



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:45 PM EDT

PDB ID : 5M2M
Title : Complex between human TNF alpha and Llama VHH3
Authors : Cambillau, C.; Spinelli, S.; Desmyter, A.; de Haard, H.
Deposited on : 2016-10-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

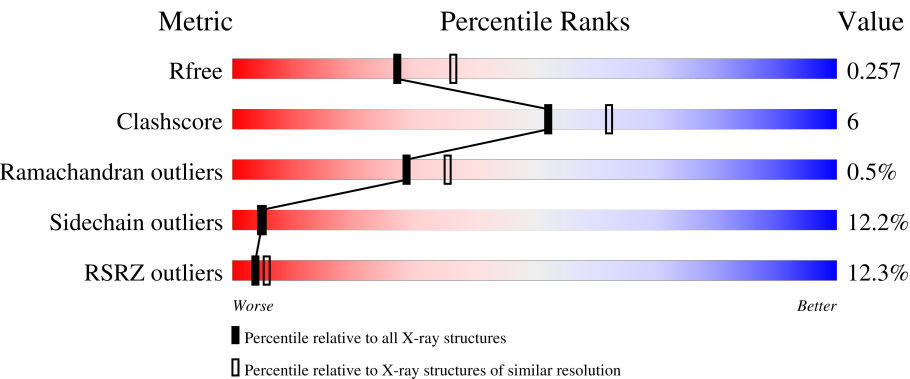
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	157	<div><div>8%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>73%18% . .</div></div>
1	B	157	<div><div>13%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>74%18% . .</div></div>
1	C	157	<div><div>11%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%18%5% .</div></div>
1	G	157	<div><div>17%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>71%20% . .</div></div>
1	I	157	<div><div>18%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>73%17%6% .</div></div>

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Mol	Chain	Length	Quality of chain
1	M	157	<div><div></div><div>20%</div><div>67%</div><div>20%</div><div>7%</div><div>6%</div></div>
2	D	129	<div><div></div><div>5%</div><div>84%</div><div>12%</div><div></div><div></div></div>
2	E	129	<div><div></div><div>2%</div><div>84%</div><div>12%</div><div></div><div></div></div>
2	F	129	<div><div></div><div>2%</div><div>84%</div><div>12%</div><div></div><div></div></div>
2	H	129	<div><div></div><div>12%</div><div>82%</div><div>16%</div><div></div><div></div></div>
2	J	129	<div><div></div><div>15%</div><div>84%</div><div>12%</div><div></div><div></div></div>
2	N	129	<div><div></div><div>16%</div><div>85%</div><div>11%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13516 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 Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1149	736	197	214	2			
1	B	151	Total	C	N	O	S	0	0	0
			1160	743	199	216	2			
1	C	150	Total	C	N	O	S	0	0	0
			1154	740	198	214	2			
1	G	150	Total	C	N	O	S	0	0	0
			1154	740	198	214	2			
1	I	150	Total	C	N	O	S	0	0	0
			1157	740	198	217	2			
1	M	148	Total	C	N	O	S	0	0	0
			1131	724	195	210	2			

- Molecule 2 is a protein called Llama nanobody VHH3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	127	Total	C	N	O	S	0	0	0
			984	612	173	196	3			
2	E	127	Total	C	N	O	S	0	0	0
			984	612	173	196	3			
2	F	127	Total	C	N	O	S	0	0	0
			984	612	173	196	3			
2	H	127	Total	C	N	O	S	0	0	0
			984	612	173	196	3			
2	J	127	Total	C	N	O	S	0	0	0
			984	612	173	196	3			
2	N	127	Total	C	N	O	S	0	0	0
			980	611	170	196	3			

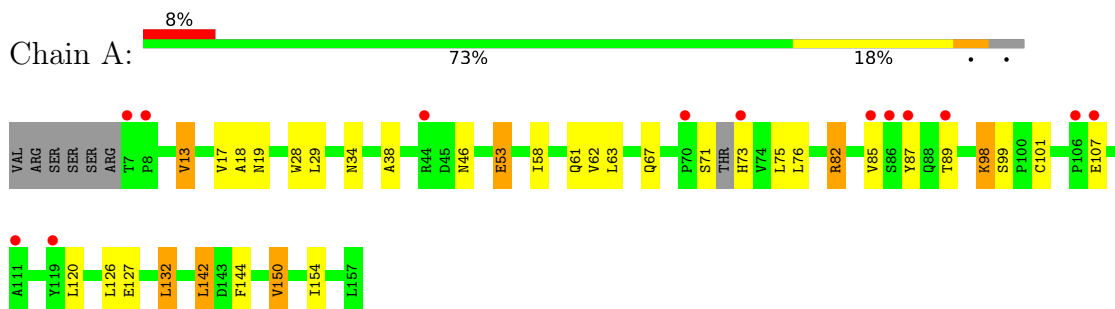
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total 92	O 92	0	0
3	B	93	Total 93	O 93	0	0
3	C	94	Total 94	O 94	0	0
3	D	78	Total 78	O 78	0	0
3	E	88	Total 88	O 88	0	0
3	F	86	Total 86	O 86	0	0
3	G	36	Total 36	O 36	0	0
3	H	23	Total 23	O 23	0	0
3	I	36	Total 36	O 36	0	0
3	J	31	Total 31	O 31	0	0
3	M	32	Total 32	O 32	0	0
3	N	22	Total 22	O 22	0	0

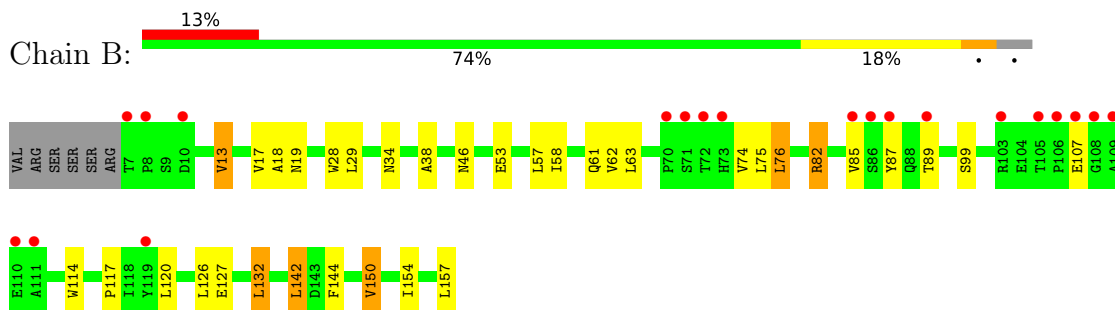
3 Residue-property plots [i](#)

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.

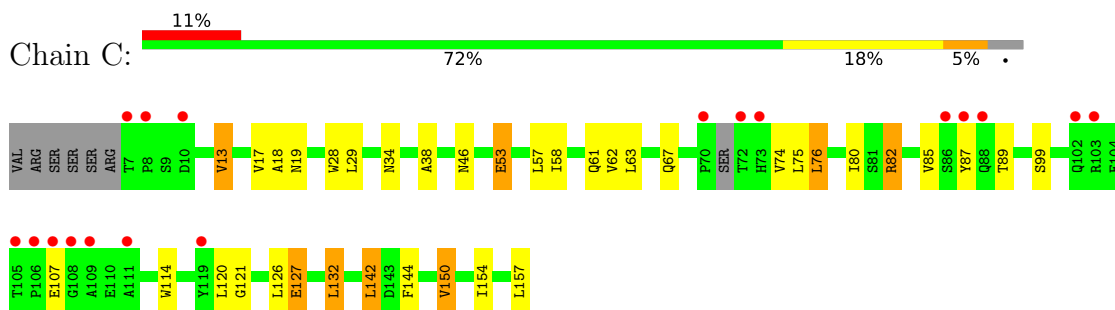
- Molecule 1: Tumor necrosis factor



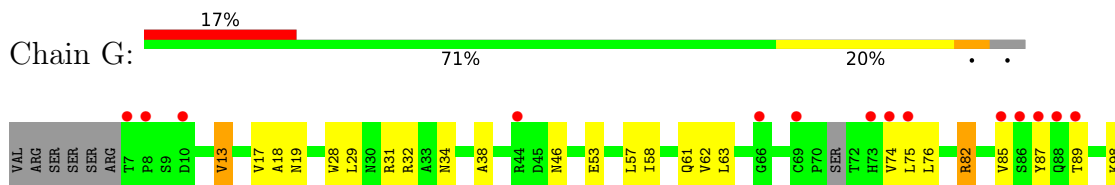
- Molecule 1: Tumor necrosis factor

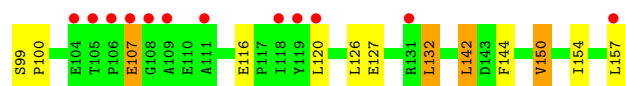


- Molecule 1: Tumor necrosis factor



- Molecule 1: Tumor necrosis factor





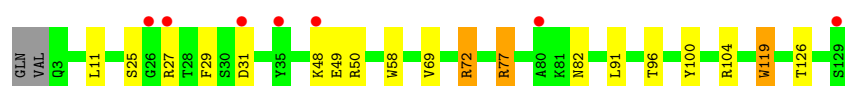
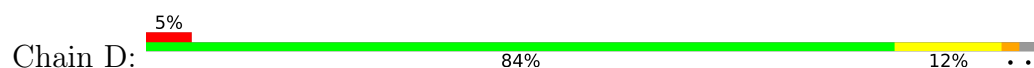
- Molecule 1: Tumor necrosis factor



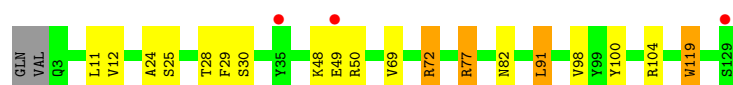
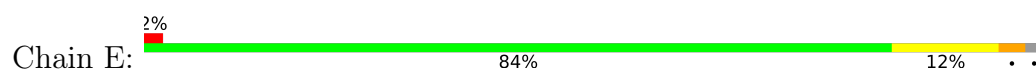
- Molecule 1: Tumor necrosis factor



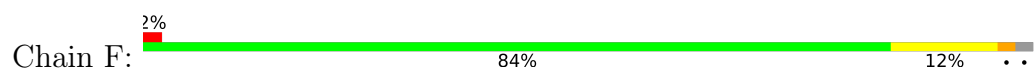
- Molecule 2: Llama nanobody VHH3



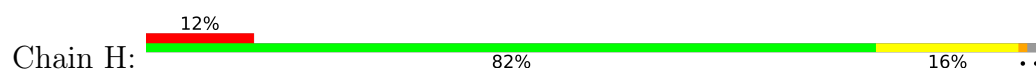
- Molecule 2: Llama nanobody VHH3

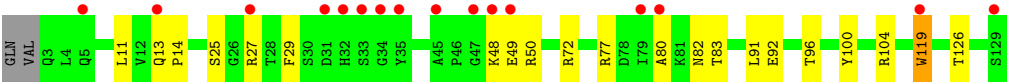


- Molecule 2: Llama nanobody VHH3

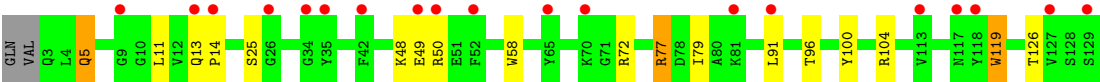
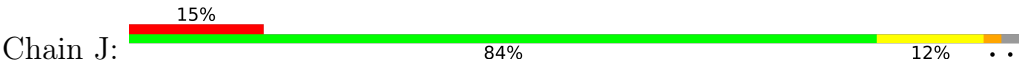


- Molecule 2: Llama nanobody VHH3

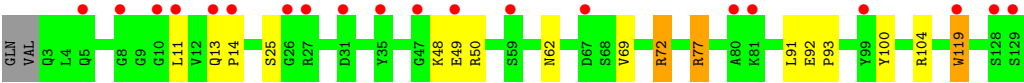
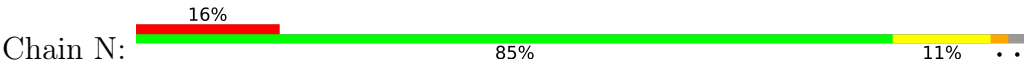




● Molecule 2: Llama nanobody VHH3



● Molecule 2: Llama nanobody VHH3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.38Å 83.84Å 150.06Å 90.00° 128.77° 90.00°	Depositor
Resolution (Å)	29.59 – 2.30 29.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.59-2.30) 100.0 (29.59-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.31Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.211 , 0.247 0.222 , 0.257	Depositor DCC
R_{free} test set	3229 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+3/2*k, 1/2*h-1/2*k, -h-k-l 0.000 for 1/2*h-3/2*k, -1/2*h-1/2*k, -h+k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13516	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 89.13 % 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 3.8166e-08. 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 [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	0.45	0/1175	0.73	0/1603
1	B	0.50	0/1187	0.73	0/1620
1	C	0.49	0/1180	0.75	0/1609
1	G	0.42	0/1180	0.71	0/1609
1	I	0.42	0/1184	0.72	0/1616
1	M	0.46	0/1154	0.71	0/1571
2	D	0.41	0/1007	0.68	0/1366
2	E	0.39	0/1007	0.68	0/1366
2	F	0.40	0/1007	0.67	0/1366
2	H	0.37	0/1007	0.62	0/1366
2	J	0.37	0/1007	0.63	0/1366
2	N	0.37	0/1003	0.62	0/1361
All	All	0.43	0/13098	0.69	0/17819

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	1149	0	1128	21	0
1	B	1160	0	1147	20	0
1	C	1154	0	1141	21	0
1	G	1154	0	1141	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1157	0	1139	19	0
1	M	1131	0	1112	26	0
2	D	984	0	922	6	0
2	E	984	0	922	7	0
2	F	984	0	922	6	0
2	H	984	0	922	5	0
2	J	984	0	922	6	0
2	N	980	0	915	6	0
3	A	92	0	0	2	0
3	B	93	0	0	0	0
3	C	94	0	0	0	0
3	D	78	0	0	0	0
3	E	88	0	0	0	0
3	F	86	0	0	0	0
3	G	36	0	0	0	0
3	H	23	0	0	0	0
3	I	36	0	0	0	0
3	J	31	0	0	0	0
3	M	32	0	0	0	0
3	N	22	0	0	0	0
All	All	13516	0	12333	139	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 6.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:TRP:H	1:G:46:ASN:HD21	1.20	0.90
1:A:28:TRP:H	1:A:46:ASN:HD21	1.19	0.90
1:C:28:TRP:H	1:C:46:ASN:HD21	1.19	0.90
1:I:28:TRP:H	1:I:46:ASN:HD21	1.20	0.89
1:B:28:TRP:H	1:B:46:ASN:HD21	1.19	0.89
1:M:28:TRP:H	1:M:46:ASN:HD21	1.21	0.86
1:B:99:SER:OG	1:C:114:TRP:HA	1.83	0.78
1:A:142:LEU:HD12	1:A:144:PHE:HD1	1.50	0.77
1:I:114:TRP:HA	1:M:99:SER:OG	1.84	0.77
1:C:142:LEU:HD12	1:C:144:PHE:HD1	1.49	0.76
1:I:142:LEU:HD12	1:I:144:PHE:HD1	1.51	0.75
1:B:142:LEU:HD12	1:B:144:PHE:HD1	1.51	0.74
1:M:142:LEU:HD12	1:M:144:PHE:HD1	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:LEU:HD12	1:G:144:PHE:HD1	1.52	0.74
1:A:58:ILE:HD11	1:A:126:LEU:HD11	1.77	0.67
1:I:58:ILE:HD11	1:I:126:LEU:HD11	1.77	0.67
1:B:28:TRP:H	1:B:46:ASN:ND2	1.92	0.66
1:M:28:TRP:H	1:M:46:ASN:ND2	1.93	0.66
1:B:58:ILE:HD11	1:B:126:LEU:HD11	1.78	0.66
1:G:58:ILE:HD11	1:G:126:LEU:HD11	1.79	0.65
1:C:28:TRP:H	1:C:46:ASN:ND2	1.93	0.64
2:D:69:VAL:HA	2:D:72:ARG:HD3	1.80	0.63
1:C:58:ILE:HD11	1:C:126:LEU:HD11	1.80	0.63
2:D:29:PHE:H	2:D:82:ASN:HD21	1.45	0.63
1:G:99:SER:OG	1:M:114:TRP:HA	1.97	0.63
1:A:28:TRP:H	1:A:46:ASN:ND2	1.93	0.63
1:I:28:TRP:H	1:I:46:ASN:ND2	1.93	0.63
1:G:120:LEU:HD23	1:M:61:GLN:HE22	1.64	0.62
2:H:29:PHE:H	2:H:82:ASN:HD21	1.47	0.62
1:G:98:LYS:HD3	1:G:116:GLU:HB3	1.83	0.60
1:M:19:ASN:HB2	1:M:29:LEU:HD13	1.84	0.60
1:G:28:TRP:H	1:G:46:ASN:ND2	1.94	0.60
1:M:58:ILE:HD11	1:M:126:LEU:HD11	1.83	0.59
1:B:142:LEU:HD12	1:B:144:PHE:CD1	2.37	0.58
1:G:142:LEU:HD12	1:G:144:PHE:CD1	2.37	0.58
2:N:92:GLU:HG2	2:N:93:PRO:HD2	1.84	0.58
2:F:32:HIS:HD2	2:F:34:GLY:O	1.86	0.57
1:A:34:ASN:HD21	1:C:82:ARG:HH21	1.52	0.57
1:I:19:ASN:HB2	1:I:29:LEU:HD13	1.85	0.57
1:A:142:LEU:HD12	1:A:144:PHE:CD1	2.36	0.57
2:D:58:TRP:CZ3	2:D:77:ARG:HG3	2.40	0.57
1:A:73:HIS:HE1	1:A:101:CYS:O	1.89	0.56
1:I:142:LEU:HD12	1:I:144:PHE:CD1	2.37	0.55
1:C:142:LEU:HD12	1:C:144:PHE:CD1	2.35	0.54
1:M:142:LEU:HD12	1:M:144:PHE:CD1	2.37	0.53
1:G:107:GLU:O	2:H:80:ALA:HB2	2.07	0.53
1:C:18:ALA:HB2	1:C:150:VAL:HG22	1.91	0.53
1:A:99:SER:HB2	3:A:226:HOH:O	2.08	0.53
1:A:82:ARG:HH21	1:B:34:ASN:HD21	1.56	0.52
1:A:18:ALA:HB2	1:A:150:VAL:HG22	1.90	0.52
2:F:29:PHE:H	2:F:82:ASN:HD21	1.58	0.52
2:D:58:TRP:CE3	2:D:77:ARG:HG3	2.43	0.52
1:M:18:ALA:HB2	1:M:150:VAL:HG22	1.92	0.52
2:J:13:GLN:HG2	2:J:14:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ALA:HB2	1:B:150:VAL:HG22	1.92	0.51
1:I:18:ALA:HB2	1:I:150:VAL:HG22	1.92	0.51
1:M:17:VAL:HG11	1:M:32:ARG:HH11	1.75	0.50
1:G:18:ALA:HB2	1:G:150:VAL:HG22	1.92	0.50
2:E:69:VAL:HA	2:E:72:ARG:HD3	1.94	0.50
1:I:34:ASN:HD21	1:M:82:ARG:HH21	1.61	0.48
1:A:99:SER:HB3	1:B:114:TRP:HA	1.96	0.48
1:B:82:ARG:HH21	1:C:34:ASN:HD21	1.62	0.48
1:M:65:LYS:HG3	2:N:62:ASN:OD1	2.14	0.48
1:G:82:ARG:HH21	1:M:34:ASN:HD21	1.62	0.48
2:E:28:THR:HA	2:E:82:ASN:HD21	1.78	0.47
1:A:98:LYS:HE3	1:B:117:PRO:HD2	1.97	0.47
1:A:73:HIS:CE1	1:A:101:CYS:O	2.67	0.47
2:J:96:THR:HG23	2:J:126:THR:HA	1.97	0.47
1:B:74:VAL:HG12	1:B:76:LEU:HD13	1.96	0.47
1:C:62:VAL:HA	1:C:150:VAL:HB	1.97	0.47
1:G:132:LEU:HD23	1:G:154:ILE:HG21	1.96	0.47
1:A:132:LEU:HD23	1:A:154:ILE:HG21	1.97	0.46
1:M:106:PRO:C	1:M:109:ALA:H	2.18	0.46
1:C:132:LEU:HD23	1:C:154:ILE:HG21	1.96	0.46
1:I:132:LEU:HD23	1:I:154:ILE:HG21	1.98	0.46
1:G:34:ASN:HD21	1:I:82:ARG:HH21	1.63	0.46
1:A:62:VAL:HA	1:A:150:VAL:HB	1.97	0.46
1:B:132:LEU:HD23	1:B:154:ILE:HG21	1.97	0.46
1:I:74:VAL:HG12	1:I:76:LEU:HD13	1.97	0.46
1:B:19:ASN:HB2	1:B:29:LEU:HD13	1.98	0.46
1:G:19:ASN:HB2	1:G:29:LEU:HD13	1.97	0.46
1:M:62:VAL:HA	1:M:150:VAL:HB	1.98	0.46
1:C:19:ASN:HB2	1:C:29:LEU:HD13	1.97	0.45
1:G:62:VAL:HA	1:G:150:VAL:HB	1.98	0.45
1:C:67:GLN:HB3	2:E:77:ARG:NH2	2.31	0.45
1:M:132:LEU:HD23	1:M:154:ILE:HG21	1.97	0.45
1:B:62:VAL:HA	1:B:150:VAL:HB	1.98	0.45
1:I:62:VAL:HA	1:I:150:VAL:HB	1.98	0.45
1:A:67:GLN:HB3	2:F:77:ARG:NH2	2.31	0.44
2:D:96:THR:HG23	2:D:126:THR:HA	1.99	0.44
1:B:13:VAL:HG23	1:B:38:ALA:HB3	1.99	0.44
1:C:58:ILE:O	1:C:121:GLY:HA2	2.18	0.44
1:M:67:GLN:HB3	2:N:77:ARG:NH2	2.33	0.44
2:N:69:VAL:HA	2:N:72:ARG:HD3	2.00	0.44
2:F:100:TYR:HB3	2:F:119:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:HB2	1:A:29:LEU:HD13	1.99	0.43
2:E:100:TYR:HB3	2:E:119:TRP:CD1	2.54	0.43
2:E:24:ALA:HB2	2:E:29:PHE:CZ	2.53	0.43
2:N:100:TYR:HB3	2:N:119:TRP:CD1	2.54	0.43
2:J:58:TRP:CZ2	2:J:79:ILE:HA	2.52	0.43
2:J:100:TYR:HB3	2:J:119:TRP:CD1	2.54	0.43
2:D:100:TYR:HB3	2:D:119:TRP:CD1	2.53	0.43
1:C:74:VAL:HG12	1:C:76:LEU:HD13	2.00	0.43
1:A:61:GLN:HE22	1:C:120:LEU:HD23	1.83	0.43
1:I:67:GLN:HB3	2:J:77:ARG:NH2	2.34	0.43
1:M:76:LEU:HD22	1:M:100:PRO:HG3	2.01	0.43
1:A:120:LEU:HD23	1:B:61:GLN:HE22	1.84	0.42
1:M:98:LYS:HB2	1:M:118:ILE:HD11	2.01	0.42
1:C:13:VAL:HG23	1:C:38:ALA:HB3	2.01	0.42
1:M:13:VAL:HG23	1:M:38:ALA:HB3	2.01	0.42
1:A:13:VAL:HG23	1:A:38:ALA:HB3	2.01	0.42
2:F:58:TRP:CZ2	2:F:79:ILE:HA	2.55	0.41
1:C:58:ILE:HG22	1:C:80:ILE:HD13	2.02	0.41
1:M:31:ARG:O	1:M:31:ARG:HG3	2.20	0.41
1:B:28:TRP:N	1:B:46:ASN:HD21	2.01	0.41
2:E:24:ALA:HB3	2:E:82:ASN:ND2	2.35	0.41
2:H:100:TYR:HB3	2:H:119:TRP:CD1	2.55	0.41
1:B:57:LEU:HB2	1:B:157:LEU:HD11	2.02	0.41
1:C:57:LEU:HB2	1:C:157:LEU:HD11	2.03	0.41
2:E:12:VAL:HG11	2:E:91:LEU:HD23	2.02	0.41
2:F:69:VAL:HA	2:F:72:ARG:HD3	2.03	0.41
1:I:32:ARG:HH11	1:I:32:ARG:HB3	1.85	0.41
1:I:61:GLN:HE22	1:M:120:LEU:HD23	1.86	0.41
1:M:53:GLU:HG2	1:M:127:GLU:HA	2.02	0.41
2:N:13:GLN:HG2	2:N:14:PRO:HD2	2.02	0.41
1:G:28:TRP:N	1:G:46:ASN:HD21	2.02	0.41
1:G:61:GLN:HE22	1:I:120:LEU:HD23	1.86	0.41
1:M:57:LEU:HB2	1:M:157:LEU:HD11	2.03	0.40
1:B:120:LEU:HD23	1:C:61:GLN:HE22	1.86	0.40
1:C:53:GLU:HG2	1:C:127:GLU:HA	2.03	0.40
1:I:13:VAL:HG23	1:I:38:ALA:HB3	2.03	0.40
1:A:53:GLU:HG3	3:A:245:HOH:O	2.21	0.40
1:I:53:GLU:HG2	1:I:127:GLU:HA	2.03	0.40
1:M:28:TRP:HZ3	1:M:151:TYR:HA	1.87	0.40
1:G:13:VAL:HG23	1:G:38:ALA:HB3	2.03	0.40
1:G:57:LEU:HB2	1:G:157:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:GLN:HG2	2:H:14:PRO:HD2	2.03	0.40
2:H:96:THR:HG23	2:H:126:THR:HA	2.03	0.40
2:J:5:GLN:HE21	2:J:5:GLN:HB3	1.64	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	A	146/157 (93%)	137 (94%)	8 (6%)	1 (1%)	22	26
1	B	149/157 (95%)	142 (95%)	6 (4%)	1 (1%)	22	26
1	C	146/157 (93%)	139 (95%)	6 (4%)	1 (1%)	22	26
1	G	146/157 (93%)	137 (94%)	7 (5%)	2 (1%)	11	11
1	I	148/157 (94%)	138 (93%)	8 (5%)	2 (1%)	11	11
1	M	140/157 (89%)	132 (94%)	7 (5%)	1 (1%)	22	26
2	D	125/129 (97%)	123 (98%)	2 (2%)	0	100	100
2	E	125/129 (97%)	124 (99%)	1 (1%)	0	100	100
2	F	125/129 (97%)	123 (98%)	2 (2%)	0	100	100
2	H	125/129 (97%)	122 (98%)	3 (2%)	0	100	100
2	J	125/129 (97%)	123 (98%)	2 (2%)	0	100	100
2	N	125/129 (97%)	121 (97%)	4 (3%)	0	100	100
All	All	1625/1716 (95%)	1561 (96%)	56 (3%)	8 (0%)	29	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLU

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Mol	Chain	Res	Type
1	B	107	GLU
1	I	71	SER
1	C	107	GLU
1	G	107	GLU
1	I	70	PRO
1	M	102	GLN
1	G	100	PRO

5.3.2 Protein sidechains ⓘ

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	121/133 (91%)	105 (87%)	16 (13%)	4	4
1	B	123/133 (92%)	109 (89%)	14 (11%)	5	6
1	C	122/133 (92%)	107 (88%)	15 (12%)	4	5
1	G	122/133 (92%)	105 (86%)	17 (14%)	3	3
1	I	123/133 (92%)	106 (86%)	17 (14%)	3	3
1	M	119/133 (90%)	103 (87%)	16 (13%)	4	4
2	D	103/105 (98%)	91 (88%)	12 (12%)	5	6
2	E	103/105 (98%)	91 (88%)	12 (12%)	5	6
2	F	103/105 (98%)	92 (89%)	11 (11%)	6	7
2	H	103/105 (98%)	90 (87%)	13 (13%)	4	4
2	J	103/105 (98%)	92 (89%)	11 (11%)	6	7
2	N	102/105 (97%)	92 (90%)	10 (10%)	8	9
All	All	1347/1428 (94%)	1183 (88%)	164 (12%)	5	5

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	17	VAL
1	A	53	GLU

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Mol	Chain	Res	Type
1	A	63	LEU
1	A	71	SER
1	A	75	LEU
1	A	76	LEU
1	A	82	ARG
1	A	85	VAL
1	A	87	TYR
1	A	89	THR
1	A	98	LYS
1	A	127	GLU
1	A	132	LEU
1	A	142	LEU
1	A	150	VAL
1	B	13	VAL
1	B	17	VAL
1	B	53	GLU
1	B	63	LEU
1	B	75	LEU
1	B	76	LEU
1	B	82	ARG
1	B	85	VAL
1	B	87	TYR
1	B	89	THR
1	B	127	GLU
1	B	132	LEU
1	B	142	LEU
1	B	150	VAL
1	C	13	VAL
1	C	17	VAL
1	C	53	GLU
1	C	63	LEU
1	C	75	LEU
1	C	76	LEU
1	C	82	ARG
1	C	85	VAL
1	C	87	TYR
1	C	89	THR
1	C	99	SER
1	C	127	GLU
1	C	132	LEU
1	C	142	LEU
1	C	150	VAL

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Mol	Chain	Res	Type
2	D	11	LEU
2	D	25	SER
2	D	27	ARG
2	D	31	ASP
2	D	48	LYS
2	D	49	GLU
2	D	50	ARG
2	D	72	ARG
2	D	77	ARG
2	D	91	LEU
2	D	104	ARG
2	D	119	TRP
2	E	11	LEU
2	E	25	SER
2	E	30	SER
2	E	48	LYS
2	E	49	GLU
2	E	50	ARG
2	E	72	ARG
2	E	77	ARG
2	E	91	LEU
2	E	98	VAL
2	E	104	ARG
2	E	119	TRP
2	F	11	LEU
2	F	27	ARG
2	F	48	LYS
2	F	49	GLU
2	F	50	ARG
2	F	72	ARG
2	F	77	ARG
2	F	91	LEU
2	F	98	VAL
2	F	104	ARG
2	F	119	TRP
1	G	13	VAL
1	G	17	VAL
1	G	31	ARG
1	G	32	ARG
1	G	53	GLU
1	G	63	LEU
1	G	74	VAL

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Mol	Chain	Res	Type
1	G	75	LEU
1	G	76	LEU
1	G	82	ARG
1	G	85	VAL
1	G	87	TYR
1	G	89	THR
1	G	127	GLU
1	G	132	LEU
1	G	142	LEU
1	G	150	VAL
2	H	11	LEU
2	H	25	SER
2	H	27	ARG
2	H	48	LYS
2	H	49	GLU
2	H	50	ARG
2	H	72	ARG
2	H	77	ARG
2	H	83	THR
2	H	91	LEU
2	H	92	GLU
2	H	104	ARG
2	H	119	TRP
1	I	13	VAL
1	I	17	VAL
1	I	32	ARG
1	I	53	GLU
1	I	63	LEU
1	I	75	LEU
1	I	76	LEU
1	I	82	ARG
1	I	85	VAL
1	I	87	TYR
1	I	89	THR
1	I	99	SER
1	I	102	GLN
1	I	127	GLU
1	I	132	LEU
1	I	142	LEU
1	I	150	VAL
2	J	5	GLN
2	J	11	LEU

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Mol	Chain	Res	Type
2	J	25	SER
2	J	48	LYS
2	J	49	GLU
2	J	50	ARG
2	J	72	ARG
2	J	77	ARG
2	J	91	LEU
2	J	104	ARG
2	J	119	TRP
1	M	13	VAL
1	M	17	VAL
1	M	53	GLU
1	M	63	LEU
1	M	65	LYS
1	M	75	LEU
1	M	76	LEU
1	M	82	ARG
1	M	85	VAL
1	M	87	TYR
1	M	89	THR
1	M	98	LYS
1	M	127	GLU
1	M	132	LEU
1	M	142	LEU
1	M	150	VAL
2	N	11	LEU
2	N	25	SER
2	N	48	LYS
2	N	49	GLU
2	N	50	ARG
2	N	72	ARG
2	N	77	ARG
2	N	91	LEU
2	N	104	ARG
2	N	119	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	46	ASN
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	67	GLN
1	A	73	HIS
1	B	34	ASN
1	B	46	ASN
1	B	61	GLN
1	C	34	ASN
1	C	46	ASN
1	C	61	GLN
2	D	5	GLN
2	D	82	ASN
2	E	32	HIS
2	F	32	HIS
2	F	82	ASN
1	G	34	ASN
1	G	46	ASN
1	G	61	GLN
2	H	82	ASN
1	I	34	ASN
1	I	46	ASN
1	I	61	GLN
1	I	102	GLN
2	J	5	GLN
1	M	34	ASN
1	M	46	ASN
1	M	61	GLN
2	N	3	GLN
2	N	5	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	106:PRO	C	107:GLU	N	2.95

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	A	150/157 (95%)	0.38	13 (8%) 10 14	8, 19, 82, 96	0
1	B	151/157 (96%)	0.54	20 (13%) 3 4	8, 18, 85, 107	0
1	C	150/157 (95%)	0.55	18 (12%) 4 6	9, 20, 85, 106	0
1	G	150/157 (95%)	1.10	26 (17%) 1 1	31, 52, 144, 199	0
1	I	150/157 (95%)	1.02	28 (18%) 1 1	34, 50, 134, 184	0
1	M	148/157 (94%)	1.16	32 (21%) 0 1	35, 53, 170, 207	0
2	D	127/129 (98%)	0.01	7 (5%) 25 31	9, 25, 59, 83	0
2	E	127/129 (98%)	0.16	3 (2%) 59 66	9, 29, 57, 107	0
2	F	127/129 (98%)	-0.03	3 (2%) 59 66	9, 28, 54, 86	0
2	H	127/129 (98%)	0.77	16 (12%) 3 5	34, 50, 86, 104	0
2	J	127/129 (98%)	0.95	19 (14%) 2 3	35, 54, 77, 111	0
2	N	127/129 (98%)	1.04	20 (15%) 2 2	32, 58, 89, 149	0
All	All	1661/1716 (96%)	0.65	205 (12%) 4 6	8, 43, 98, 207	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	87	TYR	16.7
1	I	87	TYR	12.9
1	M	87	TYR	12.5
1	B	87	TYR	12.3
1	C	87	TYR	11.6
1	G	86	SER	9.5
1	A	87	TYR	9.4
1	B	71	SER	9.0
1	I	8	PRO	8.7
1	M	8	PRO	8.1
1	C	107	GLU	7.3

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Mol	Chain	Res	Type	RSRZ
1	I	7	THR	7.2
1	C	106	PRO	6.9
1	C	108	GLY	6.7
1	B	86	SER	6.6
1	I	86	SER	6.2
1	M	73	HIS	6.1
1	A	7	THR	5.9
1	A	8	PRO	5.8
2	N	35	TYR	5.6
2	N	129	SER	5.6
1	M	107	GLU	5.6
1	C	102	GLN	5.6
1	G	108	GLY	5.3
1	G	8	PRO	5.1
1	I	108	GLY	5.1
1	M	86	SER	5.1
2	N	26	GLY	5.1
1	C	8	PRO	5.0
1	M	119	TYR	4.9
1	M	103	ARG	4.9
1	B	107	GLU	4.9
1	C	73	HIS	4.7
1	M	74	VAL	4.7
2	J	35	TYR	4.6
1	B	7	THR	4.5
1	G	89	THR	4.5
1	A	86	SER	4.4
1	M	67	GLN	4.4
1	B	108	GLY	4.4
1	I	106	PRO	4.3
1	I	119	TYR	4.3
1	I	44	ARG	4.2
1	G	85	VAL	4.2
1	C	109	ALA	4.2
1	M	89	THR	4.1
2	H	35	TYR	4.1
2	H	129	SER	4.1
1	I	107	GLU	4.1
1	A	107	GLU	4.1
1	G	69	CYS	4.1
2	N	80	ALA	4.0
1	B	103	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	105	THR	4.0
1	C	86	SER	3.9
1	G	109	ALA	3.9
1	B	106	PRO	3.9
1	G	107	GLU	3.8
1	A	111	ALA	3.8
2	N	49	GLU	3.8
2	H	31	ASP	3.8
2	H	34	GLY	3.8
1	I	89	THR	3.7
1	C	72	THR	3.7
1	M	104	GLU	3.7
1	I	109	ALA	3.6
2	H	48	LYS	3.6
2	H	79	ILE	3.6
2	H	47	GLY	3.6
1	B	72	THR	3.6
1	I	102	GLN	3.5
2	D	31	ASP	3.5
1	A	73	HIS	3.5
2	N	5	GLN	3.5
1	G	105	THR	3.4
2	N	27	ARG	3.4
2	E	129	SER	3.3
2	J	49	GLU	3.3
1	M	70	PRO	3.3
1	G	7	THR	3.3
1	G	10	ASP	3.2
1	B	8	PRO	3.2
1	G	106	PRO	3.2
1	B	110	GLU	3.2
2	J	129	SER	3.2
2	J	34	GLY	3.2
2	H	80	ALA	3.2
2	J	91	LEU	3.2
2	N	10	GLY	3.2
2	N	128	SER	3.1
1	M	101	CYS	3.1
1	G	73	HIS	3.1
1	I	111	ALA	3.1
1	B	105	THR	3.0
1	A	106	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	100	PRO	3.0
2	H	119	TRP	3.0
1	C	111	ALA	3.0
1	I	73	HIS	2.9
2	H	32	HIS	2.9
1	B	109	ALA	2.9
2	N	119	TRP	2.9
1	M	106	PRO	2.9
1	C	105	THR	2.9
1	B	85	VAL	2.9
1	G	88	GLN	2.9
2	J	117	ASN	2.9
1	I	83	ILE	2.9
2	D	26	GLY	2.9
1	A	70	PRO	2.8
2	N	13	GLN	2.8
1	C	103	ARG	2.8
1	B	70	PRO	2.8
1	M	75	LEU	2.8
1	G	120	LEU	2.8
2	H	27	ARG	2.8
1	M	108	GLY	2.7
2	H	49	GLU	2.7
1	B	111	ALA	2.7
1	G	74	VAL	2.7
2	J	52	PHE	2.7
2	N	14	PRO	2.7
1	C	119	TYR	2.7
1	I	105	THR	2.7
2	J	26	GLY	2.7
1	I	88	GLN	2.7
1	I	128	LYS	2.6
2	N	47	GLY	2.6
2	F	129	SER	2.6
1	M	68	GLY	2.6
1	M	145	ALA	2.6
1	G	44	ARG	2.6
1	I	70	PRO	2.5
1	B	73	HIS	2.5
2	H	45	ALA	2.5
1	I	85	VAL	2.5
2	J	81	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	103	ARG	2.5
1	G	119	TYR	2.5
1	G	131	ARG	2.5
2	J	118	TYR	2.5
2	J	9	GLY	2.5
1	G	104	GLU	2.4
1	I	104	GLU	2.4
1	I	75	LEU	2.4
2	D	27	ARG	2.4
1	A	85	VAL	2.4
1	M	44	ARG	2.4
1	I	131	ARG	2.4
1	M	115	TYR	2.3
1	M	7	THR	2.3
2	J	70	LYS	2.3
1	I	120	LEU	2.3
1	M	121	GLY	2.3
2	H	5	GLN	2.3
1	C	7	THR	2.3
1	M	88	GLN	2.3
1	M	85	VAL	2.3
1	G	118	ILE	2.3
1	M	120	LEU	2.2
1	I	71	SER	2.2
2	J	50	ARG	2.2
1	C	88	GLN	2.2
1	I	91	VAL	2.2
1	M	118	ILE	2.2
2	N	99	TYR	2.2
2	J	127	VAL	2.2
2	N	8	GLY	2.2
1	B	10	ASP	2.2
2	N	31	ASP	2.2
2	N	67	ASP	2.2
1	A	44	ARG	2.2
1	G	75	LEU	2.2
2	N	11	LEU	2.2
1	G	66	GLY	2.2
2	F	26	GLY	2.2
1	G	111	ALA	2.2
2	D	48	LYS	2.2
1	I	58	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	110	GLU	2.2
1	M	102	GLN	2.2
2	E	35	TYR	2.1
1	M	91	VAL	2.1
2	E	49	GLU	2.1
1	C	70	PRO	2.1
2	H	13	GLN	2.1
2	H	33	SER	2.1
2	J	14	PRO	2.1
2	N	81	LYS	2.1
2	D	80	ALA	2.1
2	J	113	VAL	2.1
1	A	89	THR	2.1
1	G	157	LEU	2.1
2	J	13	GLN	2.1
1	B	119	TYR	2.1
2	J	65	TYR	2.1
2	D	129	SER	2.1
1	A	119	TYR	2.1
2	F	49	GLU	2.0
1	B	89	THR	2.0
2	N	59	SER	2.0
1	C	10	ASP	2.0
2	D	35	TYR	2.0
2	J	42	PHE	2.0
1	M	99	SER	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.