



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:48 PM UTC

PDB ID : 9GV6 / pdb_00009gv6
Title : Structure of TCR in complex with peptide-HLA
Authors : Karuppiah, V.
Deposited on : 2024-09-23
Resolution : 2.77 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	:	9.0.010 (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

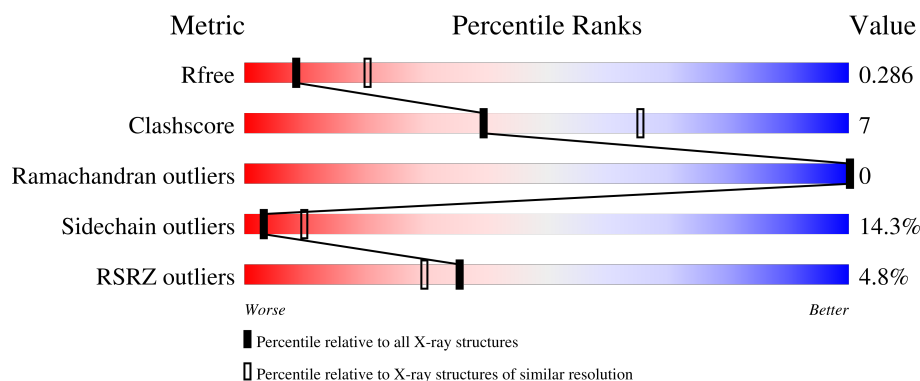
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	276	2% 75% 21% • •
1	G	276	4% 75% 19% 5% •
2	B	100	8% 82% 13% 5%
2	H	100	3% 83% 14% • •
3	C	9	11% 33% 44% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	9	44%44%11%
4	D	196	5% 67%22%5% • 6%
4	J	196	9% 68%20%5% • 6%
5	E	247	3% 72%22% • •
5	K	247	5% 70%22%6% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13165 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	G	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	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	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			79	52	13	14			
3	I	9	Total	C	N	O	0	0	0
			79	52	13	14			

- Molecule 4 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	185	Total	C	N	O	S	0	0	0
			1452	911	242	290	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	185	Total	C	N	O	S	0	0	0
			1452	911	242	290	9			

- Molecule 5 is a protein called TCR Beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1955	1241	341	368	5			
5	K	245	Total	C	N	O	S	0	0	0
			1955	1241	341	368	5			

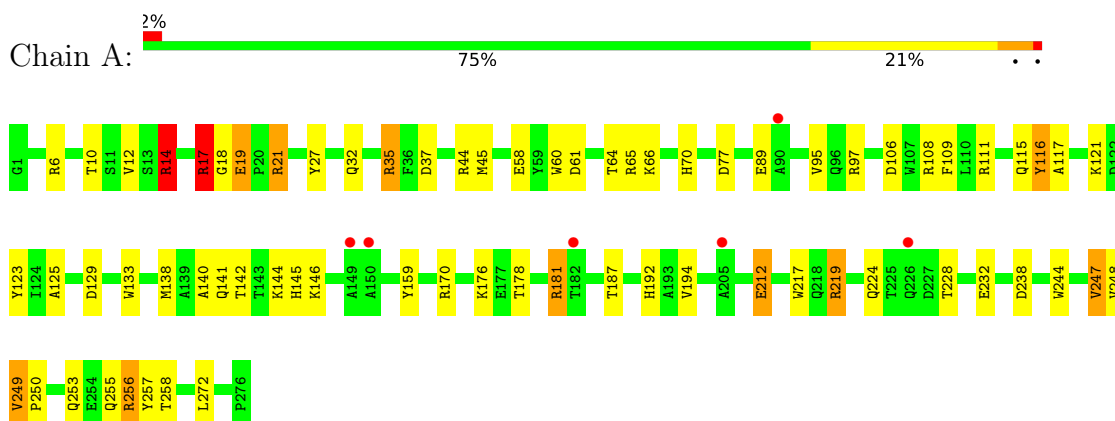
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		
6	E	1	Total	O	0	0
			1	1		
6	K	2	Total	O	0	0
			2	2		

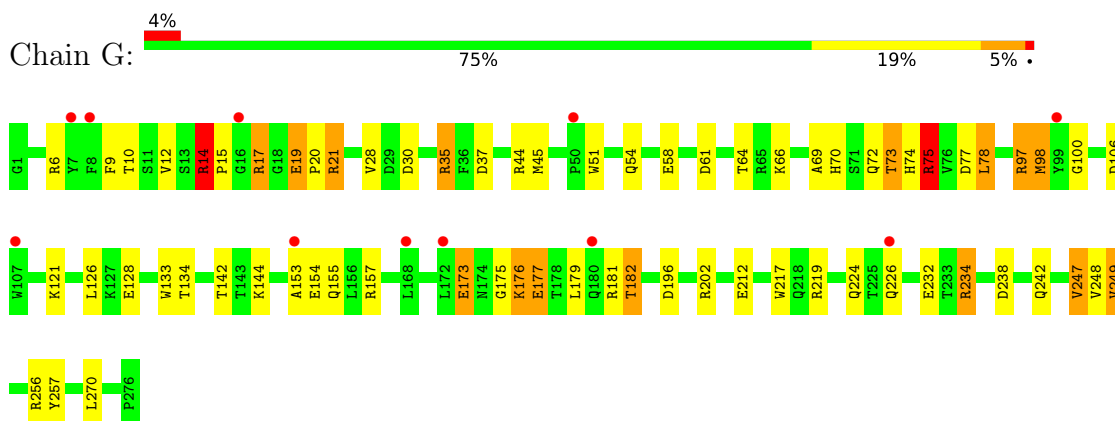
3 Residue-property plots [i](#)

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.

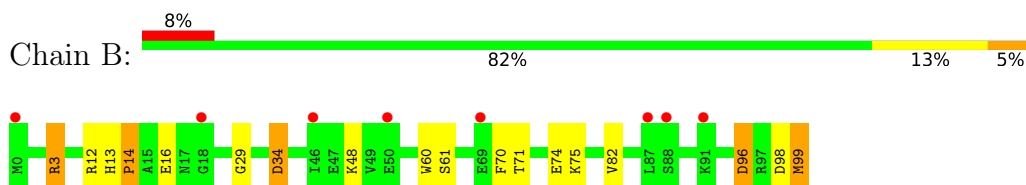
- Molecule 1: MHC class I antigen



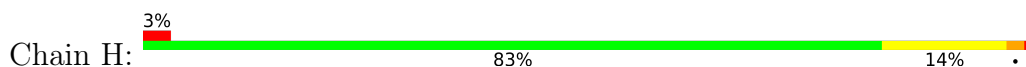
- Molecule 1: MHC class I antigen

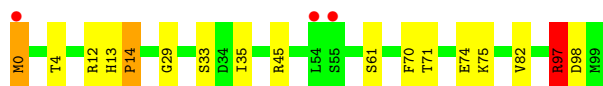


- Molecule 2: Beta-2-microglobulin

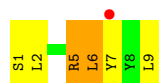


- Molecule 2: Beta-2-microglobulin





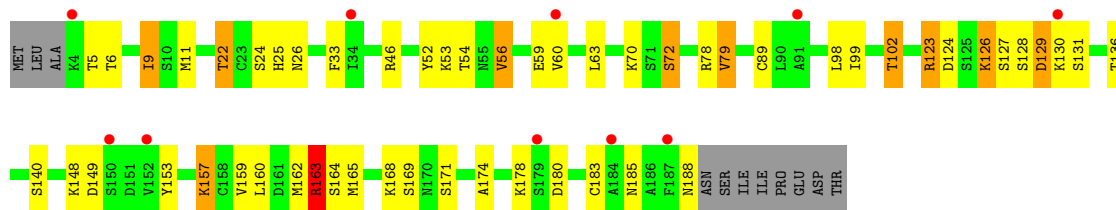
- Molecule 3: Peptide



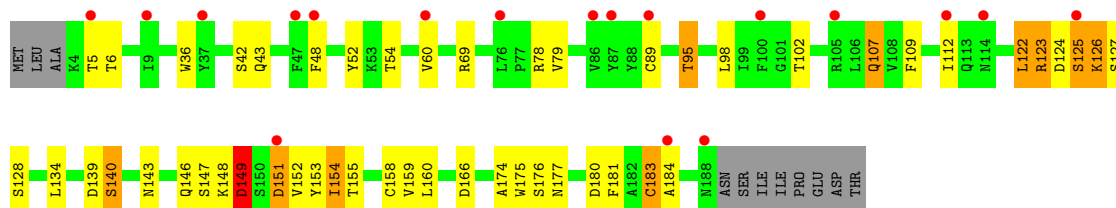
- Molecule 3: Peptide



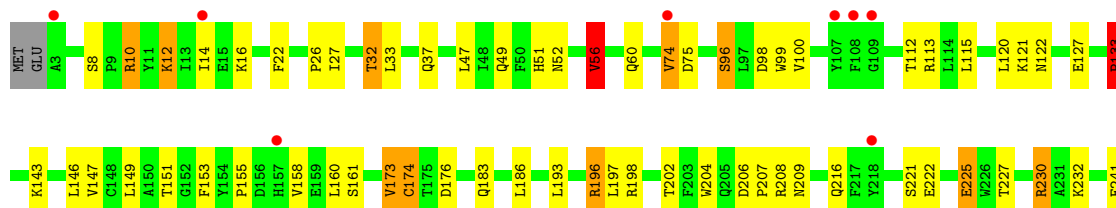
- Molecule 4: TCR alpha



- Molecule 4: TCR alpha



- Molecule 5: TCR Beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.12Å 93.53Å 388.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.94 – 2.77 90.94 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.3 (90.94-2.77) 97.6 (90.94-2.77)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.217 , 0.274 0.237 , 0.286	Depositor DCC
R_{free} test set	3492 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13165	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	A	0.65	0/2320	1.19	7/3149 (0.2%)
1	G	0.64	0/2320	1.14	8/3149 (0.3%)
2	B	0.63	0/860	1.14	4/1162 (0.3%)
2	H	0.64	0/860	1.06	2/1162 (0.2%)
3	C	0.77	0/80	1.22	1/107 (0.9%)
3	I	0.65	0/80	1.25	0/107
4	D	0.80	0/1486	1.26	5/2019 (0.2%)
4	J	0.68	0/1486	1.21	5/2019 (0.2%)
5	E	0.74	0/2009	1.29	7/2734 (0.3%)
5	K	0.70	0/2009	1.23	10/2734 (0.4%)
All	All	0.69	0/13510	1.20	49/18342 (0.3%)

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	7
1	G	0	6
2	B	0	2
2	H	0	2
3	C	0	1
3	I	0	1
4	D	0	3
5	E	0	4
5	K	0	4
All	All	0	30

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	74	VAL	CB-CA-C	-7.82	98.47	111.29
5	E	74	VAL	N-CA-C	7.70	125.36	109.34
2	B	96	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	61	ASP	CA-CB-CG	6.63	119.23	112.60
1	G	61	ASP	CA-CB-CG	6.62	119.22	112.60
4	J	151	ASP	CA-CB-CG	6.61	119.20	112.60
1	A	238	ASP	CA-CB-CG	6.32	118.92	112.60
4	D	79	VAL	N-CA-C	6.31	117.72	109.58
1	G	106	ASP	CA-CB-CG	6.21	118.81	112.60
5	K	218	TYR	CB-CA-C	6.19	119.95	109.80
1	A	129	ASP	CA-CB-CG	6.04	118.64	112.60
5	E	153	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	212	GLU	CB-CG-CD	-5.94	102.50	112.60
5	E	56	VAL	N-CA-CB	-5.93	100.66	110.56
5	K	60	GLN	N-CA-CB	-5.86	102.03	110.65
5	K	227	THR	CA-CB-OG1	-5.79	100.92	109.60
1	A	106	ASP	CA-CB-CG	5.70	118.30	112.60
1	G	58	GLU	N-CA-CB	5.67	119.07	110.28
2	B	34	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	146	LYS	N-CA-CB	5.49	118.03	110.07
5	E	133	PRO	N-CA-CB	-5.46	98.73	103.32
5	K	98	ASP	CA-CB-CG	5.44	118.04	112.60
1	G	30	ASP	CA-CB-CG	5.44	118.04	112.60
2	B	71	THR	CA-CB-OG1	-5.43	101.46	109.60
5	K	247	ASP	CA-CB-CG	5.40	118.00	112.60
4	D	102	THR	CA-CB-OG1	-5.38	101.52	109.60
3	C	9	LEU	CA-C-O	-5.37	111.67	120.80
5	E	98	ASP	CA-CB-CG	5.35	117.95	112.60
5	K	202	THR	CA-CB-OG1	-5.35	101.57	109.60
5	K	60	GLN	CB-CA-C	5.35	118.53	109.55
1	G	238	ASP	CA-CB-CG	5.34	117.94	112.60
4	D	78	ARG	CB-CA-C	-5.32	104.45	111.42
5	K	155	PRO	N-CA-CB	-5.31	96.76	102.60
2	H	71	THR	CA-CB-OG1	-5.30	101.65	109.60
1	G	134	THR	CA-CB-OG1	-5.28	101.67	109.60
4	D	22	THR	CA-CB-OG1	-5.26	101.71	109.60
2	B	48	LYS	N-CA-CB	-5.26	101.61	110.49
4	D	33	PHE	CA-CB-CG	5.19	118.99	113.80
4	J	149	ASP	CA-CB-CG	5.18	117.78	112.60
4	J	102	THR	CA-CB-OG1	-5.17	101.84	109.60
4	J	78	ARG	CB-CA-C	-5.17	105.02	111.43
5	K	58	ASP	CA-CB-CG	5.13	117.73	112.60
2	H	4	THR	CB-CA-C	5.12	116.45	108.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	225	GLU	CB-CA-C	5.12	118.96	109.54
4	J	166	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	17	ARG	N-CA-C	-5.08	107.05	113.20
5	E	202	THR	CA-CB-OG1	-5.03	102.05	109.60
1	G	196	ASP	CA-CB-CG	5.03	117.62	112.60
1	G	126	LEU	N-CA-CB	-5.02	101.88	110.16

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	17	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	181	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	256	ARG	Sidechain
1	A	35	ARG	Sidechain
2	B	12	ARG	Sidechain
2	B	3	ARG	Sidechain
3	C	5	ARG	Sidechain
4	D	123	ARG	Sidechain
4	D	163	ARG	Sidechain
4	D	46	ARG	Sidechain
5	E	113	ARG	Sidechain
5	E	196	ARG	Sidechain
5	E	198	ARG	Sidechain
5	E	230	ARG	Sidechain
1	G	14	ARG	Sidechain
1	G	157	ARG	Sidechain
1	G	181	ARG	Sidechain
1	G	234	ARG	Sidechain
1	G	35	ARG	Sidechain
1	G	75	ARG	Sidechain
2	H	12	ARG	Sidechain
2	H	97	ARG	Sidechain
3	I	5	ARG	Sidechain
5	K	10	ARG	Sidechain
5	K	17	ARG	Sidechain
5	K	196	ARG	Sidechain
5	K	70	ARG	Sidechain

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	2254	0	2103	31	0
1	G	2254	0	2103	32	0
2	B	837	0	805	8	0
2	H	837	0	805	4	0
3	C	79	0	82	4	0
3	I	79	0	82	5	0
4	D	1452	0	1372	18	0
4	J	1452	0	1372	25	0
5	E	1955	0	1880	30	0
5	K	1955	0	1880	31	0
6	A	6	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	K	2	0	0	0	0
All	All	13165	0	12484	167	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 7.

All (167) 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)
5:E:26:PRO:CD	5:E:74:VAL:O	2.22	0.88
5:E:10:ARG:HB2	5:E:10:ARG:HH11	1.41	0.86
4:D:52:TYR:CE2	4:D:53:LYS:HD2	2.27	0.70
5:K:232:LYS:HG2	5:K:234:VAL:HG13	1.74	0.69
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.29	0.68
1:G:6:ARG:HD3	1:G:100:GLY:HA3	1.76	0.66
5:E:26:PRO:CG	5:E:74:VAL:O	2.43	0.66
4:J:160:LEU:HA	5:K:174:CYS:HB2	1.76	0.65
5:E:26:PRO:HD2	5:E:74:VAL:O	1.98	0.64
5:K:186:LEU:HD23	5:K:187:ASN:H	1.62	0.63
4:D:25:HIS:NE2	4:D:72:SER:HB3	2.14	0.62
1:A:97:ARG:NH1	1:A:116:TYR:HE2	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:149:ASP:HB2	4:J:152:VAL:HG22	1.82	0.62
4:J:109:PHE:HB3	4:J:140:SER:OG	2.00	0.61
5:K:65:ARG:NH2	5:K:87:ASP:OD1	2.34	0.60
1:G:217:TRP:CE2	1:G:247:VAL:HG22	2.37	0.60
4:J:112:ILE:HG13	4:J:139:ASP:HA	1.82	0.60
5:K:226:TRP:HB2	5:K:232:LYS:HD3	1.84	0.60
5:K:60:GLN:HA	5:K:60:GLN:OE1	2.02	0.59
5:K:170:HIS:O	5:K:173:VAL:HG13	2.04	0.58
5:K:207:PRO:HA	5:K:244:GLY:O	2.04	0.58
1:A:217:TRP:CE2	1:A:247:VAL:HG22	2.38	0.57
4:J:158:CYS:HB3	5:K:196:ARG:NH1	2.19	0.57
5:E:74:VAL:HG12	5:E:75:ASP:N	2.16	0.56
4:J:160:LEU:HA	5:K:174:CYS:CB	2.35	0.56
5:E:207:PRO:HA	5:E:244:GLY:O	2.05	0.56
5:E:26:PRO:HG3	5:E:74:VAL:O	2.06	0.56
1:G:173:GLU:HA	1:G:176:LYS:HD3	1.91	0.53
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.74	0.53
1:G:77:ASP:HB3	3:I:9:LEU:HD12	1.89	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.52
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.91	0.52
2:B:98:ASP:C	2:B:99:MET:HG2	2.35	0.52
1:A:70:HIS:CD2	3:C:6:LEU:HD21	2.46	0.51
1:G:153:ALA:O	1:G:154:GLU:C	2.53	0.51
2:H:29:GLY:HA2	2:H:61:SER:OG	2.09	0.51
1:A:17:ARG:HE	1:A:17:ARG:H	1.59	0.51
1:A:77:ASP:OD2	1:A:116:TYR:OH	2.23	0.51
5:E:204:TRP:O	5:E:204:TRP:CG	2.64	0.51
5:K:157:HIS:HB3	5:K:218:TYR:HB2	1.93	0.51
5:K:13:ILE:HG23	5:K:117:LEU:HD23	1.93	0.50
5:K:133:PRO:HD2	5:K:204:TRP:CZ2	2.46	0.50
5:E:221:SER:O	5:E:232:LYS:NZ	2.44	0.50
4:D:9:ILE:HD12	4:D:9:ILE:H	1.76	0.50
4:D:26:ASN:HD22	4:D:70:LYS:HB3	1.77	0.49
1:G:70:HIS:CD2	3:I:6:LEU:HD21	2.47	0.49
1:G:66:LYS:HG3	4:J:95:THR:HG21	1.95	0.49
1:G:234:ARG:HG2	1:G:242:GLN:HB2	1.95	0.49
1:G:175:GLY:O	1:G:176:LYS:C	2.56	0.49
5:E:133:PRO:HD3	5:E:146:LEU:HG	1.93	0.49
2:B:96:ASP:CG	2:B:99:MET:HG3	2.38	0.49
1:A:65:ARG:NH1	5:E:49:GLN:OE1	2.46	0.48
4:D:162:MET:O	4:D:163:ARG:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:ASP:C	4:D:126:LYS:H	2.22	0.48
1:G:51:TRP:O	1:G:54:GLN:HG2	2.13	0.48
4:J:122:LEU:HD23	5:K:133:PRO:HA	1.95	0.48
1:G:17:ARG:C	1:G:19:GLU:H	2.22	0.48
1:A:27:TYR:CE2	1:A:32:GLN:HB2	2.49	0.48
1:A:187:THR:HB	1:A:272:LEU:HD11	1.95	0.48
1:A:219:ARG:HD2	1:A:256:ARG:CZ	2.44	0.48
1:A:95:VAL:HG11	1:A:116:TYR:HE1	1.78	0.47
4:D:163:ARG:O	4:D:164:SER:C	2.56	0.47
5:E:10:ARG:HH11	5:E:10:ARG:CB	2.20	0.47
5:K:35:TRP:O	5:K:47:LEU:HB2	2.15	0.47
5:E:22:PHE:HD2	5:E:112:THR:HG21	1.80	0.47
5:K:212:ARG:HD2	5:K:239:SER:OG	2.14	0.47
5:K:22:PHE:CD1	5:K:22:PHE:N	2.83	0.47
5:K:229:ASP:OD1	5:K:229:ASP:N	2.44	0.47
1:G:28:VAL:HG11	1:G:179:LEU:HD13	1.95	0.47
1:G:21:ARG:NH1	1:G:37:ASP:OD1	2.48	0.47
2:B:3:ARG:HH11	2:B:3:ARG:CG	2.28	0.46
5:E:22:PHE:N	5:E:22:PHE:CD1	2.83	0.46
5:K:204:TRP:O	5:K:204:TRP:CG	2.67	0.46
1:A:21:ARG:NH1	1:A:37:ASP:OD1	2.49	0.46
2:B:29:GLY:HA2	2:B:61:SER:OG	2.15	0.46
1:G:133:TRP:HB2	1:G:144:LYS:HG3	1.97	0.46
4:D:185:ASN:O	4:D:188:ASN:HB2	2.16	0.46
1:G:73:THR:HG21	3:I:6:LEU:HB3	1.98	0.45
4:J:5:THR:HG21	4:J:89:CYS:O	2.17	0.45
1:G:44:ARG:HA	1:G:64:THR:HG23	1.97	0.45
1:G:45:MET:CE	3:I:2:LEU:HD11	2.46	0.45
5:E:51:HIS:O	5:E:52:ASN:C	2.59	0.45
1:G:74:HIS:O	1:G:75:ARG:C	2.60	0.45
4:J:122:LEU:HD11	4:J:134:LEU:HB2	1.97	0.45
1:G:98:MET:HE3	1:G:98:MET:HB3	1.84	0.45
1:G:72:GLN:O	1:G:75:ARG:HG2	2.17	0.45
2:H:13:HIS:O	2:H:14:PRO:C	2.60	0.44
1:G:176:LYS:O	1:G:177:GLU:C	2.61	0.44
5:K:160:LEU:C	5:K:160:LEU:HD23	2.43	0.44
4:D:11:MET:HE3	4:D:11:MET:HB2	1.73	0.44
4:D:56:VAL:HG23	4:D:63:LEU:HB3	1.98	0.44
4:D:153:TYR:O	4:D:174:ALA:HA	2.17	0.44
4:J:124:ASP:O	4:J:125:SER:C	2.60	0.44
4:J:153:TYR:O	4:J:174:ALA:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:SER:O	4:D:129:ASP:C	2.60	0.44
1:A:123:TYR:CE1	1:A:140:ALA:HB2	2.53	0.44
4:D:127:SER:O	4:D:128:SER:C	2.61	0.44
5:E:12:LYS:HA	5:E:12:LYS:HD2	1.72	0.44
1:G:219:ARG:HD2	1:G:256:ARG:CZ	2.48	0.44
4:J:147:SER:HB3	4:J:154:ILE:HG13	2.00	0.44
1:A:44:ARG:HA	1:A:64:THR:HG23	1.99	0.44
5:E:225:GLU:H	5:E:225:GLU:HG2	1.54	0.44
2:B:13:HIS:O	2:B:14:PRO:C	2.60	0.44
4:D:157:LYS:H	4:D:157:LYS:HG2	1.44	0.44
4:J:122:LEU:HB3	5:K:132:GLU:O	2.18	0.44
5:E:26:PRO:HD3	5:E:74:VAL:O	2.13	0.43
1:G:77:ASP:O	1:G:78:LEU:C	2.61	0.43
2:H:97:ARG:HE	2:H:97:ARG:HB3	1.60	0.43
1:A:45:MET:CE	3:C:2:LEU:HD11	2.48	0.43
4:D:126:LYS:HE2	4:D:126:LYS:HB3	1.52	0.43
5:E:32:THR:HG23	5:E:96:SER:CB	2.48	0.43
4:J:123:ARG:HA	4:J:123:ARG:HD3	1.36	0.43
1:A:18:GLY:O	1:A:19:GLU:C	2.61	0.43
3:C:5:ARG:HB3	3:C:7:TYR:HE1	1.82	0.43
4:J:183:CYS:O	4:J:184:ALA:C	2.61	0.43
1:G:72:GLN:O	1:G:73:THR:C	2.61	0.43
3:I:4:ASN:HA	4:J:95:THR:HG22	2.00	0.43
1:A:14:ARG:HB2	1:A:17:ARG:HB2	2.01	0.43
1:A:138:MET:O	1:A:141:GLN:HB3	2.18	0.43
1:A:253:GLN:HB3	1:A:256:ARG:HD3	2.01	0.43
5:E:174:CYS:O	5:E:174:CYS:SG	2.76	0.43
1:G:19:GLU:HA	1:G:20:PRO:HD2	1.91	0.43
4:J:126:LYS:HB3	4:J:127:SER:H	1.62	0.43
5:K:55:VAL:HG11	5:K:58:ASP:HB3	2.00	0.43
5:K:65:ARG:HH21	5:K:87:ASP:CG	2.27	0.43
5:K:115:LEU:HD12	5:K:115:LEU:HA	1.87	0.43
5:E:121:LYS:HZ2	5:E:227:THR:H	1.66	0.42
1:G:69:ALA:HB2	5:K:99:TRP:CH2	2.54	0.42
1:G:182:THR:O	1:G:182:THR:CG2	2.66	0.42
1:A:44:ARG:HH12	1:A:60:TRP:HB3	1.84	0.42
1:A:133:TRP:O	1:A:144:LYS:HE3	2.19	0.42
1:A:244:TRP:CZ2	2:B:99:MET:CE	3.02	0.42
2:H:0:MET:HE3	2:H:0:MET:HB3	1.59	0.42
5:E:206:ASP:HB3	5:E:209:ASN:ND2	2.34	0.42
1:A:115:GLN:HG2	1:A:125:ALA:HB1	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:VAL:HG22	1:G:257:TYR:CE1	2.54	0.42
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.55	0.42
1:G:9:PHE:HB2	1:G:97:ARG:HB3	2.02	0.42
5:K:226:TRP:CZ2	5:K:233:PRO:HD3	2.55	0.42
5:K:135:GLU:HA	5:K:138:ILE:HG12	2.02	0.42
5:E:160:LEU:C	5:E:160:LEU:HD23	2.45	0.42
5:E:221:SER:OG	5:E:222:GLU:N	2.47	0.42
4:J:155:THR:HG23	4:J:175:TRP:HZ3	1.85	0.41
5:K:120:LEU:HD12	5:K:120:LEU:HA	1.83	0.41
1:A:97:ARG:NH1	1:A:116:TYR:CE2	2.84	0.41
4:J:176:SER:HB3	4:J:181:PHE:HB2	2.01	0.41
1:A:249:VAL:HA	1:A:250:PRO:HD2	1.81	0.41
4:J:107:GLN:HE21	4:J:107:GLN:HB2	1.57	0.41
1:A:159:TYR:OH	3:C:1:SER:O	2.37	0.41
5:E:173:VAL:HA	5:E:196:ARG:O	2.20	0.41
4:D:9:ILE:HG23	4:D:102:THR:HG21	2.03	0.41
4:D:163:ARG:HE	4:D:163:ARG:HB3	1.67	0.41
4:J:125:SER:HA	5:K:130:VAL:O	2.20	0.41
1:A:244:TRP:CZ2	2:B:99:MET:HE3	2.56	0.41
5:E:26:PRO:HB3	5:E:33:LEU:HD12	2.02	0.41
5:E:176:ASP:HB2	5:E:193:LEU:HD12	2.02	0.41
4:D:5:THR:HG21	4:D:89:CYS:O	2.21	0.41
1:G:14:ARG:O	1:G:15:PRO:C	2.64	0.41
4:J:36:TRP:O	4:J:48:PHE:HB3	2.21	0.41
4:J:52:TYR:O	4:J:69:ARG:NH1	2.48	0.41
5:E:56:VAL:HG13	5:E:99:TRP:CH2	2.57	0.40
5:K:23:TRP:CH2	5:K:25:ASN:HB2	2.56	0.40
5:K:69:GLU:OE2	5:K:72:LYS:NZ	2.53	0.40
1:A:109:PHE:CE1	1:A:111:ARG:C	2.99	0.40
5:E:37:GLN:HB2	5:E:47:LEU:HD11	2.03	0.40
5:E:173:VAL:HG12	5:E:197:LEU:HD13	2.02	0.40
1:G:66:LYS:HG3	4:J:95:THR:CG2	2.52	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	A	274/276 (99%)	256 (93%)	18 (7%)	0	100	100
1	G	274/276 (99%)	250 (91%)	24 (9%)	0	100	100
2	B	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
2	H	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	183/196 (93%)	160 (87%)	23 (13%)	0	100	100
4	J	183/196 (93%)	167 (91%)	16 (9%)	0	100	100
5	E	243/247 (98%)	227 (93%)	16 (7%)	0	100	100
5	K	243/247 (98%)	223 (92%)	20 (8%)	0	100	100
All	All	1610/1656 (97%)	1478 (92%)	132 (8%)	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	A	232/232 (100%)	203 (88%)	29 (12%)	4	13
1	G	232/232 (100%)	203 (88%)	29 (12%)	4	13
2	B	95/95 (100%)	87 (92%)	8 (8%)	10	29
2	H	95/95 (100%)	84 (88%)	11 (12%)	5	16
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	18
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	18
4	D	166/176 (94%)	134 (81%)	32 (19%)	1	4
4	J	166/176 (94%)	141 (85%)	25 (15%)	3	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	211/213 (99%)	178 (84%)	33 (16%)	2	8
5	K	211/213 (99%)	176 (83%)	35 (17%)	2	7
All	All	1426/1450 (98%)	1222 (86%)	204 (14%)	3	10

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	12	VAL
1	A	14	ARG
1	A	17	ARG
1	A	19	GLU
1	A	21	ARG
1	A	35	ARG
1	A	58	GLU
1	A	66	LYS
1	A	89	GLU
1	A	108	ARG
1	A	116	TYR
1	A	121	LYS
1	A	142	THR
1	A	145	HIS
1	A	176	LYS
1	A	178	THR
1	A	181	ARG
1	A	192	HIS
1	A	194	VAL
1	A	212	GLU
1	A	224	GLN
1	A	228	THR
1	A	232	GLU
1	A	247	VAL
1	A	248	VAL
1	A	249	VAL
1	A	255	GLN
1	A	258	THR
2	B	14	PRO
2	B	16	GLU
2	B	34	ASP
2	B	70	PHE
2	B	74	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	75	LYS
2	B	82	VAL
2	B	99	MET
3	C	6	LEU
4	D	6	THR
4	D	9	ILE
4	D	22	THR
4	D	24	SER
4	D	54	THR
4	D	56	VAL
4	D	59	GLU
4	D	60	VAL
4	D	72	SER
4	D	79	VAL
4	D	98	LEU
4	D	99	ILE
4	D	123	ARG
4	D	126	LYS
4	D	129	ASP
4	D	130	LYS
4	D	131	SER
4	D	136	THR
4	D	140	SER
4	D	148	LYS
4	D	149	ASP
4	D	157	LYS
4	D	159	VAL
4	D	160	LEU
4	D	163	ARG
4	D	165	MET
4	D	168	LYS
4	D	169	SER
4	D	171	SER
4	D	178	LYS
4	D	180	ASP
4	D	183	CYS
5	E	8	SER
5	E	10	ARG
5	E	12	LYS
5	E	14	ILE
5	E	16	LYS
5	E	27	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	32	THR
5	E	56	VAL
5	E	60	GLN
5	E	96	SER
5	E	100	VAL
5	E	115	LEU
5	E	120	LEU
5	E	122	ASN
5	E	127	GLU
5	E	133	PRO
5	E	143	LYS
5	E	147	VAL
5	E	149	LEU
5	E	151	THR
5	E	155	PRO
5	E	158	VAL
5	E	161	SER
5	E	173	VAL
5	E	174	CYS
5	E	183	GLN
5	E	186	LEU
5	E	208	ARG
5	E	216	GLN
5	E	225	GLU
5	E	230	ARG
5	E	241	GLU
5	E	245	ARG
1	G	10	THR
1	G	12	VAL
1	G	14	ARG
1	G	17	ARG
1	G	19	GLU
1	G	21	ARG
1	G	35	ARG
1	G	73	THR
1	G	75	ARG
1	G	78	LEU
1	G	97	ARG
1	G	98	MET
1	G	121	LYS
1	G	128	GLU
1	G	142	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	155	GLN
1	G	173	GLU
1	G	176	LYS
1	G	177	GLU
1	G	182	THR
1	G	202	ARG
1	G	212	GLU
1	G	224	GLN
1	G	226	GLN
1	G	232	GLU
1	G	247	VAL
1	G	248	VAL
1	G	249	VAL
1	G	270	LEU
2	H	0	MET
2	H	14	PRO
2	H	33	SER
2	H	35	ILE
2	H	45	ARG
2	H	70	PHE
2	H	74	GLU
2	H	75	LYS
2	H	82	VAL
2	H	97	ARG
2	H	98	ASP
3	I	6	LEU
4	J	6	THR
4	J	42	SER
4	J	43	GLN
4	J	54	THR
4	J	60	VAL
4	J	79	VAL
4	J	95	THR
4	J	98	LEU
4	J	107	GLN
4	J	122	LEU
4	J	123	ARG
4	J	125	SER
4	J	126	LYS
4	J	128	SER
4	J	140	SER
4	J	143	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	146	GLN
4	J	148	LYS
4	J	149	ASP
4	J	151	ASP
4	J	154	ILE
4	J	159	VAL
4	J	177	ASN
4	J	180	ASP
4	J	183	CYS
5	K	8	SER
5	K	14	ILE
5	K	16	LYS
5	K	18	GLN
5	K	32	THR
5	K	53	ASN
5	K	56	VAL
5	K	60	GLN
5	K	65	ARG
5	K	69	GLU
5	K	71	LEU
5	K	79	LYS
5	K	84	LYS
5	K	100	VAL
5	K	115	LEU
5	K	117	LEU
5	K	118	GLU
5	K	120	LEU
5	K	127	GLU
5	K	134	SER
5	K	151	THR
5	K	155	PRO
5	K	157	HIS
5	K	158	VAL
5	K	173	VAL
5	K	178	GLN
5	K	180	LEU
5	K	186	LEU
5	K	222	GLU
5	K	224	ASP
5	K	225	GLU
5	K	229	ASP
5	K	234	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	K	239	SER
5	K	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	180	GLN
1	A	192	HIS
2	B	83	ASN
4	D	20	ASN
4	D	26	ASN
4	D	43	GLN
5	E	7	GLN
5	E	60	GLN
5	E	106	GLN
5	E	170	HIS
5	E	223	ASN
1	G	43	GLN
1	G	114	HIS
1	G	192	HIS
2	H	83	ASN
4	J	107	GLN
4	J	111	ASN
5	K	7	GLN
5	K	228	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	276/276 (100%)	0.06	6 (2%) 62 55	65, 97, 141, 179	0
1	G	276/276 (100%)	0.40	11 (3%) 42 36	104, 124, 149, 171	0
2	B	100/100 (100%)	0.31	8 (8%) 18 14	76, 101, 134, 146	0
2	H	100/100 (100%)	0.33	3 (3%) 52 45	105, 132, 165, 183	0
3	C	9/9 (100%)	0.66	1 (11%) 10 8	73, 75, 80, 83	0
3	I	9/9 (100%)	0.64	0 100 100	92, 101, 112, 122	0
4	D	185/196 (94%)	0.43	10 (5%) 31 26	62, 88, 159, 202	0
4	J	185/196 (94%)	0.71	18 (9%) 13 10	30, 120, 173, 196	0
5	E	245/247 (99%)	0.15	8 (3%) 49 42	63, 86, 135, 174	1 (0%)
5	K	245/247 (99%)	0.45	13 (5%) 32 26	75, 104, 143, 175	1 (0%)
All	All	1630/1656 (98%)	0.34	78 (4%) 35 30	30, 109, 154, 202	2 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	K	167	LYS	5.8
4	J	114	ASN	5.0
5	K	163	TRP	4.4
5	K	166	GLY	4.3
4	J	105	ARG	4.3
4	J	48	PHE	4.1
1	A	150	ALA	4.1
1	G	107	TRP	4.0
5	E	107	TYR	3.6
1	G	172	LEU	3.6
4	J	188	ASN	3.5
5	K	178	GLN	3.5
5	E	108	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	150	SER	3.4
2	B	18	GLY	3.3
2	B	0	MET	3.2
4	J	47	PHE	3.2
4	D	91	ALA	3.2
4	J	87	TYR	3.2
5	K	177	PRO	3.1
4	J	125	SER	3.1
4	D	184	ALA	3.1
1	G	180	GLN	3.0
1	A	149	ALA	3.0
4	D	179	SER	3.0
5	E	14	ILE	2.9
4	J	76	LEU	2.9
1	G	226	GLN	2.9
1	A	205	ALA	2.8
2	B	69	GLU	2.8
4	J	100	PHE	2.8
5	K	169	VAL	2.7
4	J	86	VAL	2.7
4	J	37	TYR	2.7
2	H	0	MET	2.7
5	K	186	LEU	2.6
1	G	8	PHE	2.6
4	J	9	ILE	2.6
4	D	60	VAL	2.6
5	E	218	TYR	2.5
1	G	50	PRO	2.5
5	E	3	ALA	2.5
2	H	55	SER	2.5
5	K	156	ASP	2.5
5	E	109	GLY	2.5
5	K	65	ARG	2.4
1	G	168	LEU	2.4
4	J	5	THR	2.4
5	K	188	ASP	2.4
4	J	60	VAL	2.4
4	J	184	ALA	2.4
4	D	187	PHE	2.3
1	G	7	TYR	2.3
2	B	88	SER	2.3
5	K	238	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	54	LEU	2.3
5	E	157	HIS	2.3
1	A	182	THR	2.2
2	B	50	GLU	2.2
1	G	16	GLY	2.2
2	B	91	LYS	2.2
1	G	153	ALA	2.2
4	D	4	LYS	2.2
4	J	112	ILE	2.2
1	A	226	GLN	2.1
4	D	130	LYS	2.1
1	G	99	TYR	2.1
5	E	74	VAL	2.1
2	B	46	ILE	2.1
5	K	215	VAL	2.1
1	A	90	ALA	2.1
5	K	107	TYR	2.1
4	J	151	ASP	2.0
4	D	34	ILE	2.0
4	J	89	CYS	2.0
2	B	87	LEU	2.0
4	D	152	VAL	2.0
3	C	7	TYR	2.0

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 [i](#)

There are no such residues in this entry.