



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:20 PM UTC

PDB ID : 6LEW / pdb_00006lew
Title : RVD HA specifically contacts 5mC through van der Waals interactions
Authors : Liu, L.; Yi, C.
Deposited on : 2019-11-27
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:

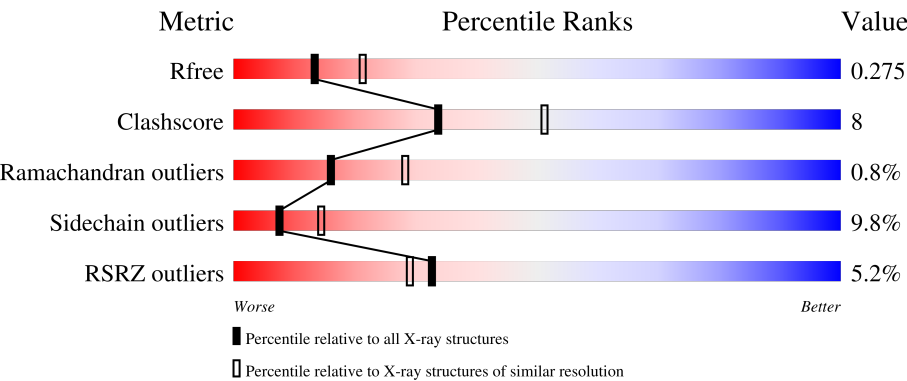
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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.



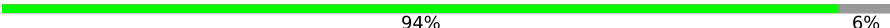
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	2% 79% 14% • 5%
1	B	499	8% 67% 14% • • 14%
2	C	17	76% 18% 6%
2	I	17	6% 71% 24% 6%
3	D	17	88% 6% 6%

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Mol	Chain	Length	Quality of chain
3	J	17	 94%6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7965 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	476	Total	C	N	O	S	0	0	0
			3445	2150	643	641	11			
1	B	427	Total	C	N	O	S	0	0	0
			3081	1932	567	572	10			

- 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	16	Total	C	N	O	P	0	0	0
			317	154	48	100	15			

- Molecule 3 is a DNA chain called DNA (5'-D(P*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	16	Total	C	N	O	P	0	0	0
			337	157	74	90	16			
3	D	16	Total	C	N	O	P	0	0	0
			337	157	74	90	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	I	17	Total	O	0	0
			17	17		
4	B	33	Total	O	0	0
			33	33		

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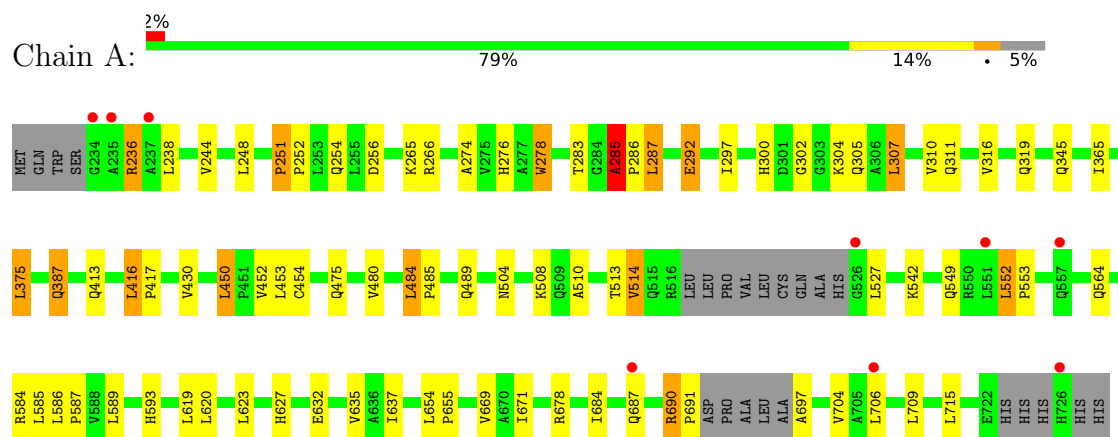
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	13	Total	O	0	0
			13	13		

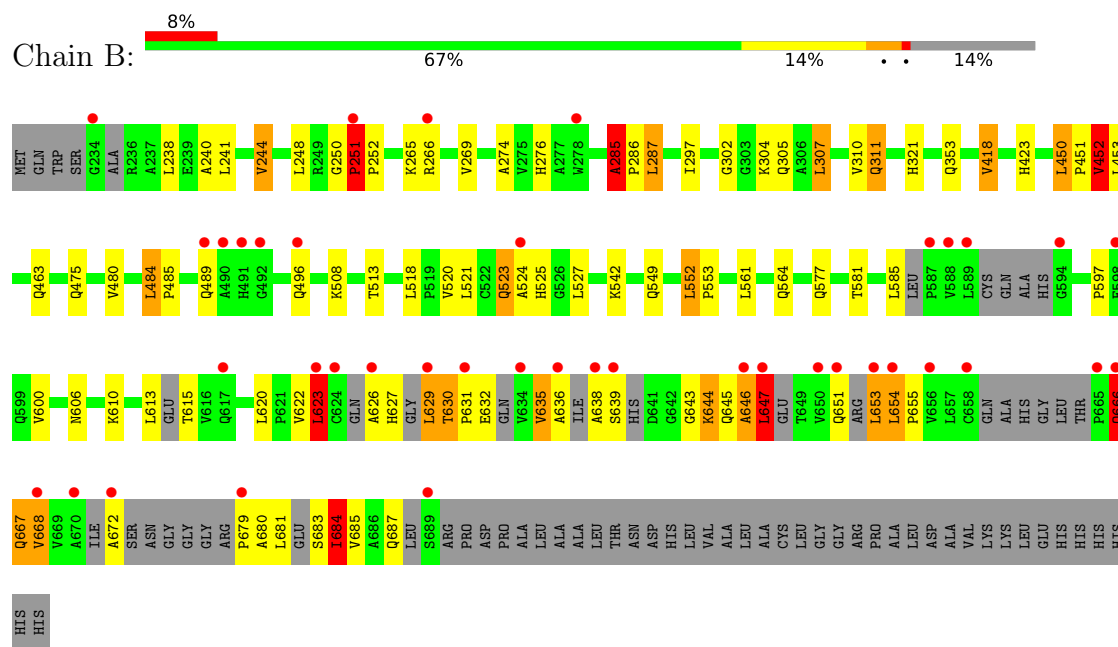
3 Residue-property plots [i](#)

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



• Molecule 1: TAL effector



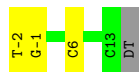
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*T)-3')





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

Chain C: 76% 18% 6%



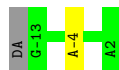
- Molecule 3: DNA (5'-D(P*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain J: 94% 6%



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

Chain D: 88% 6% 6%



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)	86.40 – 2.48 86.40 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.8 (86.40-2.48) 91.8 (86.40-2.48)	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 5.8.0049	Depositor
R, R_{free}	0.231 , 0.279 0.232 , 0.275	Depositor DCC
R_{free} test set	2095 reflections (4.60%)	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)	0.31 , 31.4	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	0.91	EDS
Total number of atoms	7965	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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

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	0.87	0/3490	1.05	8/4760 (0.2%)
1	B	0.90	0/3108	1.09	16/4222 (0.4%)
2	C	0.44	0/328	0.96	0/501
2	I	0.43	0/349	0.95	1/533 (0.2%)
3	D	0.40	0/381	0.73	0/587
3	J	0.40	0/381	0.75	0/587
All	All	0.82	0/8037	1.03	25/11190 (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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	PRO	CA-C-N	11.40	134.09	119.84
1	A	251	PRO	C-N-CA	11.40	134.09	119.84
1	B	250	GLY	CA-C-N	9.75	130.42	120.38
1	B	250	GLY	C-N-CA	9.75	130.42	120.38
1	B	635	VAL	N-CA-C	-9.28	99.73	110.21
1	B	251	PRO	N-CA-C	7.82	120.24	110.70
1	B	666	GLN	N-CA-C	-7.79	97.33	109.25
1	B	285	ALA	CA-C-N	-7.70	111.72	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ALA	C-N-CA	-7.70	111.72	121.04
1	A	285	ALA	CA-C-N	-7.39	112.52	120.94
1	A	285	ALA	C-N-CA	-7.39	112.52	120.94
1	B	418	VAL	CB-CA-C	-7.39	102.03	112.22
2	I	-2	DT	C2'-C3'-O3'	7.18	122.28	111.50
1	A	278	TRP	CA-CB-CG	6.83	126.57	113.60
1	A	251	PRO	C-N-CD	-5.90	100.81	125.00
1	B	452	VAL	CB-CA-C	-5.89	104.19	112.14
1	A	292	GLU	CB-CG-CD	5.81	122.48	112.60
1	B	623	LEU	N-CA-C	-5.78	102.35	110.50
1	A	635	VAL	N-CA-C	5.72	116.46	110.62
1	B	251	PRO	CA-C-N	-5.27	113.25	119.84
1	B	251	PRO	C-N-CA	-5.27	113.25	119.84
1	B	684	ILE	N-CA-C	-5.26	98.39	109.34
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	647	LEU	N-CA-C	-5.16	106.18	113.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Peptide
1	A	251	PRO	Peptide,Mainchain
1	B	630	THR	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	3445	0	3584	42	0
1	B	3081	0	3216	72	0
2	C	317	0	186	1	0
2	I	336	0	195	4	0
3	D	337	0	177	2	0
3	J	337	0	177	0	0
4	A	49	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	33	0	0	5	0
4	C	13	0	0	0	0
4	I	17	0	0	1	0
All	All	7965	0	7535	119	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 8.

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:629:LEU:HB3	1:B:631:PRO:HD3	1.53	0.88
1:B:622:VAL:O	1:B:626:ALA:HB3	1.85	0.76
1:B:647:LEU:CD2	1:B:679:PRO:HD3	2.15	0.75
1:B:597:PRO:O	1:B:600:VAL:HG12	1.88	0.74
1:B:613:LEU:O	1:B:615:THR:N	2.22	0.72
1:B:636:ALA:C	1:B:638:ALA:N	2.48	0.71
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.22	0.70
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.24	0.67
1:A:632:GLU:OE2	4:A:801:HOH:O	2.15	0.64
1:B:645:GLN:HG2	1:B:646:ALA:H	1.64	0.63
1:B:666:GLN:O	1:B:667:GLN:HB2	1.97	0.63
1:A:274:ALA:HB2	1:A:304:LYS:HG3	1.82	0.62
1:A:285:ALA:CB	1:A:286:PRO:CD	2.78	0.62
1:B:463:GLN:HE21	1:B:496:GLN:NE2	1.98	0.62
1:B:452:VAL:HG23	4:B:808:HOH:O	2.01	0.61
1:A:513:THR:OG1	1:A:542:LYS:HG3	2.00	0.61
2:I:-2:DT:H2"	2:I:-1:DG:OP2	2.02	0.60
1:B:513:THR:OG1	1:B:542:LYS:HG3	2.02	0.60
1:A:475:GLN:HB3	1:A:508:LYS:HD2	1.84	0.60
1:B:285:ALA:CB	1:B:286:PRO:CD	2.79	0.59
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.84	0.59
1:A:285:ALA:HB1	1:A:286:PRO:HD3	1.85	0.58
1:B:523:GLN:O	1:B:524:ALA:HB3	2.04	0.58
1:B:285:ALA:HB1	1:B:286:PRO:HD3	1.84	0.58
1:B:645:GLN:CG	1:B:646:ALA:H	2.17	0.58
1:A:365:ILE:HG22	1:A:375:LEU:HD13	1.85	0.57
1:B:631:PRO:C	1:B:632:GLU:OE1	2.47	0.56
1:B:645:GLN:CG	1:B:646:ALA:N	2.69	0.56
1:A:297:ILE:CG2	1:A:307:LEU:HD13	2.35	0.56
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HD13	1:A:454:CYS:SG	2.45	0.55
1:B:552:LEU:HB3	1:B:553:PRO:HD3	1.88	0.55
1:B:620:LEU:O	1:B:623:LEU:O	2.24	0.55
1:B:643:GLY:HA2	4:B:803:HOH:O	2.06	0.54
1:B:475:GLN:HB3	1:B:508:LYS:HD2	1.88	0.54
1:A:287:LEU:HD21	1:A:311:GLN:HA	1.90	0.54
1:B:654:LEU:N	1:B:654:LEU:HD23	2.23	0.53
1:B:666:GLN:O	1:B:667:GLN:CB	2.56	0.53
1:B:240:ALA:CB	1:B:269:VAL:HG23	2.38	0.53
1:A:552:LEU:HB3	1:A:553:PRO:HD3	1.90	0.52
1:A:690:ARG:O	1:A:691:PRO:O	2.28	0.52
1:B:523:GLN:O	1:B:524:ALA:CB	2.57	0.52
1:B:423:HIS:HB3	1:B:450:LEU:CD2	2.40	0.52
1:A:297:ILE:HG22	1:A:307:LEU:HD13	1.93	0.51
1:B:297:ILE:CG2	1:B:307:LEU:HD13	2.41	0.51
1:B:653:LEU:O	1:B:653:LEU:HD23	2.12	0.50
1:B:672:ALA:HB2	1:B:680:ALA:HB2	1.93	0.50
1:B:321:HIS:CD2	4:B:830:HOH:O	2.64	0.50
1:B:647:LEU:HD21	1:B:679:PRO:HD3	1.94	0.49
1:B:265:LYS:HE2	3:D:-4:DA:OP2	2.12	0.49
1:A:584:ARG:O	1:A:585:LEU:HD23	2.13	0.49
1:A:416:LEU:HD13	1:A:416:LEU:O	2.12	0.49
1:B:524:ALA:O	1:B:525:HIS:HB2	2.12	0.49
1:B:287:LEU:HD21	1:B:311:GLN:HA	1.95	0.49
1:B:647:LEU:HD23	1:B:679:PRO:HD3	1.90	0.48
1:A:387:GLN:HG3	4:A:812:HOH:O	2.12	0.48
1:B:653:LEU:HD23	1:B:653:LEU:C	2.37	0.48
1:B:654:LEU:HB2	1:B:655:PRO:HD3	1.95	0.48
1:A:413:GLN:HG3	4:A:808:HOH:O	2.14	0.48
1:B:520:VAL:HG11	1:B:549:GLN:HE21	1.79	0.47
1:A:319:GLN:NE2	4:A:804:HOH:O	2.45	0.47
1:B:631:PRO:HG2	4:B:832:HOH:O	2.14	0.47
1:B:684:ILE:O	1:B:685:VAL:HB	2.14	0.47
1:B:297:ILE:HG22	1:B:307:LEU:HD13	1.96	0.47
1:A:690:ARG:O	1:A:691:PRO:C	2.57	0.47
1:B:635:VAL:HG11	1:B:645:GLN:HB2	1.97	0.47
1:B:552:LEU:C	1:B:552:LEU:HD13	2.40	0.46
1:A:484:LEU:N	1:A:485:PRO:HD2	2.31	0.46
1:B:683:SER:C	1:B:684:ILE:O	2.53	0.46
2:I:13:DC:H2''	2:I:14:DT:O5'	2.16	0.46
1:B:635:VAL:CG1	1:B:645:GLN:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:LEU:HB2	1:B:655:PRO:CD	2.46	0.46
1:A:450:LEU:HD12	1:A:450:LEU:C	2.42	0.45
2:C:-2:DT:H1'	2:C:-1:DG:C8	2.51	0.45
1:A:627:HIS:HB3	1:A:654:LEU:CD2	2.46	0.45
1:A:654:LEU:N	1:A:655:PRO:HD2	2.32	0.45
1:B:484:LEU:N	1:B:485:PRO:HD2	2.32	0.45
1:B:636:ALA:O	1:B:638:ALA:N	2.48	0.45
1:B:644:LYS:O	1:B:647:LEU:HB3	2.17	0.45
1:B:630:THR:HG22	1:B:630:THR:O	2.17	0.45
1:B:681:LEU:O	1:B:683:SER:N	2.50	0.45
1:A:450:LEU:CD1	1:A:454:CYS:SG	3.05	0.44
1:B:606:ASN:HD21	1:B:638:ALA:CB	2.29	0.44
1:A:504:ASN:HB2	4:A:827:HOH:O	2.16	0.44
1:B:635:VAL:HG12	1:B:645:GLN:HB3	1.99	0.44
2:I:13:DC:H2''	2:I:14:DT:C5'	2.48	0.44
1:B:248:LEU:HD21	1:B:276:HIS:HA	1.99	0.44
1:A:256:ASP:OD1	1:A:256:ASP:C	2.61	0.44
1:A:697:ALA:N	4:A:806:HOH:O	2.51	0.44
1:A:510:ALA:O	1:A:514:VAL:HG13	2.18	0.43
1:A:416:LEU:HB3	1:A:417:PRO:HD3	1.99	0.43
1:B:654:LEU:HD23	1:B:654:LEU:H	1.82	0.43
1:B:244:VAL:O	1:B:244:VAL:HG13	2.19	0.43
1:B:244:VAL:HG22	1:B:276:HIS:CD2	2.54	0.43
1:A:416:LEU:CD1	1:A:416:LEU:C	2.92	0.42
1:B:668:VAL:O	4:B:801:HOH:O	2.21	0.42
1:B:684:ILE:HG22	1:B:685:VAL:HG23	2.01	0.42
1:A:416:LEU:HD22	1:A:430:VAL:HG11	2.01	0.42
1:B:251:PRO:O	1:B:252:PRO:C	2.59	0.42
1:B:450:LEU:HB3	1:B:451:PRO:HD3	2.01	0.42
1:B:480:VAL:O	1:B:484:LEU:HB2	2.20	0.42
1:A:480:VAL:O	1:A:484:LEU:HB2	2.20	0.42
1:B:654:LEU:N	1:B:654:LEU:CD2	2.82	0.42
1:A:302:GLY:O	1:A:305:GLN:N	2.53	0.42
1:A:593:HIS:HB3	1:A:620:LEU:HD23	2.02	0.42
1:B:265:LYS:CE	3:D:-4:DA:OP2	2.68	0.41
1:A:248:LEU:HD21	1:A:276:HIS:HA	2.02	0.41
1:A:586:LEU:N	1:A:587:PRO:HD2	2.35	0.41
1:A:637:ILE:HD11	1:A:669:VAL:HG22	2.03	0.41
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.93	0.41
2:I:14:DT:H1'	4:I:106:HOH:O	2.20	0.41
1:B:629:LEU:HD22	1:B:630:THR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:THR:HG22	1:B:585:LEU:HD12	2.03	0.41
1:A:654:LEU:HB3	1:A:655:PRO:HD3	2.02	0.40
1:B:302:GLY:O	1:B:305:GLN:N	2.54	0.40
1:A:416:LEU:HD13	1:A:416:LEU:C	2.47	0.40
1:B:629:LEU:HB3	1:B:631:PRO:CD	2.38	0.40
1:A:671:ILE:HD11	1:A:704:VAL:HG22	2.03	0.40
1:B:577:GLN:HB3	1:B:610:LYS:HD3	2.02	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	469/499 (94%)	450 (96%)	16 (3%)	3 (1%)	21	35
1	B	396/499 (79%)	372 (94%)	20 (5%)	4 (1%)	12	22
All	All	865/998 (87%)	822 (95%)	36 (4%)	7 (1%)	16	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	PRO
1	A	285	ALA
1	B	285	ALA
1	B	667	GLN
1	A	236	ARG
1	B	646	ALA
1	B	251	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	363/384 (94%)	328 (90%)	35 (10%)	8	15
1	B	328/384 (85%)	295 (90%)	33 (10%)	7	13
All	All	691/768 (90%)	623 (90%)	68 (10%)	7	14

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LEU
1	A	244	VAL
1	A	254	GLN
1	A	265	LYS
1	A	278	TRP
1	A	283	THR
1	A	287	LEU
1	A	292	GLU
1	A	307	LEU
1	A	310	VAL
1	A	316	VAL
1	A	345	GLN
1	A	375	LEU
1	A	387	GLN
1	A	416	LEU
1	A	450	LEU
1	A	452	VAL
1	A	453	LEU
1	A	484	LEU
1	A	489	GLN
1	A	514	VAL
1	A	527	LEU
1	A	549	GLN
1	A	552	LEU
1	A	564	GLN
1	A	589	LEU
1	A	619	LEU

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Mol	Chain	Res	Type
1	A	623	LEU
1	A	678	ARG
1	A	684	ILE
1	A	687	GLN
1	A	690	ARG
1	A	706	LEU
1	A	709	LEU
1	A	715	LEU
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	310	VAL
1	B	311	GLN
1	B	353	GLN
1	B	418	VAL
1	B	450	LEU
1	B	452	VAL
1	B	453	LEU
1	B	484	LEU
1	B	489	GLN
1	B	518	LEU
1	B	523	GLN
1	B	527	LEU
1	B	552	LEU
1	B	561	LEU
1	B	564	GLN
1	B	623	LEU
1	B	627	HIS
1	B	629	LEU
1	B	639	SER
1	B	647	LEU
1	B	651	GLN
1	B	653	LEU
1	B	654	LEU
1	B	666	GLN
1	B	668	VAL
1	B	684	ILE
1	B	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	276	HIS
1	A	319	GLN
1	A	353	GLN
1	A	407	GLN
1	A	457	HIS
1	A	481	GLN
1	A	491	HIS
1	A	549	GLN
1	A	593	HIS
1	A	640	HIS
1	B	321	HIS
1	B	355	HIS
1	B	407	GLN
1	B	423	HIS
1	B	457	HIS
1	B	481	GLN
1	B	491	HIS
1	B	496	GLN
1	B	549	GLN
1	B	564	GLN
1	B	599	GLN
1	B	606	ASN
1	B	651	GLN

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	C	6	2,3	18,21,22	2.36	2 (11%)	24,30,33	1.80	4 (16%)
2	5CM	I	6	2,3	18,21,22	1.28	2 (11%)	24,30,33	1.66	4 (16%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	5CM	C5-C4	9.35	1.51	1.44
2	I	6	5CM	C5-C4	3.62	1.46	1.44
2	I	6	5CM	C6-N1	-3.22	1.32	1.38
2	C	6	5CM	C6-C5	2.26	1.38	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	C5A-C5-C6	-5.16	115.87	122.85
2	I	6	5CM	C5-C4-N3	-4.35	117.30	121.75
2	C	6	5CM	C5A-C5-C4	4.20	127.41	120.51
2	I	6	5CM	C5A-C5-C6	-3.92	117.54	122.85
2	C	6	5CM	C5-C6-N1	-3.29	119.74	123.31
2	I	6	5CM	C5-C4-N4	2.85	125.41	121.39
2	I	6	5CM	O2-C2-N3	-2.44	118.48	122.33
2	C	6	5CM	O2-C2-N3	-2.21	118.85	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 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	476/499 (95%)	0.24	9 (1%) 66 63	19, 38, 63, 88	0
1	B	427/499 (85%)	0.56	40 (9%) 14 12	20, 39, 70, 80	0
2	C	15/17 (88%)	-0.48	0 100 100	22, 31, 52, 70	0
2	I	16/17 (94%)	-0.45	1 (6%) 26 23	21, 27, 74, 94	0
3	D	16/17 (94%)	-0.06	0 100 100	31, 44, 66, 71	0
3	J	16/17 (94%)	0.07	0 100 100	27, 40, 66, 71	0
All	All	966/1066 (90%)	0.35	50 (5%) 33 29	19, 38, 67, 94	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	7.4
1	B	634	VAL	5.9
1	B	638	ALA	4.9
1	B	672	ALA	4.6
1	B	689	SER	4.5
1	B	278	TRP	4.5
1	B	491	HIS	4.2
1	B	629	LEU	4.2
1	B	646	ALA	4.2
1	B	665	PRO	4.0
1	B	647	LEU	3.9
1	B	658	CYS	3.5
1	B	589	LEU	3.5
1	A	687	GLN	3.4
1	B	670	ALA	3.4
1	B	492	GLY	3.2
1	B	636	ALA	3.0
1	B	594	GLY	3.0
1	B	624	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	666	GLN	3.0
1	A	235	ALA	2.9
1	B	668	VAL	2.9
1	A	237	ALA	2.9
1	A	726	HIS	2.8
1	B	489	GLN	2.8
1	A	234	GLY	2.7
1	B	251	PRO	2.7
1	B	496	GLN	2.7
1	B	490	ALA	2.6
1	B	631	PRO	2.5
1	B	524	ALA	2.5
1	A	526	GLY	2.3
1	B	588	VAL	2.3
1	B	266	ARG	2.3
1	B	598	GLU	2.3
1	B	679	PRO	2.3
1	A	551	LEU	2.3
1	B	651	GLN	2.2
1	B	626	ALA	2.2
1	B	639	SER	2.2
1	B	587	PRO	2.2
1	A	557	GLN	2.2
1	B	623	LEU	2.1
1	B	654	LEU	2.1
1	B	653	LEU	2.1
1	B	650	VAL	2.1
1	B	617	GLN	2.0
1	B	656	VAL	2.0
2	I	14	DT	2.0
1	A	706	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5CM	C	6	20/21	0.96	0.07	23,24,25,25	0
2	5CM	I	6	20/21	0.97	0.06	22,25,29,30	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.