Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 01:40 AM EDT

PDB ID	:	6X04
Title	:	Nup133 (aa55-481) from S. cerevisiae bound by VHH-SAN5
Authors	:	Nordeen, S.A.; Schwartz, T.U.
Deposited on	:	2020-05-15
Resolution	:	2.68 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:

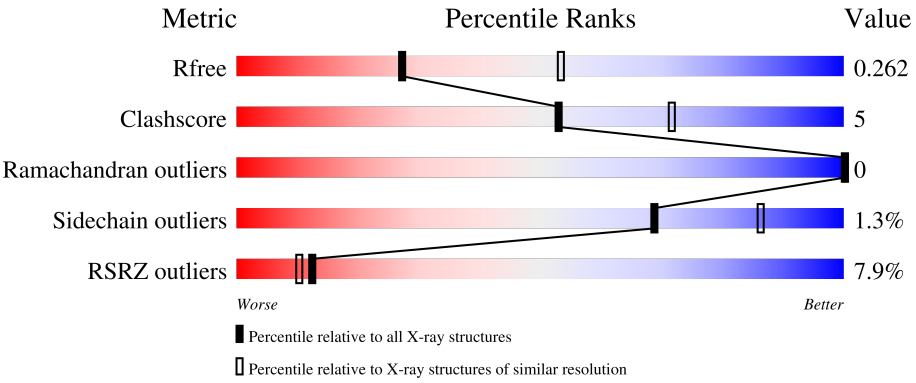
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	428	3% 75% 10% 14%
1	C	428	9% 75% 21%
1	E	428	11% 64% 9% 26%
1	G	428	10% 67% 11% 22%
1	I	428	7% 71% 10% 19%

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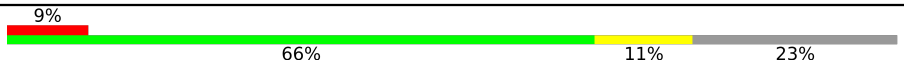
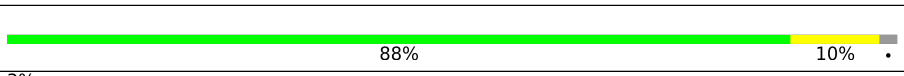
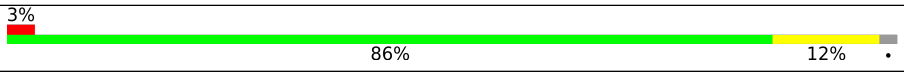
Mol	Chain	Length	Quality of chain
1	K	428	
2	B	118	
2	D	118	
2	F	118	
2	H	118	
2	J	118	
2	L	118	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20015 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 Nucleoporin NUP133.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2739	1769	435	525	10			
1	C	337	Total	C	N	O	S	0	0	0
			2405	1546	384	466	9			
1	E	315	Total	C	N	O	S	0	0	0
			2305	1491	363	442	9			
1	G	334	Total	C	N	O	S	0	0	0
			2486	1613	391	473	9			
1	I	346	Total	C	N	O	S	0	0	0
			2569	1660	410	488	11			
1	K	328	Total	C	N	O	S	0	0	0
			2414	1564	382	459	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	expression tag	UNP P36161
C	54	GLY	-	expression tag	UNP P36161
E	54	GLY	-	expression tag	UNP P36161
G	54	GLY	-	expression tag	UNP P36161
I	54	GLY	-	expression tag	UNP P36161
K	54	GLY	-	expression tag	UNP P36161

- Molecule 2 is a protein called VHH-SAN5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			853	534	152	162	5			
2	D	116	Total	C	N	O	S	0	0	0
			852	534	150	163	5			
2	F	116	Total	C	N	O	S	0	0	0
			844	528	149	162	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	116	Total	C	N	O	S	0	0	0
			847	531	149	162	5			
2	J	116	Total	C	N	O	S	0	0	0
			844	527	149	163	5			
2	L	116	Total	C	N	O	S	0	0	0
			842	528	146	163	5			

- Molecule 3 is water.

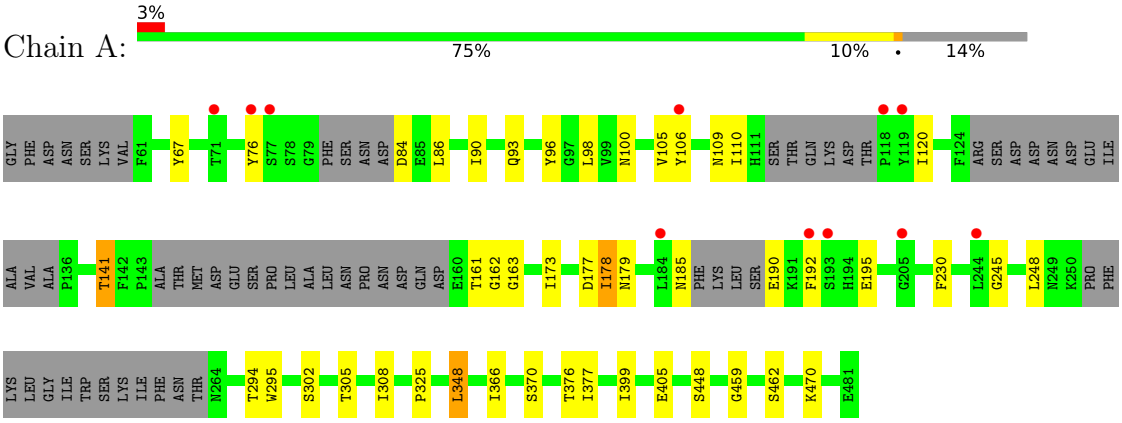
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	1	Total	O	0	0
			1	1		
3	E	1	Total	O	0	0
			1	1		
3	G	3	Total	O	0	0
			3	3		
3	I	3	Total	O	0	0
			3	3		
3	J	1	Total	O	0	0
			1	1		
3	K	2	Total	O	0	0
			2	2		

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.

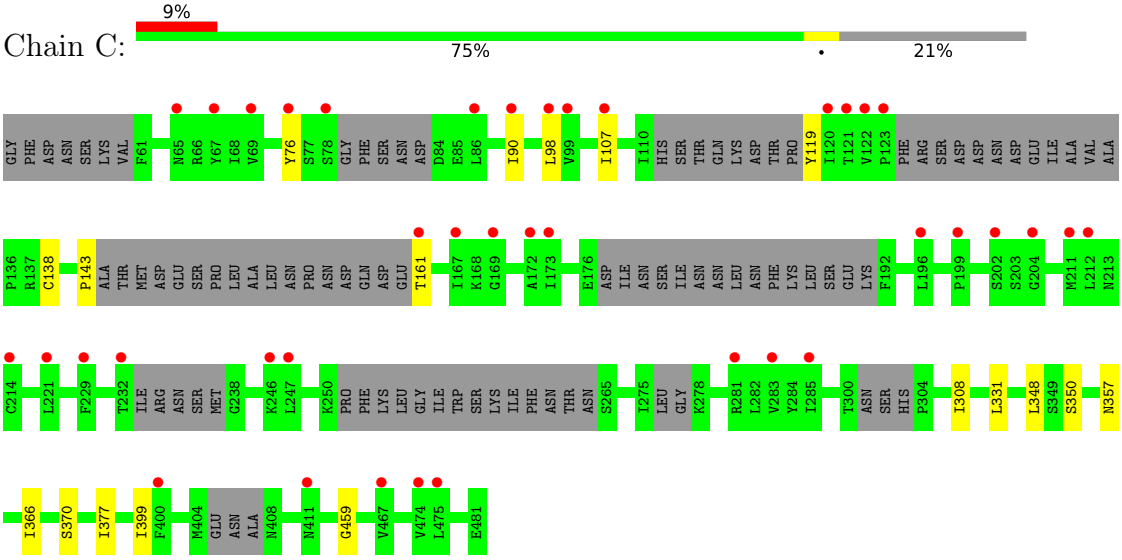
• Molecule 1: Nucleoporin NUP133

Chain A:



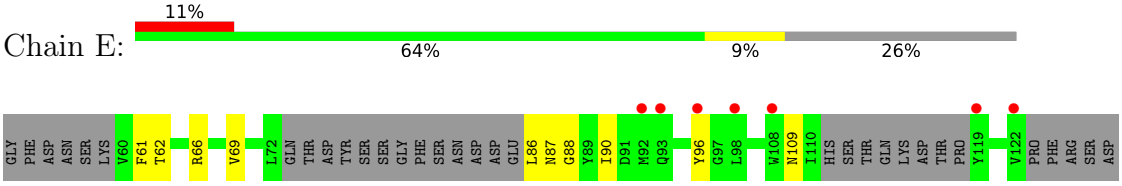
• Molecule 1: Nucleoporin NUP133

Chain C:



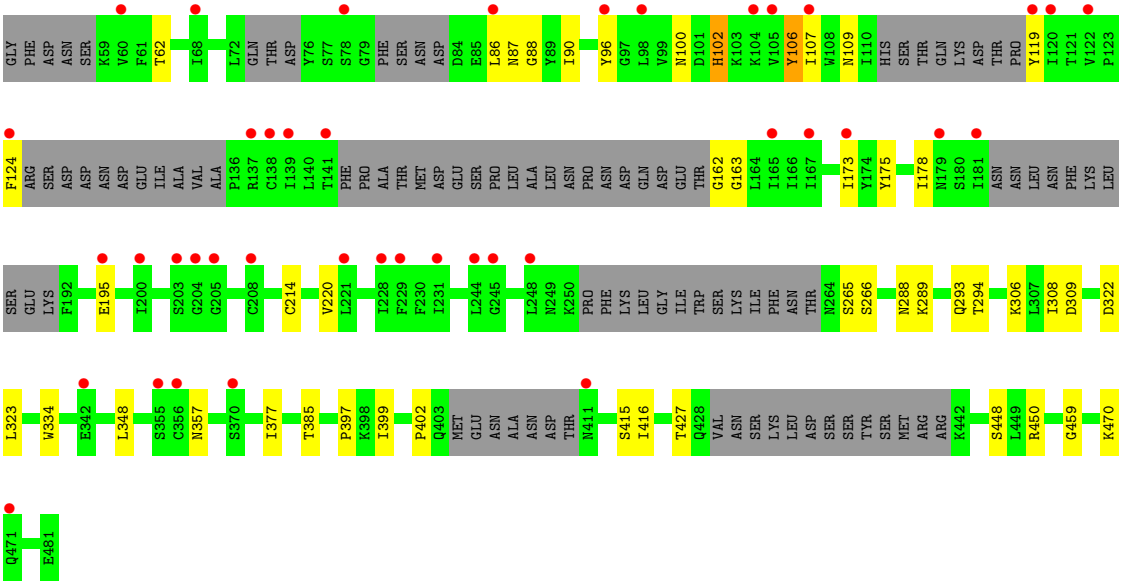
• Molecule 1: Nucleoporin NUP133

Chain E:



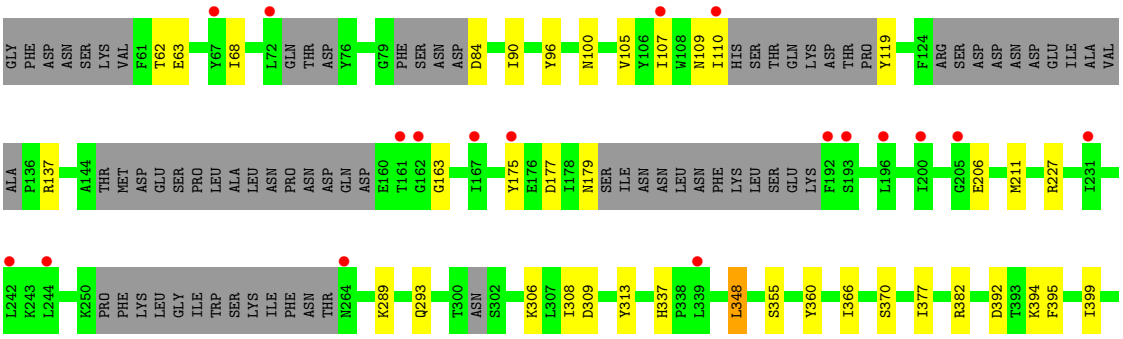
• Molecule 1: Nucleoporin NUP133

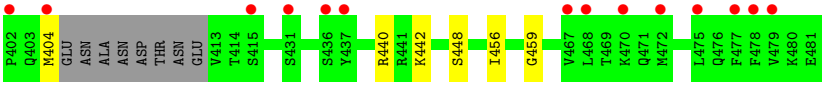
Chain G:



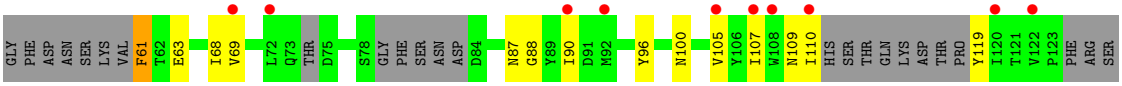
• Molecule 1: Nucleoporin NUP133

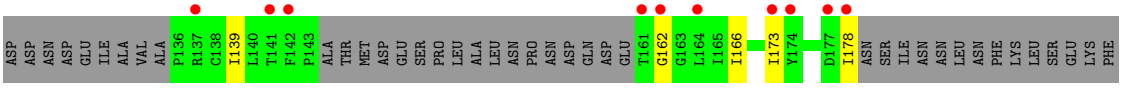
Chain I:

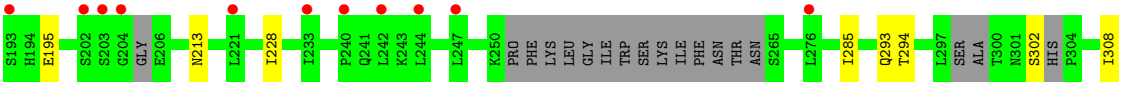


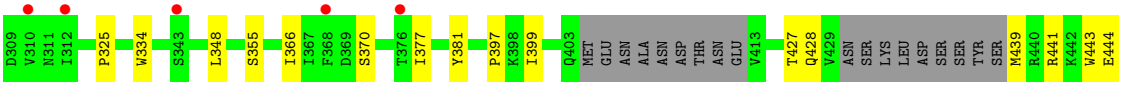


• Molecule 1: Nucleoporin NUP133

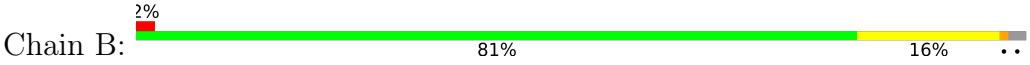




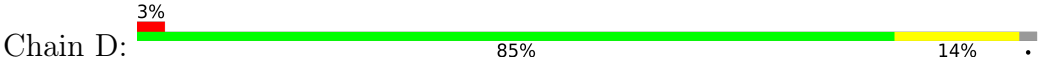


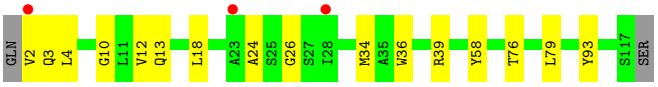


• Molecule 2: VHH-SAN5

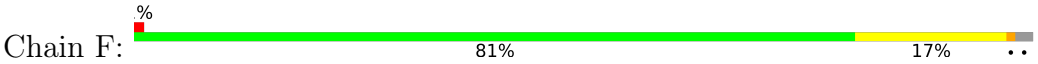


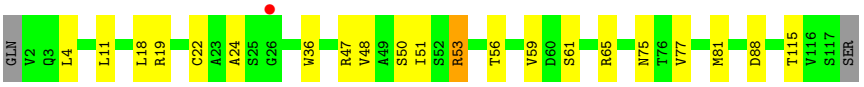
• Molecule 2: VHH-SAN5



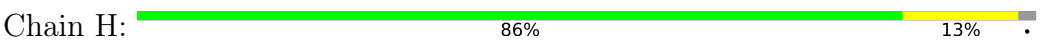


• Molecule 2: VHH-SAN5



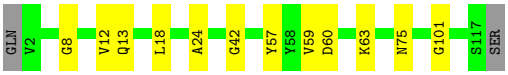


• Molecule 2: VHH-SAN5



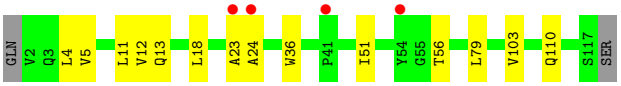
• Molecule 2: VHH-SAN5

Chain J:



• Molecule 2: VHH-SAN5

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.80Å 204.76Å 205.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.68 49.68 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.68-2.68) 98.1 (49.68-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.243 , 0.261 0.243 , 0.262	Depositor DCC
R_{free} test set	1999 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20015	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.35	0/2795	0.53	0/3812
1	C	0.26	0/2446	0.47	0/3338
1	E	0.25	0/2345	0.47	0/3193
1	G	0.29	0/2533	0.49	0/3450
1	I	0.33	0/2616	0.50	0/3560
1	K	0.27	0/2455	0.48	0/3339
2	B	0.31	0/867	0.49	0/1174
2	D	0.54	0/866	0.51	0/1172
2	F	0.30	0/858	0.48	0/1163
2	H	0.27	0/861	0.48	0/1167
2	J	0.50	0/858	0.52	0/1164
2	L	0.26	0/856	0.48	0/1161
All	All	0.32	0/20356	0.49	0/27693

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2739	0	2518	25	1
1	C	2405	0	2125	12	0
1	E	2305	0	2086	24	0
1	G	2486	0	2289	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2569	0	2371	25	0
1	K	2414	0	2212	33	0
2	B	853	0	817	14	0
2	D	852	0	820	17	0
2	F	844	0	797	13	0
2	H	847	0	806	12	0
2	J	844	0	792	8	1
2	L	842	0	798	13	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	3	0	0	0	0
3	I	3	0	0	0	0
3	J	1	0	0	0	0
3	K	2	0	0	0	0
All	All	20015	0	18431	207	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 5.

All (207) 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:G:265:SER:CA	1:G:288:ASN:HD21	1.31	1.42
1:G:265:SER:HA	1:G:288:ASN:ND2	1.43	1.28
1:C:143:PRO:HB3	1:C:161:THR:O	1.32	1.25
1:G:266:SER:H	1:G:288:ASN:ND2	1.54	1.06
1:C:143:PRO:CB	1:C:161:THR:O	2.03	1.05
1:G:266:SER:N	1:G:288:ASN:ND2	2.06	1.04
2:D:4:LEU:HD22	2:D:24:ALA:HB3	1.41	0.99
2:F:53:ARG:H	2:F:53:ARG:HD2	1.31	0.96
2:D:4:LEU:CD2	2:D:24:ALA:HB3	1.95	0.95
2:D:4:LEU:HA	2:D:24:ALA:CB	1.98	0.92
2:D:3:GLN:O	2:D:24:ALA:HB1	1.78	0.83
1:G:106:TYR:CE1	1:G:119:TYR:HB2	2.15	0.81
1:G:265:SER:HA	1:G:288:ASN:HD21	0.63	0.78
1:G:162:GLY:HA2	1:G:178:ILE:HG22	1.66	0.77
1:I:392:ASP:OD1	1:I:394:LYS:N	2.18	0.76
1:C:143:PRO:CA	1:C:161:THR:O	2.35	0.75
1:G:265:SER:C	1:G:288:ASN:HD21	1.91	0.72
1:G:265:SER:C	1:G:288:ASN:ND2	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:348:LEU:HB2	1:I:399:ILE:HD11	1.72	0.71
1:K:439:MET:HE2	2:L:103:VAL:HG13	1.73	0.70
1:A:448:SER:HB2	2:D:12:VAL:HG22	1.72	0.70
1:A:173:ILE:HG22	1:A:195:GLU:HG2	1.73	0.70
1:E:86:LEU:HD12	1:E:470:LYS:HG3	1.75	0.69
2:D:4:LEU:HA	2:D:24:ALA:HB2	1.75	0.69
1:E:348:LEU:HB2	1:E:399:ILE:HD11	1.76	0.67
1:G:86:LEU:HD12	1:G:470:LYS:HG3	1.77	0.66
2:D:4:LEU:HD23	2:D:24:ALA:HB3	1.79	0.65
1:A:90:ILE:HG23	1:A:459:GLY:HA3	1.78	0.65
1:I:163:GLY:HA2	1:I:175:TYR:O	1.97	0.65
1:E:355:SER:HA	1:K:325:PRO:HB2	1.78	0.64
1:G:265:SER:CA	1:G:288:ASN:ND2	2.16	0.64
1:G:288:ASN:OD1	1:G:289:LYS:N	2.31	0.64
2:B:5:VAL:HG22	2:B:24:ALA:HB2	1.81	0.63
1:K:173:ILE:HG22	1:K:195:GLU:HG2	1.80	0.63
2:F:53:ARG:H	2:F:53:ARG:CD	1.98	0.63
1:G:173:ILE:HG22	1:G:195:GLU:HG2	1.80	0.62
2:F:53:ARG:HD2	2:F:53:ARG:N	2.11	0.61
1:K:107:ILE:O	1:K:119:TYR:HA	2.01	0.61
1:G:266:SER:N	1:G:288:ASN:HD22	1.98	0.60
1:I:177:ASP:OD1	1:I:179:ASN:ND2	2.34	0.60
1:I:306:LYS:HD2	1:I:309:ASP:HB2	1.84	0.59
1:G:90:ILE:HG23	1:G:459:GLY:HA3	1.84	0.59
2:J:12:VAL:HG21	2:J:18:LEU:HG	1.84	0.59
2:L:12:VAL:HG21	2:L:18:LEU:HG	1.85	0.58
2:D:4:LEU:HD23	2:D:24:ALA:CB	2.34	0.58
1:E:90:ILE:HG23	1:E:459:GLY:HA3	1.84	0.58
2:L:51:ILE:HG13	2:L:56:THR:HG22	1.85	0.58
2:L:4:LEU:HA	2:L:24:ALA:HB3	1.86	0.58
2:B:36:TRP:HE1	2:B:77:VAL:HG12	1.68	0.58
2:F:65:ARG:NH2	2:F:88:ASP:OD2	2.37	0.57
1:G:107:ILE:O	1:G:119:TYR:HA	2.04	0.57
2:F:47:ARG:HD2	2:F:50:SER:HB3	1.86	0.57
1:C:357:ASN:O	2:H:63:LYS:NZ	2.37	0.57
1:C:90:ILE:HG23	1:C:459:GLY:HA3	1.86	0.57
2:B:51:ILE:HG13	2:B:56:THR:HG22	1.85	0.57
1:I:90:ILE:HG23	1:I:459:GLY:HA3	1.86	0.56
2:B:34:MET:HB3	2:B:77:VAL:HG21	1.87	0.56
2:J:24:ALA:HB3	2:J:75:ASN:HB3	1.87	0.56
1:E:415:SER:HA	1:E:428:GLN:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:TRP:HB3	1:G:397:PRO:HG2	1.87	0.56
1:I:440:ARG:O	1:I:442:LYS:NZ	2.33	0.56
1:A:308:ILE:HD11	1:A:370:SER:HA	1.88	0.55
1:A:178:ILE:HD12	1:A:178:ILE:O	2.06	0.55
2:D:39:ARG:NH1	2:D:93:TYR:OH	2.35	0.55
1:G:448:SER:HB2	2:J:12:VAL:HA	1.88	0.54
1:A:325:PRO:HB2	1:I:355:SER:HA	1.90	0.54
1:G:385:THR:HG22	2:J:8:GLY:HA2	1.90	0.54
2:F:59:VAL:HG12	2:F:61:SER:H	1.73	0.54
1:A:86:LEU:HD12	1:A:470:LYS:HG3	1.90	0.54
1:A:348:LEU:HB2	1:A:399:ILE:HD11	1.90	0.53
1:K:308:ILE:HD11	1:K:370:SER:HA	1.90	0.53
1:A:96:TYR:HH	1:A:161:THR:HG1	1.53	0.53
2:H:13:GLN:NE2	1:K:448:SER:O	2.39	0.53
1:K:162:GLY:HA2	1:K:178:ILE:HG22	1.91	0.53
2:F:51:ILE:HG13	2:F:56:THR:HG22	1.90	0.53
2:D:58:TYR:O	1:G:357:ASN:ND2	2.41	0.52
1:G:87:ASN:OD1	1:G:88:GLY:N	2.41	0.52
2:B:8:GLY:HA2	1:E:385:THR:HG22	1.92	0.52
1:E:66:ARG:O	1:E:480:LYS:N	2.43	0.52
2:J:101:GLY:HA2	2:L:23:ALA:HB3	1.92	0.52
2:D:4:LEU:CD2	2:D:24:ALA:CB	2.78	0.52
1:G:416:ILE:HG23	1:G:427:THR:HG23	1.93	0.51
1:C:308:ILE:HD11	1:C:370:SER:HA	1.93	0.51
2:B:4:LEU:HA	2:B:24:ALA:HB3	1.92	0.51
1:K:366:ILE:HG12	1:K:377:ILE:HD13	1.92	0.50
1:C:143:PRO:HA	1:C:161:THR:O	2.09	0.50
1:E:308:ILE:HD11	1:E:370:SER:HA	1.93	0.50
1:A:162:GLY:HA2	1:A:178:ILE:HG22	1.94	0.50
2:B:13:GLN:HG3	1:E:450:ARG:HA	1.94	0.49
1:I:392:ASP:OD1	1:I:395:PHE:N	2.45	0.49
1:C:107:ILE:O	1:C:119:TYR:HA	2.12	0.49
1:A:93:GLN:NE2	1:A:405:GLU:OE2	2.45	0.49
1:I:293:GLN:HA	1:I:308:ILE:O	2.13	0.49
2:J:60:ASP:HA	2:J:63:LYS:HE3	1.95	0.48
1:G:102:HIS:CD2	1:G:102:HIS:C	2.87	0.48
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.95	0.48
1:K:439:MET:CE	2:L:103:VAL:HG13	2.42	0.48
1:K:100:ASN:HB3	1:K:105:VAL:HG23	1.96	0.48
2:H:12:VAL:HG12	2:H:13:GLN:O	2.14	0.48
1:I:63:GLU:HG3	1:I:68:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:PRO:HB2	1:K:355:SER:HA	1.96	0.48
1:G:402:PRO:HD2	1:G:415:SER:O	2.14	0.48
2:B:81:MET:HE2	2:B:84:LEU:HD21	1.96	0.48
1:C:366:ILE:HG12	1:C:377:ILE:HD13	1.95	0.48
1:I:360:TYR:HD1	1:I:382:ARG:HD2	1.79	0.48
1:I:107:ILE:O	1:I:119:TYR:HA	2.14	0.47
1:I:137:ARG:HH21	1:I:211:MET:HG2	1.78	0.47
1:K:87:ASN:OD1	1:K:88:GLY:N	2.46	0.47
1:K:428:GLN:OE1	1:K:443:TRP:NE1	2.44	0.47
1:I:289:LYS:O	1:I:313:TYR:HB2	2.14	0.47
1:E:220:VAL:HA	1:E:229:PHE:O	2.15	0.47
1:A:185:ASN:HD22	1:A:190:GLU:N	2.12	0.47
2:L:5:VAL:HG23	2:L:110:GLN:HE22	1.79	0.47
1:G:163:GLY:HA2	1:G:175:TYR:O	2.15	0.47
2:H:24:ALA:HB3	2:H:75:ASN:HB3	1.96	0.47
1:K:61:PHE:HA	1:K:69:VAL:O	2.15	0.46
1:K:162:GLY:HA2	1:K:178:ILE:H	1.80	0.46
1:K:348:LEU:HB2	1:K:399:ILE:HD11	1.96	0.46
1:K:427:THR:HG22	1:K:444:GLU:HG3	1.96	0.46
1:E:96:TYR:HA	1:E:109:ASN:HA	1.98	0.46
1:A:405:GLU:HB2	1:A:462:SER:HA	1.98	0.46
1:E:139:ILE:HD11	1:E:213:ASN:HB2	1.98	0.46
1:I:90:ILE:HD11	1:I:110:ILE:HG21	1.98	0.46
1:A:366:ILE:HG12	1:A:377:ILE:HD13	1.97	0.46
1:A:177:ASP:OD1	1:A:179:ASN:CB	2.64	0.45
1:E:231:ILE:HG23	1:E:243:LYS:O	2.16	0.45
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.97	0.45
1:C:348:LEU:HB2	1:C:399:ILE:HD11	1.98	0.45
1:A:90:ILE:HD11	1:A:110:ILE:HG21	1.97	0.45
1:A:98:LEU:HA	1:A:106:TYR:O	2.15	0.45
1:E:214:CYS:SG	1:E:220:VAL:HG23	2.57	0.45
1:I:337:HIS:HE1	1:I:404:MET:HG3	1.81	0.45
1:K:90:ILE:HG23	1:K:459:GLY:HA3	1.98	0.45
1:I:360:TYR:CD1	1:I:382:ARG:HD2	2.51	0.45
1:G:322:ASP:HB2	2:H:97:VAL:HG21	1.98	0.45
1:K:90:ILE:HD11	1:K:110:ILE:HG21	1.98	0.45
1:A:230:PHE:O	1:A:245:GLY:N	2.47	0.44
1:G:306:LYS:HE3	1:G:309:ASP:HB2	1.99	0.44
1:E:366:ILE:HG12	1:E:377:ILE:HD13	1.98	0.44
2:B:12:VAL:HG21	2:B:18:LEU:HG	1.99	0.44
1:E:87:ASN:OD1	1:E:88:GLY:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:MET:HB2	2:F:81:MET:HE2	1.92	0.44
1:E:294:THR:HB	1:E:308:ILE:HB	1.99	0.43
1:K:439:MET:CE	2:L:103:VAL:HG22	2.47	0.43
2:B:11:LEU:HD13	1:E:62:THR:OG1	2.18	0.43
1:A:141:THR:OG1	1:A:163:GLY:HA3	2.19	0.43
1:E:61:PHE:HB3	1:E:69:VAL:O	2.18	0.43
1:G:100:ASN:C	1:G:100:ASN:ND2	2.71	0.43
1:I:62:THR:HG22	2:L:11:LEU:HD13	2.00	0.43
1:G:294:THR:HB	1:G:308:ILE:HB	2.00	0.43
1:K:139:ILE:HD11	1:K:213:ASN:HB2	2.00	0.43
1:K:439:MET:HE2	1:K:439:MET:HB3	1.88	0.43
1:G:214:CYS:SG	1:G:220:VAL:HG23	2.58	0.43
1:G:323:LEU:HB2	2:H:97:VAL:HG11	2.01	0.43
2:D:34:MET:HE1	2:D:76:THR:C	2.39	0.43
1:E:198:LEU:HD21	1:E:231:ILE:HD11	2.01	0.43
1:K:302:SER:O	1:K:302:SER:OG	2.31	0.43
1:K:69:VAL:HA	1:K:476:GLN:O	2.18	0.42
2:J:57:TYR:OH	2:J:59:VAL:HG22	2.19	0.42
2:B:59:VAL:HG12	2:B:61:SER:H	1.83	0.42
2:B:70:ARG:HB2	2:B:77:VAL:HG22	2.01	0.42
2:D:2:VAL:HG13	2:D:26:GLY:HA3	2.01	0.42
2:D:12:VAL:HG21	2:D:18:LEU:HG	2.01	0.42
1:A:294:THR:HB	1:A:308:ILE:HB	2.01	0.42
1:G:323:LEU:HD21	2:H:99:GLU:HB2	2.02	0.42
2:H:59:VAL:HG12	2:H:62:VAL:HG22	2.02	0.42
2:D:12:VAL:HG12	2:D:13:GLN:O	2.19	0.42
1:E:248:LEU:HD22	1:E:295:TRP:CZ3	2.55	0.42
2:F:24:ALA:HB3	2:F:75:ASN:HB3	2.02	0.42
1:K:166:ILE:HB	1:K:173:ILE:HG13	2.01	0.42
1:I:206:GLU:OE1	1:I:227:ARG:NH2	2.53	0.42
2:D:36:TRP:CD1	2:D:79:LEU:HB2	2.55	0.41
1:I:366:ILE:HG12	1:I:377:ILE:HD13	2.02	0.41
1:I:448:SER:HB2	2:L:12:VAL:HG22	2.02	0.41
1:K:228:ILE:HD13	1:K:285:ILE:HD13	2.02	0.41
2:L:12:VAL:HG12	2:L:13:GLN:O	2.19	0.41
2:B:12:VAL:HA	1:E:448:SER:HB2	2.02	0.41
1:I:100:ASN:HB3	1:I:105:VAL:HG23	2.02	0.41
1:K:294:THR:HB	1:K:308:ILE:HB	2.02	0.41
2:L:36:TRP:CD1	2:L:79:LEU:HB2	2.55	0.41
2:F:18:LEU:HD23	2:F:19:ARG:N	2.35	0.41
1:I:308:ILE:HD11	1:I:370:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:11:LEU:HD13	2:F:115:THR:HB	2.02	0.41
2:H:89:THR:HG23	2:H:115:THR:HA	2.02	0.41
1:K:96:TYR:HA	1:K:109:ASN:HA	2.02	0.41
1:E:221:LEU:HB2	1:E:229:PHE:HB2	2.02	0.41
1:K:63:GLU:HG3	1:K:68:ILE:HG23	2.03	0.41
1:A:96:TYR:HA	1:A:109:ASN:HA	2.03	0.41
1:C:331:LEU:HA	1:C:350:SER:O	2.21	0.41
1:G:293:GLN:HA	1:G:308:ILE:O	2.20	0.41
1:K:334:TRP:HB3	1:K:397:PRO:HG2	2.03	0.41
1:A:67:TYR:OH	2:D:10:GLY:HA2	2.21	0.41
2:F:4:LEU:HD22	2:F:22:CYS:SG	2.61	0.41
1:A:100:ASN:HB3	1:A:105:VAL:HG23	2.01	0.40
2:F:36:TRP:O	2:F:48:VAL:HG12	2.20	0.40
1:G:348:LEU:HB2	1:G:399:ILE:HD11	2.03	0.40
2:H:81:MET:HB2	2:H:81:MET:HE2	1.81	0.40
1:A:96:TYR:CZ	1:A:109:ASN:HB3	2.56	0.40
1:G:450:ARG:HA	2:J:13:GLN:HG3	2.02	0.40
2:H:53:ARG:NH2	2:H:54:TYR:OH	2.54	0.40
1:K:381:TYR:CE1	1:K:441:ARG:HG3	2.56	0.40
1:G:96:TYR:HA	1:G:109:ASN:HA	2.03	0.40
1:I:96:TYR:CZ	1:I:109:ASN:HB3	2.57	0.40
1:A:248:LEU:HD22	1:A:295:TRP:CZ3	2.57	0.40
1:C:98:LEU:HD21	1:C:138:CYS:HB2	2.03	0.40
1:K:293:GLN:HA	1:K:308:ILE:O	2.21	0.40
1:K:439:MET:HE1	2:L:103:VAL:HG22	2.04	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:A:179:ASN:ND2	2:J:42:GLY:O[4_456]	1.59	0.61

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	353/428 (82%)	328 (93%)	25 (7%)	0	100	100
1	C	315/428 (74%)	302 (96%)	13 (4%)	0	100	100
1	E	293/428 (68%)	278 (95%)	15 (5%)	0	100	100
1	G	314/428 (73%)	294 (94%)	20 (6%)	0	100	100
1	I	326/428 (76%)	310 (95%)	16 (5%)	0	100	100
1	K	302/428 (71%)	288 (95%)	14 (5%)	0	100	100
2	B	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
2	D	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
2	F	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
2	H	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
2	J	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
2	L	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
All	All	2587/3276 (79%)	2461 (95%)	126 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	280/394 (71%)	270 (96%)	10 (4%)	35	61
1	C	230/394 (58%)	229 (100%)	1 (0%)	91	96
1	E	228/394 (58%)	226 (99%)	2 (1%)	78	91
1	G	252/394 (64%)	247 (98%)	5 (2%)	55	79
1	I	260/394 (66%)	257 (99%)	3 (1%)	71	87
1	K	242/394 (61%)	241 (100%)	1 (0%)	91	96
2	B	83/94 (88%)	82 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	84/94 (89%)	84 (100%)	0	100 100
2	F	81/94 (86%)	79 (98%)	2 (2%)	47 74
2	H	82/94 (87%)	82 (100%)	0	100 100
2	J	81/94 (86%)	81 (100%)	0	100 100
2	L	82/94 (87%)	82 (100%)	0	100 100
All	All	1985/2928 (68%)	1960 (99%)	25 (1%)	69 86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	84	ASP
1	A	120	ILE
1	A	141	THR
1	A	178	ILE
1	A	192	PHE
1	A	302	SER
1	A	305	THR
1	A	348	LEU
1	A	376	THR
2	B	11	LEU
1	C	76	TYR
1	E	348	LEU
1	E	349	SER
2	F	53	ARG
2	F	77	VAL
1	G	62	THR
1	G	102	HIS
1	G	106	TYR
1	G	124	PHE
1	G	377	ILE
1	I	84	ASP
1	I	348	LEU
1	I	456	ILE
1	K	61	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
2	D	3	GLN
1	G	102	HIS
1	G	288	ASN

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 monosaccharides 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	367/428 (85%)	0.18	11 (2%) 50 49	36, 70, 112, 161	0
1	C	337/428 (78%)	0.62	39 (11%) 4 3	54, 112, 166, 201	0
1	E	315/428 (73%)	0.86	45 (14%) 2 1	65, 117, 175, 218	0
1	G	334/428 (78%)	0.66	41 (12%) 4 3	43, 96, 164, 228	0
1	I	346/428 (80%)	0.47	32 (9%) 9 7	36, 80, 152, 191	0
1	K	328/428 (76%)	0.56	37 (11%) 5 4	57, 100, 154, 217	0
2	B	116/118 (98%)	0.13	2 (1%) 70 71	43, 65, 132, 176	0
2	D	116/118 (98%)	-0.00	3 (2%) 56 55	42, 59, 95, 170	0
2	F	116/118 (98%)	0.06	1 (0%) 84 85	70, 86, 116, 144	0
2	H	116/118 (98%)	0.09	0 100 100	48, 65, 102, 152	0
2	J	116/118 (98%)	-0.06	0 100 100	36, 48, 89, 168	0
2	L	116/118 (98%)	0.22	4 (3%) 45 44	58, 77, 113, 138	0
All	All	2723/3276 (83%)	0.43	215 (7%) 12 10	36, 84, 154, 228	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	229	PHE	7.8
1	E	231	ILE	7.4
1	G	471	GLN	4.7
1	I	264	ASN	4.6
1	G	205	GLY	4.5
1	K	122	VAL	4.4
1	G	411	ASN	4.2
1	G	124	PHE	4.2
1	E	297	LEU	4.2
1	K	173	ILE	4.1
1	I	478	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	105	VAL	4.1
1	C	214	CYS	4.0
1	C	172	ALA	4.0
1	A	119	TYR	4.0
1	E	142	PHE	4.0
1	E	122	VAL	3.9
1	K	240	PRO	3.9
1	K	203	SER	3.9
2	L	23	ALA	3.9
1	C	123	PRO	3.8
1	E	221	LEU	3.8
1	G	98	LEU	3.8
1	E	217	ALA	3.8
1	C	167	ILE	3.7
1	G	107	ILE	3.7
1	I	475	LEU	3.7
1	I	193	SER	3.7
1	G	86	LEU	3.7
1	K	368	PHE	3.7
1	I	72	LEU	3.7
1	K	193	SER	3.6
1	G	139	ILE	3.5
1	C	76	TYR	3.5
1	E	472	MET	3.5
1	K	242	LEU	3.5
1	E	298	SER	3.5
1	E	143	PRO	3.5
1	E	471	GLN	3.4
1	C	78	SER	3.4
1	I	472	MET	3.4
1	G	181	ILE	3.4
1	I	200	ILE	3.4
1	C	90	ILE	3.3
1	E	195	GLU	3.3
1	E	92	MET	3.3
1	C	161	THR	3.3
1	E	370	SER	3.3
1	I	205	GLY	3.3
1	E	108	TRP	3.3
1	K	174	TYR	3.3
1	C	411	ASN	3.2
1	I	477	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	167	ILE	3.2
1	I	110	ILE	3.2
1	A	184	LEU	3.2
1	G	244	LEU	3.2
1	I	242	LEU	3.2
1	G	138	CYS	3.2
1	I	415	SER	3.2
1	G	356	CYS	3.1
1	I	431	SER	3.1
1	I	162	GLY	3.1
1	E	463	LYS	3.1
1	E	204	GLY	3.0
1	C	122	VAL	3.0
1	E	167	ILE	3.0
1	K	276	LEU	3.0
1	C	204	GLY	3.0
1	A	192	PHE	3.0
1	C	202	SER	3.0
1	G	231	ILE	3.0
1	I	196	LEU	3.0
1	C	246	LYS	2.9
2	B	23	ALA	2.9
1	G	120	ILE	2.9
1	C	121	THR	2.9
1	C	169	GLY	2.9
1	G	195	GLU	2.9
1	K	90	ILE	2.9
1	G	248	LEU	2.9
1	A	71	THR	2.9
1	C	86	LEU	2.9
1	E	203	SER	2.9
1	G	165	ILE	2.9
1	K	107	ILE	2.9
1	A	205	GLY	2.8
1	E	214	CYS	2.8
1	I	402	PRO	2.8
1	G	229	PHE	2.7
1	G	96	TYR	2.7
1	K	161	THR	2.7
1	C	65	ASN	2.7
2	L	41	PRO	2.7
1	I	192	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	122	VAL	2.7
1	C	67	TYR	2.7
1	E	318	GLU	2.6
1	E	466	TYR	2.6
1	C	98	LEU	2.6
1	C	199	PRO	2.6
1	G	342	GLU	2.6
1	E	198	LEU	2.6
1	K	343	SER	2.6
2	L	24	ALA	2.6
1	E	119	TYR	2.6
1	G	137	ARG	2.6
1	C	467	VAL	2.6
1	I	470	LYS	2.5
1	C	247	LEU	2.5
1	A	118	PRO	2.5
2	L	54	TYR	2.5
1	E	220	VAL	2.5
1	E	247	LEU	2.5
1	G	141	THR	2.5
1	G	173	ILE	2.5
1	E	245	GLY	2.5
1	G	200	ILE	2.5
1	A	193	SER	2.5
1	G	208	CYS	2.5
1	I	404	MET	2.5
1	G	68	ILE	2.5
1	A	106	TYR	2.5
1	E	448	SER	2.5
1	K	162	GLY	2.5
1	E	280	THR	2.5
1	K	110	ILE	2.5
1	I	468	LEU	2.5
1	K	202	SER	2.5
1	K	137	ARG	2.4
1	G	119	TYR	2.4
1	I	67	TYR	2.4
1	I	244	LEU	2.4
1	E	479	VAL	2.4
1	G	105	VAL	2.4
1	C	400	PHE	2.4
1	E	219	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	211	MET	2.4
1	C	281	ARG	2.4
1	K	120	ILE	2.4
1	C	474	VAL	2.4
1	E	427	THR	2.4
1	K	72	LEU	2.4
1	I	231	ILE	2.4
1	C	69	VAL	2.4
1	A	77	SER	2.3
1	E	244	LEU	2.3
1	K	312	ILE	2.3
1	I	437	TYR	2.3
1	K	164	LEU	2.3
1	C	99	VAL	2.3
1	E	98	LEU	2.3
1	I	175	TYR	2.3
1	E	480	LYS	2.3
2	D	23	ALA	2.3
1	C	120	ILE	2.3
1	E	228	ILE	2.3
2	B	5	VAL	2.3
1	G	204	GLY	2.3
1	E	93	GLN	2.3
1	I	107	ILE	2.3
1	C	232	THR	2.3
1	C	475	LEU	2.3
1	C	283	VAL	2.3
1	G	60	VAL	2.3
1	K	108	TRP	2.2
1	K	204	GLY	2.2
1	E	475	LEU	2.2
1	K	247	LEU	2.2
1	E	96	TYR	2.2
1	G	245	GLY	2.2
1	K	92	MET	2.2
1	A	76	TYR	2.2
1	E	139	ILE	2.2
1	K	221	LEU	2.2
1	G	104	LYS	2.2
1	G	179	ASN	2.2
1	G	203	SER	2.2
2	D	28	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	376	THR	2.2
1	C	285	ILE	2.2
1	C	221	LEU	2.2
1	K	244	LEU	2.1
1	G	370	SER	2.1
1	K	69	VAL	2.1
2	D	2	VAL	2.1
1	I	436	SER	2.1
1	C	107	ILE	2.1
1	C	211	MET	2.1
1	I	161	THR	2.1
1	E	460	TYR	2.1
1	I	167	ILE	2.1
1	I	339	LEU	2.1
1	I	467	VAL	2.1
1	K	310	VAL	2.1
2	F	26	GLY	2.1
1	K	142	PHE	2.1
1	G	228	ILE	2.1
1	C	212	LEU	2.1
1	E	212	LEU	2.1
1	C	173	ILE	2.1
1	G	78	SER	2.1
1	C	229	PHE	2.1
1	C	196	LEU	2.0
1	K	141	THR	2.0
1	G	355	SER	2.0
1	K	445	ASP	2.0
1	E	368	PHE	2.0
1	A	244	LEU	2.0
1	G	221	LEU	2.0
1	K	178	ILE	2.0
1	K	233	ILE	2.0
1	K	177	ASP	2.0
1	E	248	LEU	2.0
1	I	479	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.