



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:56 PM EDT

PDB ID : 1NAK / pdb_00001nak
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

<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:

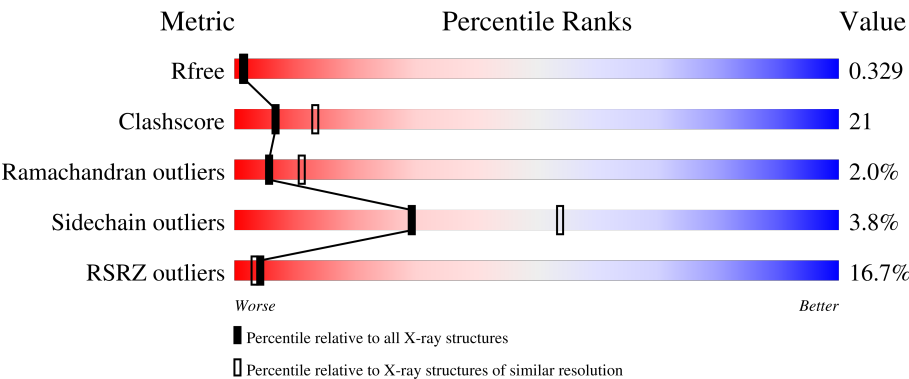
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 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 $\leq 5\%$. 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	17% 57% 38% 5% .
1	M	219	17% 56% 39% 5% .
2	H	214	14% 61% 35% . .
2	I	214	12% 61% 36% .
3	P	16	62% 19% 31% 12% 38%

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Mol	Chain	Length	Quality of chain
3	Q	16	44% 31% 31% 38%

2 Entry composition

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			

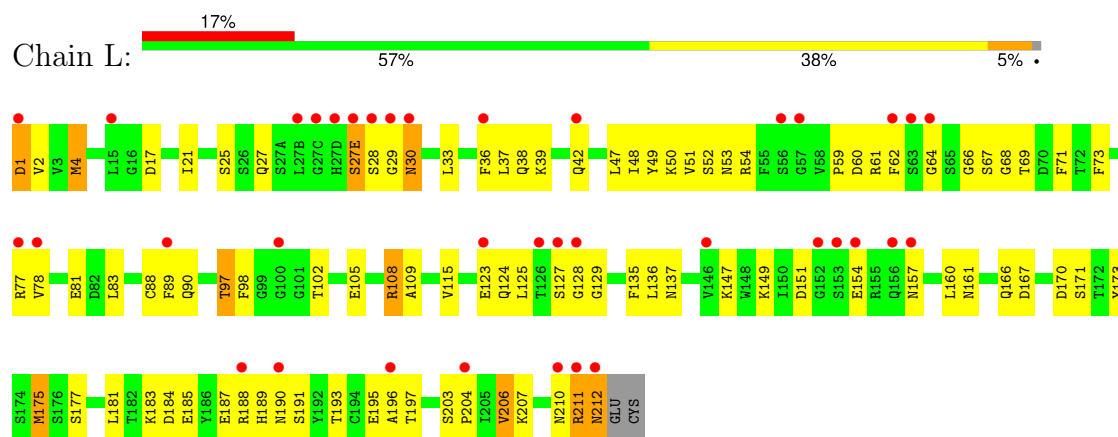
- Molecule 4 is water.

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

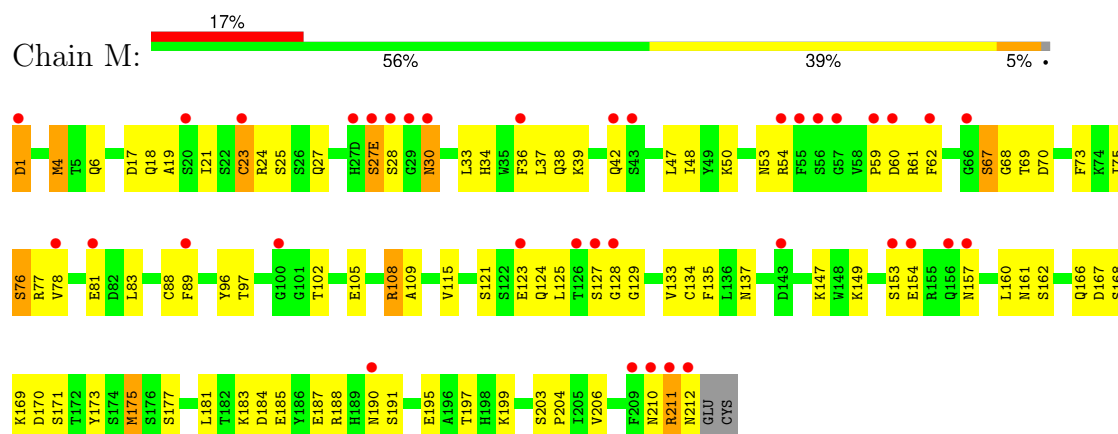
3 Residue-property plots [i](#)

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.

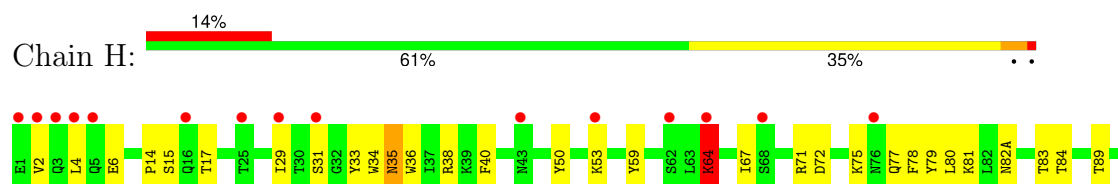
- Molecule 1: Fab 83.1 - light chain

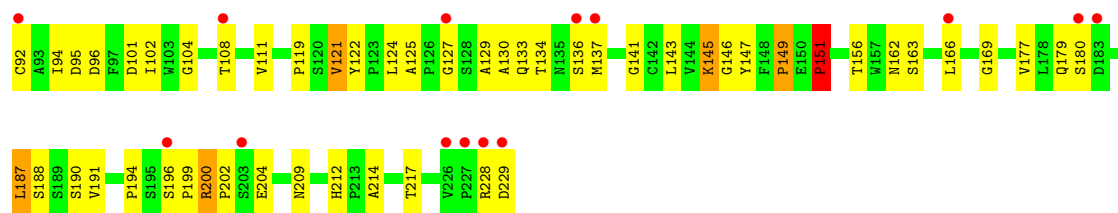


- Molecule 1: Fab 83.1 - light chain

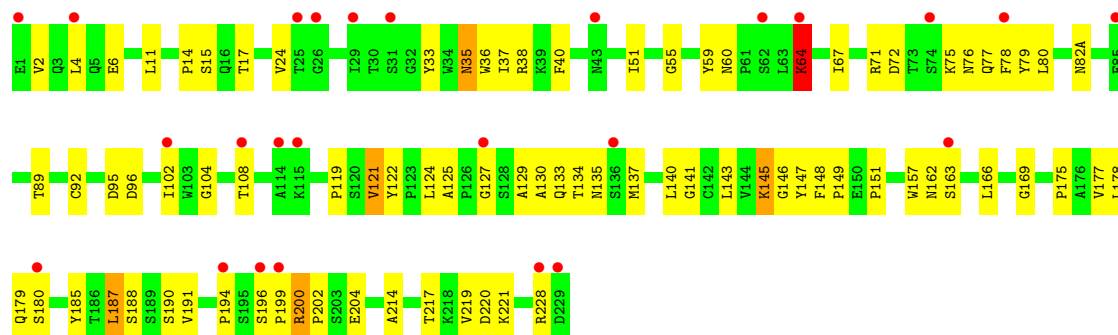


- Molecule 2: Fab 83.1 - heavy chain

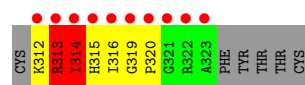




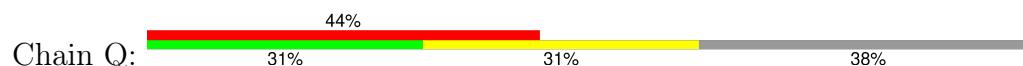
● Molecule 2: Fab 83.1 - heavy chain



● Molecule 3: Peptide MP1



● Molecule 3: Peptide MP1



4 Data and refinement statistics

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) 97.1 (48.08-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ 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%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.44	0/1724	0.92	8/2338 (0.3%)
1	M	0.42	0/1724	0.90	5/2338 (0.2%)
2	H	0.49	0/1668	1.16	15/2282 (0.7%)
2	I	0.47	0/1668	1.16	15/2282 (0.7%)
3	P	0.93	0/78	2.25	5/102 (4.9%)
3	Q	0.78	0/78	2.11	5/102 (4.9%)
All	All	0.47	0/6940	1.08	53/9444 (0.6%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	133	GLN	N-CA-C	23.04	137.48	108.45
2	H	133	GLN	N-CA-C	19.83	136.82	108.86
3	P	313	ARG	N-CA-C	13.94	140.49	110.80
2	H	130	ALA	N-CA-C	-12.93	88.25	109.07
2	I	130	ALA	N-CA-C	-12.51	87.82	108.34
2	H	2	VAL	N-CA-C	11.10	124.30	109.21
2	I	2	VAL	N-CA-C	10.62	123.65	109.21
3	Q	313	ARG	N-CA-C	-7.69	97.49	109.25
3	Q	312	LYS	CA-C-N	-7.67	110.60	121.72
3	Q	312	LYS	C-N-CA	-7.67	110.60	121.72
2	H	130	ALA	CA-C-N	-7.54	110.40	122.53
2	H	130	ALA	C-N-CA	-7.54	110.40	122.53
3	Q	319	GLY	N-CA-C	7.16	120.59	112.00
3	P	314	ILE	N-CA-C	7.12	122.00	112.04
2	I	125	ALA	CA-C-N	6.92	126.88	119.76
2	I	125	ALA	C-N-CA	6.92	126.88	119.76
2	I	130	ALA	CA-C-N	-6.87	110.39	122.20
2	I	130	ALA	C-N-CA	-6.87	110.39	122.20
2	I	133	GLN	CA-C-N	6.72	134.38	121.54
2	I	133	GLN	C-N-CA	6.72	134.38	121.54
2	H	145	LYS	N-CA-C	6.60	120.28	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	136	SER	N-CA-C	-6.54	104.91	114.39
2	H	133	GLN	CA-C-N	6.47	133.90	121.54
2	H	133	GLN	C-N-CA	6.47	133.90	121.54
2	I	145	LYS	N-CA-C	6.34	119.97	110.14
3	P	319	GLY	N-CA-C	6.24	119.78	112.23
3	P	315	HIS	N-CA-C	6.16	118.11	110.91
2	I	60	ASN	N-CA-C	-5.99	102.71	109.60
1	M	30	ASN	N-CA-C	-5.96	105.75	114.39
1	M	88	CYS	N-CA-C	-5.95	101.20	110.42
1	L	30	ASN	N-CA-C	-5.94	105.78	114.39
1	L	137	ASN	N-CA-C	5.92	119.48	109.76
2	I	35	ASN	N-CA-C	5.84	118.99	109.59
2	I	64	LYS	N-CA-C	5.60	122.74	110.80
2	H	64	LYS	N-CA-C	5.60	122.73	110.80
3	Q	313	ARG	CB-CA-C	5.58	119.45	110.29
2	H	125	ALA	CA-C-N	5.56	125.32	119.76
2	H	125	ALA	C-N-CA	5.56	125.32	119.76
1	M	128	GLY	N-CA-C	5.51	122.42	115.42
2	H	104	GLY	N-CA-C	-5.48	104.22	112.60
1	M	191	SER	N-CA-C	5.47	117.65	108.96
2	H	129	ALA	N-CA-C	5.43	122.37	110.80
1	L	88	CYS	N-CA-C	-5.43	102.01	110.42
1	L	29	GLY	N-CA-C	-5.41	106.39	115.80
1	L	128	GLY	N-CA-C	5.34	122.20	115.42
3	P	312	LYS	N-CA-C	5.31	125.86	111.00
2	I	104	GLY	N-CA-C	-5.30	104.52	112.89
2	I	133	GLN	CA-C-O	5.25	126.55	121.14
1	M	137	ASN	N-CA-C	5.23	118.59	110.17
1	L	211	ARG	N-CA-C	-5.06	102.80	110.24
1	L	206	VAL	N-CA-C	5.06	115.19	108.11
1	L	191	SER	N-CA-C	5.05	117.84	109.46
2	H	35	ASN	N-CA-C	5.02	117.94	109.95

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	L	1683	0	1612	73	0
1	M	1683	0	1612	76	0
2	H	1625	0	1594	78	0
2	I	1625	0	1594	67	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	283	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 (283) 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:CG	2:H:200:ARG:HH11	1.83	0.90
1:M:50:LYS:HB2	1:M:53:ASN:HD22	1.32	0.89
2:I:200:ARG:HH11	2:I:200:ARG:CG	1.86	0.88
1:M:190:ASN:HD21	1:M:212:ASN:ND2	1.73	0.87
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:4:MET:HE1	1:M:25:SER:HB3	1.63	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:HH11	2:H:200:ARG:HG3	1.47	0.80
1:L:4:MET:HE1	1:L:25:SER:HB3	1.64	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
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:124:LEU:HB2	2:H:141:GLY:C	2.17	0.69
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:HH11	2:H:200:ARG:HG2	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
1:L:4:MET:HE2	1:L:4:MET:HA	1.78	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:I:194:PRO:HB2	2:I:199:PRO:CD	2.26	0.65
2:H:94:ILE:HD11	2:H:101:ASP:CG	2.22	0.64
1:M:39:LYS:HE2	1:M:81:GLU:O	1.96	0.64
2:H:194:PRO:C	2:H:199:PRO:HD2	2.24	0.63
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
1:M:4:MET:HA	1:M:4:MET:HE2	1.82	0.61
1:M:161:ASN:HB3	1:M:175:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:200:ARG:HG3	2:I:200:ARG:NH1	2.00	0.61
2:I:124:LEU:HB2	2:I:141:GLY:C	2.26	0.60
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
3:P:314:ILE:HG13	3:P:316:ILE:HG23	1.82	0.60
2:I:35:ASN:O	2:I:92:CYS:HA	2.02	0.60
1:L:27(E):SER:O	1:L:28:SER:HB3	2.01	0.60
2:H:75:LYS:HE3	2:H:79:TYR:OH	2.02	0.60
2:H:200:ARG:HG3	2:H:200:ARG:NH1	2.16	0.60
2:H:121:VAL:HA	2:H:143:LEU:O	2.02	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:HG2	1:L:211:ARG:NH1	2.11	0.59
2:I:96:ASP:O	3:Q:316:ILE:HD11	2.02	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
1:L:212:ASN:C	1:L:212:ASN:OD1	2.45	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:175:MET:HE1	1:L:177:SER:HB2	1.86	0.57
1:L:61:ARG:HG2	1:L:77:ARG:NH2	2.19	0.57
2:I:137:MET:HE1	2:I:194:PRO:HG3	1.86	0.57
1:L:4:MET:CE	1:L:25:SER:HB3	2.34	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:H:137:MET:HE2	2:H:194:PRO:HA	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:167:ASP:HB3	1:M:170:ASP:OD2	2.05	0.55
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.89	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
1:L:50:LYS:CB	1:L:53:ASN:HD22	2.14	0.54
2:H:145:LYS:HG2	2:H:146:GLY:N	2.21	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: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:61:ARG:HD2	1:L:77:ARG:HB2	1.89	0.53
1:L:49:TYR:O	1:L:53:ASN:HB2	2.08	0.53
2:H:149:PRO:HD2	2:H:214:ALA:CB	2.38	0.53
1:M:17:ASP:O	1:M:78:VAL:HG23	2.08	0.53
2:H:187:LEU:HD23	2:H:187:LEU:C	2.33	0.53
2:H:64:LYS:HA	2:H:67:ILE:CG2	2.36	0.53
2:H:229:ASP:OXT	2:H:229:ASP:OD1	2.26	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:H:80:LEU:C	2:H:80:LEU:HD23	2.34	0.52
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
1:M:33:LEU:HD13	1:M:33:LEU:C	2.35	0.52
2:I:149:PRO:HD2	2:I:214:ALA:CB	2.40	0.52
2:I:187:LEU:C	2:I:187:LEU:HD23	2.35	0.52
1:L:181:LEU:HD22	1:L:185:GLU:OE1	2.10	0.52
2:I:194:PRO:C	2:I:199:PRO:HD2	2.34	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
1:M:4:MET:CE	1:M:4:MET:HA	2.41	0.51
2:I:71:ARG:HA	2:I:78:PHE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:137:MET:HE2	2:I:194:PRO:HA	1.93	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
2:I:199:PRO:O	2:I:204:GLU:HB2	2.11	0.50
1:L:175:MET:CE	1:L:177:SER:HB2	2.42	0.50
1:M:211:ARG:HG2	1:M:211:ARG:NH1	2.26	0.50
2:I:36:TRP:C	2:I:37:ILE:HG13	2.37	0.50
2:I:162:ASN:HD22	2:I:166:LEU:HG	1.77	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:80:LEU:C	2:I:80:LEU:HD23	2.36	0.49
1:M:67:SER:O	1:M:69:THR:N	2.45	0.49
2:I:59:TYR:CB	2:I:64:LYS:HB3	2.42	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:I:124:LEU:HB2	2:I:141:GLY:CA	2.43	0.49
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
1:L:1:ASP:O	1:L:2:VAL:C	2.53	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:M:27(E):SER:O	1:M:28:SER:CB	2.61	0.48
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
1:L:48:ILE:HD12	1:L:73:PHE:CE1	2.49	0.47
2:H:94:ILE:HD13	2:H:102:ILE:HD12	1.96	0.47
1:L:67:SER:O	1:L:69:THR:N	2.47	0.47
2:H:137:MET:HE1	2:H:194:PRO:HG3	1.95	0.47
1:M:133:VAL:HG12	1:M:134:CYS:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:ILE:HD12	1:M:73:PHE:CE1	2.50	0.47
1:M:123:GLU:OE2	2:I:221:LYS:HE2	2.15	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:175:MET:HE1	1:M:177:SER:HB2	1.96	0.46
2:I:72:ASP:CG	2:I:75:LYS:HE2	2.41	0.46
1:M:115:VAL:HA	1:M:135:PHE:O	2.15	0.46
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:125:LEU:C	1:L:127:SER:H	2.22	0.46
1:L:211:ARG:O	1:L:212:ASN:CB	2.63	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
1:M:125:LEU:C	1:M:127:SER:H	2.24	0.45
1:L:136:LEU:HD21	1:L:196:ALA:HB2	1.98	0.45
2:H:169:GLY:O	2:H:191:VAL:HA	2.16	0.45
1:M:19:ALA:HB3	1:M:75:ILE:HB	1.99	0.45
1:M:30:ASN:O	1:M:30:ASN:ND2	2.49	0.45
2:I:67:ILE:HD11	2:I:80:LEU:HG	1.99	0.45
1:M:36:PHE:HE1	1:M:89:PHE:HD2	1.63	0.45
1:M:37:LEU:HD12	1:M:47:LEU:HD11	1.98	0.45
2:I:178:LEU:HB2	2:I:185:TYR:CE1	2.52	0.45
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
1:L:4:MET:HB2	1:L:98:PHE:O	2.17	0.44
1:L:115:VAL:HA	1:L:135:PHE:O	2.18	0.44
2:I:187:LEU:HD23	2:I:188:SER:N	2.33	0.44
1:L:52:SER:HB3	1:L:64:GLY:O	2.18	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:51:ILE:HD11	2:I:55:GLY:HA2	2.00	0.44
2:I:219:VAL:HG12	2:I:220:ASP:N	2.33	0.44
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:I:75:LYS:O	2:I:77:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:84:THR:HA	2:H:111:VAL:HB	2.01	0.42
1:L:37:LEU:HD12	1:L:47:LEU:HD11	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: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
1:M:24:ARG:HA	1:M:69:THR:O	2.18	0.42
1:M:50:LYS:HB2	1:M:53:ASN:ND2	2.14	0.42
2:I:24:VAL:O	2:I:76:ASN:ND2	2.52	0.42
1:L:187:GLU:O	1:L:211:ARG:NH2	2.53	0.42
2:H:81:LYS:HE2	2:H:82(A):ASN:HD21	1.84	0.42
1:M:37:LEU:HD23	1:M:37:LEU:C	2.44	0.42
2:H:83:THR:C	2:H:111:VAL:HG11	2.45	0.42
1:L:33:LEU:HD13	1:L:33:LEU:C	2.44	0.42
1:L:206:VAL:O	1:L:207:LYS:HD2	2.20	0.42
2:H:72:ASP:CG	2:H:75:LYS:HE2	2.45	0.42
1:L:203:SER:HA	1:L:204:PRO:HD3	1.85	0.42
1:L:135:PHE:CZ	2:H:190:SER:HB3	2.54	0.42
2:H:14:PRO:O	2:H:15:SER:CB	2.61	0.42
2:H:179:GLN:O	2:H:180:SER:HB2	2.19	0.42
2:I:38:ARG:HD3	2:I:40:PHE:CZ	2.55	0.42
2:H:95:ASP:O	3:P:320:PRO:HD3	2.20	0.41
2:H:156:THR:OG1	2:H:209:ASN:HB2	2.20	0.41
2:H:101:ASP:C	2:H:102:ILE:HG13	2.46	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:L:125:LEU:C	1:L:127:SER:N	2.79	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
1:M:210:ASN:O	1:M:211:ARG:C	2.64	0.41
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.56	0.41
2:H:89:THR:HA	2:H:108:THR:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:ARG:HD2	2:H:202:PRO:HA	2.02	0.41
2:I:148:PHE:CE1	2:I:149:PRO:HB3	2.56	0.41
1:L:161:ASN:CB	1:L:175:MET:HE3	2.51	0.41
2:H:187:LEU:HD23	2:H:188:SER:N	2.36	0.41
1:L:62:PHE:CD1	1:L:62:PHE:N	2.88	0.40
2:I:89:THR:HA	2:I:108:THR:HA	2.03	0.40
1:L:37:LEU:HD23	1:L:37:LEU:C	2.45	0.40
1:L:147:LYS:HG2	1:L:154:GLU:OE1	2.21	0.40
2:H:127:GLY:CA	2:H:228:ARG:HD2	2.40	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
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%)	14	29
1	M	215/219 (98%)	200 (93%)	9 (4%)	6 (3%)	4	6
2	H	212/214 (99%)	192 (91%)	17 (8%)	3 (1%)	9	18
2	I	212/214 (99%)	192 (91%)	15 (7%)	5 (2%)	4	8
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%)	6	11

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
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%)	185 (95%)	9 (5%)	24	47
1	M	194/196 (99%)	185 (95%)	9 (5%)	24	47
2	H	190/190 (100%)	184 (97%)	6 (3%)	34	59
2	I	190/190 (100%)	186 (98%)	4 (2%)	47	71
3	P	7/13 (54%)	5 (71%)	2 (29%)	0	0
3	Q	7/13 (54%)	7 (100%)	0	100	100
All	All	782/798 (98%)	752 (96%)	30 (4%)	29	54

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	4	MET

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Mol	Chain	Res	Type
1	L	97	THR
1	L	105	GLU
1	L	108	ARG
1	L	157	ASN
1	L	175	MET
1	L	210	ASN
1	L	212	ASN
2	H	121	VAL
2	H	149	PRO
2	H	151	PRO
2	H	187	LEU
2	H	200	ARG
2	H	217	THR
3	P	313	ARG
3	P	314	ILE
1	M	1	ASP
1	M	4	MET
1	M	23	CYS
1	M	70	ASP
1	M	97	THR
1	M	105	GLU
1	M	108	ARG
1	M	157	ASN
1	M	175	MET
2	I	121	VAL
2	I	187	LEU
2	I	200	ARG
2	I	217	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	42	GLN
1	L	53	ASN
1	L	93	HIS
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

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Mol	Chain	Res	Type
2	H	172	HIS
2	H	179	GLN
1	M	18	GLN
1	M	30	ASN
1	M	42	GLN
1	M	53	ASN
1	M	137	ASN
1	M	190	ASN
2	I	16	GLN
2	I	82(A)	ASN
2	I	162	ASN
2	I	172	HIS
2	I	179	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	L	217/219 (99%)	1.14	37 (17%) 4 3	6, 28, 44, 51	2 (0%)
1	M	217/219 (99%)	1.23	37 (17%) 4 3	5, 29, 45, 61	2 (0%)
2	H	208/214 (97%)	1.03	29 (13%) 6 5	7, 26, 43, 59	4 (1%)
2	I	208/214 (97%)	1.15	25 (12%) 9 7	9, 29, 47, 67	4 (1%)
3	P	10/16 (62%)	3.46	10 (100%) 0 0	33, 41, 45, 52	0
3	Q	10/16 (62%)	2.52	7 (70%) 0 0	26, 36, 44, 50	0
All	All	870/898 (96%)	1.18	145 (16%) 4 3	5, 28, 45, 67	12 (1%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	31	SER	9.6
2	H	31	SER	8.8
2	I	62	SER	8.5
2	H	62	SER	8.4
2	H	108	THR	6.9
2	I	108	THR	6.7
2	I	4	LEU	6.5
1	L	42	GLN	6.1
3	P	323	ALA	5.9
2	H	1	GLU	5.8
2	I	1	GLU	5.0
2	H	229	ASP	4.7
3	P	320	PRO	4.7
1	M	143	ASP	4.7
1	L	100	GLY	4.6
1	M	42	GLN	4.3
1	M	100	GLY	4.3
3	Q	323	ALA	4.3
2	I	136	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	28	SER	4.2
1	M	66	GLY	4.2
1	M	210	ASN	4.1
1	M	57	GLY	4.1
3	P	321	GLY	4.1
1	L	57	GLY	3.9
3	Q	321	GLY	3.8
1	M	23	CYS	3.7
1	M	212	ASN	3.7
2	H	180	SER	3.7
2	H	136	SER	3.6
3	P	312	LYS	3.6
1	M	190	ASN	3.6
2	H	2	VAL	3.6
2	I	199	PRO	3.5
1	L	30	ASN	3.5
2	H	29	ILE	3.5
2	H	4	LEU	3.4
2	I	64	LYS	3.4
3	P	319	GLY	3.3
1	L	153	SER	3.3
1	L	27(D)	HIS	3.3
1	L	123	GLU	3.3
1	M	89	PHE	3.3
1	L	27(E)	SER	3.2
1	L	190	ASN	3.2
2	I	229	ASP	3.1
1	M	27(D)	HIS	3.1
1	L	89	PHE	3.1
1	M	27(E)	SER	3.1
2	I	127	GLY	3.1
2	H	64	LYS	3.0
1	M	36	PHE	3.0
1	M	153	SER	3.0
2	I	29	ILE	3.0
1	M	157	ASN	3.0
1	L	63	SER	3.0
1	M	211	ARG	2.9
1	L	128	GLY	2.9
1	M	128	GLY	2.9
1	M	123	GLU	2.9
1	L	62	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	29	GLY	2.9
2	I	196	SER	2.9
1	M	29	GLY	2.9
1	M	56	SER	2.8
3	Q	312	LYS	2.8
3	P	313	ARG	2.8
1	L	27(C)	GLY	2.7
1	M	30	ASN	2.7
2	I	115	LYS	2.7
1	L	156	GLN	2.7
2	I	43	ASN	2.7
1	L	212	ASN	2.7
3	P	314	ILE	2.7
3	P	322	ARG	2.7
1	L	146	VAL	2.6
1	L	157	ASN	2.6
1	L	154	GLU	2.6
2	I	85	GLU	2.6
1	L	28	SER	2.6
1	M	1	ASP	2.6
2	I	180	SER	2.6
2	H	166	LEU	2.6
1	M	126	THR	2.6
3	Q	313	ARG	2.5
2	H	127	GLY	2.5
1	M	154	GLU	2.5
2	I	25	THR	2.5
2	H	3	GLN	2.5
2	I	114	ALA	2.5
1	M	127	SER	2.5
3	Q	314	ILE	2.4
2	H	228	ARG	2.4
2	I	228	ARG	2.4
1	L	1	ASP	2.4
1	M	55	PHE	2.4
3	Q	322	ARG	2.4
3	P	316	ILE	2.4
1	M	43	SER	2.4
2	H	203	SER	2.4
3	P	315	HIS	2.4
1	L	204	PRO	2.3
1	M	156	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	74	SER	2.3
1	L	211	ARG	2.3
2	H	68	SER	2.3
1	M	60	ASP	2.3
1	L	15	LEU	2.2
1	M	81	GLU	2.2
1	L	78	VAL	2.2
1	L	64	GLY	2.2
1	L	27(B)	LEU	2.2
1	L	127	SER	2.2
1	M	20	SER	2.2
1	M	59	PRO	2.2
2	I	194	PRO	2.2
1	L	196	ALA	2.2
2	H	137	MET	2.2
1	L	36	PHE	2.2
2	I	78	PHE	2.2
1	L	188	ARG	2.1
2	I	163	SER	2.1
2	H	43	ASN	2.1
2	I	26	GLY	2.1
1	L	56	SER	2.1
2	H	5	GLN	2.1
2	H	76	ASN	2.1
1	L	126	THR	2.1
1	M	54	ARG	2.1
2	I	102	ILE	2.1
2	H	227	PRO	2.1
1	M	62	PHE	2.1
2	H	183	ASP	2.1
2	H	196	SER	2.1
2	H	16	GLN	2.0
1	L	210	ASN	2.0
3	Q	319	GLY	2.0
2	H	92	CYS	2.0
1	L	77	ARG	2.0
1	M	78	VAL	2.0
1	M	209	PHE	2.0
2	H	226	VAL	2.0
1	L	152	GLY	2.0
2	H	53	LYS	2.0
2	H	25	THR	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 oligosaccharides 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.