/23/24	0/2/2/2
2	5HC	I	6	2,3	-	0/9/23/24	0/2/2/2
2	5HC	C	6	2,3	-	1/9/23/24	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	5HC	C6-N1	-3.96	1.31	1.38
2	K	6	5HC	O5'-C5'	-3.42	1.36	1.44
2	K	6	5HC	C6-N1	-2.98	1.33	1.38
2	I	6	5HC	C6-N1	-2.81	1.33	1.38
2	C	6	5HC	C6-N1	-2.06	1.34	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	6	5HC	O4'-C4'-C5'	-6.22	88.91	109.37
2	F	6	5HC	C5-C6-N1	-3.93	117.63	122.91
2	F	6	5HC	O2-C2-N3	-3.19	117.14	122.33
2	C	6	5HC	C5-C6-N1	-2.80	119.15	122.91
2	F	6	5HC	C4-N3-C2	-2.59	117.19	120.69
2	F	6	5HC	N1-C2-N3	2.53	123.41	118.81
2	K	6	5HC	C5-C6-N1	-2.50	119.55	122.91
2	F	6	5HC	O5-C5M-C5	-2.34	104.92	111.03
2	K	6	5HC	C2'-C3'-C4'	2.29	107.53	102.76
2	K	6	5HC	O4'-C1'-C2'	2.18	110.37	106.25
2	K	6	5HC	O2-C2-N3	-2.16	118.82	122.33
2	K	6	5HC	O5-C5M-C5	-2.05	105.69	111.03
2	F	6	5HC	C2'-C1'-N1	2.05	118.48	113.77
2	K	6	5HC	N1-C2-N3	2.02	122.48	118.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	6	5HC	O4'-C4'-C5'-O5'
2	K	6	5HC	C3'-C4'-C5'-O5'
2	C	6	5HC	O4'-C4'-C5'-O5'
2	F	6	5HC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	6	5HC	3	0

5.5 Carbohydrates (i)

There are no monosaccharides 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

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^{th} 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%)	-0.07	10 (2%) 65 36	28, 56, 101, 177	0
1	B	493/498 (98%)	0.04	20 (4%) 37 15	30, 57, 122, 219	0
1	E	493/498 (98%)	-0.02	15 (3%) 50 22	34, 65, 113, 199	0
1	H	493/498 (98%)	0.04	13 (2%) 56 27	37, 78, 128, 198	0
2	C	16/17 (94%)	-0.26	0 100 100	31, 39, 103, 121	0
2	F	16/17 (94%)	-0.05	2 (12%) 3 1	27, 42, 135, 144	0
2	I	16/17 (94%)	-0.35	0 100 100	24, 37, 84, 115	0
2	K	16/17 (94%)	0.18	2 (12%) 3 1	32, 55, 156, 183	0
3	D	17/17 (100%)	-0.41	0 100 100	35, 49, 85, 103	0
3	G	17/17 (100%)	-0.13	1 (5%) 22 7	31, 48, 130, 146	0
3	J	17/17 (100%)	-0.41	0 100 100	32, 45, 86, 95	0
3	L	17/17 (100%)	0.01	1 (5%) 22 7	43, 64, 121, 141	0
All	All	2104/2128 (98%)	-0.01	64 (3%) 50 22	24, 63, 121, 219	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	14.4
1	B	233	SER	11.1
1	E	236	ARG	9.2
1	B	232	TRP	7.0
1	A	233	SER	6.6
1	A	722	HIS	6.6
1	H	233	SER	6.1
1	B	693	ALA	6.1
1	A	230	MET	6.0
1	E	235	ALA	5.9
1	E	234	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	5.8
1	E	232	TRP	5.5
1	E	237	ALA	5.4
1	H	234	GLY	5.4
1	H	230	MET	5.3
1	A	232	TRP	4.9
1	B	231	GLN	4.8
1	E	239	GLU	4.8
1	A	234	GLY	4.8
1	A	524	HIS	4.8
1	E	240	ALA	4.7
1	A	692	PRO	4.7
1	B	692	PRO	4.5
1	B	722	HIS	4.2
1	B	691	ASP	4.0
1	E	233	SER	4.0
1	H	692	PRO	3.6
3	L	2	DA	3.3
1	B	261	LEU	3.3
1	H	232	TRP	3.2
1	B	262	LYS	3.2
3	G	2	DA	3.1
1	B	230	MET	3.1
1	A	691	ASP	3.1
1	A	231	GLN	3.0
1	E	692	PRO	3.0
1	B	239	GLU	3.0
2	K	14	DT	2.9
1	B	258	GLY	2.8
1	H	691	ASP	2.8
2	K	-2	DT	2.7
1	H	235	ALA	2.7
1	A	243	THR	2.6
1	E	230	MET	2.6
1	B	694	LEU	2.5
1	E	686	GLN	2.4
1	H	231	GLN	2.4
1	B	257	THR	2.4
1	H	722	HIS	2.4
1	B	236	ARG	2.3
1	E	492	LEU	2.3
1	B	719	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	238	LEU	2.3
1	H	236	ARG	2.3
1	B	238	LEU	2.3
1	B	237	ALA	2.3
1	E	722	HIS	2.2
2	F	-2	DT	2.2
2	F	14	DT	2.2
1	E	719	LYS	2.1
1	H	524	HIS	2.1
1	H	686	GLN	2.1
1	H	693	ALA	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, 95^{th} 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	0.96	0.16	39,41,45,47	0
2	5HC	F	6	21/22	0.97	0.15	27,32,42,45	0
2	5HC	I	6	21/22	0.98	0.16	21,22,26,27	0
2	5HC	C	6	21/22	0.98	0.15	27,29,32,34	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.