



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:13 AM UTC

PDB ID : 8RLU / pdb_00008rlu
Title : TCR in complex with HLA-E*01:03 bound to HBV envelope 371-379 S3N peptide
Authors : Pengelly, R.J.; Godinho, L.F.
Deposited on : 2024-01-03
Resolution : 2.35 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

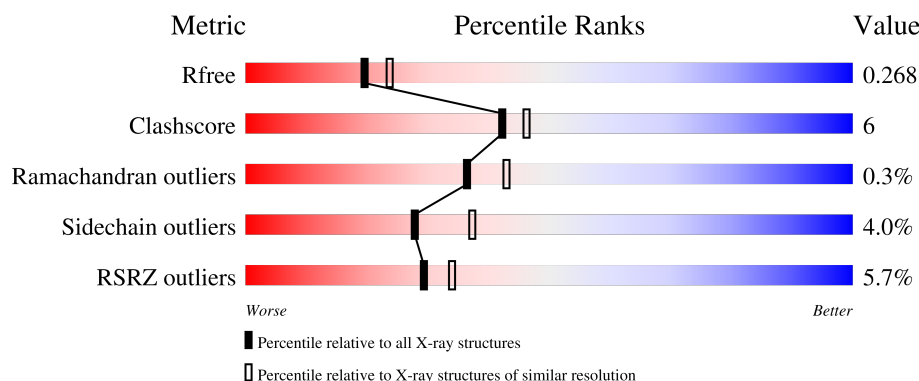
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	83% 14% .
1	F	276	3% 86% 12% ..
2	B	100	% 88% 12%
2	G	100	82% 15% .
3	C	9	89% 11%

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Mol	Chain	Length	Quality of chain
3	H	9	89%11%
4	D	199	% 74%19%5%
4	I	199	12% 79%11%10%
5	E	243	% 81%16%..
5	J	243	23% 72%20%6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25369 atoms, of which 12254 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	H	N	O	S	79	1	0
			4360	1408	2107	403	435	7			
1	F	273	Total	C	H	N	O	S	75	0	0
			4310	1393	2084	397	429	7			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	100	Total	C	H	N	O	S	28	0	0
			1644	533	807	141	159	4			
2	G	100	Total	C	H	N	O	S	28	0	0
			1644	533	807	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Large envelope protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O		0	0	0
			160	53	86	10	11				
3	H	9	Total	C	H	N	O		0	0	0
			160	53	86	10	11				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ASN	SER	engineered mutation	UNP Q67953
H	3	ASN	SER	engineered mutation	UNP Q67953

- Molecule 4 is a protein called T cell receptor alpha variable 12-2,T cell receptor alpha chain MC.7.G5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	189	Total	C	H	N	O	S	48	0	0
			2857	907	1396	249	295	10			
4	I	180	Total	C	H	N	O	S	45	0	0
			2714	863	1325	237	279	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP A0A075B6T6
D	1	ALA	-	expression tag	UNP A0A075B6T6
D	31	VAL	GLN	variant	UNP A0A075B6T6
D	49	SER	PHE	variant	UNP A0A075B6T6
D	52	LEU	SER	variant	UNP A0A075B6T6
D	55	LEU	ASP	variant	UNP A0A075B6T6
D	92	GLY	-	variant	UNP A0A075B6T6
D	93	ASN	-	variant	UNP A0A075B6T6
D	94	HIS	-	variant	UNP A0A075B6T6
D	95	ASN	-	variant	UNP A0A075B6T6
D	96	THR	-	variant	UNP A0A075B6T6
D	97	GLY	-	variant	UNP A0A075B6T6
D	98	ASN	-	variant	UNP A0A075B6T6
D	99	MET	-	variant	UNP A0A075B6T6
D	100	LEU	-	variant	UNP A0A075B6T6
D	101	THR	-	variant	UNP A0A075B6T6
D	102	PHE	-	variant	UNP A0A075B6T6
D	103	GLY	-	variant	UNP A0A075B6T6
D	104	GLY	-	variant	UNP A0A075B6T6
D	105	GLY	-	variant	UNP A0A075B6T6
D	106	THR	-	variant	UNP A0A075B6T6
D	107	ARG	-	variant	UNP A0A075B6T6
D	108	LEU	-	variant	UNP A0A075B6T6
D	109	MET	-	variant	UNP A0A075B6T6
D	113	HIS	ASN	variant	UNP P0DTU3
D	160	CYS	THR	variant	UNP P0DTU3
I	0	MET	-	initiating methionine	UNP A0A075B6T6
I	1	ALA	-	expression tag	UNP A0A075B6T6
I	31	VAL	GLN	variant	UNP A0A075B6T6
I	49	SER	PHE	variant	UNP A0A075B6T6
I	52	LEU	SER	variant	UNP A0A075B6T6
I	55	LEU	ASP	variant	UNP A0A075B6T6
I	92	GLY	-	variant	UNP A0A075B6T6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	93	ASN	-	variant	UNP A0A075B6T6
I	94	HIS	-	variant	UNP A0A075B6T6
I	95	ASN	-	variant	UNP A0A075B6T6
I	96	THR	-	variant	UNP A0A075B6T6
I	97	GLY	-	variant	UNP A0A075B6T6
I	98	ASN	-	variant	UNP A0A075B6T6
I	99	MET	-	variant	UNP A0A075B6T6
I	100	LEU	-	variant	UNP A0A075B6T6
I	101	THR	-	variant	UNP A0A075B6T6
I	102	PHE	-	variant	UNP A0A075B6T6
I	103	GLY	-	variant	UNP A0A075B6T6
I	104	GLY	-	variant	UNP A0A075B6T6
I	105	GLY	-	variant	UNP A0A075B6T6
I	106	THR	-	variant	UNP A0A075B6T6
I	107	ARG	-	variant	UNP A0A075B6T6
I	108	LEU	-	variant	UNP A0A075B6T6
I	109	MET	-	variant	UNP A0A075B6T6
I	113	HIS	ASN	variant	UNP P0DTU3
I	160	CYS	THR	variant	UNP P0DTU3

- Molecule 5 is a protein called T cell receptor beta variable 6-5,T cell receptor beta chain MC.7.G5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	240	Total	C	H	N	O	S	59	0	0
			3728	1200	1818	333	368	9			
5	J	229	Total	C	H	N	O	S	57	0	0
			3555	1146	1738	312	350	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP A0A0K0K1A5
E	29	TYR	HIS	variant	UNP A0A0K0K1A5
E	51	SER	GLY	variant	UNP A0A0K0K1A5
E	54	LEU	ILE	variant	UNP A0A0K0K1A5
E	94	HIS	-	variant	UNP A0A0K0K1A5
E	95	ARG	-	variant	UNP A0A0K0K1A5
E	96	ASN	-	variant	UNP A0A0K0K1A5
E	97	ARG	-	variant	UNP A0A0K0K1A5
E	98	LEU	-	variant	UNP A0A0K0K1A5
E	99	THR	-	variant	UNP A0A0K0K1A5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	100	GLU	-	variant	UNP A0A0K0K1A5
E	101	ALA	-	variant	UNP A0A0K0K1A5
E	102	PHE	-	variant	UNP A0A0K0K1A5
E	105	GLN	PRO	variant	UNP P0DTU4
E	112	VAL	LEU	variant	UNP P0DTU4
E	169	CYS	SER	variant	UNP P0DTU4
E	187	ALA	CYS	variant	UNP P0DTU4
E	201	ASP	ASN	variant	UNP P0DTU4
J	0	MET	-	initiating methionine	UNP A0A0K0K1A5
J	29	TYR	HIS	variant	UNP A0A0K0K1A5
J	51	SER	GLY	variant	UNP A0A0K0K1A5
J	54	LEU	ILE	variant	UNP A0A0K0K1A5
J	94	HIS	-	variant	UNP A0A0K0K1A5
J	95	ARG	-	variant	UNP A0A0K0K1A5
J	96	ASN	-	variant	UNP A0A0K0K1A5
J	97	ARG	-	variant	UNP A0A0K0K1A5
J	98	LEU	-	variant	UNP A0A0K0K1A5
J	99	THR	-	variant	UNP A0A0K0K1A5
J	100	GLU	-	variant	UNP A0A0K0K1A5
J	101	ALA	-	variant	UNP A0A0K0K1A5
J	102	PHE	-	variant	UNP A0A0K0K1A5
J	105	GLN	PRO	variant	UNP P0DTU4
J	112	VAL	LEU	variant	UNP P0DTU4
J	169	CYS	SER	variant	UNP P0DTU4
J	187	ALA	CYS	variant	UNP P0DTU4
J	201	ASP	ASN	variant	UNP P0DTU4

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	21	Total O 21 21	0	0
6	C	2	Total O 2 2	0	0
6	D	22	Total O 22 22	0	0
6	E	31	Total O 31 31	0	0
6	F	61	Total O 61 61	0	0

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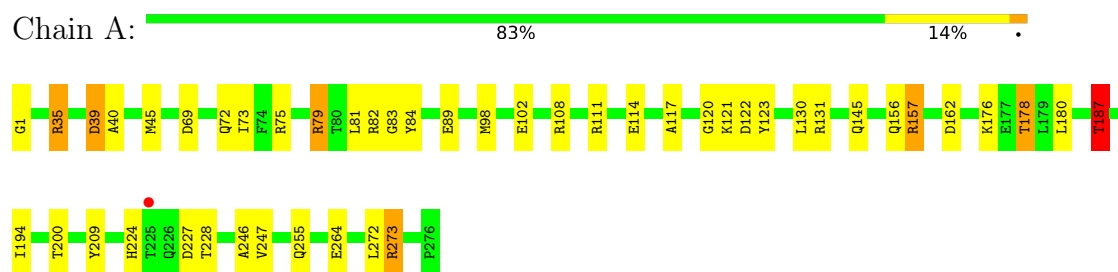
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	15	Total 15	O 15	0	0
6	H	4	Total 4	O 4	0	0
6	I	15	Total 15	O 15	0	0
6	J	5	Total 5	O 5	0	0

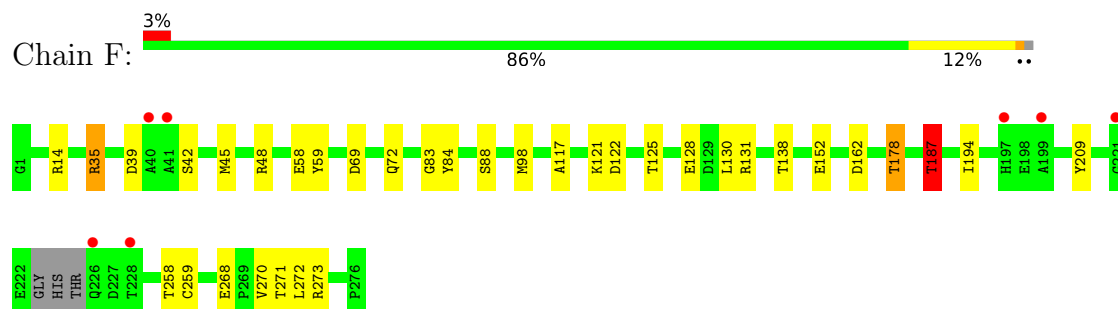
3 Residue-property plots [i](#)

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.

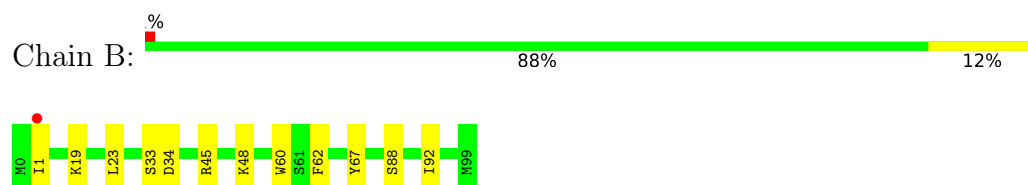
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



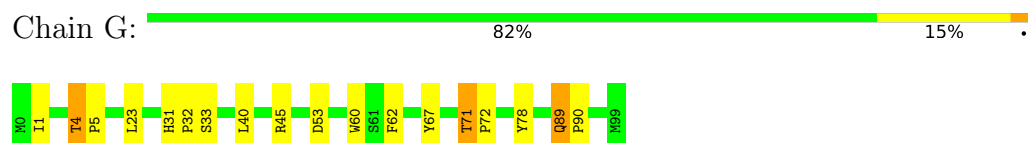
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Large envelope protein

Chain C:  89% 11%



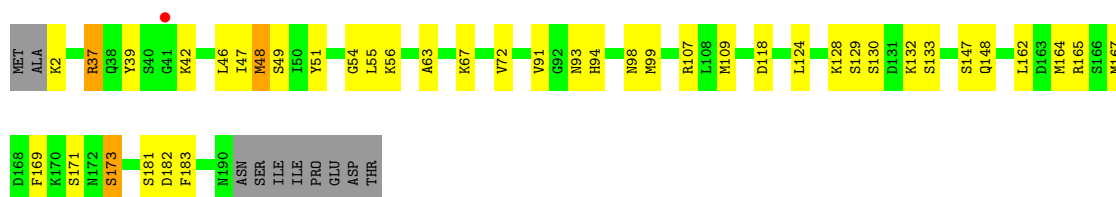
- Molecule 3: Large envelope protein

Chain H:  89% 11%



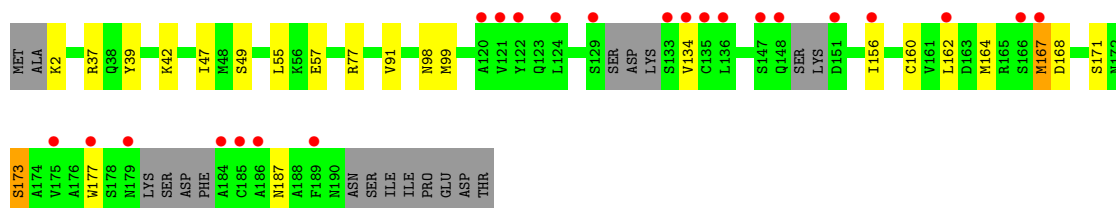
- Molecule 4: T cell receptor alpha variable 12-2,T cell receptor alpha chain MC.7.G5

Chain D:  % 74% 19% • 5%



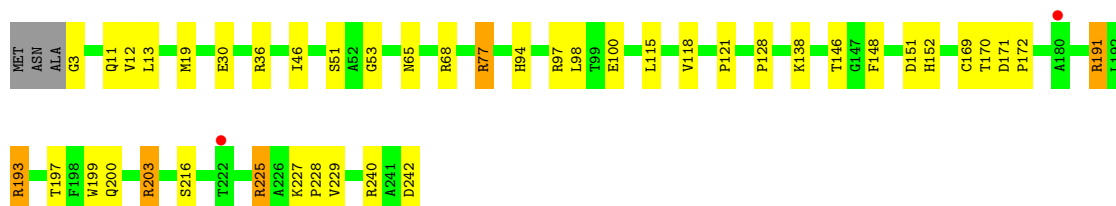
- Molecule 4: T cell receptor alpha variable 12-2,T cell receptor alpha chain MC.7.G5

Chain I:  12% 79% 11% • 10%



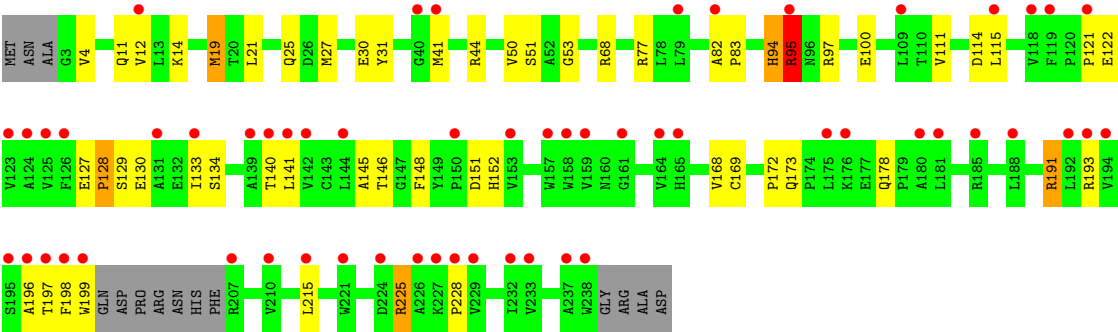
- Molecule 5: T cell receptor beta variable 6-5,T cell receptor beta chain MC.7.G5

Chain E:  % 81% 16% • •



- Molecule 5: T cell receptor beta variable 6-5,T cell receptor beta chain MC.7.G5

Chain J:  23% 72% 20% • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.42Å 147.84Å 91.91Å 90.00° 99.03° 90.00°	Depositor
Resolution (Å)	65.51 – 2.35 65.51 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (65.51-2.35) 99.1 (65.51-2.35)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.208 , 0.261 0.214 , 0.268	Depositor DCC
R_{free} test set	4289 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25369	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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	0.66	0/2320	1.12	6/3154 (0.2%)
1	F	0.65	0/2291	1.12	6/3113 (0.2%)
2	B	0.66	0/860	1.07	0/1162
2	G	0.58	0/860	1.01	1/1162 (0.1%)
3	C	0.69	0/76	1.26	0/103
3	H	0.71	0/76	1.20	0/103
4	D	0.66	0/1490	1.07	0/2015
4	I	0.63	0/1414	1.08	0/1911
5	E	0.62	0/1961	1.09	3/2670 (0.1%)
5	J	0.55	0/1864	1.07	3/2539 (0.1%)
All	All	0.63	0/13212	1.09	19/17932 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	F	0	3
2	B	0	1
2	G	0	1
4	D	0	1
4	I	0	1
5	E	0	4
5	J	0	4
All	All	0	21

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	THR	CA-CB-OG1	-7.78	97.94	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	162	ASP	CA-CB-CG	7.13	119.73	112.60
1	F	178	THR	CA-CB-OG1	-6.96	99.16	109.60
5	J	94	HIS	CA-CB-CG	6.73	120.53	113.80
5	E	197	THR	CA-CB-OG1	-6.42	99.97	109.60
5	E	200	GLN	CB-CA-C	6.07	121.37	109.72
5	E	152	HIS	CB-CA-C	-5.78	103.82	112.09
1	A	187	THR	CB-CA-C	5.72	119.66	109.65
5	J	152	HIS	CB-CA-C	-5.72	103.92	112.09
1	F	187	THR	CB-CA-C	5.56	119.39	109.65
2	G	71	THR	CA-CB-OG1	-5.31	101.64	109.60
1	F	125	THR	CA-CB-OG1	-5.30	101.64	109.60
1	A	224	HIS	CA-CB-CG	-5.25	108.55	113.80
5	J	198	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	264	GLU	CB-CG-CD	5.11	121.28	112.60
1	F	138	THR	CA-CB-OG1	-5.08	101.98	109.60
1	F	194	ILE	N-CA-C	-5.03	106.90	111.67
1	A	111	ARG	CA-C-N	5.01	126.22	121.46
1	A	111	ARG	C-N-CA	5.01	126.22	121.46

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	35	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	82	ARG	Sidechain
2	B	45	ARG	Sidechain
4	D	37	ARG	Sidechain
5	E	191	ARG	Sidechain
5	E	193	ARG	Sidechain
5	E	203	ARG	Sidechain
5	E	225	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	14	ARG	Sidechain
1	F	35	ARG	Sidechain
2	G	45	ARG	Sidechain
4	I	77	ARG	Sidechain
5	J	191	ARG	Sidechain
5	J	225	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	J	44	ARG	Sidechain
5	J	95	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	2107	2092	27	0
1	F	2226	2084	2070	20	0
2	B	837	807	803	5	0
2	G	837	807	803	12	0
3	C	74	86	86	1	0
3	H	74	86	86	1	0
4	D	1461	1396	1393	35	0
4	I	1389	1325	1319	12	0
5	E	1910	1818	1811	31	0
5	J	1817	1738	1731	43	0
6	A	61	0	0	3	0
6	B	21	0	0	0	0
6	C	2	0	0	0	0
6	D	22	0	0	3	0
6	E	31	0	0	2	0
6	F	61	0	0	1	0
6	G	15	0	0	0	0
6	H	4	0	0	0	0
6	I	15	0	0	1	0
6	J	5	0	0	0	0
All	All	13115	12254	12194	159	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 (159) 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:129:SER:O	5:J:133:ILE:HG12	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HD3	6:A:326:HOH:O	1.72	0.87
5:E:225:ARG:NH1	5:E:228:PRO:HG3	1.92	0.82
1:F:35:ARG:HG3	2:G:53:ASP:CG	2.08	0.78
5:J:82:ALA:O	5:J:111:VAL:HG21	1.84	0.77
5:J:128:PRO:HD2	5:J:199:TRP:CZ2	2.22	0.74
5:E:240:ARG:HH21	5:E:242:ASP:C	1.96	0.74
4:D:162:LEU:HB3	5:E:169:CYS:HB2	1.69	0.74
5:E:77:ARG:HG2	5:E:77:ARG:HH11	1.53	0.73
4:I:164:MET:HE3	5:J:193:ARG:HB3	1.70	0.73
5:J:83:PRO:HA	5:J:111:VAL:CG2	2.18	0.73
5:J:83:PRO:HA	5:J:111:VAL:HG23	1.73	0.71
5:E:30:GLU:OE1	5:E:51:SER:HB3	1.91	0.71
5:J:82:ALA:C	5:J:111:VAL:HG21	2.15	0.71
4:D:164:MET:HE1	5:E:138:LYS:HD3	1.74	0.68
1:F:187:THR:HG23	1:F:272:LEU:HD13	1.77	0.66
5:E:115:LEU:O	5:E:118:VAL:HG22	1.96	0.65
5:J:115:LEU:HD23	5:J:215:LEU:CD2	2.27	0.65
1:A:145:GLN:HG2	6:A:314:HOH:O	1.98	0.64
4:D:109:MET:HG2	6:D:220:HOH:O	1.97	0.64
5:J:115:LEU:HD23	5:J:215:LEU:HD22	1.80	0.64
5:E:240:ARG:NH2	5:E:242:ASP:OXT	2.31	0.63
5:J:128:PRO:HD3	5:J:141:LEU:HD23	1.79	0.63
4:D:2:LYS:N	6:D:204:HOH:O	2.32	0.62
5:J:11:GLN:HG2	5:J:19:MET:SD	2.40	0.62
1:A:176:LYS:HG3	1:A:180:LEU:HD12	1.83	0.61
5:J:25:GLN:HB2	5:J:27:MET:CE	2.31	0.60
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.37	0.60
5:E:77:ARG:HH11	5:E:77:ARG:CG	2.13	0.59
1:F:35:ARG:NH1	2:G:53:ASP:OD1	2.32	0.59
5:E:118:VAL:HG23	5:E:228:PRO:HG2	1.85	0.59
4:D:48:MET:HE2	4:D:63:ALA:HB3	1.84	0.59
4:I:173:SER:HB2	5:J:191:ARG:HE	1.67	0.59
4:D:54:GLY:C	4:D:55:LEU:HD22	2.28	0.58
4:D:48:MET:CE	4:D:63:ALA:HB3	2.34	0.58
1:F:72:GLN:NE2	5:J:30:GLU:OE1	2.28	0.58
5:J:127:GLU:O	5:J:128:PRO:O	2.21	0.58
5:J:215:LEU:HD12	5:J:228:PRO:HD2	1.86	0.57
4:D:128:LYS:O	4:D:130:SER:N	2.35	0.57
4:D:164:MET:CE	5:E:193:ARG:HD3	2.34	0.57
4:I:2:LYS:N	6:I:202:HOH:O	2.39	0.55
4:I:134:VAL:HG22	4:I:177:TRP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:MET:HB2	6:F:341:HOH:O	2.06	0.55
4:D:107:ARG:HG2	4:D:107:ARG:HH11	1.71	0.54
5:J:25:GLN:HB2	5:J:27:MET:HE2	1.90	0.53
4:D:128:LYS:C	4:D:130:SER:H	2.17	0.53
4:I:167:MET:O	4:I:168:ASP:HB3	2.09	0.53
1:F:35:ARG:HG3	2:G:53:ASP:OD1	2.08	0.53
4:I:37:ARG:HB2	4:I:47:ILE:HD11	1.91	0.53
1:A:255:GLN:OE1	1:A:273:ARG:HD3	2.09	0.52
4:D:37:ARG:HB2	4:D:47:ILE:HD11	1.90	0.52
4:D:164:MET:HE2	5:E:193:ARG:HD3	1.92	0.52
2:G:4:THR:HG22	2:G:5:PRO:HD2	1.92	0.52
1:A:194:ILE:HD11	1:A:200:THR:OG1	2.10	0.52
4:D:173:SER:HB2	5:E:191:ARG:HE	1.75	0.51
5:J:77:ARG:HH11	5:J:77:ARG:HG2	1.75	0.51
4:D:48:MET:HE2	4:D:63:ALA:CB	2.40	0.51
1:F:258:THR:CG2	1:F:273:ARG:HH21	2.24	0.51
1:A:130:LEU:HB2	1:A:157:ARG:HD2	1.91	0.51
5:E:30:GLU:OE1	5:E:51:SER:CB	2.59	0.51
5:E:128:PRO:HD2	5:E:199:TRP:CZ2	2.48	0.49
4:D:94:HIS:HA	5:E:98:LEU:HD11	1.94	0.49
5:E:227:LYS:O	5:E:229:VAL:N	2.43	0.49
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.49	0.48
4:D:98:ASN:O	4:D:99:MET:C	2.55	0.48
1:A:228:THR:HA	1:A:246:ALA:O	2.13	0.48
4:D:164:MET:HE3	4:D:169:PHE:CD1	2.49	0.48
5:E:11:GLN:HG2	5:E:19:MET:SD	2.53	0.48
5:J:14:LYS:HD2	5:J:115:LEU:HD11	1.95	0.48
4:I:39:TYR:O	4:I:42:LYS:HB2	2.14	0.48
1:F:83:GLY:O	1:F:84:TYR:C	2.56	0.47
4:D:118:ASP:CB	6:D:202:HOH:O	2.63	0.47
2:G:1:ILE:C	2:G:1:ILE:HD12	2.39	0.47
5:E:3:GLY:N	6:E:304:HOH:O	2.48	0.47
1:F:58:GLU:HG3	1:F:59:TYR:N	2.30	0.47
1:F:152:GLU:OE1	5:J:95:ARG:NH1	2.47	0.47
5:J:114:ASP:OD1	5:J:115:LEU:N	2.48	0.47
1:A:39:ASP:O	1:A:40:ALA:HB2	2.15	0.47
1:A:1:GLY:N	1:A:102:GLU:OE1	2.48	0.47
1:A:162:ASP:OD2	4:D:67:LYS:NZ	2.45	0.46
4:D:48:MET:HE1	4:D:56:LYS:O	2.14	0.46
4:D:165:ARG:HH11	4:D:165:ARG:HG3	1.80	0.46
4:D:181:SER:C	4:D:183:PHE:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:VAL:HG23	5:E:228:PRO:CB	2.45	0.46
5:J:115:LEU:CD2	5:J:215:LEU:HD22	2.45	0.46
5:J:133:ILE:HG23	5:J:196:ALA:HB1	1.96	0.46
1:A:83:GLY:O	1:A:84:TYR:C	2.59	0.46
5:E:118:VAL:HG23	5:E:228:PRO:HB2	1.98	0.46
2:G:40:LEU:O	2:G:78:TYR:HA	2.16	0.46
4:D:49:SER:OG	4:D:51:TYR:CE1	2.69	0.46
1:A:209:TYR:CD1	1:A:209:TYR:C	2.94	0.45
1:A:121:LYS:O	1:A:122:ASP:C	2.60	0.45
1:A:162:ASP:OD2	4:D:67:LYS:CE	2.63	0.45
1:A:73:ILE:HG12	6:E:308:HOH:O	2.16	0.45
4:I:160:CYS:C	5:J:169:CYS:SG	2.99	0.45
5:J:31:TYR:CE2	5:J:50:VAL:HG13	2.51	0.45
4:I:134:VAL:HG22	4:I:177:TRP:CB	2.46	0.45
1:A:75:ARG:HH11	1:A:79:ARG:HH11	1.65	0.45
5:E:36:ARG:HB3	5:E:46:ILE:HD11	1.99	0.45
5:E:77:ARG:CG	5:E:77:ARG:NH1	2.72	0.44
1:F:121:LYS:O	1:F:122:ASP:C	2.58	0.44
5:E:121:PRO:HB3	5:E:148:PHE:HB3	1.99	0.44
4:I:187:ASN:OD1	4:I:187:ASN:C	2.60	0.44
2:G:33:SER:HB3	2:G:62:PHE:CE2	2.53	0.44
1:A:162:ASP:OD2	4:D:67:LYS:HE3	2.18	0.44
4:D:48:MET:CE	4:D:63:ALA:CB	2.96	0.44
4:I:98:ASN:O	4:I:99:MET:C	2.61	0.44
5:J:53:GLY:N	5:J:68:ARG:O	2.47	0.43
2:B:19:LYS:HE2	2:B:19:LYS:HB3	1.88	0.43
1:F:128:GLU:O	1:F:130:LEU:HD13	2.17	0.43
1:A:79:ARG:HG3	6:A:323:HOH:O	2.18	0.43
1:A:120:GLY:O	2:B:1:ILE:HD12	2.19	0.43
5:J:4:VAL:HG22	5:J:27:MET:HE1	2.00	0.43
5:J:100:GLU:H	5:J:100:GLU:CD	2.27	0.43
1:F:209:TYR:CD1	1:F:209:TYR:C	2.97	0.43
5:J:121:PRO:HB3	5:J:148:PHE:HB3	2.01	0.43
5:J:83:PRO:CA	5:J:111:VAL:CG2	2.94	0.43
4:D:132:LYS:HB2	4:D:132:LYS:HE2	1.80	0.43
4:D:46:LEU:HD22	5:E:100:GLU:CD	2.43	0.43
1:F:69:ASP:CG	5:J:97:ARG:HH21	2.27	0.43
1:F:72:GLN:OE1	5:J:50:VAL:HG12	2.19	0.43
5:J:140:THR:OG1	5:J:193:ARG:NE	2.41	0.43
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.54	0.42
5:E:13:LEU:HD11	5:E:19:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:CYS:O	1:F:271:THR:HA	2.19	0.42
5:E:118:VAL:HG23	5:E:228:PRO:CG	2.48	0.42
1:F:45:MET:CE	3:H:2:LEU:HD11	2.50	0.42
5:J:151:ASP:CG	5:J:151:ASP:O	2.63	0.42
5:J:111:VAL:HG23	5:J:111:VAL:O	2.20	0.42
1:A:75:ARG:HH11	1:A:79:ARG:NH1	2.17	0.42
4:D:49:SER:OG	4:D:51:TYR:HE1	2.03	0.42
2:G:89:GLN:O	2:G:90:PRO:C	2.63	0.42
1:A:114:GLU:OE1	1:A:156:GLN:OE1	2.38	0.42
4:D:124:LEU:O	4:D:133:SER:HB2	2.20	0.42
1:F:72:GLN:NE2	5:J:51:SER:HB2	2.35	0.42
5:J:168:VAL:HG12	5:J:169:CYS:N	2.35	0.42
5:J:130:GLU:HA	5:J:133:ILE:HB	2.00	0.41
5:J:4:VAL:CG2	5:J:27:MET:HE1	2.51	0.41
5:J:225:ARG:CB	5:J:225:ARG:HH11	2.33	0.41
1:F:35:ARG:HB2	1:F:48:ARG:HG3	2.03	0.41
5:E:53:GLY:N	5:E:68:ARG:O	2.51	0.41
2:B:23:LEU:O	2:B:67:TYR:HA	2.21	0.41
2:G:71:THR:HA	2:G:72:PRO:HD2	1.93	0.41
1:A:45:MET:CE	3:C:2:LEU:HD11	2.50	0.41
1:A:69:ASP:CG	5:E:97:ARG:HH21	2.28	0.41
5:E:151:ASP:O	5:E:151:ASP:CG	2.63	0.41
2:G:31:HIS:ND1	2:G:32:PRO:HA	2.36	0.41
1:A:176:LYS:HE2	1:A:180:LEU:HD12	2.03	0.41
5:J:19:MET:HE2	5:J:21:LEU:HG	2.02	0.41
5:J:122:GLU:O	5:J:145:ALA:HA	2.21	0.41
5:E:170:THR:O	5:E:171:ASP:C	2.65	0.40
2:G:23:LEU:O	2:G:67:TYR:HA	2.22	0.40
4:I:162:LEU:HB3	5:J:169:CYS:HB2	2.03	0.40
4:D:128:LYS:C	4:D:130:SER:N	2.79	0.40
4:D:93:ASN:C	4:D:93:ASN:OD1	2.64	0.40
4:D:107:ARG:HG2	4:D:107:ARG:NH1	2.35	0.40
1:A:81:LEU:HD21	1:A:123:TYR:CZ	2.57	0.40
1:A:187:THR:HG23	1:A:272:LEU:HD22	2.04	0.40
4:D:39:TYR:O	4:D:42:LYS:HB2	2.21	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	275/276 (100%)	267 (97%)	8 (3%)	0	100	100
1	F	269/276 (98%)	264 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	G	98/100 (98%)	96 (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
4	D	187/199 (94%)	177 (95%)	8 (4%)	2 (1%)	11	11
4	I	172/199 (86%)	161 (94%)	11 (6%)	0	100	100
5	E	238/243 (98%)	220 (92%)	17 (7%)	1 (0%)	30	34
5	J	225/243 (93%)	204 (91%)	19 (8%)	2 (1%)	14	14
All	All	1576/1654 (95%)	1499 (95%)	72 (5%)	5 (0%)	36	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	128	PRO
4	D	182	ASP
4	D	129	SER
5	J	172	PRO
5	E	172	PRO

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	238/237 (100%)	228 (96%)	10 (4%)	26	35
1	F	235/237 (99%)	228 (97%)	7 (3%)	36	48
2	B	95/95 (100%)	91 (96%)	4 (4%)	26	35
2	G	95/95 (100%)	93 (98%)	2 (2%)	47	61
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	166/175 (95%)	158 (95%)	8 (5%)	23	29
4	I	157/175 (90%)	149 (95%)	8 (5%)	21	26
5	E	209/211 (99%)	202 (97%)	7 (3%)	33	44
5	J	200/211 (95%)	190 (95%)	10 (5%)	22	27
All	All	1413/1454 (97%)	1357 (96%)	56 (4%)	28	37

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	39	ASP
1	A	72	GLN
1	A	89	GLU
1	A	98	MET
1	A	178	THR
1	A	187	THR
1	A	227	ASP
1	A	247	VAL
1	A	273	ARG
2	B	34	ASP
2	B	48	LYS
2	B	88	SER
2	B	92	ILE
4	D	48	MET
4	D	72	VAL
4	D	91	VAL
4	D	147	SER
4	D	148	GLN
4	D	167	MET
4	D	171	SER
4	D	173	SER
5	E	12	VAL
5	E	65	ASN

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Mol	Chain	Res	Type
5	E	77	ARG
5	E	94	HIS
5	E	146	THR
5	E	203	ARG
5	E	216	SER
1	F	39	ASP
1	F	42	SER
1	F	88	SER
1	F	178	THR
1	F	187	THR
1	F	268	GLU
1	F	270	VAL
2	G	4	THR
2	G	89	GLN
4	I	49	SER
4	I	55	LEU
4	I	57	GLU
4	I	91	VAL
4	I	156	ILE
4	I	167	MET
4	I	171	SER
4	I	173	SER
5	J	12	VAL
5	J	19	MET
5	J	41	MET
5	J	94	HIS
5	J	95	ARG
5	J	134	SER
5	J	146	THR
5	J	173	GLN
5	J	178	GLN
5	J	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	I	38	GLN
5	J	37	GLN
5	J	223	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	276/276 (100%)	-0.21	1 (0%) 88 91	25, 46, 80, 151	1 (0%)
1	F	273/276 (98%)	-0.04	7 (2%) 57 63	32, 48, 93, 121	0
2	B	100/100 (100%)	-0.31	1 (1%) 79 83	35, 45, 76, 92	0
2	G	100/100 (100%)	-0.02	0 100 100	37, 54, 86, 107	0
3	C	9/9 (100%)	-0.59	0 100 100	37, 39, 45, 46	0
3	H	9/9 (100%)	-0.61	0 100 100	36, 37, 44, 51	0
4	D	189/199 (94%)	-0.09	1 (0%) 87 90	33, 49, 94, 121	0
4	I	180/199 (90%)	0.52	23 (12%) 7 9	30, 54, 120, 143	0
5	E	240/243 (98%)	-0.03	2 (0%) 82 86	35, 53, 91, 122	0
5	J	229/243 (94%)	1.32	57 (24%) 2 1	39, 83, 122, 139	0
All	All	1605/1654 (97%)	0.16	92 (5%) 29 34	25, 52, 107, 151	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	194	VAL	5.3
5	J	198	PHE	5.2
5	J	215	LEU	4.9
5	J	238	TRP	4.7
5	J	199	TRP	4.6
4	I	121	VAL	4.4
5	J	232	ILE	4.4
5	J	142	VAL	4.3
5	J	197	THR	4.3
5	J	141	LEU	4.1
5	J	79	LEU	4.0
5	J	139	ALA	4.0
5	J	140	THR	3.8

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Mol	Chain	Res	Type	RSRZ
5	J	221	TRP	3.8
5	J	159	VAL	3.8
4	I	167	MET	3.8
5	J	196	ALA	3.7
5	J	125	VAL	3.6
5	J	41	MET	3.6
5	J	157	TRP	3.5
5	J	195	SER	3.5
5	J	124	ALA	3.5
4	I	122	TYR	3.3
4	I	148	GLN	3.3
5	J	228	PRO	3.2
5	J	131	ALA	3.1
5	J	175	LEU	3.1
4	I	186	ALA	3.1
4	I	133	SER	3.0
4	D	41	GLY	3.0
4	I	136	LEU	3.0
4	I	179	ASN	3.0
1	A	225	THR	3.0
4	I	120	ALA	2.9
4	I	124	LEU	2.9
5	J	161	GLY	2.9
5	J	158	TRP	2.9
5	J	210	VAL	2.9
5	J	229	VAL	2.8
4	I	156	ILE	2.8
4	I	134	VAL	2.8
5	J	133	ILE	2.8
2	B	1	ILE	2.7
4	I	177	TRP	2.7
4	I	151	ASP	2.7
5	J	126	PHE	2.7
5	J	188	LEU	2.7
4	I	189	PHE	2.6
1	F	228	THR	2.6
5	J	40	GLY	2.6
4	I	185	CYS	2.5
4	I	166	SER	2.5
5	J	193	ARG	2.5
4	I	162	LEU	2.5
5	J	180	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
5	J	164	VAL	2.5
5	J	237	ALA	2.5
5	J	144	LEU	2.5
5	J	150	PRO	2.4
4	I	184	ALA	2.4
5	J	233	VAL	2.4
5	J	119	PHE	2.3
5	J	192	LEU	2.3
5	J	118	VAL	2.3
5	J	181	LEU	2.3
1	F	199	ALA	2.3
5	J	95	ARG	2.3
5	E	222	THR	2.3
4	I	175	VAL	2.2
5	J	123	VAL	2.2
5	J	121	PRO	2.2
4	I	129	SER	2.2
4	I	135	CYS	2.1
4	I	147	SER	2.1
5	J	185	ARG	2.1
5	J	224	ASP	2.1
1	F	221	GLY	2.1
5	J	207	ARG	2.1
5	J	153	VAL	2.1
5	J	226	ALA	2.1
5	J	227	LYS	2.1
5	J	115	LEU	2.1
1	F	41	ALA	2.0
5	E	180	ALA	2.0
1	F	197	HIS	2.0
1	F	226	GLN	2.0
5	J	165	HIS	2.0
5	J	12	VAL	2.0
1	F	40	ALA	2.0
5	J	82	ALA	2.0
5	J	109	LEU	2.0
5	J	176	LYS	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.