Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 02:58 pm BST

PDB ID	:	8RLV
Title	:	TCR in complex with HLA-E*01:03 bound to HBV envelope 371-379 L6I peptide
Authors	:	Pengelly, R.J.; Godinho, L.F.
Deposited on	:	2024-01-03
Resolution	:	2.61 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:

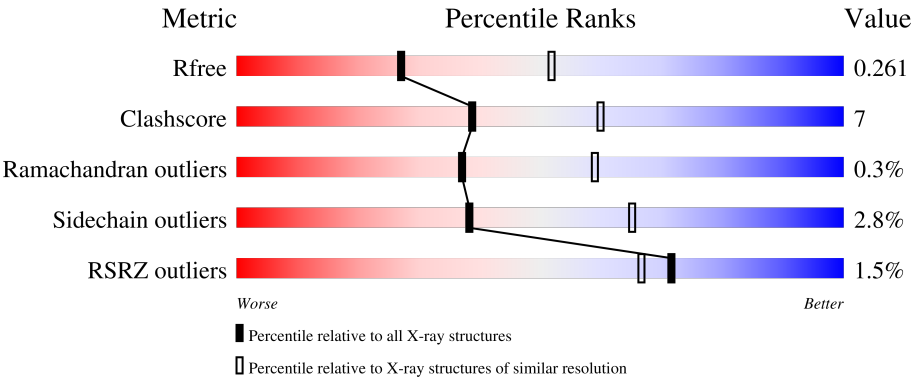
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 <=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	80% 19%
1	F	276	2% 80% 17%
2	B	100	83% 17%
2	G	100	85% 15%
3	C	9	78% 22%

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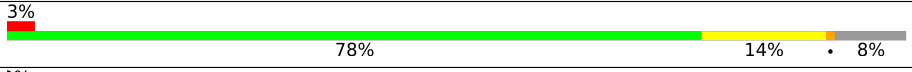
Mol	Chain	Length	Quality of chain
3	H	9	
4	D	199	
4	I	199	
5	E	243	
5	J	243	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25338 atoms, of which 12292 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	271	Total	C	H	N	O	S	75	0	0
			4278	1383	2070	394	424	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	1	0	0
			157	52	85	9	11			
3	H	9	Total	C	H	N	O	1	0	0
			157	52	85	9	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ILE	LEU	variant	UNP Q67953
H	6	ILE	LEU	variant	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	184	Total	C	H	N	O	S	47	0	0
			2778	884	1357	242	285	10			
4	I	184	Total	C	H	N	O	S	46	0	0
			2781	882	1360	243	286	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	237	Total	C	H	N	O	S	59	0	0
			3681	1187	1796	327	362	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	37	Total O 37 37	0	0
6	B	17	Total O 17 17	0	0
6	D	11	Total O 11 11	0	0
6	E	5	Total O 5 5	0	0
6	F	35	Total O 35 35	0	0
6	G	12	Total O 12 12	0	0

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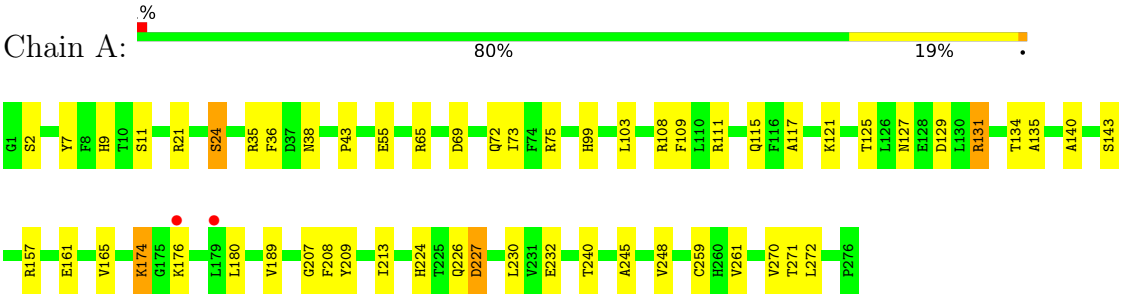
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O 1 1	0	0
6	I	8	Total O 8 8	0	0
6	J	4	Total O 4 4	0	0

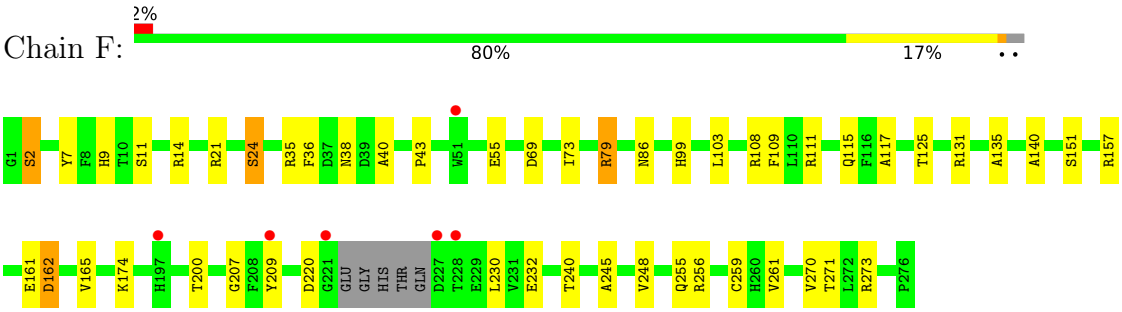
3 Residue-property plots (i)

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.

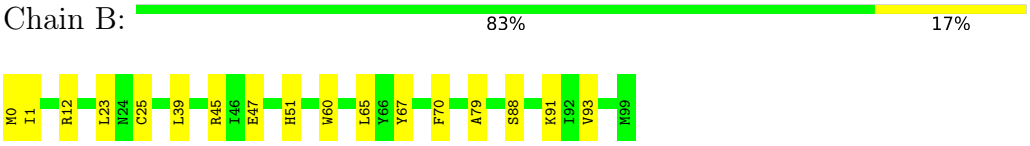
• Molecule 1: HLA class I histocompatibility antigen, alpha chain E



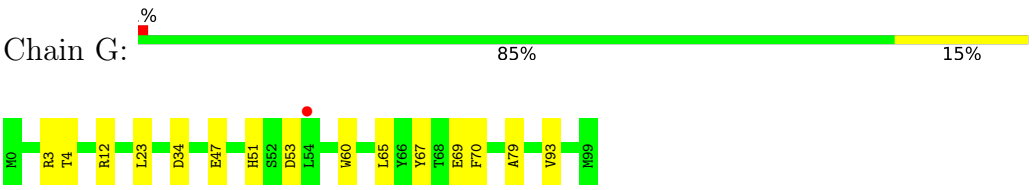
• Molecule 1: HLA class I histocompatibility antigen, alpha chain E



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 3: Large envelope protein

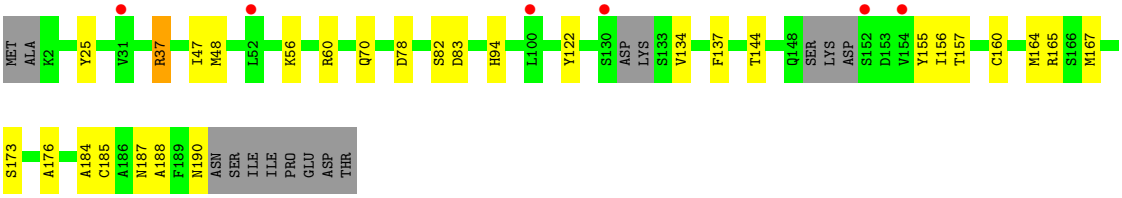
Chain C:

• Molecule 3: Large envelope protein

Chain H:

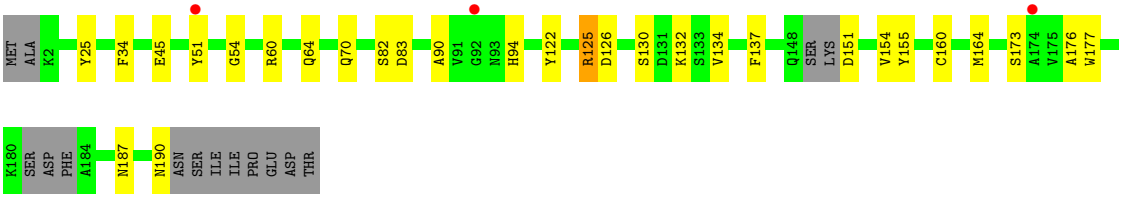
• Molecule 4: T cell receptor alpha variable 12-2,T cell receptor alpha chain MC.7.G5

Chain D:



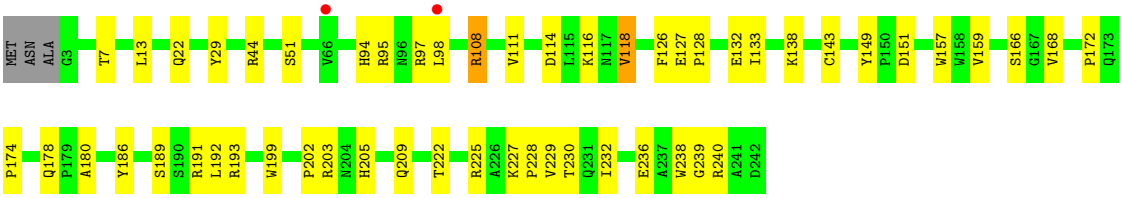
• Molecule 4: T cell receptor alpha variable 12-2,T cell receptor alpha chain MC.7.G5

Chain I:



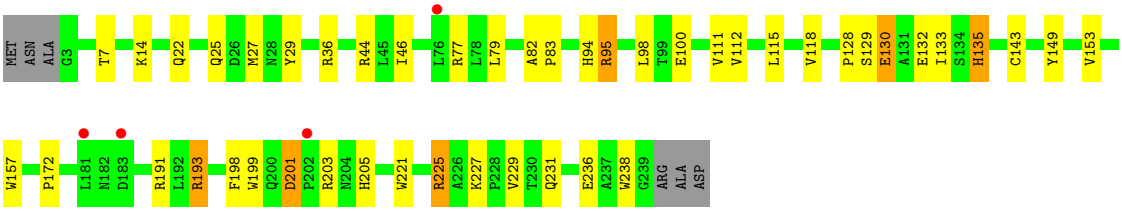
• Molecule 5: T cell receptor beta variable 6-5,T cell receptor beta chain MC.7.G5

Chain E:



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

Chain J:


MET
ASN
ALA
G3
T7
K14
Q22
Q25
D26
M27
N28
Y29
R36
R44
L45
I46
L76
R77
L78
L79
A82
P83
H94
R95
L98
T99
E100
V111
V112
L115
V118
P128
S129
E130
A131
E132
I133
S134
H135
C143
Y149
V153
W157
P172
L181
N182
D183
R191
L192
R193
F198
W199
Q200
D201
P202
R203
N204
H205
W221
R225
A226
K227
P228
V229
T230
Q231
E236
A237
W238
G239
ARG
ALA
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.19Å 153.81Å 93.40Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	79.65 – 2.61 79.65 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.1 (79.65-2.61) 98.4 (79.65-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.198 , 0.251 0.209 , 0.261	Depositor DCC
R_{free} test set	3362 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	70.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25338	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/2320	0.91	0/3154
1	F	0.51	1/2273 (0.0%)	0.89	2/3089 (0.1%)
2	B	0.50	0/860	0.88	0/1162
2	G	0.50	0/860	0.86	0/1162
3	C	0.63	0/74	0.82	0/100
3	H	0.54	0/74	0.91	0/100
4	D	0.48	0/1448	0.85	1/1957 (0.1%)
4	I	0.54	1/1447 (0.1%)	0.86	0/1955
5	E	0.43	0/1961	0.83	0/2670
5	J	0.43	0/1936	0.85	0/2638
All	All	0.49	2/13253 (0.0%)	0.87	3/17987 (0.0%)

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	2
1	F	0	4
2	B	0	1
2	G	0	2
4	D	0	1
4	I	0	1
5	E	0	3
5	J	0	4
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	45	GLU	CD-OE1	6.93	1.33	1.25
1	F	161	GLU	CD-OE2	5.06	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	162	ASP	N-CA-CB	5.22	120.00	110.60
1	F	157	ARG	NE-CZ-NH1	5.13	122.86	120.30
4	D	78	ASP	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	131	ARG	Sidechain
2	B	12	ARG	Sidechain
4	D	37	ARG	Sidechain
5	E	191	ARG	Sidechain
5	E	225	ARG	Sidechain
5	E	44	ARG	Sidechain
1	F	111	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	14	ARG	Sidechain
1	F	79	ARG	Sidechain
2	G	12	ARG	Sidechain
2	G	3	ARG	Sidechain
4	I	125	ARG	Sidechain
5	J	193	ARG	Sidechain
5	J	225	ARG	Sidechain
5	J	44	ARG	Sidechain
5	J	95	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	2107	2092	40	0
1	F	2208	2070	2056	28	0
2	B	837	807	803	8	0
2	G	837	807	803	6	0
3	C	72	85	85	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	72	85	85	1	0
4	D	1421	1357	1352	18	0
4	I	1421	1360	1355	18	0
5	E	1910	1818	1811	37	0
5	J	1885	1796	1789	35	0
6	A	37	0	0	1	0
6	B	17	0	0	0	0
6	D	11	0	0	0	0
6	E	5	0	0	1	0
6	F	35	0	0	1	0
6	G	12	0	0	0	0
6	H	1	0	0	1	0
6	I	8	0	0	0	0
6	J	4	0	0	0	0
All	All	13046	12292	12231	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (169) 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)
1:A:176:LYS:HG2	1:A:180:LEU:HD12	1.60	0.82
4:I:134:VAL:HG23	4:I:177:TRP:HB3	1.66	0.77
1:F:40:ALA:HB2	6:F:327:HOH:O	1.91	0.70
5:J:128:PRO:HD2	5:J:199:TRP:CZ2	2.27	0.69
5:E:108:ARG:HG3	5:E:108:ARG:HH11	1.59	0.67
1:A:224:HIS:ND1	1:A:226:GLN:HB2	2.13	0.63
5:E:128:PRO:HD2	5:E:199:TRP:CZ2	2.35	0.62
1:A:73:ILE:HG23	3:C:8:LEU:CD2	2.29	0.62
2:G:23:LEU:O	2:G:67:TYR:HA	2.00	0.61
5:J:201:ASP:OD2	5:J:203:ARG:HB3	2.00	0.61
2:B:23:LEU:O	2:B:67:TYR:HA	1.99	0.61
1:F:2:SER:HA	1:F:103:LEU:O	2.01	0.61
1:A:73:ILE:HG23	3:C:8:LEU:HD23	1.84	0.59
4:D:165:ARG:HH11	4:D:165:ARG:HG3	1.68	0.59
5:J:118:VAL:O	5:J:225:ARG:NH2	2.36	0.58
1:A:143:SER:OG	3:C:9:LEU:O	2.15	0.58
5:J:221:TRP:CZ3	5:J:227:LYS:HA	2.38	0.58
4:D:157:THR:HG21	5:E:189:SER:OG	2.04	0.57
5:J:82:ALA:C	5:J:111:VAL:HG21	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HB	1:A:270:VAL:HG22	1.87	0.57
5:J:221:TRP:CE3	5:J:227:LYS:HA	2.39	0.57
1:A:103:LEU:HD21	1:A:165:VAL:HG13	1.87	0.56
1:F:261:VAL:HB	1:F:270:VAL:HG22	1.87	0.56
1:F:220:ASP:OD2	1:F:256:ARG:NH2	2.39	0.56
5:E:118:VAL:HG23	5:E:228:PRO:HB2	1.87	0.55
1:F:103:LEU:HD21	1:F:165:VAL:HG13	1.88	0.55
5:J:82:ALA:O	5:J:111:VAL:HG21	2.07	0.55
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.42	0.54
1:F:21:ARG:HG2	1:F:21:ARG:HH11	1.72	0.54
4:D:155:TYR:O	4:D:176:ALA:HA	2.07	0.54
5:E:209:GLN:HG3	5:E:232:ILE:HG21	1.91	0.53
2:B:79:ALA:HB1	2:B:93:VAL:O	2.08	0.53
5:E:159:VAL:O	5:E:159:VAL:HG13	2.09	0.53
4:D:164:MET:CE	5:E:193:ARG:HD3	2.39	0.53
5:E:13:LEU:HB2	5:E:111:VAL:HG22	1.91	0.53
5:J:205:HIS:NE2	5:J:236:GLU:OE2	2.41	0.52
6:H:101:HOH:O	4:I:94:HIS:HE1	1.91	0.52
1:A:109:PHE:CD2	1:A:161:GLU:HA	2.45	0.52
4:I:155:TYR:O	4:I:176:ALA:HA	2.10	0.52
4:I:126:ASP:HB2	4:I:132:LYS:HB2	1.92	0.51
1:A:72:GLN:NE2	5:E:51:SER:HB3	2.25	0.51
1:F:255:GLN:OE1	1:F:273:ARG:HD3	2.11	0.51
1:A:11:SER:HA	1:A:21:ARG:O	2.12	0.50
5:J:25:GLN:HB2	5:J:27:MET:CE	2.42	0.50
1:F:35:ARG:HG2	1:F:36:PHE:N	2.27	0.50
1:A:21:ARG:HG2	1:A:21:ARG:NH1	2.27	0.49
4:D:187:ASN:HB2	4:D:190:ASN:HD21	1.78	0.49
1:A:2:SER:HA	1:A:103:LEU:O	2.13	0.49
1:A:72:GLN:HG3	1:A:75:ARG:NH2	2.28	0.49
5:E:29:TYR:CE1	5:E:95:ARG:HG2	2.48	0.49
1:F:11:SER:HA	1:F:21:ARG:O	2.13	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
1:A:35:ARG:HG2	1:A:36:PHE:N	2.26	0.48
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.77	0.48
1:F:21:ARG:HG2	1:F:21:ARG:NH1	2.26	0.48
4:D:157:THR:HG21	5:E:189:SER:HG	1.79	0.48
4:D:185:CYS:HA	4:D:188:ALA:HB2	1.96	0.48
5:E:205:HIS:NE2	5:E:236:GLU:OE1	2.47	0.48
4:I:51:TYR:OH	5:J:100:GLU:OE2	2.28	0.47
5:J:29:TYR:CZ	5:J:95:ARG:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:VAL:HG13	5:E:126:PHE:CE2	2.49	0.47
5:J:130:GLU:HA	5:J:133:ILE:HD12	1.96	0.47
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.95	0.47
4:D:164:MET:HE2	5:E:193:ARG:HD3	1.96	0.47
5:E:209:GLN:HG3	5:E:232:ILE:CG2	2.44	0.47
4:D:122:TYR:CD2	5:E:132:GLU:HB2	2.49	0.47
1:F:261:VAL:HB	1:F:270:VAL:CG2	2.44	0.47
4:I:122:TYR:CD2	5:J:132:GLU:HB2	2.49	0.47
5:J:77:ARG:NH2	5:J:79:LEU:HA	2.30	0.47
5:E:118:VAL:CG2	5:E:228:PRO:HB2	2.45	0.47
5:E:178:GLN:OE1	5:E:180:ALA:HB3	2.15	0.47
5:J:205:HIS:HB2	5:J:238:TRP:CE3	2.51	0.46
1:F:7:TYR:HB2	1:F:99:HIS:CE1	2.50	0.46
5:E:128:PRO:HD2	5:E:199:TRP:CH2	2.50	0.46
5:E:205:HIS:HB2	5:E:238:TRP:CZ3	2.51	0.46
5:J:205:HIS:HB2	5:J:238:TRP:CZ3	2.50	0.46
1:F:115:GLN:HG2	1:F:125:THR:HG23	1.97	0.46
1:A:189:VAL:HG23	1:A:272:LEU:HD23	1.98	0.46
1:F:108:ARG:O	1:F:109:PHE:C	2.54	0.46
4:I:34:PHE:HB2	4:I:90:ALA:HB3	1.97	0.46
5:J:14:LYS:HB2	5:J:115:LEU:HD11	1.97	0.46
5:E:202:PRO:HA	5:E:239:GLY:O	2.16	0.46
4:D:94:HIS:HA	5:E:98:LEU:HD11	1.98	0.46
1:A:227:ASP:OD1	1:A:227:ASP:N	2.48	0.46
4:I:187:ASN:HB2	4:I:190:ASN:HD21	1.80	0.46
2:B:51:HIS:HA	2:B:65:LEU:O	2.16	0.45
2:G:79:ALA:HB1	2:G:93:VAL:O	2.16	0.45
5:E:127:GLU:OE1	5:E:240:ARG:NH1	2.49	0.45
4:I:122:TYR:HB3	5:J:129:SER:HB2	1.99	0.45
5:J:83:PRO:HA	5:J:111:VAL:CG2	2.46	0.45
5:E:203:ARG:NH1	6:E:301:HOH:O	2.49	0.45
1:F:117:ALA:HB2	2:G:60:TRP:CZ2	2.51	0.45
5:E:151:ASP:HB2	5:E:186:TYR:CE2	2.52	0.45
4:D:167:MET:CE	5:E:138:LYS:HE3	2.47	0.45
1:F:35:ARG:HD3	2:G:53:ASP:CG	2.37	0.45
5:J:135:HIS:O	5:J:135:HIS:ND1	2.47	0.45
1:A:209:TYR:CD1	1:A:209:TYR:C	2.90	0.45
5:E:7:THR:OG1	5:E:22:GLN:HB2	2.16	0.45
4:D:156:ILE:HD13	4:D:176:ALA:HB1	1.99	0.44
5:J:7:THR:OG1	5:J:22:GLN:HB2	2.17	0.44
5:J:27:MET:H	5:J:27:MET:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HB	1:A:270:VAL:CG2	2.46	0.44
1:F:200:THR:OG1	1:F:248:VAL:HG12	2.17	0.44
5:J:227:LYS:O	5:J:229:VAL:N	2.50	0.44
2:G:51:HIS:HA	2:G:65:LEU:O	2.17	0.44
1:F:73:ILE:HG23	3:H:8:LEU:CD2	2.48	0.44
1:F:55:GLU:OE2	1:F:174:LYS:NZ	2.47	0.44
1:F:69:ASP:O	1:F:73:ILE:HG12	2.18	0.44
5:E:151:ASP:OD1	5:E:174:PRO:HG3	2.18	0.44
1:A:108:ARG:O	1:A:109:PHE:C	2.54	0.43
1:A:208:PHE:CE2	1:A:213:ILE:HD13	2.53	0.43
5:E:227:LYS:O	5:E:229:VAL:N	2.50	0.43
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.99	0.43
4:I:151:ASP:HB3	4:I:154:VAL:HB	1.99	0.43
5:E:118:VAL:HG23	5:E:228:PRO:CB	2.48	0.43
4:D:25:TYR:CZ	4:D:70:GLN:HA	2.53	0.43
1:A:55:GLU:OE2	1:A:174:LYS:NZ	2.43	0.43
2:B:45:ARG:HH12	2:B:47:GLU:HG2	1.83	0.43
1:F:9:HIS:ND1	1:F:24:SER:OG	2.51	0.43
1:F:230:LEU:HD12	1:F:245:ALA:HB2	2.01	0.43
5:J:149:TYR:C	5:J:149:TYR:CD1	2.92	0.43
1:A:207:GLY:HA2	1:A:240:THR:OG1	2.19	0.43
4:I:25:TYR:CZ	4:I:70:GLN:HA	2.53	0.42
4:I:94:HIS:HA	5:J:98:LEU:HD11	2.01	0.42
1:A:115:GLN:HG2	1:A:125:THR:HG23	2.01	0.42
4:I:122:TYR:HB3	5:J:129:SER:CB	2.49	0.42
1:F:135:ALA:HB1	1:F:140:ALA:HB3	2.00	0.42
5:J:112:VAL:HG11	5:J:149:TYR:HE1	1.84	0.42
2:B:91:LYS:HE3	2:B:91:LYS:HB2	1.82	0.42
5:E:108:ARG:HG3	5:E:108:ARG:NH1	2.30	0.42
5:E:114:ASP:OD2	5:E:116:LYS:HE3	2.19	0.42
1:A:135:ALA:HB1	1:A:140:ALA:CB	2.50	0.42
5:E:143:CYS:HB2	5:E:157:TRP:CZ2	2.55	0.42
1:F:259:CYS:O	1:F:271:THR:HA	2.19	0.42
5:J:83:PRO:HA	5:J:111:VAL:HG22	2.02	0.42
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.00	0.42
1:A:38:ASN:HA	1:A:43:PRO:HB3	2.02	0.42
1:A:259:CYS:O	1:A:271:THR:HA	2.19	0.42
4:D:60:ARG:HH22	4:D:83:ASP:CG	2.23	0.42
5:E:168:VAL:HG22	5:E:192:LEU:HD13	2.02	0.42
1:A:69:ASP:O	1:A:73:ILE:HG12	2.19	0.41
1:F:209:TYR:CD1	1:F:209:TYR:C	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:60:ARG:HH22	4:I:83:ASP:CG	2.23	0.41
1:A:157:ARG:NH2	6:A:302:HOH:O	2.54	0.41
5:E:149:TYR:C	5:E:149:TYR:CD1	2.94	0.41
1:F:38:ASN:HA	1:F:43:PRO:HB3	2.03	0.41
4:I:54:GLY:O	4:I:64:GLN:HA	2.20	0.41
5:J:198:PHE:O	5:J:199:TRP:HB3	2.20	0.41
4:D:48:MET:HE3	4:D:56:LYS:HD3	2.02	0.41
1:A:7:TYR:HB2	1:A:99:HIS:CE1	2.56	0.41
1:F:207:GLY:HA2	1:F:240:THR:OG1	2.21	0.41
4:D:37:ARG:HB2	4:D:47:ILE:HD11	2.02	0.41
4:I:164:MET:HE2	5:J:193:ARG:HB3	2.03	0.41
5:J:77:ARG:HH21	5:J:79:LEU:HA	1.85	0.41
4:I:126:ASP:OD2	4:I:132:LYS:HD2	2.20	0.41
1:A:232:GLU:HA	1:A:232:GLU:OE1	2.21	0.41
5:J:77:ARG:CZ	5:J:79:LEU:HD23	2.51	0.41
1:A:127:ASN:ND2	1:A:134:THR:OG1	2.42	0.40
5:J:112:VAL:CG1	5:J:149:TYR:HE1	2.34	0.40
1:A:65:ARG:HD2	5:E:97:ARG:CZ	2.52	0.40
5:J:36:ARG:HB3	5:J:46:ILE:HD11	2.02	0.40
1:A:73:ILE:CG2	3:C:8:LEU:HD23	2.52	0.40
1:A:129:ASP:OD1	1:A:131:ARG:N	2.48	0.40
5:J:143:CYS:HB2	5:J:157:TRP:CH2	2.56	0.40
1:A:9:HIS:ND1	1:A:24:SER:OG	2.53	0.40
1:A:121:LYS:HG2	2:B:1:ILE:HD11	2.02	0.40
4:D:37:ARG:HB2	4:D:47:ILE:CD1	2.52	0.40
5:E:229:VAL:HG12	5:E:230:THR:N	2.36	0.40
4:I:125:ARG:NH2	4:I:130:SER:O	2.38	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%)	260 (94%)	15 (6%)	0	100	100
1	F	267/276 (97%)	253 (95%)	14 (5%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	G	98/100 (98%)	93 (95%)	5 (5%)	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	178/199 (89%)	159 (89%)	18 (10%)	1 (1%)	22	43
4	I	178/199 (89%)	163 (92%)	15 (8%)	0	100	100
5	E	238/243 (98%)	216 (91%)	21 (9%)	1 (0%)	30	52
5	J	235/243 (97%)	216 (92%)	17 (7%)	2 (1%)	14	31
All	All	1581/1654 (96%)	1469 (93%)	108 (7%)	4 (0%)	37	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	184	ALA
5	J	231	GLN
5	E	172	PRO
5	J	172	PRO

5.3.2 Protein sidechains (i)

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%)	234 (98%)	4 (2%)	56	78
1	F	233/237 (98%)	226 (97%)	7 (3%)	36	63
2	B	95/95 (100%)	92 (97%)	3 (3%)	34	60
2	G	95/95 (100%)	90 (95%)	5 (5%)	19	40
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	161/175 (92%)	156 (97%)	5 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	161/175 (92%)	157 (98%)	4 (2%)	42	68
5	E	209/211 (99%)	203 (97%)	6 (3%)	37	64
5	J	207/211 (98%)	201 (97%)	6 (3%)	37	64
All	All	1417/1454 (98%)	1377 (97%)	40 (3%)	38	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	174	LYS
1	A	227	ASP
1	A	248	VAL
2	B	0	MET
2	B	70	PHE
2	B	88	SER
4	D	82	SER
4	D	137	PHE
4	D	144	THR
4	D	160	CYS
4	D	173	SER
5	E	94	HIS
5	E	108	ARG
5	E	118	VAL
5	E	133	ILE
5	E	166	SER
5	E	222	THR
1	F	2	SER
1	F	24	SER
1	F	79	ARG
1	F	86	ASN
1	F	151	SER
1	F	162	ASP
1	F	232	GLU
2	G	4	THR
2	G	34	ASP
2	G	47	GLU
2	G	69	GLU
2	G	70	PHE
4	I	82	SER
4	I	137	PHE
4	I	160	CYS

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Mol	Chain	Res	Type
4	I	173	SER
5	J	94	HIS
5	J	130	GLU
5	J	135	HIS
5	J	153	VAL
5	J	191	ARG
5	J	201	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	65	ASN
1	F	156	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.49	2 (0%) 84 81	40, 79, 125, 159	1 (0%)
1	F	271/276 (98%)	-0.41	6 (2%) 62 57	57, 78, 128, 149	0
2	B	100/100 (100%)	-0.44	0 100 100	62, 79, 110, 125	0
2	G	100/100 (100%)	-0.19	1 (1%) 79 75	59, 91, 125, 138	0
3	C	9/9 (100%)	-0.38	0 100 100	56, 64, 75, 78	0
3	H	9/9 (100%)	-0.63	0 100 100	52, 60, 67, 70	0
4	D	184/199 (92%)	-0.02	6 (3%) 49 43	57, 88, 163, 187	0
4	I	184/199 (92%)	-0.10	3 (1%) 70 65	53, 84, 144, 165	0
5	E	240/243 (98%)	-0.11	2 (0%) 82 79	61, 109, 160, 197	0
5	J	237/243 (97%)	-0.06	4 (1%) 69 64	59, 106, 154, 166	0
All	All	1610/1654 (97%)	-0.24	24 (1%) 71 67	40, 88, 146, 197	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	100	LEU	4.4
1	F	221	GLY	4.3
2	G	54	LEU	3.4
5	J	181	LEU	3.3
1	F	227	ASP	3.0
5	J	183	ASP	2.9
5	J	202	PRO	2.8
4	D	52	LEU	2.8
1	A	179	LEU	2.7
4	I	51	TYR	2.6
4	D	130	SER	2.6
4	D	152	SER	2.6
1	F	197	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
4	I	92	GLY	2.5
4	I	174	ALA	2.5
1	A	176	LYS	2.4
5	E	98	LEU	2.4
5	E	66	VAL	2.3
5	J	76	LEU	2.3
1	F	209	TYR	2.2
1	F	228	THR	2.2
4	D	31	VAL	2.1
4	D	154	VAL	2.0
1	F	51	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.