



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 01:18 PM EDT

PDB ID : 8EN8 / pdb_00008en8
Title : Cross-reactive 3180 TCR recognition of HLA-B*35:01-NP4 epitope from 1972 influenza strain
Authors : Littler, D.R.; Rossjohn, J.
Deposited on : 2022-09-29
Resolution : 2.70 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

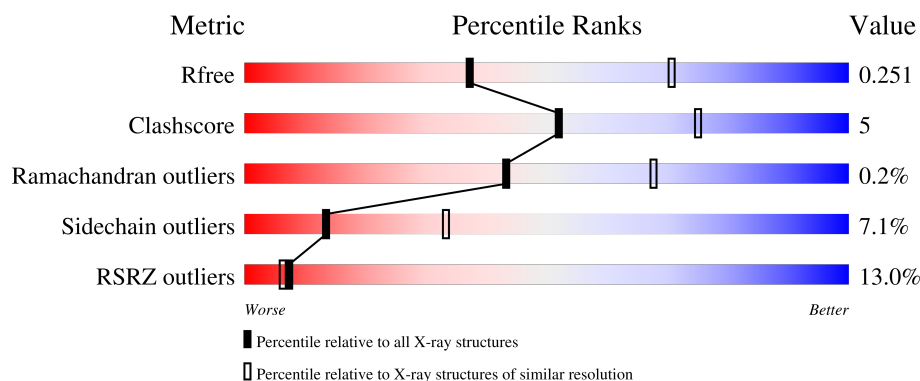
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	11% 88% 10% .
1	F	276	7% 88% 12% .
2	B	100	7% 92% 6% ..
2	G	100	2% 89% 9% ..
3	C	9	67% 33%

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Mol	Chain	Length	Quality of chain
3	H	9	56% 44%
4	D	205	2% 88% 11%
4	I	205	33% 86% 12%
5	E	245	2% 80% 16%
5	J	245	33% 75% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13859 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	1	0
			2262	1409	413	433	7			
1	F	276	Total	C	N	O	S	0	1	0
			2262	1409	413	433	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			

There are 2 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

- Molecule 3 is a protein called Nucleoprotein NP4 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			73	48	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
			1594	994	266	326	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	205	Total	C	N	O	S	0	0	0
			1594	994	266	326	8			

- Molecule 5 is a protein called 3180 TCR beta 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	245	Total	C	N	O	S	0	0	0
			1937	1219	334	375	9			

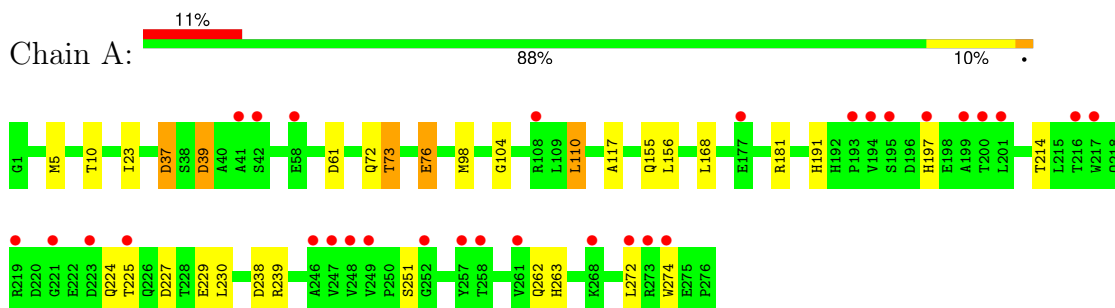
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	14	Total	O	0	0
			14	14		
6	C	3	Total	O	0	0
			3	3		
6	D	51	Total	O	0	0
			51	51		
6	E	80	Total	O	0	0
			80	80		
6	F	110	Total	O	0	0
			110	110		
6	G	36	Total	O	0	0
			36	36		
6	H	8	Total	O	0	0
			8	8		
6	I	34	Total	O	0	0
			34	34		
6	J	54	Total	O	0	0
			54	54		

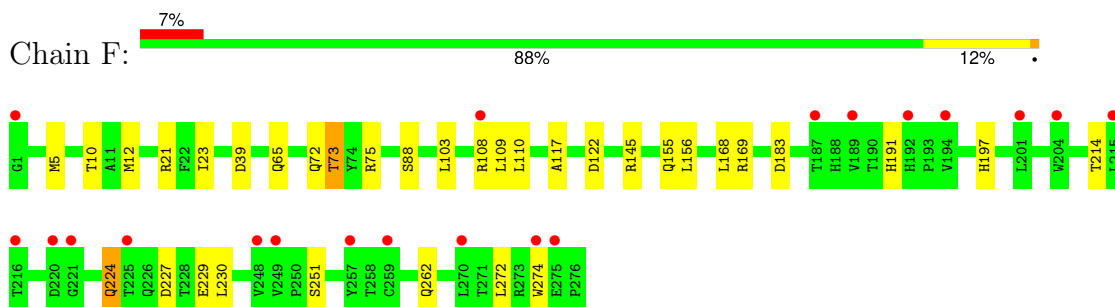
3 Residue-property plots [i](#)

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.

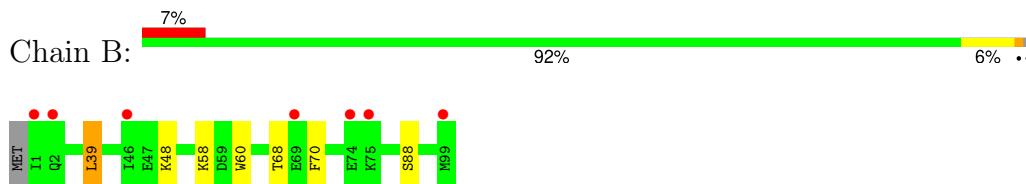
- Molecule 1: MHC class I antigen



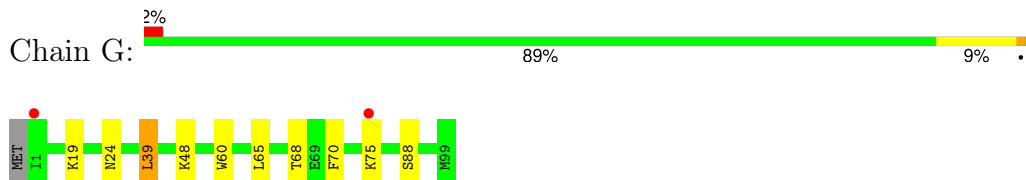
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin

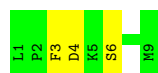


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein NP4 epitope

Chain C:  67% 33%



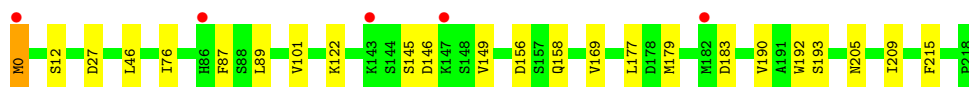
- Molecule 3: Nucleoprotein NP4 epitope

Chain H:  56% 44%



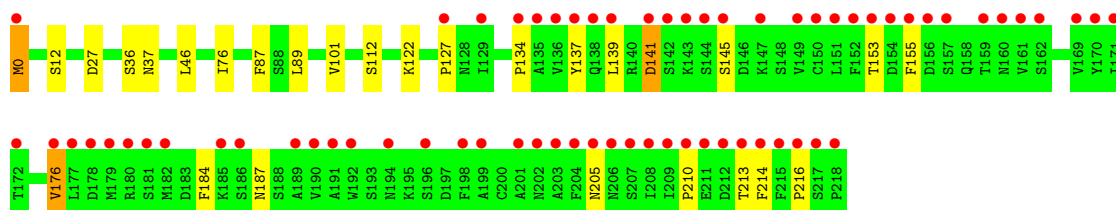
- Molecule 4: 3180 TCR alpha chain

Chain D:  2% 88% 11%



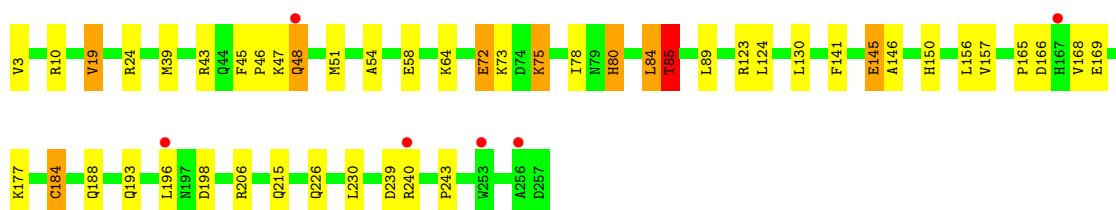
- Molecule 4: 3180 TCR alpha chain

Chain I:  33% 86% 12%



- Molecule 5: 3180 TCR beta chain

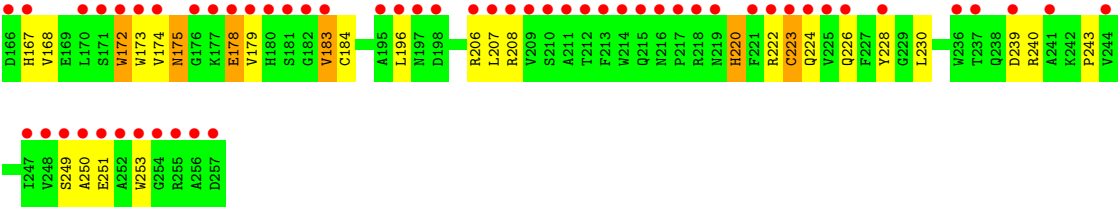
Chain E:  2% 80% 16%



- Molecule 5: 3180 TCR beta chain

Chain J:  33% 75% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.77Å 116.69Å 253.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.20 – 2.70 27.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.20-2.70) 99.8 (27.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.72Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.207 , 0.249 0.211 , 0.251	Depositor DCC
R_{free} test set	3281 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13859	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.79	3/2325 (0.1%)	1.21	4/3161 (0.1%)
1	F	0.80	1/2325 (0.0%)	1.22	7/3161 (0.2%)
2	B	0.75	0/852	1.10	1/1152 (0.1%)
2	G	0.73	0/852	1.12	1/1152 (0.1%)
3	C	1.15	0/74	1.23	1/97 (1.0%)
3	H	0.68	0/74	1.24	1/97 (1.0%)
4	D	0.72	0/1628	1.17	4/2205 (0.2%)
4	I	0.78	0/1628	1.16	2/2205 (0.1%)
5	E	0.69	0/1988	1.15	6/2705 (0.2%)
5	J	0.77	0/1988	1.17	5/2705 (0.2%)
All	All	0.76	4/13734 (0.0%)	1.18	32/18640 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ILE	C-O	-5.69	1.18	1.24
1	A	37	ASP	C-O	-5.22	1.18	1.23
1	F	23	ILE	C-O	-5.21	1.18	1.24
1	A	10	THR	C-O	-5.06	1.18	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	165	PRO	CA-C-N	6.44	131.00	120.63
5	E	165	PRO	C-N-CA	6.44	131.00	120.63
5	J	178	GLU	CB-CG-CD	6.12	123.01	112.60
3	H	4	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	70	PHE	CA-CB-CG	5.90	119.70	113.80
4	D	179	MET	CA-C-N	5.84	128.90	120.38
4	D	179	MET	C-N-CA	5.84	128.90	120.38
2	G	70	PHE	CA-CB-CG	5.79	119.59	113.80
5	J	72	GLU	CB-CG-CD	5.72	122.33	112.60
4	D	215	PHE	CA-CB-CG	5.72	119.52	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	ASP	CA-CB-CG	5.67	118.27	112.60
4	I	87	PHE	CA-CB-CG	5.56	119.36	113.80
4	D	87	PHE	CA-CB-CG	5.35	119.15	113.80
5	E	80	HIS	CA-C-N	5.35	127.71	120.44
5	E	80	HIS	C-N-CA	5.35	127.71	120.44
5	E	85	THR	CB-CA-C	5.32	116.02	109.16
1	F	122	ASP	CA-CB-CG	5.25	117.85	112.60
1	F	169	ARG	CA-C-N	5.25	127.26	120.44
1	F	169	ARG	C-N-CA	5.25	127.26	120.44
5	E	47	LYS	N-CA-C	-5.24	102.10	109.96
5	J	85	THR	CB-CA-C	5.23	115.91	109.16
1	F	72	GLN	CA-C-N	5.18	127.53	120.54
1	F	72	GLN	C-N-CA	5.18	127.53	120.54
1	F	224	GLN	CA-C-N	5.14	127.94	120.79
1	F	224	GLN	C-N-CA	5.14	127.94	120.79
4	I	155	PHE	CA-CB-CG	5.03	118.83	113.80
5	J	172	TRP	CA-C-N	-5.01	116.32	122.84
5	J	172	TRP	C-N-CA	-5.01	116.32	122.84
1	A	72	GLN	CA-C-N	5.00	126.95	120.44
1	A	72	GLN	C-N-CA	5.00	126.95	120.44
1	A	263	HIS	CA-C-N	5.00	126.99	120.28
1	A	263	HIS	C-N-CA	5.00	126.99	120.28

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	2262	0	2122	14	0
1	F	2262	0	2122	10	0
2	B	829	0	794	3	0
2	G	829	0	794	3	0
3	C	73	0	78	2	0
3	H	73	0	78	3	0
4	D	1594	0	1521	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1594	0	1521	27	0
5	E	1937	0	1856	30	0
5	J	1937	0	1856	59	0
6	A	79	0	0	0	0
6	B	14	0	0	0	0
6	C	3	0	0	0	0
6	D	51	0	0	0	0
6	E	80	0	0	2	0
6	F	110	0	0	0	0
6	G	36	0	0	0	0
6	H	8	0	0	0	0
6	I	34	0	0	1	0
6	J	54	0	0	0	0
All	All	13859	0	12742	132	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 5.

All (132) 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:J:147:GLU:O	5:J:148:ILE:CG1	1.95	1.14
5:J:147:GLU:O	5:J:148:ILE:HG12	1.52	1.06
5:J:147:GLU:C	5:J:148:ILE:HG12	1.77	1.06
4:I:127:PRO:HG3	4:I:176:VAL:HG11	1.40	1.03
5:J:175:ASN:H	5:J:220:HIS:HD2	1.08	1.00
5:J:147:GLU:O	5:J:148:ILE:HG13	1.67	0.93
5:J:175:ASN:N	5:J:220:HIS:HD2	1.69	0.89
5:J:140:VAL:HG23	5:J:158:CYS:SG	2.15	0.86
4:I:176:VAL:HG12	4:I:187:ASN:OD1	1.82	0.80
5:J:175:ASN:N	5:J:220:HIS:CD2	2.52	0.77
5:J:175:ASN:H	5:J:220:HIS:CD2	2.00	0.74
5:E:46:PRO:O	5:E:48:GLN:NE2	2.22	0.73
4:I:214:PHE:HE2	5:J:146:ALA:HB1	1.53	0.72
5:J:142:GLU:HB2	5:J:143:PRO:HD2	1.71	0.71
5:J:173:TRP:CZ2	5:J:178:GLU:HG3	2.25	0.70
5:E:72:GLU:HB3	6:E:301:HOH:O	1.92	0.69
4:I:0:MET:HE1	4:I:112:SER:O	1.93	0.69
5:J:72:GLU:H	5:J:72:GLU:CD	2.02	0.68
5:J:175:ASN:CA	5:J:220:HIS:CD2	2.76	0.68
5:E:157:VAL:HG12	5:E:206:ARG:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:175:ASN:HA	5:J:220:HIS:CD2	2.30	0.66
5:E:48:GLN:HE21	5:E:48:GLN:N	1.96	0.64
5:J:183:VAL:HG13	5:J:207:LEU:HB2	1.79	0.63
4:I:0:MET:N	4:I:0:MET:HE2	2.13	0.63
5:E:39:MET:HG3	5:E:80:HIS:HE1	1.65	0.62
3:H:5:LYS:HE3	5:J:114:ASP:OD1	2.00	0.62
4:I:137:TYR:CE1	5:J:146:ALA:HB3	2.34	0.62
5:J:157:VAL:HG12	5:J:206:ARG:HG2	1.82	0.62
5:J:158:CYS:HB2	5:J:172:TRP:CZ2	2.35	0.61
4:I:141:ASP:HB3	4:I:145:SER:H	1.65	0.61
4:I:137:TYR:HB3	5:J:144:SER:CB	2.32	0.60
5:E:24:ARG:HH11	5:E:85:THR:CG2	2.15	0.59
5:J:24:ARG:HH11	5:J:85:THR:CG2	2.15	0.59
5:J:151:THR:O	5:J:152:GLN:HB2	2.02	0.58
5:E:58:GLU:HG2	5:E:80:HIS:HD2	1.67	0.58
1:F:73:THR:HG21	3:H:6:SER:OG	2.04	0.57
1:A:181:ARG:HH21	1:A:239:ARG:HH21	1.51	0.57
5:J:148:ILE:HG23	5:J:154:ALA:HB2	1.86	0.56
5:J:174:VAL:HG23	5:J:179:VAL:HG21	1.87	0.56
5:E:39:MET:HG3	5:E:80:HIS:CE1	2.41	0.56
4:I:139:LEU:HD12	5:J:144:SER:HB2	1.88	0.56
5:J:167:HIS:HB3	5:J:228:TYR:HB2	1.89	0.55
5:J:224:GLN:NE2	5:J:226:GLN:HB2	2.21	0.55
4:I:139:LEU:HD22	5:J:157:VAL:HG22	1.89	0.55
5:E:58:GLU:HG2	5:E:80:HIS:CD2	2.41	0.55
5:J:223:CYS:HB3	5:J:250:ALA:O	2.07	0.54
1:F:155:GLN:HB3	3:H:3:PHE:HZ	1.72	0.54
1:A:155:GLN:HB3	3:C:3:PHE:HZ	1.73	0.54
4:I:214:PHE:CE2	5:J:146:ALA:HB1	2.39	0.53
5:E:58:GLU:HG3	5:E:84:LEU:HD13	1.90	0.53
5:J:147:GLU:C	5:J:149:SER:H	2.15	0.53
1:A:37:ASP:OD1	1:A:39:ASP:HB2	2.09	0.53
4:I:137:TYR:CE1	5:J:146:ALA:O	2.62	0.53
5:J:183:VAL:CG1	5:J:207:LEU:HB2	2.38	0.53
5:E:230:LEU:HD12	5:E:243:PRO:HD2	1.90	0.52
1:A:73:THR:HG21	3:C:6:SER:OG	2.10	0.52
5:J:230:LEU:HD12	5:J:243:PRO:HD2	1.92	0.52
5:E:145:GLU:H	5:E:145:GLU:CD	2.17	0.51
1:F:108:ARG:HG2	1:F:109:LEU:H	1.76	0.51
5:E:48:GLN:HE21	5:E:48:GLN:CA	2.23	0.50
5:J:148:ILE:CG2	5:J:154:ALA:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:HA2	1:A:110:LEU:HD12	1.93	0.49
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.93	0.49
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.94	0.49
1:F:10:THR:HG22	1:F:12:MET:HE2	1.93	0.49
5:E:45:PHE:HB3	5:E:46:PRO:HD2	1.94	0.48
4:D:205:ASN:O	4:D:209:ILE:HG12	2.13	0.48
5:J:147:GLU:C	5:J:148:ILE:CG1	2.48	0.48
4:D:177:LEU:HB3	5:E:184:CYS:HB3	1.94	0.47
1:A:76:GLU:HA	1:A:76:GLU:OE1	2.13	0.47
1:A:181:ARG:NH2	1:A:239:ARG:HH21	2.12	0.47
5:J:175:ASN:CA	5:J:220:HIS:HD2	2.22	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.46
4:I:37:ASN:HB2	6:I:308:HOH:O	2.15	0.46
4:I:216:PRO:HG3	5:J:146:ALA:HB3	1.97	0.46
4:I:137:TYR:CZ	5:J:146:ALA:O	2.69	0.46
5:E:48:GLN:NE2	5:E:48:GLN:CA	2.79	0.46
1:F:224:GLN:HB3	1:F:227:ASP:HB2	1.98	0.46
5:E:10:ARG:HG2	5:E:123:ARG:HB3	1.98	0.46
4:I:137:TYR:HB3	5:J:144:SER:OG	2.15	0.46
4:I:139:LEU:CD1	5:J:144:SER:HB2	2.45	0.46
5:J:39:MET:HG3	5:J:80:HIS:CE1	2.51	0.45
1:F:21:ARG:HG3	1:F:39:ASP:HB2	1.98	0.45
4:I:137:TYR:HB3	5:J:144:SER:HB3	1.99	0.45
1:A:238:ASP:O	1:A:239:ARG:HG2	2.16	0.45
4:D:190:VAL:HG23	5:E:206:ARG:HH11	1.81	0.45
5:E:43:ARG:HD2	6:E:309:HOH:O	2.17	0.45
1:A:224:GLN:HB3	1:A:227:ASP:HB2	1.99	0.45
4:D:169:VAL:HG12	4:D:193:SER:HB2	1.99	0.45
5:J:173:TRP:CE2	5:J:178:GLU:HG3	2.52	0.45
4:D:149:VAL:HG21	5:E:157:VAL:HG21	1.99	0.44
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.99	0.44
4:I:216:PRO:HG3	5:J:146:ALA:CB	2.48	0.44
5:J:45:PHE:HB3	5:J:46:PRO:HD2	2.00	0.44
1:A:214:THR:HB	1:A:262:GLN:HB3	1.99	0.44
4:I:134:PRO:O	4:I:213:THR:HA	2.18	0.44
1:A:98:MET:HE1	2:B:58:LYS:HG2	1.99	0.44
5:J:222:ARG:HG3	5:J:251:GLU:HB3	1.99	0.44
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.53	0.43
5:E:24:ARG:HH11	5:E:85:THR:HG23	1.84	0.43
4:D:101:VAL:HG22	4:D:122:LYS:HD2	2.00	0.43
4:I:137:TYR:CD1	5:J:146:ALA:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:174:VAL:HG12	5:J:175:ASN:ND2	2.34	0.43
4:I:134:PRO:HG3	4:I:210:PRO:HG2	2.00	0.43
2:B:39:LEU:HD23	2:B:68:THR:HG22	2.01	0.43
4:D:0:MET:HE3	4:D:0:MET:HB3	1.86	0.43
4:I:184:PHE:HE2	5:J:208:ARG:NH1	2.16	0.43
1:A:191:HIS:HB2	1:A:274:TRP:NE1	2.34	0.42
4:I:153:THR:HG21	5:J:147:GLU:OE1	2.18	0.42
5:E:24:ARG:HD3	5:E:85:THR:HG23	2.00	0.42
4:I:0:MET:HE2	4:I:0:MET:H2	1.83	0.42
5:E:141:PHE:HB2	5:E:157:VAL:CG2	2.50	0.42
5:J:183:VAL:HG13	5:J:207:LEU:HD13	2.00	0.42
5:J:142:GLU:CB	5:J:143:PRO:HD2	2.45	0.42
1:F:214:THR:HB	1:F:262:GLN:HB3	2.01	0.42
5:J:24:ARG:CD	5:J:85:THR:HG23	2.50	0.42
5:J:24:ARG:HD3	5:J:85:THR:HG23	2.02	0.41
5:E:146:ALA:O	5:E:150:HIS:HB2	2.20	0.41
5:E:19:VAL:HG11	5:E:124:LEU:HD11	2.02	0.41
5:E:24:ARG:CD	5:E:85:THR:HG23	2.50	0.41
5:J:223:CYS:O	5:J:223:CYS:SG	2.79	0.41
5:J:140:VAL:HG21	5:J:223:CYS:HB3	2.02	0.41
5:E:48:GLN:NE2	5:E:48:GLN:HA	2.36	0.41
5:E:54:ALA:HB3	5:E:78:ILE:CD1	2.50	0.41
2:G:39:LEU:HD23	2:G:68:THR:HG22	2.02	0.41
5:E:169:GLU:HG3	5:E:226:GLN:HB3	2.03	0.41
1:F:191:HIS:HB2	1:F:274:TRP:NE1	2.35	0.41
4:I:36:SER:C	4:I:37:ASN:HD22	2.29	0.41
4:I:101:VAL:HG22	4:I:122:LYS:HD2	2.02	0.40
5:J:147:GLU:C	5:J:149:SER:N	2.79	0.40
4:D:149:VAL:HG12	4:D:192:TRP:HB3	2.03	0.40
5:E:72:GLU:HB2	5:E:75:LYS:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	275/276 (100%)	265 (96%)	9 (3%)	1 (0%)	30	54
1	F	275/276 (100%)	262 (95%)	12 (4%)	1 (0%)	30	54
2	B	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	G	97/100 (97%)	96 (99%)	1 (1%)	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
4	D	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
4	I	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
5	E	243/245 (99%)	232 (96%)	10 (4%)	1 (0%)	30	54
5	J	243/245 (99%)	224 (92%)	18 (7%)	1 (0%)	30	54
All	All	1650/1670 (99%)	1574 (95%)	72 (4%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	148	ILE
1	A	251	SER
5	E	166	ASP
1	F	251	SER

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%)	224 (95%)	11 (5%)	23	51
1	F	235/234 (100%)	222 (94%)	13 (6%)	19	45
2	B	94/95 (99%)	91 (97%)	3 (3%)	34	64
2	G	94/95 (99%)	89 (95%)	5 (5%)	20	46
3	C	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	182/182 (100%)	171 (94%)	11 (6%)	17	41
4	I	182/182 (100%)	173 (95%)	9 (5%)	22	49
5	E	216/216 (100%)	192 (89%)	24 (11%)	6	15
5	J	216/216 (100%)	187 (87%)	29 (13%)	4	9
All	All	1472/1472 (100%)	1367 (93%)	105 (7%)	13	33

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	61	ASP
1	A	73	THR
1	A	76	GLU
1	A	110	LEU
1	A	156	LEU
1	A	197	HIS
1	A	225	THR
1	A	229	GLU
1	A	230	LEU
1	A	272	LEU
2	B	39	LEU
2	B	48	LYS
2	B	88	SER
4	D	0	MET
4	D	12	SER
4	D	27	ASP
4	D	46	LEU
4	D	76	ILE
4	D	89	LEU
4	D	145	SER
4	D	146	ASP
4	D	156	ASP
4	D	158	GLN
4	D	183	ASP
5	E	3	VAL
5	E	19	VAL
5	E	48	GLN
5	E	51	MET
5	E	64	LYS

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Mol	Chain	Res	Type
5	E	72	GLU
5	E	73	LYS
5	E	75	LYS
5	E	84	LEU
5	E	85	THR
5	E	89	LEU
5	E	130	LEU
5	E	145	GLU
5	E	156	LEU
5	E	168	VAL
5	E	177	LYS
5	E	184	CYS
5	E	188	GLN
5	E	193	GLN
5	E	196	LEU
5	E	198	ASP
5	E	215	GLN
5	E	239	ASP
5	E	240	ARG
1	F	65	GLN
1	F	73	THR
1	F	75	ARG
1	F	88	SER
1	F	103	LEU
1	F	110	LEU
1	F	145	ARG
1	F	156	LEU
1	F	183	ASP
1	F	197	HIS
1	F	229	GLU
1	F	230	LEU
1	F	272	LEU
2	G	19	LYS
2	G	39	LEU
2	G	48	LYS
2	G	75	LYS
2	G	88	SER
4	I	0	MET
4	I	12	SER
4	I	27	ASP
4	I	46	LEU
4	I	76	ILE

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Mol	Chain	Res	Type
4	I	89	LEU
4	I	141	ASP
4	I	176	VAL
4	I	205	ASN
5	J	3	VAL
5	J	19	VAL
5	J	47	LYS
5	J	48	GLN
5	J	64	LYS
5	J	72	GLU
5	J	73	LYS
5	J	75	LYS
5	J	84	LEU
5	J	85	THR
5	J	89	LEU
5	J	130	LEU
5	J	140	VAL
5	J	147	GLU
5	J	148	ILE
5	J	158	CYS
5	J	159	LEU
5	J	161	THR
5	J	168	VAL
5	J	175	ASN
5	J	183	VAL
5	J	184	CYS
5	J	196	LEU
5	J	220	HIS
5	J	223	CYS
5	J	239	ASP
5	J	240	ARG
5	J	249	SER
5	J	253	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	180	GLN
1	A	255	GLN
4	D	14	GLN
4	D	86	HIS

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Mol	Chain	Res	Type
4	D	138	GLN
4	D	163	GLN
4	D	202	ASN
5	E	48	GLN
5	E	132	ASN
5	E	150	HIS
5	E	215	GLN
5	E	220	HIS
5	E	238	GLN
5	E	246	GLN
1	F	155	GLN
1	F	180	GLN
1	F	218	GLN
2	G	17	ASN
4	I	14	GLN
4	I	37	ASN
4	I	138	GLN
5	J	132	ASN
5	J	175	ASN
5	J	220	HIS

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 [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	276/276 (100%)	0.52	30 (10%) 10 9	20, 66, 177, 207	8 (2%)
1	F	276/276 (100%)	0.22	20 (7%) 21 18	17, 52, 185, 205	9 (3%)
2	B	99/100 (99%)	0.85	7 (7%) 22 19	47, 87, 127, 138	6 (6%)
2	G	99/100 (99%)	0.20	2 (2%) 65 62	32, 62, 99, 115	6 (6%)
3	C	9/9 (100%)	-0.60	0 100 100	29, 34, 43, 50	0
3	H	9/9 (100%)	-0.36	0 100 100	26, 32, 36, 39	0
4	D	205/205 (100%)	0.18	5 (2%) 59 56	32, 61, 105, 139	1 (0%)
4	I	205/205 (100%)	1.38	67 (32%) 1 1	32, 91, 226, 253	0
5	E	245/245 (100%)	0.13	6 (2%) 59 56	27, 57, 103, 144	0
5	J	245/245 (100%)	1.35	80 (32%) 1 1	27, 107, 230, 263	0
All	All	1668/1670 (99%)	0.59	217 (13%) 7 6	17, 66, 193, 263	30 (1%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	156	LEU	8.3
2	B	1	ILE	8.0
5	J	256	ALA	7.8
4	I	151	LEU	7.0
4	I	209	ILE	6.9
2	G	1	ILE	6.9
4	I	204	PHE	6.6
5	J	155	THR	6.4
4	I	136	VAL	6.2
5	J	207	LEU	5.9
4	I	208	ILE	5.8
4	I	150	CYS	5.7
5	J	214	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
5	J	257	ASP	5.5
5	J	140	VAL	5.5
5	J	157	VAL	5.4
4	I	178	ASP	5.2
4	I	192	TRP	5.2
5	J	179	VAL	5.2
4	I	198	PHE	5.1
5	J	252	ALA	5.1
5	J	216	ASN	4.9
5	J	212	THR	4.9
5	J	141	PHE	4.6
5	J	213	PHE	4.6
5	J	139	ALA	4.5
5	J	211	ALA	4.5
4	I	217	SER	4.5
5	J	253	TRP	4.4
5	J	153	LYS	4.4
5	J	142	GLU	4.4
4	I	205	ASN	4.4
1	A	257	TYR	4.4
4	I	206	ASN	4.3
5	J	210	SER	4.3
1	F	1	GLY	4.2
5	J	217	PRO	4.2
5	J	221	PHE	4.0
4	I	199	ALA	4.0
4	I	203	ALA	4.0
4	I	149	VAL	4.0
5	J	143	PRO	4.0
5	J	148	ILE	4.0
5	J	174	VAL	4.0
4	I	207	SER	3.9
5	J	208	ARG	3.9
4	I	201	ALA	3.9
4	I	177	LEU	3.8
5	J	209	VAL	3.8
4	I	152	PHE	3.8
5	J	248	VAL	3.8
5	J	223	CYS	3.7
5	J	171	SER	3.7
5	J	251	GLU	3.7
4	I	157	SER	3.7

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Mol	Chain	Res	Type	RSRZ
5	J	218	ARG	3.7
5	J	249	SER	3.7
4	I	210	PRO	3.6
5	J	224	GLN	3.6
2	G	75	LYS	3.6
4	I	161	VAL	3.5
1	A	258	THR	3.5
4	I	135	ALA	3.5
1	A	261	VAL	3.5
1	F	257	TYR	3.5
5	J	151	THR	3.4
4	I	218	PRO	3.4
4	I	139	LEU	3.4
2	B	74	GLU	3.3
4	I	156	ASP	3.3
4	I	143	LYS	3.3
4	I	137	TYR	3.3
5	J	254	GLY	3.3
4	I	216	PRO	3.2
5	J	222	ARG	3.2
1	F	248	VAL	3.2
2	B	99	MET	3.1
4	I	215	PHE	3.1
5	J	225	VAL	3.1
4	I	214	PHE	3.1
1	A	252	GLY	3.1
1	A	199	ALA	3.1
1	F	270	LEU	3.1
1	A	268	LYS	3.1
5	J	172	TRP	3.1
5	J	183	VAL	3.1
5	J	173	TRP	3.0
5	J	226	GLN	3.0
5	J	250	ALA	3.0
1	A	201	LEU	3.0
5	J	181	SER	3.0
5	J	228	TYR	3.0
4	D	182	MET	3.0
1	A	248	VAL	3.0
4	I	0	MET	3.0
4	I	182	MET	3.0
4	I	211	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
4	I	141	ASP	2.9
5	J	178	GLU	2.9
1	A	247	VAL	2.9
4	I	213	THR	2.9
5	J	180	HIS	2.9
5	J	146	ALA	2.8
1	A	195	SER	2.8
1	F	189	VAL	2.8
2	B	75	LYS	2.8
1	A	217	TRP	2.8
1	F	274	TRP	2.8
4	I	194	ASN	2.8
4	I	185	LYS	2.7
4	I	202	ASN	2.7
5	J	59	GLY	2.7
4	I	212	ASP	2.7
5	J	154	ALA	2.7
5	J	239	ASP	2.7
4	I	129	ILE	2.7
4	I	155	PHE	2.7
4	I	179	MET	2.6
4	I	169	VAL	2.6
2	B	46	ILE	2.6
2	B	69	GLU	2.6
5	J	197	ASN	2.6
5	J	219	ASN	2.6
5	J	149	SER	2.6
5	J	176	GLY	2.6
1	A	193	PRO	2.6
1	F	201	LEU	2.6
1	F	192	HIS	2.6
5	J	147	GLU	2.6
5	J	182	GLY	2.6
5	J	247	ILE	2.5
4	I	190	VAL	2.5
5	J	170	LEU	2.5
1	A	221	GLY	2.5
5	J	49	SER	2.5
4	I	170	TYR	2.5
1	A	194	VAL	2.5
1	A	249	VAL	2.5
4	D	0	MET	2.5

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Mol	Chain	Res	Type	RSRZ
5	J	241	ALA	2.5
1	A	200	THR	2.5
1	A	219	ARG	2.5
5	J	206	ARG	2.5
5	J	163	PHE	2.5
1	F	259	CYS	2.4
4	I	154	ASP	2.4
1	F	194	VAL	2.4
5	J	150	HIS	2.4
4	D	143	LYS	2.4
4	I	142	SER	2.4
4	I	134	PRO	2.4
4	I	147	LYS	2.4
5	J	255	ARG	2.4
1	A	216	THR	2.4
1	F	187	THR	2.4
4	I	171	ILE	2.4
5	E	196	LEU	2.4
1	F	108	ARG	2.4
1	A	246	ALA	2.4
2	B	2	GLN	2.3
4	I	138	GLN	2.3
4	I	153	THR	2.3
4	I	189	ALA	2.3
5	J	196	LEU	2.3
4	I	181	SER	2.3
5	J	144	SER	2.3
5	E	253	TRP	2.3
5	J	236	TRP	2.3
1	F	215	LEU	2.3
1	F	249	VAL	2.3
5	J	158	CYS	2.2
5	E	240	ARG	2.2
1	F	220	ASP	2.2
5	E	48	GLN	2.2
5	J	152	GLN	2.2
5	J	166	ASP	2.2
1	A	272	LEU	2.2
1	A	274	TRP	2.2
5	J	167	HIS	2.2
1	A	225	THR	2.2
4	I	159	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	223	ASP	2.2
4	I	162	SER	2.2
5	J	198	ASP	2.2
5	E	256	ALA	2.2
1	F	225	THR	2.2
1	A	273	ARG	2.2
1	A	42	SER	2.2
4	I	144	SER	2.2
5	E	167	HIS	2.2
4	I	191	ALA	2.1
1	A	177	GLU	2.1
4	I	172	THR	2.1
5	J	237	THR	2.1
5	J	215	GLN	2.1
1	F	221	GLY	2.1
1	A	197	HIS	2.1
4	I	127	PRO	2.1
4	I	160	ASN	2.1
1	A	41	ALA	2.1
4	I	196	SER	2.1
1	F	275	GLU	2.1
1	F	204	TRP	2.1
4	D	147	LYS	2.1
1	A	58	GLU	2.0
4	I	180	ARG	2.0
5	J	145	GLU	2.0
4	I	145	SER	2.0
5	J	195	ALA	2.0
5	J	177	LYS	2.0
1	F	216	THR	2.0
5	J	161	THR	2.0
4	D	86	HIS	2.0
4	I	176	VAL	2.0
5	J	244	VAL	2.0
4	I	186	SER	2.0
1	A	108	ARG	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 [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.