Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 07:32 am GMT

PDB ID	:	1NAK
Title	:	IGG1 FAB FRAGMENT (83.1) COMPLEX WITH 16-RESIDUE PEPTIDE (RESIDUES 304-321 OF HIV-1 GP120 (MN ISOLATE))
Authors	:	Stanfield, R.L.; Ghiara, J.B.; Saphire, E.O.; Profy, A.T.; Wilson, I.A.
Deposited on	:	2002-11-27
Resolution	:	2.57 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

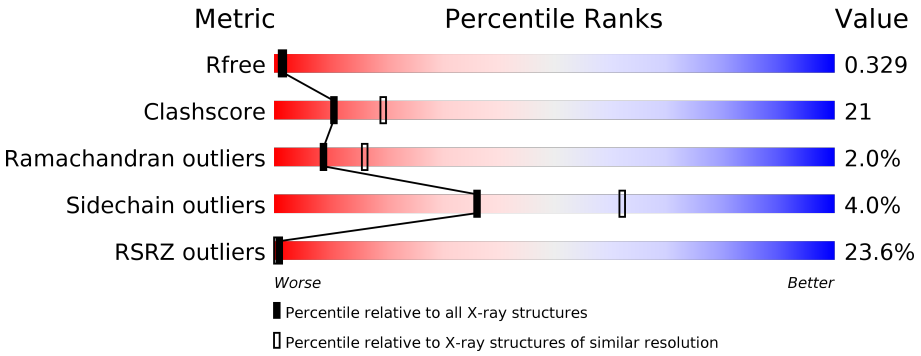
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.57 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}	100719	2899 (2.60-2.56)
Clashscore	112137	3268 (2.60-2.56)
Ramachandran outliers	110173	3218 (2.60-2.56)
Sidechain outliers	110143	3218 (2.60-2.56)
RSRZ outliers	101464	2907 (2.60-2.56)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	L	219	20% 60% 36%
1	M	219	30% 58% 36% 5%
2	H	214	16% 64% 33%
2	I	214	23% 63% 35%
3	P	16	38% 31% 19% 13% 38%
3	Q	16	31% 44% 19% 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6877 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 Fab 83.1 - light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1683	1053	286	338	6			
1	M	217	Total	C	N	O	S	0	0	0
			1683	1053	286	338	6			

- Molecule 2 is a protein called Fab 83.1 - heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	40	0	0
			1625	1030	263	326	6			
2	I	214	Total	C	N	O	S	40	0	0
			1625	1030	263	326	6			

- Molecule 3 is a protein called Peptide MP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			77	48	19	10			
3	Q	10	Total	C	N	O	0	0	0
			77	48	19	10			

- Molecule 4 is water.

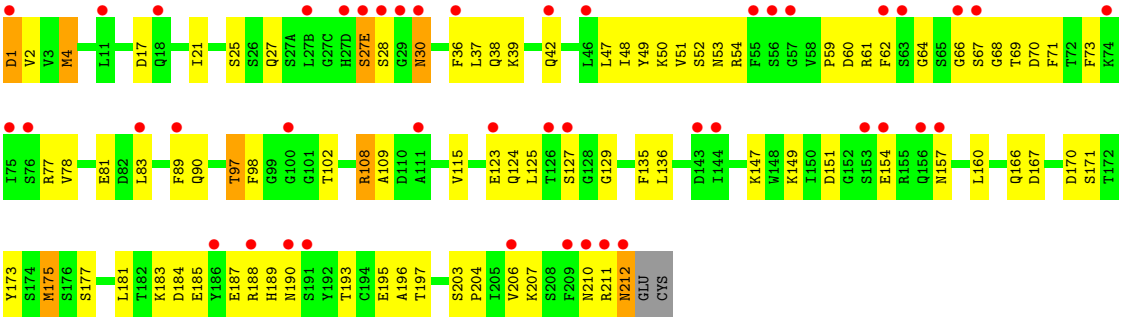
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	22	Total	O	0	0
			22	22		
4	I	19	Total	O	0	0
			19	19		
4	L	32	Total	O	0	0
			32	32		
4	M	34	Total	O	0	0
			34	34		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

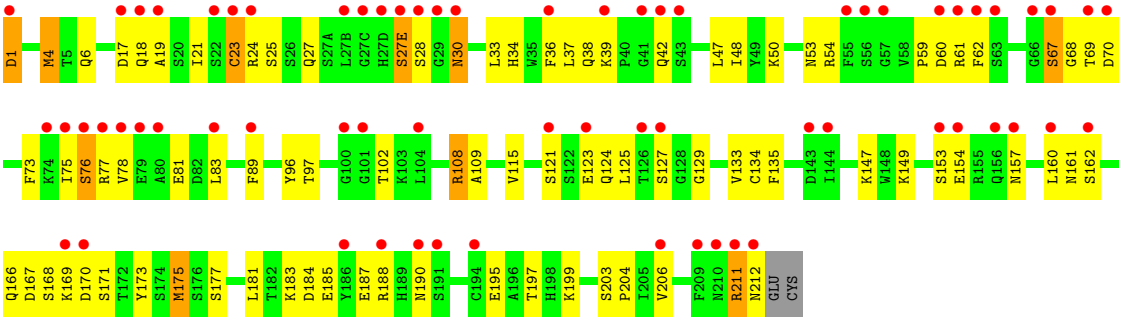
• Molecule 1: Fab 83.1 - light chain

Chain L:



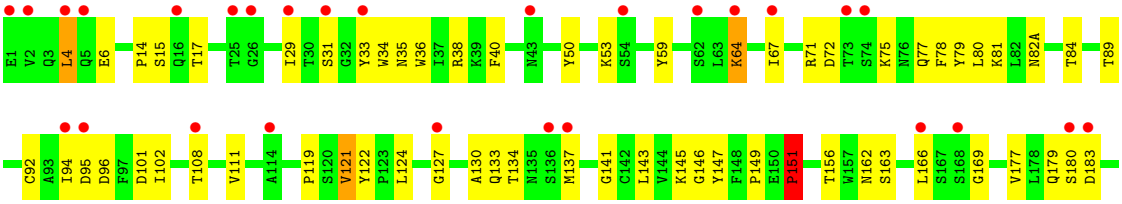
• Molecule 1: Fab 83.1 - light chain

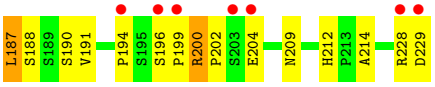
Chain M:



• Molecule 2: Fab 83.1 - heavy chain

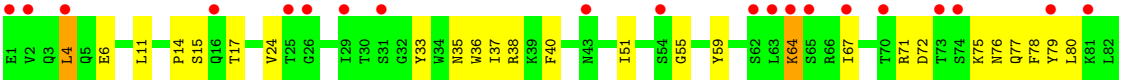
Chain H:

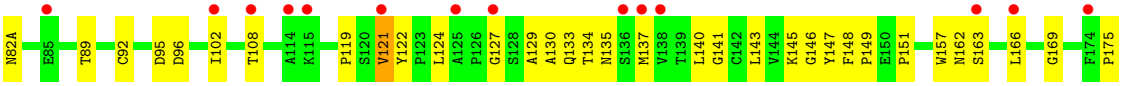


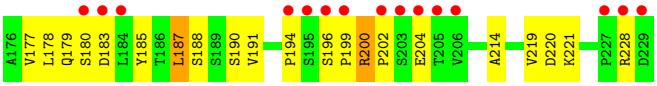


• Molecule 2: Fab 83.1 - heavy chain

Chain I:

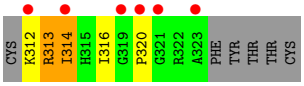






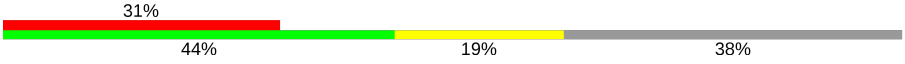
• Molecule 3: Peptide MP1

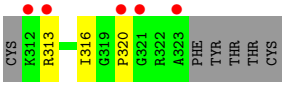
Chain P:



• Molecule 3: Peptide MP1

Chain Q:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.51Å 122.60Å 69.46Å 90.00° 108.54° 90.00°	Depositor
Resolution (Å)	48.08 – 2.57 48.08 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.08-2.57) 96.9 (48.08-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.288 , 0.326 0.290 , 0.329	Depositor DCC
R_{free} test set	1469 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6877	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 30.65 % 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 1.2623e-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

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	L	0.36	0/1724	0.64	0/2338
1	M	0.36	0/1724	0.64	0/2338
2	H	0.38	0/1668	0.78	3/2282 (0.1%)
2	I	0.37	0/1668	0.78	4/2282 (0.2%)
3	P	0.82	0/78	1.66	2/102 (2.0%)
3	Q	0.64	0/78	1.39	1/102 (1.0%)
All	All	0.38	0/6940	0.74	10/9444 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	313	ARG	N-CA-C	10.92	140.49	111.00
2	I	133	GLN	N-CA-C	9.81	137.48	111.00
2	H	133	GLN	N-CA-C	9.56	136.82	111.00
2	I	130	ALA	N-CA-C	-8.59	87.82	111.00
2	H	130	ALA	N-CA-C	-8.43	88.25	111.00
2	H	133	GLN	CA-C-N	-6.00	104.00	117.20
2	I	133	GLN	CA-C-N	-5.80	104.44	117.20
3	P	312	LYS	N-CA-C	5.50	125.86	111.00
2	I	133	GLN	C-N-CA	5.07	134.38	121.70
3	Q	313	ARG	N-CA-C	-5.00	97.49	111.00

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	L	1683	0	1612	68	0
1	M	1683	0	1612	74	0
2	H	1625	0	1594	74	0
2	I	1625	0	1594	66	0
3	P	77	0	85	7	0
3	Q	77	0	85	4	0
4	H	22	0	0	0	0
4	I	19	0	0	0	0
4	L	32	0	0	1	0
4	M	34	0	0	2	0
All	All	6877	0	6582	271	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (271) 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)
2:I:200:ARG:HG3	2:I:200:ARG:HH11	1.21	1.02
1:M:21:ILE:HD12	1:M:102:THR:HG21	1.46	0.95
1:L:50:LYS:HB2	1:L:53:ASN:HD22	1.34	0.93
2:H:200:ARG:HH11	2:H:200:ARG:CG	1.83	0.90
1:M:50:LYS:HB2	1:M:53:ASN:HD22	1.32	0.89
2:I:200:ARG:CG	2:I:200:ARG:HH11	1.86	0.88
1:L:4:MET:HE1	1:L:25:SER:HB3	1.56	0.88
1:M:190:ASN:HD21	1:M:212:ASN:ND2	1.73	0.87
1:M:4:MET:HE1	1:M:25:SER:HB3	1.57	0.86
1:L:21:ILE:HD12	1:L:102:THR:HG21	1.56	0.86
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.56	0.85
2:H:64:LYS:HA	2:H:67:ILE:HG22	1.59	0.85
2:H:127:GLY:HA2	2:H:228:ARG:HD2	1.58	0.84
1:M:54:ARG:CZ	1:M:60:ASP:HA	2.06	0.84
1:L:54:ARG:CZ	1:L:60:ASP:HA	2.06	0.84
2:I:64:LYS:HA	2:I:67:ILE:HG22	1.58	0.83
2:I:127:GLY:HA2	2:I:228:ARG:HD2	1.62	0.81
1:M:195:GLU:HG2	1:M:206:VAL:HG22	1.62	0.80
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.46	0.80
2:H:200:ARG:HG3	2:H:200:ARG:HH11	1.47	0.80
1:L:160:LEU:HD22	2:H:177:VAL:HG11	1.64	0.80
1:L:183:LYS:HE2	1:L:187:GLU:OE2	1.81	0.80
1:M:183:LYS:HE2	1:M:187:GLU:OE2	1.83	0.79
1:M:54:ARG:NH1	1:M:60:ASP:HA	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:14:PRO:O	2:I:15:SER:HB3	1.83	0.78
2:H:59:TYR:HB2	2:H:64:LYS:HB3	1.67	0.76
2:H:194:PRO:HB2	2:H:199:PRO:CD	2.16	0.76
2:H:95:ASP:OD1	3:P:320:PRO:HD2	1.85	0.75
1:M:190:ASN:ND2	1:M:212:ASN:ND2	2.35	0.74
2:I:137:MET:HE2	2:I:194:PRO:HA	1.70	0.74
1:M:190:ASN:HD21	1:M:212:ASN:HD21	1.34	0.72
2:I:59:TYR:HB2	2:I:64:LYS:HB3	1.72	0.72
1:M:61:ARG:HG2	1:M:77:ARG:NH2	2.05	0.71
1:M:160:LEU:HD22	2:I:177:VAL:HG11	1.73	0.71
2:H:14:PRO:O	2:H:15:SER:HB3	1.90	0.70
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.33	0.69
1:L:54:ARG:NH1	1:L:60:ASP:HA	2.07	0.69
2:H:29:ILE:HD11	2:H:78:PHE:HB3	1.75	0.69
1:M:4:MET:CE	1:M:25:SER:HB3	2.21	0.69
2:H:72:ASP:OD2	2:H:75:LYS:HE2	1.94	0.68
2:H:29:ILE:CD1	2:H:78:PHE:HB3	2.23	0.68
2:I:200:ARG:HD2	2:I:202:PRO:HA	1.75	0.68
3:P:314:ILE:HD11	3:P:316:ILE:HD13	1.77	0.67
1:M:211:ARG:HG2	1:M:211:ARG:HH11	1.58	0.67
2:I:72:ASP:OD2	2:I:75:LYS:HE2	1.95	0.67
2:H:200:ARG:HG2	2:H:200:ARG:HH11	1.59	0.66
1:M:181:LEU:HD22	1:M:185:GLU:OE1	1.95	0.66
1:L:39:LYS:HE2	1:L:81:GLU:O	1.95	0.65
2:I:75:LYS:HE3	2:I:79:TYR:OH	1.97	0.65
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.79	0.65
2:H:124:LEU:HB2	2:H:141:GLY:C	2.17	0.65
2:I:194:PRO:HB2	2:I:199:PRO:CD	2.26	0.65
1:M:39:LYS:HE2	1:M:81:GLU:O	1.96	0.64
2:I:6:GLU:HG3	2:I:92:CYS:SG	2.38	0.63
2:I:194:PRO:HD2	2:I:199:PRO:HG3	1.80	0.63
2:H:4:LEU:HD11	2:H:94:ILE:HG23	1.80	0.63
2:H:4:LEU:HD12	2:H:102:ILE:HG22	1.80	0.62
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.34	0.62
1:M:166:GLN:HG3	1:M:173:TYR:CZ	2.34	0.62
2:H:162:ASN:HD22	2:H:166:LEU:HG	1.64	0.62
2:H:194:PRO:HD2	2:H:199:PRO:HG3	1.81	0.61
2:I:200:ARG:HG3	2:I:200:ARG:NH1	2.00	0.61
1:M:135:PHE:CE2	2:I:190:SER:HB3	2.36	0.60
1:M:61:ARG:HG2	1:M:77:ARG:HH21	1.67	0.60
2:I:35:ASN:O	2:I:92:CYS:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:314:ILE:HG13	3:P:316:ILE:HG23	1.82	0.60
1:L:27(E):SER:O	1:L:28:SER:HB3	2.01	0.60
2:H:200:ARG:HG3	2:H:200:ARG:NH1	2.16	0.60
2:H:75:LYS:HE3	2:H:79:TYR:OH	2.02	0.60
2:H:121:VAL:HA	2:H:143:LEU:O	2.02	0.60
2:H:94:ILE:HD11	2:H:101:ASP:CG	2.22	0.60
1:L:124:GLN:HG2	1:L:129:GLY:O	2.01	0.60
1:L:37:LEU:HD23	1:L:38:GLN:N	2.17	0.59
1:L:184:ASP:O	1:L:188:ARG:HG3	2.02	0.59
1:L:211:ARG:NH1	1:L:211:ARG:HG2	2.11	0.59
2:I:96:ASP:O	3:Q:316:ILE:HD11	2.02	0.59
2:H:194:PRO:C	2:H:199:PRO:HD2	2.24	0.59
1:L:135:PHE:CE2	2:H:190:SER:HB3	2.38	0.59
1:M:83:LEU:HD21	1:M:166:GLN:O	2.02	0.59
1:M:197:THR:HG22	1:M:204:PRO:HG3	1.85	0.58
2:H:194:PRO:O	2:H:199:PRO:HD2	2.04	0.58
1:M:27(E):SER:O	1:M:28:SER:HB3	2.04	0.58
1:L:17:ASP:O	1:L:78:VAL:HG23	2.04	0.58
1:L:61:ARG:HG2	1:L:77:ARG:NH2	2.19	0.57
2:I:119:PRO:HB3	2:I:147:TYR:HB3	1.86	0.57
1:M:147:LYS:HG2	1:M:154:GLU:OE1	2.05	0.57
2:H:31:SER:O	2:H:53:LYS:HE3	2.05	0.57
2:H:71:ARG:HA	2:H:78:PHE:HA	1.87	0.57
2:I:95:ASP:OD1	3:Q:320:PRO:HD2	2.05	0.56
2:H:124:LEU:HB2	2:H:141:GLY:CA	2.35	0.56
2:H:35:ASN:OD1	3:P:320:PRO:HG3	2.06	0.56
1:L:167:ASP:HB3	1:L:170:ASP:OD2	2.05	0.56
2:I:124:LEU:HB2	2:I:141:GLY:C	2.26	0.56
1:M:37:LEU:HD23	1:M:38:GLN:N	2.20	0.56
1:M:108:ARG:HD3	1:M:109:ALA:O	2.05	0.56
2:H:96:ASP:O	3:P:316:ILE:HD11	2.06	0.56
2:H:33:TYR:HB2	2:H:95:ASP:OD1	2.05	0.55
2:I:4:LEU:HD12	2:I:102:ILE:HG22	1.88	0.55
1:L:108:ARG:HD3	1:L:109:ALA:O	2.07	0.55
1:M:167:ASP:HB3	1:M:170:ASP:OD2	2.05	0.55
2:H:35:ASN:O	2:H:92:CYS:HA	2.07	0.55
1:M:190:ASN:ND2	1:M:212:ASN:HD21	1.98	0.55
1:L:27(E):SER:O	1:L:28:SER:CB	2.54	0.54
1:M:39:LYS:HB2	1:M:42:GLN:NE2	2.22	0.54
1:M:21:ILE:CD1	1:M:102:THR:HG21	2.30	0.54
2:H:145:LYS:HG2	2:H:146:GLY:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:LYS:CB	1:L:53:ASN:HD22	2.14	0.54
1:M:184:ASP:O	1:M:188:ARG:HG3	2.07	0.54
1:M:27:GLN:HG3	4:M:215:HOH:O	2.07	0.54
1:M:4:MET:HE2	1:M:4:MET:HA	1.89	0.54
1:L:83:LEU:HD21	1:L:166:GLN:O	2.07	0.54
1:L:50:LYS:O	1:L:51:VAL:HB	2.07	0.54
2:H:50:TYR:CD2	3:P:320:PRO:HB3	2.43	0.54
1:L:190:ASN:HD21	1:L:212:ASN:ND2	2.06	0.54
1:L:123:GLU:HG3	2:H:122:TYR:HD1	1.73	0.54
2:I:64:LYS:HA	2:I:67:ILE:CG2	2.35	0.54
1:L:212:ASN:OD1	1:L:212:ASN:C	2.45	0.54
1:L:61:ARG:HD2	1:L:77:ARG:HB2	1.89	0.53
2:H:149:PRO:HD2	2:H:214:ALA:CB	2.38	0.53
1:L:49:TYR:O	1:L:53:ASN:HB2	2.08	0.53
1:M:17:ASP:O	1:M:78:VAL:HG23	2.08	0.53
2:H:229:ASP:OXT	2:H:229:ASP:OD1	2.26	0.53
2:H:64:LYS:HA	2:H:67:ILE:CG2	2.36	0.53
2:H:194:PRO:HB2	2:H:199:PRO:HD3	1.90	0.53
1:M:187:GLU:O	1:M:211:ARG:NH2	2.42	0.53
2:I:196:SER:N	2:I:199:PRO:HD2	2.25	0.52
1:M:123:GLU:HG3	2:I:122:TYR:HD1	1.75	0.52
2:I:149:PRO:HD2	2:I:214:ALA:CB	2.40	0.52
1:L:181:LEU:HD22	1:L:185:GLU:OE1	2.10	0.52
1:L:39:LYS:HB2	1:L:42:GLN:NE2	2.26	0.51
2:H:200:ARG:CG	2:H:200:ARG:NH1	2.53	0.51
1:M:96:TYR:OH	3:Q:320:PRO:HA	2.10	0.51
2:H:194:PRO:HB2	2:H:199:PRO:HD2	1.90	0.51
2:H:199:PRO:O	2:H:204:GLU:HB2	2.10	0.51
2:I:71:ARG:HA	2:I:78:PHE:HA	1.93	0.51
1:M:4:MET:CE	1:M:4:MET:HA	2.41	0.51
2:H:196:SER:N	2:H:199:PRO:HD2	2.26	0.51
2:I:17:THR:HG22	2:I:82(A):ASN:HA	1.92	0.50
1:L:175:MET:CE	1:L:177:SER:HB2	2.42	0.50
1:L:4:MET:CE	1:L:25:SER:HB3	2.34	0.50
2:I:199:PRO:O	2:I:204:GLU:HB2	2.11	0.50
2:I:162:ASN:HD22	2:I:166:LEU:HG	1.77	0.50
1:M:211:ARG:HG2	1:M:211:ARG:NH1	2.26	0.50
2:I:11:LEU:HD22	2:I:149:PRO:HD3	1.92	0.49
2:I:194:PRO:HB2	2:I:199:PRO:HD2	1.94	0.49
1:L:30:ASN:O	1:L:30:ASN:ND2	2.44	0.49
2:I:59:TYR:CB	2:I:64:LYS:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:67:SER:O	1:M:69:THR:N	2.45	0.49
1:L:197:THR:HG22	1:L:204:PRO:HG3	1.95	0.49
1:M:175:MET:CE	1:M:177:SER:HB2	2.42	0.49
2:H:137:MET:HE1	2:H:194:PRO:HG3	1.95	0.49
2:I:124:LEU:HB2	2:I:141:GLY:CA	2.43	0.49
2:H:80:LEU:HD23	2:H:80:LEU:C	2.34	0.48
1:L:59:PRO:HG2	1:L:62:PHE:CD1	2.49	0.48
1:M:50:LYS:CB	1:M:53:ASN:HD22	2.16	0.48
2:H:187:LEU:HD23	2:H:187:LEU:C	2.33	0.48
2:I:121:VAL:HA	2:I:143:LEU:O	2.13	0.48
1:M:1:ASP:HB3	4:M:226:HOH:O	2.13	0.48
1:L:125:LEU:HD22	1:L:183:LYS:HG3	1.96	0.48
1:L:190:ASN:ND2	1:L:212:ASN:ND2	2.62	0.48
1:M:59:PRO:HG2	1:M:62:PHE:CD1	2.48	0.48
1:M:81:GLU:OE2	1:M:168:SER:O	2.32	0.48
1:M:125:LEU:HD22	1:M:183:LYS:HG3	1.96	0.48
1:L:27:GLN:HG3	4:L:219:HOH:O	2.14	0.48
1:L:175:MET:HE2	1:L:177:SER:HB2	1.96	0.48
1:M:27(E):SER:O	1:M:28:SER:CB	2.61	0.48
1:M:33:LEU:HD13	1:M:33:LEU:C	2.35	0.47
2:H:67:ILE:HD11	2:H:80:LEU:HG	1.96	0.47
1:M:36:PHE:CE1	1:M:89:PHE:HD2	2.32	0.47
1:L:66:GLY:HA3	1:L:71:PHE:CD1	2.50	0.47
1:M:124:GLN:HG2	1:M:129:GLY:O	2.13	0.47
1:M:167:ASP:OD2	1:M:169:LYS:HB2	2.14	0.47
2:H:94:ILE:HD13	2:H:102:ILE:HD12	1.96	0.47
1:L:48:ILE:HD12	1:L:73:PHE:CE1	2.49	0.47
2:I:187:LEU:C	2:I:187:LEU:HD23	2.35	0.47
1:M:133:VAL:HG12	1:M:134:CYS:N	2.28	0.47
2:I:194:PRO:C	2:I:199:PRO:HD2	2.34	0.47
1:L:67:SER:O	1:L:69:THR:N	2.47	0.47
1:M:149:LYS:HA	1:M:153:SER:O	2.14	0.47
2:H:89:THR:OG1	2:H:108:THR:HG22	2.14	0.47
1:M:123:GLU:OE2	2:I:221:LYS:HE2	2.15	0.47
1:M:48:ILE:HD12	1:M:73:PHE:CE1	2.50	0.47
2:H:163:SER:HB3	2:I:163:SER:HB3	1.96	0.46
1:M:123:GLU:HG3	2:I:122:TYR:CD1	2.50	0.46
2:I:145:LYS:HG2	2:I:146:GLY:N	2.31	0.46
2:I:194:PRO:O	2:I:199:PRO:HD2	2.15	0.46
2:I:200:ARG:CG	2:I:200:ARG:NH1	2.55	0.46
1:M:115:VAL:HA	1:M:135:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:35:ASN:OD1	3:Q:320:PRO:HG3	2.16	0.46
2:I:179:GLN:O	2:I:180:SER:HB2	2.16	0.46
1:L:211:ARG:O	1:L:212:ASN:CB	2.63	0.46
1:M:161:ASN:HB3	1:M:175:MET:HE3	1.98	0.46
2:H:34:TRP:CZ3	2:H:94:ILE:HG22	2.51	0.45
1:L:54:ARG:HD2	1:L:59:PRO:O	2.16	0.45
2:H:169:GLY:O	2:H:191:VAL:HA	2.16	0.45
1:L:136:LEU:HD21	1:L:196:ALA:HB2	1.98	0.45
2:I:67:ILE:HD11	2:I:80:LEU:HG	1.99	0.45
1:M:19:ALA:HB3	1:M:75:ILE:HB	1.99	0.45
1:M:30:ASN:ND2	1:M:30:ASN:O	2.49	0.45
2:I:178:LEU:HB2	2:I:185:TYR:CE1	2.52	0.45
1:M:175:MET:HE2	1:M:177:SER:HB2	1.97	0.45
1:M:37:LEU:HD12	1:M:47:LEU:HD11	1.98	0.45
1:M:36:PHE:HE1	1:M:89:PHE:HD2	1.63	0.45
2:I:36:TRP:C	2:I:37:ILE:HG13	2.37	0.44
2:I:80:LEU:C	2:I:80:LEU:HD23	2.36	0.44
2:H:17:THR:HG22	2:H:82(A):ASN:HA	1.98	0.44
2:I:140:LEU:HD11	2:I:200:ARG:HG2	2.00	0.44
2:I:169:GLY:O	2:I:191:VAL:HA	2.18	0.44
2:H:59:TYR:CB	2:H:64:LYS:HB3	2.40	0.44
2:I:33:TYR:HB2	2:I:95:ASP:OD1	2.16	0.44
2:I:187:LEU:HD23	2:I:188:SER:N	2.33	0.44
1:L:115:VAL:HA	1:L:135:PHE:O	2.18	0.44
1:L:4:MET:HB2	1:L:98:PHE:O	2.17	0.44
1:L:52:SER:HB3	1:L:64:GLY:O	2.18	0.44
2:I:51:ILE:HD11	2:I:55:GLY:HA2	2.00	0.44
1:M:6:GLN:HG3	1:M:23:CYS:SG	2.57	0.44
1:M:36:PHE:CE1	1:M:89:PHE:CD2	3.05	0.44
2:I:219:VAL:HG12	2:I:220:ASP:N	2.33	0.44
1:L:1:ASP:O	1:L:2:VAL:C	2.53	0.44
2:I:75:LYS:O	2:I:77:GLN:HG3	2.18	0.43
1:L:149:LYS:HB2	1:L:193:THR:HB	1.98	0.43
1:L:167:ASP:O	1:L:171:SER:HA	2.18	0.43
2:H:38:ARG:HD3	2:H:40:PHE:CZ	2.53	0.43
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.18	0.43
1:M:61:ARG:HD2	1:M:77:ARG:HB2	1.99	0.43
2:H:94:ILE:HD11	2:H:101:ASP:OD1	2.17	0.43
2:I:14:PRO:O	2:I:15:SER:CB	2.56	0.43
1:L:36:PHE:CE1	1:L:89:PHE:HD2	2.37	0.43
1:M:203:SER:HA	1:M:204:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:THR:HA	2:H:111:VAL:HB	2.01	0.42
2:H:151:PRO:O	2:H:212:HIS:HD2	2.02	0.42
2:I:157:TRP:HB2	2:I:166:LEU:HB2	2.00	0.42
1:L:37:LEU:HD12	1:L:47:LEU:HD11	2.01	0.42
1:M:33:LEU:HD13	1:M:34:HIS:N	2.34	0.42
2:H:4:LEU:CD1	2:H:102:ILE:HG22	2.48	0.42
2:H:179:GLN:O	2:H:180:SER:HB2	2.19	0.42
2:I:24:VAL:O	2:I:76:ASN:ND2	2.52	0.42
1:M:50:LYS:HB2	1:M:53:ASN:ND2	2.14	0.42
1:M:24:ARG:HA	1:M:69:THR:O	2.18	0.42
2:H:81:LYS:HE2	2:H:82(A):ASN:HD21	1.84	0.42
1:L:187:GLU:O	1:L:211:ARG:NH2	2.53	0.42
1:L:4:MET:CE	1:L:4:MET:HA	2.50	0.42
1:L:206:VAL:O	1:L:207:LYS:HD2	2.20	0.42
1:L:203:SER:HA	1:L:204:PRO:HD3	1.85	0.42
2:H:14:PRO:O	2:H:15:SER:CB	2.61	0.42
1:L:135:PHE:CZ	2:H:190:SER:HB3	2.54	0.42
2:I:38:ARG:HD3	2:I:40:PHE:CZ	2.55	0.42
2:H:156:THR:OG1	2:H:209:ASN:HB2	2.20	0.41
2:H:95:ASP:O	3:P:320:PRO:HD3	2.20	0.41
2:I:72:ASP:CG	2:I:75:LYS:HE2	2.41	0.41
1:L:36:PHE:CE1	1:L:89:PHE:CD2	3.09	0.41
1:L:36:PHE:HE1	1:L:89:PHE:HD2	1.68	0.41
1:M:121:SER:OG	2:I:122:TYR:HB3	2.20	0.41
1:M:167:ASP:O	1:M:171:SER:HA	2.19	0.41
2:H:89:THR:HA	2:H:108:THR:HA	2.02	0.41
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.56	0.41
1:L:125:LEU:C	1:L:127:SER:H	2.22	0.41
2:H:75:LYS:O	2:H:77:GLN:HG3	2.20	0.41
1:M:162:SER:OG	2:I:175:PRO:HD2	2.20	0.41
2:I:148:PHE:CE1	2:I:149:PRO:HB3	2.56	0.41
2:H:200:ARG:HD2	2:H:202:PRO:HA	2.02	0.41
2:H:187:LEU:HD23	2:H:188:SER:N	2.36	0.41
1:M:125:LEU:C	1:M:127:SER:H	2.24	0.41
2:I:89:THR:HA	2:I:108:THR:HA	2.03	0.40
1:L:62:PHE:N	1:L:62:PHE:CD1	2.88	0.40
2:H:127:GLY:CA	2:H:228:ARG:HD2	2.40	0.40
1:L:147:LYS:HG2	1:L:154:GLU:OE1	2.21	0.40
2:I:36:TRP:CE2	2:I:80:LEU:HB2	2.56	0.40
1:L:123:GLU:HG3	2:H:122:TYR:CD1	2.55	0.40
1:L:90:GLN:NE2	1:L:97:THR:OG1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:18:GLN:HA	1:M:76:SER:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	215/219 (98%)	200 (93%)	13 (6%)	2 (1%)	20 39
1	M	215/219 (98%)	200 (93%)	9 (4%)	6 (3%)	6 9
2	H	212/214 (99%)	192 (91%)	17 (8%)	3 (1%)	13 25
2	I	212/214 (99%)	192 (91%)	15 (7%)	5 (2%)	7 12
3	P	8/16 (50%)	4 (50%)	3 (38%)	1 (12%)	0 0
3	Q	8/16 (50%)	5 (62%)	3 (38%)	0	100 100
All	All	870/898 (97%)	793 (91%)	60 (7%)	17 (2%)	9 16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	134	THR
3	P	313	ARG
1	M	68	GLY
2	I	134	THR
2	I	135	ASN
1	L	68	GLY
2	H	64	LYS
1	M	199	LYS
1	L	27(E)	SER
1	M	27(E)	SER
2	I	64	LYS

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Mol	Chain	Res	Type
2	I	129	ALA
1	M	76	SER
1	M	211	ARG
1	M	67	SER
2	H	151	PRO
2	I	151	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	194/196 (99%)	184 (95%)	10 (5%)	27 50
1	M	194/196 (99%)	185 (95%)	9 (5%)	31 56
2	H	190/190 (100%)	184 (97%)	6 (3%)	44 70
2	I	190/190 (100%)	185 (97%)	5 (3%)	51 76
3	P	7/13 (54%)	6 (86%)	1 (14%)	4 6
3	Q	7/13 (54%)	7 (100%)	0	100 100
All	All	782/798 (98%)	751 (96%)	31 (4%)	36 62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	4	MET
1	L	30	ASN
1	L	70	ASP
1	L	97	THR
1	L	108	ARG
1	L	157	ASN
1	L	175	MET
1	L	210	ASN
1	L	212	ASN
2	H	4	LEU
2	H	121	VAL

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Mol	Chain	Res	Type
2	H	151	PRO
2	H	183	ASP
2	H	187	LEU
2	H	200	ARG
3	P	314	ILE
1	M	1	ASP
1	M	4	MET
1	M	23	CYS
1	M	30	ASN
1	M	70	ASP
1	M	97	THR
1	M	108	ARG
1	M	157	ASN
1	M	175	MET
2	I	4	LEU
2	I	121	VAL
2	I	183	ASP
2	I	187	LEU
2	I	200	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	27(D)	HIS
1	L	30	ASN
1	L	42	GLN
1	L	53	ASN
1	L	137	ASN
1	L	157	ASN
1	L	190	ASN
2	H	16	GLN
2	H	82(A)	ASN
2	H	162	ASN
2	H	172	HIS
1	M	18	GLN
1	M	30	ASN
1	M	42	GLN
1	M	53	ASN
1	M	190	ASN
2	I	16	GLN
2	I	82(A)	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 carbohydrates 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	L	217/219 (99%)	1.33	44 (20%)	1	0	11, 28, 44, 51	2 (0%)
1	M	217/219 (99%)	1.51	66 (30%)	0	0	9, 29, 45, 61	2 (0%)
2	H	208/214 (97%)	1.30	35 (16%)	2	1	12, 26, 43, 59	4 (1%)
2	I	208/214 (97%)	1.45	49 (23%)	1	0	13, 29, 47, 67	4 (1%)
3	P	10/16 (62%)	2.42	6 (60%)	0	0	33, 41, 45, 52	0
3	Q	10/16 (62%)	2.21	5 (50%)	0	0	26, 36, 44, 50	0
All	All	870/898 (96%)	1.42	205 (23%)	1	0	9, 28, 45, 67	12 (1%)

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	GLU	6.9
2	I	4	LEU	6.4
2	I	199	PRO	6.3
2	H	108	THR	6.2
2	H	229	ASP	6.1
2	I	229	ASP	6.0
2	I	1	GLU	5.9
2	I	64	LYS	5.9
2	I	108	THR	5.8
2	I	31	SER	5.7
1	M	143	ASP	5.5
2	H	64	LYS	5.3
2	H	228	ARG	5.3
1	M	66	GLY	5.3
2	I	196	SER	5.1
1	M	76	SER	5.0
1	M	190	ASN	5.0
1	L	62	PHE	4.9
1	L	18	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	M	210	ASN	4.8
1	L	210	ASN	4.6
2	I	67	ILE	4.6
2	H	62	SER	4.6
1	L	42	GLN	4.5
2	H	31	SER	4.5
1	L	57	GLY	4.5
1	M	23	CYS	4.4
1	M	62	PHE	4.4
2	I	228	ARG	4.3
2	I	62	SER	4.2
1	L	190	ASN	4.2
2	H	180	SER	4.1
1	M	89	PHE	4.0
1	M	27(E)	SER	3.9
1	L	28	SER	3.9
2	H	136	SER	3.8
1	L	156	GLN	3.8
3	P	320	PRO	3.8
1	L	212	ASN	3.7
2	H	199	PRO	3.7
2	H	67	ILE	3.5
2	H	4	LEU	3.5
2	H	204	GLU	3.5
1	M	169	LYS	3.5
2	I	194	PRO	3.5
1	L	30	ASN	3.5
1	M	30	ASN	3.4
1	M	42	GLN	3.4
1	M	28	SER	3.4
1	M	186	TYR	3.4
2	H	73	THR	3.3
2	H	2	VAL	3.3
1	M	55	PHE	3.3
2	H	114	ALA	3.3
1	M	56	SER	3.3
2	H	54	SER	3.3
1	M	75	ILE	3.2
1	M	212	ASN	3.2
1	M	43	SER	3.2
1	L	89	PHE	3.2
2	H	127	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	191	SER	3.2
1	M	1	ASP	3.1
1	M	144	ILE	3.1
1	L	29	GLY	3.1
1	M	19	ALA	3.1
2	I	205	THR	3.1
3	Q	312	LYS	3.1
1	L	63	SER	3.1
2	I	138	VAL	3.1
1	M	157	ASN	3.1
1	M	27(D)	HIS	3.1
2	H	183	ASP	3.0
2	I	81	LYS	3.0
1	M	79	GLU	3.0
2	I	85	GLU	3.0
1	M	17	ASP	3.0
1	L	74	LYS	3.0
3	P	323	ALA	3.0
3	P	321	GLY	3.0
1	L	27(D)	HIS	2.9
1	M	36	PHE	2.9
1	M	104	LEU	2.9
1	L	56	SER	2.9
2	H	203	SER	2.9
2	I	25	THR	2.9
3	Q	321	GLY	2.9
2	H	137	MET	2.9
1	M	18	GLN	2.8
3	Q	323	ALA	2.8
2	I	26	GLY	2.8
1	M	206	VAL	2.8
1	L	55	PHE	2.8
1	M	57	GLY	2.8
1	M	22	SER	2.8
2	H	29	ILE	2.8
1	M	69	THR	2.8
2	I	202	PRO	2.7
1	M	211	ARG	2.7
2	H	196	SER	2.7
3	P	312	LYS	2.7
2	I	43	ASN	2.7
2	H	168	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	61	ARG	2.6
2	H	74	SER	2.6
1	M	80	ALA	2.6
2	H	16	GLN	2.6
1	M	170	ASP	2.6
1	M	29	GLY	2.6
2	I	74	SER	2.6
1	M	194	CYS	2.6
2	I	114	ALA	2.6
1	M	123	GLU	2.6
1	L	100	GLY	2.6
1	M	63	SER	2.6
2	I	163	SER	2.6
2	I	79	TYR	2.6
1	L	111	ALA	2.5
2	H	194	PRO	2.5
2	I	115	LYS	2.5
3	P	319	GLY	2.5
1	M	100	GLY	2.5
2	H	166	LEU	2.5
2	I	63	LEU	2.5
1	M	27(C)	GLY	2.5
2	I	29	ILE	2.5
1	L	67	SER	2.5
1	L	1	ASP	2.5
1	L	143	ASP	2.5
2	I	2	VAL	2.5
1	L	11	LEU	2.4
2	I	166	LEU	2.4
3	Q	313	ARG	2.4
1	L	75	ILE	2.4
1	L	211	ARG	2.4
1	M	101	GLY	2.4
1	M	126	THR	2.4
1	L	76	SER	2.4
1	L	154	GLU	2.4
2	H	94	ILE	2.4
1	L	36	PHE	2.4
2	I	70	THR	2.4
1	L	27(E)	SER	2.4
1	L	46	LEU	2.4
1	L	144	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	102	ILE	2.3
2	I	203	SER	2.3
2	I	184	LEU	2.3
2	I	137	MET	2.3
1	L	127	SER	2.3
2	I	65	SER	2.3
1	L	157	ASN	2.3
1	M	156	GLN	2.3
2	I	206	VAL	2.3
1	M	67	SER	2.3
1	M	191	SER	2.3
2	H	33	TYR	2.3
2	I	180	SER	2.3
1	M	24	ARG	2.3
1	M	27(B)	LEU	2.3
3	Q	320	PRO	2.3
1	L	209	PHE	2.3
2	I	136	SER	2.3
2	I	204	GLU	2.3
1	M	74	LYS	2.3
1	L	27(B)	LEU	2.3
1	L	153	SER	2.2
2	I	183	ASP	2.2
1	M	162	SER	2.2
1	L	126	THR	2.2
1	M	39	LYS	2.2
1	M	154	GLU	2.2
2	I	54	SER	2.2
2	I	125	ALA	2.2
2	I	16	GLN	2.2
1	L	66	GLY	2.2
1	M	41	GLY	2.2
1	L	186	TYR	2.2
1	M	127	SER	2.2
1	M	153	SER	2.2
2	I	73	THR	2.2
1	L	188	ARG	2.2
1	M	121	SER	2.2
1	M	160	LEU	2.2
1	M	70	ASP	2.1
2	I	127	GLY	2.1
1	L	123	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	209	PHE	2.1
2	H	25	THR	2.1
2	I	195	SER	2.1
1	M	77	ARG	2.1
2	H	43	ASN	2.1
2	H	26	GLY	2.1
2	I	174	PHE	2.1
1	M	60	ASP	2.1
2	H	95	ASP	2.1
2	H	5	GLN	2.1
1	L	206	VAL	2.0
1	L	83	LEU	2.0
1	M	83	LEU	2.0
1	M	188	ARG	2.0
2	I	227	PRO	2.0
1	M	78	VAL	2.0
3	P	314	ILE	2.0
2	I	121	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 carbohydrates 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.