Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 06:38 PM JST

PDB ID	:	6JVZ
Title	:	RVD HA specifically contacts 5mC through van der Waals interactions
Authors	:	Liu, L.; Yi, C.
Deposited on	:	2019-04-18
Resolution	:	2.48 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 (i) 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 (1)) were used in the production of this report:

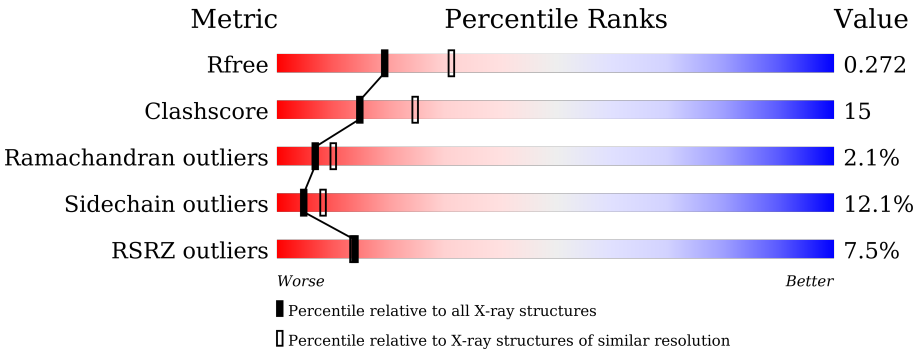
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	499	2% 78% 17% ·
1	B	499	13% 70% 21% 7% ·
2	C	17	6% 65% 35%
2	I	17	71% 24% 6%
3	D	17	6% 82% 18%
3	J	17	6% 82% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8705 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
			3610	2256	675	667	12			
1	B	497	Total	C	N	O	S	0	0	0
			3605	2253	673	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			

- 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			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	I	16	Total	O	0	0
			16	16		
4	B	31	Total	O	0	0
			31	31		

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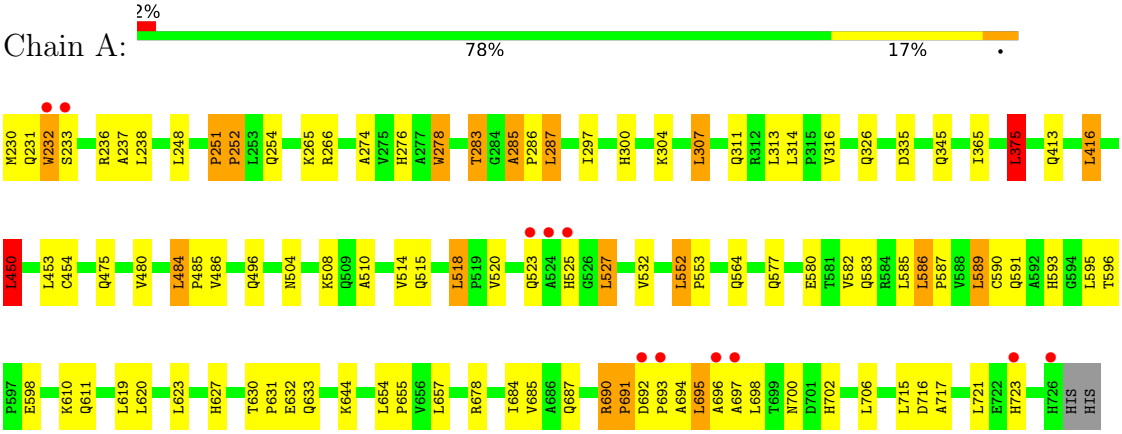
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	13	Total O 13 13	0	0

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:

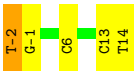


• Molecule 1: TAL effector

Chain B:

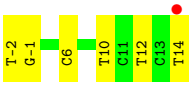
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*T)-3')

Chain I:



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

Chain C:

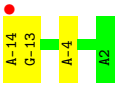


• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.79Å 88.02Å 89.35Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	86.40 – 2.48 43.20 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.8 (86.40-2.48) 91.8 (43.20-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.223 , 0.275 0.225 , 0.272	Depositor DCC
R_{free} test set	2095 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8705	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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: 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	0.59	0/3666	0.77	6/5009 (0.1%)
1	B	0.68	2/3660 (0.1%)	0.89	9/5001 (0.2%)
2	C	0.50	0/349	1.02	1/533 (0.2%)
2	I	0.52	0/349	0.97	1/533 (0.2%)
3	D	0.51	0/402	0.77	0/620
3	J	0.49	0/402	0.75	0/620
All	All	0.61	2/8828 (0.0%)	0.84	17/12316 (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	A	0	5
1	B	0	12
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	595	LEU	N-CA	8.35	1.63	1.46
1	B	725	HIS	CA-C	6.19	1.69	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	677	GLY	N-CA-C	-9.10	90.34	113.10
1	B	663	LEU	CA-CB-CG	7.46	132.46	115.30
1	B	725	HIS	CB-CA-C	7.08	124.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	LEU	CA-CB-CG	6.71	130.73	115.30
2	I	-2	DT	C5'-C4'-C3'	5.86	124.65	114.10
1	B	706	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	A	335	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	278	TRP	CA-CB-CG	5.75	124.62	113.70
1	B	516	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	450	LEU	CB-CG-CD1	5.58	120.48	111.00
1	B	234	GLY	N-CA-C	5.39	126.59	113.10
1	B	418	VAL	CB-CA-C	-5.39	101.17	111.40
1	A	335	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	678	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	C	10	DT	O5'-P-OP1	-5.15	101.07	105.70
1	A	251	PRO	C-N-CD	-5.12	109.33	120.60
1	B	285	ALA	C-N-CA	-5.12	100.51	122.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Peptide
1	A	237	ALA	Peptide
1	A	251	PRO	Mainchain,Peptide
1	A	694	ALA	Peptide
1	B	284	GLY	Peptide
1	B	285	ALA	Peptide
1	B	625	GLN	Peptide
1	B	629	LEU	Peptide
1	B	631	PRO	Peptide
1	B	640	HIS	Peptide
1	B	664	THR	Peptide
1	B	672	ALA	Peptide
1	B	676	GLY	Peptide
1	B	678	ARG	Peptide
1	B	692	ASP	Peptide
1	B	702	HIS	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	3610	0	3739	67	4
1	B	3605	0	3734	190	16
2	C	336	0	195	5	0
2	I	336	0	195	3	0
3	D	355	0	189	3	0
3	J	355	0	189	2	0
4	A	48	0	0	7	0
4	B	31	0	0	3	0
4	C	13	0	0	0	0
4	I	16	0	0	0	0
All	All	8705	0	8241	256	16

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 15.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:ILE:HG22	1:B:638:ALA:H	1.24	1.02
1:B:702:HIS:HB2	1:B:705:ALA:O	1.64	0.98
1:B:629:LEU:HG	1:B:631:PRO:HG3	1.45	0.97
1:B:655:PRO:O	1:B:659:GLN:N	2.00	0.94
1:B:648:GLU:OE1	1:B:652:ARG:C	2.09	0.90
1:A:285:ALA:HB1	1:A:286:PRO:HD3	1.55	0.89
1:B:678:ARG:HG2	1:B:681:LEU:HD12	1.55	0.89
1:B:637:ILE:HG22	1:B:638:ALA:N	1.90	0.86
1:B:662:GLY:O	1:B:663:LEU:HD12	1.76	0.85
1:B:702:HIS:CB	1:B:705:ALA:O	2.25	0.84
1:B:648:GLU:OE2	1:B:652:ARG:CB	2.25	0.84
1:B:633:GLN:O	1:B:637:ILE:HG13	1.77	0.84
1:B:702:HIS:HB2	1:B:703:LEU:HA	1.60	0.84
1:B:637:ILE:CG2	1:B:638:ALA:H	1.92	0.82
1:A:695:LEU:O	4:A:801:HOH:O	1.96	0.82
1:B:673:SER:OG	1:B:703:LEU:C	2.19	0.81
1:B:635:VAL:HG12	1:B:645:GLN:HB3	1.64	0.80
1:B:646:ALA:C	1:B:648:GLU:H	1.83	0.79
1:B:678:ARG:CG	1:B:681:LEU:HD12	2.12	0.79
1:B:632:GLU:N	1:B:632:GLU:OE1	2.16	0.78
1:B:648:GLU:OE2	1:B:652:ARG:HB2	1.85	0.76
1:B:648:GLU:OE2	1:B:652:ARG:HB3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:LEU:HB3	1:B:595:LEU:HD21	1.69	0.75
1:B:673:SER:OG	1:B:703:LEU:O	2.05	0.75
1:B:675:GLY:O	2:C:12:DT:OP2	2.05	0.74
1:B:674:ASN:HB3	1:B:683:SER:OG	1.88	0.73
1:B:692:ASP:HB2	1:B:693:PRO:HD3	1.70	0.73
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.18	0.72
1:B:675:GLY:HA2	1:B:679:PRO:HB2	1.70	0.72
1:B:629:LEU:CG	1:B:631:PRO:HG3	2.20	0.71
1:B:635:VAL:CG1	1:B:645:GLN:HB3	2.20	0.70
1:B:655:PRO:O	1:B:659:GLN:HB3	1.91	0.70
1:B:648:GLU:CG	1:B:681:LEU:HD13	2.22	0.69
1:A:285:ALA:CB	1:A:286:PRO:CD	2.71	0.69
1:B:588:VAL:C	1:B:590:CYS:H	1.96	0.69
1:B:675:GLY:HA3	1:B:680:ALA:HB2	1.74	0.69
1:B:648:GLU:OE1	1:B:652:ARG:O	2.10	0.69
1:A:721:LEU:HD21	1:B:706:LEU:HD21	1.75	0.68
1:B:621:PRO:O	1:B:623:LEU:O	2.11	0.68
2:I:-2:DT:H2"	2:I:-1:DG:OP2	1.94	0.68
1:B:675:GLY:HA3	1:B:680:ALA:CA	2.24	0.67
1:B:637:ILE:O	1:B:640:HIS:O	2.12	0.67
1:B:662:GLY:O	1:B:663:LEU:CD1	2.42	0.67
1:B:463:GLN:HE21	1:B:496:GLN:NE2	1.93	0.67
1:B:718:VAL:HG12	1:B:718:VAL:O	1.95	0.67
1:B:321:HIS:CD2	4:B:830:HOH:O	2.48	0.66
1:B:648:GLU:HG2	1:B:681:LEU:HB3	1.76	0.66
1:B:672:ALA:C	1:B:674:ASN:N	2.50	0.65
1:B:674:ASN:O	1:B:674:ASN:ND2	2.28	0.65
1:B:702:HIS:HB3	1:B:705:ALA:HB3	1.78	0.65
1:B:648:GLU:CD	1:B:652:ARG:HB3	2.18	0.64
1:A:520:VAL:HA	1:A:523:GLN:HB3	1.79	0.64
2:C:14:DT:H2'	2:C:14:DT:O2	1.98	0.64
1:B:675:GLY:CA	1:B:680:ALA:N	2.61	0.63
1:B:700:ASN:OD1	1:B:702:HIS:N	2.31	0.62
1:B:675:GLY:HA2	1:B:680:ALA:N	2.15	0.62
1:B:702:HIS:HB2	1:B:703:LEU:CA	2.28	0.62
1:B:644:LYS:O	1:B:647:LEU:HB3	2.00	0.61
1:A:274:ALA:HB2	1:A:304:LYS:HG3	1.83	0.60
1:B:648:GLU:OE2	1:B:652:ARG:CZ	2.49	0.60
1:B:513:THR:OG1	1:B:542:LYS:HG3	2.01	0.60
1:B:687:GLN:HE21	1:B:687:GLN:C	2.04	0.60
1:B:648:GLU:OE1	1:B:652:ARG:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:ASP:O	1:B:704:VAL:HG13	2.02	0.59
1:B:662:GLY:O	1:B:663:LEU:CG	2.50	0.59
1:A:586:LEU:N	1:A:587:PRO:HD2	2.17	0.59
1:B:673:SER:OG	1:B:704:VAL:N	2.35	0.59
1:B:635:VAL:CG1	1:B:645:GLN:CB	2.81	0.58
1:B:629:LEU:HG	1:B:631:PRO:CG	2.25	0.58
1:B:672:ALA:CB	1:B:675:GLY:O	2.51	0.58
1:B:672:ALA:O	1:B:674:ASN:N	2.37	0.58
1:B:648:GLU:HG3	1:B:681:LEU:HD13	1.86	0.58
1:A:721:LEU:CD2	1:B:706:LEU:HD11	2.34	0.57
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.86	0.57
1:A:416:LEU:HD13	1:A:416:LEU:O	2.04	0.57
1:B:675:GLY:HA3	1:B:680:ALA:CB	2.33	0.57
1:B:646:ALA:C	1:B:648:GLU:N	2.54	0.57
1:B:452:VAL:HG23	4:B:806:HOH:O	2.04	0.57
1:B:673:SER:C	1:B:703:LEU:HB3	2.23	0.57
1:B:671:ILE:HG23	1:B:673:SER:H	1.70	0.57
1:B:583:GLN:O	1:B:587:PRO:CD	2.53	0.57
1:B:423:HIS:HB3	1:B:450:LEU:CD2	2.35	0.56
1:A:632:GLU:OE2	4:A:802:HOH:O	2.18	0.56
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.86	0.56
1:A:721:LEU:HD22	1:B:706:LEU:HD11	1.87	0.56
1:B:645:GLN:CG	1:B:646:ALA:H	2.17	0.56
1:B:637:ILE:CG2	1:B:638:ALA:N	2.58	0.56
1:B:647:LEU:O	1:B:648:GLU:CB	2.54	0.56
1:B:663:LEU:O	1:B:665:PRO:HD2	2.05	0.56
1:B:638:ALA:O	1:B:639:SER:C	2.44	0.56
1:B:645:GLN:CG	1:B:646:ALA:N	2.69	0.55
1:B:671:ILE:HG12	1:B:706:LEU:HD11	1.88	0.55
1:B:633:GLN:O	1:B:637:ILE:CG1	2.54	0.55
1:A:365:ILE:HG22	1:A:375:LEU:HD13	1.88	0.54
1:B:647:LEU:HD23	1:B:678:ARG:C	2.26	0.54
1:B:588:VAL:C	1:B:590:CYS:N	2.59	0.54
1:B:623:LEU:C	1:B:625:GLN:H	2.11	0.54
1:B:552:LEU:C	1:B:552:LEU:HD13	2.27	0.54
1:B:635:VAL:HG11	1:B:645:GLN:HB2	1.88	0.54
1:B:655:PRO:O	1:B:659:GLN:CB	2.55	0.54
1:B:702:HIS:O	1:B:703:LEU:HD12	2.06	0.54
1:A:450:LEU:CD1	1:A:454:CYS:SG	2.95	0.54
1:A:657:LEU:HD21	1:A:685:VAL:CG2	2.37	0.54
1:B:654:LEU:HD23	1:B:654:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HB3	1:B:553:PRO:HD3	1.88	0.54
1:B:648:GLU:CD	1:B:652:ARG:CB	2.75	0.54
1:A:690:ARG:O	1:A:691:PRO:C	2.45	0.54
1:B:675:GLY:HA3	1:B:680:ALA:N	2.21	0.53
2:C:14:DT:O2	2:C:14:DT:C2'	2.56	0.53
1:B:232:TRP:CD1	1:B:232:TRP:C	2.82	0.53
1:B:673:SER:CB	1:B:703:LEU:C	2.77	0.53
1:B:692:ASP:HB2	1:B:693:PRO:CD	2.38	0.53
1:B:646:ALA:O	1:B:648:GLU:N	2.30	0.53
1:A:552:LEU:HB3	1:A:553:PRO:HD3	1.90	0.53
1:A:287:LEU:HD21	1:A:311:GLN:HA	1.90	0.53
1:B:672:ALA:O	1:B:675:GLY:N	2.26	0.53
1:B:701:ASP:OD1	1:B:702:HIS:ND1	2.34	0.52
2:C:-2:DT:H4'	2:C:-1:DG:OP1	2.09	0.52
1:B:244:VAL:HG22	1:B:276:HIS:CD2	2.44	0.52
1:B:648:GLU:O	1:B:652:ARG:N	2.34	0.52
1:B:687:GLN:O	1:B:690:ARG:HB2	2.09	0.52
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.90	0.52
1:B:606:ASN:HD21	1:B:638:ALA:N	2.07	0.52
1:A:413:GLN:HG3	4:A:805:HOH:O	2.08	0.51
1:A:702:HIS:CE1	1:B:664:THR:HG22	2.46	0.51
1:B:265:LYS:HE2	3:D:-4:DA:OP2	2.10	0.51
1:B:635:VAL:HG11	1:B:645:GLN:CB	2.41	0.51
1:A:611:GLN:HB3	1:A:644:LYS:HD3	1.92	0.51
1:B:287:LEU:HD21	1:B:311:GLN:HA	1.92	0.51
1:A:475:GLN:HB3	1:A:508:LYS:HD2	1.94	0.50
1:B:671:ILE:HG13	1:B:672:ALA:N	2.27	0.50
1:B:629:LEU:C	1:B:631:PRO:HD3	2.31	0.50
1:A:657:LEU:HD21	1:A:685:VAL:HG23	1.94	0.50
1:B:648:GLU:OE2	1:B:652:ARG:NE	2.45	0.50
1:B:663:LEU:HD11	1:B:695:LEU:HD21	1.94	0.50
1:A:593:HIS:HB3	1:A:620:LEU:HD23	1.94	0.50
1:B:701:ASP:OD1	1:B:705:ALA:HB3	2.11	0.50
1:A:596:THR:HB	1:A:598:GLU:OE1	2.12	0.49
1:B:672:ALA:HB3	1:B:673:SER:O	2.12	0.49
1:B:596:THR:OG1	1:B:599:GLN:HB2	2.13	0.49
1:A:297:ILE:CG2	1:A:307:LEU:HD13	2.42	0.49
1:B:631:PRO:C	1:B:632:GLU:OE1	2.51	0.49
1:A:692:ASP:HB3	1:A:693:PRO:HD3	1.95	0.49
1:B:650:VAL:HG13	1:B:651:GLN:N	2.28	0.49
1:B:630:THR:HG22	1:B:630:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:HG11	1:A:515:GLN:HE21	1.78	0.49
1:A:514:VAL:HG23	1:A:518:LEU:HD22	1.95	0.49
1:B:265:LYS:CE	3:D:-4:DA:OP2	2.61	0.48
1:B:678:ARG:HG3	1:B:681:LEU:HD12	1.92	0.48
1:B:629:LEU:CD1	1:B:631:PRO:HG3	2.43	0.48
1:B:648:GLU:O	1:B:649:THR:C	2.51	0.48
1:B:662:GLY:O	1:B:663:LEU:HG	2.13	0.48
1:B:690:ARG:HA	1:B:690:ARG:NH2	2.28	0.48
1:A:697:ALA:HB1	1:B:666:GLN:HB3	1.95	0.48
1:B:586:LEU:N	1:B:587:PRO:HD2	2.28	0.48
1:A:721:LEU:CD1	1:B:706:LEU:HD11	2.44	0.48
1:B:484:LEU:N	1:B:485:PRO:HD2	2.29	0.48
1:B:240:ALA:CB	1:B:269:VAL:HG23	2.44	0.48
1:A:631:PRO:HD2	4:A:802:HOH:O	2.13	0.48
1:A:484:LEU:N	1:A:485:PRO:HD2	2.29	0.47
1:B:663:LEU:CD1	1:B:695:LEU:HD21	2.44	0.47
1:A:590:CYS:SG	1:A:595:LEU:O	2.70	0.47
1:B:639:SER:OG	1:B:640:HIS:N	2.47	0.47
1:B:450:LEU:HB3	1:B:451:PRO:HD3	1.97	0.47
1:B:644:LYS:N	4:B:801:HOH:O	2.34	0.47
1:B:585:LEU:HD23	1:B:588:VAL:HG12	1.96	0.47
1:B:702:HIS:HB3	1:B:705:ALA:O	2.09	0.47
1:A:695:LEU:O	1:A:697:ALA:N	2.48	0.47
1:A:721:LEU:HB3	1:B:671:ILE:HD13	1.97	0.47
1:B:633:GLN:O	1:B:634:VAL:C	2.52	0.47
1:B:647:LEU:O	1:B:648:GLU:HB3	2.14	0.47
1:A:586:LEU:N	1:A:587:PRO:CD	2.78	0.46
1:B:588:VAL:O	1:B:590:CYS:N	2.44	0.46
1:B:623:LEU:O	1:B:625:GLN:N	2.48	0.46
1:A:585:LEU:HB3	1:A:589:LEU:HD22	1.98	0.46
1:A:552:LEU:HD12	1:A:552:LEU:O	2.16	0.46
1:B:630:THR:N	1:B:631:PRO:HD3	2.31	0.45
1:A:582:VAL:O	1:A:586:LEU:HB2	2.16	0.45
1:A:252:PRO:HB2	1:A:283:THR:HG21	1.98	0.45
1:B:595:LEU:HD13	1:B:600:VAL:HB	1.99	0.45
1:B:297:ILE:CG2	1:B:307:LEU:HD13	2.47	0.45
2:I:14:DT:O3'	1:B:719:LYS:CD	2.65	0.44
1:A:232:TRP:NE1	4:A:807:HOH:O	2.49	0.44
1:B:652:ARG:HA	1:B:655:PRO:HD2	1.99	0.44
1:A:627:HIS:HB3	1:A:654:LEU:CD2	2.47	0.44
1:A:717:ALA:O	1:A:721:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:LEU:CB	1:B:595:LEU:HD21	2.43	0.44
1:B:312:ARG:NH2	1:B:342:GLU:OE2	2.51	0.44
1:B:687:GLN:O	1:B:687:GLN:NE2	2.46	0.44
1:B:648:GLU:HG2	1:B:681:LEU:HD13	1.99	0.44
1:A:504:ASN:HB2	4:A:820:HOH:O	2.17	0.44
1:A:518:LEU:HD13	1:A:532:VAL:HG11	1.99	0.44
1:A:654:LEU:HB3	1:A:655:PRO:HD3	1.99	0.44
1:A:416:LEU:CD1	1:A:416:LEU:C	2.85	0.44
1:A:580:GLU:O	1:A:583:GLN:HB3	2.17	0.44
1:A:598:GLU:CD	1:A:598:GLU:H	2.21	0.44
1:B:585:LEU:CD2	1:B:588:VAL:HG12	2.48	0.44
1:B:664:THR:HA	1:B:666:GLN:HG2	2.00	0.44
3:D:-14:DA:H5'	3:D:-13:DG:N7	2.33	0.44
1:B:673:SER:OG	1:B:704:VAL:HA	2.18	0.43
1:A:480:VAL:O	1:A:484:LEU:HB2	2.18	0.43
1:A:721:LEU:HD11	1:B:706:LEU:CD2	2.48	0.43
1:B:248:LEU:HD21	1:B:276:HIS:HA	1.99	0.43
1:B:434:ALA:HB2	1:B:443:LEU:HD11	2.00	0.43
1:B:656:VAL:HA	1:B:659:GLN:HB3	1.99	0.43
1:B:700:ASN:OD1	1:B:701:ASP:N	2.52	0.43
1:A:486:VAL:HG11	1:A:515:GLN:NE2	2.34	0.43
1:B:552:LEU:C	1:B:552:LEU:CD1	2.87	0.43
1:B:655:PRO:C	1:B:659:GLN:HB3	2.38	0.43
1:B:675:GLY:HA2	1:B:679:PRO:C	2.37	0.43
1:B:480:VAL:O	1:B:484:LEU:HB2	2.18	0.43
1:B:714:ALA:O	1:B:715:LEU:HD23	2.19	0.43
1:A:692:ASP:HB3	1:A:693:PRO:CD	2.48	0.42
1:B:718:VAL:O	1:B:718:VAL:CG1	2.65	0.42
2:C:-2:DT:H1'	2:C:-1:DG:C8	2.54	0.42
1:B:629:LEU:N	1:B:631:PRO:HD3	2.35	0.42
1:B:645:GLN:HG2	1:B:646:ALA:H	1.85	0.42
1:B:673:SER:CB	1:B:703:LEU:O	2.68	0.42
1:B:475:GLN:HB3	1:B:508:LYS:HD2	2.02	0.42
1:B:631:PRO:C	1:B:633:GLN:H	2.23	0.42
1:A:510:ALA:O	1:A:514:VAL:HG13	2.19	0.42
1:B:648:GLU:OE1	1:B:652:ARG:CB	2.68	0.42
1:B:674:ASN:HB2	1:B:703:LEU:HB2	2.01	0.42
1:A:721:LEU:HD13	1:B:706:LEU:HD11	2.02	0.42
1:B:664:THR:O	1:B:664:THR:OG1	2.33	0.42
1:A:450:LEU:HD12	1:A:450:LEU:O	2.20	0.42
1:A:630:THR:HG23	1:A:633:GLN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LEU:HB3	1:A:655:PRO:CD	2.50	0.42
1:B:552:LEU:HD13	1:B:552:LEU:O	2.19	0.42
1:A:527:LEU:HD21	1:A:552:LEU:CD2	2.50	0.41
1:B:647:LEU:HD21	1:B:679:PRO:HD3	2.02	0.41
1:B:673:SER:OG	1:B:704:VAL:CA	2.68	0.41
1:B:671:ILE:CG1	1:B:672:ALA:N	2.83	0.41
2:I:13:DC:H2"	2:I:14:DT:O5'	2.21	0.41
1:B:606:ASN:OD1	1:B:638:ALA:HA	2.19	0.41
1:B:713:PRO:O	1:B:714:ALA:HB2	2.20	0.41
3:J:-11:DG:H5"	1:B:716:ASP:OD1	2.20	0.41
1:B:577:GLN:HB3	1:B:610:LYS:HD3	2.01	0.41
1:B:673:SER:HB3	1:B:703:LEU:CB	2.49	0.41
1:B:663:LEU:HB2	1:B:664:THR:HG23	2.02	0.41
1:A:313:LEU:O	1:A:314:LEU:C	2.58	0.41
1:A:657:LEU:HD21	1:A:685:VAL:HG22	2.03	0.41
3:J:-9:DC:H2"	3:J:-8:DG:H5'	2.01	0.41
1:A:630:THR:HG22	1:A:633:GLN:CG	2.51	0.41
1:B:232:TRP:C	1:B:232:TRP:HD1	2.24	0.41
1:B:645:GLN:HG3	1:B:646:ALA:N	2.36	0.41
1:B:652:ARG:NE	1:B:685:VAL:HG21	2.36	0.41
1:B:678:ARG:CG	1:B:681:LEU:CD1	2.93	0.41
1:A:577:GLN:HB3	1:A:610:LYS:HD3	2.03	0.41
1:A:248:LEU:HD21	1:A:276:HIS:HA	2.03	0.40
1:B:586:LEU:CD1	1:B:600:VAL:HG11	2.49	0.40
1:A:698:LEU:N	4:A:801:HOH:O	2.45	0.40
1:B:583:GLN:O	1:B:587:PRO:CG	2.69	0.40
1:B:348:LEU:HD23	1:B:348:LEU:C	2.42	0.40
1:B:589:LEU:HD13	1:B:595:LEU:HD22	2.03	0.40
1:B:706:LEU:C	1:B:708:CYS:N	2.75	0.40

All (16) 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:B:595:LEU:N	1:B:725:HIS:C[2_545]	1.13	1.07
1:B:595:LEU:N	1:B:725:HIS:CA[2_545]	1.18	1.02
1:B:595:LEU:N	1:B:726:HIS:N[2_545]	1.72	0.48
1:B:594:GLY:C	1:B:725:HIS:C[2_545]	1.73	0.47
1:A:231:GLN:O	1:B:231:GLN:C[1_656]	1.77	0.43
1:B:594:GLY:C	1:B:726:HIS:N[2_545]	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:LEU:CA	1:B:726:HIS:N[2_545]	1.88	0.32
1:A:230:MET:O	1:B:233:SER:N[1_656]	1.89	0.31
1:B:594:GLY:O	1:B:726:HIS:N[2_545]	1.89	0.31
1:B:595:LEU:CA	1:B:725:HIS:C[2_545]	1.89	0.31
1:B:595:LEU:CA	1:B:725:HIS:CA[2_545]	1.90	0.30
1:B:595:LEU:N	1:B:725:HIS:CB[2_545]	1.91	0.29
1:A:231:GLN:O	1:B:231:GLN:O[1_656]	2.02	0.18
1:B:586:LEU:O	1:B:724:HIS:ND1[2_545]	2.06	0.14
1:B:586:LEU:O	1:B:724:HIS:CE1[2_545]	2.14	0.06
1:A:231:GLN:O	1:B:232:TRP:N[1_656]	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	495/499 (99%)	462 (93%)	29 (6%)	4 (1%)	19 33
1	B	495/499 (99%)	430 (87%)	48 (10%)	17 (3%)	3 4
All	All	990/998 (99%)	892 (90%)	77 (8%)	21 (2%)	7 10

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ALA
1	B	624	CYS
1	B	631	PRO
1	B	647	LEU
1	B	663	LEU
1	B	673	SER
1	A	252	PRO
1	A	696	ALA
1	B	589	LEU
1	B	648	GLU

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Mol	Chain	Res	Type
1	B	714	ALA
1	B	286	PRO
1	B	633	GLN
1	B	691	PRO
1	B	699	THR
1	B	692	ASP
1	A	691	PRO
1	B	489	GLN
1	B	285	ALA
1	B	678	ARG
1	B	251	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	380/384 (99%)	342 (90%)	38 (10%)	7 13
1	B	379/384 (99%)	325 (86%)	54 (14%)	3 5
All	All	759/768 (99%)	667 (88%)	92 (12%)	5 8

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	TRP
1	A	233	SER
1	A	238	LEU
1	A	254	GLN
1	A	265	LYS
1	A	278	TRP
1	A	283	THR
1	A	287	LEU
1	A	307	LEU
1	A	316	VAL
1	A	326	GLN
1	A	345	GLN

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	416	LEU
1	A	450	LEU
1	A	453	LEU
1	A	484	LEU
1	A	496	GLN
1	A	518	LEU
1	A	525	HIS
1	A	527	LEU
1	A	552	LEU
1	A	564	GLN
1	A	586	LEU
1	A	589	LEU
1	A	591	GLN
1	A	619	LEU
1	A	623	LEU
1	A	678	ARG
1	A	684	ILE
1	A	687	GLN
1	A	690	ARG
1	A	695	LEU
1	A	700	ASN
1	A	706	LEU
1	A	715	LEU
1	A	716	ASP
1	A	723	HIS
1	B	231	GLN
1	B	233	SER
1	B	238	LEU
1	B	241	LEU
1	B	244	VAL
1	B	266	ARG
1	B	287	LEU
1	B	307	LEU
1	B	311	GLN
1	B	353	GLN
1	B	418	VAL
1	B	453	LEU
1	B	484	LEU
1	B	518	LEU
1	B	527	LEU
1	B	542	LYS

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Mol	Chain	Res	Type
1	B	552	LEU
1	B	564	GLN
1	B	571	SER
1	B	588	VAL
1	B	590	CYS
1	B	613	LEU
1	B	623	LEU
1	B	625	GLN
1	B	627	HIS
1	B	629	LEU
1	B	631	PRO
1	B	632	GLU
1	B	633	GLN
1	B	652	ARG
1	B	653	LEU
1	B	663	LEU
1	B	666	GLN
1	B	667	GLN
1	B	668	VAL
1	B	673	SER
1	B	674	ASN
1	B	678	ARG
1	B	684	ILE
1	B	687	GLN
1	B	689	SER
1	B	690	ARG
1	B	692	ASP
1	B	695	LEU
1	B	698	LEU
1	B	701	ASP
1	B	704	VAL
1	B	706	LEU
1	B	716	ASP
1	B	719	LYS
1	B	720	LYS
1	B	721	LEU
1	B	723	HIS
1	B	724	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	591	GLN
1	A	593	HIS
1	B	321	HIS
1	B	496	GLN
1	B	659	GLN
1	B	687	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	I	6	2,3	17,21,22	0.97	1 (5%)	24,30,33	1.30	3 (12%)
2	5CM	C	6	2,3	17,21,22	0.98	1 (5%)	24,30,33	1.32	3 (12%)

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	I	6	2,3	-	0/7/21/22	0/2/2/2
2	5CM	C	6	2,3	-	0/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	5CM	C6-N1	-2.96	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	5CM	C6-C5	2.87	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	6	5CM	C5A-C5-C6	-3.55	118.11	122.85
2	I	6	5CM	C5-C4-N3	-3.29	118.13	121.67
2	C	6	5CM	C5-C6-N1	-3.01	120.24	123.34
2	I	6	5CM	O2-C2-N3	-2.74	117.88	122.33
2	I	6	5CM	C5A-C5-C6	-2.56	119.43	122.85
2	C	6	5CM	O2-C2-N3	-2.24	118.69	122.33

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 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	497/499 (99%)	0.04	11 (2%) 62 64	16, 37, 71, 126	0
1	B	497/499 (99%)	0.86	66 (13%) 3 2	16, 40, 133, 207	0
2	C	16/17 (94%)	-0.18	1 (6%) 20 20	19, 28, 68, 148	0
2	I	16/17 (94%)	-0.53	0 100 100	16, 22, 75, 94	0
3	D	17/17 (100%)	-0.19	1 (5%) 22 22	28, 41, 67, 121	0
3	J	17/17 (100%)	-0.20	1 (5%) 22 22	26, 39, 77, 126	0
All	All	1060/1066 (99%)	0.40	80 (7%) 14 13	16, 38, 105, 207	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	MET	20.2
1	B	706	LEU	19.0
1	B	699	THR	14.2
1	B	707	ALA	14.1
1	B	726	HIS	11.9
1	B	720	LYS	11.8
1	B	713	PRO	11.2
1	B	588	VAL	11.1
1	B	718	VAL	10.9
1	B	716	ASP	10.4
1	B	715	LEU	10.1
1	B	714	ALA	9.8
1	B	717	ALA	9.6
1	B	591	GLN	9.1
1	B	693	PRO	8.6
1	B	231	GLN	8.0
1	B	691	PRO	8.0
1	B	711	GLY	8.0
1	A	524	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	692	ASP	7.8
1	B	698	LEU	7.8
1	B	587	PRO	7.5
1	A	232	TRP	7.5
1	B	710	GLY	7.5
1	B	704	VAL	7.4
1	B	723	HIS	7.2
1	B	700	ASN	7.0
1	B	722	GLU	6.5
1	B	721	LEU	5.8
1	B	719	LYS	5.8
1	B	708	CYS	5.1
1	B	694	ALA	5.1
1	B	661	HIS	4.9
1	A	692	ASP	4.8
1	B	232	TRP	4.7
1	B	652	ARG	4.7
2	C	14	DT	4.7
1	A	525	HIS	4.5
1	B	712	ARG	4.5
1	B	590	CYS	4.4
1	B	638	ALA	4.4
3	D	-14	DA	4.4
1	B	627	HIS	4.1
1	B	702	HIS	4.1
1	A	693	PRO	4.0
1	B	725	HIS	4.0
1	B	709	LEU	3.7
1	B	633	GLN	3.6
1	B	672	ALA	3.5
1	B	233	SER	3.4
1	B	675	GLY	3.3
1	B	668	VAL	3.2
1	B	251	PRO	3.0
1	B	597	PRO	3.0
1	A	697	ALA	3.0
1	B	589	LEU	2.9
1	B	678	ARG	2.9
1	B	662	GLY	2.9
1	B	598	GLU	2.9
1	A	723	HIS	2.9
1	B	593	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	491	HIS	2.8
1	B	676	GLY	2.7
1	B	660	ALA	2.7
1	A	726	HIS	2.6
1	B	592	ALA	2.6
1	B	671	ILE	2.6
1	B	640	HIS	2.5
1	A	523	GLN	2.5
1	B	674	ASN	2.5
1	B	625	GLN	2.4
1	A	696	ALA	2.2
3	J	-14	DA	2.2
1	B	272	VAL	2.2
1	B	634	VAL	2.2
1	B	584	ARG	2.2
1	B	557	GLN	2.1
1	B	666	GLN	2.1
1	B	556	CYS	2.1
1	A	233	SER	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	5CM	I	6	20/21	0.98	0.13	19,22,25,26	0
2	5CM	C	6	20/21	0.98	0.12	19,21,23,23	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.