Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 02:49 PM EDT

PDB ID	:	6BZW
Title	:	Structure of the Hepatitis C virus envelope glycoprotein E2 antigenic region 412-423 bound to the GL precursor of the broadly neutralizing antibody AP33
Authors	:	Tzarum, N.; Aleman, F.; Wilson, I.A.; Law, M.
Deposited on	:	2017-12-26
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

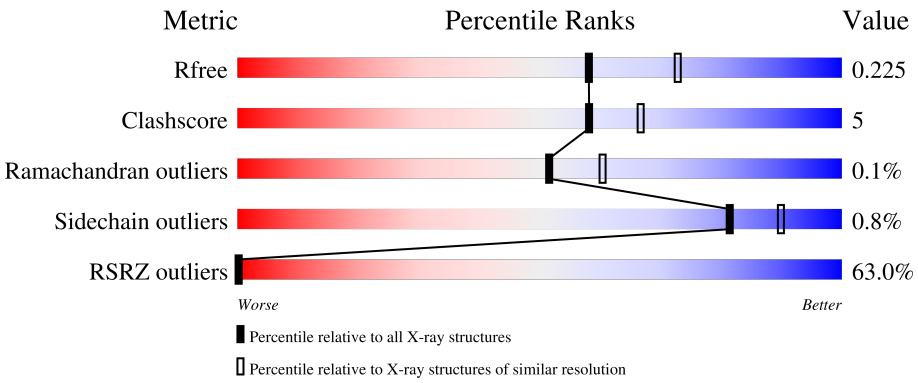
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	223	58% 88% 10% •
1	C	223	61% 86% 12% •
1	E	223	59% 84% 14% •
1	G	223	65% 86% 11% •
2	B	219	60% 88% 11% •

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Mol	Chain	Length	Quality of chain
2	D	219	62% 85% 14%
2	F	219	63% 89% 10%
2	H	219	66% 84% 16%
3	I	13	62% 62% 8% 31%
3	J	13	77% 69% 8% 23%
3	K	13	46% 69% 31%
3	L	13	46% 69% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14240 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 AP33 GL Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	218	1655	1049	267	333	6	0	0	0
1	A	219	1661	1052	268	335	6	0	0	0
1	E	219	1661	1052	268	335	6	0	0	0
1	G	219	1661	1052	268	335	6	0	0	0

- Molecule 2 is a protein called AP33 GL Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	216	1652	1028	279	339	6	0	0	0
2	B	217	1661	1033	280	342	6	0	0	0
2	F	217	1661	1033	280	343	5	0	0	0
2	H	218	1667	1036	281	344	6	0	0	0

- Molecule 3 is a protein called E2 AS412 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	9	73	46	14	13	0	0	0
3	J	10	81	52	15	14	0	0	0
3	K	9	73	46	14	13	0	0	0
3	L	9	73	46	14	13	0	0	0

- Molecule 4 is water.

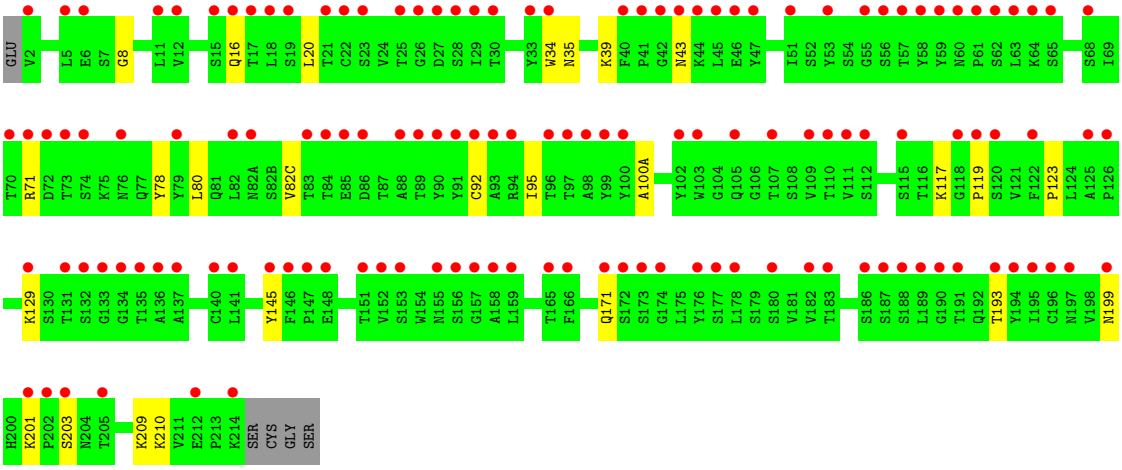
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	89	Total O 89 89	0	0
4	D	80	Total O 80 80	0	0
4	A	81	Total O 81 81	0	0
4	B	79	Total O 79 79	0	0
4	E	69	Total O 69 69	0	0
4	F	95	Total O 95 95	0	0
4	G	62	Total O 62 62	0	0
4	H	91	Total O 91 91	0	0
4	I	5	Total O 5 5	0	0
4	J	3	Total O 3 3	0	0
4	K	3	Total O 3 3	0	0
4	L	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.

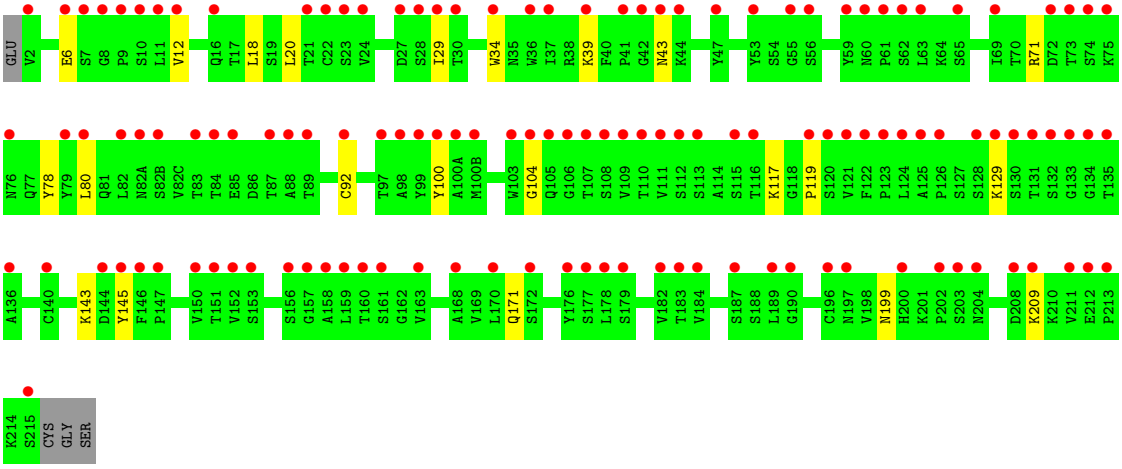
• Molecule 1: AP33 GL Heavy Chain

Chain C:



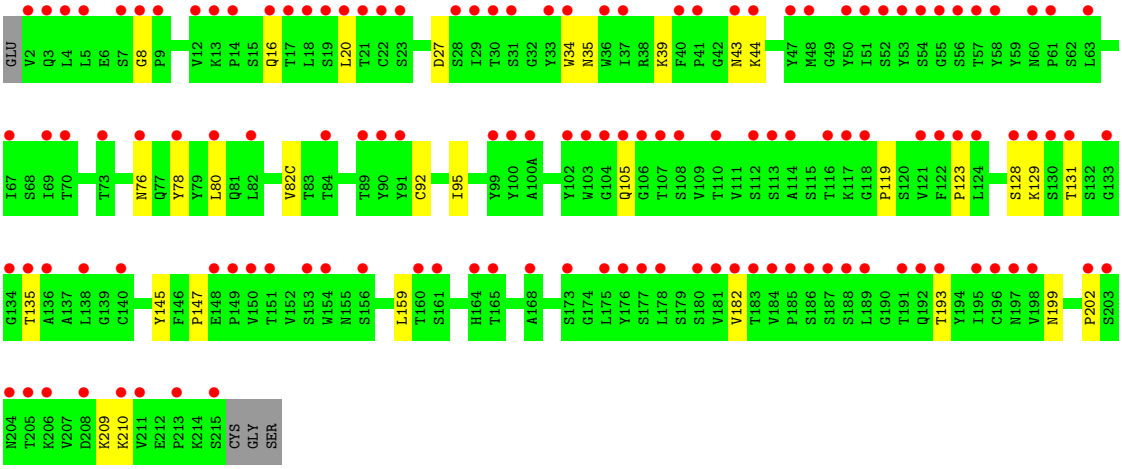
• Molecule 1: AP33 GL Heavy Chain

Chain A:



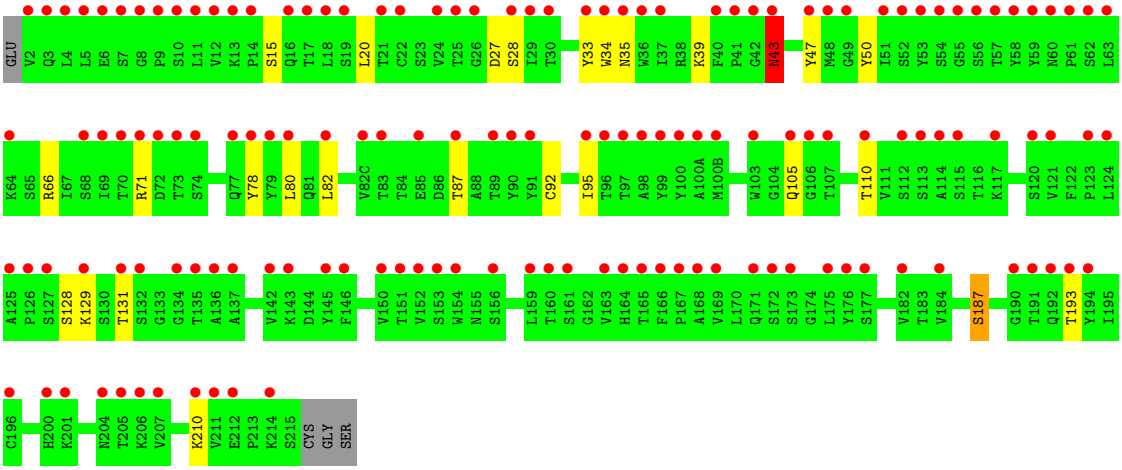
• Molecule 1: AP33 GL Heavy Chain

Chain E: 59% 84% 14%



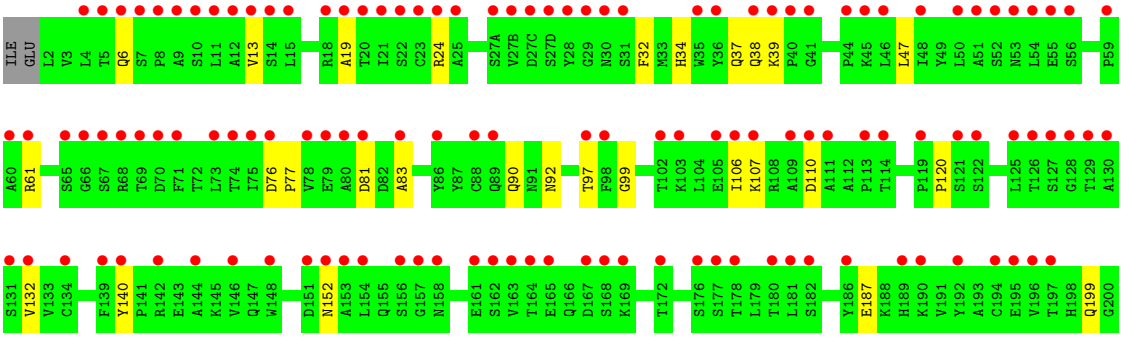
- Molecule 1: AP33 GL Heavy Chain

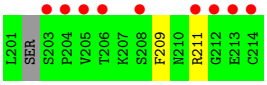
Chain G: 65% 86% 11%



- Molecule 2: AP33 GL Light Chain

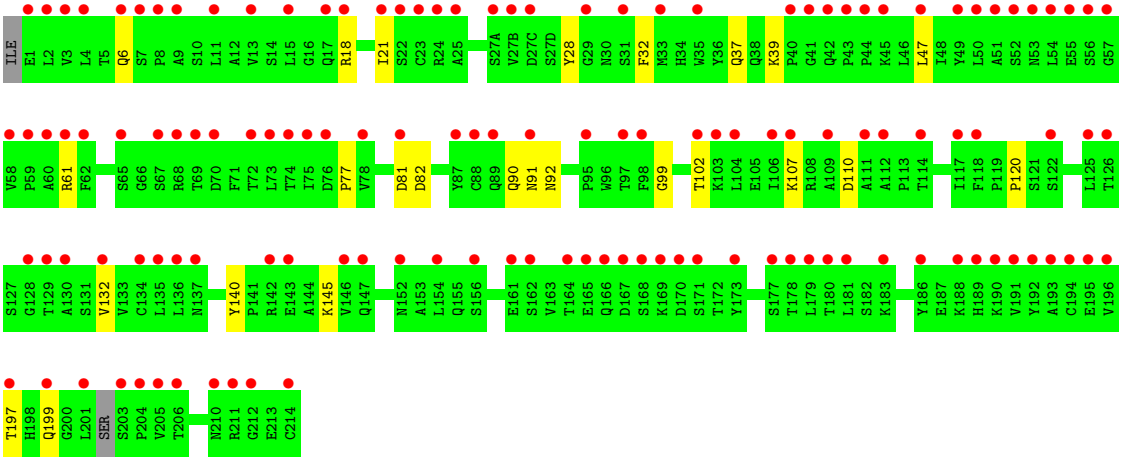
Chain D: 62% 85% 14%





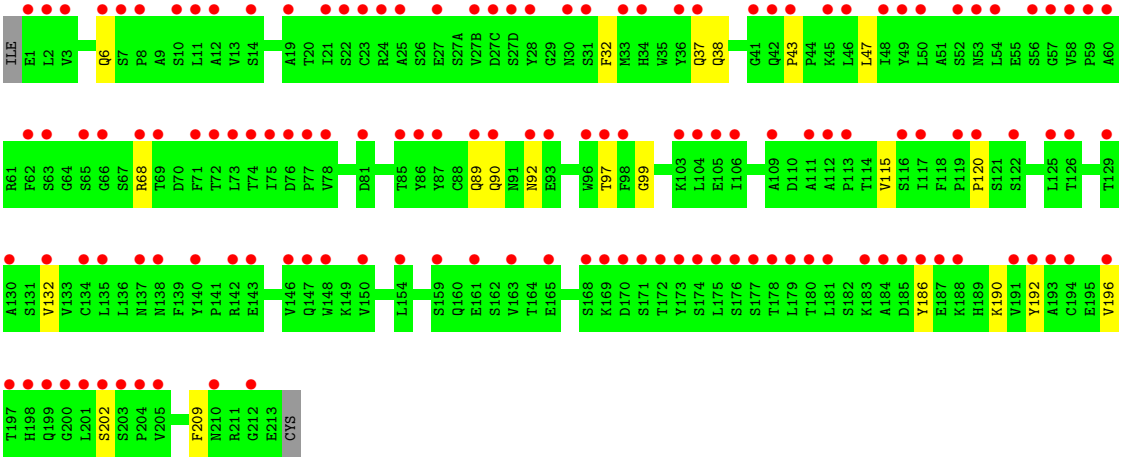
• Molecule 2: AP33 GL Light Chain

Chain B:



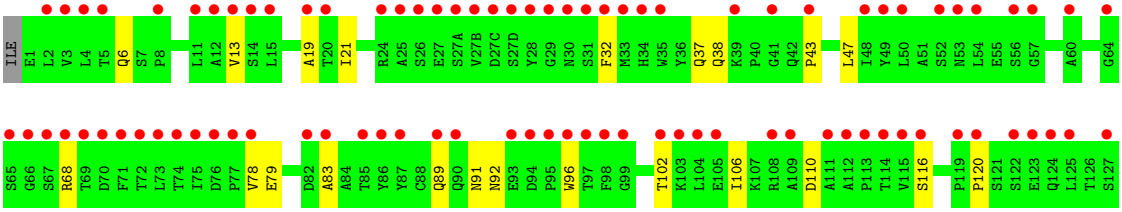
• Molecule 2: AP33 GL Light Chain

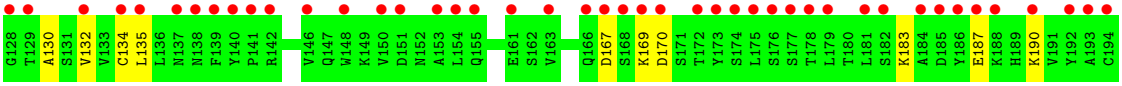
Chain F:

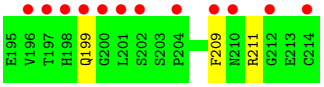


• Molecule 2: AP33 GL Light Chain

Chain H:

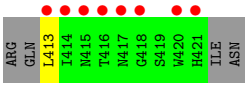






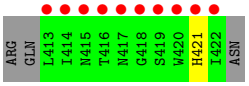
- Molecule 3: E2 AS412 peptide

Chain I:



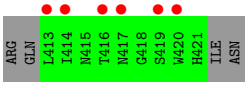
- Molecule 3: E2 AS412 peptide

Chain J:



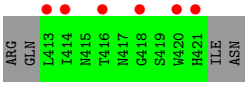
- Molecule 3: E2 AS412 peptide

Chain K:



- Molecule 3: E2 AS412 peptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.36Å 84.71Å 192.92Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	49.16 – 2.20 49.15 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.9 (49.16-2.20) 94.9 (49.15-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	113.35 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.192 , 0.231 0.190 , 0.225	Depositor DCC
R_{free} test set	4557 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 20.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14240	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8314e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	0.25	0/1703	0.49	0/2327
1	C	0.25	0/1697	0.50	0/2319
1	E	0.25	0/1703	0.49	0/2327
1	G	0.25	0/1703	0.51	0/2327
2	B	0.25	0/1696	0.46	0/2306
2	D	0.25	0/1687	0.46	0/2294
2	F	0.25	0/1697	0.47	0/2309
2	H	0.25	0/1703	0.47	0/2317
3	I	0.21	0/75	0.42	0/102
3	J	0.20	0/83	0.42	0/113
3	K	0.21	0/75	0.42	0/102
3	L	0.20	0/75	0.43	0/102
All	All	0.25	0/13897	0.48	0/18945

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 (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	1661	0	1627	12	1
1	C	1655	0	1622	18	1
1	E	1661	0	1627	20	0
1	G	1661	0	1627	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1661	0	1591	16	0
2	D	1652	0	1582	19	0
2	F	1661	0	1592	12	0
2	H	1667	0	1597	21	0
3	I	73	0	65	1	0
3	J	81	0	76	1	0
3	K	73	0	65	0	0
3	L	73	0	65	0	0
4	A	81	0	0	3	0
4	B	79	0	0	2	0
4	C	89	0	0	2	0
4	D	80	0	0	2	0
4	E	69	0	0	0	0
4	F	95	0	0	1	0
4	G	62	0	0	2	0
4	H	91	0	0	4	0
4	I	5	0	0	1	0
4	J	3	0	0	0	0
4	K	3	0	0	0	0
4	L	4	0	0	0	0
All	All	14240	0	13136	127	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 (127) 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:117:LYS:NZ	4:A:301:HOH:O	2.09	0.85
1:A:143:LYS:NZ	4:A:302:HOH:O	2.14	0.81
2:F:68:ARG:NH1	4:F:301:HOH:O	2.16	0.77
2:H:134:CYS:SG	4:H:301:HOH:O	2.43	0.76
2:H:110:ASP:OD2	2:H:199:GLN:NE2	2.17	0.71
2:B:110:ASP:OD2	2:B:199:GLN:NE2	2.24	0.70
1:C:39:LYS:NZ	2:D:38:GLN:OE1	2.26	0.68
1:E:35:ASN:HD21	1:E:95:ILE:HG13	1.60	0.67
1:E:39:LYS:HE3	1:E:43:ASN:HA	1.78	0.66
2:H:116:SER:O	4:H:301:HOH:O	2.14	0.65
1:G:39:LYS:NZ	2:H:38:GLN:OE1	2.23	0.65
1:G:129:LYS:NZ	4:G:305:HOH:O	2.29	0.65
1:E:193:THR:HG23	1:E:210:LYS:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LYS:NZ	2:F:38:GLN:OE1	2.31	0.62
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.81	0.62
1:A:39:LYS:HE3	1:A:43:ASN:HA	1.82	0.61
2:D:39:LYS:NZ	2:D:81:ASP:OD1	2.34	0.61
2:H:211:ARG:NH2	4:H:309:HOH:O	2.34	0.60
1:C:20:LEU:HD12	1:C:80:LEU:HD23	1.84	0.59
1:C:35:ASN:HD21	1:C:95:ILE:HG13	1.66	0.59
1:C:117:LYS:NZ	4:C:307:HOH:O	2.36	0.59
1:G:20:LEU:HD12	1:G:80:LEU:HD23	1.85	0.58
2:D:32:PHE:HB2	2:D:92:ASN:HB2	1.84	0.58
2:D:187:GLU:O	2:D:211:ARG:NH1	2.37	0.58
2:D:90:GLN:HE21	2:D:97:THR:HG22	1.69	0.57
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.85	0.57
1:G:39:LYS:HE3	1:G:43:ASN:HB3	1.86	0.56
3:I:413:LEU:N	4:I:502:HOH:O	2.37	0.56
1:C:71:ARG:HA	1:C:78:TYR:HA	1.86	0.56
2:H:135:LEU:N	4:H:301:HOH:O	2.37	0.56
2:D:110:ASP:OD2	2:D:199:GLN:NE2	2.39	0.55
1:G:105:GLN:HA	2:H:43:PRO:HG3	1.88	0.55
2:B:90:GLN:NE2	4:B:308:HOH:O	2.35	0.54
2:H:32:PHE:HB2	2:H:92:ASN:HB2	1.88	0.54
1:A:171:GLN:OE1	4:A:303:HOH:O	2.18	0.54
1:E:123:PRO:HD3	1:E:209:LYS:HE2	1.90	0.54
2:B:32:PHE:HB2	2:B:92:ASN:HB2	1.88	0.54
1:G:35:ASN:ND2	1:G:47:TYR:OH	2.39	0.54
2:D:61:ARG:HG2	2:D:77:PRO:HD2	1.89	0.53
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.89	0.53
2:B:61:ARG:HG2	2:B:77:PRO:HD2	1.89	0.53
1:A:78:TYR:OH	1:A:92:CYS:HB2	2.08	0.53
1:E:78:TYR:OH	1:E:92:CYS:HB2	2.09	0.53
2:F:90:GLN:HE21	2:F:97:THR:HG22	1.73	0.53
1:E:35:ASN:ND2	1:E:95:ILE:HG13	2.23	0.52
1:C:35:ASN:ND2	1:C:95:ILE:HG13	2.25	0.52
2:D:13:VAL:HG21	2:D:19:ALA:HB2	1.92	0.51
1:C:78:TYR:OH	1:C:92:CYS:HB2	2.10	0.51
1:G:27:ASP:OD1	1:G:28:SER:N	2.43	0.51
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.92	0.50
1:C:123:PRO:HD3	1:C:209:LYS:HE2	1.92	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.50
2:H:167:ASP:OD2	2:H:170:ASP:N	2.37	0.50
1:G:187:SER:O	4:G:301:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:TYR:OH	1:G:92:CYS:HB2	2.12	0.50
2:F:32:PHE:HB2	2:F:92:ASN:HB2	1.94	0.49
1:G:71:ARG:HA	1:G:78:TYR:HA	1.93	0.49
2:B:18:ARG:NH1	4:B:302:HOH:O	2.45	0.49
2:B:61:ARG:HD2	2:B:77:PRO:O	2.13	0.49
1:A:71:ARG:HA	1:A:78:TYR:HA	1.94	0.48
1:G:35:ASN:ND2	1:G:50:TYR:HB3	2.28	0.48
1:G:193:THR:HG23	1:G:210:LYS:HE3	1.96	0.48
1:G:34:TRP:HB3	1:G:78:TYR:CZ	2.49	0.48
1:C:34:TRP:HB3	1:C:78:TYR:CZ	2.49	0.47
2:H:183:LYS:O	2:H:187:GLU:HG2	2.13	0.47
2:H:167:ASP:OD2	2:H:169:LYS:N	2.44	0.47
1:C:8:GLY:HA3	1:C:20:LEU:HD23	1.96	0.47
1:A:20:LEU:HD12	1:A:80:LEU:HD23	1.97	0.47
2:B:6:GLN:HG3	2:B:99:GLY:HA3	1.96	0.47
1:C:193:THR:HG23	1:C:210:LYS:HE3	1.96	0.47
1:E:147:PRO:HD2	1:E:202:PRO:HB3	1.97	0.47
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.97	0.47
2:F:186:TYR:HA	2:F:192:TYR:OH	2.15	0.46
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.97	0.46
2:D:199:GLN:NE2	4:D:508:HOH:O	2.35	0.46
2:H:21:ILE:HG12	2:H:102:THR:HG21	1.98	0.46
1:E:129:LYS:HD3	2:F:209:PHE:HB3	1.98	0.46
1:G:129:LYS:HD3	2:H:209:PHE:HB3	1.98	0.45
2:B:39:LYS:NZ	2:B:81:ASP:OD1	2.46	0.45
2:H:190:LYS:HB2	2:H:190:LYS:HE2	1.75	0.45
2:D:6:GLN:HG3	2:D:99:GLY:HA3	1.98	0.45
1:A:12:VAL:HG21	1:A:18:LEU:HD13	1.99	0.45
1:E:27:ASP:O	1:E:76:ASN:ND2	2.49	0.45
2:H:91:ASN:HB2	2:H:96:TRP:CE2	2.52	0.45
1:A:29:ILE:HA	1:A:34:TRP:CE2	2.52	0.45
1:E:44:LYS:HA	1:E:44:LYS:HD3	1.78	0.44
1:E:105:GLN:HA	2:F:43:PRO:HG3	1.99	0.44
1:C:39:LYS:HE3	1:C:43:ASN:HA	2.00	0.44
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.99	0.44
1:E:8:GLY:HA3	1:E:20:LEU:HD23	1.98	0.44
1:E:34:TRP:HB3	1:E:78:TYR:CZ	2.53	0.44
2:F:6:GLN:HG3	2:F:99:GLY:HA3	2.00	0.44
1:C:201:LYS:NZ	4:C:311:HOH:O	2.37	0.44
2:H:13:VAL:HG21	2:H:19:ALA:HB2	1.99	0.44
2:F:115:VAL:HG21	2:F:196:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LYS:HA	2:B:140:TYR:OH	2.18	0.43
2:B:145:LYS:HB3	2:B:197:THR:HB	2.01	0.43
1:E:20:LEU:HD12	1:E:80:LEU:HD23	2.00	0.43
2:B:28:TYR:CE1	3:J:421:HIS:HA	2.53	0.43
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.99	0.43
1:E:119:PRO:HB3	1:E:145:TYR:HB3	2.01	0.43
2:H:120:PRO:HG3	2:H:130:ALA:HB1	2.01	0.43
2:D:83:ALA:HB2	2:D:106:ILE:HG12	2.01	0.43
1:C:16:GLN:O	1:C:82(C):VAL:HG22	2.19	0.43
1:E:128:SER:HA	1:E:131:THR:HG22	2.01	0.43
2:F:190:LYS:HB2	2:F:190:LYS:HE2	1.64	0.43
1:A:6:GLU:OE2	1:A:104:GLY:HA3	2.18	0.42
1:G:128:SER:HA	1:G:131:THR:HG22	2.00	0.42
1:G:33:TYR:HB2	1:G:95:ILE:HB	2.01	0.42
1:G:87:THR:HG23	1:G:110:THR:HA	2.00	0.42
1:E:16:GLN:O	1:E:82(C):VAL:HG22	2.20	0.42
1:G:66:ARG:O	1:G:82:LEU:HD12	2.20	0.42
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.02	0.41
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.48	0.41
1:E:131:THR:HA	1:E:135:THR:O	2.20	0.41
2:H:83:ALA:HB2	2:H:106:ILE:HG12	2.03	0.41
1:E:159:LEU:HD21	1:E:182:VAL:HG21	2.02	0.41
2:D:24:ARG:NH1	4:D:513:HOH:O	2.52	0.41
1:C:100(A):ALA:HB2	2:D:34:HIS:ND1	2.36	0.41
2:H:78:VAL:HG22	2:H:79:GLU:H	1.86	0.41
2:B:21:ILE:HG12	2:B:102:THR:HG21	2.03	0.40
1:C:171:GLN:HE21	1:C:171:GLN:HB2	1.63	0.40
2:D:107:LYS:HA	2:D:140:TYR:OH	2.21	0.40
1:C:129:LYS:HD3	2:D:209:PHE:HB3	2.03	0.40
2:D:76:ASP:HA	2:D:77:PRO:HA	1.94	0.40
2:D:61:ARG:HD2	2:D:77:PRO:O	2.21	0.40
1:A:100:TYR:O	2:B:91:ASN:ND2	2.43	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:C:203:SER:O	1:A:209:LYS:NZ[2_656]	2.09	0.11

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	217/223 (97%)	212 (98%)	5 (2%)	0	100	100
1	C	216/223 (97%)	210 (97%)	6 (3%)	0	100	100
1	E	217/223 (97%)	210 (97%)	7 (3%)	0	100	100
1	G	217/223 (97%)	213 (98%)	3 (1%)	1 (0%)	29	31
2	B	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
2	D	212/219 (97%)	206 (97%)	6 (3%)	0	100	100
2	F	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
2	H	216/219 (99%)	209 (97%)	6 (3%)	1 (0%)	29	31
3	I	7/13 (54%)	7 (100%)	0	0	100	100
3	J	8/13 (62%)	8 (100%)	0	0	100	100
3	K	7/13 (54%)	7 (100%)	0	0	100	100
3	L	7/13 (54%)	7 (100%)	0	0	100	100
All	All	1752/1820 (96%)	1706 (97%)	44 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	43	ASN
2	H	68	ARG

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	193/196 (98%)	191 (99%)	2 (1%)	76	86
1	C	192/196 (98%)	191 (100%)	1 (0%)	88	94
1	E	193/196 (98%)	192 (100%)	1 (0%)	88	94
1	G	193/196 (98%)	190 (98%)	3 (2%)	62	76
2	B	187/189 (99%)	187 (100%)	0	100	100
2	D	186/189 (98%)	185 (100%)	1 (0%)	88	94
2	F	187/189 (99%)	185 (99%)	2 (1%)	73	85
2	H	188/189 (100%)	186 (99%)	2 (1%)	73	85
3	I	8/12 (67%)	8 (100%)	0	100	100
3	J	9/12 (75%)	9 (100%)	0	100	100
3	K	8/12 (67%)	8 (100%)	0	100	100
3	L	8/12 (67%)	8 (100%)	0	100	100
All	All	1552/1588 (98%)	1540 (99%)	12 (1%)	81	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	ASN
2	D	152	ASN
1	A	129	LYS
1	A	199	ASN
1	E	199	ASN
2	F	89	GLN
2	F	202	SER
1	G	15	SER
1	G	43	ASN
1	G	187	SER
2	H	6	GLN
2	H	89	GLN

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

Mol	Chain	Res	Type
1	C	35	ASN
2	D	90	GLN
1	E	35	ASN
2	F	90	GLN
1	G	35	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	219/223 (98%)	2.39	130 (59%)	0	0	11, 20, 32, 43	0
1	C	218/223 (97%)	2.43	135 (61%)	0	0	11, 20, 30, 38	0
1	E	219/223 (98%)	2.41	131 (59%)	0	0	13, 21, 31, 41	0
1	G	219/223 (98%)	2.50	146 (66%)	0	0	12, 21, 33, 46	0
2	B	217/219 (99%)	2.58	132 (60%)	0	0	10, 20, 30, 58	0
2	D	216/219 (98%)	2.48	136 (62%)	0	0	11, 21, 30, 39	0
2	F	217/219 (99%)	2.49	138 (63%)	0	0	13, 22, 31, 50	0
2	H	218/219 (99%)	2.62	144 (66%)	0	0	12, 21, 29, 42	0
3	I	9/13 (69%)	3.08	8 (88%)	0	0	20, 22, 26, 26	0
3	J	10/13 (76%)	2.94	10 (100%)	0	0	21, 23, 27, 29	0
3	K	9/13 (69%)	2.67	6 (66%)	0	0	21, 23, 25, 25	0
3	L	9/13 (69%)	2.77	6 (66%)	0	0	21, 24, 27, 27	0
All	All	1780/1820 (97%)	2.49	1122 (63%)	0	0	10, 21, 31, 58	0

All (1122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	GLU	10.6
2	B	214	CYS	9.9
2	H	86	TYR	9.0
2	B	13	VAL	8.1
2	F	57	GLY	7.3
2	D	214	CYS	7.2
1	C	111	VAL	7.0
1	A	55	GLY	6.7
1	A	190	GLY	6.6
1	E	33	TYR	6.4
1	E	131	THR	6.4

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Mol	Chain	Res	Type	RSRZ
2	B	203	SER	6.4
2	H	66	GLY	6.3
1	A	6	GLU	6.3
2	H	214	CYS	6.3
1	E	211	VAL	6.3
1	C	133	GLY	6.3
1	G	98	ALA	6.2
1	G	131	THR	6.1
2	B	15	LEU	5.9
2	F	148	TRP	5.9
2	H	33	MET	5.9
2	F	86	TYR	5.8
2	D	109	ALA	5.7
2	D	212	GLY	5.7
1	C	132	SER	5.7
1	E	14	PRO	5.6
2	F	129	THR	5.6
1	A	72	ASP	5.5
2	B	125	LEU	5.5
1	E	8	GLY	5.4
1	E	34	TRP	5.4
2	H	50	LEU	5.4
2	F	2	LEU	5.4
3	K	420	TRP	5.4
2	H	57	GLY	5.3
2	H	119	PRO	5.3
1	G	30	THR	5.3
2	B	193	ALA	5.3
1	A	134	GLY	5.3
2	H	148	TRP	5.2
2	B	109	ALA	5.2
2	F	27(C)	ASP	5.2
2	F	73	LEU	5.1
2	H	202	SER	5.1
2	F	49	TYR	5.1
2	F	42	GLN	5.1
2	F	54	LEU	5.1
2	D	114	THR	5.0
2	B	170	ASP	5.0
1	E	7	SER	5.0
2	F	154	LEU	5.0
2	H	129	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	61	PRO	4.9
2	F	14	SER	4.9
2	D	15	LEU	4.9
2	F	71	PHE	4.9
2	D	111	ALA	4.9
1	A	132	SER	4.9
2	B	212	GLY	4.9
2	B	23	CYS	4.9
1	G	164	HIS	4.9
2	F	69	THR	4.9
1	A	133	GLY	4.8
1	A	82(A)	ASN	4.8
2	F	119	PRO	4.8
3	K	413	LEU	4.8
1	A	84	THR	4.8
2	D	65	SER	4.8
2	B	54	LEU	4.8
2	F	179	LEU	4.8
2	F	66	GLY	4.8
2	B	126	THR	4.8
1	G	184	VAL	4.8
1	C	65	SER	4.7
1	G	54	SER	4.7
2	B	169	LYS	4.7
1	C	203	SER	4.7
1	A	189	LEU	4.7
2	B	112	ALA	4.7
2	H	71	PHE	4.7
1	G	106	GLY	4.7
1	E	3	GLN	4.7
2	H	20	THR	4.6
2	B	57	GLY	4.6
1	C	56	SER	4.6
2	D	181	LEU	4.6
2	B	60	ALA	4.6
2	B	31	SER	4.6
2	F	200	GLY	4.6
2	D	106	ILE	4.5
3	L	416	THR	4.5
2	H	53	ASN	4.5
1	G	18	LEU	4.5
2	H	93	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	197	THR	4.4
2	F	74	THR	4.4
3	I	416	THR	4.4
1	E	106	GLY	4.4
2	H	27(D)	SER	4.4
1	C	191	THR	4.4
2	B	206	THR	4.4
1	G	79	TYR	4.4
2	D	125	LEU	4.4
2	B	130	ALA	4.4
2	H	185	ASP	4.3
1	A	2	VAL	4.3
1	G	64	LYS	4.3
1	G	90	TYR	4.3
2	H	74	THR	4.3
1	G	68	SER	4.3
3	J	418	GLY	4.3
1	C	76	ASN	4.3
1	C	19	SER	4.3
2	D	134	CYS	4.3
2	F	183	LYS	4.3
1	G	49	GLY	4.3
1	C	61	PRO	4.2
2	B	41	GLY	4.2
2	B	134	CYS	4.2
1	C	190	GLY	4.2
2	H	27(B)	VAL	4.2
1	G	42	GLY	4.2
1	G	156	SER	4.2
2	H	179	LEU	4.2
1	E	52	SER	4.2
2	H	54	LEU	4.2
1	E	91	TYR	4.2
1	G	53	TYR	4.2
2	H	25	ALA	4.2
2	H	135	LEU	4.1
1	G	48	MET	4.1
1	C	72	ASP	4.1
2	D	69	THR	4.1
2	H	43	PRO	4.1
2	H	34	HIS	4.1
2	F	188	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	190	LYS	4.1
2	D	41	GLY	4.1
1	C	202	PRO	4.1
2	B	4	LEU	4.1
2	B	142	ARG	4.1
2	B	7	SER	4.1
1	C	99	TYR	4.1
2	H	69	THR	4.1
1	G	63	LEU	4.1
1	E	114	ALA	4.0
2	D	190	LYS	4.0
1	G	33	TYR	4.0
2	D	102	THR	4.0
2	D	142	ARG	4.0
1	C	85	GLU	4.0
1	E	105	GLN	4.0
1	G	47	TYR	4.0
1	C	5	LEU	4.0
2	D	68	ARG	4.0
2	F	85	THR	4.0
2	B	106	ILE	4.0
1	E	99	TYR	4.0
1	G	97	THR	4.0
2	H	127	SER	4.0
3	I	414	ILE	4.0
1	E	138	LEU	4.0
2	H	11	LEU	4.0
2	H	105	GLU	4.0
1	G	193	THR	4.0
2	D	203	SER	4.0
2	F	31	SER	4.0
1	A	22	CYS	4.0
2	B	136	LEU	4.0
1	C	157	GLY	4.0
2	D	70	ASP	4.0
1	E	180	SER	4.0
2	B	205	VAL	4.0
1	A	131	THR	3.9
1	C	16	GLN	3.9
1	A	42	GLY	3.9
1	C	15	SER	3.9
1	G	12	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	143	LYS	3.9
1	G	28	SER	3.9
2	D	172	THR	3.9
1	E	40	PHE	3.9
2	H	27	GLU	3.9
2	D	44	PRO	3.9
1	A	115	SER	3.9
2	F	11	LEU	3.9
2	F	87	TYR	3.9
1	E	117	LYS	3.9
1	E	30	THR	3.9
2	B	35	TRP	3.9
2	B	111	ALA	3.9
2	H	15	LEU	3.9
1	G	70	THR	3.8
1	E	43	ASN	3.8
1	G	100	TYR	3.8
1	A	200	HIS	3.8
1	E	129	LYS	3.8
2	B	104	LEU	3.8
2	H	28	TYR	3.8
1	A	30	THR	3.8
2	D	126	THR	3.8
1	C	53	TYR	3.8
1	E	191	THR	3.8
2	H	76	ASP	3.8
1	C	201	LYS	3.8
1	C	22	CYS	3.8
2	F	34	HIS	3.8
1	E	90	TYR	3.8
1	E	28	SER	3.7
2	D	8	PRO	3.7
2	D	153	ALA	3.7
1	C	110	THR	3.7
2	B	114	THR	3.7
2	B	191	VAL	3.7
2	F	48	ILE	3.7
1	G	132	SER	3.7
2	D	154	LEU	3.7
2	B	59	PRO	3.7
1	A	140	CYS	3.7
2	H	194	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	129	THR	3.7
2	D	7	SER	3.7
1	G	124	LEU	3.7
2	H	137	ASN	3.7
2	D	23	CYS	3.7
2	B	194	CYS	3.7
1	E	128	SER	3.7
2	B	177	SER	3.7
2	H	200	GLY	3.7
1	C	183	THR	3.7
1	G	57	THR	3.7
2	B	88	CYS	3.7
2	F	77	PRO	3.7
2	F	194	CYS	3.7
2	D	146	VAL	3.7
1	A	63	LEU	3.7
1	A	76	ASN	3.7
1	G	35	ASN	3.7
2	H	167	ASP	3.7
1	C	112	SER	3.7
2	F	68	ARG	3.7
1	E	47	TYR	3.7
1	G	26	GLY	3.7
2	F	59	PRO	3.6
2	B	181	LEU	3.6
3	I	420	TRP	3.6
1	E	21	THR	3.6
2	H	49	TYR	3.6
2	H	163	VAL	3.6
3	L	413	LEU	3.6
2	D	113	PRO	3.6
2	F	1	GLU	3.6
1	A	75	LYS	3.6
1	E	195	ILE	3.6
1	G	34	TRP	3.6
1	G	52	SER	3.6
2	H	64	GLY	3.6
1	A	135	THR	3.6
1	E	160	THR	3.6
2	D	71	PHE	3.6
2	H	14	SER	3.6
2	H	94	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	212	GLY	3.6
2	F	96	TRP	3.6
3	L	420	TRP	3.6
1	E	9	PRO	3.6
2	D	130	ALA	3.5
2	D	206	THR	3.6
1	C	62	SER	3.5
2	D	128	GLY	3.5
1	C	96	THR	3.5
1	G	115	SER	3.5
2	D	156	SER	3.5
2	F	203	SER	3.5
2	H	26	SER	3.5
2	B	118	PHE	3.5
1	A	83	THR	3.5
1	A	160	THR	3.5
1	A	129	LYS	3.5
2	H	24	ARG	3.5
2	H	27(C)	ASP	3.5
1	E	80	LEU	3.5
2	B	186	TYR	3.5
1	C	115	SER	3.5
2	D	177	SER	3.5
1	A	124	LEU	3.5
2	F	181	LEU	3.5
2	B	76	ASP	3.5
2	F	191	VAL	3.5
1	G	171	GLN	3.5
2	B	147	GLN	3.5
2	B	128	GLY	3.5
2	F	169	LYS	3.5
2	H	70	ASP	3.5
1	A	159	LEU	3.5
2	D	165	GLU	3.5
2	F	201	LEU	3.5
2	H	3	VAL	3.5
2	D	29	GLY	3.5
1	G	194	TYR	3.5
2	F	113	PRO	3.4
2	H	2	LEU	3.4
1	G	182	VAL	3.4
2	H	150	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	86	TYR	3.4
2	H	173	TYR	3.4
1	E	130	SER	3.4
1	C	140	CYS	3.4
1	E	48	MET	3.4
1	E	56	SER	3.4
2	B	67	SER	3.4
1	E	82	LEU	3.4
1	G	142	VAL	3.4
1	A	60	ASN	3.4
1	A	79	TYR	3.4
1	A	126	PRO	3.4
1	C	25	THR	3.4
2	D	162	SER	3.4
2	F	117	ILE	3.4
3	I	413	LEU	3.4
1	E	154	TRP	3.4
2	D	205	VAL	3.4
1	E	102	TYR	3.4
1	E	187	SER	3.4
2	B	52	SER	3.4
2	D	74	THR	3.4
1	E	5	LEU	3.4
1	G	80	LEU	3.4
2	D	27(B)	VAL	3.3
2	B	27(B)	VAL	3.3
1	A	73	THR	3.3
1	E	205	THR	3.3
2	F	25	ALA	3.3
2	B	6	GLN	3.3
2	H	209	PHE	3.3
1	C	46	GLU	3.3
1	A	109	VAL	3.3
2	F	3	VAL	3.3
1	A	41	PRO	3.3
1	C	122	PHE	3.3
1	C	126	PRO	3.3
3	J	420	TRP	3.3
2	D	180	THR	3.3
2	D	46	LEU	3.3
1	E	61	PRO	3.3
1	C	120	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	187	SER	3.3
1	A	121	VAL	3.3
1	E	108	SER	3.3
1	E	203	SER	3.3
2	F	53	ASN	3.3
2	H	134	CYS	3.3
2	B	190	LYS	3.3
2	H	193	ALA	3.3
2	D	61	ARG	3.3
1	A	11	LEU	3.3
2	D	4	LEU	3.3
1	C	147	PRO	3.3
1	E	67	ILE	3.3
1	G	19	SER	3.3
2	B	156	SER	3.3
2	H	31	SER	3.3
2	B	81	ASP	3.3
1	C	84	THR	3.3
1	G	89	THR	3.3
1	A	36	TRP	3.3
1	E	134	GLY	3.3
2	F	143	GLU	3.3
2	H	87	TYR	3.3
1	E	153	SER	3.3
2	D	67	SER	3.3
2	B	22	SER	3.3
1	G	6	GLU	3.3
2	D	161	GLU	3.3
2	B	195	GLU	3.3
1	C	55	GLY	3.2
1	C	88	ALA	3.2
2	B	154	LEU	3.2
1	C	109	VAL	3.2
2	H	178	THR	3.2
1	A	88	ALA	3.2
1	C	186	SER	3.2
1	G	5	LEU	3.2
2	H	175	LEU	3.2
2	B	75	ILE	3.2
2	F	106	ILE	3.2
2	B	89	GLN	3.2
2	H	78	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	105	GLU	3.2
2	H	12	ALA	3.2
1	A	82(B)	SER	3.2
1	E	54	SER	3.2
2	D	24	ARG	3.2
2	F	159	SER	3.2
2	H	113	PRO	3.2
2	H	141	PRO	3.2
1	C	63	LEU	3.2
1	G	51	ILE	3.2
2	B	161	GLU	3.2
1	A	98	ALA	3.2
1	A	187	SER	3.2
1	G	58	TYR	3.2
2	D	157	GLY	3.2
1	A	144	ASP	3.2
2	F	185	ASP	3.2
1	C	83	THR	3.2
2	B	129	THR	3.2
2	B	146	VAL	3.2
2	F	58	VAL	3.2
1	E	161	SER	3.2
2	D	131	SER	3.2
2	F	112	ALA	3.2
3	J	419	SER	3.2
2	D	55	GLU	3.2
2	F	33	MET	3.2
2	D	81	ASP	3.2
1	E	69	ILE	3.2
1	E	135	THR	3.2
2	D	98	PHE	3.2
1	A	111	VAL	3.2
1	C	196	CYS	3.2
1	A	136	ALA	3.2
1	G	9	PRO	3.2
2	H	68	ARG	3.2
2	B	188	LYS	3.2
1	G	110	THR	3.1
1	A	179	SER	3.1
2	H	186	TYR	3.1
1	G	82(C)	VAL	3.1
2	F	146	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	184	ALA	3.1
1	G	8	GLY	3.1
1	G	105	GLN	3.1
2	D	105	GLU	3.1
2	B	2	LEU	3.1
1	E	57	THR	3.1
1	G	165	THR	3.1
1	E	113	SER	3.1
2	D	27(D)	SER	3.1
2	B	171	SER	3.1
1	G	14	PRO	3.1
2	D	45	LYS	3.1
2	H	169	LYS	3.1
1	C	82(A)	ASN	3.1
1	G	4	LEU	3.1
1	G	62	SER	3.1
2	F	63	SER	3.1
3	J	416	THR	3.1
1	E	2	VAL	3.1
1	G	24	VAL	3.1
2	B	17	GLN	3.1
1	G	159	LEU	3.1
1	A	153	SER	3.1
2	B	98	PHE	3.1
2	B	199	GLN	3.1
1	C	98	ALA	3.1
1	C	136	ALA	3.1
1	A	182	VAL	3.1
1	E	198	VAL	3.1
2	F	132	VAL	3.1
2	F	193	ALA	3.1
2	F	28	TYR	3.1
2	H	192	TYR	3.1
2	B	201	LEU	3.1
1	C	195	ILE	3.1
3	J	422	ILE	3.1
2	H	128	GLY	3.1
1	G	40	PHE	3.1
3	I	421	HIS	3.1
2	F	202	SER	3.1
1	A	178	LEU	3.1
1	E	4	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	104	GLY	3.1
1	A	196	CYS	3.1
2	D	144	ALA	3.1
1	A	152	VAL	3.0
1	G	78	TYR	3.0
1	G	201	LYS	3.0
2	B	74	THR	3.0
2	H	108	ARG	3.0
1	G	176	TYR	3.0
1	C	30	THR	3.0
2	F	43	PRO	3.0
1	E	208	ASP	3.0
1	A	177	SER	3.0
1	E	12	VAL	3.0
1	G	10	SER	3.0
1	G	56	SER	3.0
1	G	153	SER	3.0
2	B	162	SER	3.0
2	F	134	CYS	3.0
1	A	99	TYR	3.0
1	G	205	THR	3.0
1	C	141	LEU	3.0
1	C	29	ILE	3.0
2	H	75	ILE	3.0
2	B	24	ARG	3.0
2	H	177	SER	3.0
1	C	2	VAL	3.0
1	E	184	VAL	3.0
1	A	106	GLY	3.0
1	E	13	LYS	3.0
1	A	53	TYR	3.0
1	E	84	THR	3.0
1	E	89	THR	3.0
2	F	192	TYR	3.0
1	C	43	ASN	3.0
1	G	37	ILE	3.0
1	G	121	VAL	3.0
1	C	17	THR	3.0
1	G	126	PRO	3.0
1	A	145	TYR	3.0
2	B	192	TYR	3.0
1	C	82	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	165	GLU	3.0
1	A	105	GLN	3.0
1	C	103	TRP	3.0
1	C	119	PRO	3.0
1	A	21	THR	3.0
1	A	89	THR	3.0
2	D	97	THR	3.0
2	B	102	THR	3.0
1	C	90	TYR	2.9
2	F	98	PHE	2.9
1	C	199	ASN	2.9
2	H	142	ARG	2.9
2	B	69	THR	2.9
2	D	140	TYR	2.9
2	H	29	GLY	2.9
1	A	123	PRO	2.9
1	C	21	THR	2.9
2	F	198	HIS	2.9
1	A	103	TRP	2.9
1	G	113	SER	2.9
2	D	54	LEU	2.9
1	A	125	ALA	2.9
2	B	9	ALA	2.9
2	B	143	GLU	2.9
2	H	109	ALA	2.9
1	E	123	PRO	2.9
2	D	204	PRO	2.9
2	D	110	ASP	2.9
1	G	172	SER	2.9
2	F	65	SER	2.9
2	H	56	SER	2.9
1	C	178	LEU	2.9
1	C	176	TYR	2.9
1	E	100(A)	ALA	2.9
2	H	153	ALA	2.9
1	C	197	ASN	2.9
2	F	138	ASN	2.9
2	D	59	PRO	2.9
3	J	421	HIS	2.9
1	G	160	THR	2.9
2	B	180	THR	2.9
1	A	65	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	56	SER	2.9
1	C	134	GLY	2.9
3	J	413	LEU	2.9
1	G	125	ALA	2.9
2	F	184	ALA	2.9
1	E	41	PRO	2.9
2	F	41	GLY	2.9
1	E	204	ASN	2.9
1	C	159	LEU	2.9
2	B	47	LEU	2.9
2	B	103	LYS	2.9
1	G	136	ALA	2.9
2	D	40	PRO	2.9
2	D	189	HIS	2.9
2	H	140	TYR	2.9
1	A	146	PHE	2.8
1	G	212	GLU	2.8
2	D	76	ASP	2.8
2	F	81	ASP	2.8
1	G	135	THR	2.8
2	D	21	ILE	2.8
1	G	11	LEU	2.8
1	C	129	LYS	2.8
1	E	149	PRO	2.8
1	E	213	PRO	2.8
1	G	21	THR	2.8
1	G	134	GLY	2.8
2	D	75	ILE	2.8
2	D	186	TYR	2.8
1	C	40	PHE	2.8
1	E	122	PHE	2.8
2	D	39	LYS	2.8
2	B	78	VAL	2.8
2	F	27(B)	VAL	2.8
1	C	92	CYS	2.8
3	I	415	ASN	2.8
1	C	118	GLY	2.8
1	E	116	THR	2.8
2	H	35	TRP	2.8
1	A	100(A)	ALA	2.8
1	C	41	PRO	2.8
2	B	210	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	26	GLY	2.8
1	C	173	SER	2.8
1	A	172	SER	2.8
2	D	66	GLY	2.8
1	C	193	THR	2.8
1	C	212	GLU	2.8
1	E	17	THR	2.8
1	G	210	LYS	2.8
2	H	72	THR	2.8
2	B	49	TYR	2.8
2	B	117	ILE	2.8
2	F	75	ILE	2.8
2	D	19	ALA	2.8
2	H	138	ASN	2.8
2	H	204	PRO	2.8
1	A	161	SER	2.8
1	G	175	LEU	2.8
2	F	135	LEU	2.8
1	G	16	GLN	2.8
2	D	30	ASN	2.8
2	B	43	PRO	2.7
1	C	174	GLY	2.7
2	F	78	VAL	2.7
1	A	62	SER	2.7
1	A	113	SER	2.7
3	L	418	GLY	2.7
2	F	180	THR	2.7
2	H	5	THR	2.7
3	K	414	ILE	2.7
2	B	211	ARG	2.7
2	D	151	ASP	2.7
2	B	8	PRO	2.7
1	A	74	SER	2.7
2	D	27(A)	SER	2.7
2	F	60	ALA	2.7
1	E	182	VAL	2.7
2	F	126	THR	2.7
1	C	71	ARG	2.7
2	F	30	ASN	2.7
2	F	92	ASN	2.7
2	D	27(C)	ASP	2.7
1	C	145	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	77	GLN	2.7
2	D	25	ALA	2.7
1	C	11	LEU	2.7
2	H	4	LEU	2.7
2	D	31	SER	2.7
2	F	111	ALA	2.7
2	H	146	VAL	2.7
2	B	91	ASN	2.7
1	G	129	LYS	2.7
1	E	185	PRO	2.7
1	G	123	PRO	2.7
2	B	65	SER	2.7
2	B	168	SER	2.7
2	H	77	PRO	2.7
2	H	176	SER	2.7
1	G	100(A)	ALA	2.7
1	C	33	TYR	2.7
1	G	59	TYR	2.7
2	F	36	TYR	2.7
1	A	122	PHE	2.7
1	C	105	GLN	2.7
1	C	107	THR	2.7
2	F	125	LEU	2.7
2	D	213	GLU	2.7
2	H	89	GLN	2.7
1	A	203	SER	2.7
2	H	174	SER	2.7
3	L	414	ILE	2.7
1	G	114	ALA	2.7
3	K	417	ASN	2.7
2	F	27	GLU	2.7
2	H	187	GLU	2.7
1	E	73	THR	2.7
2	D	11	LEU	2.7
2	H	32	PHE	2.7
2	H	73	LEU	2.7
2	D	122	SER	2.6
2	D	168	SER	2.6
2	F	171	SER	2.6
2	F	93	GLU	2.6
2	H	123	GLU	2.6
1	E	136	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	192	GLN	2.6
2	F	62	PHE	2.6
2	H	102	THR	2.6
2	H	197	THR	2.6
2	D	38	GLN	2.6
2	H	19	ALA	2.6
2	B	18	ARG	2.6
1	A	85	GLU	2.6
2	B	97	THR	2.6
1	C	152	VAL	2.6
1	C	153	SER	2.6
1	G	7	SER	2.6
2	B	44	PRO	2.6
1	C	125	ALA	2.6
1	E	29	ILE	2.6
2	D	60	ALA	2.6
1	A	157	GLY	2.6
2	D	103	LYS	2.6
1	A	97	THR	2.6
1	G	191	THR	2.6
1	C	12	VAL	2.6
2	B	3	VAL	2.6
3	I	418	GLY	2.6
1	C	89	THR	2.6
1	C	131	THR	2.6
1	A	183	THR	2.6
1	E	151	THR	2.6
1	G	96	THR	2.6
2	B	166	GLN	2.6
2	H	97	THR	2.6
2	D	139	PHE	2.6
2	B	179	LEU	2.6
2	F	46	LEU	2.6
1	A	163	VAL	2.6
1	E	150	VAL	2.6
2	D	18	ARG	2.6
1	C	156	SER	2.6
1	A	110	THR	2.6
2	D	35	TRP	2.6
2	D	176	SER	2.6
2	B	178	THR	2.6
2	F	178	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	94	ARG	2.6
1	A	92	CYS	2.6
1	E	22	CYS	2.6
1	G	196	CYS	2.6
1	G	61	PRO	2.6
2	H	201	LEU	2.6
1	G	211	VAL	2.6
2	B	62	PHE	2.6
2	F	109	ALA	2.6
2	H	111	ALA	2.6
1	C	57	THR	2.5
1	C	70	THR	2.5
2	D	5	THR	2.5
1	A	119	PRO	2.5
1	E	20	LEU	2.5
1	C	182	VAL	2.5
1	A	100(B)	MET	2.5
1	E	140	CYS	2.5
2	B	58	VAL	2.5
2	B	27(C)	ASP	2.5
1	E	44	LYS	2.5
2	F	137	ASN	2.5
2	H	60	ALA	2.5
1	A	28	SER	2.5
1	A	29	ILE	2.5
1	E	37	ILE	2.5
1	E	177	SER	2.5
1	G	107	THR	2.5
2	B	21	ILE	2.5
2	F	97	THR	2.5
1	A	34	TRP	2.5
1	E	103	TRP	2.5
1	G	152	VAL	2.5
2	B	107	LYS	2.5
1	E	53	TYR	2.5
1	E	78	TYR	2.5
1	A	168	ALA	2.5
2	B	25	ALA	2.5
1	G	74	SER	2.5
1	E	110	THR	2.5
1	A	147	PRO	2.5
2	B	40	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	178	LEU	2.5
2	B	11	LEU	2.5
2	H	210	ASN	2.5
1	C	91	TYR	2.5
1	A	10	SER	2.5
1	E	186	SER	2.5
1	G	168	ALA	2.5
2	D	121	SER	2.5
2	F	165	GLU	2.5
2	H	27(A)	SER	2.5
2	D	169	LYS	2.5
1	A	116	THR	2.5
1	E	107	THR	2.5
1	G	87	THR	2.5
2	D	20	THR	2.5
1	G	100(B)	MET	2.5
1	A	12	VAL	2.5
2	H	161	GLU	2.5
2	D	89	GLN	2.5
2	D	107	LYS	2.5
2	D	192	TYR	2.5
2	F	186	TYR	2.5
1	C	18	LEU	2.5
1	E	210	LYS	2.5
2	H	125	LEU	2.5
1	G	3	GLN	2.5
2	F	199	GLN	2.5
2	H	199	GLN	2.5
2	B	122	SER	2.5
2	B	132	VAL	2.5
2	F	76	ASP	2.5
2	H	67	SER	2.5
1	A	59	TYR	2.5
2	B	197	THR	2.5
1	E	16	GLN	2.5
1	C	189	LEU	2.5
1	E	175	LEU	2.5
1	E	189	LEU	2.5
2	H	181	LEU	2.5
1	C	74	SER	2.4
1	C	172	SER	2.4
2	F	174	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	116	SER	2.4
2	D	132	VAL	2.4
2	D	211	ARG	2.4
2	H	172	THR	2.4
3	I	417	ASN	2.4
1	G	145	TYR	2.4
2	H	41	GLY	2.4
1	A	16	GLN	2.4
2	H	48	ILE	2.4
2	H	166	GLN	2.4
1	A	82	LEU	2.4
1	G	127	SER	2.4
1	A	211	VAL	2.4
2	D	53	ASN	2.4
3	J	415	ASN	2.4
1	G	83	THR	2.4
2	D	6	GLN	2.4
1	C	79	TYR	2.4
2	D	36	TYR	2.4
2	B	87	TYR	2.4
1	C	51	ILE	2.4
2	B	68	ARG	2.4
1	C	214	LYS	2.4
2	D	208	SER	2.4
1	E	124	LEU	2.4
2	D	73	LEU	2.4
1	E	192	GLN	2.4
1	G	41	PRO	2.4
2	D	163	VAL	2.4
2	F	8	PRO	2.4
2	H	98	PHE	2.4
1	A	151	THR	2.4
1	E	193	THR	2.4
1	G	103	TRP	2.4
2	F	45	LYS	2.4
2	F	21	ILE	2.4
2	F	168	SER	2.4
2	F	37	GLN	2.4
1	C	42	GLY	2.4
1	C	64	LYS	2.4
1	C	97	THR	2.4
2	D	178	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	151	ASP	2.4
1	C	47	TYR	2.4
1	G	177	SER	2.4
2	H	65	SER	2.4
1	A	212	GLU	2.4
1	C	27	ASP	2.4
1	G	13	LYS	2.4
1	G	117	LYS	2.4
2	H	198	HIS	2.4
2	H	120	PRO	2.4
1	E	70	THR	2.4
1	E	112	SER	2.4
2	D	22	SER	2.4
2	F	140	TYR	2.4
1	E	36	TRP	2.4
1	A	80	LEU	2.4
1	C	158	ALA	2.4
2	D	12	ALA	2.4
2	H	95	PRO	2.4
1	G	73	THR	2.4
1	G	2	VAL	2.4
2	H	196	VAL	2.4
1	C	23	SER	2.4
1	C	28	SER	2.4
1	E	156	SER	2.4
1	G	43	ASN	2.4
1	A	37	ILE	2.3
1	C	194	TYR	2.3
1	A	47	TYR	2.3
2	D	195	GLU	2.3
2	F	50	LEU	2.3
2	F	204	PRO	2.3
1	C	73	THR	2.3
2	D	164	THR	2.3
1	A	204	ASN	2.3
1	G	166	PHE	2.3
2	D	78	VAL	2.3
2	F	7	SER	2.3
2	F	27(D)	SER	2.3
1	G	72	ASP	2.3
2	B	70	ASP	2.3
2	H	170	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	202	PRO	2.3
1	G	99	TYR	2.3
2	D	28	TYR	2.3
1	E	18	LEU	2.3
1	G	151	THR	2.3
2	B	137	ASN	2.3
1	A	128	SER	2.3
2	H	182	SER	2.3
2	F	150	VAL	2.3
1	E	148	GLU	2.3
1	A	104	GLY	2.3
2	B	45	LYS	2.3
1	A	69	ILE	2.3
2	B	204	PRO	2.3
1	C	60	ASN	2.3
1	E	176	TYR	2.3
1	E	197	ASN	2.3
1	E	31	SER	2.3
1	G	85	GLU	2.3
1	G	173	SER	2.3
1	C	34	TRP	2.3
2	F	161	GLU	2.3
1	A	150	VAL	2.3
1	A	184	VAL	2.3
1	E	164	HIS	2.3
2	H	124	GLN	2.3
1	G	60	ASN	2.3
1	C	6	GLU	2.3
2	F	170	ASP	2.3
1	C	59	TYR	2.3
1	C	100	TYR	2.3
1	C	102	TYR	2.3
1	G	161	SER	2.3
2	D	10	SER	2.3
2	F	176	SER	2.3
2	D	148	TRP	2.3
2	B	29	GLY	2.3
1	E	181	VAL	2.3
2	F	196	VAL	2.3
2	H	13	VAL	2.3
3	L	421	HIS	2.3
1	G	71	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	152	ASN	2.3
2	H	8	PRO	2.3
2	H	30	ASN	2.3
1	C	44	LYS	2.3
1	A	56	SER	2.3
1	A	87	THR	2.3
2	D	50	LEU	2.3
2	D	127	SER	2.3
2	F	52	SER	2.3
2	F	72	THR	2.3
2	F	177	SER	2.3
2	H	122	SER	2.3
1	C	58	TYR	2.3
1	E	50	TYR	2.3
1	E	196	CYS	2.3
1	G	200	HIS	2.3
2	D	196	VAL	2.3
1	C	155	ASN	2.3
2	B	152	ASN	2.3
2	B	167	ASP	2.3
1	A	9	PRO	2.3
1	C	171	GLN	2.3
1	C	180	SER	2.3
2	D	83	ALA	2.3
2	F	56	SER	2.3
2	H	85	THR	2.2
2	B	55	GLU	2.2
2	H	96	TRP	2.2
1	A	23	SER	2.2
1	A	120	SER	2.2
1	G	69	ILE	2.2
2	D	51	ALA	2.2
2	F	142	ARG	2.2
2	H	112	ALA	2.2
1	G	82	LEU	2.2
1	C	86	ASP	2.2
1	A	197	ASN	2.2
1	G	150	VAL	2.2
1	G	169	VAL	2.2
2	B	42	GLN	2.2
1	C	146	PHE	2.2
1	A	156	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	120	SER	2.2
2	D	56	SER	2.2
2	B	27(A)	SER	2.2
2	F	22	SER	2.2
1	C	93	ALA	2.2
1	A	39	LYS	2.2
1	E	206	LYS	2.2
1	C	205	THR	2.2
1	A	170	LEU	2.2
2	B	135	LEU	2.2
2	F	89	GLN	2.2
1	G	163	VAL	2.2
1	A	130	SER	2.2
1	E	23	SER	2.2
1	G	55	GLY	2.2
1	G	36	TRP	2.2
1	A	43	ASN	2.2
1	G	29	ILE	2.2
2	D	158	ASN	2.2
2	F	6	GLN	2.2
2	B	61	ARG	2.2
1	E	58	TYR	2.2
2	D	119	PRO	2.2
2	F	10	SER	2.2
1	C	135	THR	2.2
1	E	168	ALA	2.2
2	D	9	ALA	2.2
2	F	147	GLN	2.2
2	F	24	ARG	2.2
1	A	7	SER	2.2
1	E	173	SER	2.2
1	E	188	SER	2.2
2	H	52	SER	2.2
1	E	121	VAL	2.2
2	D	13	VAL	2.2
1	C	166	PHE	2.2
2	F	90	GLN	2.2
1	A	158	ALA	2.2
2	H	188	LYS	2.2
2	F	175	LEU	2.2
1	A	215	SER	2.2
2	F	116	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	82	ASP	2.2
2	D	80	ALA	2.1
2	F	19	ALA	2.1
2	F	187	GLU	2.1
2	D	48	ILE	2.1
2	D	88	CYS	2.1
2	H	155	GLN	2.1
1	E	60	ASN	2.1
1	G	91	TYR	2.1
2	B	189	HIS	2.1
2	F	205	VAL	2.1
1	C	151	THR	2.1
1	G	137	ALA	2.1
2	F	12	ALA	2.1
2	H	83	ALA	2.1
2	H	139	PHE	2.1
2	D	167	ASP	2.1
3	J	414	ILE	2.1
1	C	68	SER	2.1
1	E	63	LEU	2.1
1	G	112	SER	2.1
2	D	14	SER	2.1
1	E	118	GLY	2.1
1	G	190	GLY	2.1
3	J	417	ASN	2.1
1	C	165	THR	2.1
1	A	100	TYR	2.1
1	E	100	TYR	2.1
1	G	207	VAL	2.1
2	B	173	TYR	2.1
1	G	146	PHE	2.1
1	A	112	SER	2.1
1	E	76	ASN	2.1
1	E	215	SER	2.1
2	D	79	GLU	2.1
3	K	419	SER	2.1
1	A	44	LYS	2.1
2	D	194	CYS	2.1
2	H	39	LYS	2.1
1	A	208	ASP	2.1
2	F	172	THR	2.1
2	F	197	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	114	THR	2.1
1	A	24	VAL	2.1
1	A	176	TYR	2.1
2	B	196	VAL	2.1
1	E	55	GLY	2.1
2	F	122	SER	2.1
2	F	212	GLY	2.1
2	H	168	SER	2.1
1	G	214	LYS	2.1
1	A	27	ASP	2.1
2	H	90	GLN	2.1
1	A	107	THR	2.1
1	G	17	THR	2.1
1	G	22	CYS	2.1
2	F	23	CYS	2.1
2	B	51	ALA	2.1
2	B	53	ASN	2.1
2	F	130	ALA	2.1
2	F	120	PRO	2.1
2	B	50	LEU	2.1
2	H	154	LEU	2.1
1	A	209	LYS	2.1
1	E	165	THR	2.1
1	E	183	THR	2.1
1	G	25	THR	2.1
2	B	164	THR	2.1
2	F	210	ASN	2.1
1	C	177	SER	2.1
1	E	19	SER	2.1
2	H	115	VAL	2.1
2	H	132	VAL	2.1
1	G	167	PRO	2.1
2	B	95	PRO	2.1
1	C	148	GLU	2.0
1	C	45	LEU	2.0
1	E	51	ILE	2.0
2	B	73	LEU	2.0
2	F	104	LEU	2.0
1	C	188	SER	2.0
1	A	8	GLY	2.0
1	A	108	SER	2.0
1	A	213	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	163	VAL	2.0
2	B	183	LYS	2.0
2	H	104	LEU	2.0
2	B	33	MET	2.0
1	E	133	GLY	2.0
3	K	416	THR	2.0
1	C	137	ALA	2.0
2	D	52	SER	2.0
2	D	182	SER	2.0
1	E	202	PRO	2.0
2	F	103	LYS	2.0
1	G	154	TRP	2.0
1	G	204	ASN	2.0
2	F	173	TYR	2.0
1	G	95	ILE	2.0
2	H	99	GLY	2.0
1	G	206	LYS	2.0
2	B	72	THR	2.0
2	H	103	LYS	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.