



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 06:24 PM JST

PDB ID : 9VSO / pdb_00009vso
Title : Crystal structure of Fab bound to the WT1-derived RMF peptide presented by HLA-A*02:01
Authors : Oh, T.S.; Jeong, B.S.; Oh, B.H.
Deposited on : 2025-07-09
Resolution : 3.03 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:

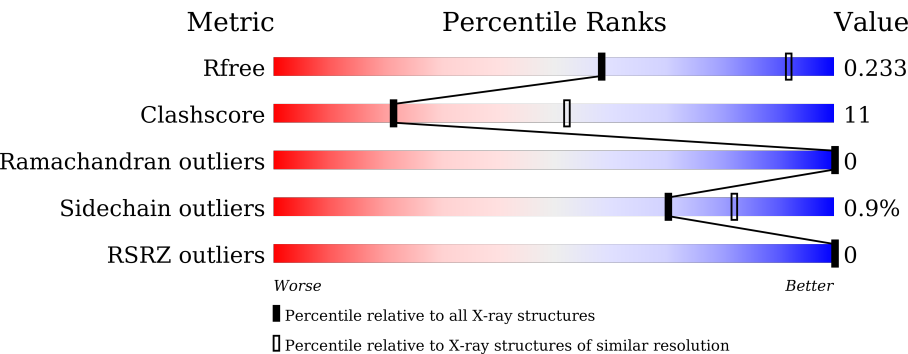
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	G	244	70%19%11%
1	I	244	70%18%11%
2	J	233	63%27%8%
2	K	233	61%29%8%
3	A	282	80%18%
3	C	282	83%14%

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Mol	Chain	Length	Quality of chain	
4	B	100		
4	D	100		
5	M	9		
5	T	9		

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12830 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 Q2L_Fab_heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	218	Total	C	N	O	S	0	0	0
			1625	1027	271	321	6			
1	I	218	Total	C	N	O	S	0	0	0
			1625	1027	271	321	6			

- Molecule 2 is a protein called Q2L_Fab_light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	214	Total	C	N	O	S	0	0	0
			1630	1016	274	334	6			
2	K	214	Total	C	N	O	S	0	0	0
			1630	1016	274	334	6			

- Molecule 3 is a protein called HLA class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
3	C	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q53Z42
A	276	HIS	-	expression tag	UNP Q53Z42
A	277	HIS	-	expression tag	UNP Q53Z42
A	278	HIS	-	expression tag	UNP Q53Z42
A	279	HIS	-	expression tag	UNP Q53Z42
A	280	HIS	-	expression tag	UNP Q53Z42
A	281	HIS	-	expression tag	UNP Q53Z42
C	0	MET	-	initiating methionine	UNP Q53Z42

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Chain	Residue	Modelled	Actual	Comment	Reference
C	276	HIS	-	expression tag	UNP Q53Z42
C	277	HIS	-	expression tag	UNP Q53Z42
C	278	HIS	-	expression tag	UNP Q53Z42
C	279	HIS	-	expression tag	UNP Q53Z42
C	280	HIS	-	expression tag	UNP Q53Z42
C	281	HIS	-	expression tag	UNP Q53Z42

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
4	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
D	0	MET	-	expression tag	UNP P61769

- Molecule 5 is a protein called Wilms tumor protein.

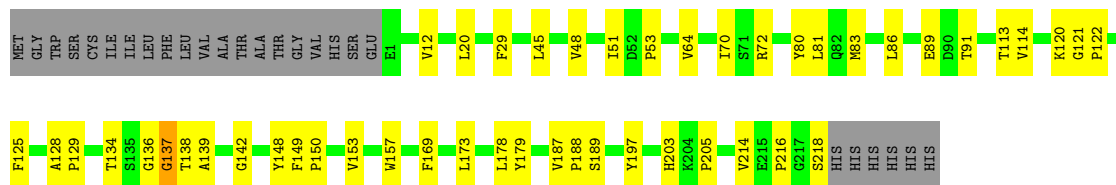
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	9	Total	C	N	O	S	0	0	0
			77	52	13	11	1			
5	M	9	Total	C	N	O	S	0	0	0
			77	52	13	11	1			

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.

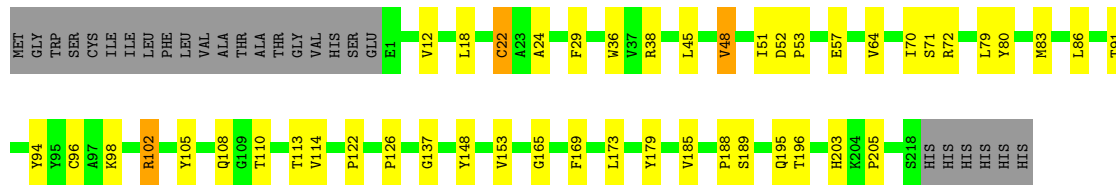
- Molecule 1: Q2L_Fab_heavy chain

Chain G: 



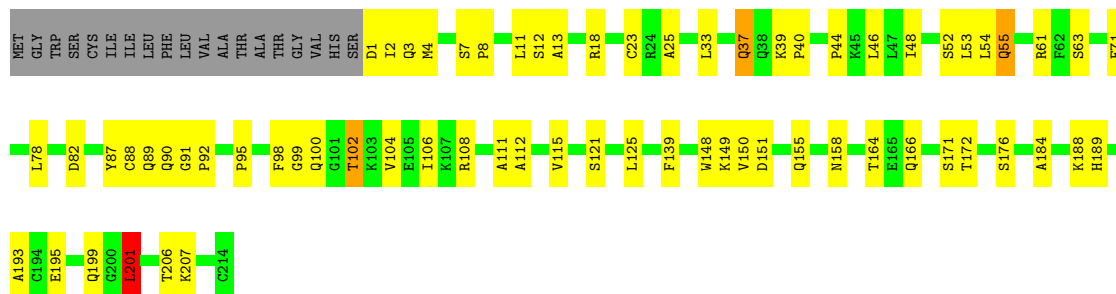
- Molecule 1: Q2L_Fab_heavy chain

Chain I: 



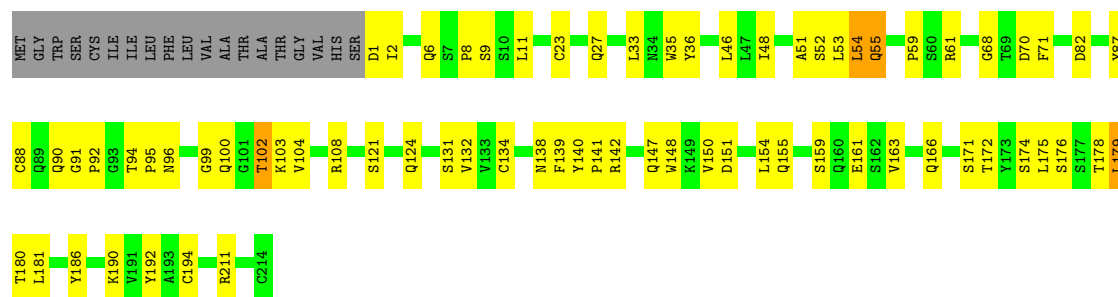
- Molecule 2: Q2L_Fab_light chain

Chain J: 



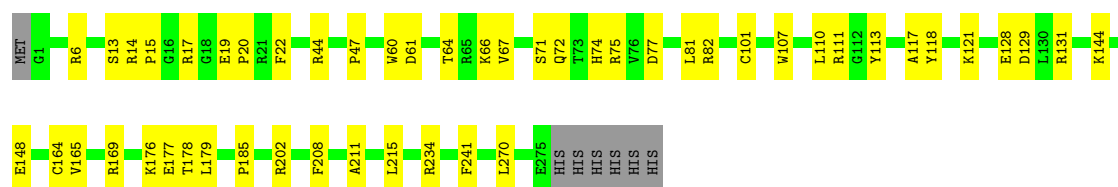
- Molecule 2: Q2L_Fab_light chain

Chain K: 



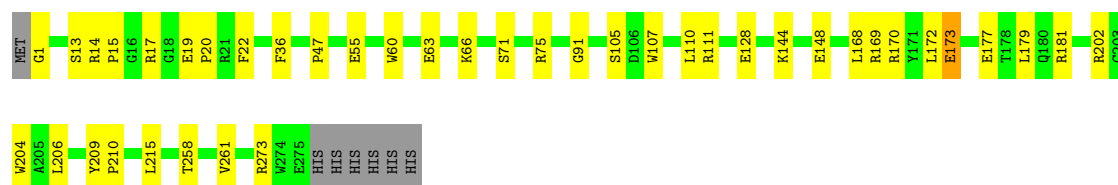
- Molecule 3: HLA class I antigen

Chain A: 80% 18%



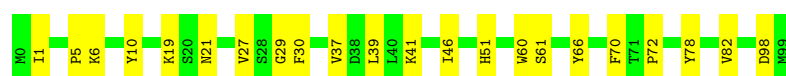
- Molecule 3: HLA class I antigen

Chain C: 83% 14%



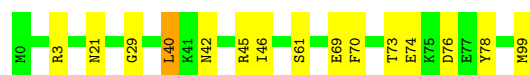
- Molecule 4: Beta-2-microglobulin

Chain B: 78% 22%



- Molecule 4: Beta-2-microglobulin

Chain D: 85% 14%



- Molecule 5: Wilms tumor protein

Chain T: 78% 22%



- Molecule 5: Wilms tumor protein

Chain M:  78% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.07Å 132.81Å 185.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 3.03 29.92 – 3.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.92-3.03) 99.8 (29.92-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.183 , 0.234 0.186 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	90.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12830	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

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	G	0.67	0/1664	0.88	4/2267 (0.2%)
1	I	0.94	4/1664 (0.2%)	0.88	2/2267 (0.1%)
2	J	0.81	0/1664	0.84	2/2259 (0.1%)
2	K	0.94	5/1664 (0.3%)	0.96	7/2259 (0.3%)
3	A	0.67	0/2311	0.80	4/3137 (0.1%)
3	C	0.59	0/2311	0.78	1/3137 (0.0%)
4	B	0.45	0/860	0.72	0/1162
4	D	0.47	0/860	0.70	1/1162 (0.1%)
5	M	0.53	0/80	0.92	0/108
5	T	1.17	0/80	1.02	0/108
All	All	0.73	9/13158 (0.1%)	0.84	21/17866 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	102	ARG	CA-C	-6.72	1.48	1.52
2	K	103	LYS	C-O	-5.71	1.17	1.24
1	I	29	PHE	C-O	-5.64	1.17	1.24
1	I	24	ALA	CA-C	-5.31	1.46	1.52
2	K	94	THR	C-O	-5.31	1.17	1.24
1	I	22	CYS	C-O	-5.29	1.17	1.24
2	K	102	THR	C-O	-5.21	1.18	1.24
2	K	95	PRO	CA-C	-5.14	1.45	1.52
2	K	103	LYS	CA-C	-5.14	1.46	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	94	THR	CA-C-N	10.53	130.48	119.85
2	K	94	THR	C-N-CA	10.53	130.48	119.85
1	G	137	GLY	N-CA-C	-10.20	101.79	115.36
3	C	179	LEU	N-CA-C	10.15	122.42	111.36
3	A	179	LEU	N-CA-C	7.39	119.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	48	VAL	N-CA-C	6.37	117.03	111.56
2	K	104	VAL	CB-CA-C	-6.00	102.84	111.19
2	J	199	GLN	N-CA-C	-6.00	101.53	110.23
3	A	178	THR	N-CA-C	5.92	117.54	111.14
2	K	91	GLY	CA-C-N	5.83	125.21	118.85
2	K	91	GLY	C-N-CA	5.83	125.21	118.85
2	K	179	LEU	CB-CG-CD2	-5.83	93.22	110.70
2	K	52	SER	N-CA-C	5.78	118.35	111.71
1	I	22	CYS	CA-CB-SG	5.68	127.47	114.40
1	G	214	VAL	CA-C-N	-5.41	109.54	122.74
1	G	214	VAL	C-N-CA	-5.41	109.54	122.74
1	G	128	ALA	N-CA-C	5.41	116.70	109.83
2	J	201	LEU	N-CA-C	-5.40	100.10	108.90
3	A	178	THR	CB-CA-C	-5.24	102.62	110.90
3	A	176	LYS	N-CA-C	5.22	116.97	111.28
4	D	40	LEU	N-CA-C	5.21	117.39	108.90

There are no chirality outliers.

There are no planarity outliers.

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	G	1625	0	1596	32	0
1	I	1625	0	1597	41	0
2	J	1630	0	1587	50	0
2	K	1630	0	1587	73	0
3	A	2246	0	2094	35	0
3	C	2246	0	2096	29	0
4	B	837	0	803	16	0
4	D	837	0	803	15	0
5	M	77	0	78	3	0
5	T	77	0	78	1	0
All	All	12830	0	12319	272	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 11.

All (272) 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:I:22:CYS:SG	1:I:96:CYS:CB	2.04	1.43
1:I:22:CYS:SG	1:I:96:CYS:SG	1.32	1.31
2:K:8:PRO:O	2:K:102:THR:HG23	1.38	1.20
2:J:100:GLN:NE2	2:K:166:GLN:OE1	1.82	1.13
1:G:137:GLY:HA2	1:G:188:PRO:HA	1.37	1.07
2:K:6:GLN:NE2	2:K:102:THR:OG1	1.88	1.05
2:K:61:ARG:NH2	2:K:82:ASP:OD2	1.89	1.05
3:A:66:LYS:NZ	1:I:57:GLU:OE1	1.91	1.03
2:J:39:LYS:HB3	2:J:40:PRO:HD2	1.50	0.90
2:J:48:ILE:HD13	2:J:54:LEU:HD12	1.56	0.88
2:K:8:PRO:O	2:K:102:THR:CG2	2.22	0.87
2:K:147:GLN:HG3	2:K:154:LEU:HD13	1.58	0.84
3:A:101:CYS:CB	3:A:164:CYS:SG	2.67	0.82
1:I:22:CYS:SG	1:I:96:CYS:HB3	2.15	0.81
2:K:132:VAL:HB	2:K:179:LEU:HD23	1.60	0.81
2:K:61:ARG:NH2	2:K:82:ASP:CG	2.38	0.81
4:D:42:ASN:ND2	4:D:76:ASP:OD1	2.14	0.81
1:I:48:VAL:HG13	1:I:64:VAL:HG21	1.63	0.80
1:I:22:CYS:SG	1:I:96:CYS:HB2	2.21	0.80
3:A:101:CYS:HB3	3:A:164:CYS:SG	2.23	0.79
2:K:96:ASN:O	2:K:96:ASN:ND2	2.15	0.78
2:K:148:TRP:CD2	2:K:179:LEU:HD21	2.19	0.77
1:G:91:THR:HG23	1:G:113:THR:HA	1.65	0.77
3:C:181:ARG:HH11	3:C:181:ARG:HG2	1.46	0.76
1:I:57:GLU:HG2	5:M:1:ARG:NH2	2.00	0.76
2:K:48:ILE:CG2	2:K:51:ALA:O	2.33	0.76
1:G:81:LEU:HD23	1:G:83:MET:HE2	1.66	0.76
2:J:100:GLN:CD	2:J:100:GLN:H	1.93	0.75
3:A:107:TRP:O	3:A:169:ARG:NH1	2.20	0.74
3:A:177:GLU:OE1	3:A:177:GLU:N	2.17	0.74
2:K:61:ARG:HH21	2:K:82:ASP:CG	1.97	0.73
3:C:19:GLU:OE2	3:C:75:ARG:HD2	1.88	0.72
1:I:45:LEU:HD11	2:K:92:PRO:HG2	1.71	0.72
2:K:148:TRP:CE3	2:K:179:LEU:HD21	2.24	0.72
2:K:11:LEU:C	2:K:11:LEU:HD12	2.14	0.71
2:J:44:PRO:HG2	2:J:98:PHE:CE2	2.25	0.71
2:K:100:GLN:N	2:K:100:GLN:OE1	2.23	0.71
1:G:45:LEU:HD11	2:J:92:PRO:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:66:LYS:HZ2	1:I:57:GLU:CD	1.96	0.70
2:J:11:LEU:HD12	2:J:11:LEU:C	2.15	0.70
2:K:108:ARG:HE	2:K:171:SER:HB2	1.57	0.68
2:K:48:ILE:HG21	2:K:51:ALA:O	1.93	0.68
2:J:89:GLN:HG2	2:J:95:PRO:HG3	1.77	0.67
2:K:59:PRO:HB2	2:K:61:ARG:HG3	1.76	0.66
2:K:8:PRO:HG2	2:K:11:LEU:HD23	1.77	0.66
3:C:177:GLU:H	3:C:177:GLU:CD	2.04	0.65
1:G:122:PRO:HB3	1:G:148:TYR:HB3	1.79	0.64
4:D:45:ARG:NH1	4:D:46:ILE:O	2.31	0.64
1:I:53:PRO:HA	1:I:72:ARG:NH1	2.12	0.64
2:J:100:GLN:OE1	2:J:100:GLN:N	2.23	0.63
1:I:51:ILE:HB	1:I:70:ILE:HD13	1.81	0.62
1:G:173:LEU:HD12	1:G:179:TYR:CE1	2.34	0.62
3:A:111:ARG:HD3	3:A:113:TYR:CZ	2.34	0.62
2:K:36:TYR:CE1	2:K:46:LEU:HB2	2.35	0.62
2:K:61:ARG:NH2	2:K:82:ASP:OD1	2.31	0.62
4:D:70:PHE:HE1	4:D:78:TYR:CZ	2.18	0.61
3:C:63:GLU:OE1	3:C:66:LYS:NZ	2.34	0.61
1:G:139:ALA:HB2	1:G:189:SER:HB3	1.84	0.60
2:J:108:ARG:NH2	2:J:111:ALA:HB2	2.16	0.60
3:C:144:LYS:O	3:C:148:GLU:HG3	2.00	0.60
1:I:45:LEU:HD11	2:K:92:PRO:CG	2.31	0.60
1:I:91:THR:HG23	1:I:113:THR:HA	1.85	0.59
2:J:48:ILE:HG23	2:J:53:LEU:O	2.03	0.59
1:G:120:LYS:HG2	1:G:121:GLY:O	2.03	0.59
2:J:90:GLN:HG2	2:J:91:GLY:N	2.18	0.59
1:G:137:GLY:H	1:G:189:SER:H	1.50	0.58
3:C:181:ARG:NH1	3:C:209:TYR:CE2	2.71	0.58
2:K:134:CYS:HB2	2:K:148:TRP:CH2	2.39	0.58
4:D:69:GLU:HG2	4:D:70:PHE:H	1.68	0.58
2:K:148:TRP:CZ3	2:K:194:CYS:HB3	2.38	0.58
2:J:61:ARG:NH1	2:J:82:ASP:OD2	2.33	0.58
2:J:112:ALA:HB1	2:J:201:LEU:HD21	1.84	0.58
2:K:140:TYR:CD1	2:K:141:PRO:HA	2.39	0.58
1:I:22:CYS:CB	1:I:96:CYS:SG	2.82	0.58
3:C:181:ARG:HH11	3:C:181:ARG:CG	2.17	0.57
3:A:47:PRO:HB3	3:A:60:TRP:CH2	2.38	0.57
2:K:147:GLN:HG3	2:K:154:LEU:CD1	2.32	0.57
3:C:181:ARG:NH1	3:C:209:TYR:CD2	2.73	0.57
4:B:21:ASN:HB3	4:B:70:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:211:ARG:NH1	2:K:211:ARG:HB3	2.20	0.57
2:J:149:LYS:HB2	2:J:193:ALA:HB3	1.86	0.57
2:K:150:VAL:HB	2:K:155:GLN:HE21	1.70	0.57
2:K:11:LEU:HD12	2:K:11:LEU:O	2.05	0.57
3:C:14:ARG:HB3	3:C:17:ARG:HB2	1.87	0.56
2:J:112:ALA:HB1	2:J:201:LEU:CD2	2.35	0.56
2:K:211:ARG:HB3	2:K:211:ARG:HH11	1.70	0.56
2:J:55:GLN:OE1	2:J:55:GLN:HA	2.05	0.56
2:J:39:LYS:HB3	2:J:40:PRO:CD	2.29	0.56
2:J:195:GLU:HG3	2:J:206:THR:OG1	2.05	0.56
2:K:55:GLN:HA	2:K:55:GLN:OE1	2.04	0.56
3:A:144:LYS:O	3:A:148:GLU:HG3	2.06	0.56
3:A:177:GLU:H	3:A:177:GLU:CD	2.10	0.56
2:K:8:PRO:CG	2:K:11:LEU:HD23	2.36	0.56
2:K:150:VAL:HB	2:K:155:GLN:NE2	2.21	0.55
2:K:48:ILE:HD13	2:K:54:LEU:HD12	1.88	0.55
1:G:29:PHE:CE1	1:G:72:ARG:NH2	2.69	0.55
2:K:48:ILE:HG22	2:K:51:ALA:O	2.04	0.55
4:D:29:GLY:HA2	4:D:61:SER:HB2	1.87	0.55
4:B:5:PRO:HA	4:B:30:PHE:HB3	1.89	0.55
2:K:33:LEU:HD11	2:K:88:CYS:SG	2.47	0.55
2:K:9:SER:O	2:K:102:THR:HA	2.07	0.55
2:K:87:TYR:HE1	2:K:99:GLY:O	1.90	0.54
2:J:155:GLN:OE1	2:J:158:ASN:ND2	2.35	0.54
1:G:149:PHE:HB2	1:G:178:LEU:HD23	1.89	0.53
1:I:52:ASP:HB2	1:I:53:PRO:CD	2.38	0.53
2:J:3:GLN:HG2	2:K:142:ARG:CZ	2.38	0.53
2:K:138:ASN:H	2:K:174:SER:HB3	1.72	0.53
3:C:169:ARG:O	3:C:173:GLU:HG3	2.09	0.53
3:C:15:PRO:HG2	3:C:91:GLY:O	2.10	0.52
2:K:36:TYR:CZ	2:K:46:LEU:HD13	2.45	0.52
1:G:48:VAL:HG13	1:G:64:VAL:HG21	1.91	0.51
2:K:148:TRP:CG	2:K:179:LEU:HD11	2.45	0.51
1:G:136:GLY:C	1:G:138:THR:H	2.16	0.51
3:A:117:ALA:HB2	4:B:60:TRP:CE2	2.45	0.51
4:D:21:ASN:C	4:D:70:PHE:HB3	2.35	0.51
1:I:165:GLY:C	1:I:185:VAL:HG23	2.36	0.51
2:J:13:ALA:O	2:J:106:ILE:HA	2.11	0.51
4:B:21:ASN:HB3	4:B:70:PHE:HE1	1.76	0.51
1:G:187:VAL:HG21	1:G:197:TYR:CE2	2.46	0.50
3:A:202:ARG:NH1	4:B:98:ASP:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:48:ILE:CD1	2:K:54:LEU:HD12	2.41	0.50
2:J:48:ILE:CD1	2:J:54:LEU:HD12	2.35	0.50
2:K:96:ASN:HD22	2:K:96:ASN:C	2.02	0.50
3:C:209:TYR:CD1	3:C:210:PRO:HA	2.47	0.50
2:J:151:ASP:OD2	2:J:189:HIS:HB3	2.12	0.50
2:K:48:ILE:HG23	2:K:53:LEU:O	2.11	0.50
3:C:1:GLY:O	3:C:105:SER:HA	2.12	0.49
2:J:18:ARG:NH2	2:K:70:ASP:OD2	2.30	0.49
4:B:6:LYS:O	4:B:27:VAL:HA	2.12	0.49
1:G:125:PHE:CE2	2:K:124:GLN:HG3	2.48	0.49
3:A:64:THR:HA	3:A:67:VAL:HG12	1.95	0.49
4:B:5:PRO:CA	4:B:30:PHE:HB3	2.43	0.49
1:I:71:SER:OG	1:I:80:TYR:HB2	2.13	0.49
1:G:89:GLU:CD	1:G:89:GLU:H	2.21	0.48
2:J:46:LEU:HD23	2:J:55:GLN:HE21	1.78	0.48
1:I:108:GLN:OE1	1:I:108:GLN:N	2.47	0.48
1:G:142:GLY:HA2	1:G:157:TRP:CH2	2.49	0.48
2:J:11:LEU:C	2:J:11:LEU:CD1	2.85	0.48
3:C:55:GLU:OE1	3:C:170:ARG:NH2	2.47	0.48
3:A:82:ARG:CZ	3:A:82:ARG:HB3	2.42	0.48
3:C:181:ARG:HG3	3:C:181:ARG:O	2.14	0.47
3:C:258:THR:HG22	3:C:273:ARG:HG2	1.95	0.47
2:K:68:GLY:O	2:K:71:PHE:CE1	2.67	0.47
2:J:115:VAL:HG12	2:J:207:LYS:HG3	1.96	0.47
2:K:100:GLN:N	2:K:100:GLN:CD	2.72	0.47
2:J:33:LEU:HD11	2:J:88:CYS:SG	2.55	0.47
4:D:21:ASN:N	4:D:70:PHE:O	2.32	0.47
2:J:125:LEU:HA	2:J:125:LEU:HD23	1.65	0.47
2:J:148:TRP:HB2	2:J:155:GLN:HB2	1.97	0.47
3:A:215:LEU:HD12	3:A:215:LEU:HA	1.70	0.46
2:K:159:SER:HA	2:K:178:THR:O	2.16	0.46
2:J:87:TYR:HE1	2:J:99:GLY:O	1.97	0.46
2:J:150:VAL:HB	2:J:155:GLN:HE21	1.78	0.46
1:I:36:TRP:HE1	1:I:79:LEU:HG	1.81	0.46
2:K:179:LEU:HB3	2:K:181:LEU:CD1	2.45	0.46
2:J:90:GLN:HG2	2:J:91:GLY:H	1.80	0.46
3:A:74:HIS:HA	3:A:77:ASP:HB2	1.98	0.46
1:I:203:HIS:CD2	1:I:205:PRO:HD2	2.50	0.46
1:G:134:THR:O	1:G:134:THR:HG23	2.15	0.46
1:G:150:PRO:HD2	1:G:205:PRO:CB	2.45	0.46
1:I:12:VAL:CG1	1:I:114:VAL:HG22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:THR:O	1:I:110:THR:HG23	2.14	0.46
2:K:148:TRP:CE2	2:K:179:LEU:HD21	2.51	0.46
1:G:12:VAL:HG11	1:G:86:LEU:HD13	1.97	0.46
4:B:51:HIS:HB3	4:B:66:TYR:CD1	2.51	0.46
2:K:36:TYR:HE1	2:K:46:LEU:HB2	1.81	0.46
3:A:110:LEU:HD12	3:A:110:LEU:HA	1.68	0.45
3:C:47:PRO:HB3	3:C:60:TRP:CH2	2.51	0.45
4:B:37:VAL:HG22	4:B:82:VAL:HG22	1.98	0.45
1:I:18:LEU:HD12	1:I:18:LEU:HA	1.79	0.45
1:G:169:PHE:HE2	2:K:175:LEU:HA	1.81	0.45
2:J:176:SER:HB3	1:I:169:PHE:CE2	2.51	0.45
2:J:121:SER:CB	1:I:126:PRO:HD2	2.47	0.45
3:A:66:LYS:CE	1:I:57:GLU:OE1	2.63	0.45
4:D:74:GLU:O	4:D:74:GLU:HG2	2.16	0.45
3:A:19:GLU:HB3	3:A:75:ARG:HH22	1.82	0.45
3:A:129:ASP:O	3:A:131:ARG:HG3	2.17	0.45
1:G:136:GLY:HA2	1:G:189:SER:OG	2.17	0.45
3:A:22:PHE:CD2	3:A:71:SER:HB2	2.52	0.45
2:K:11:LEU:C	2:K:11:LEU:CD1	2.85	0.45
4:D:73:THR:HB	4:D:76:ASP:HB2	1.98	0.45
3:A:14:ARG:HB3	3:A:17:ARG:HB2	1.99	0.45
1:I:18:LEU:HB3	1:I:83:MET:HE2	1.99	0.45
2:J:7:SER:HA	2:J:8:PRO:C	2.42	0.44
2:K:2:ILE:HG12	2:K:27:GLN:HG2	1.98	0.44
2:K:140:TYR:HB2	2:K:172:THR:HG22	1.98	0.44
2:K:186:TYR:O	2:K:192:TYR:OH	2.28	0.44
1:G:53:PRO:HA	1:G:72:ARG:NH1	2.32	0.44
1:G:12:VAL:CG1	1:G:114:VAL:HG22	2.48	0.44
3:A:144:LYS:HE3	3:A:148:GLU:OE2	2.17	0.44
2:J:4:MET:HE1	2:J:25:ALA:HB2	2.00	0.44
3:A:185:PRO:HA	3:A:208:PHE:HB3	1.99	0.44
4:D:3:ARG:HH11	4:D:61:SER:HB3	1.83	0.44
1:G:129:PRO:HG2	1:G:216:PRO:HA	2.00	0.44
4:D:69:GLU:HG2	4:D:70:PHE:N	2.31	0.44
1:I:12:VAL:HG11	1:I:86:LEU:HD13	2.00	0.43
3:C:181:ARG:NH1	3:C:181:ARG:CG	2.77	0.43
1:G:125:PHE:HB3	2:K:121:SER:OG	2.19	0.43
3:A:234:ARG:HD2	4:B:10:TYR:CE1	2.53	0.43
1:I:173:LEU:HD13	1:I:179:TYR:CE1	2.52	0.43
4:B:19:LYS:O	4:B:72:PRO:HD2	2.18	0.43
2:K:131:SER:HA	2:K:179:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:148:TRP:CH2	2:K:194:CYS:HB3	2.52	0.43
1:G:148:TYR:CE2	1:G:153:VAL:HG23	2.54	0.43
4:B:39:LEU:O	4:B:46:ILE:HG13	2.19	0.43
4:D:40:LEU:HD23	4:D:45:ARG:HA	2.00	0.43
1:I:102:ARG:HB2	5:M:8:TYR:CD2	2.54	0.43
2:K:180:THR:O	2:K:181:LEU:HD12	2.19	0.43
4:B:41:LYS:HE3	4:B:78:TYR:HE1	1.84	0.42
1:I:98:LYS:HD3	1:I:105:TYR:CD2	2.54	0.42
2:K:1:ASP:HB3	2:K:2:ILE:H	1.50	0.42
3:C:111:ARG:CZ	3:C:128:GLU:HG3	2.49	0.42
2:J:8:PRO:HG2	2:J:11:LEU:HD23	2.00	0.42
2:J:102:THR:HG22	2:J:104:VAL:HG23	2.01	0.42
1:I:57:GLU:CG	5:M:1:ARG:NH2	2.77	0.42
1:I:38:ARG:HD3	1:I:94:TYR:CE2	2.55	0.42
5:T:5:ASN:OD1	5:T:6:ALA:N	2.50	0.42
1:I:98:LYS:HD3	1:I:105:TYR:HD2	1.84	0.42
2:K:151:ASP:CG	2:K:190:LYS:H	2.28	0.42
2:K:179:LEU:N	2:K:179:LEU:HD22	2.35	0.42
3:C:181:ARG:HG2	3:C:181:ARG:NH1	2.23	0.42
1:G:20:LEU:HG	1:G:83:MET:HE3	2.02	0.42
2:J:184:ALA:O	2:J:188:LYS:HG3	2.19	0.42
4:B:39:LEU:HA	4:B:39:LEU:HD23	1.83	0.42
2:K:139:PHE:O	2:K:172:THR:HB	2.20	0.42
2:K:163:VAL:HG22	2:K:175:LEU:HB3	2.00	0.42
2:J:23:CYS:HB3	2:J:71:PHE:HB2	2.01	0.42
2:K:108:ARG:NE	2:K:171:SER:HB2	2.29	0.42
1:I:52:ASP:HB2	1:I:53:PRO:HD2	2.02	0.42
3:A:13:SER:HA	3:A:20:PRO:HB3	2.01	0.42
1:I:148:TYR:CE2	1:I:153:VAL:HB	2.55	0.42
1:G:20:LEU:O	1:G:80:TYR:HA	2.20	0.42
1:I:122:PRO:HB3	1:I:148:TYR:HB3	2.01	0.42
3:C:204:TRP:CE3	3:C:206:LEU:HD21	2.55	0.42
3:A:44:ARG:NH2	3:A:61:ASP:OD1	2.50	0.41
2:J:11:LEU:HD12	2:J:11:LEU:O	2.20	0.41
3:A:121:LYS:HB2	4:B:1:ILE:HD11	2.02	0.41
1:I:137:GLY:O	1:I:188:PRO:HA	2.20	0.41
1:I:137:GLY:O	1:I:189:SER:N	2.37	0.41
3:A:6:ARG:HG2	3:A:6:ARG:HH11	1.86	0.41
4:B:29:GLY:HA2	4:B:61:SER:HB2	2.01	0.41
3:C:110:LEU:HD23	3:C:110:LEU:HA	1.93	0.41
3:C:168:LEU:O	3:C:172:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:ARG:NH1	4:D:99:MET:HG2	2.35	0.41
1:G:203:HIS:CD2	1:G:205:PRO:HD2	2.56	0.41
2:J:78:LEU:HD12	2:J:78:LEU:HA	1.72	0.41
3:A:165:VAL:O	3:A:169:ARG:HG3	2.20	0.41
2:K:23:CYS:HB2	2:K:35:TRP:CH2	2.56	0.41
2:J:1:ASP:HB3	2:J:2:ILE:H	1.34	0.41
3:C:13:SER:HA	3:C:20:PRO:HB3	2.02	0.41
1:G:136:GLY:C	1:G:138:THR:N	2.72	0.41
2:J:139:PHE:O	2:J:172:THR:HB	2.21	0.41
2:K:148:TRP:CD1	2:K:179:LEU:HD11	2.56	0.41
2:K:161:GLU:HA	2:K:176:SER:O	2.21	0.41
3:C:22:PHE:CD2	3:C:71:SER:HB2	2.55	0.41
3:C:215:LEU:CD2	3:C:261:VAL:HG22	2.51	0.41
4:D:70:PHE:CE1	4:D:78:TYR:CE2	3.09	0.41
2:J:166:GLN:HE21	2:J:171:SER:HB3	1.85	0.41
3:A:81:LEU:HD13	3:A:118:TYR:CD1	2.56	0.41
2:K:6:GLN:NE2	2:K:102:THR:HG1	2.11	0.41
3:C:107:TRP:O	3:C:169:ARG:NH1	2.46	0.41
4:D:29:GLY:HA2	4:D:61:SER:CB	2.49	0.41
3:A:111:ARG:CZ	3:A:128:GLU:HG3	2.51	0.40
3:A:270:LEU:HD23	3:A:270:LEU:HA	1.76	0.40
1:G:51:ILE:HB	1:G:70:ILE:HD13	2.03	0.40
2:J:37:GLN:O	2:J:37:GLN:HG2	2.21	0.40
2:J:164:THR:HG23	1:I:169:PHE:CE1	2.57	0.40
3:A:211:ALA:HB2	3:A:241:PHE:CE2	2.56	0.40
3:C:36:PHE:CD1	3:C:36:PHE:C	2.98	0.40
2:J:100:GLN:CD	2:J:100:GLN:N	2.71	0.40
3:A:15:PRO:O	3:A:15:PRO:HG2	2.21	0.40
1:I:195:GLN:OE1	1:I:196:THR:N	2.54	0.40

There are no symmetry-related clashes.

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	G	216/244 (88%)	208 (96%)	8 (4%)	0	100	100
1	I	216/244 (88%)	209 (97%)	7 (3%)	0	100	100
2	J	212/233 (91%)	204 (96%)	8 (4%)	0	100	100
2	K	212/233 (91%)	203 (96%)	9 (4%)	0	100	100
3	A	273/282 (97%)	268 (98%)	5 (2%)	0	100	100
3	C	273/282 (97%)	265 (97%)	8 (3%)	0	100	100
4	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
4	D	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
5	M	7/9 (78%)	7 (100%)	0	0	100	100
5	T	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1612/1736 (93%)	1564 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	G	182/204 (89%)	181 (100%)	1 (0%)	81	86
1	I	182/204 (89%)	182 (100%)	0	100	100
2	J	188/203 (93%)	181 (96%)	7 (4%)	30	61
2	K	188/203 (93%)	185 (98%)	3 (2%)	55	76
3	A	231/238 (97%)	230 (100%)	1 (0%)	84	87
3	C	231/238 (97%)	230 (100%)	1 (0%)	84	87
4	B	95/95 (100%)	95 (100%)	0	100	100
4	D	95/95 (100%)	95 (100%)	0	100	100
5	M	8/8 (100%)	8 (100%)	0	100	100
5	T	8/8 (100%)	8 (100%)	0	100	100
All	All	1408/1496 (94%)	1395 (99%)	13 (1%)	70	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	218	SER
2	J	12	SER
2	J	37	GLN
2	J	52	SER
2	J	55	GLN
2	J	63	SER
2	J	102	THR
2	J	201	LEU
3	A	72	GLN
2	K	54	LEU
2	K	55	GLN
2	K	90	GLN
3	C	173	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	89	GLN
2	J	90	GLN
2	J	160	GLN
2	J	166	GLN
3	A	72	GLN
3	A	145	HIS
3	A	188	HIS
3	A	253	GLN
4	B	83	ASN
1	I	84	ASN
1	I	174	GLN
2	K	6	GLN
2	K	90	GLN
2	K	137	ASN
2	K	155	GLN
3	C	141	GLN
3	C	218	GLN
4	D	17	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	G	218/244 (89%)	-0.57	0 100 100	54, 84, 141, 188	0
1	I	218/244 (89%)	-0.66	0 100 100	54, 79, 135, 198	0
2	J	214/233 (91%)	-0.64	0 100 100	56, 85, 127, 180	0
2	K	214/233 (91%)	-0.36	0 100 100	54, 103, 155, 194	0
3	A	275/282 (97%)	-0.71	0 100 100	53, 77, 119, 147	0
3	C	275/282 (97%)	-0.72	0 100 100	52, 77, 109, 135	0
4	B	100/100 (100%)	-0.59	0 100 100	65, 96, 131, 149	0
4	D	100/100 (100%)	-0.51	0 100 100	66, 98, 127, 140	0
5	M	9/9 (100%)	-0.54	0 100 100	58, 65, 75, 77	0
5	T	9/9 (100%)	-0.49	0 100 100	59, 63, 72, 85	0
All	All	1632/1736 (94%)	-0.61	0 100 100	52, 83, 135, 198	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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 ⓘ

There are no such residues in this entry.