Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 05:15 PM EDT

PDB ID	:	8F7Z
Title	:	VRC34.01_mm28 bound to fusion peptide
Authors	:	Olia, A.S.; Kwong, P.D.
Deposited on	:	2022-11-21
Resolution	:	2.70 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:

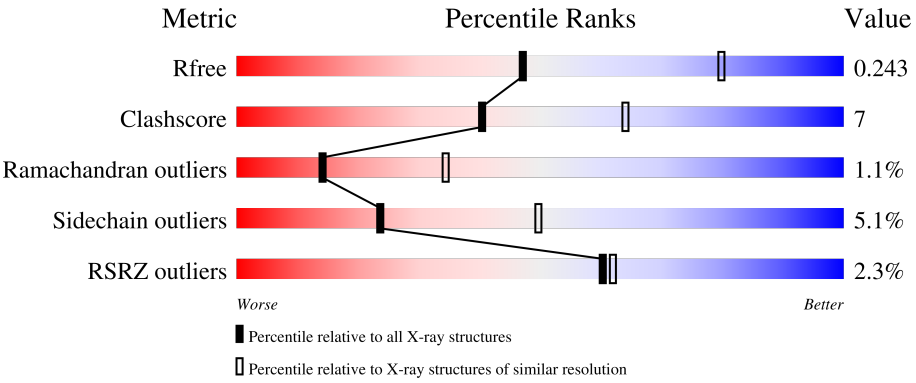
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	8	12% 75% 25%
1	K	8	62% 38%
1	L	8	12% 75% 25%
1	M	8	75% 25%
2	A	234	3% 75% 15% • 9%

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Mol	Chain	Length	Quality of chain
2	C	234	2% 73% 16% 9%
2	E	234	% 72% 18% 9%
2	G	234	3% 74% 17% 9%
3	B	214	3% 81% 16%
3	D	214	% 76% 21%
3	F	214	2% 77% 21%
3	H	214	2% 82% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13314 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 HIV-1 Env Fusion Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	8	Total	C	N	O	S	0	0	0
			48	30	8	9	1			
1	K	8	Total	C	N	O	S	0	0	0
			48	30	8	9	1			
1	L	8	Total	C	N	O	S	0	0	0
			48	30	8	9	1			
1	M	8	Total	C	N	O	S	0	0	0
			48	30	8	9	1			

- Molecule 2 is a protein called VRC34_mm28 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	213	Total	C	N	O	S	0	0	0
			1608	1022	273	307	6			
2	A	213	Total	C	N	O	S	0	0	0
			1608	1022	273	307	6			
2	C	213	Total	C	N	O	S	0	0	0
			1608	1022	273	307	6			
2	G	213	Total	C	N	O	S	0	0	0
			1608	1022	273	307	6			

- Molecule 3 is a protein called VRC34_m228 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	212	Total	C	N	O	S	0	0	0
			1586	1000	268	313	5			
3	B	212	Total	C	N	O	S	0	0	0
			1586	1000	268	313	5			
3	D	212	Total	C	N	O	S	0	0	0
			1586	1000	268	313	5			
3	H	212	Total	C	N	O	S	0	0	0
			1586	1000	268	313	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	51	Total O 51 51	0	0
4	F	34	Total O 34 34	0	0
4	A	56	Total O 56 56	0	0
4	C	44	Total O 44 44	0	0
4	G	56	Total O 56 56	0	0
4	B	36	Total O 36 36	0	0
4	D	30	Total O 30 30	0	0
4	H	35	Total O 35 35	0	0
4	K	2	Total O 2 2	0	0
4	L	2	Total O 2 2	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: HIV-1 Env Fusion Peptide

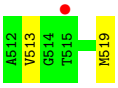
Chain I:

• Molecule 1: HIV-1 Env Fusion Peptide

Chain K:

• Molecule 1: HIV-1 Env Fusion Peptide

Chain L:

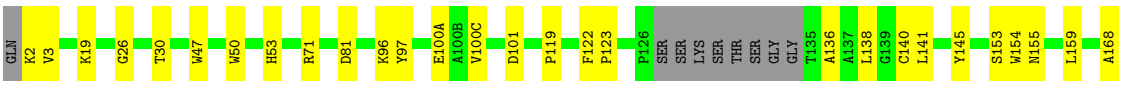


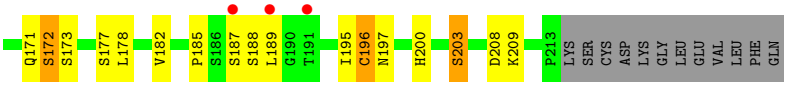
• Molecule 1: HIV-1 Env Fusion Peptide

Chain M:

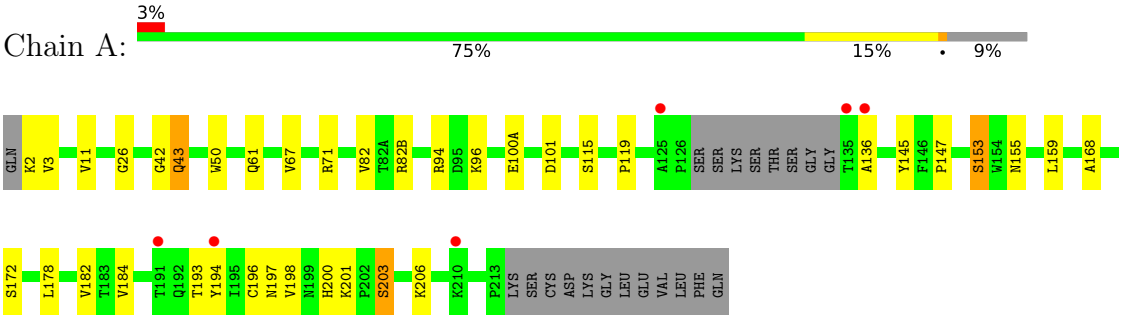
• Molecule 2: VRC34_mm28 Heavy Chain

Chain E:

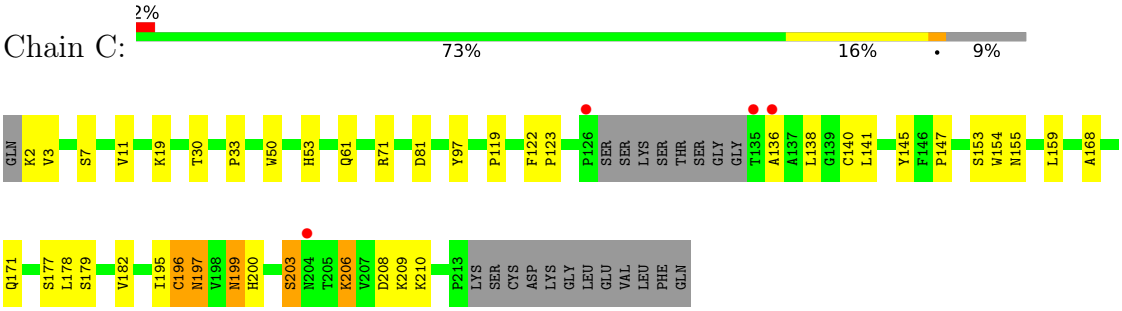




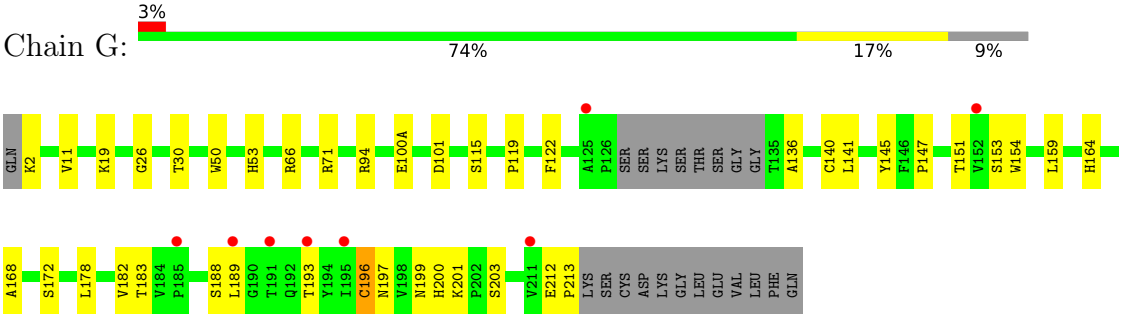
• Molecule 2: VRC34_mm28 Heavy Chain



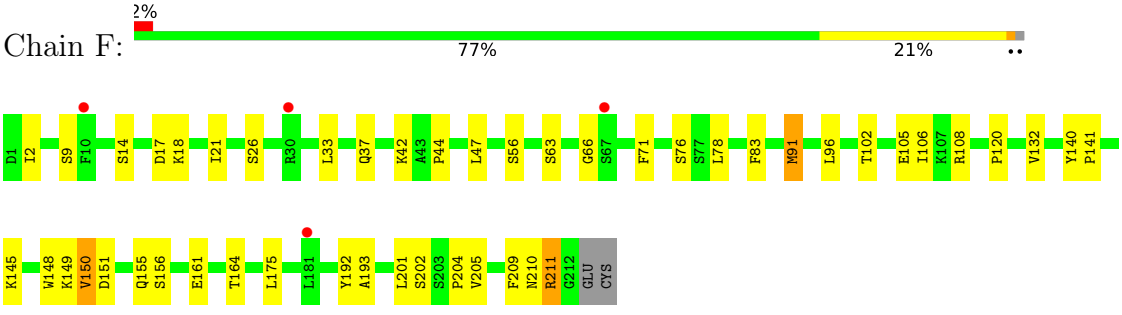
• Molecule 2: VRC34_mm28 Heavy Chain



• Molecule 2: VRC34_mm28 Heavy Chain

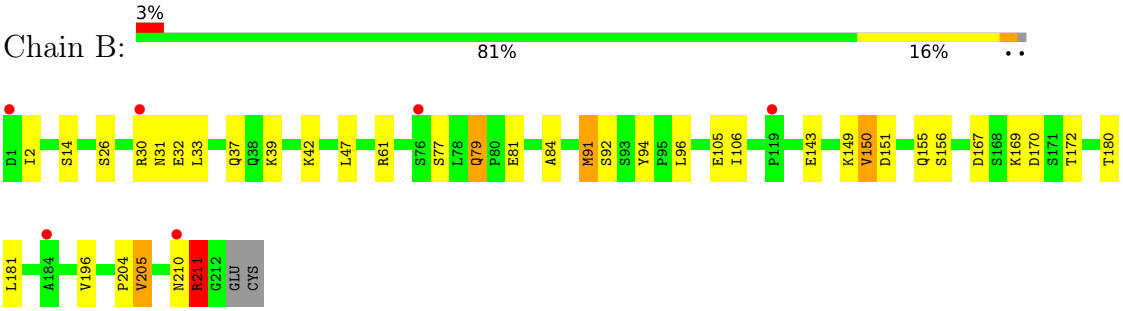


• Molecule 3: VRC34_m228 Light Chain



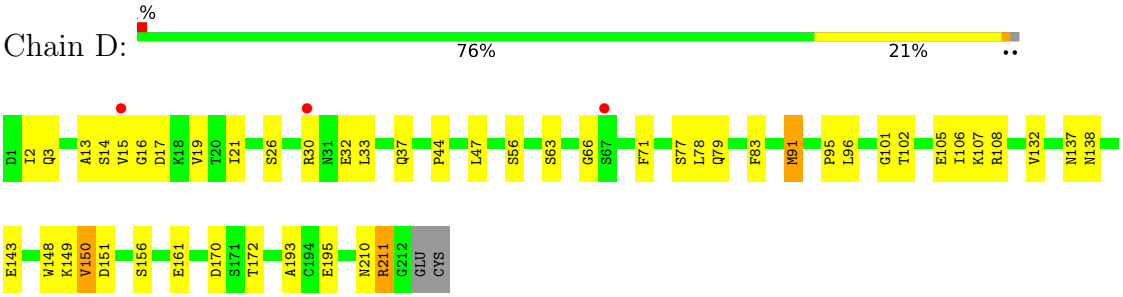
• Molecule 3: VRC34_m228 Light Chain

Chain B:



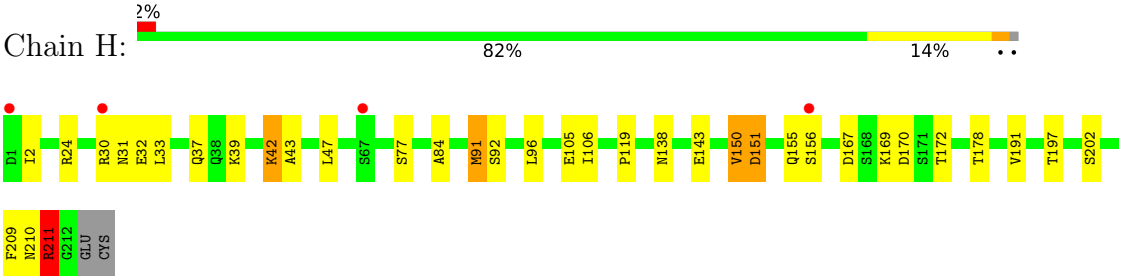
• Molecule 3: VRC34_m228 Light Chain

Chain D:



• Molecule 3: VRC34_m228 Light Chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	129.85Å 130.55Å 130.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.22 – 2.70 43.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (36.22-2.70) 95.3 (43.42-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.210 , 0.243 0.210 , 0.243	Depositor DCC
R_{free} test set	2010 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.439 for -h,l,k 0.004 for -l,-k,-h 0.006 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13314	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	I	0.27	0/47	0.57	0/62
1	K	0.31	0/47	0.65	0/62
1	L	0.34	0/47	0.68	0/62
1	M	0.28	0/47	0.51	0/62
2	A	0.42	4/1650 (0.2%)	0.61	2/2250 (0.1%)
2	C	0.32	0/1650	0.60	1/2250 (0.0%)
2	E	0.34	0/1650	0.59	2/2250 (0.1%)
2	G	0.35	0/1650	0.62	2/2250 (0.1%)
3	B	0.38	1/1623 (0.1%)	0.74	4/2213 (0.2%)
3	D	0.31	0/1623	0.61	1/2213 (0.0%)
3	F	0.31	0/1623	0.56	0/2213
3	H	0.30	0/1623	0.55	0/2213
All	All	0.34	5/13280 (0.0%)	0.61	12/18100 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	143	GLU	CD-OE2	-6.56	1.18	1.25
2	A	201	LYS	CE-NZ	6.13	1.64	1.49
2	A	201	LYS	CD-CE	5.94	1.66	1.51
2	A	201	LYS	CG-CD	5.14	1.70	1.52
2	A	201	LYS	CB-CG	5.00	1.66	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	143	GLU	CA-CB-CG	14.38	145.04	113.40
2	C	206	LYS	CD-CE-NZ	11.39	137.89	111.70
3	B	143	GLU	N-CA-CB	8.32	125.58	110.60
2	G	201	LYS	CA-CB-CG	6.99	128.77	113.40
3	B	205	VAL	CG1-CB-CG2	6.96	122.04	110.90
2	A	201	LYS	CG-CD-CE	6.64	131.81	111.90
2	G	201	LYS	CD-CE-NZ	6.56	126.78	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	143	GLU	N-CA-CB	6.30	121.95	110.60
2	E	172	SER	C-N-CA	6.14	137.06	121.70
2	A	201	LYS	N-CA-CB	5.30	120.14	110.60
3	B	143	GLU	CB-CA-C	-5.15	100.11	110.40
2	E	173	SER	N-CA-CB	-5.08	102.87	110.50

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	I	48	0	51	2	0
1	K	48	0	51	3	0
1	L	48	0	51	2	0
1	M	48	0	51	1	0
2	A	1608	0	1569	20	0
2	C	1608	0	1569	24	0
2	E	1608	0	1569	25	0
2	G	1608	0	1569	20	0
3	B	1586	0	1507	21	0
3	D	1586	0	1507	26	0
3	F	1586	0	1507	27	0
3	H	1586	0	1507	24	0
4	A	56	0	0	3	1
4	B	36	0	0	1	0
4	C	44	0	0	2	0
4	D	30	0	0	5	0
4	E	51	0	0	2	0
4	F	34	0	0	6	0
4	G	56	0	0	5	1
4	H	35	0	0	3	0
4	K	2	0	0	0	0
4	L	2	0	0	2	0
All	All	13314	0	12508	183	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (183) 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:C:2:LYS:N	4:C:301:HOH:O	1.96	0.98
1:L:513:VAL:O	4:L:601:HOH:O	1.82	0.98
3:H:39:LYS:H	3:H:42:LYS:HE3	1.34	0.91
3:D:195:GLU:O	4:D:301:HOH:O	1.90	0.88
2:G:159:LEU:HD11	2:G:182:VAL:HG21	1.59	0.84
3:F:42:LYS:NZ	4:F:304:HOH:O	2.09	0.84
2:A:2:LYS:N	4:A:302:HOH:O	2.12	0.82
2:A:159:LEU:HD11	2:A:182:VAL:HG21	1.61	0.82
3:B:39:LYS:H	3:B:42:LYS:HE2	1.47	0.79
3:F:161:GLU:OE1	4:F:301:HOH:O	2.01	0.79
3:F:44:PRO:O	4:F:302:HOH:O	2.03	0.77
2:C:199:ASN:ND2	2:C:206:LYS:HD3	2.00	0.76
3:B:42:LYS:NZ	4:B:301:HOH:O	2.20	0.74
2:C:171:GLN:HE22	2:C:177:SER:HB3	1.53	0.74
3:D:161:GLU:OE1	4:D:302:HOH:O	2.06	0.73
2:E:171:GLN:HE22	2:E:177:SER:HB3	1.53	0.73
2:C:61:GLN:HE22	3:D:95:PRO:HD3	1.52	0.72
3:H:178:THR:O	4:H:301:HOH:O	2.06	0.72
3:H:39:LYS:HB2	3:H:42:LYS:HE2	1.71	0.71
3:F:96:LEU:O	4:F:303:HOH:O	2.07	0.71
2:G:200:HIS:ND1	2:G:203:SER:OG	2.21	0.70
2:E:100(C):VAL:O	4:E:301:HOH:O	2.09	0.70
2:C:199:ASN:HD21	2:C:206:LYS:HD3	1.56	0.70
2:E:2:LYS:HG3	2:E:3:VAL:HG23	1.74	0.69
2:G:164:HIS:HE1	3:H:138:ASN:HD21	1.38	0.68
2:C:7:SER:O	4:C:302:HOH:O	2.11	0.68
3:D:101:GLY:O	4:D:303:HOH:O	2.13	0.66
3:D:91:MET:HA	3:D:96:LEU:HD22	1.78	0.65
2:A:82(B):ARG:NH1	4:A:308:HOH:O	2.29	0.65
3:H:143:GLU:OE1	3:H:143:GLU:N	2.26	0.64
3:F:91:MET:HA	3:F:96:LEU:HD22	1.78	0.64
2:G:66:ARG:NH1	4:G:307:HOH:O	2.32	0.63
3:H:24:ARG:NH2	4:H:303:HOH:O	2.31	0.63
3:B:210:ASN:O	3:B:211:ARG:HB2	1.98	0.63
3:D:210:ASN:O	3:D:211:ARG:HB2	1.99	0.63
2:G:188:SER:H	2:G:189:LEU:HD12	1.63	0.62
3:D:44:PRO:O	4:D:304:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:210:ASN:O	3:F:211:ARG:HB2	1.99	0.62
2:A:2:LYS:HG3	2:A:3:VAL:HG23	1.82	0.61
3:H:210:ASN:O	3:H:211:ARG:HB2	2.00	0.61
3:D:21:ILE:HD12	3:D:102:THR:HG21	1.83	0.60
3:H:91:MET:HA	3:H:96:LEU:HD22	1.83	0.60
3:B:39:LYS:HE2	3:B:81:GLU:O	2.01	0.59
2:E:171:GLN:NE2	2:E:177:SER:HB3	2.17	0.59
2:A:200:HIS:ND1	2:A:203:SER:HB3	2.17	0.59
2:E:97:TYR:CE2	1:L:519:MET:HE3	2.38	0.59
3:D:13:ALA:HB1	3:D:17:ASP:OD2	2.02	0.59
3:F:83:PHE:CD2	3:F:106:ILE:HG12	2.38	0.59
2:E:159:LEU:HD21	2:E:182:VAL:HG11	1.84	0.58
2:C:197:ASN:ND2	2:C:208:ASP:OD1	2.23	0.58
3:H:150:VAL:HG23	3:H:155:GLN:HG3	1.86	0.58
2:G:19:LYS:NZ	4:G:309:HOH:O	2.37	0.57
2:G:164:HIS:CE1	3:H:138:ASN:HD21	2.23	0.57
4:G:349:HOH:O	3:H:32:GLU:HG2	2.04	0.57
2:E:155:ASN:HD21	2:E:195:ILE:H	1.54	0.56
3:B:150:VAL:HG23	3:B:155:GLN:HG3	1.87	0.56
2:G:100(A):GLU:OE2	4:G:301:HOH:O	2.18	0.56
2:E:155:ASN:ND2	2:E:195:ILE:H	2.04	0.55
2:C:11:VAL:HG21	2:C:147:PRO:HG3	1.88	0.55
2:C:200:HIS:ND1	2:C:203:SER:HB3	2.22	0.55
2:E:200:HIS:ND1	2:E:203:SER:HB3	2.21	0.55
2:C:168:ALA:HA	2:C:178:LEU:HB3	1.88	0.55
3:H:39:LYS:HG3	3:H:84:ALA:HB2	1.87	0.55
2:C:2:LYS:HG3	2:C:3:VAL:HG23	1.89	0.54
3:F:149:LYS:NZ	4:F:309:HOH:O	2.33	0.54
3:F:201:LEU:HD13	3:F:205:VAL:HG13	1.89	0.53
2:E:100(A):GLU:HA	4:L:601:HOH:O	2.09	0.53
3:B:170:ASP:HB3	3:B:172:THR:HG23	1.89	0.53
2:C:155:ASN:ND2	2:C:195:ILE:H	2.07	0.53
3:B:91:MET:HA	3:B:96:LEU:HD22	1.90	0.53
2:C:33:PRO:HG3	1:K:519:MET:HE3	1.90	0.52
3:B:30:ARG:O	3:B:32:GLU:HG3	2.09	0.52
3:H:37:GLN:HB2	3:H:47:LEU:HD11	1.91	0.52
3:F:78:LEU:HD13	3:F:83:PHE:CE1	2.45	0.52
2:C:159:LEU:HD21	2:C:182:VAL:HG11	1.91	0.52
2:A:168:ALA:HA	2:A:178:LEU:HB3	1.91	0.52
2:G:183:THR:OG1	4:G:302:HOH:O	2.19	0.52
3:B:39:LYS:HD3	3:B:84:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:168:ALA:HB2	2:A:178:LEU:HD23	1.91	0.52
3:D:3:GLN:NE2	4:D:305:HOH:O	2.25	0.51
3:F:132:VAL:HG12	3:F:148:TRP:CH2	2.45	0.51
2:E:123:PRO:HD3	2:E:209:LYS:HE3	1.92	0.51
2:C:155:ASN:HD21	2:C:195:ILE:H	1.58	0.51
2:E:19:LYS:HE2	2:E:81:ASP:OD2	2.11	0.51
3:D:32:GLU:OE1	1:K:512:ALA:N	2.44	0.51
2:E:168:ALA:HA	2:E:178:LEU:HB3	1.93	0.51
3:B:167:ASP:OD1	3:B:169:LYS:N	2.38	0.51
3:D:83:PHE:CD2	3:D:106:ILE:HG12	2.47	0.50
2:G:100(A):GLU:HG2	1:M:512:ALA:HB3	1.92	0.50
3:F:149:LYS:HB2	3:F:193:ALA:HB3	1.94	0.50
2:A:42:GLY:C	2:A:43:GLN:HG2	2.32	0.50
3:D:14:SER:HB3	3:D:107:LYS:O	2.11	0.50
2:G:119:PRO:HB3	2:G:145:TYR:HB3	1.94	0.50
2:G:11:VAL:HG21	2:G:147:PRO:HG3	1.94	0.50
3:H:39:LYS:H	3:H:42:LYS:CE	2.14	0.50
3:B:37:GLN:HB2	3:B:47:LEU:HD11	1.94	0.49
3:D:78:LEU:HD13	3:D:83:PHE:CE1	2.47	0.49
2:G:154:TRP:CH2	2:G:196:CYS:HB3	2.48	0.49
3:H:156:SER:O	3:H:156:SER:OG	2.27	0.49
3:H:170:ASP:HB3	3:H:172:THR:HG23	1.95	0.49
2:A:119:PRO:HB3	2:A:145:TYR:HB3	1.94	0.49
3:D:132:VAL:HG12	3:D:148:TRP:CH2	2.48	0.48
2:E:119:PRO:HB3	2:E:145:TYR:HB3	1.94	0.48
3:F:204:PRO:HB2	3:B:204:PRO:HG2	1.95	0.48
3:F:201:LEU:O	3:B:149:LYS:NZ	2.47	0.48
3:H:30:ARG:O	3:H:32:GLU:HG3	2.14	0.48
3:H:197:THR:HA	4:H:322:HOH:O	2.14	0.48
3:F:164:THR:O	4:F:305:HOH:O	2.19	0.48
2:G:168:ALA:HA	2:G:178:LEU:HB3	1.96	0.48
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.96	0.47
3:F:105:GLU:HG2	3:F:106:ILE:N	2.28	0.47
2:C:19:LYS:HE2	2:C:81:ASP:OD2	2.15	0.47
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.96	0.47
3:D:156:SER:O	3:D:156:SER:OG	2.27	0.47
2:E:122:PHE:HD2	2:E:141:LEU:HD23	1.79	0.47
2:C:122:PHE:HD2	2:C:141:LEU:HD23	1.80	0.47
1:I:513:VAL:HG21	3:B:94:TYR:CE1	2.50	0.47
2:E:197:ASN:ND2	2:E:208:ASP:OD1	2.40	0.47
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:149:LYS:HB2	3:D:193:ALA:HB3	1.95	0.47
2:C:97:TYR:OH	1:K:517:GLY:O	2.24	0.47
2:A:94:ARG:NH2	2:A:101:ASP:OD2	2.41	0.47
3:B:156:SER:O	3:B:156:SER:OG	2.26	0.47
2:E:171:GLN:HE22	2:E:177:SER:CB	2.26	0.47
3:H:42:LYS:HD2	3:H:43:ALA:O	2.16	0.46
3:F:66:GLY:HA3	3:F:71:PHE:CD2	2.51	0.46
3:F:150:VAL:HG12	3:F:151:ASP:N	2.31	0.46
2:A:67:VAL:HG22	2:A:82:VAL:HG22	1.96	0.46
3:F:14:SER:N	3:F:17:ASP:OD2	2.49	0.46
2:G:30:THR:HB	2:G:53:HIS:HB2	1.97	0.46
3:F:161:GLU:HG2	3:F:175:LEU:HD21	1.98	0.45
2:E:185:PRO:HG2	2:E:188:SER:HB3	1.97	0.45
2:E:188:SER:H	2:E:189:LEU:HD12	1.81	0.45
3:F:156:SER:O	3:F:156:SER:OG	2.27	0.45
3:B:61:ARG:NE	3:B:79:GLN:HG3	2.32	0.45
2:E:96:LYS:HE3	2:E:101:ASP:OD2	2.17	0.45
2:E:2:LYS:HB3	2:E:26:GLY:HA3	1.99	0.45
3:B:105:GLU:HG2	3:B:106:ILE:N	2.31	0.45
3:D:30:ARG:O	3:D:32:GLU:HG3	2.17	0.45
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.99	0.45
3:B:150:VAL:HG12	3:B:151:ASP:N	2.32	0.44
3:B:196:VAL:HB	3:B:205:VAL:HG12	1.97	0.44
3:D:16:GLY:HA2	3:D:77:SER:HB2	1.99	0.44
3:H:150:VAL:HG12	3:H:151:ASP:N	2.31	0.44
2:A:193:THR:HA	4:A:301:HOH:O	2.16	0.44
2:C:154:TRP:CH2	2:C:196:CYS:HB3	2.53	0.44
3:H:167:ASP:OD1	3:H:169:LYS:N	2.41	0.44
2:A:198:VAL:O	2:A:206:LYS:HA	2.18	0.44
2:G:94:ARG:NH2	2:G:101:ASP:OD2	2.44	0.44
2:C:195:ILE:HG12	2:C:210:LYS:HA	2.00	0.43
2:E:30:THR:HB	2:E:53:HIS:HB2	2.00	0.43
2:A:2:LYS:HB3	2:A:26:GLY:HA3	2.01	0.43
2:E:168:ALA:HB2	2:E:178:LEU:HD23	2.01	0.43
2:G:151:THR:OG1	2:G:199:ASN:HB3	2.19	0.43
3:B:180:THR:C	3:B:181:LEU:HD12	2.38	0.43
2:E:47:TRP:O	4:E:302:HOH:O	2.21	0.43
2:A:155:ASN:HD21	2:A:194:TYR:HD1	1.67	0.43
2:E:154:TRP:CH2	2:E:196:CYS:HB3	2.53	0.43
1:I:512:ALA:HB3	2:A:100(A):GLU:HG2	2.01	0.43
3:H:105:GLU:HG2	3:H:106:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:THR:HB	2:C:53:HIS:HB2	2.01	0.42
2:A:11:VAL:HG21	2:A:147:PRO:HG3	2.00	0.42
3:D:150:VAL:HG12	3:D:151:ASP:N	2.35	0.42
3:D:105:GLU:HG2	3:D:106:ILE:N	2.34	0.42
2:A:184:VAL:HG11	2:A:194:TYR:CZ	2.55	0.42
2:G:122:PHE:HD2	2:G:141:LEU:HD23	1.84	0.42
3:D:66:GLY:HA3	3:D:71:PHE:CD2	2.55	0.41
3:D:137:ASN:ND2	3:D:138:ASN:OD1	2.53	0.41
2:C:61:GLN:H	2:C:61:GLN:CD	2.24	0.41
2:G:212:GLU:HA	2:G:213:PRO:HD3	1.91	0.41
3:F:21:ILE:HD12	3:F:102:THR:HG21	2.02	0.41
2:A:96:LYS:HE3	2:A:101:ASP:OD1	2.20	0.41
3:F:140:TYR:CG	3:F:141:PRO:HA	2.55	0.41
3:F:192:TYR:HB2	3:F:209:PHE:CE1	2.56	0.41
2:A:61:GLN:OE1	2:A:61:GLN:N	2.44	0.41
3:F:150:VAL:HG23	3:F:155:GLN:HG3	2.03	0.40
2:G:2:LYS:HB3	2:G:26:GLY:HA3	2.02	0.40
3:H:119:PRO:HB3	3:H:209:PHE:CE1	2.57	0.40
2:C:123:PRO:HD3	2:C:209:LYS:HE2	2.03	0.40
3:D:170:ASP:HB3	3:D:172:THR:HG23	2.03	0.40
3:H:151:ASP:OD2	3:H:191:VAL:HG12	2.21	0.40
3:B:81:GLU:H	3:B:81:GLU:HG2	1.59	0.40
3:D:15:VAL:HG13	3:D:79:GLN:HA	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:349:HOH:O	4:G:354:HOH:O[4_455]	2.01	0.19

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	I	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	K	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	L	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	M	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	A	209/234 (89%)	195 (93%)	12 (6%)	2 (1%)	15	37
2	C	209/234 (89%)	196 (94%)	12 (6%)	1 (0%)	29	54
2	E	209/234 (89%)	193 (92%)	14 (7%)	2 (1%)	15	37
2	G	209/234 (89%)	195 (93%)	12 (6%)	2 (1%)	15	37
3	B	210/214 (98%)	195 (93%)	12 (6%)	3 (1%)	11	28
3	D	210/214 (98%)	195 (93%)	12 (6%)	3 (1%)	11	28
3	F	210/214 (98%)	195 (93%)	12 (6%)	3 (1%)	11	28
3	H	210/214 (98%)	195 (93%)	12 (6%)	3 (1%)	11	28
All	All	1700/1824 (93%)	1579 (93%)	102 (6%)	19 (1%)	14	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	211	ARG
3	D	211	ARG
2	E	172	SER
3	F	150	VAL
3	F	211	ARG
3	B	2	ILE
3	B	150	VAL
3	D	150	VAL
3	H	2	ILE
3	H	150	VAL
3	H	211	ARG
3	F	2	ILE
3	D	2	ILE
2	G	136	ALA
2	E	136	ALA
2	A	136	ALA
2	C	136	ALA
2	G	153	SER
2	A	153	SER

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	I	4/4 (100%)	4 (100%)	0	100 100
1	K	4/4 (100%)	4 (100%)	0	100 100
1	L	4/4 (100%)	4 (100%)	0	100 100
1	M	4/4 (100%)	3 (75%)	1 (25%)	0 1
2	A	178/198 (90%)	169 (95%)	9 (5%)	24 50
2	C	178/198 (90%)	168 (94%)	10 (6%)	21 45
2	E	178/198 (90%)	170 (96%)	8 (4%)	27 55
2	G	178/198 (90%)	170 (96%)	8 (4%)	27 55
3	B	172/187 (92%)	163 (95%)	9 (5%)	23 49
3	D	172/187 (92%)	165 (96%)	7 (4%)	30 59
3	F	172/187 (92%)	161 (94%)	11 (6%)	17 39
3	H	172/187 (92%)	163 (95%)	9 (5%)	23 49
All	All	1416/1556 (91%)	1344 (95%)	72 (5%)	24 50

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	50	TRP
2	E	71	ARG
2	E	138	LEU
2	E	140	CYS
2	E	153	SER
2	E	187	SER
2	E	196	CYS
2	E	203	SER
3	F	9	SER
3	F	18	LYS
3	F	26	SER
3	F	33	LEU
3	F	56	SER
3	F	63	SER

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Mol	Chain	Res	Type
3	F	76	SER
3	F	91	MET
3	F	108	ARG
3	F	145	LYS
3	F	202	SER
2	A	43	GLN
2	A	50	TRP
2	A	71	ARG
2	A	115	SER
2	A	153	SER
2	A	172	SER
2	A	196	CYS
2	A	197	ASN
2	A	203	SER
2	C	50	TRP
2	C	71	ARG
2	C	138	LEU
2	C	140	CYS
2	C	153	SER
2	C	179	SER
2	C	196	CYS
2	C	197	ASN
2	C	199	ASN
2	C	203	SER
2	G	50	TRP
2	G	71	ARG
2	G	115	SER
2	G	140	CYS
2	G	172	SER
2	G	193	THR
2	G	196	CYS
2	G	197	ASN
3	B	14	SER
3	B	26	SER
3	B	31	ASN
3	B	33	LEU
3	B	77	SER
3	B	79	GLN
3	B	91	MET
3	B	92	SER
3	B	211	ARG
3	D	19	VAL

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Mol	Chain	Res	Type
3	D	26	SER
3	D	33	LEU
3	D	56	SER
3	D	63	SER
3	D	91	MET
3	D	108	ARG
3	H	31	ASN
3	H	33	LEU
3	H	42	LYS
3	H	77	SER
3	H	91	MET
3	H	92	SER
3	H	151	ASP
3	H	202	SER
3	H	211	ARG
1	M	516	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	155	ASN
2	E	171	GLN
3	F	45	ASN
2	A	76	ASN
2	A	164	HIS
2	A	171	GLN
2	C	61	GLN
2	C	155	ASN
2	C	171	GLN
2	C	199	ASN
2	G	164	HIS
3	B	31	ASN
3	D	137	ASN
3	H	70	HIS
3	H	138	ASN
3	H	160	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	I	8/8 (100%)	1.14	1 (12%) 3 3	35, 42, 53, 57	0
1	K	8/8 (100%)	0.64	0 100 100	35, 42, 49, 54	0
1	L	8/8 (100%)	1.06	1 (12%) 3 3	38, 50, 56, 56	0
1	M	8/8 (100%)	0.55	0 100 100	35, 41, 51, 55	0
2	A	213/234 (91%)	0.21	6 (2%) 53 54	21, 32, 70, 81	0
2	C	213/234 (91%)	0.13	4 (1%) 66 69	22, 32, 63, 86	0
2	E	213/234 (91%)	0.15	3 (1%) 75 77	22, 33, 63, 84	0
2	G	213/234 (91%)	0.25	8 (3%) 40 39	20, 32, 69, 81	0
3	B	212/214 (99%)	0.33	6 (2%) 53 54	25, 41, 63, 71	0
3	D	212/214 (99%)	0.36	3 (1%) 75 77	28, 45, 61, 71	0
3	F	212/214 (99%)	0.34	4 (1%) 66 69	28, 45, 59, 67	0
3	H	212/214 (99%)	0.30	4 (1%) 66 69	25, 41, 62, 75	0
All	All	1732/1824 (94%)	0.27	40 (2%) 60 62	20, 41, 63, 86	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	136	ALA	4.6
3	H	156	SER	4.4
2	E	189	LEU	4.0
2	G	189	LEU	3.6
2	E	191	THR	3.6
2	A	136	ALA	3.5
3	B	1	ASP	3.4
2	C	126	PRO	3.3
1	I	512	ALA	3.3
2	E	187	SER	3.1
2	A	194	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	30	ARG	2.9
2	G	211	VAL	2.9
3	D	15	VAL	2.8
2	G	152	VAL	2.8
3	D	67	SER	2.8
3	B	30	ARG	2.8
2	A	125	ALA	2.7
2	G	191	THR	2.7
3	F	67	SER	2.7
2	A	210	LYS	2.6
2	A	191	THR	2.6
2	G	125	ALA	2.6
3	B	210	ASN	2.6
3	B	119	PRO	2.5
3	D	30	ARG	2.5
2	A	135	THR	2.4
2	G	195	ILE	2.4
3	H	30	ARG	2.4
3	H	1	ASP	2.3
3	B	184	ALA	2.3
2	G	185	PRO	2.3
1	L	515	THR	2.3
3	F	181	LEU	2.2
2	C	204	ASN	2.2
3	B	76	SER	2.2
2	G	193	THR	2.2
3	H	67	SER	2.1
2	C	135	THR	2.1
3	F	10	PHE	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.