



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2025 – 12:14 PM JST

PDB ID : 9K2R / pdb_00009k2r
Title : Human T cell receptor (TRAV24*01/TRBV27*01) in complex with HLA-C*1202 and IY11 peptide
Authors : Chikata, T.; Kuroki, K.; Kuse, N.; Kliszczak, A.; Paes, W.; Tomioka, N.; Parker, R.; Aflalo, A.; Akahoshi, T.; Yamashita, R.; Sakata, R.; Kusaka, H.; Watanabe, Y.; Nicastrì, A.; Matsubara, H.; Ose, T.; Kita, S.; Oka, S.; Gatanaga, H.; Lin, Z.; Ternette, N.; Borrow, P.; Maenaka, K.; Takiguchi, M.
Deposited on : 2024-10-18
Resolution : 2.98 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engl & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

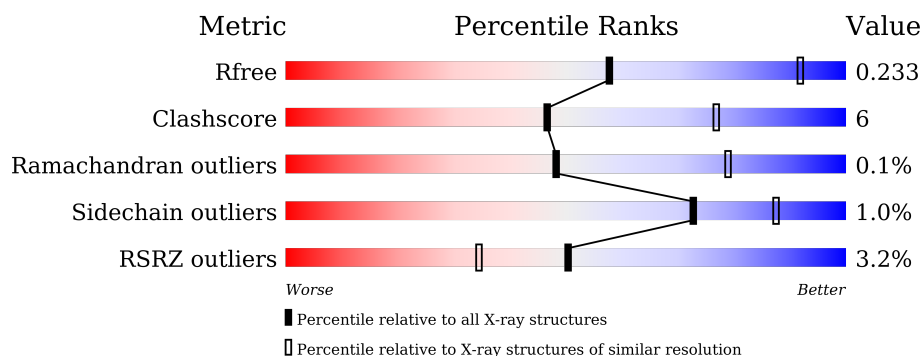
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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.



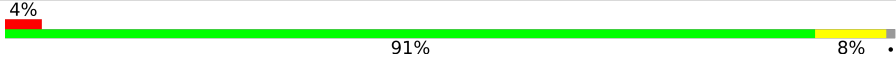




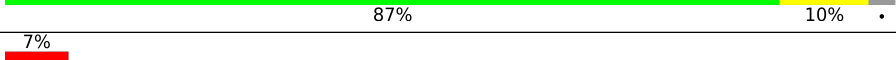

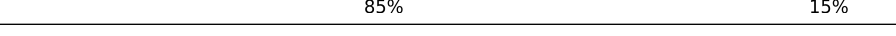
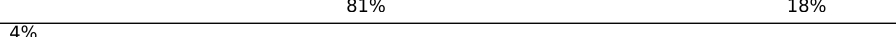

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

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	275	<div> <div>3%</div> <div>83% 16% .</div> </div>
1	D	275	<div> <div>3%</div> <div>83% 15% ..</div> </div>
1	G	275	<div> <div>4%</div> <div>88% 11% .</div> </div>
2	B	100	<div> <div>90% 10%</div> </div>
2	E	100	<div> <div>% 92% 7% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	100	
3	C	11	
3	F	11	
3	I	11	
4	J	204	
4	L	204	
4	N	204	
5	K	241	
5	M	241	
5	O	241	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19680 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	271	Total	C	N	O	S	0	0	0
			2223	1385	403	429	6			
1	D	270	Total	C	N	O	S	0	0	0
			2219	1382	405	426	6			
1	G	273	Total	C	N	O	S	0	0	0
			2238	1393	408	431	6			

- 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	E	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	H	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P61769
E	1	MET	-	expression tag	UNP P61769
H	1	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called peptide from p51 RT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			94	64	14	16			
3	F	11	Total	C	N	O	0	0	0
			94	64	14	16			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	0	0	0
			94	64	14	16			

- Molecule 4 is a protein called T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	199	Total	C	N	O	S	0	0	0
			1580	1000	254	317	9			
4	L	197	Total	C	N	O	S	0	0	0
			1564	991	251	313	9			
4	N	167	Total	C	N	O	S	0	0	0
			1336	845	216	267	8			

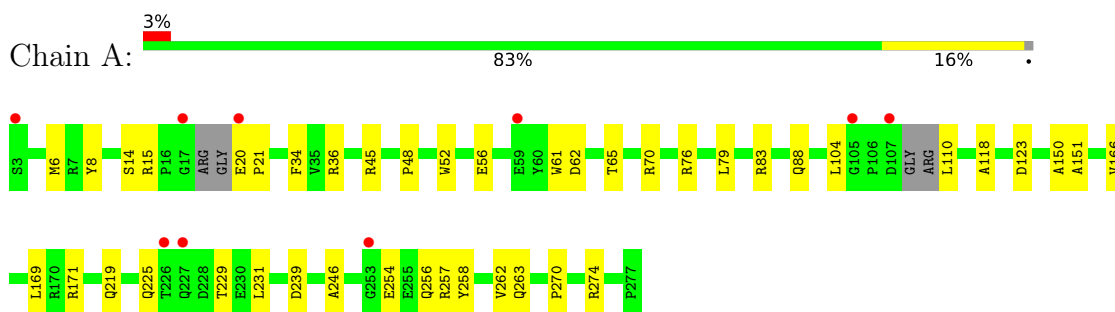
- Molecule 5 is a protein called T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	241	Total	C	N	O	S	0	0	0
			1928	1216	337	367	8			
5	M	240	Total	C	N	O	S	0	0	0
			1919	1211	335	365	8			
5	O	237	Total	C	N	O	S	0	0	0
			1898	1198	332	360	8			

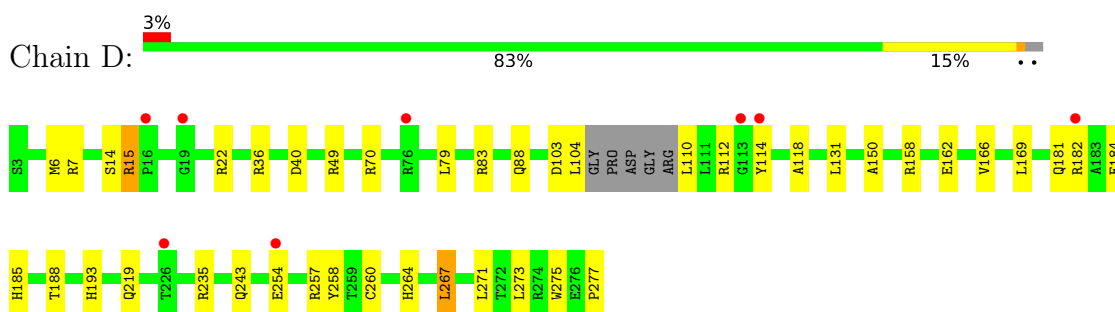
3 Residue-property plots [i](#)

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.

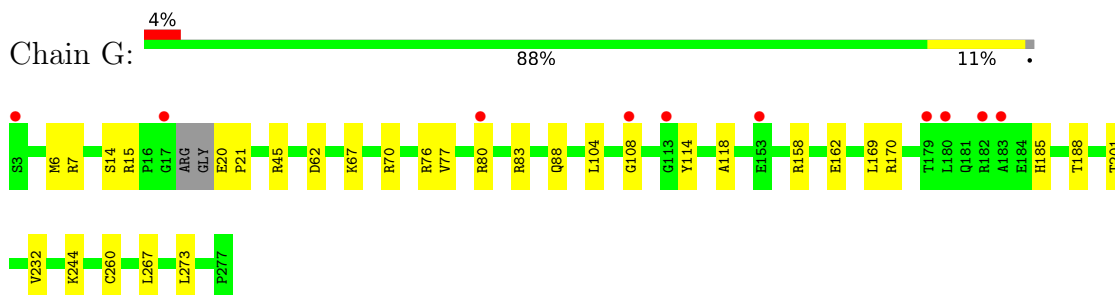
- Molecule 1: MHC class I antigen



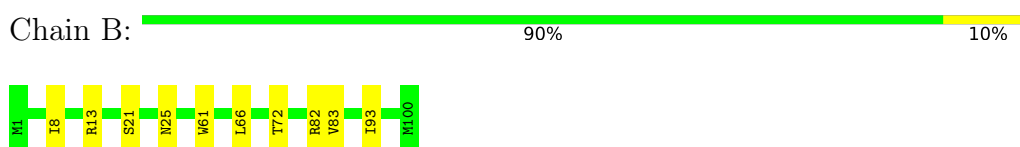
- Molecule 1: MHC class I antigen



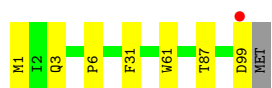
- Molecule 1: MHC class I antigen



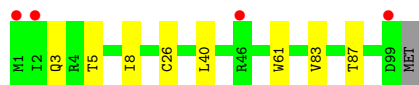
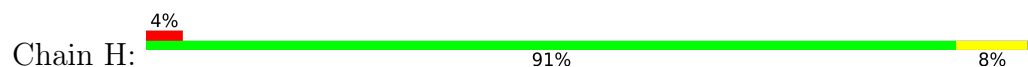
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: peptide from p51 RT



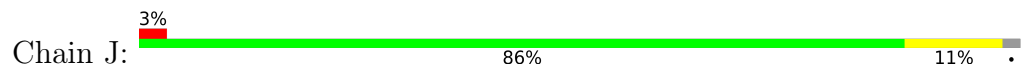
- Molecule 3: peptide from p51 RT



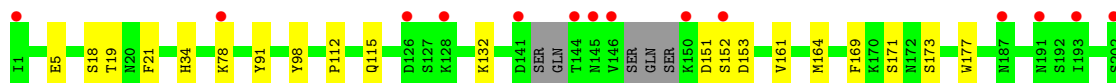
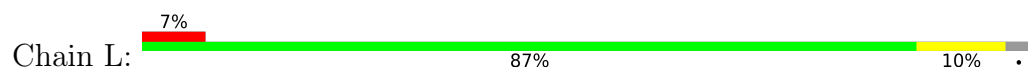
- Molecule 3: peptide from p51 RT



- Molecule 4: T cell receptor alpha chain

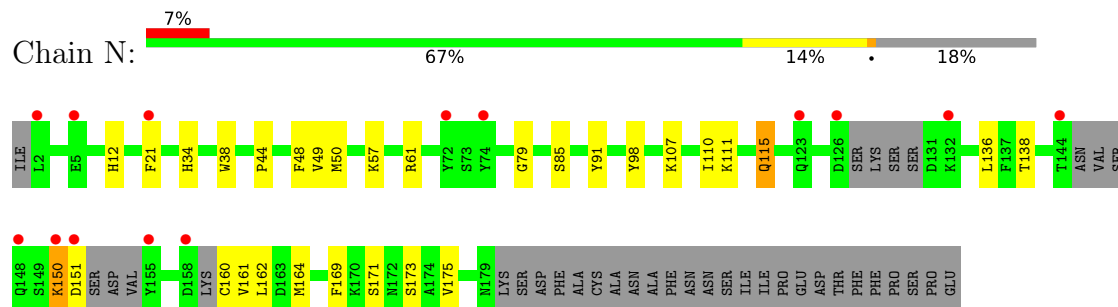


- Molecule 4: T cell receptor alpha chain

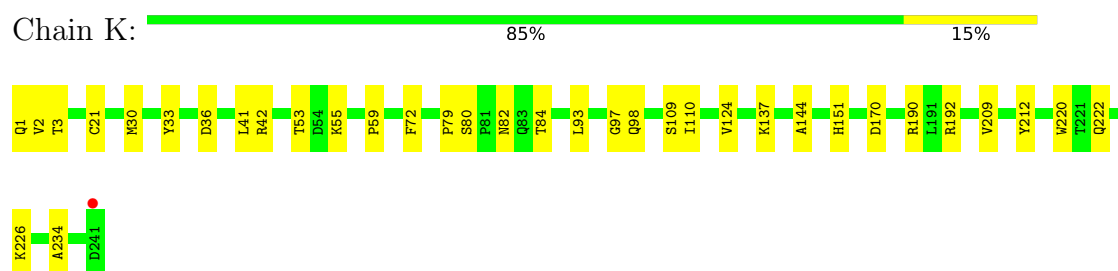


PRO
GLU

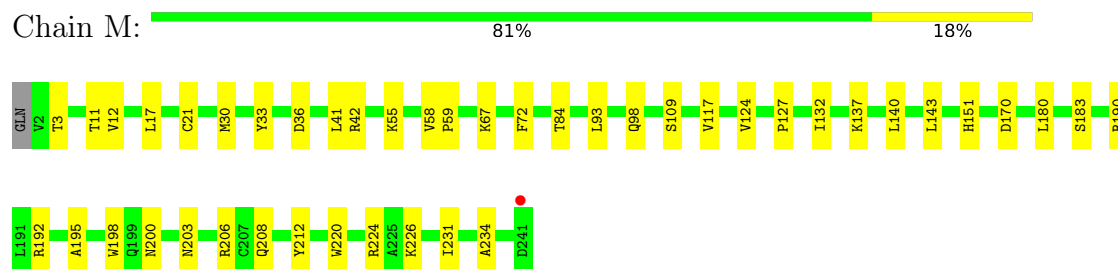
- Molecule 4: T cell receptor alpha chain



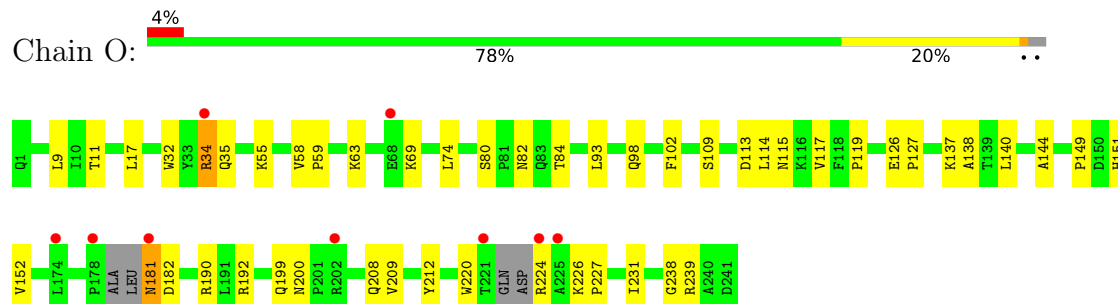
- Molecule 5: T cell receptor beta chain



- Molecule 5: T cell receptor beta chain



- Molecule 5: T cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	207.83Å 344.87Å 134.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.50 – 2.98 44.50 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.50-2.98) 99.7 (44.50-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.207 , 0.233 0.207 , 0.233	Depositor DCC
R_{free} test set	4557 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.008 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19680	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/2285	0.29	0/3105
1	D	0.12	0/2281	0.31	0/3099
1	G	0.13	0/2301	0.31	0/3127
2	B	0.11	0/860	0.28	0/1162
2	E	0.11	0/851	0.30	0/1152
2	H	0.10	0/851	0.30	0/1152
3	C	0.13	0/97	0.35	0/130
3	F	0.13	0/97	0.36	0/130
3	I	0.12	0/97	0.35	0/130
4	J	0.13	0/1619	0.33	0/2197
4	L	0.13	0/1602	0.33	0/2173
4	N	0.11	0/1366	0.29	0/1849
5	K	0.13	0/1980	0.32	0/2695
5	M	0.13	0/1971	0.33	0/2683
5	O	0.14	0/1948	0.38	2/2648 (0.1%)
All	All	0.12	0/20206	0.32	2/27432 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	181	ASN	CA-C-N	5.28	131.62	121.54
5	O	181	ASN	C-N-CA	5.28	131.62	121.54

There are no chirality outliers.

There are no planarity outliers.

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	2223	0	2058	33	0
1	D	2219	0	2061	30	0
1	G	2238	0	2075	21	0
2	B	837	0	803	7	0
2	E	828	0	794	5	0
2	H	828	0	794	5	0
3	C	94	0	96	5	0
3	F	94	0	96	3	0
3	I	94	0	96	2	0
4	J	1580	0	1497	17	0
4	L	1564	0	1481	16	0
4	N	1336	0	1260	24	0
5	K	1928	0	1853	22	0
5	M	1919	0	1842	27	0
5	O	1898	0	1823	34	0
All	All	19680	0	18629	214	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 6.

All (214) 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:O:117:VAL:O	5:O:224:ARG:NH2	2.06	0.88
5:K:93:LEU:HB3	5:K:98:GLN:HG3	1.66	0.77
5:M:11:THR:HG21	5:M:17:LEU:HD21	1.65	0.77
5:M:117:VAL:O	5:M:224:ARG:NH2	2.19	0.75
4:J:164:MET:HE1	5:K:137:LYS:HD3	1.73	0.70
4:L:151:ASP:O	4:L:153:ASP:N	2.24	0.70
5:M:93:LEU:HB3	5:M:98:GLN:HG3	1.74	0.70
5:K:36:ASP:OD2	5:K:42:ARG:NH2	2.24	0.70
1:D:182:ARG:NH1	1:D:184:GLU:HG3	2.08	0.68
4:L:34:HIS:HB2	4:L:91:TYR:HB3	1.76	0.68
4:N:34:HIS:HB2	4:N:91:TYR:HB3	1.75	0.67
4:J:34:HIS:HB2	4:J:91:TYR:HB3	1.76	0.67
5:O:126:GLU:OE1	5:O:239:ARG:NH2	2.26	0.66
1:D:131:LEU:O	1:D:158:ARG:NH1	2.29	0.66
1:D:7:ARG:NE	1:D:114:TYR:OH	2.29	0.65
5:O:9:LEU:HD21	5:O:17:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:153:ASP:HB2	4:J:180:LYS:HD2	1.80	0.64
4:N:150:LYS:HE3	4:N:151:ASP:H	1.63	0.64
4:N:175:VAL:HG23	5:O:190:ARG:HH11	1.64	0.63
1:A:20:GLU:OE2	1:A:76:ARG:HD2	1.99	0.63
1:G:14:SER:HA	1:G:21:PRO:HB3	1.82	0.62
1:D:15:ARG:HE	1:D:22:ARG:HB2	1.64	0.61
4:N:164:MET:HE1	5:O:137:LYS:HD3	1.83	0.61
5:O:80:SER:OG	5:O:82:ASN:OD1	2.17	0.61
5:O:117:VAL:HG12	5:O:149:PRO:HD3	1.83	0.61
1:A:104:LEU:HD21	1:A:166:VAL:HG13	1.83	0.60
5:M:30:MET:CE	5:M:72:PHE:HB2	2.31	0.60
5:K:42:ARG:NH1	4:L:5:GLU:OE2	2.35	0.60
4:J:8:PRO:HD2	4:J:21:PHE:HB3	1.84	0.60
2:B:8:ILE:HG12	2:B:83:VAL:HG11	1.83	0.59
5:O:84:THR:HG23	5:O:109:SER:HA	1.85	0.59
5:O:220:TRP:HB2	5:O:226:LYS:HE2	1.83	0.58
1:G:158:ARG:NH1	1:G:162:GLU:OE1	2.33	0.58
5:O:152:VAL:HG23	5:O:209:VAL:HG13	1.86	0.58
4:N:38:TRP:HH2	5:O:35:GLN:HG3	1.69	0.57
5:M:36:ASP:OD1	5:M:42:ARG:NH2	2.35	0.57
4:N:138:THR:HG22	4:N:173:SER:HB3	1.87	0.57
1:D:185:HIS:HB2	1:D:267:LEU:HD13	1.87	0.56
1:A:6:MET:HB2	1:A:169:LEU:HD13	1.88	0.56
5:O:127:PRO:HD3	5:O:140:LEU:HG	1.87	0.56
2:H:8:ILE:HG12	2:H:83:VAL:HG21	1.88	0.55
1:D:254:GLU:HB3	1:D:257:ARG:HD2	1.87	0.55
5:K:84:THR:HG23	5:K:109:SER:HA	1.89	0.54
1:A:45:ARG:NH2	1:A:62:ASP:OD1	2.36	0.54
1:G:77:VAL:HG22	1:G:80:ARG:HH21	1.74	0.53
2:H:3:GLN:HB3	2:H:87:THR:HG22	1.90	0.53
1:G:6:MET:HB2	1:G:169:LEU:HD13	1.92	0.52
1:G:70:ARG:HD2	4:N:98:TYR:CE1	2.44	0.52
4:J:164:MET:HE2	5:K:192:ARG:HD3	1.92	0.52
4:N:162:LEU:HD21	5:O:192:ARG:HB3	1.90	0.52
5:O:151:HIS:HB3	5:O:212:TYR:HB2	1.91	0.52
5:M:30:MET:HE3	5:M:72:PHE:HB2	1.89	0.52
4:N:169:PHE:HE1	4:N:171:SER:HB2	1.75	0.52
1:D:264:HIS:HB3	1:D:267:LEU:HD22	1.92	0.51
4:N:136:LEU:HG	4:N:138:THR:HG23	1.92	0.51
1:D:6:MET:HB2	1:D:169:LEU:HD13	1.92	0.51
1:G:260:CYS:HB3	1:G:273:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:120:ALA:HB2	4:J:199:PHE:HB3	1.92	0.51
1:D:188:THR:HB	1:D:273:LEU:HD11	1.91	0.51
1:G:104:LEU:HG	1:G:169:LEU:HD23	1.92	0.51
5:O:119:PRO:HD3	5:O:227:PRO:HB3	1.91	0.51
1:A:123:ASP:OD1	2:B:61:TRP:NE1	2.36	0.51
1:G:21:PRO:HG3	1:G:76:ARG:HG3	1.92	0.51
4:L:164:MET:HE1	5:M:137:LYS:HD3	1.91	0.51
4:N:160:CYS:N	4:N:173:SER:H	2.07	0.51
1:A:6:MET:HE1	3:C:1:ILE:N	2.26	0.51
1:D:110:LEU:HD22	1:D:162:GLU:HA	1.93	0.51
1:D:235:ARG:NH2	1:D:243:GLN:OE1	2.28	0.51
1:A:225:GLN:O	1:A:229:THR:HG23	2.11	0.50
1:D:70:ARG:HD3	4:L:98:TYR:CZ	2.46	0.50
1:D:275:TRP:CZ2	1:D:277:PRO:HB3	2.46	0.50
1:D:70:ARG:HD3	4:L:98:TYR:CE2	2.47	0.50
5:K:124:VAL:HG23	5:K:234:ALA:HB3	1.93	0.50
1:A:6:MET:HE2	1:A:8:TYR:CE2	2.47	0.50
4:J:21:PHE:CE2	4:J:75:LEU:HD23	2.46	0.50
2:H:26:CYS:HB2	2:H:40:LEU:HD21	1.94	0.50
5:M:84:THR:HG23	5:M:109:SER:HA	1.93	0.50
1:G:83:ARG:HG3	1:G:88:GLN:HB2	1.92	0.50
1:A:118:ALA:HB2	2:B:61:TRP:CE2	2.47	0.49
1:D:260:CYS:HB3	1:D:273:LEU:HB2	1.93	0.49
5:K:80:SER:OG	5:K:82:ASN:OD1	2.27	0.49
5:K:55:LYS:HB3	5:K:59:PRO:HG3	1.93	0.49
4:N:48:PHE:HD1	4:N:57:LYS:HE2	1.78	0.49
2:B:25:ASN:HB3	2:B:66:LEU:HD11	1.94	0.49
3:C:6:VAL:O	3:C:9:VAL:HG22	2.11	0.49
5:M:55:LYS:HB3	5:M:59:PRO:HG3	1.95	0.49
5:M:33:TYR:HB3	5:M:41:LEU:HD22	1.94	0.49
1:A:150:ALA:O	5:K:98:GLN:NE2	2.40	0.49
4:N:50:MET:HG2	4:N:57:LYS:HD3	1.93	0.49
1:D:182:ARG:HH12	1:D:184:GLU:HG3	1.76	0.49
1:G:21:PRO:CG	1:G:76:ARG:HG3	2.42	0.48
3:F:6:VAL:O	3:F:9:VAL:HG22	2.13	0.48
4:L:18:SER:OG	4:L:78:LYS:HG3	2.12	0.48
1:G:188:THR:HB	1:G:273:LEU:HD11	1.96	0.48
4:N:38:TRP:CH2	5:O:35:GLN:HG3	2.49	0.48
5:O:181:ASN:O	5:O:182:ASP:CG	2.57	0.48
1:A:104:LEU:HG	1:A:169:LEU:HD23	1.96	0.47
1:D:36:ARG:HH21	1:D:49:ARG:NH1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:44:PRO:HG2	5:O:102:PHE:CG	2.48	0.47
2:B:21:SER:HA	2:B:72:THR:HG22	1.96	0.47
5:K:170:ASP:OD1	5:K:190:ARG:NH2	2.47	0.47
4:N:175:VAL:HG23	5:O:190:ARG:NH1	2.29	0.47
1:A:6:MET:HE3	1:A:34:PHE:HZ	1.80	0.47
1:G:185:HIS:HB2	1:G:267:LEU:HD23	1.97	0.47
5:O:144:ALA:HB2	5:O:209:VAL:HG21	1.96	0.46
5:M:170:ASP:OD1	5:M:190:ARG:NH2	2.48	0.46
5:K:30:MET:HE3	5:K:72:PHE:HB2	1.97	0.46
5:O:93:LEU:HB3	5:O:98:GLN:HG3	1.96	0.46
4:J:131:ASP:OD1	4:J:131:ASP:N	2.46	0.46
5:K:220:TRP:CE2	5:K:222:GLN:HB2	2.51	0.46
5:O:224:ARG:HH22	5:O:227:PRO:HG3	1.80	0.46
1:D:193:HIS:NE2	2:E:99:ASP:HB3	2.30	0.46
3:F:7:HIS:HB2	4:L:98:TYR:CD2	2.50	0.45
1:D:118:ALA:HB2	2:E:61:TRP:CE2	2.51	0.45
1:A:56:GLU:OE2	1:A:171:ARG:NH1	2.49	0.45
1:A:231:LEU:HD23	1:A:246:ALA:HB2	1.98	0.45
1:D:83:ARG:HG3	1:D:88:GLN:HB2	1.99	0.45
4:L:132:LYS:HD2	4:L:177:TRP:CD1	2.52	0.45
1:A:6:MET:HE1	3:C:1:ILE:H2	1.80	0.45
1:A:254:GLU:HB3	1:A:257:ARG:HD3	1.99	0.45
2:E:6:PRO:HB3	2:E:31:PHE:HB3	1.99	0.45
4:J:94:MET:HB2	4:J:99:GLN:HB2	1.99	0.45
5:K:151:HIS:HB3	5:K:212:TYR:HB2	1.98	0.45
5:M:67:LYS:HA	5:M:67:LYS:HD3	1.85	0.45
5:M:220:TRP:HB2	5:M:226:LYS:HE2	1.99	0.45
4:N:49:VAL:H	4:N:57:LYS:NZ	2.15	0.45
1:A:70:ARG:HD3	4:J:98:TYR:CZ	2.52	0.45
2:E:3:GLN:HB3	2:E:87:THR:HG22	1.98	0.45
2:H:5:THR:HG22	2:H:87:THR:HB	1.99	0.45
3:I:6:VAL:O	3:I:9:VAL:HG22	2.16	0.45
4:L:169:PHE:CE2	4:L:171:SER:HB3	2.52	0.45
5:K:220:TRP:HB2	5:K:226:LYS:HE2	1.99	0.44
5:K:144:ALA:HB2	5:K:209:VAL:HG21	1.98	0.44
1:D:104:LEU:HD21	1:D:166:VAL:HG13	1.99	0.44
1:G:45:ARG:NH2	1:G:62:ASP:OD1	2.33	0.44
4:L:164:MET:HE2	5:M:192:ARG:HD3	2.00	0.44
5:M:208:GLN:HG3	5:M:231:ILE:HG23	1.99	0.44
1:G:118:ALA:HB2	2:H:61:TRP:CE2	2.53	0.44
5:O:114:LEU:O	5:O:117:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:115:GLN:H	4:N:115:GLN:HG2	1.61	0.44
1:A:239:ASP:HB3	2:B:13:ARG:HD3	2.00	0.43
1:G:70:ARG:HD2	4:N:98:TYR:CZ	2.53	0.43
5:O:32:TRP:CE2	5:O:74:LEU:HB2	2.52	0.43
4:N:160:CYS:SG	5:O:190:ARG:NH2	2.91	0.43
1:A:14:SER:HB3	1:A:79:LEU:HD13	1.99	0.43
1:D:219:GLN:O	1:D:258:TYR:HA	2.17	0.43
5:K:33:TYR:HB3	5:K:41:LEU:HD22	1.99	0.43
5:K:79:PRO:HB2	5:K:110:ILE:HD13	2.00	0.43
1:D:110:LEU:HB2	1:D:166:VAL:HG21	2.00	0.43
3:F:7:HIS:HB2	4:L:98:TYR:CG	2.54	0.43
1:A:6:MET:HE3	1:A:34:PHE:CZ	2.53	0.43
1:A:15:ARG:NH2	1:A:20:GLU:O	2.52	0.43
1:A:70:ARG:HD3	4:J:98:TYR:CE2	2.53	0.43
1:A:263:GLN:HG2	1:A:270:PRO:HB3	2.00	0.43
1:G:15:ARG:NH2	1:G:20:GLU:O	2.50	0.43
5:M:3:THR:O	5:M:21:CYS:HA	2.19	0.43
5:M:17:LEU:HD23	5:M:17:LEU:HA	1.79	0.43
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.90	0.43
5:M:132:ILE:HG23	5:M:195:ALA:HB1	2.01	0.43
1:A:83:ARG:HG3	1:A:88:GLN:HB2	2.01	0.42
3:C:7:HIS:HB2	4:J:98:TYR:CD2	2.54	0.42
5:M:127:PRO:HD2	5:M:198:TRP:CZ2	2.54	0.42
4:N:12:HIS:CD2	4:N:111:LYS:HE3	2.54	0.42
4:N:61:ARG:NH1	4:N:79:GLY:O	2.52	0.42
4:N:107:LYS:HE2	4:N:107:LYS:HB3	1.82	0.42
4:L:169:PHE:HE2	4:L:171:SER:HB3	1.84	0.42
5:M:200:ASN:HB3	5:M:203:ASN:ND2	2.34	0.42
5:O:63:LYS:HA	5:O:63:LYS:HD3	1.90	0.42
4:J:164:MET:HE3	4:J:169:PHE:CD2	2.54	0.42
5:M:124:VAL:HG23	5:M:234:ALA:HB3	2.01	0.42
1:D:15:ARG:NH2	1:D:40:ASP:OD1	2.52	0.42
2:E:1:MET:HE2	2:E:1:MET:HB2	1.94	0.42
5:M:127:PRO:HD3	5:M:140:LEU:HG	2.01	0.42
1:A:52:TRP:CD1	1:A:52:TRP:H	2.37	0.42
1:A:110:LEU:HB2	1:A:166:VAL:HG21	2.02	0.42
1:G:104:LEU:HD23	1:G:104:LEU:HA	1.91	0.42
4:J:162:LEU:HD21	5:K:192:ARG:HB3	2.02	0.42
4:N:85:SER:HB2	4:N:110:ILE:HG12	2.01	0.42
4:L:115:GLN:H	4:L:115:GLN:HG2	1.67	0.42
1:D:267:LEU:HG	1:D:271:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:113:ASP:OD2	5:O:115:ASN:ND2	2.52	0.42
1:D:103:ASP:O	1:D:110:LEU:HD12	2.20	0.42
1:D:112:ARG:NH1	1:D:114:TYR:CD2	2.88	0.42
4:L:112:PRO:HG3	4:L:161:VAL:HG13	2.02	0.42
5:O:55:LYS:HB3	5:O:59:PRO:HG3	2.01	0.41
1:D:14:SER:HB3	1:D:79:LEU:HD13	2.02	0.41
1:A:45:ARG:HA	1:A:65:THR:HG23	2.02	0.41
1:A:151:ALA:HA	5:K:97:GLY:HA3	2.03	0.41
1:D:150:ALA:O	5:M:98:GLN:NE2	2.43	0.41
5:K:3:THR:O	5:K:21:CYS:HA	2.21	0.41
1:A:20:GLU:HA	1:A:21:PRO:HD3	1.96	0.41
5:O:127:PRO:HG3	5:O:138:ALA:HB1	2.03	0.41
5:O:208:GLN:HG3	5:O:231:ILE:HG23	2.03	0.41
1:A:256:GLN:O	1:A:274:ARG:NH1	2.53	0.41
5:M:206:ARG:NH1	5:M:208:GLN:HB2	2.36	0.41
5:O:200:ASN:O	5:O:238:GLY:HA3	2.21	0.41
5:O:9:LEU:HD11	5:O:11:THR:HG23	2.02	0.41
5:M:180:LEU:HB2	5:M:183:SER:HB2	2.03	0.41
5:O:34:ARG:HD2	5:O:58:VAL:HG11	2.03	0.41
1:A:48:PRO:HB3	1:A:61:TRP:CZ2	2.56	0.41
1:G:7:ARG:NE	1:G:114:TYR:OH	2.33	0.41
1:G:67:LYS:HD3	3:I:4:GLU:OE2	2.20	0.41
1:A:219:GLN:O	1:A:258:TYR:HA	2.21	0.41
1:G:108:GLY:O	1:G:170:ARG:NH2	2.51	0.40
4:J:50:MET:HG2	4:J:57:LYS:HD3	2.02	0.40
5:K:1:GLN:HB3	5:K:2:VAL:H	1.66	0.40
4:J:21:PHE:HE2	4:J:75:LEU:HD23	1.83	0.40
5:O:199:GLN:HA	5:O:239:ARG:O	2.21	0.40
4:L:173:SER:OG	5:M:190:ARG:HD2	2.21	0.40
2:B:82:ARG:HB2	2:B:93:ILE:HG12	2.03	0.40
1:D:49:ARG:HA	1:D:49:ARG:HD2	1.97	0.40
3:C:7:HIS:HB2	4:J:98:TYR:CG	2.56	0.40
1:G:232:VAL:O	1:G:244:LYS:NZ	2.54	0.40
5:M:151:HIS:HB3	5:M:212:TYR:HB2	2.03	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	265/275 (96%)	259 (98%)	6 (2%)	0	100	100
1	D	266/275 (97%)	259 (97%)	7 (3%)	0	100	100
1	G	269/275 (98%)	263 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
2	H	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
3	C	9/11 (82%)	9 (100%)	0	0	100	100
3	F	9/11 (82%)	9 (100%)	0	0	100	100
3	I	9/11 (82%)	9 (100%)	0	0	100	100
4	J	195/204 (96%)	185 (95%)	9 (5%)	1 (0%)	25	59
4	L	191/204 (94%)	181 (95%)	9 (5%)	1 (0%)	25	59
4	N	157/204 (77%)	149 (95%)	7 (4%)	1 (1%)	22	55
5	K	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
5	M	238/241 (99%)	233 (98%)	5 (2%)	0	100	100
5	O	231/241 (96%)	227 (98%)	4 (2%)	0	100	100
All	All	2370/2493 (95%)	2300 (97%)	67 (3%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	152	SER
4	J	148	GLN
4	N	161	VAL

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	228/230 (99%)	226 (99%)	2 (1%)	75	88
1	D	227/230 (99%)	224 (99%)	3 (1%)	65	84
1	G	229/230 (100%)	228 (100%)	1 (0%)	89	95
2	B	95/95 (100%)	95 (100%)	0	100	100
2	E	94/95 (99%)	94 (100%)	0	100	100
2	H	94/95 (99%)	94 (100%)	0	100	100
3	C	10/10 (100%)	10 (100%)	0	100	100
3	F	10/10 (100%)	10 (100%)	0	100	100
3	I	10/10 (100%)	10 (100%)	0	100	100
4	J	180/185 (97%)	175 (97%)	5 (3%)	38	69
4	L	178/185 (96%)	176 (99%)	2 (1%)	70	86
4	N	151/185 (82%)	148 (98%)	3 (2%)	50	76
5	K	214/214 (100%)	213 (100%)	1 (0%)	86	94
5	M	213/214 (100%)	210 (99%)	3 (1%)	62	83
5	O	211/214 (99%)	209 (99%)	2 (1%)	75	88
All	All	2144/2202 (97%)	2122 (99%)	22 (1%)	73	87

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	262	VAL
1	D	15	ARG
1	D	181	GLN
1	D	267	LEU
1	G	201	THR
4	J	13	VAL
4	J	19	THR
4	J	21	PHE
4	J	175	VAL

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Mol	Chain	Res	Type
4	J	194	ILE
5	K	53	THR
4	L	19	THR
4	L	21	PHE
5	M	12	VAL
5	M	58	VAL
5	M	143	LEU
4	N	21	PHE
4	N	115	GLN
4	N	150	LYS
5	O	34	ARG
5	O	69	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3	GLN
1	D	71	GLN
1	D	225	GLN
1	G	4	HIS
1	G	128	ASN
1	G	181	GLN
1	G	225	GLN
2	H	3	GLN
4	J	29	ASN
4	J	172	ASN
5	K	43	GLN
5	K	222	GLN
4	L	145	ASN
5	M	115	ASN
5	M	181	ASN
5	M	222	GLN
4	N	29	ASN
5	O	43	GLN
5	O	100	GLN

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

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	271/275 (98%)	0.02	9 (3%)	49	34	46, 66, 104, 152	0
1	D	270/275 (98%)	0.02	8 (2%)	52	36	45, 69, 101, 137	0
1	G	273/275 (99%)	0.20	10 (3%)	45	31	56, 74, 109, 143	0
2	B	100/100 (100%)	-0.19	0	100	100	50, 63, 84, 108	0
2	E	99/100 (99%)	0.05	1 (1%)	79	65	49, 77, 116, 134	0
2	H	99/100 (99%)	0.33	4 (4%)	43	29	57, 82, 125, 140	0
3	C	11/11 (100%)	-0.26	0	100	100	48, 53, 58, 62	0
3	F	11/11 (100%)	-0.30	0	100	100	48, 55, 62, 63	0
3	I	11/11 (100%)	-0.21	0	100	100	66, 67, 71, 75	0
4	J	199/204 (97%)	0.06	6 (3%)	52	36	43, 58, 99, 131	0
4	L	197/204 (96%)	0.22	14 (7%)	23	15	46, 66, 109, 135	0
4	N	167/204 (81%)	0.71	14 (8%)	18	12	70, 100, 131, 160	0
5	K	241/241 (100%)	-0.31	1 (0%)	89	80	41, 54, 87, 127	0
5	M	240/241 (99%)	-0.28	1 (0%)	89	80	41, 56, 83, 120	0
5	O	237/241 (98%)	0.28	9 (3%)	44	30	60, 79, 105, 130	0
All	All	2426/2493 (97%)	0.07	77 (3%)	50	34	41, 68, 111, 160	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	202	SER	4.9
2	E	99	ASP	4.9
5	O	178	PRO	4.9
4	J	190	ASN	4.6
1	G	17	GLY	4.6
1	G	182	ARG	4.3
4	N	151	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
4	L	145	ASN	3.9
1	A	107	ASP	3.8
4	N	126	ASP	3.7
1	A	17	GLY	3.6
1	D	182	ARG	3.5
1	A	105	GLY	3.4
5	O	181	ASN	3.4
1	A	3	SER	3.4
4	L	146	VAL	3.3
5	O	224	ARG	3.3
4	N	2	LEU	3.2
4	L	144	THR	3.2
2	H	1	MET	3.2
4	J	195	PRO	3.2
1	A	253	GLY	3.2
4	J	1	ILE	3.1
1	D	254	GLU	3.1
4	N	148	GLN	3.0
1	D	19	GLY	2.9
1	G	153	GLU	2.8
4	N	155	TYR	2.8
1	D	114	TYR	2.8
4	L	191	ASN	2.7
4	N	158	ASP	2.7
4	N	21	PHE	2.7
1	D	16	PRO	2.6
4	L	128	LYS	2.6
4	L	1	ILE	2.5
4	L	141	ASP	2.5
2	H	99	ASP	2.5
1	G	113	GLY	2.5
1	D	226	THR	2.5
5	O	221	THR	2.5
5	M	241	ASP	2.4
1	G	180	LEU	2.4
4	N	74	TYR	2.4
4	L	126	ASP	2.4
5	O	68	GLU	2.4
1	A	226	THR	2.4
1	G	3	SER	2.3
1	G	179	THR	2.3
1	D	113	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	L	150	LYS	2.3
4	L	193	ILE	2.3
5	O	202	ARG	2.3
5	O	174	LEU	2.3
4	N	132	LYS	2.3
1	A	227	GLN	2.3
2	H	2	ILE	2.3
4	J	201	PRO	2.3
1	A	20	GLU	2.2
1	A	59	GLU	2.2
4	L	152	SER	2.2
4	N	72	TYR	2.2
1	G	80	ARG	2.2
4	N	144	THR	2.2
4	L	187	ASN	2.2
1	D	76	ARG	2.1
4	J	193	ILE	2.1
2	H	46	ARG	2.1
4	N	123	GLN	2.1
4	J	182	ASP	2.1
4	N	5	GLU	2.1
4	N	150	LYS	2.1
1	G	183	ALA	2.1
5	O	34	ARG	2.1
1	G	108	GLY	2.1
5	K	241	ASP	2.0
5	O	225	ALA	2.0
4	L	78	LYS	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.