



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:32 AM UTC

PDB ID : 6JW5 / pdb_00006jw5
Title : RVD Q* recognizes 5hmC through water-mediated H bonds
Authors : Liu, L.; Yi, C.
Deposited on : 2019-04-18
Resolution : 2.99 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

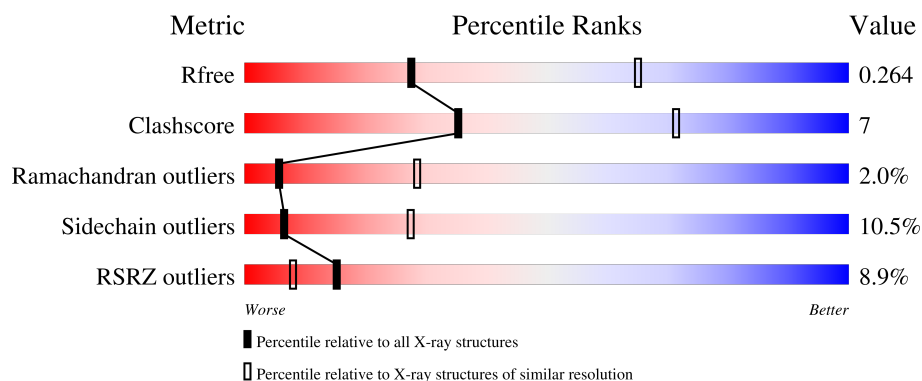
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	498	6% 78% 17% • •
1	B	498	7% 77% 17% • •
1	E	498	10% 81% 14% • •
1	H	498	12% 80% 16% • •
2	C	17	6% 53% 41% 6%

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Mol	Chain	Length	Quality of chain
2	F	17	
2	I	17	
2	K	17	
3	D	17	
3	G	17	
3	J	17	
3	L	17	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17094 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TAL effector.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			
1	B	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			
1	E	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			
1	H	493	Total	C	N	O	S	0	0	0
			3580	2237	667	664	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	C	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	F	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	K	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	D	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	G	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	17	Total 355	C 167	N 79	O 93	P 16	0	0	0

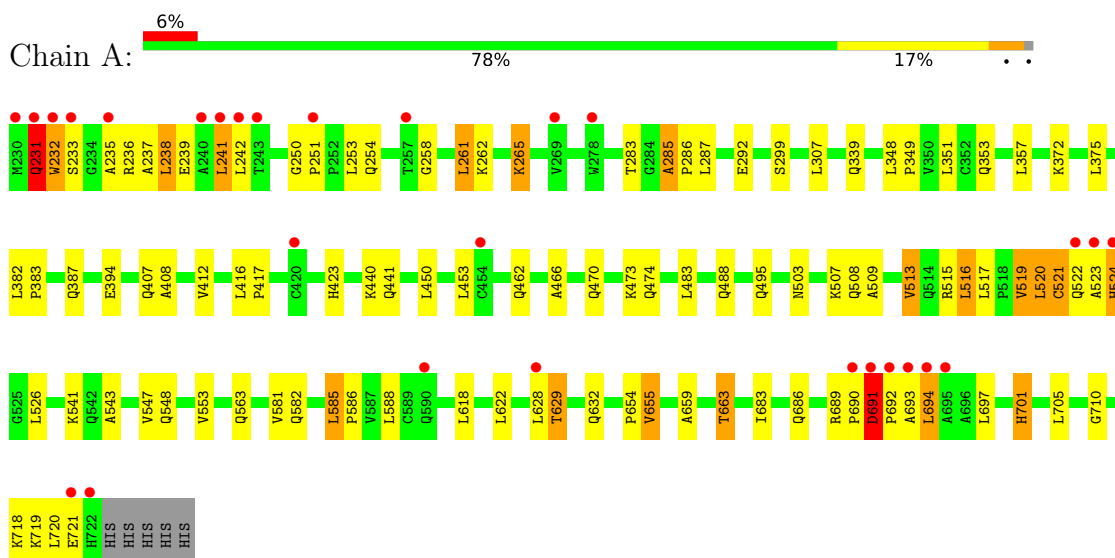
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	I	1	Total 1	O 1	0	0
4	C	1	Total 1	O 1	0	0
4	H	1	Total 1	O 1	0	0

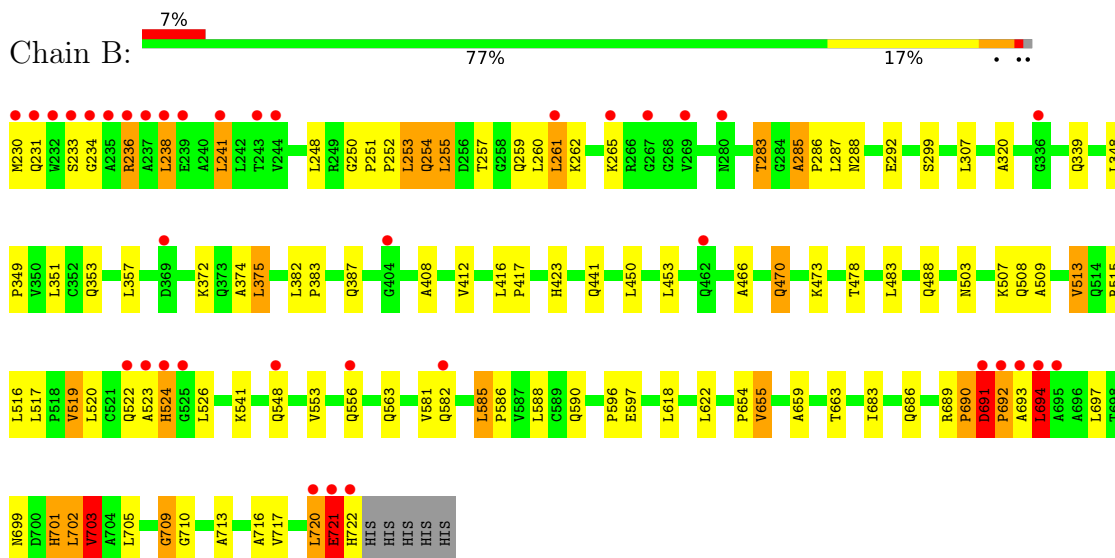
3 Residue-property plots

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.

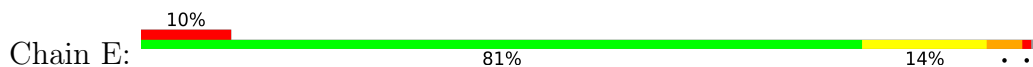
• Molecule 1: TAL effector

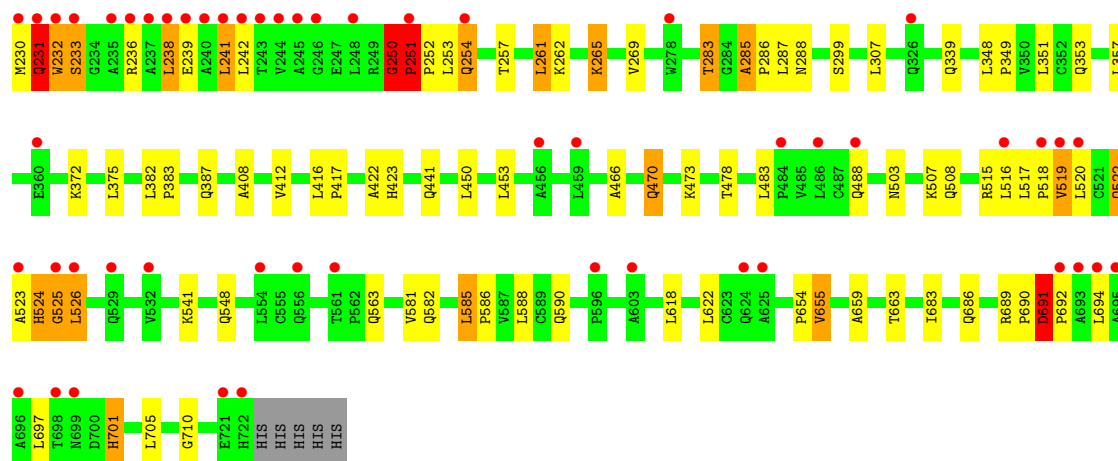


• Molecule 1: TAL effector

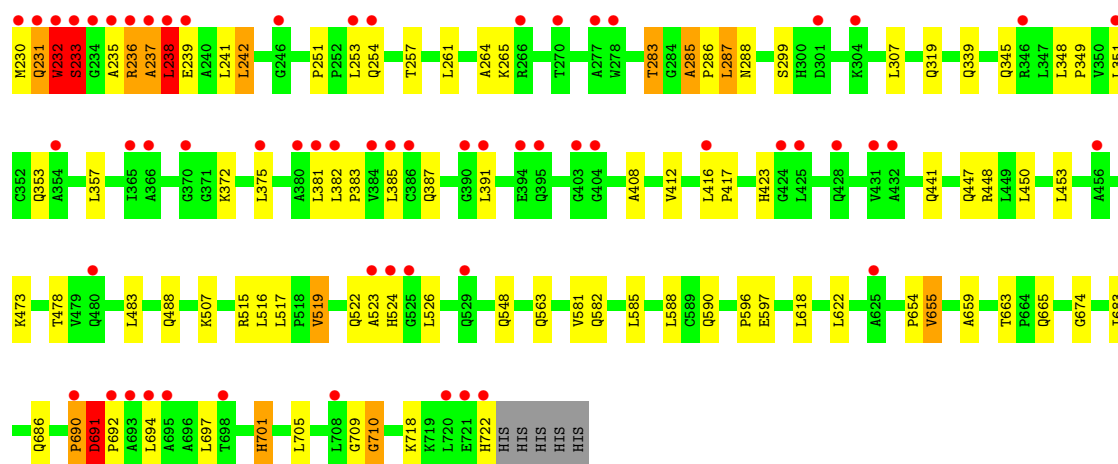
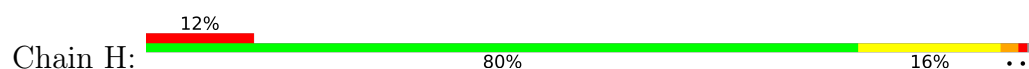


• Molecule 1: TAL effector

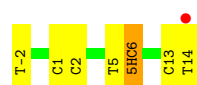




• Molecule 1: TAL effector



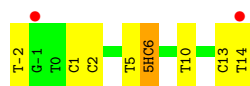
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



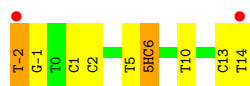
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



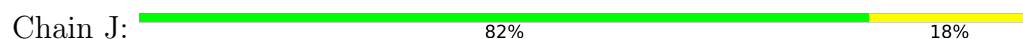
- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



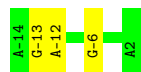
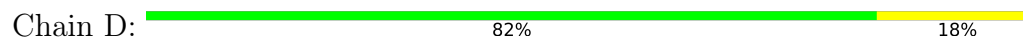
- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



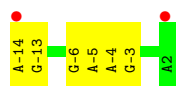
- Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')



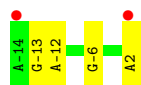
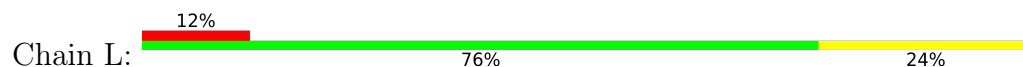
- Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')



- 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	94.42Å 93.78Å 168.16Å 90.00° 102.73° 90.00°	Depositor
Resolution (Å)	164.03 – 2.99 164.03 – 2.99	Depositor EDS
% Data completeness (in resolution range)	84.3 (164.03-2.99) 84.4 (164.03-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.244 , 0.267 0.240 , 0.264	Depositor DCC
R_{free} test set	2485 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.4	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	0.89	EDS
Total number of atoms	17094	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% 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: 5HC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	0/3632	0.99	12/4961 (0.2%)
1	B	0.82	3/3632 (0.1%)	1.01	14/4961 (0.3%)
1	E	0.77	4/3632 (0.1%)	0.96	6/4961 (0.1%)
1	H	0.73	1/3632 (0.0%)	0.96	7/4961 (0.1%)
2	C	0.56	0/349	0.90	0/533
2	F	0.61	1/349 (0.3%)	0.89	0/533
2	I	0.59	0/349	0.90	0/533
2	K	0.59	1/349 (0.3%)	0.91	1/533 (0.2%)
3	D	0.44	0/402	0.74	1/620 (0.2%)
3	G	0.48	0/402	0.83	1/620 (0.2%)
3	J	0.45	0/402	0.78	0/620
3	L	0.43	0/402	0.82	1/620 (0.2%)
All	All	0.74	10/17532 (0.1%)	0.96	43/24456 (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	B	0	1
1	E	0	3
1	H	0	1
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	251	PRO	CA-C	6.55	1.58	1.52
1	E	232	TRP	N-CA	5.97	1.53	1.45
1	E	232	TRP	CA-C	5.77	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	709	GLY	C-O	-5.77	1.16	1.23
1	E	231	GLN	CA-C	5.70	1.60	1.52
1	B	234	GLY	N-CA	5.41	1.50	1.45
2	K	10	DT	O3'-P	-5.30	1.53	1.61
1	B	694	LEU	CA-C	5.22	1.59	1.52
1	H	233	SER	N-CA	5.21	1.52	1.46
2	F	10	DT	O3'-P	-5.14	1.53	1.61

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	251	PRO	N-CA-C	10.64	123.69	110.70
1	H	251	PRO	CA-C-N	-10.61	107.28	118.85
1	H	251	PRO	C-N-CA	-10.61	107.28	118.85
1	H	251	PRO	N-CA-C	10.09	123.01	110.70
1	B	703	VAL	N-CA-CB	9.24	126.48	111.23
1	A	251	PRO	N-CA-C	8.83	121.47	110.70
1	B	251	PRO	N-CA-C	8.69	121.30	110.70
1	E	522	GLN	N-CA-C	-8.60	97.03	110.36
1	A	251	PRO	CA-C-N	-8.34	109.79	119.05
1	A	251	PRO	C-N-CA	-8.34	109.79	119.05
1	A	520	LEU	N-CA-C	-8.18	98.38	110.48
1	A	232	TRP	N-CA-C	7.99	121.51	110.24
1	B	691	ASP	CA-C-N	-7.69	110.22	119.84
1	B	691	ASP	C-N-CA	-7.69	110.22	119.84
1	B	703	VAL	N-CA-C	-7.65	93.42	109.34
1	B	250	GLY	CA-C-N	7.16	127.76	120.38
1	B	250	GLY	C-N-CA	7.16	127.76	120.38
1	B	694	LEU	N-CA-C	7.07	121.04	109.24
1	H	232	TRP	N-CA-C	6.96	119.85	107.80
1	B	251	PRO	CA-C-N	-6.89	111.23	119.84
1	B	251	PRO	C-N-CA	-6.89	111.23	119.84
1	A	231	GLN	CA-C-N	6.64	130.26	120.90
1	A	231	GLN	C-N-CA	6.64	130.26	120.90
1	E	250	GLY	CA-C-N	6.22	126.79	120.38
1	E	250	GLY	C-N-CA	6.22	126.79	120.38
1	E	253	LEU	N-CA-C	5.86	121.31	114.04
1	B	253	LEU	CB-CA-C	-5.81	103.80	111.82
1	A	231	GLN	CB-CA-C	5.80	121.95	110.42
3	G	-6	DG	C4'-C3'-O3'	-5.60	101.60	110.00
1	A	250	GLY	CA-C-N	5.56	126.10	120.38
1	A	250	GLY	C-N-CA	5.56	126.10	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	TRP	N-CA-C	5.50	117.75	109.23
1	H	253	LEU	N-CA-C	5.50	120.85	114.04
2	K	-2	DT	C2'-C3'-O3'	5.34	119.52	111.50
1	A	253	LEU	N-CA-C	5.29	120.60	114.04
1	H	242	LEU	N-CA-C	-5.26	105.61	112.23
3	L	-6	DG	C4'-C3'-O3'	-5.22	102.17	110.00
1	B	694	LEU	CA-CB-CG	5.15	134.33	116.30
1	B	702	LEU	N-CA-C	-5.09	99.95	110.80
1	A	524	HIS	N-CA-C	-5.08	99.98	110.80
3	D	-6	DG	C4'-C3'-O3'	-5.03	102.45	110.00
1	H	674	GLY	N-CA-C	-5.03	106.80	112.33
1	B	721	GLU	N-CA-C	5.01	115.91	108.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	MET	Peptide
1	E	250	GLY	Peptide
1	E	251	PRO	Peptide
1	E	525	GLY	Peptide
1	H	232	TRP	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	3580	0	3725	59	10
1	B	3580	0	3725	66	6
1	E	3580	0	3725	50	17
1	H	3580	0	3725	39	5
2	C	337	0	195	4	1
2	F	337	0	195	6	0
2	I	337	0	195	6	0
2	K	337	0	195	17	0
3	D	355	0	189	1	0
3	G	355	0	189	5	10

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	355	0	189	1	8
3	L	355	0	189	7	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
All	All	17094	0	16436	246	33

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 (246) 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:-2:DT:O4	3:L:2:DA:N1	1.70	1.23
2:K:-2:DT:O4	3:L:2:DA:C6	1.95	1.17
2:K:-2:DT:C4	3:L:2:DA:N1	2.17	1.13
2:K:13:DC:H2''	2:K:14:DT:H5'	1.46	0.97
1:A:258:GLY:O	1:A:261:LEU:HD12	1.63	0.97
1:A:233:SER:OG	2:I:-2:DT:O5'	1.60	0.92
1:B:255:LEU:HD23	1:B:259:GLN:HB2	1.55	0.86
1:A:629:THR:HG22	1:A:632:GLN:OE1	1.77	0.84
1:A:238:LEU:HA	1:A:241:LEU:HD23	1.60	0.84
2:K:13:DC:C2'	2:K:14:DT:H5'	2.07	0.83
1:B:255:LEU:CD2	1:B:259:GLN:HB2	2.10	0.82
1:A:285:ALA:HB1	1:A:286:PRO:HD2	1.63	0.80
1:E:285:ALA:HB1	1:E:286:PRO:HD2	1.65	0.79
1:E:231:GLN:O	1:E:232:TRP:HD1	1.66	0.78
1:H:285:ALA:HB1	1:H:286:PRO:HD2	1.64	0.78
1:E:518:PRO:O	1:E:522:GLN:CB	2.31	0.77
1:B:285:ALA:HB1	1:B:286:PRO:HD2	1.67	0.77
1:B:702:LEU:O	1:B:703:VAL:HG23	1.86	0.75
1:A:692:PRO:HD2	1:A:718:LYS:HE3	1.68	0.74
1:B:692:PRO:O	1:B:722:HIS:CD2	2.40	0.74
1:B:691:ASP:C	1:B:693:ALA:H	1.94	0.74
1:E:231:GLN:O	1:E:232:TRP:CD1	2.41	0.73
1:E:525:GLY:CA	1:E:526:LEU:HD13	2.18	0.73
1:H:236:ARG:O	1:H:237:ALA:O	2.06	0.72
1:B:691:ASP:HB3	1:B:692:PRO:CD	2.20	0.71
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.20	0.71
1:E:285:ALA:HB1	1:E:286:PRO:CD	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:NE	1:B:236:ARG:HA	2.05	0.71
1:A:520:LEU:O	1:A:521:CYS:CB	2.38	0.70
1:H:285:ALA:HB1	1:H:286:PRO:CD	2.21	0.70
1:A:233:SER:CB	2:I:-2:DT:O5'	2.38	0.70
1:E:518:PRO:O	1:E:522:GLN:HB3	1.91	0.70
1:A:258:GLY:O	1:A:261:LEU:CD1	2.41	0.69
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.23	0.69
1:B:692:PRO:O	1:B:722:HIS:CG	2.47	0.67
1:B:694:LEU:HD13	1:B:722:HIS:CE1	2.29	0.67
3:L:-13:DG:H5'	3:L:-13:DG:C8	2.30	0.66
1:A:233:SER:HG	2:I:-2:DT:HO5'	0.89	0.66
2:K:13:DC:C5	2:K:14:DT:C5	2.84	0.66
1:A:520:LEU:O	1:A:521:CYS:HB2	1.95	0.66
1:B:694:LEU:H	1:B:722:HIS:CE1	2.14	0.65
1:B:716:ALA:O	1:B:720:LEU:HG	1.98	0.64
1:E:238:LEU:HD22	1:E:242:LEU:HG	1.80	0.64
1:B:721:GLU:HG2	1:B:722:HIS:N	2.14	0.63
1:A:235:ALA:O	1:A:236:ARG:HB2	1.99	0.63
1:B:691:ASP:C	1:B:693:ALA:N	2.57	0.62
1:A:663:THR:HG21	1:B:320:ALA:HB1	1.83	0.61
1:E:520:LEU:O	1:E:524:HIS:O	2.20	0.60
1:B:255:LEU:CD2	1:B:259:GLN:CB	2.79	0.59
1:A:509:ALA:O	1:A:513:VAL:HG13	2.03	0.59
2:K:-2:DT:C4	3:L:2:DA:C2	2.89	0.59
1:B:509:ALA:O	1:B:513:VAL:HG13	2.03	0.58
1:A:691:ASP:HB3	1:A:692:PRO:HD2	1.86	0.58
1:B:691:ASP:HB3	1:B:692:PRO:HD2	1.84	0.58
1:E:262:LYS:HE3	3:G:-5:DA:OP1	2.03	0.58
2:K:13:DC:C1'	2:K:14:DT:H5'	2.33	0.57
1:B:694:LEU:HD13	1:B:722:HIS:HE1	1.69	0.57
2:K:13:DC:H1'	2:K:14:DT:H5'	1.86	0.57
1:E:238:LEU:HD23	1:E:241:LEU:HD23	1.87	0.56
1:E:518:PRO:O	1:E:522:GLN:HB2	2.05	0.56
1:A:238:LEU:HD22	1:A:242:LEU:HG	1.87	0.56
1:E:691:ASP:HB3	1:E:692:PRO:HD2	1.87	0.56
2:K:-2:DT:O2	2:K:-1:DG:O4'	2.24	0.56
1:B:701:HIS:CE1	1:E:701:HIS:CE1	2.95	0.55
1:B:339:GLN:HB3	1:B:372:LYS:HD3	1.87	0.55
1:H:238:LEU:CD2	1:H:242:LEU:HG	2.36	0.55
1:A:407:GLN:HB3	1:A:440:LYS:HD3	1.87	0.55
1:H:339:GLN:HB3	1:H:372:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LYS:O	1:A:720:LEU:N	2.41	0.54
1:E:339:GLN:HB3	1:E:372:LYS:HD3	1.89	0.54
1:A:231:GLN:O	1:A:231:GLN:HG2	2.07	0.54
1:A:339:GLN:HB3	1:A:372:LYS:HD3	1.88	0.54
1:H:382:LEU:N	1:H:383:PRO:HD2	2.23	0.54
1:A:261:LEU:HD13	1:A:262:LYS:N	2.23	0.54
1:A:517:LEU:O	1:A:520:LEU:O	2.25	0.54
1:A:382:LEU:N	1:A:383:PRO:HD2	2.23	0.53
1:A:522:GLN:O	1:A:523:ALA:HB3	2.08	0.53
1:E:519:VAL:O	1:E:523:ALA:HB3	2.08	0.53
1:H:236:ARG:O	1:H:237:ALA:C	2.51	0.53
1:H:522:GLN:O	1:H:523:ALA:HB3	2.08	0.53
1:A:694:LEU:HD13	1:A:694:LEU:O	2.09	0.53
1:E:422:ALA:HB2	1:H:319:GLN:HB3	1.90	0.53
1:B:522:GLN:O	1:B:523:ALA:HB3	2.09	0.53
2:K:13:DC:H5	2:K:14:DT:C5	2.27	0.53
1:A:474:GLN:HB3	1:A:507:LYS:HD2	1.90	0.53
1:B:699:ASN:O	1:B:702:LEU:O	2.27	0.52
1:E:525:GLY:C	1:E:526:LEU:HD13	2.35	0.52
2:K:13:DC:HI'	2:K:14:DT:C5'	2.38	0.52
1:A:718:LYS:C	1:A:720:LEU:H	2.17	0.52
1:A:261:LEU:CD2	1:A:265:LYS:HD3	2.40	0.52
1:H:691:ASP:HB3	1:H:692:PRO:HD2	1.91	0.52
1:E:518:PRO:O	1:E:522:GLN:N	2.41	0.52
1:B:694:LEU:H	1:B:722:HIS:HE1	1.56	0.51
1:A:441:GLN:HB3	1:A:473:LYS:HD2	1.93	0.51
1:B:382:LEU:N	1:B:383:PRO:HD2	2.26	0.51
1:B:441:GLN:HB3	1:B:473:LYS:HD2	1.93	0.50
1:H:441:GLN:HB3	1:H:473:LYS:HD2	1.93	0.50
1:B:709:GLY:O	1:B:713:ALA:HB3	2.11	0.50
1:E:516:LEU:HA	1:E:519:VAL:CG1	2.42	0.50
1:A:232:TRP:H	1:A:232:TRP:CD1	2.28	0.50
1:H:285:ALA:CB	1:H:286:PRO:CD	2.90	0.50
1:A:285:ALA:CB	1:A:286:PRO:CD	2.90	0.49
1:B:416:LEU:N	1:B:417:PRO:CD	2.75	0.49
1:B:236:ARG:NE	1:B:236:ARG:CA	2.75	0.49
1:A:394:GLU:OE1	1:A:394:GLU:N	2.44	0.49
1:B:255:LEU:HD21	1:B:259:GLN:CB	2.41	0.49
1:B:515:ARG:O	1:B:517:LEU:N	2.43	0.49
1:H:516:LEU:HA	1:H:519:VAL:CG1	2.43	0.49
1:H:237:ALA:O	1:H:239:GLU:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:HIS:HB3	1:A:450:LEU:HD23	1.94	0.49
1:B:238:LEU:O	1:B:241:LEU:HB3	2.13	0.49
1:E:285:ALA:CB	1:E:286:PRO:CD	2.90	0.49
1:E:382:LEU:N	1:E:383:PRO:HD2	2.27	0.49
1:E:515:ARG:HB3	1:E:516:LEU:HD12	1.94	0.49
1:B:423:HIS:HB3	1:B:450:LEU:HD23	1.95	0.48
1:E:441:GLN:HB3	1:E:473:LYS:HD2	1.93	0.48
1:B:236:ARG:HA	1:B:236:ARG:HE	1.78	0.48
1:B:515:ARG:NH2	1:B:516:LEU:CD1	2.76	0.48
1:E:515:ARG:O	1:E:517:LEU:N	2.45	0.48
1:B:285:ALA:CB	1:B:286:PRO:CD	2.92	0.48
1:A:515:ARG:O	1:A:517:LEU:N	2.43	0.48
1:A:516:LEU:HA	1:A:519:VAL:CG1	2.43	0.48
1:B:255:LEU:HD21	1:B:259:GLN:HB3	1.95	0.48
1:E:423:HIS:HB3	1:E:450:LEU:HD23	1.95	0.48
1:E:265:LYS:NZ	3:G:-4:DA:OP2	2.33	0.48
2:K:-2:DT:H71	3:L:2:DA:H61	1.77	0.48
1:B:516:LEU:HA	1:B:519:VAL:CG1	2.44	0.48
1:B:716:ALA:O	1:B:720:LEU:CG	2.62	0.48
1:E:233:SER:HB2	2:F:-2:DT:O5'	2.14	0.47
1:A:416:LEU:N	1:A:417:PRO:CD	2.78	0.47
1:A:285:ALA:CB	1:A:286:PRO:HD2	2.40	0.47
1:B:702:LEU:O	1:B:703:VAL:CG2	2.61	0.47
1:E:525:GLY:HA3	1:E:526:LEU:HD13	1.95	0.47
3:L:-13:DG:H2''	3:L:-12:DA:OP2	2.15	0.47
2:I:1:DC:H2''	2:I:2:DC:O5'	2.15	0.46
1:B:248:LEU:O	1:B:253:LEU:O	2.33	0.46
1:B:348:LEU:N	1:B:349:PRO:CD	2.78	0.46
3:G:-14:DA:N7	3:G:-13:DG:N1	2.64	0.46
1:H:232:TRP:CE3	1:H:233:SER:HA	2.50	0.46
1:H:348:LEU:N	1:H:349:PRO:CD	2.79	0.46
1:A:470:GLN:HB2	1:A:503:ASN:N	2.31	0.46
1:H:381:LEU:HB3	1:H:385:LEU:HD12	1.98	0.46
1:B:285:ALA:CB	1:B:286:PRO:HD2	2.43	0.46
1:H:718:LYS:HB3	1:H:722:HIS:CE1	2.51	0.46
1:A:520:LEU:O	1:A:521:CYS:SG	2.74	0.46
2:K:1:DC:H2''	2:K:2:DC:O5'	2.16	0.46
1:B:697:LEU:HD23	1:B:701:HIS:CD2	2.51	0.46
1:A:348:LEU:N	1:A:349:PRO:CD	2.79	0.46
2:I:5:DT:H2''	2:I:6:5HC:O5'	2.17	0.45
1:A:232:TRP:H	1:A:232:TRP:HD1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:-2:DT:H1'	2:K:-1:DG:O5'	2.15	0.45
1:H:351:LEU:HB3	1:H:357:LEU:HD12	1.98	0.45
2:K:5:DT:H2''	2:K:6:5HC:O5'	2.16	0.45
1:E:470:GLN:HB2	1:E:503:ASN:N	2.32	0.45
1:B:238:LEU:CD2	1:B:241:LEU:HD22	2.46	0.45
1:E:526:LEU:HD13	1:E:526:LEU:N	2.31	0.45
1:H:423:HIS:HB3	1:H:450:LEU:HD23	1.98	0.45
1:B:520:LEU:C	1:B:522:GLN:H	2.25	0.45
1:H:230:MET:O	1:H:231:GLN:HG3	2.17	0.45
1:H:385:LEU:HD23	1:H:391:LEU:HD12	1.98	0.45
1:B:690:PRO:O	1:B:691:ASP:O	2.34	0.45
1:E:691:ASP:HB3	1:E:692:PRO:CD	2.47	0.45
2:F:5:DT:H2''	2:F:6:5HC:O5'	2.17	0.45
2:C:1:DC:H2''	2:C:2:DC:O5'	2.17	0.44
1:B:508:GLN:HB3	1:B:541:LYS:HD3	2.00	0.44
1:B:697:LEU:HD23	1:B:701:HIS:HD2	1.83	0.44
2:F:1:DC:H2''	2:F:2:DC:O5'	2.17	0.44
1:E:348:LEU:N	1:E:349:PRO:CD	2.81	0.44
1:A:581:VAL:O	1:A:582:GLN:C	2.59	0.44
1:A:655:VAL:O	1:A:659:ALA:HB3	2.18	0.44
1:H:416:LEU:N	1:H:417:PRO:CD	2.80	0.44
1:A:237:ALA:O	1:A:238:LEU:C	2.61	0.43
1:A:720:LEU:O	1:A:721:GLU:HG3	2.18	0.43
1:A:232:TRP:CD1	1:A:232:TRP:N	2.87	0.43
1:A:408:ALA:O	1:A:412:VAL:HG23	2.18	0.43
1:B:408:ALA:O	1:B:412:VAL:HG23	2.18	0.43
2:C:5:DT:H2''	2:C:6:5HC:O5'	2.18	0.43
1:E:416:LEU:N	1:E:417:PRO:CD	2.82	0.43
1:A:261:LEU:HD22	1:A:265:LYS:HD3	2.00	0.43
1:B:238:LEU:HD23	1:B:241:LEU:HD22	1.99	0.43
1:B:466:ALA:O	1:B:470:GLN:HG2	2.17	0.43
1:B:351:LEU:HB3	1:B:357:LEU:HD12	2.00	0.43
1:B:478:THR:OG1	1:B:507:LYS:HG3	2.19	0.43
2:C:13:DC:C5	2:C:14:DT:C4	3.07	0.43
1:A:697:LEU:HD23	1:A:701:HIS:CD2	2.54	0.43
1:E:508:GLN:HB3	1:E:541:LYS:HD3	2.01	0.43
1:B:470:GLN:HB2	1:B:503:ASN:N	2.34	0.43
2:C:-2:DT:H2''	2:C:-1:DG:OP2	2.18	0.43
1:E:241:LEU:HD11	1:E:269:VAL:HB	2.01	0.43
1:A:466:ALA:O	1:A:470:GLN:HG2	2.18	0.43
1:B:515:ARG:NH2	1:B:516:LEU:HD11	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:THR:OG1	1:E:507:LYS:HG3	2.19	0.43
2:F:14:DT:C4	3:G:-14:DA:N6	2.87	0.43
1:H:655:VAL:O	1:H:659:ALA:HB3	2.19	0.43
1:B:655:VAL:O	1:B:659:ALA:HB3	2.19	0.43
1:E:351:LEU:HB3	1:E:357:LEU:HD12	2.00	0.43
1:E:466:ALA:O	1:E:470:GLN:HG2	2.19	0.43
1:E:581:VAL:O	1:E:582:GLN:C	2.60	0.43
1:E:655:VAL:O	1:E:659:ALA:HB3	2.19	0.43
1:E:697:LEU:HD23	1:E:701:HIS:CD2	2.54	0.43
1:A:629:THR:CG2	1:A:632:GLN:OE1	2.57	0.42
1:H:478:THR:OG1	1:H:507:LYS:HG3	2.19	0.42
2:F:13:DC:H1'	2:F:14:DT:O4'	2.19	0.42
1:H:408:ALA:O	1:H:412:VAL:HG23	2.19	0.42
1:H:447:GLN:OE1	1:H:448:ARG:N	2.52	0.42
3:D:-13:DG:H2''	3:D:-12:DA:OP2	2.18	0.42
1:H:515:ARG:O	1:H:517:LEU:N	2.47	0.42
1:H:581:VAL:O	1:H:582:GLN:C	2.59	0.42
1:H:691:ASP:HB3	1:H:692:PRO:CD	2.49	0.42
1:H:692:PRO:HG2	1:H:722:HIS:NE2	2.34	0.42
1:H:697:LEU:HD23	1:H:701:HIS:CD2	2.54	0.42
1:B:581:VAL:O	1:B:582:GLN:C	2.63	0.42
1:E:408:ALA:O	1:E:412:VAL:HG23	2.19	0.42
1:A:508:GLN:HB3	1:A:541:LYS:HD3	2.02	0.42
1:B:596:PRO:O	1:B:597:GLU:C	2.63	0.42
1:B:374:ALA:O	1:B:375:LEU:C	2.63	0.42
1:H:285:ALA:CB	1:H:286:PRO:HD2	2.41	0.42
1:A:351:LEU:HB3	1:A:357:LEU:HD12	2.00	0.41
1:B:261:LEU:HG	1:B:262:LYS:N	2.35	0.41
1:H:697:LEU:HD23	1:H:701:HIS:HD2	1.85	0.41
3:J:-13:DG:H2''	3:J:-12:DA:OP2	2.20	0.41
1:A:693:ALA:CB	1:A:721:GLU:OE2	2.68	0.41
1:H:690:PRO:O	1:H:691:ASP:O	2.38	0.41
1:E:515:ARG:CB	1:E:516:LEU:HD12	2.50	0.41
1:A:543:ALA:O	1:A:547:VAL:HG23	2.20	0.41
1:H:709:GLY:O	1:H:710:GLY:C	2.64	0.41
1:H:283:THR:O	1:H:288:ASN:HA	2.20	0.41
1:B:255:LEU:HD22	1:B:260:LEU:HG	2.01	0.41
3:G:-14:DA:C8	3:G:-13:DG:C2	3.09	0.41
2:I:13:DC:C5	2:I:14:DT:O4	2.74	0.41
1:E:230:MET:HA	1:E:238:LEU:HD12	2.03	0.41
1:E:697:LEU:HD23	1:E:701:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:LEU:HD23	1:A:701:HIS:HD2	1.86	0.41
1:E:261:LEU:HG	1:E:262:LYS:N	2.36	0.40
1:E:283:THR:O	1:E:288:ASN:HA	2.20	0.40
1:A:629:THR:HG23	1:A:632:GLN:HG3	2.02	0.40
1:E:522:GLN:O	1:E:523:ALA:C	2.64	0.40
2:F:14:DT:O2	2:F:14:DT:H2'	2.20	0.40
2:K:-2:DT:C2	2:K:-1:DG:C4	3.10	0.40
1:A:585:LEU:HB3	1:A:586:PRO:CD	2.52	0.40
1:B:283:THR:O	1:B:288:ASN:HA	2.22	0.40
1:B:585:LEU:HB3	1:B:586:PRO:CD	2.51	0.40
1:E:585:LEU:HB3	1:E:586:PRO:CD	2.51	0.40
1:H:287:LEU:O	1:H:288:ASN:C	2.65	0.40
1:B:523:ALA:O	1:B:524:HIS:HB2	2.22	0.40
1:H:596:PRO:O	1:H:597:GLU:C	2.64	0.40

All (33) 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:236:ARG:CZ	3:G:-3:DG:OP2[2_445]	0.57	1.63
1:A:236:ARG:NH2	3:G:-3:DG:OP2[2_445]	0.85	1.35
1:B:236:ARG:NH2	1:H:264:ALA:O[2_556]	1.23	0.97
3:J:-3:DG:OP1	1:E:236:ARG:NH1[2_445]	1.39	0.81
1:E:251:PRO:CA	1:E:524:HIS:NE2[2_455]	1.39	0.81
1:A:236:ARG:NH1	3:G:-3:DG:P[2_445]	1.47	0.73
1:A:236:ARG:CZ	3:G:-3:DG:P[2_445]	1.50	0.70
1:A:236:ARG:NE	3:G:-3:DG:OP2[2_445]	1.50	0.70
1:A:236:ARG:NH2	3:G:-3:DG:P[2_445]	1.51	0.69
1:A:236:ARG:NH1	3:G:-3:DG:OP1[2_445]	1.52	0.68
1:E:250:GLY:C	1:E:524:HIS:CE1[2_455]	1.56	0.64
1:E:251:PRO:CA	1:E:524:HIS:CD2[2_455]	1.56	0.64
1:E:250:GLY:O	1:E:524:HIS:CE1[2_455]	1.58	0.62
1:B:236:ARG:CZ	1:H:264:ALA:O[2_556]	1.59	0.61
3:J:-3:DG:OP2	1:E:236:ARG:CZ[2_445]	1.63	0.57
3:J:-3:DG:OP2	1:E:236:ARG:NH2[2_445]	1.66	0.54
1:E:251:PRO:N	1:E:524:HIS:NE2[2_455]	1.72	0.48
1:B:236:ARG:NH2	1:H:264:ALA:C[2_556]	1.73	0.47
3:J:-3:DG:P	1:E:236:ARG:NH2[2_445]	1.77	0.43
1:B:236:ARG:NH1	1:H:264:ALA:O[2_556]	1.82	0.38
1:A:236:ARG:NH1	3:G:-3:DG:OP2[2_445]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:GLN:OE1	1:E:524:HIS:ND1[2_455]	1.87	0.33
3:J:-3:DG:P	1:E:236:ARG:NH1[2_445]	1.90	0.30
1:E:250:GLY:C	1:E:524:HIS:NE2[2_455]	1.96	0.24
3:J:-3:DG:P	1:E:236:ARG:CZ[2_445]	1.97	0.23
1:E:250:GLY:O	1:E:524:HIS:NE2[2_455]	1.98	0.22
3:J:-3:DG:O5'	1:E:236:ARG:NH2[2_445]	1.99	0.21
1:A:236:ARG:NH2	3:G:-3:DG:O5'[2_445]	2.03	0.17
3:J:-3:DG:OP1	1:E:236:ARG:CZ[2_445]	2.03	0.17
1:E:251:PRO:N	1:E:524:HIS:CE1[2_455]	2.12	0.08
1:A:236:ARG:NH1	3:G:-4:DA:O3'[2_445]	2.13	0.07
1:B:556:GLN:OE1	2:C:-2:DT:O4[2_556]	2.13	0.07
1:B:524:HIS:N	1:H:231:GLN:OE1[1_565]	2.19	0.01

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	491/498 (99%)	445 (91%)	38 (8%)	8 (2%)	7	34
1	B	491/498 (99%)	447 (91%)	32 (6%)	12 (2%)	4	24
1	E	491/498 (99%)	453 (92%)	30 (6%)	8 (2%)	7	34
1	H	491/498 (99%)	446 (91%)	34 (7%)	11 (2%)	5	26
All	All	1964/1992 (99%)	1791 (91%)	134 (7%)	39 (2%)	6	28

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ALA
1	B	285	ALA
1	B	691	ASP
1	B	703	VAL
1	E	233	SER

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Mol	Chain	Res	Type
1	E	252	PRO
1	E	285	ALA
1	H	231	GLN
1	H	233	SER
1	H	237	ALA
1	H	285	ALA
1	A	524	HIS
1	A	710	GLY
1	B	233	SER
1	B	236	ARG
1	B	254	GLN
1	B	710	GLY
1	E	710	GLY
1	H	710	GLY
1	A	521	CYS
1	A	690	PRO
1	B	252	PRO
1	E	231	GLN
1	E	690	PRO
1	H	238	LEU
1	H	690	PRO
1	A	691	ASP
1	B	524	HIS
1	E	691	ASP
1	H	524	HIS
1	H	691	ASP
1	A	719	LYS
1	B	690	PRO
1	H	235	ALA
1	B	692	PRO
1	E	654	PRO
1	H	654	PRO
1	A	654	PRO
1	B	654	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	378/384 (98%)	336 (89%)	42 (11%)	6	25
1	B	378/384 (98%)	336 (89%)	42 (11%)	6	25
1	E	378/384 (98%)	340 (90%)	38 (10%)	7	29
1	H	378/384 (98%)	341 (90%)	37 (10%)	7	30
All	All	1512/1536 (98%)	1353 (90%)	159 (10%)	6	27

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	238	LEU
1	A	239	GLU
1	A	241	LEU
1	A	254	GLN
1	A	261	LEU
1	A	265	LYS
1	A	283	THR
1	A	287	LEU
1	A	292	GLU
1	A	299	SER
1	A	307	LEU
1	A	353	GLN
1	A	375	LEU
1	A	387	GLN
1	A	453	LEU
1	A	462	GLN
1	A	483	LEU
1	A	488	GLN
1	A	495	GLN
1	A	513	VAL
1	A	516	LEU
1	A	519	VAL
1	A	526	LEU
1	A	548	GLN
1	A	553	VAL
1	A	563	GLN
1	A	585	LEU
1	A	588	LEU
1	A	618	LEU
1	A	622	LEU
1	A	628	LEU
1	A	629	THR

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Mol	Chain	Res	Type
1	A	655	VAL
1	A	663	THR
1	A	683	ILE
1	A	686	GLN
1	A	689	ARG
1	A	691	ASP
1	A	694	LEU
1	A	701	HIS
1	A	705	LEU
1	B	231	GLN
1	B	238	LEU
1	B	241	LEU
1	B	254	GLN
1	B	255	LEU
1	B	257	THR
1	B	261	LEU
1	B	265	LYS
1	B	283	THR
1	B	287	LEU
1	B	292	GLU
1	B	299	SER
1	B	307	LEU
1	B	353	GLN
1	B	375	LEU
1	B	387	GLN
1	B	453	LEU
1	B	470	GLN
1	B	483	LEU
1	B	488	GLN
1	B	513	VAL
1	B	519	VAL
1	B	526	LEU
1	B	548	GLN
1	B	553	VAL
1	B	563	GLN
1	B	585	LEU
1	B	588	LEU
1	B	590	GLN
1	B	618	LEU
1	B	622	LEU
1	B	655	VAL
1	B	663	THR

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Mol	Chain	Res	Type
1	B	683	ILE
1	B	686	GLN
1	B	689	ARG
1	B	694	LEU
1	B	701	HIS
1	B	705	LEU
1	B	717	VAL
1	B	720	LEU
1	B	721	GLU
1	E	231	GLN
1	E	238	LEU
1	E	239	GLU
1	E	241	LEU
1	E	254	GLN
1	E	257	THR
1	E	261	LEU
1	E	265	LYS
1	E	283	THR
1	E	287	LEU
1	E	299	SER
1	E	307	LEU
1	E	353	GLN
1	E	375	LEU
1	E	387	GLN
1	E	453	LEU
1	E	470	GLN
1	E	483	LEU
1	E	488	GLN
1	E	519	VAL
1	E	524	HIS
1	E	526	LEU
1	E	548	GLN
1	E	563	GLN
1	E	585	LEU
1	E	588	LEU
1	E	590	GLN
1	E	618	LEU
1	E	622	LEU
1	E	655	VAL
1	E	663	THR
1	E	683	ILE
1	E	686	GLN

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Mol	Chain	Res	Type
1	E	689	ARG
1	E	691	ASP
1	E	694	LEU
1	E	701	HIS
1	E	705	LEU
1	H	232	TRP
1	H	236	ARG
1	H	238	LEU
1	H	241	LEU
1	H	254	GLN
1	H	257	THR
1	H	261	LEU
1	H	265	LYS
1	H	283	THR
1	H	287	LEU
1	H	299	SER
1	H	307	LEU
1	H	345	GLN
1	H	353	GLN
1	H	375	LEU
1	H	387	GLN
1	H	453	LEU
1	H	483	LEU
1	H	488	GLN
1	H	519	VAL
1	H	526	LEU
1	H	548	GLN
1	H	563	GLN
1	H	585	LEU
1	H	588	LEU
1	H	590	GLN
1	H	618	LEU
1	H	622	LEU
1	H	655	VAL
1	H	663	THR
1	H	665	GLN
1	H	683	ILE
1	H	686	GLN
1	H	691	ASP
1	H	694	LEU
1	H	701	HIS
1	H	705	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	300	HIS
1	A	311	GLN
1	A	457	HIS
1	A	488	GLN
1	A	490	HIS
1	A	522	GLN
1	A	616	GLN
1	A	686	GLN
1	A	699	ASN
1	A	701	HIS
1	B	254	GLN
1	B	276	HIS
1	B	280	ASN
1	B	300	HIS
1	B	311	GLN
1	B	321	HIS
1	B	353	GLN
1	B	457	HIS
1	B	490	HIS
1	B	522	GLN
1	B	616	GLN
1	B	658	GLN
1	B	686	GLN
1	B	699	ASN
1	B	701	HIS
1	B	722	HIS
1	E	280	ASN
1	E	300	HIS
1	E	311	GLN
1	E	321	HIS
1	E	339	GLN
1	E	428	GLN
1	E	455	GLN
1	E	457	HIS
1	E	490	HIS
1	E	590	GLN
1	E	616	GLN
1	E	686	GLN
1	E	699	ASN
1	E	701	HIS

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Mol	Chain	Res	Type
1	E	722	HIS
1	H	276	HIS
1	H	280	ASN
1	H	300	HIS
1	H	311	GLN
1	H	321	HIS
1	H	339	GLN
1	H	457	HIS
1	H	490	HIS
1	H	616	GLN
1	H	686	GLN
1	H	699	ASN
1	H	701	HIS
1	H	722	HIS

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	5HC	K	6	2,3	18,22,23	1.00	1 (5%)	22,31,34	1.42	3 (13%)
2	5HC	C	6	2,3	18,22,23	1.07	1 (5%)	22,31,34	1.04	0
2	5HC	I	6	2,3	18,22,23	1.13	1 (5%)	22,31,34	1.16	2 (9%)
2	5HC	F	6	2,3	18,22,23	1.08	1 (5%)	22,31,34	1.33	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5HC	K	6	2,3	-	1/9/23/24	0/2/2/2
2	5HC	C	6	2,3	-	1/9/23/24	0/2/2/2
2	5HC	I	6	2,3	-	1/9/23/24	0/2/2/2
2	5HC	F	6	2,3	-	1/9/23/24	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	5HC	C6-N1	-3.36	1.32	1.38
2	I	6	5HC	C6-N1	-3.17	1.32	1.38
2	K	6	5HC	C6-N1	-2.64	1.33	1.38
2	C	6	5HC	C6-N1	-2.56	1.33	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	6	5HC	C2'-C3'-C4'	2.94	108.76	102.80
2	F	6	5HC	C5-C6-N1	-2.81	119.15	122.94
2	I	6	5HC	O2-C2-N3	-2.72	118.04	122.33
2	F	6	5HC	O2-C2-N3	-2.53	118.33	122.33
2	I	6	5HC	O5-C5M-C5	-2.22	104.12	111.64
2	F	6	5HC	C1'-N1-C6	-2.15	117.13	120.74
2	K	6	5HC	O4'-C1'-C2'	2.09	110.15	106.25
2	K	6	5HC	O2-C2-N3	-2.08	119.06	122.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	6	5HC	1	0
2	C	6	5HC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	6	5HC	1	0
2	F	6	5HC	1	0

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	493/498 (98%)	0.49	28 (5%) 29 15	21, 48, 82, 122	0
1	B	493/498 (98%)	0.63	37 (7%) 20 10	22, 47, 97, 161	0
1	E	493/498 (98%)	0.90	52 (10%) 11 6	30, 61, 103, 131	0
1	H	493/498 (98%)	0.92	61 (12%) 8 5	28, 62, 104, 147	0
2	C	16/17 (94%)	0.05	1 (6%) 26 13	24, 32, 85, 89	0
2	F	16/17 (94%)	0.58	2 (12%) 8 5	24, 38, 105, 114	0
2	I	16/17 (94%)	0.00	1 (6%) 26 13	20, 29, 67, 85	0
2	K	16/17 (94%)	0.55	2 (12%) 8 5	26, 42, 112, 117	0
3	D	17/17 (100%)	-0.11	0 100 100	25, 43, 77, 87	0
3	G	17/17 (100%)	0.57	2 (11%) 9 5	23, 42, 98, 111	0
3	J	17/17 (100%)	-0.00	0 100 100	27, 37, 76, 83	0
3	L	17/17 (100%)	0.86	2 (11%) 9 5	32, 53, 111, 118	0
All	All	2104/2128 (98%)	0.71	188 (8%) 15 8	20, 54, 100, 161	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	9.9
1	B	722	HIS	8.1
1	B	233	SER	8.0
3	L	-14	DA	7.3
1	H	234	GLY	7.1
1	B	235	ALA	7.0
1	E	232	TRP	6.9
1	E	235	ALA	6.7
1	B	692	PRO	6.5
1	A	230	MET	6.4
1	B	523	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	H	233	SER	5.8
1	H	232	TRP	5.8
1	E	230	MET	5.5
1	B	694	LEU	5.4
1	H	722	HIS	5.4
1	E	237	ALA	5.2
1	H	235	ALA	5.2
1	A	692	PRO	4.8
1	H	720	LEU	4.6
1	A	722	HIS	4.6
1	E	245	ALA	4.6
1	B	231	GLN	4.5
1	B	556	GLN	4.5
1	H	524	HIS	4.5
1	B	524	HIS	4.5
1	H	230	MET	4.5
1	H	694	LEU	4.4
1	B	232	TRP	4.4
1	A	693	ALA	4.4
1	E	240	ALA	4.3
1	A	721	GLU	4.2
1	B	236	ARG	4.1
1	H	239	GLU	4.1
1	A	243	THR	4.0
1	A	523	ALA	4.0
1	H	523	ALA	4.0
1	B	238	LEU	4.0
1	A	232	TRP	3.9
1	E	254	GLN	3.9
1	E	722	HIS	3.8
1	B	241	LEU	3.8
1	H	301	ASP	3.8
1	E	520	LEU	3.8
2	F	14	DT	3.8
1	A	694	LEU	3.6
1	A	233	SER	3.6
1	E	694	LEU	3.6
1	E	692	PRO	3.6
1	E	241	LEU	3.5
1	B	522	GLN	3.5
1	H	277	ALA	3.5
1	H	692	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	391	LEU	3.3
1	E	238	LEU	3.3
1	H	525	GLY	3.3
1	H	354	ALA	3.3
1	A	524	HIS	3.3
3	G	-14	DA	3.2
1	H	236	ARG	3.2
2	K	14	DT	3.2
1	B	525	GLY	3.2
2	K	-2	DT	3.2
1	H	404	GLY	3.2
1	E	233	SER	3.2
1	B	462	GLN	3.2
1	H	238	LEU	3.1
1	H	386	CYS	3.1
1	B	239	GLU	3.1
1	E	243	THR	3.1
1	H	346	ARG	3.1
1	E	251	PRO	3.1
1	A	695	ALA	3.0
1	H	425	LEU	3.0
1	B	280	ASN	3.0
1	B	336	GLY	3.0
1	E	248	LEU	3.0
1	E	242	LEU	3.0
1	H	721	GLU	3.0
1	H	270	THR	2.9
1	E	246	GLY	2.9
1	B	269	VAL	2.9
1	E	693	ALA	2.9
1	A	235	ALA	2.9
1	E	695	ALA	2.9
1	A	269	VAL	2.8
1	E	236	ARG	2.8
1	H	254	GLN	2.8
1	H	365	ILE	2.8
1	A	231	GLN	2.8
1	H	266	ARG	2.8
1	E	484	PRO	2.8
1	E	518	PRO	2.8
1	H	384	VAL	2.7
1	B	230	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	721	GLU	2.7
1	A	242	LEU	2.7
1	E	239	GLU	2.7
1	A	251	PRO	2.6
1	A	241	LEU	2.6
1	B	691	ASP	2.6
1	H	370	GLY	2.6
2	C	14	DT	2.5
1	H	351	LEU	2.5
1	H	381	LEU	2.5
1	E	523	ALA	2.5
1	A	278	TRP	2.5
1	E	231	GLN	2.5
1	E	696	ALA	2.5
1	H	237	ALA	2.5
1	H	480	GLN	2.5
1	B	261	LEU	2.5
1	E	278	TRP	2.5
1	H	231	GLN	2.5
3	G	2	DA	2.5
1	A	420	CYS	2.5
1	A	690	PRO	2.4
1	H	382	LEU	2.4
1	B	267	GLY	2.4
1	E	519	VAL	2.4
1	B	237	ALA	2.4
1	B	693	ALA	2.4
1	E	625	ALA	2.4
1	E	486	LEU	2.4
1	B	244	VAL	2.4
1	B	695	ALA	2.4
1	E	624	GLN	2.4
1	E	516	LEU	2.4
1	H	304	LYS	2.3
2	I	14	DT	2.3
1	E	244	VAL	2.3
1	H	695	ALA	2.3
1	E	488	GLN	2.3
1	H	253	LEU	2.3
1	A	454	CYS	2.3
1	E	529	GLN	2.3
1	B	720	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	416	LEU	2.3
1	E	698	THR	2.3
3	L	2	DA	2.3
1	H	246	GLY	2.3
2	F	-1	DG	2.3
1	H	380	ALA	2.3
1	H	385	LEU	2.3
1	H	431	VAL	2.3
1	H	625	ALA	2.3
1	A	590	GLN	2.3
1	A	628	LEU	2.3
1	H	395	GLN	2.3
1	H	366	ALA	2.2
1	A	257	THR	2.2
1	A	691	ASP	2.2
1	E	525	GLY	2.2
1	E	360	GLU	2.2
1	H	394	GLU	2.2
1	E	699	ASN	2.2
1	E	556	GLN	2.2
1	H	690	PRO	2.2
1	B	265	LYS	2.2
1	H	708	LEU	2.2
1	H	432	ALA	2.2
1	A	522	GLN	2.2
1	E	603	ALA	2.2
1	B	582	GLN	2.1
1	E	561	THR	2.1
1	H	403	GLY	2.1
1	E	596	PRO	2.1
1	H	390	GLY	2.1
1	H	698	THR	2.1
1	A	240	ALA	2.1
1	H	428	GLN	2.1
1	E	459	LEU	2.1
1	H	424	GLY	2.1
1	B	243	THR	2.1
1	H	693	ALA	2.1
1	H	529	GLN	2.1
1	E	526	LEU	2.1
1	H	375	LEU	2.1
1	B	369	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	721	GLU	2.1
1	B	548	GLN	2.0
1	E	326	GLN	2.0
1	B	404	GLY	2.0
1	E	456	ALA	2.0
1	H	456	ALA	2.0
1	E	532	VAL	2.0
1	E	554	LEU	2.0
1	H	278	TRP	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	5HC	C	6	21/22	0.97	0.08	22,25,30,33	0
2	5HC	F	6	21/22	0.97	0.07	22,27,37,40	0
2	5HC	K	6	21/22	0.97	0.07	27,31,38,41	0
2	5HC	I	6	21/22	0.98	0.07	17,20,24,26	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.