



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:49 pm BST

PDB ID : 6JW3
Title : Degenerate RVD RG forms a distinct loop conformation
Authors : Liu, L.; Yi, C.
Deposited on : 2019-04-18
Resolution : 3.10 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

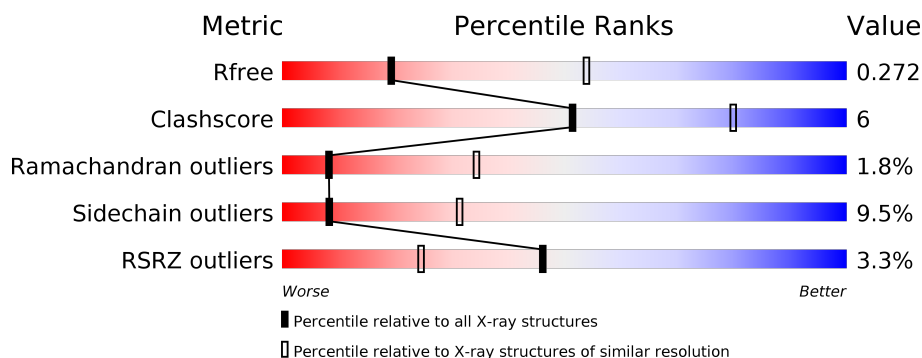
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	499	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	499	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	E	499	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	H	499	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
2	C	17	<div> <div></div> <div> <div>65%</div> <div>35%</div> </div> </div>
2	F	17	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>35%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	17	 71% 29%
2	K	17	 59% 41%
3	D	17	 82% 18%
3	G	17	 6% 88% 12%
3	J	17	 88% 12%
3	L	17	 6% 82% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17194 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	497	Total	C	N	O	S	0	0	0
			3605	2252	674	667	12			
1	B	497	Total	C	N	O	S	0	0	0
			3605	2252	674	667	12			
1	E	497	Total	C	N	O	S	0	0	0
			3605	2252	674	667	12			
1	H	497	Total	C	N	O	S	0	0	0
			3605	2252	674	667	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)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
			336	163	50	107	16			
2	C	17	Total	C	N	O	P	0	0	0
			336	163	50	107	16			
2	F	17	Total	C	N	O	P	0	0	0
			336	163	50	107	16			
2	K	17	Total	C	N	O	P	0	0	0
			336	163	50	107	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			

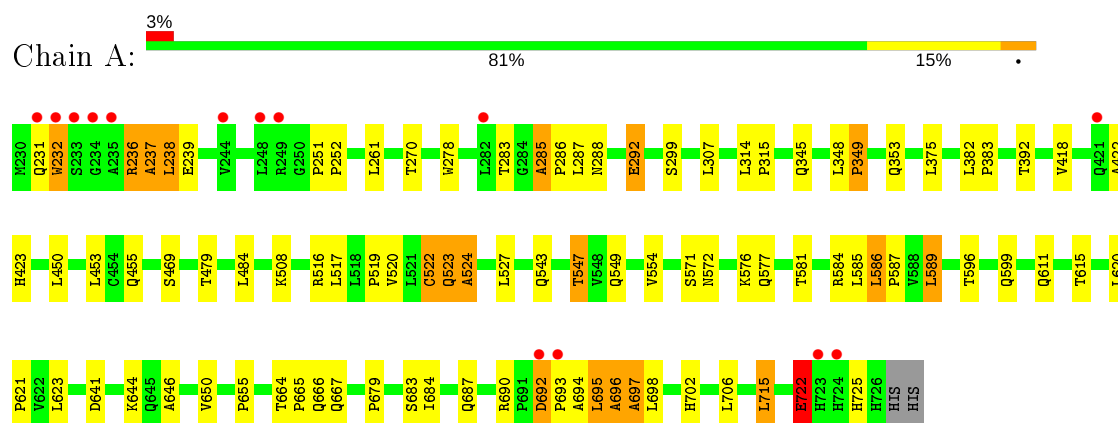
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	4	Total	O	0	0
			4	4		

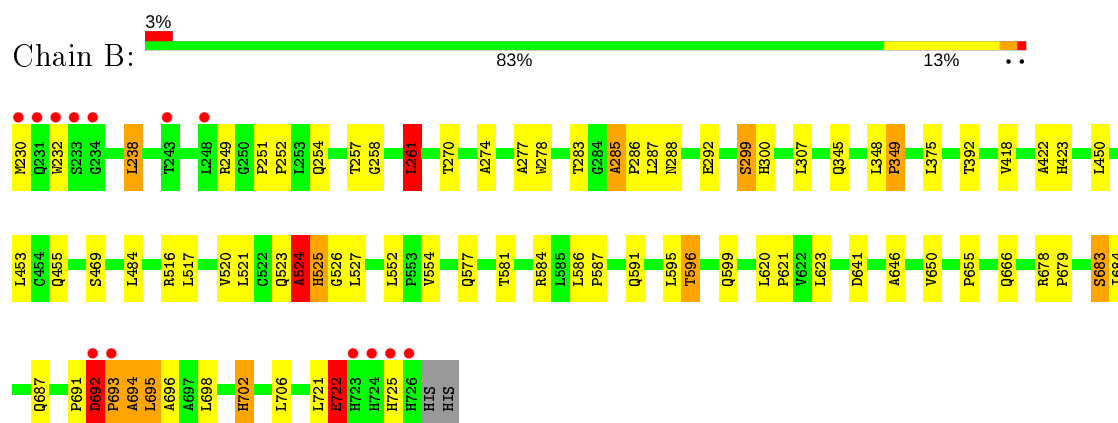
3 Residue-property plots

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 ($RSRZ > 2$). 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.

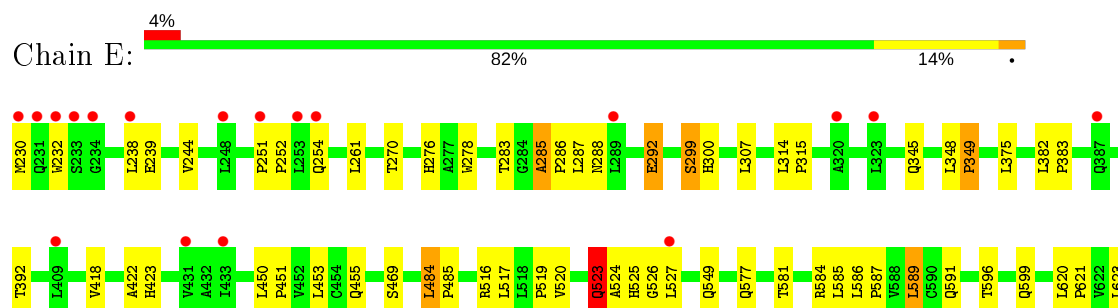
• Molecule 1: TAL effector

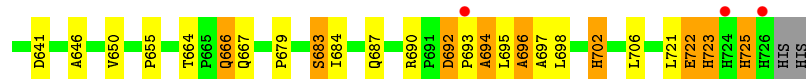


• Molecule 1: TAL effector

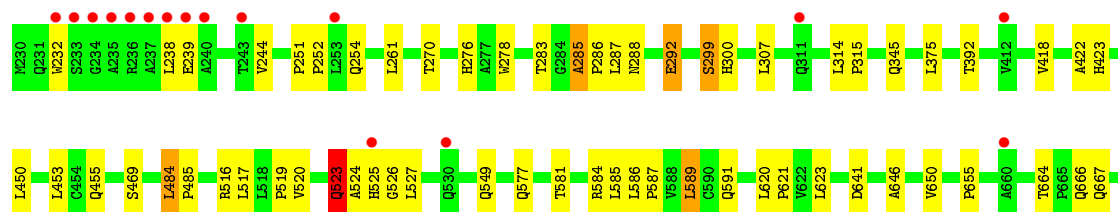
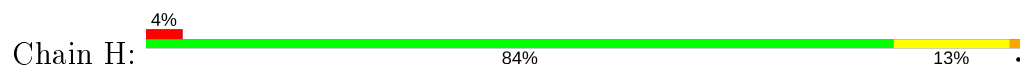


• Molecule 1: TAL effector





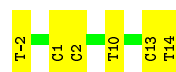
- Molecule 1: TAL effector



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



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




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



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




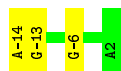
- Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain J:  88% 12%




- 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:  82% 18%




- 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:  6% 88% 12%



- 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:  6% 82% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.17Å 93.62Å 167.63Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 47.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-3.10) 89.0 (47.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.243 , 0.278 0.238 , 0.272	Depositor DCC
R_{free} test set	2348 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.5	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	0.90	EDS
Total number of atoms	17194	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0295e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 5CM

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	1/3659 (0.0%)	0.69	1/4998 (0.0%)
1	B	0.55	0/3659	0.68	3/4998 (0.1%)
1	E	0.50	0/3659	0.64	0/4998
1	H	0.51	0/3659	0.65	2/4998 (0.0%)
2	C	0.85	1/349 (0.3%)	0.91	1/533 (0.2%)
2	F	0.80	1/349 (0.3%)	0.90	2/533 (0.4%)
2	I	0.81	0/349	0.90	1/533 (0.2%)
2	K	0.91	2/349 (0.6%)	0.88	1/533 (0.2%)
3	D	0.65	1/402 (0.2%)	0.74	0/620
3	G	0.53	0/402	0.78	0/620
3	J	0.62	0/402	0.84	0/620
3	L	0.66	1/402 (0.2%)	0.80	0/620
All	All	0.56	7/17640 (0.0%)	0.70	11/24604 (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	B	0	2
1	E	0	2
1	H	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	-6	DG	O3'-P	-5.82	1.54	1.61
2	K	9	DG	O3'-P	-5.76	1.54	1.61
2	C	10	DT	O3'-P	-5.63	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	CYS	CB-SG	-5.54	1.72	1.81
2	K	10	DT	O3'-P	-5.39	1.54	1.61
2	F	9	DG	O3'-P	-5.38	1.54	1.61
3	D	-6	DG	O3'-P	-5.30	1.54	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	678	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	H	695	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	522	CYS	CB-CA-C	6.14	122.68	110.40
2	F	-2	DT	O4'-C4'-C3'	6.08	109.65	106.00
1	B	695	LEU	CA-CB-CG	5.79	128.62	115.30
2	C	-2	DT	C5'-C4'-O4'	5.77	120.27	109.30
2	F	-2	DT	C5'-C4'-O4'	5.62	119.97	109.30
1	B	261	LEU	CA-CB-CG	5.53	128.03	115.30
1	B	678	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	I	-2	DT	C5'-C4'-C3'	5.14	123.35	114.10
2	K	-2	DT	C5'-C4'-C3'	5.03	123.15	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	MET	Peptide
1	B	524	ALA	Peptide
1	E	230	MET	Peptide
1	E	523	GLN	Peptide
1	H	523	GLN	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	3605	0	3738	45	0
1	B	3605	0	3738	44	0
1	E	3605	0	3738	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3605	0	3738	28	0
2	C	336	0	195	3	0
2	F	336	0	195	7	0
2	I	336	0	195	4	0
2	K	336	0	195	12	0
3	D	355	0	189	1	0
3	G	355	0	189	4	0
3	J	355	0	189	1	0
3	L	355	0	189	5	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
All	All	17194	0	16488	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (187) 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:14:DT:C4	3:L:-14:DA:N6	2.21	1.09
1:B:721:LEU:HD23	2:F:14:DT:C5	1.96	1.00
1:B:694:ALA:HA	1:B:722:GLU:CD	1.82	0.98
1:E:721:LEU:O	1:E:722:GLU:HB3	1.64	0.94
1:B:694:ALA:HA	1:B:722:GLU:OE2	1.70	0.92
2:K:13:DC:N4	2:K:14:DT:O4	2.04	0.89
2:K:13:DC:C4	2:K:14:DT:C4	2.62	0.88
3:J:-14:DA:H2"	3:J:-13:DG:O5'	1.74	0.88
1:E:722:GLU:HB2	1:E:725:HIS:CD2	2.10	0.87
2:K:13:DC:C4	2:K:14:DT:O4	2.35	0.80
1:E:694:ALA:HB2	1:E:722:GLU:OE1	1.83	0.78
1:B:721:LEU:CD2	2:F:14:DT:C5	2.69	0.75
2:K:13:DC:C4	2:K:14:DT:C5	2.74	0.75
2:K:13:DC:N3	2:K:14:DT:C4	2.57	0.72
1:H:285:ALA:HB1	1:H:286:PRO:CD	2.22	0.69
1:B:702:HIS:CE1	1:E:702:HIS:CE1	2.81	0.69
1:E:285:ALA:HB1	1:E:286:PRO:CD	2.23	0.68
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.24	0.68
2:K:13:DC:C5	2:K:14:DT:C5	2.82	0.67
1:B:277:ALA:O	1:B:278:TRP:CD1	2.48	0.67
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.24	0.66
1:B:722:GLU:HA	1:B:725:HIS:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLN:O	1:A:547:THR:HG23	1.97	0.65
1:B:694:ALA:HB2	1:B:722:GLU:HB3	1.79	0.65
1:E:722:GLU:HG2	1:E:723:HIS:O	1.97	0.64
2:K:14:DT:O4	3:L:-14:DA:N6	2.31	0.63
1:E:694:ALA:CB	1:E:722:GLU:OE1	2.47	0.63
1:B:274:ALA:HB1	1:B:278:TRP:CZ3	2.34	0.62
1:A:722:GLU:HA	1:A:725:HIS:HB3	1.83	0.61
1:E:695:LEU:O	1:E:696:ALA:C	2.39	0.60
1:E:285:ALA:HB1	1:E:286:PRO:HD2	1.84	0.60
1:B:285:ALA:HB1	1:B:286:PRO:HD2	1.84	0.60
1:H:285:ALA:HB1	1:H:286:PRO:HD2	1.83	0.59
1:A:285:ALA:HB1	1:A:286:PRO:HD2	1.85	0.58
1:H:722:GLU:HA	1:H:725:HIS:HB3	1.85	0.57
1:E:695:LEU:O	1:E:696:ALA:O	2.24	0.56
1:H:244:VAL:HG13	1:H:276:HIS:HB2	1.87	0.56
1:E:418:VAL:O	1:E:422:ALA:HB3	2.06	0.56
1:E:244:VAL:HG13	1:E:276:HIS:HB2	1.88	0.56
1:B:418:VAL:O	1:B:422:ALA:HB3	2.06	0.55
1:H:418:VAL:O	1:H:422:ALA:HB3	2.06	0.55
1:E:517:LEU:HA	1:E:520:VAL:HG12	1.88	0.55
1:A:586:LEU:HB3	1:A:587:PRO:CD	2.37	0.55
1:B:702:HIS:ND1	1:E:702:HIS:CE1	2.75	0.55
2:F:13:DC:C5	2:F:14:DT:N3	2.75	0.54
1:A:418:VAL:O	1:A:422:ALA:HB3	2.06	0.54
1:E:679:PRO:O	1:E:683:SER:HB2	2.07	0.54
1:E:696:ALA:O	1:E:698:LEU:N	2.41	0.54
1:A:517:LEU:HA	1:A:520:VAL:HG12	1.90	0.54
1:H:679:PRO:O	1:H:683:SER:HB2	2.08	0.54
2:K:14:DT:C5	3:L:-14:DA:N6	2.75	0.54
1:A:693:PRO:O	1:A:695:LEU:N	2.41	0.53
1:B:679:PRO:O	1:B:683:SER:HB2	2.08	0.53
1:E:620:LEU:HB3	1:E:621:PRO:HD3	1.90	0.53
1:A:237:ALA:O	1:A:238:LEU:CB	2.56	0.53
1:A:523:GLN:O	1:A:524:ALA:HB2	2.09	0.53
1:H:517:LEU:HA	1:H:520:VAL:HG12	1.89	0.53
2:I:14:DT:OP2	2:I:14:DT:H3'	2.08	0.53
1:A:423:HIS:HB3	1:A:450:LEU:HD23	1.91	0.53
1:B:524:ALA:O	1:B:526:GLY:N	2.42	0.53
1:A:679:PRO:O	1:A:683:SER:HB2	2.09	0.52
1:B:292:GLU:OE1	1:B:292:GLU:N	2.42	0.52
1:A:543:GLN:O	1:A:547:THR:CG2	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LEU:HA	1:B:520:VAL:HG12	1.89	0.52
1:H:423:HIS:HB3	1:H:450:LEU:HD23	1.92	0.52
1:B:696:ALA:O	1:B:698:LEU:N	2.41	0.52
1:B:702:HIS:CE1	1:E:702:HIS:ND1	2.78	0.52
1:H:696:ALA:O	1:H:698:LEU:N	2.42	0.52
1:A:695:LEU:O	1:A:697:ALA:N	2.44	0.51
1:H:251:PRO:O	1:H:252:PRO:C	2.48	0.51
1:H:524:ALA:O	1:H:526:GLY:N	2.44	0.50
1:A:620:LEU:HB3	1:A:621:PRO:HD3	1.93	0.50
1:H:620:LEU:HB3	1:H:621:PRO:HD3	1.92	0.50
1:B:694:ALA:H	1:B:722:GLU:HG2	1.77	0.50
1:B:251:PRO:O	1:B:252:PRO:C	2.49	0.50
1:E:721:LEU:O	1:E:722:GLU:CB	2.43	0.50
1:H:519:PRO:O	1:H:523:GLN:HB3	2.11	0.49
1:B:423:HIS:HB3	1:B:450:LEU:HD23	1.93	0.49
2:F:1:DC:H2"	2:F:2:DC:O5'	2.11	0.49
1:B:725:HIS:ND1	3:G:-14:DA:N1	2.56	0.49
2:C:1:DC:H2"	2:C:2:DC:O5'	2.12	0.49
2:K:1:DC:H2"	2:K:2:DC:O5'	2.12	0.49
1:E:423:HIS:HB3	1:E:450:LEU:HD23	1.94	0.49
1:E:577:GLN:O	1:E:581:THR:OG1	2.23	0.49
1:E:251:PRO:O	1:E:252:PRO:C	2.50	0.49
1:E:524:ALA:O	1:E:526:GLY:N	2.45	0.49
1:A:646:ALA:O	1:A:650:VAL:HG23	2.13	0.48
1:A:547:THR:HG21	1:A:576:LYS:HG3	1.96	0.48
2:I:13:DC:C4	2:I:14:DT:C4	3.01	0.48
2:I:1:DC:H2"	2:I:2:DC:O5'	2.12	0.48
1:B:620:LEU:HB3	1:B:621:PRO:HD3	1.95	0.48
1:E:646:ALA:O	1:E:650:VAL:HG23	2.13	0.48
1:H:577:GLN:O	1:H:581:THR:OG1	2.24	0.48
1:H:244:VAL:HG13	1:H:276:HIS:CB	2.43	0.48
1:B:596:THR:OG1	1:B:599:GLN:HG3	2.14	0.47
1:A:231:GLN:HB3	1:A:232:TRP:CD1	2.49	0.47
1:E:519:PRO:O	1:E:523:GLN:HB3	2.13	0.47
1:B:646:ALA:O	1:B:650:VAL:HG23	2.14	0.47
1:B:277:ALA:O	1:B:278:TRP:CG	2.68	0.47
1:E:244:VAL:HG13	1:E:276:HIS:CB	2.44	0.47
1:H:646:ALA:O	1:H:650:VAL:HG23	2.13	0.47
1:B:249:ARG:HH12	1:B:257:THR:HG22	1.78	0.47
1:B:258:GLY:O	1:B:261:LEU:HD22	2.14	0.47
1:A:577:GLN:O	1:A:581:THR:OG1	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PRO:O	1:A:252:PRO:C	2.53	0.46
3:L:-14:DA:H2"	3:L:-13:DG:C8	2.51	0.46
1:E:722:GLU:OE2	1:E:723:HIS:N	2.43	0.46
2:K:13:DC:N3	2:K:14:DT:O4	2.47	0.46
1:E:585:LEU:HB3	1:E:589:LEU:HD22	1.98	0.46
1:H:283:THR:O	1:H:288:ASN:HA	2.16	0.46
1:A:571:SER:O	1:A:572:ASN:ND2	2.50	0.45
1:H:585:LEU:HB3	1:H:589:LEU:HD22	1.98	0.45
2:F:13:DC:C5	2:F:14:DT:C4	3.04	0.45
1:A:585:LEU:HB3	1:A:589:LEU:HD22	1.99	0.45
1:A:283:THR:O	1:A:288:ASN:HA	2.16	0.45
1:B:577:GLN:O	1:B:581:THR:OG1	2.23	0.45
1:B:586:LEU:HB3	1:B:587:PRO:CD	2.47	0.45
1:E:292:GLU:H	1:E:292:GLU:CD	2.20	0.45
1:A:232:TRP:CD1	1:A:232:TRP:N	2.86	0.44
1:A:314:LEU:N	1:A:315:PRO:CD	2.81	0.44
1:B:722:GLU:O	1:B:722:GLU:HG3	2.16	0.44
1:E:692:ASP:HB3	1:E:693:PRO:HD2	2.00	0.44
1:A:547:THR:HG21	1:A:576:LYS:CB	2.48	0.44
1:H:299:SER:O	1:H:300:HIS:CG	2.70	0.44
1:A:698:LEU:HD23	1:A:702:HIS:ND1	2.33	0.44
1:E:283:THR:O	1:E:288:ASN:HA	2.18	0.44
1:A:523:GLN:O	1:A:524:ALA:CB	2.66	0.43
1:A:692:ASP:HB3	1:A:693:PRO:HD2	1.99	0.43
1:B:725:HIS:HA	3:G:-14:DA:C6	2.52	0.43
1:H:520:VAL:O	1:H:523:GLN:O	2.36	0.43
1:E:299:SER:O	1:E:300:HIS:CG	2.71	0.43
2:F:13:DC:C5	2:F:14:DT:C2	3.06	0.43
1:H:314:LEU:N	1:H:315:PRO:CD	2.82	0.43
1:A:292:GLU:CD	1:A:292:GLU:H	2.22	0.43
1:A:664:THR:O	1:A:667:GLN:N	2.52	0.43
1:A:696:ALA:O	1:A:698:LEU:N	2.49	0.43
1:B:238:LEU:HG	1:B:238:LEU:O	2.18	0.43
1:B:283:THR:O	1:B:288:ASN:HA	2.18	0.43
1:A:285:ALA:CB	1:A:286:PRO:CD	2.96	0.43
2:F:13:DC:H2"	2:F:14:DT:C5'	2.48	0.43
3:G:-14:DA:H2"	3:G:-13:DG:C8	2.54	0.43
1:A:698:LEU:HD22	1:A:702:HIS:CG	2.54	0.42
1:E:520:VAL:O	1:E:523:GLN:O	2.37	0.42
1:E:586:LEU:HB3	1:E:587:PRO:CD	2.49	0.42
1:A:664:THR:O	1:A:665:PRO:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LEU:HA	1:B:525:HIS:CB	2.49	0.42
1:H:586:LEU:HB3	1:H:587:PRO:CD	2.50	0.42
2:C:13:DC:C2'	2:C:14:DT:H2'	2.49	0.42
1:E:484:LEU:N	1:E:485:PRO:HD2	2.35	0.42
2:I:13:DC:N4	2:I:14:DT:O4	2.52	0.42
1:E:664:THR:O	1:E:667:GLN:N	2.52	0.42
1:H:484:LEU:N	1:H:485:PRO:HD2	2.35	0.42
1:A:382:LEU:N	1:A:383:PRO:CD	2.83	0.42
1:B:725:HIS:HA	3:G:-14:DA:N6	2.35	0.42
1:H:285:ALA:CB	1:H:286:PRO:CD	2.94	0.42
1:H:292:GLU:H	1:H:292:GLU:CD	2.23	0.42
2:K:14:DT:O4	3:L:-14:DA:C6	2.73	0.42
1:B:692:ASP:HB3	1:B:693:PRO:HD2	2.02	0.42
1:E:666:GLN:H	1:E:666:GLN:CD	2.22	0.42
1:A:519:PRO:O	1:A:523:GLN:HB3	2.20	0.41
1:E:314:LEU:N	1:E:315:PRO:CD	2.82	0.41
1:E:382:LEU:N	1:E:383:PRO:CD	2.83	0.41
1:A:547:THR:HG21	1:A:576:LYS:CG	2.50	0.41
1:B:299:SER:O	1:B:300:HIS:CG	2.73	0.41
1:A:236:ARG:O	1:A:237:ALA:O	2.39	0.41
1:A:692:ASP:CB	1:A:693:PRO:HD2	2.50	0.41
2:C:13:DC:H2''	2:C:14:DT:H2'	2.02	0.41
1:E:722:GLU:N	1:E:722:GLU:OE2	2.54	0.41
1:A:237:ALA:O	1:A:238:LEU:HB2	2.21	0.41
1:B:525:HIS:HA	1:B:552:LEU:HD23	2.01	0.41
3:D:-14:DA:H2''	3:D:-13:DG:C8	2.55	0.41
1:E:596:THR:OG1	1:E:599:GLN:HG3	2.20	0.41
1:A:611:GLN:O	1:A:615:THR:OG1	2.37	0.41
1:A:348:LEU:N	1:A:349:PRO:CD	2.84	0.41
1:B:348:LEU:N	1:B:349:PRO:CD	2.84	0.41
1:H:692:ASP:HB3	1:H:693:PRO:HD2	2.03	0.41
1:H:664:THR:O	1:H:667:GLN:N	2.53	0.41
1:E:692:ASP:CB	1:E:693:PRO:HD2	2.51	0.41
1:B:694:ALA:CA	1:B:722:GLU:CD	2.71	0.41
1:E:348:LEU:N	1:E:349:PRO:CD	2.84	0.40
1:E:450:LEU:HB3	1:E:451:PRO:HD3	2.03	0.40
1:B:520:VAL:O	1:B:523:GLN:O	2.39	0.40
1:B:692:ASP:CB	1:B:693:PRO:HD2	2.52	0.40
1:H:692:ASP:OD1	1:H:693:PRO:HD2	2.21	0.40
1:A:596:THR:OG1	1:A:599:GLN:HG3	2.21	0.40
1:A:479:THR:OG1	1:A:508:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:ALA:CB	1:E:286:PRO:CD	2.95	0.40

There are no symmetry-related clashes.

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	495/499 (99%)	450 (91%)	33 (7%)	12 (2%)	6	27
1	B	495/499 (99%)	447 (90%)	38 (8%)	10 (2%)	7	31
1	E	495/499 (99%)	448 (90%)	38 (8%)	9 (2%)	8	34
1	H	495/499 (99%)	447 (90%)	43 (9%)	5 (1%)	15	49
All	All	1980/1996 (99%)	1792 (90%)	152 (8%)	36 (2%)	8	34

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ALA
1	A	285	ALA
1	A	523	GLN
1	A	694	ALA
1	B	285	ALA
1	B	525	HIS
1	B	692	ASP
1	B	693	PRO
1	B	694	ALA
1	E	285	ALA
1	E	525	HIS
1	E	696	ALA
1	H	285	ALA
1	H	525	HIS

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Mol	Chain	Res	Type
1	A	524	ALA
1	E	694	ALA
1	E	722	GLU
1	A	696	ALA
1	E	697	ALA
1	H	722	GLU
1	A	722	GLU
1	E	523	GLN
1	H	523	GLN
1	A	236	ARG
1	A	655	PRO
1	A	697	ALA
1	A	715	LEU
1	B	524	ALA
1	B	655	PRO
1	B	722	GLU
1	E	655	PRO
1	H	655	PRO
1	B	691	PRO
1	A	349	PRO
1	B	349	PRO
1	E	349	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	379/384 (99%)	340 (90%)	39 (10%)	7	27
1	B	379/384 (99%)	346 (91%)	33 (9%)	10	36
1	E	379/384 (99%)	343 (90%)	36 (10%)	8	31
1	H	379/384 (99%)	343 (90%)	36 (10%)	8	31
All	All	1516/1536 (99%)	1372 (90%)	144 (10%)	8	31

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	TRP
1	A	238	LEU
1	A	239	GLU
1	A	261	LEU
1	A	270	THR
1	A	278	TRP
1	A	287	LEU
1	A	292	GLU
1	A	299	SER
1	A	307	LEU
1	A	345	GLN
1	A	353	GLN
1	A	375	LEU
1	A	392	THR
1	A	453	LEU
1	A	455	GLN
1	A	469	SER
1	A	484	LEU
1	A	516	ARG
1	A	522	CYS
1	A	527	LEU
1	A	547	THR
1	A	549	GLN
1	A	554	VAL
1	A	584	ARG
1	A	586	LEU
1	A	589	LEU
1	A	623	LEU
1	A	641	ASP
1	A	644	LYS
1	A	666	GLN
1	A	684	ILE
1	A	687	GLN
1	A	690	ARG
1	A	692	ASP
1	A	695	LEU
1	A	706	LEU
1	A	715	LEU
1	A	722	GLU
1	B	232	TRP
1	B	238	LEU
1	B	254	GLN
1	B	261	LEU

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Mol	Chain	Res	Type
1	B	270	THR
1	B	287	LEU
1	B	299	SER
1	B	307	LEU
1	B	345	GLN
1	B	375	LEU
1	B	392	THR
1	B	453	LEU
1	B	455	GLN
1	B	469	SER
1	B	484	LEU
1	B	516	ARG
1	B	527	LEU
1	B	554	VAL
1	B	584	ARG
1	B	591	GLN
1	B	595	LEU
1	B	596	THR
1	B	623	LEU
1	B	641	ASP
1	B	666	GLN
1	B	683	SER
1	B	684	ILE
1	B	687	GLN
1	B	692	ASP
1	B	695	LEU
1	B	702	HIS
1	B	706	LEU
1	B	722	GLU
1	E	232	TRP
1	E	238	LEU
1	E	239	GLU
1	E	254	GLN
1	E	261	LEU
1	E	270	THR
1	E	278	TRP
1	E	287	LEU
1	E	292	GLU
1	E	299	SER
1	E	307	LEU
1	E	345	GLN
1	E	375	LEU

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Mol	Chain	Res	Type
1	E	392	THR
1	E	453	LEU
1	E	455	GLN
1	E	469	SER
1	E	484	LEU
1	E	516	ARG
1	E	527	LEU
1	E	549	GLN
1	E	584	ARG
1	E	589	LEU
1	E	591	GLN
1	E	623	LEU
1	E	641	ASP
1	E	666	GLN
1	E	683	SER
1	E	684	ILE
1	E	687	GLN
1	E	690	ARG
1	E	692	ASP
1	E	702	HIS
1	E	706	LEU
1	E	723	HIS
1	E	725	HIS
1	H	232	TRP
1	H	238	LEU
1	H	239	GLU
1	H	254	GLN
1	H	261	LEU
1	H	270	THR
1	H	278	TRP
1	H	287	LEU
1	H	292	GLU
1	H	299	SER
1	H	307	LEU
1	H	345	GLN
1	H	375	LEU
1	H	392	THR
1	H	453	LEU
1	H	455	GLN
1	H	469	SER
1	H	484	LEU
1	H	516	ARG

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Mol	Chain	Res	Type
1	H	527	LEU
1	H	549	GLN
1	H	584	ARG
1	H	589	LEU
1	H	591	GLN
1	H	623	LEU
1	H	641	ASP
1	H	666	GLN
1	H	683	SER
1	H	684	ILE
1	H	687	GLN
1	H	690	ARG
1	H	692	ASP
1	H	695	LEU
1	H	702	HIS
1	H	706	LEU
1	H	722	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	ASN
1	A	633	GLN
1	A	667	GLN
1	A	687	GLN
1	A	700	ASN
1	B	591	GLN
1	B	687	GLN
1	B	700	ASN
1	E	591	GLN
1	E	687	GLN
1	E	700	ASN
1	H	591	GLN
1	H	687	GLN
1	H	700	ASN

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	5CM	C	6	3,2	15,21,22	1.02	1 (6%)	19,30,33	1.53	2 (10%)
2	5CM	K	6	3,2	15,21,22	1.43	2 (13%)	19,30,33	1.05	1 (5%)
2	5CM	F	6	3,2	15,21,22	1.35	1 (6%)	19,30,33	1.09	1 (5%)
2	5CM	I	6	3,2	15,21,22	1.31	1 (6%)	19,30,33	1.02	2 (10%)

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	5CM	C	6	3,2	-	0/4/21/22	0/2/2/2
2	5CM	K	6	3,2	-	0/4/21/22	0/2/2/2
2	5CM	F	6	3,2	-	0/4/21/22	0/2/2/2
2	5CM	I	6	3,2	-	0/4/21/22	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	5CM	C5-C4	4.53	1.48	1.41
2	I	6	5CM	C5-C4	4.22	1.47	1.41
2	K	6	5CM	C5-C4	3.66	1.47	1.41
2	K	6	5CM	C2-N3	-2.52	1.33	1.38
2	C	6	5CM	C5-C4	2.37	1.45	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	C2-N3-C4	5.40	122.54	116.02
2	K	6	5CM	C5-C6-N1	-3.03	118.93	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	5CM	C2-N3-C4	2.83	119.44	116.02
2	C	6	5CM	C5-C4-N3	-2.46	117.37	121.26
2	I	6	5CM	C2-N3-C4	2.41	118.92	116.02
2	I	6	5CM	C5A-C5-C4	2.13	123.89	121.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/499 (99%)	0.17	14 (2%) 53 30	35, 60, 113, 177	0
1	B	497/499 (99%)	0.06	13 (2%) 56 33	32, 59, 101, 155	0
1	E	497/499 (99%)	0.28	21 (4%) 36 18	38, 77, 121, 160	0
1	H	497/499 (99%)	0.21	20 (4%) 38 19	37, 68, 114, 152	0
2	C	16/17 (94%)	-0.20	0 100 100	28, 43, 78, 105	0
2	F	16/17 (94%)	0.45	1 (6%) 20 8	40, 59, 137, 145	0
2	I	16/17 (94%)	-0.13	0 100 100	39, 46, 103, 104	0
2	K	16/17 (94%)	0.01	0 100 100	30, 48, 114, 139	0
3	D	17/17 (100%)	-0.45	0 100 100	32, 48, 79, 92	0
3	G	17/17 (100%)	-0.13	1 (5%) 22 10	43, 62, 112, 130	0
3	J	17/17 (100%)	-0.32	0 100 100	34, 55, 85, 100	0
3	L	17/17 (100%)	-0.03	1 (5%) 22 10	36, 56, 113, 122	0
All	All	2120/2132 (99%)	0.16	71 (3%) 46 24	28, 66, 115, 177	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	10.3
1	H	235	ALA	9.5
1	H	232	TRP	9.5
1	E	233	SER	9.5
1	B	233	SER	9.4
1	A	724	HIS	8.6
1	A	723	HIS	8.5
1	B	230	MET	8.3
1	B	723	HIS	7.8
1	H	234	GLY	7.5
1	H	239	GLU	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	233	SER	7.4
1	B	724	HIS	7.1
1	E	726	HIS	7.1
1	H	233	SER	6.8
1	H	693	PRO	6.7
1	E	232	TRP	6.0
1	A	231	GLN	5.6
2	F	14	DT	5.4
1	A	248	LEU	5.2
1	H	238	LEU	5.0
1	A	232	TRP	5.0
1	E	253	LEU	4.7
1	A	693	PRO	4.4
1	E	724	HIS	4.4
1	H	236	ARG	4.4
1	B	231	GLN	3.8
1	B	693	PRO	3.7
1	A	282	LEU	3.7
1	E	234	GLY	3.6
1	E	251	PRO	3.6
1	E	230	MET	3.3
1	H	243	THR	3.3
1	H	525	HIS	3.3
1	B	232	TRP	3.2
1	E	693	PRO	3.0
1	E	323	LEU	2.9
1	H	726	HIS	2.9
1	E	320	ALA	2.9
1	A	244	VAL	2.7
3	G	2	DA	2.7
1	E	248	LEU	2.7
1	E	289	LEU	2.7
1	B	243	THR	2.6
1	A	235	ALA	2.6
1	H	240	ALA	2.6
1	B	726	HIS	2.6
1	E	433	ILE	2.5
1	E	231	GLN	2.4
1	A	249	ARG	2.4
1	E	431	VAL	2.4
1	H	692	ASP	2.4
1	E	254	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	660	ALA	2.3
1	B	234	GLY	2.3
1	E	238	LEU	2.3
1	E	409	LEU	2.3
1	E	527	LEU	2.3
1	H	530	GLN	2.3
1	H	237	ALA	2.2
1	B	725	HIS	2.2
3	L	2	DA	2.2
1	A	692	ASP	2.1
1	B	692	ASP	2.1
1	A	421	GLN	2.0
1	H	724	HIS	2.1
1	H	412	VAL	2.0
1	B	248	LEU	2.0
1	H	253	LEU	2.0
1	H	311	GLN	2.0
1	E	387	GLN	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	5CM	K	6	20/21	0.97	0.15	29,34,43,46	0
2	5CM	F	6	20/21	0.97	0.18	41,44,50,50	0
2	5CM	I	6	20/21	0.97	0.20	35,39,42,44	0
2	5CM	C	6	20/21	0.99	0.16	26,28,31,32	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.