Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 11:17 PM EDT

PDB ID	:	3WUV
Title	:	Structure basis of inactivating cell abscission with chimera peptide 2
Authors	:	Kim, H.J.; Matsuura, A.; Lee, H.H.
Deposited on	:	2014-05-05
Resolution	:	2.79 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:

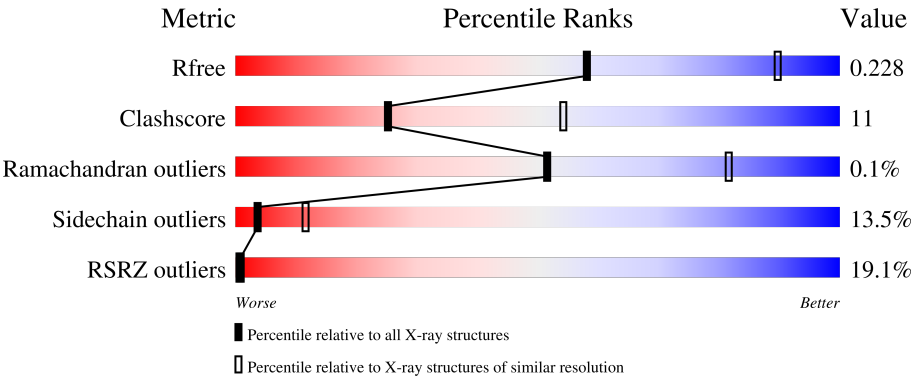
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	63	14% 65% 19% 5% 11%
1	B	63	21% 65% 24% 6% 5%
1	D	63	21% 49% 25% 5% 21%
1	E	63	25% 71% 13% • 13%
1	G	63	14% 57% 16% 6% 21%

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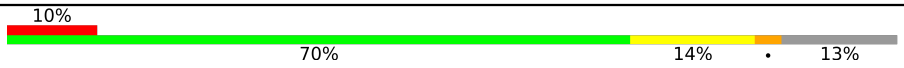
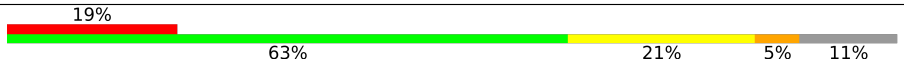
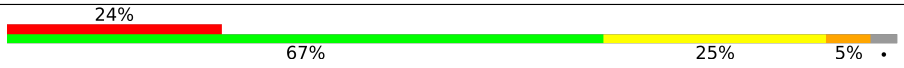
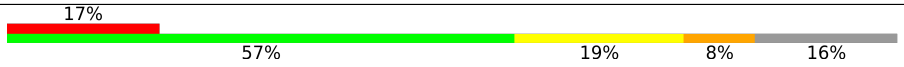
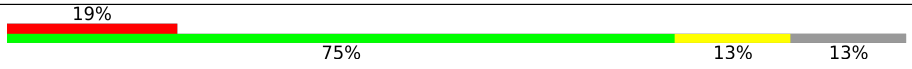
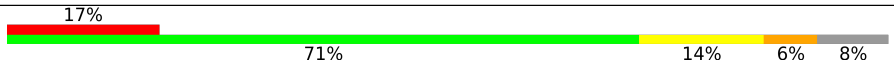
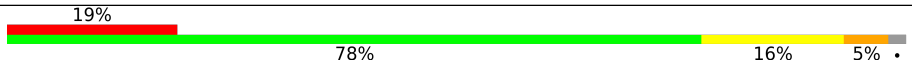
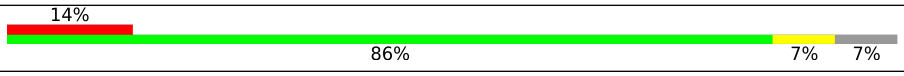
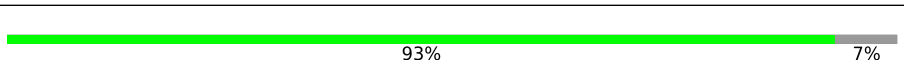
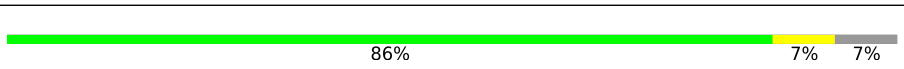
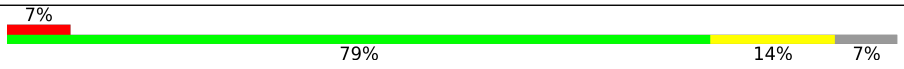
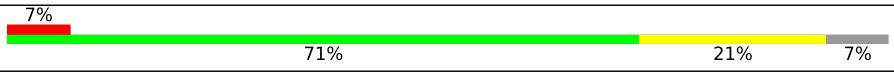
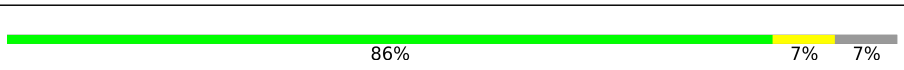
Mol	Chain	Length	Quality of chain
1	H	63	
1	J	63	
1	K	63	
1	M	63	
1	N	63	
1	P	63	
1	Q	63	
2	C	14	
2	F	14	
2	I	14	
2	L	14	
2	O	14	
2	R	14	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6299 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 Centrosomal protein of 55 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	0	0
			460	292	77	89	2			
1	B	60	Total	C	N	O	S	0	0	0
			489	309	83	95	2			
1	D	50	Total	C	N	O	S	0	0	0
			424	272	71	80	1			
1	E	55	Total	C	N	O	S	0	0	0
			451	287	76	86	2			
1	G	50	Total	C	N	O	S	0	0	0
			424	272	71	80	1			
1	H	55	Total	C	N	O	S	0	0	0
			451	287	76	86	2			
1	J	56	Total	C	N	O	S	0	0	0
			460	292	77	89	2			
1	K	61	Total	C	N	O	S	0	0	0
			497	315	84	96	2			
1	M	53	Total	C	N	O	S	0	0	0
			443	282	74	86	1			
1	N	55	Total	C	N	O	S	0	0	0
			451	287	76	86	2			
1	P	58	Total	C	N	O	S	0	0	0
			472	299	79	92	2			
1	Q	62	Total	C	N	O	S	0	0	0
			501	317	85	97	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	-	expression tag	UNP Q53EZ4
A	156	ALA	-	expression tag	UNP Q53EZ4
A	157	MET	-	expression tag	UNP Q53EZ4
A	158	GLY	-	expression tag	UNP Q53EZ4
A	159	SER	-	expression tag	UNP Q53EZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	155	GLY	-	expression tag	UNP Q53EZ4
B	156	ALA	-	expression tag	UNP Q53EZ4
B	157	MET	-	expression tag	UNP Q53EZ4
B	158	GLY	-	expression tag	UNP Q53EZ4
B	159	SER	-	expression tag	UNP Q53EZ4
D	155	GLY	-	expression tag	UNP Q53EZ4
D	156	ALA	-	expression tag	UNP Q53EZ4
D	157	MET	-	expression tag	UNP Q53EZ4
D	158	GLY	-	expression tag	UNP Q53EZ4
D	159	SER	-	expression tag	UNP Q53EZ4
E	155	GLY	-	expression tag	UNP Q53EZ4
E	156	ALA	-	expression tag	UNP Q53EZ4
E	157	MET	-	expression tag	UNP Q53EZ4
E	158	GLY	-	expression tag	UNP Q53EZ4
E	159	SER	-	expression tag	UNP Q53EZ4
G	155	GLY	-	expression tag	UNP Q53EZ4
G	156	ALA	-	expression tag	UNP Q53EZ4
G	157	MET	-	expression tag	UNP Q53EZ4
G	158	GLY	-	expression tag	UNP Q53EZ4
G	159	SER	-	expression tag	UNP Q53EZ4
H	155	GLY	-	expression tag	UNP Q53EZ4
H	156	ALA	-	expression tag	UNP Q53EZ4
H	157	MET	-	expression tag	UNP Q53EZ4
H	158	GLY	-	expression tag	UNP Q53EZ4
H	159	SER	-	expression tag	UNP Q53EZ4
J	155	GLY	-	expression tag	UNP Q53EZ4
J	156	ALA	-	expression tag	UNP Q53EZ4
J	157	MET	-	expression tag	UNP Q53EZ4
J	158	GLY	-	expression tag	UNP Q53EZ4
J	159	SER	-	expression tag	UNP Q53EZ4
K	155	GLY	-	expression tag	UNP Q53EZ4
K	156	ALA	-	expression tag	UNP Q53EZ4
K	157	MET	-	expression tag	UNP Q53EZ4
K	158	GLY	-	expression tag	UNP Q53EZ4
K	159	SER	-	expression tag	UNP Q53EZ4
M	155	GLY	-	expression tag	UNP Q53EZ4
M	156	ALA	-	expression tag	UNP Q53EZ4
M	157	MET	-	expression tag	UNP Q53EZ4
M	158	GLY	-	expression tag	UNP Q53EZ4
M	159	SER	-	expression tag	UNP Q53EZ4
N	155	GLY	-	expression tag	UNP Q53EZ4
N	156	ALA	-	expression tag	UNP Q53EZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
N	157	MET	-	expression tag	UNP Q53EZ4
N	158	GLY	-	expression tag	UNP Q53EZ4
N	159	SER	-	expression tag	UNP Q53EZ4
P	155	GLY	-	expression tag	UNP Q53EZ4
P	156	ALA	-	expression tag	UNP Q53EZ4
P	157	MET	-	expression tag	UNP Q53EZ4
P	158	GLY	-	expression tag	UNP Q53EZ4
P	159	SER	-	expression tag	UNP Q53EZ4
Q	155	GLY	-	expression tag	UNP Q53EZ4
Q	156	ALA	-	expression tag	UNP Q53EZ4
Q	157	MET	-	expression tag	UNP Q53EZ4
Q	158	GLY	-	expression tag	UNP Q53EZ4
Q	159	SER	-	expression tag	UNP Q53EZ4

- Molecule 2 is a protein called peptide from Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			101	68	15	18			
2	F	13	Total	C	N	O	0	0	0
			101	68	15	18			
2	I	13	Total	C	N	O	0	0	0
			101	68	15	18			
2	L	13	Total	C	N	O	0	0	0
			101	68	15	18			
2	O	13	Total	C	N	O	0	0	0
			101	68	15	18			
2	R	13	Total	C	N	O	0	0	0
			101	68	15	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	796	ASP	PRO	engineered mutation	UNP Q8WUM4
C	807	ILE	PRO	engineered mutation	UNP Q8WUM4
C	808	PRO	GLY	engineered mutation	UNP Q8WUM4
C	809	PRO	TYR	engineered mutation	UNP Q8WUM4
F	796	ASP	PRO	engineered mutation	UNP Q8WUM4
F	807	ILE	PRO	engineered mutation	UNP Q8WUM4
F	808	PRO	GLY	engineered mutation	UNP Q8WUM4
F	809	PRO	TYR	engineered mutation	UNP Q8WUM4
I	796	ASP	PRO	engineered mutation	UNP Q8WUM4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	807	ILE	PRO	engineered mutation	UNP Q8WUM4
I	808	PRO	GLY	engineered mutation	UNP Q8WUM4
I	809	PRO	TYR	engineered mutation	UNP Q8WUM4
L	796	ASP	PRO	engineered mutation	UNP Q8WUM4
L	807	ILE	PRO	engineered mutation	UNP Q8WUM4
L	808	PRO	GLY	engineered mutation	UNP Q8WUM4
L	809	PRO	TYR	engineered mutation	UNP Q8WUM4
O	796	ASP	PRO	engineered mutation	UNP Q8WUM4
O	807	ILE	PRO	engineered mutation	UNP Q8WUM4
O	808	PRO	GLY	engineered mutation	UNP Q8WUM4
O	809	PRO	TYR	engineered mutation	UNP Q8WUM4
R	796	ASP	PRO	engineered mutation	UNP Q8WUM4
R	807	ILE	PRO	engineered mutation	UNP Q8WUM4
R	808	PRO	GLY	engineered mutation	UNP Q8WUM4
R	809	PRO	TYR	engineered mutation	UNP Q8WUM4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	12	Total O 12 12	0	0
3	C	4	Total O 4 4	0	0
3	D	8	Total O 8 8	0	0
3	E	12	Total O 12 12	0	0
3	F	7	Total O 7 7	0	0
3	G	12	Total O 12 12	0	0
3	H	15	Total O 15 15	0	0
3	I	5	Total O 5 5	0	0
3	J	7	Total O 7 7	0	0
3	K	13	Total O 13 13	0	0
3	L	3	Total O 3 3	0	0

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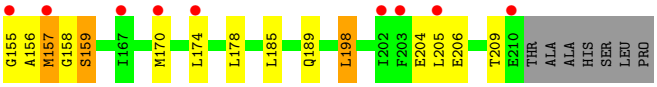
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	14	Total O 14 14	0	0
3	N	7	Total O 7 7	0	0
3	O	4	Total O 4 4	0	0
3	P	13	Total O 13 13	0	0
3	Q	12	Total O 12 12	0	0
3	R	6	Total O 6 6	0	0

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.

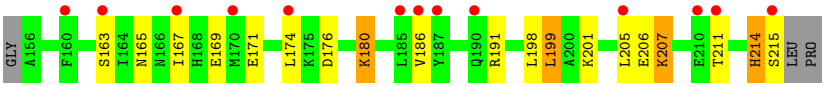
• Molecule 1: Centrosomal protein of 55 kDa

Chain A:



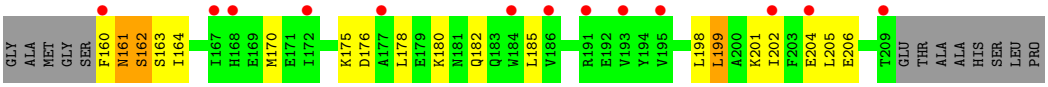
• Molecule 1: Centrosomal protein of 55 kDa

Chain B:



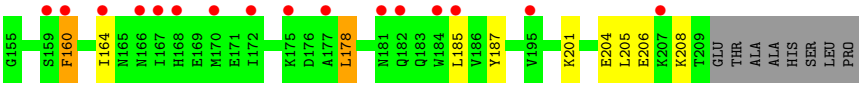
• Molecule 1: Centrosomal protein of 55 kDa

Chain D:



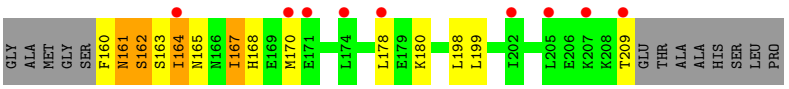
• Molecule 1: Centrosomal protein of 55 kDa

Chain E:



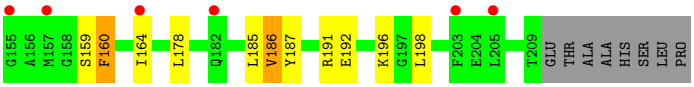
• Molecule 1: Centrosomal protein of 55 kDa

Chain G:



• Molecule 1: Centrosomal protein of 55 kDa

Chain H:

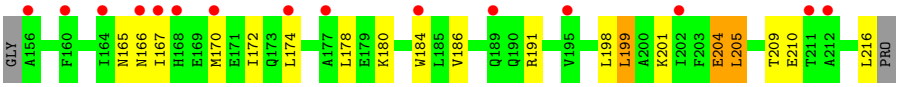


• Molecule 1: Centrosomal protein of 55 kDa

Chain J:

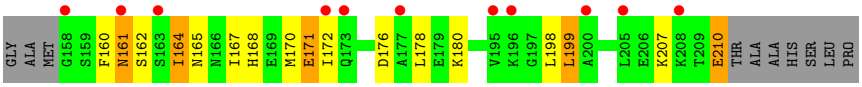
• Molecule 1: Centrosomal protein of 55 kDa

Chain K:



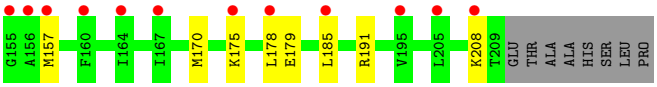
• Molecule 1: Centrosomal protein of 55 kDa

Chain M:



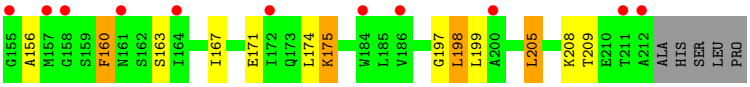
• Molecule 1: Centrosomal protein of 55 kDa

Chain N:



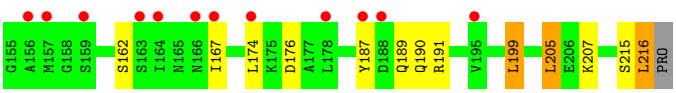
• Molecule 1: Centrosomal protein of 55 kDa

Chain P:



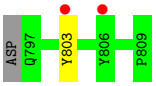
• Molecule 1: Centrosomal protein of 55 kDa

Chain Q:



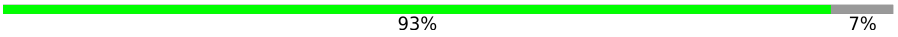
• Molecule 2: peptide from Programmed cell death 6-interacting protein

Chain C:



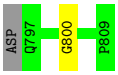
• Molecule 2: peptide from Programmed cell death 6-interacting protein

Chain F:



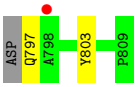
• Molecule 2: peptide from Programmed cell death 6-interacting protein

Chain I:



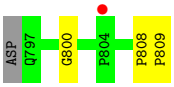
• Molecule 2: peptide from Programmed cell death 6-interacting protein

Chain L:



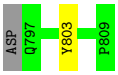
• Molecule 2: peptide from Programmed cell death 6-interacting protein

Chain O:



• Molecule 2: peptide from Programmed cell death 6-interacting protein

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.07Å 134.67Å 88.33Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	48.64 – 2.79 48.66 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.64-2.79) 99.3 (48.66-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.201 , 0.227 0.208 , 0.228	Depositor DCC
R_{free} test set	2011 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.020 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.460 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.467 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6299	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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	0.39	0/466	0.43	0/623
1	B	0.26	0/496	0.46	0/665
1	D	0.27	0/430	0.50	0/576
1	E	0.26	0/457	0.45	0/611
1	G	0.49	0/430	0.57	1/576 (0.2%)
1	H	0.34	0/457	0.44	0/611
1	J	0.40	0/466	0.49	0/623
1	K	0.61	0/504	0.53	0/676
1	M	0.29	0/449	0.42	0/601
1	N	0.27	0/457	0.44	0/611
1	P	0.31	0/478	0.44	0/640
1	Q	0.24	0/508	0.43	0/681
2	C	0.23	0/107	0.48	0/150
2	F	0.23	0/107	0.53	0/150
2	I	0.24	0/107	0.53	0/150
2	L	0.21	0/107	0.51	0/150
2	O	0.26	0/107	0.58	0/150
2	R	0.22	0/107	0.49	0/150
All	All	0.35	0/6240	0.48	1/8394 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	162	SER	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	460	0	458	22	0
1	B	489	0	484	13	1
1	D	424	0	427	18	0
1	E	451	0	452	9	0
1	G	424	0	427	24	0
1	H	451	0	452	7	0
1	J	460	0	458	16	0
1	K	497	0	495	14	0
1	M	443	0	441	9	0
1	N	451	0	452	3	0
1	P	472	0	470	10	0
1	Q	501	0	498	9	0
2	C	101	0	94	0	0
2	F	101	0	94	0	0
2	I	101	0	94	1	0
2	L	101	0	94	0	0
2	O	101	0	94	2	0
2	R	101	0	94	0	0
3	A	16	0	0	0	0
3	B	12	0	0	0	0
3	C	4	0	0	0	0
3	D	8	0	0	0	0
3	E	12	0	0	0	0
3	F	7	0	0	0	0
3	G	12	0	0	0	0
3	H	15	0	0	0	0
3	I	5	0	0	0	0
3	J	7	0	0	0	0
3	K	13	0	0	1	0
3	L	3	0	0	0	0
3	M	14	0	0	0	1
3	N	7	0	0	0	0
3	O	4	0	0	0	0
3	P	13	0	0	0	0
3	Q	12	0	0	0	0
3	R	6	0	0	0	0
All	All	6299	0	6078	130	1

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 11.

All (130) 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:157:MET:H	1:A:157:MET:CE	1.44	1.28
1:G:167:ILE:HG22	1:G:168:HIS:N	1.62	1.11
1:A:157:MET:H	1:A:157:MET:HE3	0.99	1.09
1:A:157:MET:HE3	1:A:157:MET:N	1.75	1.01
1:A:157:MET:HG2	1:A:158:GLY:HA2	1.41	0.97
1:A:157:MET:CE	1:A:157:MET:N	2.30	0.92
1:J:207:LYS:O	1:J:210:GLU:CB	2.20	0.89
1:G:162:SER:O	1:G:165:ASN:HB2	1.71	0.89
1:G:161:ASN:O	1:G:164:ILE:HG22	1.74	0.88
1:J:210:GLU:H	1:J:210:GLU:CD	1.79	0.86
1:A:157:MET:H	1:A:157:MET:HE2	1.40	0.85
1:J:210:GLU:CD	1:J:210:GLU:N	2.30	0.85
1:G:167:ILE:CG2	1:G:168:HIS:N	2.39	0.84
1:G:160:PHE:CD1	1:G:160:PHE:O	2.31	0.83
1:G:161:ASN:ND2	1:G:161:ASN:C	2.30	0.82
1:D:205:LEU:HD23	1:E:205:LEU:HB3	1.61	0.80
1:J:209:THR:N	1:J:210:GLU:HA	2.00	0.76
1:A:157:MET:HG2	1:A:158:GLY:CA	2.16	0.76
1:A:157:MET:N	1:A:158:GLY:HA3	2.03	0.73
1:A:157:MET:CG	1:A:158:GLY:HA2	2.17	0.73
1:J:207:LYS:O	1:J:210:GLU:HB3	1.88	0.72
1:D:160:PHE:HB3	1:D:163:SER:H	1.55	0.71
1:A:206:GLU:HG3	1:B:205:LEU:HD21	1.72	0.69
1:J:207:LYS:O	1:J:210:GLU:HB2	1.93	0.69
1:G:160:PHE:O	1:G:160:PHE:HD1	1.75	0.69
1:A:157:MET:N	1:A:158:GLY:CA	2.57	0.67
1:G:164:ILE:O	1:G:167:ILE:HB	1.94	0.67
1:G:160:PHE:O	1:G:161:ASN:ND2	2.30	0.64
1:M:176:ASP:OD2	1:M:180:LYS:NZ	2.28	0.63
1:M:161:ASN:O	1:M:164:ILE:HG22	1.99	0.63
1:G:167:ILE:HG22	1:G:168:HIS:CA	2.29	0.63
1:G:162:SER:O	1:G:165:ASN:N	2.33	0.62
1:D:206:GLU:HG3	1:E:205:LEU:HD21	1.81	0.62
1:G:164:ILE:HG23	1:G:165:ASN:N	2.15	0.61
1:A:155:GLY:O	1:A:159:SER:N	2.35	0.60
1:J:162:SER:O	1:J:166:ASN:ND2	2.35	0.60
1:G:167:ILE:O	1:G:170:MET:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:ILE:CG2	1:G:165:ASN:N	2.65	0.59
1:G:161:ASN:O	1:G:161:ASN:CG	2.41	0.59
1:D:160:PHE:HB3	1:D:162:SER:N	2.17	0.59
1:A:156:ALA:C	1:A:158:GLY:HA3	2.23	0.58
1:M:161:ASN:O	1:M:165:ASN:ND2	2.37	0.57
1:K:209:THR:O	1:K:210:GLU:HB2	2.03	0.57
1:K:165:ASN:OD1	1:K:166:ASN:N	2.40	0.55
1:A:156:ALA:N	1:A:157:MET:HE3	2.20	0.55
1:J:181:ASN:HB3	1:K:180:LYS:HE3	1.90	0.54
1:K:180:LYS:HE3	1:K:184:TRP:HE1	1.71	0.54
1:A:198:LEU:HD21	1:B:199:LEU:HD13	1.89	0.54
1:D:160:PHE:CB	1:D:163:SER:H	2.21	0.53
1:E:160:PHE:O	1:E:164:ILE:HG12	2.09	0.53
1:G:161:ASN:C	1:G:161:ASN:HD22	2.12	0.53
1:A:156:ALA:N	1:A:157:MET:CE	2.73	0.52
1:G:160:PHE:O	1:G:161:ASN:CB	2.57	0.52
1:J:210:GLU:N	1:J:210:GLU:OE1	2.30	0.52
1:M:207:LYS:O	1:M:210:GLU:N	2.43	0.52
1:A:174:LEU:HD13	1:B:174:LEU:HA	1.92	0.52
1:J:173:GLN:HG2	1:K:174:LEU:HD21	1.92	0.52
1:D:185:LEU:HD21	1:P:205:LEU:HD13	1.93	0.51
1:A:157:MET:N	1:A:157:MET:HE2	2.11	0.51
1:J:198:LEU:HD21	1:K:199:LEU:HD13	1.93	0.50
1:P:198:LEU:HD21	1:Q:199:LEU:HD13	1.93	0.49
1:D:201:LYS:O	1:D:204:GLU:N	2.45	0.49
1:J:206:GLU:O	1:J:209:THR:OG1	2.30	0.49
1:P:163:SER:O	1:P:167:ILE:HG12	2.12	0.49
1:Q:187:TYR:CZ	1:Q:191:ARG:HD2	2.47	0.49
1:A:155:GLY:O	1:A:158:GLY:HA3	2.12	0.49
1:Q:207:LYS:N	1:Q:207:LYS:HD2	2.28	0.48
1:H:160:PHE:HD1	1:H:160:PHE:N	2.11	0.48
1:D:205:LEU:HD21	1:E:206:GLU:HG3	1.95	0.48
1:E:187:TYR:CD1	1:P:197:GLY:HA3	2.49	0.47
1:G:162:SER:O	1:G:165:ASN:CB	2.52	0.47
1:D:205:LEU:HB3	1:E:205:LEU:HD23	1.97	0.47
1:A:170:MET:HG3	1:B:174:LEU:HD22	1.96	0.47
1:H:186:VAL:HG23	1:J:193:VAL:HG13	1.96	0.47
1:H:160:PHE:N	1:H:160:PHE:CD1	2.82	0.47
1:D:202:ILE:HD13	1:E:201:LYS:HD3	1.97	0.47
1:K:167:ILE:O	1:K:170:MET:HB2	2.15	0.47
1:M:199:LEU:HD12	1:M:199:LEU:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:ARG:NH2	3:K:301:HOH:O	2.48	0.46
1:B:205:LEU:HD12	1:B:205:LEU:HA	1.80	0.46
1:B:191:ARG:HD2	1:B:191:ARG:HA	1.70	0.46
1:P:174:LEU:HD13	1:Q:174:LEU:HA	1.97	0.46
1:G:161:ASN:O	1:G:161:ASN:ND2	2.47	0.46
1:H:192:GLU:O	1:H:196:LYS:HG2	2.15	0.46
1:B:201:LYS:O	1:B:205:LEU:HB2	2.15	0.46
1:G:160:PHE:O	1:G:161:ASN:HB3	2.14	0.46
1:M:168:HIS:CE1	1:M:172:ILE:HD11	2.50	0.46
1:B:205:LEU:O	1:B:207:LYS:N	2.49	0.45
1:D:182:GLN:NE2	1:P:208:LYS:HE2	2.32	0.45
1:E:178:LEU:HD12	1:E:178:LEU:HA	1.83	0.45
1:G:162:SER:OG	1:G:163:SER:N	2.50	0.45
1:J:167:ILE:HG21	1:K:167:ILE:HD12	1.99	0.44
1:Q:205:LEU:HD12	1:Q:205:LEU:HA	1.79	0.44
1:K:205:LEU:HD12	1:K:205:LEU:HA	1.82	0.44
1:M:167:ILE:O	1:M:170:MET:HB3	2.18	0.44
1:M:171:GLU:HB2	1:N:170:MET:CE	2.48	0.44
1:K:180:LYS:CE	1:K:184:TRP:HE1	2.30	0.44
1:B:171:GLU:O	1:B:171:GLU:HG2	2.18	0.43
1:K:201:LYS:O	1:K:205:LEU:HB2	2.18	0.43
1:D:160:PHE:N	1:D:161:ASN:HA	2.32	0.43
1:D:176:ASP:OD2	1:D:180:LYS:HE2	2.19	0.43
1:B:180:LYS:HZ1	1:Q:216:LEU:HD11	1.84	0.43
1:H:187:TYR:CD1	1:J:197:GLY:HA3	2.53	0.43
1:H:191:ARG:HA	1:H:191:ARG:HD2	1.78	0.43
1:P:167:ILE:HG21	1:Q:167:ILE:HD13	2.00	0.43
1:B:180:LYS:NZ	1:Q:216:LEU:HD11	2.32	0.43
1:P:175:LYS:HD3	1:P:175:LYS:HA	1.27	0.43
1:D:161:ASN:H	1:D:161:ASN:HD22	1.66	0.43
1:N:191:ARG:HA	1:N:191:ARG:HD2	1.84	0.42
1:D:160:PHE:N	1:D:163:SER:HB2	2.33	0.42
1:P:156:ALA:O	1:P:160:PHE:CD1	2.73	0.42
1:P:160:PHE:CD1	1:P:160:PHE:N	2.88	0.42
1:B:163:SER:O	1:B:167:ILE:HG12	2.19	0.42
1:Q:187:TYR:OH	1:Q:191:ARG:HD2	2.20	0.42
1:K:199:LEU:HD12	1:K:199:LEU:HA	1.93	0.42
2:O:808:PRO:HA	2:O:809:PRO:HA	1.81	0.42
1:K:204:GLU:HG3	1:K:205:LEU:N	2.34	0.42
1:G:161:ASN:HD22	1:G:162:SER:N	2.17	0.42
1:N:208:LYS:HD2	1:N:208:LYS:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:180:LYS:HD3	2:O:800:GLY:N	2.35	0.41
1:G:180:LYS:HD3	2:I:800:GLY:N	2.35	0.41
1:A:170:MET:SD	1:B:171:GLU:HB2	2.60	0.41
1:E:204:GLU:O	1:E:208:LYS:HD3	2.21	0.41
1:J:209:THR:N	1:J:210:GLU:CA	2.80	0.41
1:D:160:PHE:HB3	1:D:162:SER:H	1.84	0.41
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.86	0.40
1:D:205:LEU:HD12	1:D:205:LEU:HA	1.92	0.40
1:H:160:PHE:O	1:H:164:ILE:HG12	2.22	0.40
1:A:185:LEU:O	1:A:189:GLN:HG3	2.22	0.40
1:G:161:ASN:ND2	1:G:162:SER:N	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:HIS:O	3:M:312:HOH:O[1_556]	2.03	0.17

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	54/63 (86%)	54 (100%)	0	0	100	100
1	B	58/63 (92%)	56 (97%)	1 (2%)	1 (2%)	9	29
1	D	48/63 (76%)	46 (96%)	2 (4%)	0	100	100
1	E	53/63 (84%)	51 (96%)	2 (4%)	0	100	100
1	G	48/63 (76%)	46 (96%)	2 (4%)	0	100	100
1	H	53/63 (84%)	52 (98%)	1 (2%)	0	100	100
1	J	54/63 (86%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	59/63 (94%)	58 (98%)	1 (2%)	0	100 100
1	M	51/63 (81%)	49 (96%)	2 (4%)	0	100 100
1	N	53/63 (84%)	53 (100%)	0	0	100 100
1	P	56/63 (89%)	56 (100%)	0	0	100 100
1	Q	60/63 (95%)	59 (98%)	1 (2%)	0	100 100
2	C	11/14 (79%)	11 (100%)	0	0	100 100
2	F	11/14 (79%)	11 (100%)	0	0	100 100
2	I	11/14 (79%)	11 (100%)	0	0	100 100
2	L	11/14 (79%)	11 (100%)	0	0	100 100
2	O	11/14 (79%)	11 (100%)	0	0	100 100
2	R	11/14 (79%)	11 (100%)	0	0	100 100
All	All	713/840 (85%)	700 (98%)	12 (2%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	206	GLU

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	50/55 (91%)	43 (86%)	7 (14%)	3 11
1	B	53/55 (96%)	42 (79%)	11 (21%)	1 3
1	D	47/55 (86%)	39 (83%)	8 (17%)	2 6
1	E	49/55 (89%)	46 (94%)	3 (6%)	18 48
1	G	47/55 (86%)	40 (85%)	7 (15%)	3 9
1	H	49/55 (89%)	43 (88%)	6 (12%)	5 15
1	J	50/55 (91%)	43 (86%)	7 (14%)	3 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	54/55 (98%)	46 (85%)	8 (15%)	3 9
1	M	49/55 (89%)	40 (82%)	9 (18%)	1 5
1	N	49/55 (89%)	44 (90%)	5 (10%)	7 22
1	P	51/55 (93%)	44 (86%)	7 (14%)	3 11
1	Q	54/55 (98%)	46 (85%)	8 (15%)	3 9
2	C	11/12 (92%)	10 (91%)	1 (9%)	9 27
2	F	11/12 (92%)	11 (100%)	0	100 100
2	I	11/12 (92%)	11 (100%)	0	100 100
2	L	11/12 (92%)	9 (82%)	2 (18%)	1 5
2	O	11/12 (92%)	11 (100%)	0	100 100
2	R	11/12 (92%)	10 (91%)	1 (9%)	9 27
All	All	668/732 (91%)	578 (86%)	90 (14%)	4 11

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	MET
1	A	159	SER
1	A	178	LEU
1	A	198	LEU
1	A	204	GLU
1	A	205	LEU
1	A	209	THR
1	B	165	ASN
1	B	169	GLU
1	B	176	ASP
1	B	180	LYS
1	B	186	VAL
1	B	198	LEU
1	B	199	LEU
1	B	207	LYS
1	B	211	THR
1	B	214	HIS
1	B	215	SER
2	C	803	TYR
1	D	161	ASN
1	D	162	SER
1	D	164	ILE

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Mol	Chain	Res	Type
1	D	170	MET
1	D	175	LYS
1	D	178	LEU
1	D	198	LEU
1	D	199	LEU
1	E	160	PHE
1	E	178	LEU
1	E	185	LEU
1	G	161	ASN
1	G	164	ILE
1	G	167	ILE
1	G	178	LEU
1	G	198	LEU
1	G	199	LEU
1	G	209	THR
1	H	159	SER
1	H	160	PHE
1	H	178	LEU
1	H	185	LEU
1	H	186	VAL
1	H	198	LEU
1	J	169	GLU
1	J	171	GLU
1	J	178	LEU
1	J	199	LEU
1	J	207	LYS
1	J	209	THR
1	J	210	GLU
1	K	172	ILE
1	K	178	LEU
1	K	186	VAL
1	K	198	LEU
1	K	199	LEU
1	K	204	GLU
1	K	205	LEU
1	K	216	LEU
2	L	797	GLN
2	L	803	TYR
1	M	160	PHE
1	M	161	ASN
1	M	162	SER
1	M	164	ILE

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Mol	Chain	Res	Type
1	M	171	GLU
1	M	178	LEU
1	M	198	LEU
1	M	199	LEU
1	M	210	GLU
1	N	157	MET
1	N	175	LYS
1	N	178	LEU
1	N	179	GLU
1	N	185	LEU
1	P	160	PHE
1	P	171	GLU
1	P	175	LYS
1	P	198	LEU
1	P	199	LEU
1	P	205	LEU
1	P	209	THR
1	Q	162	SER
1	Q	176	ASP
1	Q	189	GLN
1	Q	190	GLN
1	Q	199	LEU
1	Q	205	LEU
1	Q	215	SER
1	Q	216	LEU
2	R	803	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	161	ASN
1	G	161	ASN
1	J	166	ASN
1	M	168	HIS
1	Q	214	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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	56/63 (88%)	1.34	9 (16%) 1 1	29, 57, 118, 153	0
1	B	60/63 (95%)	1.17	13 (21%) 0 0	31, 64, 100, 113	0
1	D	50/63 (79%)	1.27	13 (26%) 0 0	31, 57, 112, 128	0
1	E	55/63 (87%)	1.50	16 (29%) 0 0	32, 61, 107, 130	0
1	G	50/63 (79%)	1.14	9 (18%) 1 1	31, 55, 105, 112	0
1	H	55/63 (87%)	1.09	6 (10%) 5 3	31, 61, 116, 126	0
1	J	56/63 (88%)	1.41	12 (21%) 0 0	29, 56, 123, 138	0
1	K	61/63 (96%)	1.45	15 (24%) 0 0	30, 56, 100, 111	0
1	M	53/63 (84%)	1.53	11 (20%) 1 0	33, 59, 126, 136	0
1	N	55/63 (87%)	1.32	12 (21%) 0 0	29, 62, 113, 140	0
1	P	58/63 (92%)	1.53	11 (18%) 1 1	30, 58, 123, 135	0
1	Q	62/63 (98%)	1.10	12 (19%) 1 0	30, 58, 95, 118	0
2	C	13/14 (92%)	0.94	2 (15%) 2 1	38, 49, 69, 83	0
2	F	13/14 (92%)	0.99	0 100 100	32, 35, 56, 86	0
2	I	13/14 (92%)	0.80	0 100 100	30, 35, 56, 80	0
2	L	13/14 (92%)	1.06	1 (7%) 13 7	37, 53, 73, 84	0
2	O	13/14 (92%)	0.92	1 (7%) 13 7	33, 37, 57, 80	0
2	R	13/14 (92%)	0.64	0 100 100	42, 48, 71, 85	0
All	All	749/840 (89%)	1.28	143 (19%) 1 1	29, 57, 113, 153	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	156	ALA	8.9
1	A	210	GLU	8.1
1	P	211	THR	7.8

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Mol	Chain	Res	Type	RSRZ
1	P	212	ALA	7.4
1	J	157	MET	6.7
1	E	167	ILE	6.0
1	M	158	GLY	6.0
1	M	208	LYS	5.6
1	M	173	GLN	5.1
1	P	157	MET	5.0
1	N	155	GLY	4.9
1	J	164	ILE	4.9
1	A	167	ILE	4.8
1	Q	167	ILE	4.7
1	H	205	LEU	4.7
1	K	164	ILE	4.6
1	M	200	ALA	4.4
1	N	167	ILE	4.3
1	G	205	LEU	4.2
1	A	155	GLY	4.1
1	A	157	MET	4.0
1	P	158	GLY	3.9
1	E	170	MET	3.8
1	N	156	ALA	3.7
1	N	164	ILE	3.6
1	M	195	VAL	3.5
1	P	161	ASN	3.5
1	G	170	MET	3.5
1	E	181	ASN	3.5
1	B	160	PHE	3.4
1	D	184	TRP	3.4
1	K	170	MET	3.4
1	G	171	GLU	3.4
1	J	172	ILE	3.3
1	P	155	GLY	3.3
1	A	170	MET	3.2
1	P	186	VAL	3.2
2	L	798	ALA	3.2
1	P	164	ILE	3.2
1	B	211	THR	3.2
1	E	160	PHE	3.1
1	H	203	PHE	3.1
1	E	164	ILE	3.1
1	K	160	PHE	3.1
1	P	172	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	163	SER	2.9
1	N	208	LYS	2.9
1	N	205	LEU	2.9
1	Q	156	ALA	2.9
1	J	161	ASN	2.9
1	G	209	THR	2.9
1	B	205	LEU	2.9
1	E	175	LYS	2.8
1	N	178	LEU	2.8
1	B	167	ILE	2.8
1	K	202	ILE	2.8
2	C	806	TYR	2.8
1	H	164	ILE	2.7
1	K	167	ILE	2.7
1	E	159	SER	2.7
1	K	166	ASN	2.7
1	M	205	LEU	2.7
1	N	160	PHE	2.7
1	J	167	ILE	2.7
1	B	215	SER	2.7
1	H	157	MET	2.7
1	D	191	ARG	2.7
1	A	174	LEU	2.6
1	K	195	VAL	2.6
1	B	174	LEU	2.6
1	K	189	GLN	2.6
1	K	168	HIS	2.6
1	Q	164	ILE	2.6
1	B	186	VAL	2.6
1	E	195	VAL	2.6
1	J	186	VAL	2.6
1	M	196	LYS	2.6
1	D	172	ILE	2.5
1	K	184	TRP	2.5
1	N	195	VAL	2.5
1	N	175	LYS	2.5
1	P	184	TRP	2.5
1	M	161	ASN	2.5
1	D	167	ILE	2.5
1	B	170	MET	2.5
1	D	160	PHE	2.5
1	G	164	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	202	ILE	2.5
1	B	210	GLU	2.5
1	A	205	LEU	2.5
1	B	185	LEU	2.5
1	D	177	ALA	2.4
1	M	177	ALA	2.4
1	A	203	PHE	2.4
1	N	157	MET	2.4
1	D	168	HIS	2.4
1	E	185	LEU	2.4
1	J	158	GLY	2.4
1	K	211	THR	2.4
1	Q	159	SER	2.3
1	J	195	VAL	2.3
1	Q	157	MET	2.3
1	E	172	ILE	2.3
1	Q	174	LEU	2.3
1	Q	166	ASN	2.3
1	B	190	GLN	2.3
1	D	209	THR	2.3
1	B	163	SER	2.3
1	E	207	LYS	2.3
1	G	207	LYS	2.3
1	D	186	VAL	2.3
1	Q	195	VAL	2.2
1	H	155	GLY	2.2
1	E	177	ALA	2.2
1	J	198	LEU	2.2
2	C	803	TYR	2.2
1	D	202	ILE	2.2
1	G	174	LEU	2.2
1	G	178	LEU	2.2
1	K	174	LEU	2.2
1	D	195	VAL	2.2
1	M	163	SER	2.2
1	J	175	LYS	2.2
1	H	182	GLN	2.2
1	K	177	ALA	2.2
1	K	212	ALA	2.2
1	E	166	ASN	2.1
1	D	193	VAL	2.1
1	E	184	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	188	ASP	2.1
2	O	804	PRO	2.1
1	P	200	ALA	2.1
1	N	185	LEU	2.1
1	Q	187	TYR	2.1
1	Q	178	LEU	2.1
1	B	187	TYR	2.1
1	E	182	GLN	2.1
1	J	209	THR	2.1
1	A	202	ILE	2.1
1	M	172	ILE	2.1
1	E	168	HIS	2.0
1	D	204	GLU	2.0
1	J	193	VAL	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.