



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:44 PM UTC

PDB ID : 6JTQ / pdb_00006jtq
Title : RVD HA specifically contacts 5mC through van der Waals interactions
Authors : Liu, L.; Yi, C.
Deposited on : 2019-04-11
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

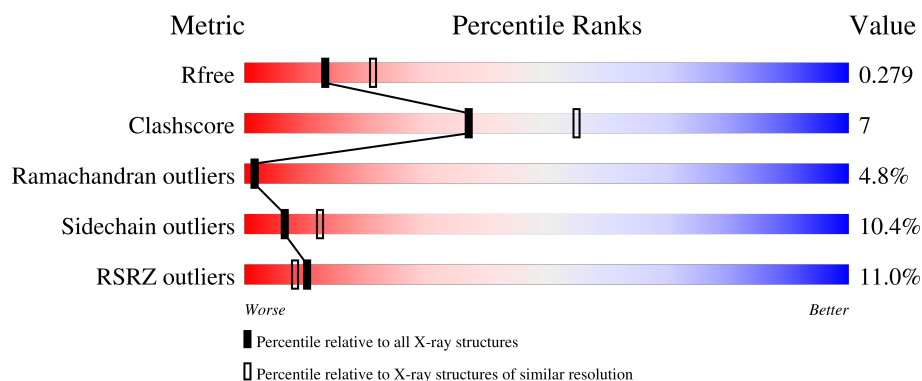
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 $\leq 5\%$. 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	
1	B	499	
2	C	17	
2	I	17	
3	D	17	

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Mol	Chain	Length	Quality of chain
3	J	17	6% 82% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8704 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	2253	673	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	51	Total	O	0	0
			51	51		
4	I	13	Total	O	0	0
			13	13		
4	J	1	Total	O	0	0
			1	1		

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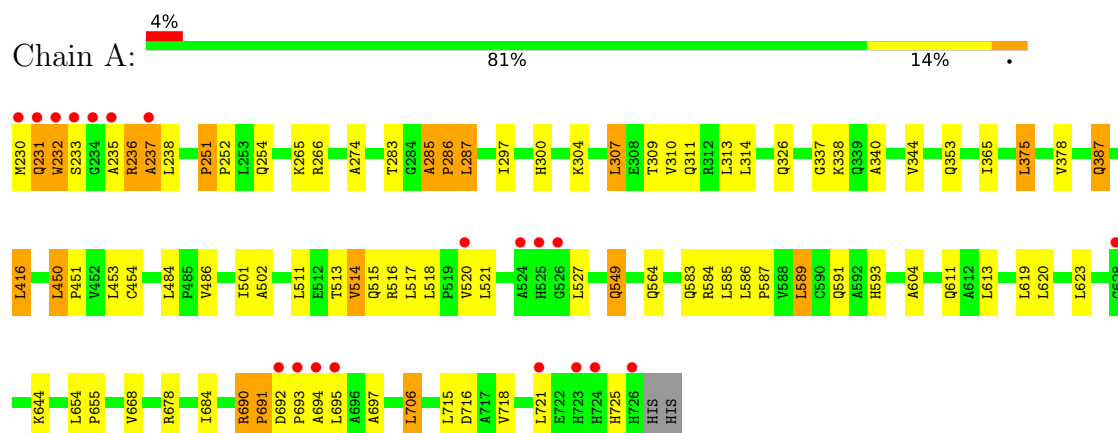
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	33	Total 33	O 33	0	0
4	C	14	Total 14	O 14	0	0

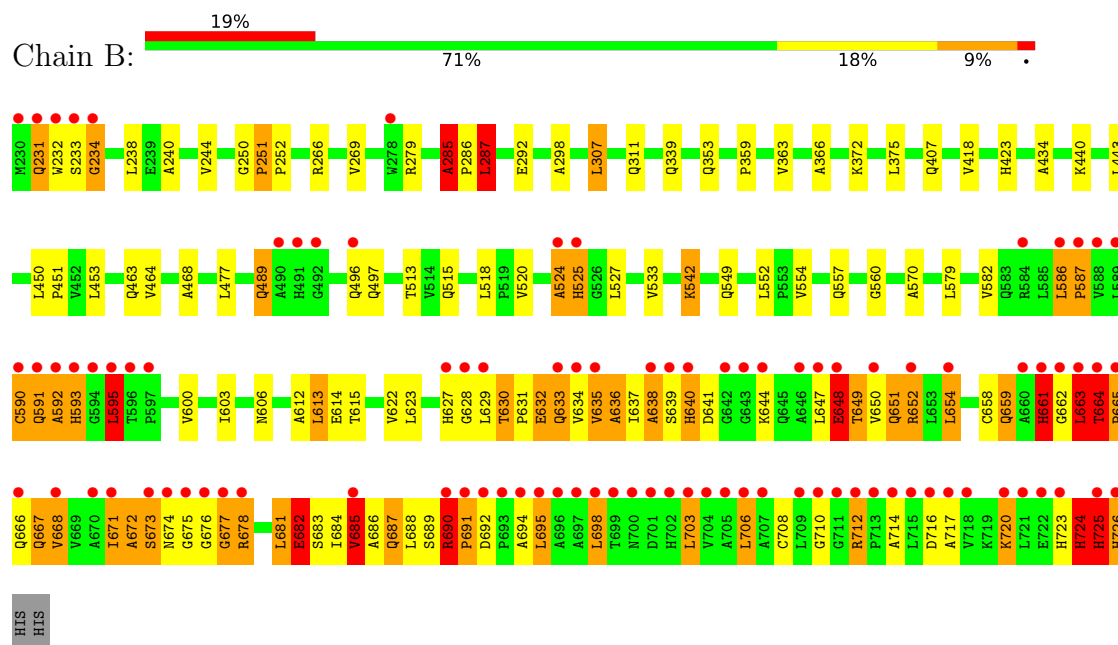
3 Residue-property plots

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.

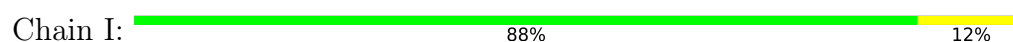
• Molecule 1: TAL effector



• Molecule 1: TAL effector

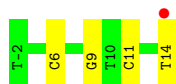
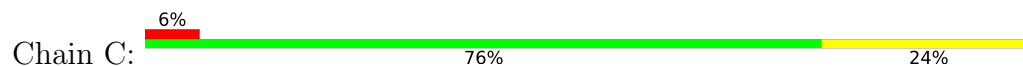


• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*T)-3')

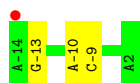
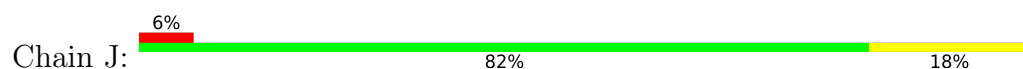




- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.79Å 88.02Å 89.35Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.48 50.00 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.8 (50.00-2.48) 91.8 (50.00-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.218 , 0.283 0.220 , 0.279	Depositor DCC
R_{free} test set	2095 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8704	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.96	2/3660 (0.1%)	1.10	3/5001 (0.1%)
1	B	1.07	7/3660 (0.2%)	1.26	23/5001 (0.5%)
2	C	0.42	0/349	1.11	2/533 (0.4%)
2	I	0.43	0/349	1.00	1/533 (0.2%)
3	D	0.40	0/402	0.80	0/620
3	J	0.43	0/402	0.81	1/620 (0.2%)
All	All	0.94	9/8822 (0.1%)	1.14	30/12308 (0.2%)

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	4
1	B	0	15
All	All	0	19

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	640	HIS	CA-C	6.91	1.61	1.52
1	B	592	ALA	N-CA	6.72	1.54	1.46
1	A	237	ALA	CA-C	6.39	1.61	1.52
1	B	592	ALA	CA-C	6.18	1.61	1.52
1	B	593	HIS	N-CA	6.05	1.53	1.46
1	B	591	GLN	CA-C	5.64	1.59	1.52
1	A	231	GLN	N-CA	5.07	1.52	1.45
1	B	590	CYS	CA-C	5.04	1.57	1.52
1	B	661	HIS	N-CA	5.01	1.52	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	GLY	CA-C-N	9.68	130.35	120.38
1	B	250	GLY	C-N-CA	9.68	130.35	120.38
1	B	251	PRO	N-CA-C	8.98	121.65	110.70
2	I	-2	DT	C2'-C3'-O3'	8.79	124.69	111.50
1	B	285	ALA	CA-C-N	-8.56	110.99	119.64
1	B	285	ALA	C-N-CA	-8.56	110.99	119.64
1	B	632	GLU	N-CA-C	-7.75	100.89	110.65
1	B	234	GLY	N-CA-C	7.45	121.62	110.75
1	B	724	HIS	N-CA-CB	7.07	122.41	111.39
1	B	591	GLN	N-CA-C	6.91	120.11	108.02
1	B	633	GLN	N-CA-C	-6.77	96.38	110.80
1	B	592	ALA	N-CA-C	6.64	124.95	110.80
2	C	9	DG	C2'-C3'-O3'	6.64	121.46	111.50
2	C	11	DC	C2'-C3'-O3'	6.61	121.41	111.50
3	J	-13	DG	C2'-C3'-O3'	6.29	120.93	111.50
1	B	681	LEU	N-CA-C	-6.07	99.27	108.67
1	B	686	ALA	N-CA-C	-5.99	104.66	111.07
1	B	665	PRO	N-CA-C	-5.89	106.44	114.80
1	B	725	HIS	N-CA-C	-5.88	98.27	110.80
1	A	235	ALA	N-CA-C	5.81	117.96	108.55
1	B	279	ARG	N-CA-C	5.60	118.11	111.33
1	B	287	LEU	N-CA-C	5.38	116.95	111.14
1	B	648	GLU	N-CA-CB	5.25	119.37	110.49
1	B	661	HIS	N-CA-C	5.20	121.87	110.80
1	B	644	LYS	CA-C-N	5.17	127.52	120.54
1	B	644	LYS	C-N-CA	5.17	127.52	120.54
1	B	724	HIS	CA-CB-CG	5.14	118.94	113.80
1	A	251	PRO	N-CA-C	5.10	116.92	110.70
1	A	232	TRP	N-CA-C	5.08	116.54	108.67
1	B	595	LEU	CA-CB-CG	5.04	133.95	116.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Peptide
1	A	237	ALA	Peptide
1	A	251	PRO	Peptide
1	A	694	ALA	Peptide
1	B	234	GLY	Peptide
1	B	524	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	B	525	HIS	Peptide
1	B	622	VAL	Peptide
1	B	630	THR	Peptide
1	B	631	PRO	Peptide
1	B	648	GLU	Peptide
1	B	658	CYS	Peptide
1	B	661	HIS	Peptide
1	B	664	THR	Peptide
1	B	671	ILE	Peptide
1	B	672	ALA	Peptide
1	B	678	ARG	Peptide
1	B	723	HIS	Peptide
1	B	724	HIS	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	3734	42	3
1	B	3605	0	3734	80	4
2	C	336	0	195	2	0
2	I	336	0	195	0	0
3	D	355	0	189	0	0
3	J	355	0	189	1	0
4	A	51	0	0	0	0
4	B	33	0	0	2	0
4	C	14	0	0	0	0
4	I	13	0	0	0	0
4	J	1	0	0	0	0
All	All	8704	0	8236	119	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (119) 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:613:LEU:O	1:B:615:THR:N	2.13	0.80
1:B:672:ALA:HB3	1:B:675:GLY:HA3	1.66	0.77
1:B:648:GLU:HA	1:B:652:ARG:HB2	1.67	0.77
1:B:678:ARG:HG2	1:B:681:LEU:HD12	1.65	0.77
1:A:274:ALA:HB2	1:A:304:LYS:HG3	1.69	0.75
1:B:434:ALA:HB2	1:B:443:LEU:HD11	1.71	0.72
1:B:672:ALA:HB3	1:B:675:GLY:CA	2.22	0.69
1:B:724:HIS:O	1:B:726:HIS:N	2.27	0.68
1:B:659:GLN:HE22	1:B:688:LEU:HB3	1.59	0.68
1:B:676:GLY:O	1:B:677:GLY:C	2.40	0.64
1:B:637:ILE:HG22	1:B:638:ALA:N	2.12	0.64
1:B:287:LEU:HD21	1:B:311:GLN:HA	1.79	0.63
1:B:672:ALA:O	1:B:674:ASN:C	2.42	0.63
1:B:648:GLU:O	1:B:651:GLN:N	2.32	0.62
1:B:678:ARG:CG	1:B:681:LEU:HD12	2.29	0.62
1:B:638:ALA:O	1:B:639:SER:OG	2.16	0.61
1:B:681:LEU:O	1:B:682:GLU:HB2	1.98	0.61
1:A:365:ILE:HD13	1:A:378:VAL:HG21	1.82	0.60
1:B:463:GLN:HE21	1:B:496:GLN:NE2	2.00	0.60
1:A:721:LEU:HB3	1:B:671:ILE:HB	1.86	0.57
1:A:501:ILE:HD13	1:A:514:VAL:HG11	1.86	0.56
1:B:632:GLU:N	1:B:632:GLU:OE1	2.40	0.55
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.37	0.55
1:B:520:VAL:HG11	1:B:549:GLN:HE21	1.73	0.54
1:B:662:GLY:C	1:B:663:LEU:HD12	2.33	0.54
1:A:309:THR:OG1	1:A:338:LYS:HG3	2.08	0.53
1:B:637:ILE:C	1:B:638:ALA:O	2.49	0.53
1:A:486:VAL:HG11	1:A:515:GLN:HE21	1.73	0.53
1:A:365:ILE:HG22	1:A:375:LEU:HD13	1.92	0.52
1:B:633:GLN:HA	1:B:637:ILE:HG13	1.91	0.52
1:A:584:ARG:O	1:A:585:LEU:HD23	2.10	0.52
1:B:637:ILE:CG2	1:B:638:ALA:N	2.73	0.52
1:A:593:HIS:HB3	1:A:620:LEU:HD23	1.92	0.52
1:B:648:GLU:CG	1:B:681:LEU:HD13	2.40	0.52
1:A:585:LEU:HB3	1:A:589:LEU:HD22	1.91	0.51
1:B:587:PRO:O	1:B:590:CYS:N	2.43	0.51
1:B:339:GLN:HB3	1:B:372:LYS:HD2	1.92	0.51
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.93	0.50
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.94	0.50
1:B:659:GLN:CD	4:B:804:HOH:O	2.55	0.50
1:B:298:ALA:HB2	1:B:307:LEU:HD21	1.93	0.49
1:B:662:GLY:O	1:B:664:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ALA:O	1:B:674:ASN:N	2.45	0.49
1:B:606:ASN:HD21	1:B:638:ALA:N	2.11	0.49
1:A:287:LEU:HD21	1:A:311:GLN:HA	1.95	0.49
1:A:521:LEU:HD21	1:A:549:GLN:HB2	1.93	0.49
1:B:674:ASN:CG	1:B:703:LEU:HD22	2.38	0.49
1:B:663:LEU:HD13	1:B:695:LEU:HD11	1.96	0.48
1:A:697:ALA:HB1	1:B:666:GLN:HB3	1.96	0.48
1:B:654:LEU:N	1:B:654:LEU:HD23	2.28	0.48
1:B:366:ALA:HB2	1:B:375:LEU:HD11	1.96	0.47
2:C:14:DT:O2	2:C:14:DT:H2'	2.15	0.47
1:B:423:HIS:HB3	1:B:450:LEU:CD2	2.44	0.46
1:B:690:ARG:HG2	1:B:691:PRO:CD	2.45	0.46
1:A:706:LEU:HD21	1:A:718:VAL:HG21	1.97	0.46
1:B:633:GLN:O	1:B:634:VAL:C	2.57	0.46
3:J:-10:DA:H2'	3:J:-9:DC:C6	2.50	0.46
1:B:652:ARG:CZ	1:B:685:VAL:HG11	2.46	0.46
1:A:285:ALA:CB	1:A:286:PRO:CD	2.93	0.46
1:B:648:GLU:CG	1:B:649:THR:N	2.79	0.46
1:B:662:GLY:O	1:B:665:PRO:HD3	2.16	0.46
1:B:285:ALA:CB	1:B:286:PRO:CD	2.94	0.46
1:B:552:LEU:C	1:B:552:LEU:HD13	2.40	0.46
1:B:717:ALA:HB3	1:B:720:LYS:HG3	1.97	0.46
1:A:313:LEU:O	1:A:314:LEU:C	2.58	0.45
1:A:450:LEU:HD13	1:A:454:CYS:SG	2.56	0.45
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.46	0.45
1:B:635:VAL:O	1:B:636:ALA:HB3	2.16	0.45
1:B:648:GLU:O	1:B:649:THR:C	2.58	0.45
1:A:517:LEU:HA	1:A:520:VAL:HG12	1.97	0.45
1:B:497:GLN:NE2	1:B:533:VAL:HG21	2.32	0.45
1:B:666:GLN:O	1:B:667:GLN:HB2	2.15	0.45
1:A:604:ALA:HB2	1:A:613:LEU:HD11	1.97	0.45
1:B:450:LEU:HB3	1:B:451:PRO:HD3	1.99	0.45
1:A:513:THR:O	1:A:517:LEU:HB2	2.17	0.45
1:B:240:ALA:CB	1:B:269:VAL:HG23	2.47	0.45
1:B:687:GLN:HE21	1:B:690:ARG:HD2	1.81	0.45
1:B:630:THR:HG22	1:B:630:THR:O	2.17	0.44
1:A:654:LEU:HD12	1:A:668:VAL:HG11	1.99	0.44
1:B:612:ALA:C	1:B:613:LEU:O	2.60	0.44
1:B:232:TRP:CD1	1:B:232:TRP:C	2.96	0.44
1:A:297:ILE:CG2	1:A:307:LEU:HD13	2.48	0.44
1:A:690:ARG:O	1:A:691:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:THR:OG1	1:B:542:LYS:HG3	2.18	0.43
1:B:468:ALA:HB2	1:B:477:LEU:HD11	2.00	0.43
1:B:647:LEU:HD23	1:B:678:ARG:C	2.43	0.43
1:A:706:LEU:CD2	1:A:718:VAL:HG21	2.48	0.43
1:A:450:LEU:HD12	1:A:450:LEU:C	2.43	0.43
1:A:654:LEU:HB3	1:A:655:PRO:HD3	2.00	0.43
1:B:407:GLN:HB3	1:B:440:LYS:HD3	2.00	0.43
1:B:603:ILE:HG13	1:B:637:ILE:HD13	1.99	0.43
1:A:502:ALA:HB2	1:A:511:LEU:HD11	2.01	0.43
1:A:516:ARG:O	1:A:518:LEU:N	2.49	0.43
1:B:648:GLU:HA	1:B:652:ARG:CB	2.42	0.43
1:A:721:LEU:HD21	1:B:706:LEU:HB3	2.01	0.42
1:B:649:THR:O	1:B:650:VAL:C	2.62	0.42
1:B:668:VAL:HA	1:B:672:ALA:HA	2.02	0.42
1:B:672:ALA:HB3	1:B:675:GLY:HA2	2.00	0.42
1:B:638:ALA:O	1:B:639:SER:CB	2.67	0.42
1:A:514:VAL:O	1:A:516:ARG:O	2.38	0.42
2:C:14:DT:O2	2:C:14:DT:C2'	2.68	0.42
1:A:340:ALA:O	1:A:344:VAL:HG23	2.20	0.42
1:A:450:LEU:N	1:A:451:PRO:CD	2.82	0.42
1:B:668:VAL:O	1:B:671:ILE:O	2.38	0.42
1:B:285:ALA:HB1	1:B:286:PRO:HD3	2.02	0.41
1:B:570:ALA:HB2	1:B:579:LEU:HD11	2.02	0.41
1:B:647:LEU:HD23	1:B:678:ARG:O	2.20	0.41
1:A:692:ASP:HB3	1:A:693:PRO:CD	2.51	0.41
1:B:659:GLN:NE2	4:B:804:HOH:O	2.53	0.41
1:A:721:LEU:HD22	1:B:671:ILE:HG12	2.01	0.41
1:B:606:ASN:HB3	1:B:641:ASP:OD1	2.21	0.41
1:A:285:ALA:HB1	1:A:286:PRO:HD3	2.02	0.41
1:B:359:PRO:O	1:B:363:VAL:HG23	2.20	0.41
1:B:450:LEU:HD12	1:B:464:VAL:HG11	2.02	0.41
1:A:654:LEU:CD1	1:A:668:VAL:HG11	2.52	0.41
1:A:416:LEU:HD13	1:A:416:LEU:C	2.47	0.40
1:A:586:LEU:N	1:A:587:PRO:HD2	2.36	0.40
1:A:721:LEU:HD13	1:B:671:ILE:HG21	2.04	0.40
1:A:721:LEU:HD11	1:B:706:LEU:HA	2.04	0.40

All (4) 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:230:MET:O	1:B:233:SER:N[1_656]	1.95	0.25
1:A:231:GLN:O	1:B:231:GLN:C[1_656]	1.98	0.22
1:A:231:GLN:O	1:B:231:GLN:O[1_656]	2.00	0.20
1:B:595:LEU:N	1:B:725:HIS:O[2_545]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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%)	454 (92%)	32 (6%)	9 (2%)	6	11
1	B	495/499 (99%)	401 (81%)	55 (11%)	39 (8%)	1	0
All	All	990/998 (99%)	855 (86%)	87 (9%)	48 (5%)	2	2

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ALA
1	B	285	ALA
1	B	524	ALA
1	B	586	LEU
1	B	592	ALA
1	B	628	GLY
1	B	638	ALA
1	B	648	GLU
1	B	661	HIS
1	B	663	LEU
1	B	667	GLN
1	B	673	SER
1	B	685	VAL
1	B	690	ARG
1	B	691	PRO
1	B	695	LEU
1	B	698	LEU

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Mol	Chain	Res	Type
1	B	720	LYS
1	A	233	SER
1	A	252	PRO
1	B	613	LEU
1	B	636	ALA
1	B	677	GLY
1	B	682	GLU
1	B	708	CYS
1	B	716	ASP
1	B	725	HIS
1	A	236	ARG
1	A	387	GLN
1	A	691	PRO
1	A	725	HIS
1	B	489	GLN
1	B	593	HIS
1	B	614	GLU
1	B	649	THR
1	B	694	ALA
1	B	252	PRO
1	B	525	HIS
1	B	582	VAL
1	B	560	GLY
1	B	587	PRO
1	B	692	ASP
1	B	714	ALA
1	A	337	GLY
1	B	712	ARG
1	B	251	PRO
1	B	710	GLY
1	A	286	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/384 (99%)	345 (91%)	34 (9%)	9	17
1	B	379/384 (99%)	334 (88%)	45 (12%)	5	9
All	All	758/768 (99%)	679 (90%)	79 (10%)	7	12

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	TRP
1	A	238	LEU
1	A	254	GLN
1	A	265	LYS
1	A	283	THR
1	A	287	LEU
1	A	307	LEU
1	A	310	VAL
1	A	326	GLN
1	A	353	GLN
1	A	375	LEU
1	A	387	GLN
1	A	416	LEU
1	A	450	LEU
1	A	453	LEU
1	A	484	LEU
1	A	514	VAL
1	A	527	LEU
1	A	549	GLN
1	A	564	GLN
1	A	583	GLN
1	A	589	LEU
1	A	591	GLN
1	A	611	GLN
1	A	619	LEU
1	A	623	LEU
1	A	644	LYS
1	A	678	ARG
1	A	684	ILE
1	A	690	ARG
1	A	695	LEU
1	A	706	LEU

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Mol	Chain	Res	Type
1	A	715	LEU
1	A	716	ASP
1	B	231	GLN
1	B	238	LEU
1	B	244	VAL
1	B	266	ARG
1	B	287	LEU
1	B	292	GLU
1	B	307	LEU
1	B	353	GLN
1	B	418	VAL
1	B	453	LEU
1	B	489	GLN
1	B	515	GLN
1	B	518	LEU
1	B	527	LEU
1	B	542	LYS
1	B	554	VAL
1	B	557	GLN
1	B	591	GLN
1	B	595	LEU
1	B	623	LEU
1	B	627	HIS
1	B	629	LEU
1	B	635	VAL
1	B	640	HIS
1	B	651	GLN
1	B	652	ARG
1	B	654	LEU
1	B	659	GLN
1	B	663	LEU
1	B	664	THR
1	B	668	VAL
1	B	673	SER
1	B	682	GLU
1	B	683	SER
1	B	684	ILE
1	B	685	VAL
1	B	687	GLN
1	B	689	SER
1	B	690	ARG
1	B	698	LEU

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Mol	Chain	Res	Type
1	B	703	LEU
1	B	706	LEU
1	B	712	ARG
1	B	725	HIS
1	B	726	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	HIS
1	A	321	HIS
1	A	345	GLN
1	A	373	GLN
1	A	423	HIS
1	A	428	GLN
1	A	475	GLN
1	A	489	GLN
1	A	491	HIS
1	A	515	GLN
1	A	559	HIS
1	A	591	GLN
1	A	611	GLN
1	A	617	GLN
1	A	640	HIS
1	A	661	HIS
1	A	700	ASN
1	B	231	GLN
1	B	288	ASN
1	B	305	GLN
1	B	321	HIS
1	B	345	GLN
1	B	355	HIS
1	B	407	GLN
1	B	413	GLN
1	B	457	HIS
1	B	491	HIS
1	B	496	GLN
1	B	509	GLN
1	B	549	GLN
1	B	564	GLN
1	B	633	GLN
1	B	659	GLN

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Mol	Chain	Res	Type
1	B	667	GLN
1	B	687	GLN
1	B	723	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	18,21,22	1.63	3 (16%)	24,30,33	1.65	5 (20%)
2	5CM	C	6	2,3	18,21,22	1.73	2 (11%)	24,30,33	1.28	2 (8%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	5CM	C5-C4	6.38	1.48	1.44
2	I	6	5CM	C5-C4	5.65	1.48	1.44
2	C	6	5CM	C6-C5	2.99	1.39	1.34
2	I	6	5CM	C6-N1	-2.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	5CM	C6-C5	2.25	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	5CM	C5-C4-N3	-4.14	117.51	121.75
2	I	6	5CM	C5A-C5-C6	-3.35	118.31	122.85
2	C	6	5CM	C5A-C5-C6	-3.31	118.38	122.85
2	C	6	5CM	C5A-C5-C4	2.75	125.03	120.51
2	I	6	5CM	C5-C4-N4	2.74	125.25	121.39
2	I	6	5CM	O2-C2-N3	-2.72	118.04	122.33
2	I	6	5CM	O4'-C1'-N1	2.12	111.62	107.86

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 oligosaccharides 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%)	0.16	20 (4%) 42 38	17, 38, 76, 130	0
1	B	497/499 (99%)	0.79	94 (18%) 3 2	17, 41, 136, 282	0
2	C	16/17 (94%)	-0.47	1 (6%) 26 23	20, 28, 73, 155	0
2	I	16/17 (94%)	-0.60	0 100 100	19, 25, 72, 100	0
3	D	17/17 (100%)	-0.10	1 (5%) 28 25	28, 42, 74, 130	0
3	J	17/17 (100%)	0.11	1 (5%) 28 25	27, 41, 82, 145	0
All	All	1060/1066 (99%)	0.43	117 (11%) 10 8	17, 39, 106, 282	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	TRP	7.4
1	B	648	GLU	7.1
1	B	706	LEU	6.1
1	B	634	VAL	6.0
1	B	588	VAL	6.0
1	A	232	TRP	5.9
1	B	704	VAL	5.7
1	B	677	GLY	5.6
1	B	230	MET	5.6
1	B	705	ALA	5.5
1	B	652	ARG	5.3
1	B	715	LEU	5.3
1	B	678	ARG	5.1
1	B	676	GLY	5.1
1	B	695	LEU	5.0
1	B	524	ALA	4.7
1	B	698	LEU	4.7
1	B	726	HIS	4.6
1	B	663	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	707	ALA	4.6
1	B	721	LEU	4.6
1	B	660	ALA	4.5
1	B	675	GLY	4.5
1	A	524	ALA	4.5
1	B	718	VAL	4.5
1	B	697	ALA	4.5
1	B	595	LEU	4.5
1	B	593	HIS	4.3
1	A	526	GLY	4.3
1	B	640	HIS	4.3
1	B	671	ILE	4.2
1	A	692	ASP	4.2
1	B	696	ALA	4.0
1	B	720	LYS	4.0
1	B	703	LEU	4.0
1	B	691	PRO	4.0
1	A	525	HIS	3.9
1	A	693	PRO	3.9
1	A	694	ALA	3.9
1	B	693	PRO	3.9
3	J	-14	DA	3.8
1	B	629	LEU	3.8
1	B	646	ALA	3.8
1	B	234	GLY	3.8
1	B	662	GLY	3.8
1	B	233	SER	3.7
1	B	694	ALA	3.7
1	B	661	HIS	3.7
1	B	723	HIS	3.7
1	B	701	ASP	3.7
1	A	230	MET	3.6
1	B	713	PRO	3.6
1	B	664	THR	3.6
1	B	278	TRP	3.5
1	B	717	ALA	3.5
1	B	638	ALA	3.4
1	B	647	LEU	3.3
1	B	710	GLY	3.3
1	A	235	ALA	3.3
1	B	628	GLY	3.3
1	B	673	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	589	LEU	3.2
1	B	594	GLY	3.2
1	B	231	GLN	3.2
1	B	674	ASN	3.2
1	B	690	ARG	3.2
1	B	650	VAL	3.2
1	B	590	CYS	3.2
1	B	591	GLN	3.1
1	B	699	THR	3.1
2	C	14	DT	3.1
1	A	231	GLN	3.1
1	B	712	ARG	3.1
1	B	643	GLY	3.1
1	B	716	ASP	3.0
1	B	496	GLN	3.0
3	D	-14	DA	3.0
1	B	700	ASN	3.0
1	A	237	ALA	3.0
1	B	525	HIS	3.0
1	B	711	GLY	3.0
1	B	633	GLN	2.9
1	B	725	HIS	2.8
1	B	709	LEU	2.8
1	A	695	LEU	2.8
1	B	722	GLU	2.8
1	B	490	ALA	2.8
1	A	726	HIS	2.8
1	B	702	HIS	2.8
1	B	592	ALA	2.6
1	B	714	ALA	2.6
1	A	724	HIS	2.6
1	B	597	PRO	2.6
1	B	666	GLN	2.5
1	A	520	VAL	2.5
1	A	233	SER	2.5
1	B	596	THR	2.5
1	B	635	VAL	2.5
1	B	668	VAL	2.5
1	B	639	SER	2.4
1	B	586	LEU	2.4
1	B	587	PRO	2.4
1	B	654	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	491	HIS	2.4
1	B	627	HIS	2.3
1	B	692	ASP	2.3
1	B	492	GLY	2.3
1	A	723	HIS	2.3
1	B	670	ALA	2.3
1	B	584	ARG	2.2
1	B	685	VAL	2.2
1	B	644	LYS	2.2
1	A	628	GLY	2.2
1	A	721	LEU	2.1
1	A	234	GLY	2.1
1	B	665	PRO	2.1
1	B	642	GLY	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($\text{\AA}^2$)	Q<0.9
2	5CM	I	6	20/21	0.97	0.06	21,24,27,28	0
2	5CM	C	6	20/21	0.97	0.05	20,22,25,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.