



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:23 AM UTC

PDB ID : 8ENH / pdb_00008enh
Title : Cross-reactive 3180 TCR recognition of HLA-B*35:01-NP7 epitope from 2002 H3N2 influenza strain
Authors : Littler, D.R.; Rossjohn, J.
Deposited on : 2022-09-30
Resolution : 2.50 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

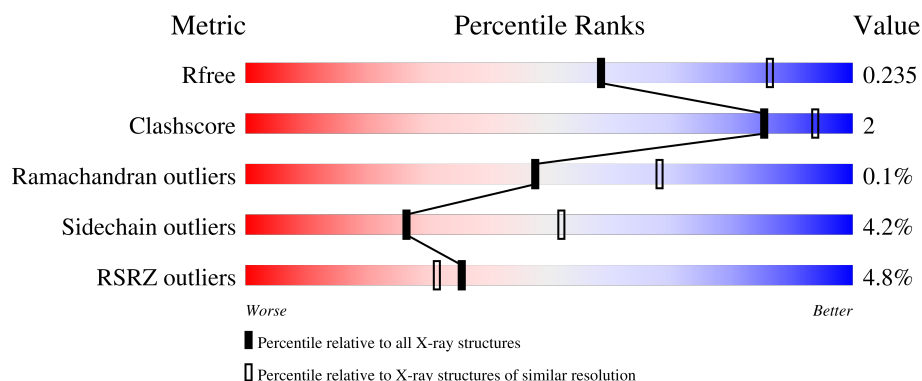
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	7% 90% 8% .
1	F	276	% 92% 7%
1	K	276	10% 84% 7% 9%
1	P	276	5% 90% 9% .
2	B	100	% 88% 9% ..

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Mol	Chain	Length	Quality of chain
2	G	100	92% 7% 2%
2	L	100	91% 7% 3%
2	Q	100	88% 11% 2%
3	C	9	78% 22%
3	H	9	100%
3	M	9	89% 11%
3	R	9	78% 22%
4	D	206	94% 5% 6%
4	I	206	92% 8% 2%
4	N	206	88% 7% 3%
4	S	206	89% 7% 3%
5	E	246	86% 13% 12%
5	J	246	89% 9% 5%
5	O	246	89% 8% 3%
5	T	246	89% 9% 3%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27676 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	275	Total	C	N	O	S	0	1	0
			2258	1408	411	431	8			
1	F	275	Total	C	N	O	S	0	0	0
			2250	1403	410	430	7			
1	K	252	Total	C	N	O	S	0	0	0
			2069	1299	379	384	7			
1	P	275	Total	C	N	O	S	0	0	0
			2250	1403	410	430	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Nucleoprotein NP7 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	M	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	R	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			

- Molecule 4 is a protein called 3180 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1591	992	266	326	7			
4	I	205	Total	C	N	O	S	0	0	0
			1591	992	266	326	7			
4	N	198	Total	C	N	O	S	0	0	0
			1530	951	259	313	7			
4	S	199	Total	C	N	O	S	0	0	0
			1539	956	260	316	7			

- Molecule 5 is a protein called 3180 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1937	1219	334	375	9			
5	J	246	Total	C	N	O	S	0	0	0
			1942	1222	335	376	9			
5	O	246	Total	C	N	O	S	0	0	0
			1942	1222	335	376	9			
5	T	244	Total	C	N	O	S	0	0	0
			1928	1215	333	371	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		
6	B	48	Total	O	0	0
			48	48		
6	C	8	Total	O	0	0
			8	8		

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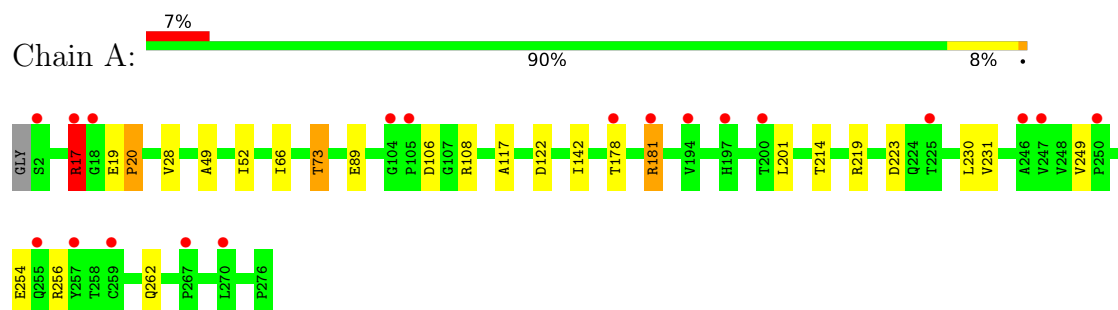
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	39	Total 39	O 39	0	0
6	E	70	Total 70	O 70	0	0
6	F	138	Total 138	O 138	0	0
6	G	66	Total 66	O 66	0	0
6	H	6	Total 6	O 6	0	0
6	I	57	Total 57	O 57	0	0
6	J	78	Total 78	O 78	0	0
6	K	118	Total 118	O 118	0	0
6	L	59	Total 59	O 59	0	0
6	M	5	Total 5	O 5	0	0
6	N	66	Total 66	O 66	0	0
6	O	78	Total 78	O 78	0	0
6	P	116	Total 116	O 116	0	0
6	Q	51	Total 51	O 51	0	0
6	R	4	Total 4	O 4	0	0
6	S	50	Total 50	O 50	0	0
6	T	70	Total 70	O 70	0	0

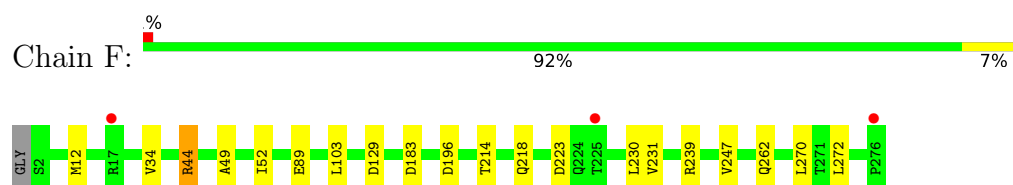
3 Residue-property plots [i](#)

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.

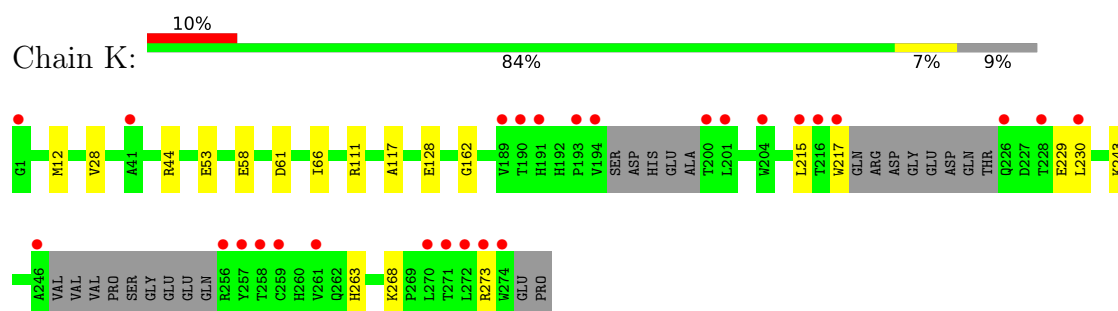
- Molecule 1: MHC class I antigen



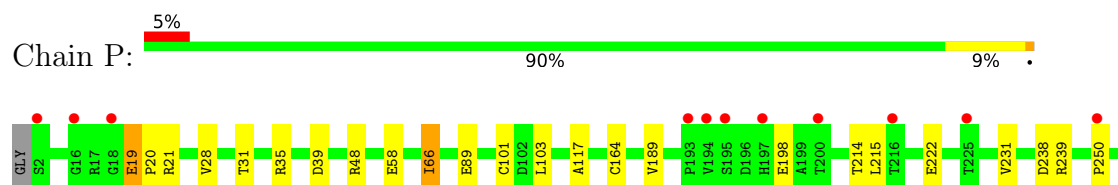
- Molecule 1: MHC class I antigen

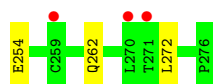


- Molecule 1: MHC class I antigen

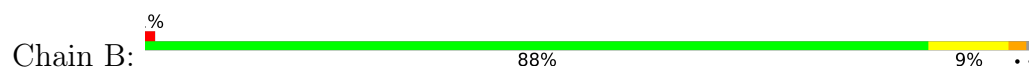


- Molecule 1: MHC class I antigen





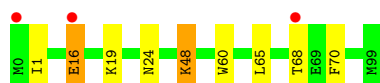
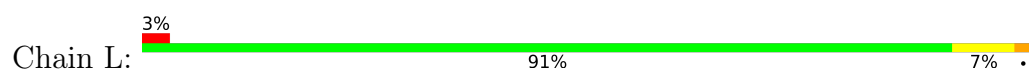
- Molecule 2: Beta-2-microglobulin



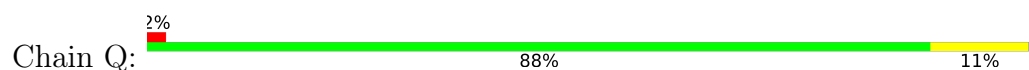
- Molecule 2: Beta-2-microglobulin



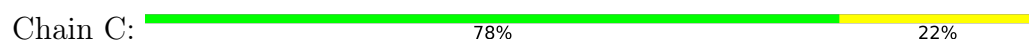
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein NP7 epitope



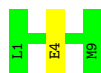
- Molecule 3: Nucleoprotein NP7 epitope



There are no outlier residues recorded for this chain.

- Molecule 3: Nucleoprotein NP7 epitope





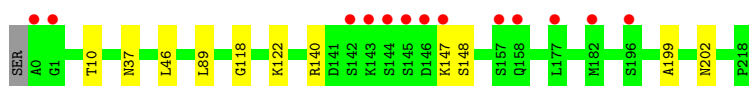
- Molecule 3: Nucleoprotein NP7 epitope

Chain R: 78% 22%



- Molecule 4: 3180 TCR alpha chain

Chain D: 6% 94% 5%



- Molecule 4: 3180 TCR alpha chain

Chain I: 2% 92% 8%



- Molecule 4: 3180 TCR alpha chain

Chain N: 3% 88% 7%



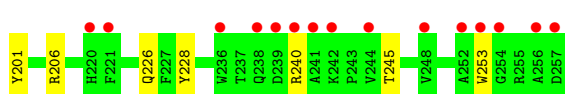
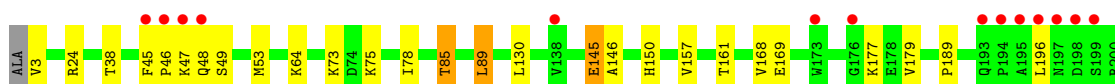
- Molecule 4: 3180 TCR alpha chain

Chain S: 3% 89% 7%

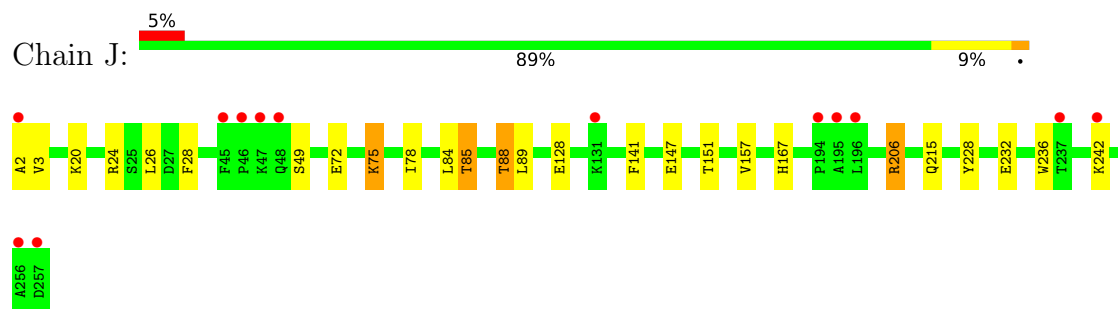


- Molecule 5: 3180 TCR alpha chain

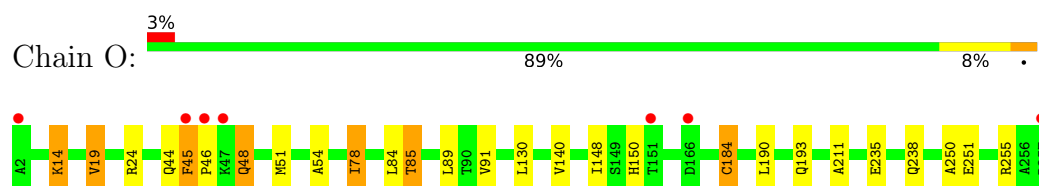
Chain E: 12% 86% 13%



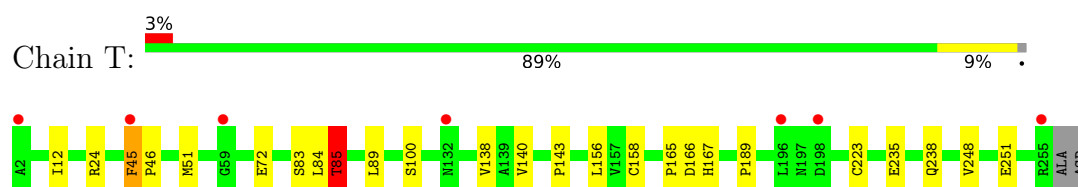
● Molecule 5: 3180 TCR alpha chain



● Molecule 5: 3180 TCR alpha chain



● Molecule 5: 3180 TCR alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.15Å 79.55Å 172.19Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	49.47 – 2.50 49.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.47-2.50) 99.7 (49.47-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.51Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.191 , 0.230 0.196 , 0.235	Depositor DCC
R_{free} test set	7850 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27676	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4455e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.77	0/2321	1.19	4/3155 (0.1%)
1	F	0.73	0/2313	1.16	1/3145 (0.0%)
1	K	0.71	0/2126	1.18	9/2886 (0.3%)
1	P	0.80	2/2313 (0.1%)	1.20	4/3145 (0.1%)
2	B	0.76	0/852	1.09	0/1152
2	G	0.69	0/852	1.09	0/1152
2	L	0.71	0/860	1.13	1/1162 (0.1%)
2	Q	0.72	0/852	1.10	0/1152
3	C	0.82	0/75	1.07	0/98
3	H	0.66	0/75	1.08	0/98
3	M	0.78	0/75	1.20	0/98
3	R	0.68	0/75	1.09	0/98
4	D	0.70	0/1625	1.11	2/2202 (0.1%)
4	I	0.70	0/1625	1.19	3/2202 (0.1%)
4	N	0.71	0/1560	1.08	1/2113 (0.0%)
4	S	0.71	0/1569	1.11	4/2125 (0.2%)
5	E	0.71	0/1988	1.13	3/2705 (0.1%)
5	J	0.69	0/1993	1.13	1/2712 (0.0%)
5	O	0.70	0/1993	1.13	2/2712 (0.1%)
5	T	0.69	0/1979	1.10	1/2694 (0.0%)
All	All	0.72	2/27121 (0.0%)	1.14	36/36806 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	58	GLU	C-O	-5.31	1.18	1.24
1	P	21	ARG	C-O	-5.05	1.17	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	28	VAL	N-CA-C	-7.10	96.87	107.37
4	I	81	ASN	CA-C-N	6.96	129.91	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	81	ASN	C-N-CA	6.96	129.91	120.38
1	K	162	GLY	N-CA-C	6.58	116.19	110.21
1	P	28	VAL	N-CA-C	-6.25	98.12	107.37
5	J	49	SER	N-CA-C	6.12	118.91	110.35
5	E	49	SER	N-CA-C	5.79	118.22	110.35
5	O	48	GLN	N-CA-C	5.78	117.58	111.28
1	A	20	PRO	N-CA-C	5.49	119.94	111.21
1	K	53	GLU	CA-C-N	5.48	127.62	120.28
1	K	53	GLU	C-N-CA	5.48	127.62	120.28
1	P	19	GLU	N-CA-C	5.42	118.50	110.32
1	K	263	HIS	CA-C-N	5.36	127.72	120.38
1	K	263	HIS	C-N-CA	5.36	127.72	120.38
1	F	129	ASP	CA-CB-CG	5.33	117.93	112.60
1	P	20	PRO	CA-N-CD	-5.30	104.58	112.00
4	I	209	ILE	N-CA-C	5.27	113.92	109.02
5	T	85	THR	CB-CA-C	5.26	115.94	109.16
1	K	61	ASP	CA-C-N	5.23	127.29	120.28
1	K	61	ASP	C-N-CA	5.23	127.29	120.28
4	S	209	ILE	N-CA-CB	-5.23	107.23	111.67
4	D	37	ASN	CA-CB-CG	5.19	117.79	112.60
2	L	70	PHE	CA-CB-CG	5.17	118.97	113.80
4	N	37	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	28	VAL	N-CA-C	-5.14	99.11	107.28
1	A	17	ARG	N-CA-C	5.13	119.17	113.01
1	P	238	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	122	ASP	CA-CB-CG	5.12	117.72	112.60
4	S	145	SER	CA-C-N	5.11	127.64	120.28
4	S	145	SER	C-N-CA	5.11	127.64	120.28
5	O	150	HIS	N-CA-C	5.10	116.92	111.36
1	K	58	GLU	CB-CG-CD	5.09	121.25	112.60
4	S	37	ASN	CA-CB-CG	5.09	117.69	112.60
5	E	145	GLU	CA-C-N	5.06	127.06	120.28
5	E	145	GLU	C-N-CA	5.06	127.06	120.28
4	D	118	GLY	N-CA-C	-5.03	105.88	112.82

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	A	2258	0	2121	12	0
1	F	2250	0	2111	5	0
1	K	2069	0	1959	5	0
1	P	2250	0	2115	11	0
2	B	829	0	794	3	0
2	G	829	0	794	4	0
2	L	837	0	803	4	0
2	Q	829	0	796	4	0
3	C	74	0	80	2	0
3	H	74	0	80	0	0
3	M	74	0	80	1	0
3	R	74	0	80	3	0
4	D	1591	0	1520	3	0
4	I	1591	0	1518	6	0
4	N	1530	0	1470	6	0
4	S	1539	0	1475	2	0
5	E	1937	0	1857	10	0
5	J	1942	0	1862	14	0
5	O	1942	0	1861	13	0
5	T	1928	0	1855	15	0
6	A	102	0	0	0	0
6	B	48	0	0	1	0
6	C	8	0	0	0	0
6	D	39	0	0	0	0
6	E	70	0	0	1	0
6	F	138	0	0	0	0
6	G	66	0	0	0	0
6	H	6	0	0	0	0
6	I	57	0	0	0	0
6	J	78	0	0	1	0
6	K	118	0	0	0	0
6	L	59	0	0	0	0
6	M	5	0	0	0	0
6	N	66	0	0	0	0
6	O	78	0	0	0	0
6	P	116	0	0	0	0
6	Q	51	0	0	0	0
6	R	4	0	0	0	0
6	S	50	0	0	0	0
6	T	70	0	0	0	0
All	All	27676	0	25231	108	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 2.

All (108) 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:45:PHE:HB3	5:O:46:PRO:CD	1.94	0.98
5:T:45:PHE:HB3	5:T:46:PRO:HD2	1.50	0.93
1:A:106:ASP:OD2	1:A:108:ARG:HB2	1.85	0.76
1:A:17:ARG:HG3	1:A:17:ARG:O	1.87	0.74
5:O:45:PHE:HB3	5:O:46:PRO:HD2	1.74	0.67
5:E:45:PHE:HB3	5:E:46:PRO:HD2	1.77	0.64
2:B:2:GLN:NE2	6:B:101:HOH:O	2.30	0.63
5:J:24:ARG:HH11	5:J:85:THR:HG23	1.63	0.63
5:J:72:GLU:HB2	5:J:75:LYS:HB2	1.79	0.63
5:E:228:TYR:HA	5:E:245:THR:HG23	1.81	0.63
5:J:3:VAL:HG13	5:J:26:LEU:HD12	1.81	0.62
4:N:143:LYS:HE3	5:O:251:GLU:H	1.63	0.62
5:T:158:CYS:HG	5:T:223:CYS:HG	1.43	0.61
5:T:24:ARG:HH11	5:T:85:THR:CG2	2.12	0.61
5:T:24:ARG:HD2	5:T:85:THR:HG23	1.83	0.61
1:A:214:THR:HB	1:A:262:GLN:HB2	1.83	0.60
5:O:44:GLN:NE2	5:O:48:GLN:O	2.34	0.60
5:E:169:GLU:HG3	5:E:226:GLN:HB3	1.82	0.60
5:J:24:ARG:HH11	5:J:85:THR:CG2	2.14	0.60
4:N:150:CYS:HG	4:N:200:CYS:HG	1.49	0.58
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.85	0.57
5:E:157:VAL:HG12	5:E:206:ARG:HG2	1.90	0.54
1:K:66:ILE:HG12	3:M:4:GLU:HA	1.90	0.54
1:F:214:THR:HB	1:F:262:GLN:HB2	1.90	0.54
4:N:140:ARG:HD3	4:N:148:SER:HB3	1.90	0.53
5:O:54:ALA:HB3	5:O:78:ILE:HD13	1.90	0.53
1:K:111:ARG:CZ	1:K:128:GLU:HG2	2.39	0.53
4:N:177:LEU:HB3	5:O:184:CYS:HB3	1.89	0.53
1:P:66:ILE:HG21	3:R:4:GLU:HA	1.90	0.53
5:J:88:THR:HG22	6:J:311:HOH:O	2.09	0.52
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.92	0.52
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.45	0.52
5:T:45:PHE:HB3	5:T:46:PRO:CD	2.30	0.52
4:S:168:ASP:HB3	4:S:195:LYS:HD2	1.90	0.51
4:I:188:SER:OG	5:J:206:ARG:HD3	2.10	0.51
1:A:49:ALA:O	1:A:52:ILE:HG22	2.10	0.51
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:166:ASP:HB2	5:T:189:PRO:HG2	1.92	0.50
5:E:189:PRO:HB2	5:E:201:TYR:HB3	1.93	0.50
5:T:24:ARG:CD	5:T:85:THR:HG23	2.42	0.49
4:N:6:GLN:HG3	4:N:23:CYS:SG	2.52	0.49
5:E:24:ARG:HH11	5:E:85:THR:HG23	1.77	0.49
1:P:89:GLU:H	1:P:89:GLU:CD	2.21	0.49
5:T:138:VAL:HG12	5:T:248:VAL:HG12	1.94	0.48
4:D:10:THR:HG22	4:D:122:LYS:HB3	1.94	0.48
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.96	0.48
1:P:66:ILE:CD1	3:R:2:PRO:HG2	2.44	0.48
1:F:49:ALA:O	1:F:52:ILE:HG22	2.15	0.47
5:J:147:GLU:O	5:J:151:THR:HG22	2.15	0.47
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.96	0.47
5:O:24:ARG:HH11	5:O:85:THR:CG2	2.27	0.47
4:D:140:ARG:HD2	4:D:148:SER:HB3	1.97	0.47
2:G:39:LEU:HB3	2:G:46:ILE:HD12	1.97	0.46
5:T:143:PRO:HD3	5:T:156:LEU:HG	1.97	0.46
5:J:167:HIS:HB3	5:J:228:TYR:HB2	1.97	0.46
2:G:46:ILE:HG21	2:G:68:THR:HG21	1.98	0.46
1:P:214:THR:HB	1:P:262:GLN:HB2	1.97	0.46
1:P:189:VAL:HG23	1:P:272:LEU:HD23	1.97	0.46
5:J:236:TRP:CD1	5:J:242:LYS:HG3	2.50	0.46
1:A:73:THR:HG21	3:C:6:SER:HB2	1.98	0.45
5:O:19:VAL:HG13	5:O:91:VAL:HB	1.98	0.45
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.51	0.45
5:T:140:VAL:HG22	5:T:223:CYS:SG	2.55	0.45
4:I:6:GLN:HG3	4:I:23:CYS:SG	2.56	0.45
1:A:219:ARG:HD2	1:A:256:ARG:HD3	1.97	0.45
4:D:199:ALA:H	4:D:202:ASN:HD22	1.65	0.45
4:I:149:VAL:HG21	5:J:157:VAL:HG21	1.99	0.44
1:K:217:TRP:HZ3	1:K:273:ARG:HG2	1.82	0.44
1:A:142:ILE:HD11	5:T:24:ARG:HD2	2.00	0.44
5:T:12:ILE:HG12	5:T:165:PRO:HG2	2.00	0.44
5:T:83:SER:C	5:T:85:THR:H	2.25	0.44
1:F:44:ARG:HE	1:F:44:ARG:HB2	1.58	0.44
5:O:148:ILE:HG23	5:O:211:ALA:HB1	1.99	0.44
1:F:49:ALA:HA	1:F:239:ARG:HH12	1.82	0.43
2:L:48:LYS:O	2:L:68:THR:HG22	2.19	0.43
1:P:101:CYS:CB	1:P:164:CYS:HG	2.25	0.43
1:K:230:LEU:HD22	1:K:243:LYS:HE3	2.00	0.43
2:L:16:GLU:HB2	2:L:19:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:139:LEU:HD22	5:J:157:VAL:HG22	2.01	0.42
5:O:45:PHE:HB3	5:O:46:PRO:HD3	1.88	0.42
5:E:38:THR:HG21	6:E:353:HOH:O	2.19	0.42
5:J:2:ALA:HB1	5:J:28:PHE:CE1	2.54	0.42
1:P:66:ILE:HD11	3:R:2:PRO:HG2	2.01	0.42
1:P:198:GLU:HG2	1:P:250:PRO:HA	2.01	0.42
5:E:146:ALA:O	5:E:150:HIS:HB2	2.20	0.42
4:I:141:ASP:HB3	4:I:144:SER:O	2.20	0.42
5:O:14:LYS:HG3	5:O:130:LEU:HG	2.02	0.42
5:E:24:ARG:HH11	5:E:85:THR:CG2	2.33	0.42
2:G:3:ARG:HB3	2:G:29:GLY:O	2.20	0.42
1:F:218:GLN:HG2	1:F:223:ASP:HA	2.02	0.42
1:A:66:ILE:HG12	3:C:4:GLU:HA	2.02	0.41
5:T:24:ARG:HH11	5:T:85:THR:HG22	1.85	0.41
5:O:140:VAL:HG23	5:O:250:ALA:HB3	2.02	0.41
1:P:35:ARG:HG2	1:P:48:ARG:HD3	2.01	0.41
2:G:49:VAL:HG22	2:G:68:THR:OG1	2.21	0.41
1:A:19:GLU:HG3	1:A:20:PRO:CD	2.50	0.41
1:A:178:THR:HA	1:A:181:ARG:HD2	2.02	0.41
5:J:242:LYS:H	5:J:242:LYS:HD3	1.85	0.41
2:Q:41:LYS:HG3	2:Q:78:TYR:CE1	2.56	0.41
5:E:53:MET:HE1	5:E:89:LEU:HD11	2.02	0.41
4:N:21:ILE:HG12	4:N:121:THR:HG21	2.02	0.41
5:T:165:PRO:HB2	5:T:167:HIS:HD2	1.86	0.41
2:Q:3:ARG:HB3	2:Q:29:GLY:O	2.21	0.41
5:O:45:PHE:O	5:O:46:PRO:C	2.62	0.40
4:S:141:ASP:HB3	4:S:144:SER:O	2.21	0.40
1:P:31:THR:HG23	1:P:239:ARG:HD3	2.03	0.40
4:I:169:VAL:HG12	4:I:193:SER:HB2	2.04	0.40
5:J:141:PHE:HB2	5:J:157:VAL:CG2	2.51	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%)	269 (98%)	5 (2%)	0	100	100
1	F	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
1	K	244/276 (88%)	238 (98%)	6 (2%)	0	100	100
1	P	273/276 (99%)	266 (97%)	7 (3%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	G	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	L	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	Q	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	D	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
4	I	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
4	N	196/206 (95%)	188 (96%)	8 (4%)	0	100	100
4	S	197/206 (96%)	189 (96%)	8 (4%)	0	100	100
5	E	243/246 (99%)	231 (95%)	11 (4%)	1 (0%)	30	49
5	J	244/246 (99%)	235 (96%)	9 (4%)	0	100	100
5	O	244/246 (99%)	236 (97%)	7 (3%)	1 (0%)	30	49
5	T	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	30	49
All	All	3253/3348 (97%)	3152 (97%)	98 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	48	GLN
5	O	45	PHE
5	T	45	PHE

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	235/234 (100%)	227 (97%)	8 (3%)	32	60
1	F	234/234 (100%)	222 (95%)	12 (5%)	21	43
1	K	213/234 (91%)	208 (98%)	5 (2%)	44	72
1	P	234/234 (100%)	226 (97%)	8 (3%)	32	60
2	B	94/95 (99%)	85 (90%)	9 (10%)	8	17
2	G	94/95 (99%)	93 (99%)	1 (1%)	65	84
2	L	95/95 (100%)	92 (97%)	3 (3%)	34	62
2	Q	94/95 (99%)	90 (96%)	4 (4%)	26	51
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100
4	D	181/182 (100%)	178 (98%)	3 (2%)	53	78
4	I	181/182 (100%)	176 (97%)	5 (3%)	38	66
4	N	174/182 (96%)	168 (97%)	6 (3%)	32	60
4	S	175/182 (96%)	166 (95%)	9 (5%)	21	43
5	E	216/216 (100%)	199 (92%)	17 (8%)	11	24
5	J	216/216 (100%)	205 (95%)	11 (5%)	21	43
5	O	216/216 (100%)	203 (94%)	13 (6%)	17	36
5	T	215/216 (100%)	206 (96%)	9 (4%)	26	52
All	All	2903/2944 (99%)	2780 (96%)	123 (4%)	26	52

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	73	THR
1	A	89	GLU
1	A	181	ARG
1	A	223	ASP
1	A	230	LEU
1	A	231	VAL

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Mol	Chain	Res	Type
1	A	254	GLU
2	B	1	ILE
2	B	2	GLN
2	B	4	THR
2	B	6	LYS
2	B	39	LEU
2	B	45	ARG
2	B	47	GLU
2	B	77	GLU
2	B	85	VAL
4	D	46	LEU
4	D	89	LEU
4	D	147	LYS
5	E	3	VAL
5	E	47	LYS
5	E	64	LYS
5	E	73	LYS
5	E	75	LYS
5	E	78	ILE
5	E	85	THR
5	E	89	LEU
5	E	130	LEU
5	E	145	GLU
5	E	161	THR
5	E	168	VAL
5	E	177	LYS
5	E	179	VAL
5	E	196	LEU
5	E	240	ARG
5	E	253	TRP
1	F	12	MET
1	F	34	VAL
1	F	44	ARG
1	F	89	GLU
1	F	103	LEU
1	F	183	ASP
1	F	196	ASP
1	F	230	LEU
1	F	231	VAL
1	F	247	VAL
1	F	270	LEU
1	F	272	LEU

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Mol	Chain	Res	Type
2	G	70	PHE
4	I	65	GLU
4	I	76	ILE
4	I	156	ASP
4	I	180	ARG
4	I	194	ASN
5	J	20	LYS
5	J	75	LYS
5	J	78	ILE
5	J	84	LEU
5	J	85	THR
5	J	88	THR
5	J	89	LEU
5	J	128	GLU
5	J	206	ARG
5	J	215	GLN
5	J	232	GLU
1	K	12	MET
1	K	44	ARG
1	K	215	LEU
1	K	229	GLU
1	K	268	LYS
2	L	1	ILE
2	L	16	GLU
2	L	48	LYS
4	N	76	ILE
4	N	92	THR
4	N	97	GLU
4	N	143	LYS
4	N	208	ILE
4	N	209	ILE
5	O	14	LYS
5	O	19	VAL
5	O	51	MET
5	O	78	ILE
5	O	84	LEU
5	O	85	THR
5	O	89	LEU
5	O	184	CYS
5	O	190	LEU
5	O	193	GLN
5	O	235	GLU

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Mol	Chain	Res	Type
5	O	238	GLN
5	O	255	ARG
1	P	19	GLU
1	P	39	ASP
1	P	66	ILE
1	P	103	LEU
1	P	215	LEU
1	P	222	GLU
1	P	231	VAL
1	P	254	GLU
2	Q	1	ILE
2	Q	35	ILE
2	Q	47	GLU
2	Q	83	ASN
4	S	27	ASP
4	S	46	LEU
4	S	79	THR
4	S	89	LEU
4	S	156	ASP
4	S	160	ASN
4	S	175	CYS
4	S	208	ILE
4	S	209	ILE
5	T	51	MET
5	T	72	GLU
5	T	84	LEU
5	T	85	THR
5	T	89	LEU
5	T	100	SER
5	T	235	GLU
5	T	238	GLN
5	T	251	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	144	GLN
1	A	155	GLN
1	A	188	HIS
1	A	262	GLN
2	B	8	GLN

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Mol	Chain	Res	Type
2	B	13	HIS
2	B	17	ASN
4	D	14	GLN
4	D	44	GLN
4	D	95	GLN
5	E	44	GLN
5	E	48	GLN
5	E	95	HIS
5	E	132	ASN
5	E	220	HIS
5	E	238	GLN
1	F	63	ASN
1	F	72	GLN
1	F	141	GLN
1	F	188	HIS
1	F	197	HIS
2	G	13	HIS
4	I	44	GLN
4	I	51	GLN
4	I	90	HIS
4	I	138	GLN
5	J	7	HIS
5	J	44	GLN
5	J	57	ASN
5	J	116	GLN
5	J	193	GLN
5	J	215	GLN
5	J	238	GLN
1	K	63	ASN
1	K	113	HIS
1	K	180	GLN
4	N	14	GLN
4	N	138	GLN
5	O	57	ASN
5	O	116	GLN
5	O	150	HIS
5	O	193	GLN
5	O	216	ASN
1	P	63	ASN
1	P	72	GLN
1	P	113	HIS
1	P	192	HIS

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Mol	Chain	Res	Type
1	P	255	GLN
2	Q	83	ASN
2	Q	84	HIS
2	Q	89	GLN
4	S	114	GLN
4	S	160	ASN
5	T	57	ASN
5	T	116	GLN
5	T	132	ASN
5	T	152	GLN
5	T	193	GLN
5	T	226	GLN

5.3.3 RNA [i](#)

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	275/276 (99%)	0.22	19 (6%) 23 20	15, 40, 106, 119	1 (0%)
1	F	275/276 (99%)	-0.12	3 (1%) 78 75	18, 30, 88, 106	0
1	K	252/276 (91%)	0.21	27 (10%) 11 9	19, 35, 104, 127	0
1	P	275/276 (99%)	0.10	14 (5%) 33 29	17, 37, 102, 115	0
2	B	99/100 (99%)	0.06	1 (1%) 79 76	31, 48, 68, 77	0
2	G	99/100 (99%)	-0.21	2 (2%) 65 61	26, 39, 58, 64	0
2	L	100/100 (100%)	0.09	3 (3%) 52 48	28, 45, 66, 73	0
2	Q	99/100 (99%)	0.12	2 (2%) 65 61	27, 46, 69, 73	0
3	C	9/9 (100%)	-0.32	0 100 100	27, 27, 30, 31	0
3	H	9/9 (100%)	-0.83	0 100 100	19, 20, 23, 24	0
3	M	9/9 (100%)	-0.82	0 100 100	19, 20, 23, 24	0
3	R	9/9 (100%)	-0.33	0 100 100	19, 21, 24, 25	0
4	D	205/206 (99%)	0.35	13 (6%) 26 23	28, 53, 88, 100	0
4	I	205/206 (99%)	0.13	4 (1%) 65 61	23, 46, 75, 84	0
4	N	198/206 (96%)	0.17	6 (3%) 52 48	22, 45, 79, 90	0
4	S	199/206 (96%)	0.27	7 (3%) 47 42	23, 51, 90, 101	0
5	E	245/246 (99%)	0.63	29 (11%) 9 7	21, 60, 93, 117	0
5	J	246/246 (100%)	0.25	13 (5%) 32 28	20, 48, 81, 98	0
5	O	246/246 (100%)	0.10	7 (2%) 55 50	20, 44, 77, 93	1 (0%)
5	T	244/246 (99%)	0.25	7 (2%) 53 49	20, 51, 81, 96	1 (0%)
All	All	3298/3348 (98%)	0.18	157 (4%) 35 31	15, 44, 88, 127	3 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	274	TRP	7.9
5	O	2	ALA	6.2
4	I	0	ALA	5.4
4	D	0	ALA	5.2
5	T	45	PHE	5.1
5	J	196	LEU	4.8
5	J	45	PHE	4.5
1	K	257	TYR	4.3
2	Q	1	ILE	4.2
5	E	253	TRP	4.1
1	K	191	HIS	4.1
1	K	194	VAL	4.0
5	E	196	LEU	4.0
5	J	46	PRO	4.0
1	K	272	LEU	3.9
5	T	2	ALA	3.8
5	T	196	LEU	3.7
4	I	1	GLY	3.6
4	S	182	MET	3.6
1	A	246	ALA	3.6
1	K	258	THR	3.5
5	J	2	ALA	3.5
4	D	145	SER	3.5
5	E	48	GLN	3.4
1	K	1	GLY	3.4
5	O	45	PHE	3.4
1	K	190	THR	3.3
5	E	45	PHE	3.3
4	N	168	ASP	3.3
4	N	145	SER	3.3
1	A	2	SER	3.2
4	D	147	LYS	3.2
1	F	225	THR	3.2
1	K	271	THR	3.1
1	K	246	ALA	3.1
1	A	105	PRO	3.0
2	G	1	ILE	2.9
4	S	209	ILE	2.9
1	K	273	ARG	2.9
5	E	241	ALA	2.9
1	A	259	CYS	2.9
5	E	46	PRO	2.9
1	K	217	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	216	THR	2.8
1	P	197	HIS	2.8
5	J	131	LYS	2.8
1	P	195	SER	2.8
1	P	270	LEU	2.8
1	A	197	HIS	2.8
2	B	1	ILE	2.7
5	O	46	PRO	2.7
1	P	216	THR	2.7
4	D	182	MET	2.7
1	A	194	VAL	2.7
4	S	208	ILE	2.6
5	E	138	VAL	2.6
5	E	256	ALA	2.6
1	A	18	GLY	2.6
1	K	256	ARG	2.6
4	D	1	GLY	2.6
4	D	157	SER	2.6
5	E	257	ASP	2.6
2	L	16	GLU	2.6
5	E	197	ASN	2.6
1	K	259	CYS	2.6
5	E	238	GLN	2.6
1	A	267	PRO	2.5
1	P	193	PRO	2.5
5	T	198	ASP	2.5
1	A	225	THR	2.5
1	K	193	PRO	2.5
5	O	166	ASP	2.5
1	K	270	LEU	2.5
2	Q	2	GLN	2.5
2	G	2	GLN	2.5
4	N	160	ASN	2.5
1	K	228	THR	2.5
1	P	225	THR	2.5
5	E	199	SER	2.5
5	E	195	ALA	2.5
1	P	250	PRO	2.4
5	E	254	GLY	2.4
4	D	146	ASP	2.4
4	N	197	ASP	2.4
4	S	197	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	2.4
5	E	194	PRO	2.4
1	A	257	TYR	2.4
1	K	200	THR	2.4
5	E	239	ASP	2.4
1	K	201	LEU	2.4
1	K	230	LEU	2.4
1	K	204	TRP	2.4
1	K	215	LEU	2.4
4	D	158	GLN	2.4
4	S	201	ALA	2.4
5	J	242	LYS	2.4
1	P	259	CYS	2.3
5	J	47	LYS	2.3
4	D	196	SER	2.3
1	A	104	GLY	2.3
2	L	0	MET	2.3
4	S	211	GLU	2.3
5	J	256	ALA	2.3
1	A	178	THR	2.3
1	A	181	ARG	2.3
1	A	255	GLN	2.3
5	E	220	HIS	2.3
5	O	257	ASP	2.3
5	E	242	LYS	2.3
1	F	276	PRO	2.3
1	P	200	THR	2.3
1	K	226	GLN	2.3
1	K	189	VAL	2.2
5	E	176	GLY	2.2
5	T	59	GLY	2.2
5	E	244	VAL	2.2
4	N	194	ASN	2.2
4	D	143	LYS	2.2
1	P	271	THR	2.2
1	P	16	GLY	2.2
4	D	142	SER	2.2
1	K	261	VAL	2.2
5	J	48	GLN	2.2
5	E	198	ASP	2.2
5	E	236	TRP	2.2
5	J	194	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	194	VAL	2.1
5	E	193	GLN	2.1
5	T	132	ASN	2.1
2	L	68	THR	2.1
4	D	144	SER	2.1
4	I	145	SER	2.1
4	I	156	ASP	2.1
5	E	47	LYS	2.1
5	E	221	PHE	2.1
1	A	247	VAL	2.1
1	A	200	THR	2.1
1	P	18	GLY	2.1
1	A	17	ARG	2.1
4	N	167	SER	2.1
5	J	257	ASP	2.1
1	A	250	PRO	2.1
1	K	41	ALA	2.1
5	E	173	TRP	2.1
1	F	17	ARG	2.1
5	E	248	VAL	2.1
4	D	177	LEU	2.1
5	J	237	THR	2.1
1	P	2	SER	2.1
5	E	252	ALA	2.0
5	T	255	ARG	2.0
5	E	240	ARG	2.0
5	J	195	ALA	2.0
5	O	47	LYS	2.0
5	O	151	THR	2.0
4	S	210	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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.