



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:33 PM UTC

PDB ID : 6BZU / pdb_00006bzu
Title : Structure of the Hepatitis C virus envelope glycoprotein E2 antigenic region
412-423 bound to the broadly neutralizing antibody 19B3
Authors : Tzarum, N.; Aleman, F.; Kong, L.; Wilson, I.A.; Law, M.
Deposited on : 2017-12-26
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 : 4-5-2 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

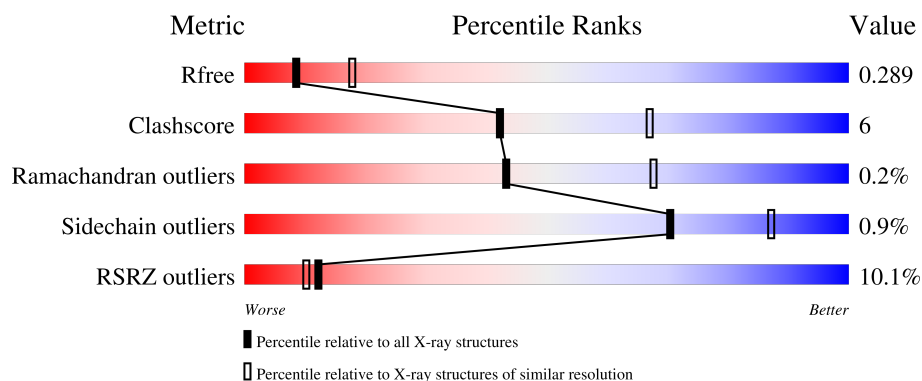
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	223	9% 85%13%
1	C	223	9% 85%13%
1	E	223	13% 72%14%14%
1	G	223	6% 80%18%
2	B	219	8% 79%20%

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Mol	Chain	Length	Quality of chain
2	D	219	
2	F	219	
2	H	219	
3	I	13	
3	J	13	
3	K	13	
3	L	13	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13547 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 19B3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1644	1035	270	332	7			
1	C	218	Total	C	N	O	S	0	0	0
			1646	1035	270	334	7			
1	E	192	Total	C	N	O	S	0	0	0
			1482	937	242	296	7			
1	G	220	Total	C	N	O	S	0	0	0
			1661	1044	273	337	7			

- Molecule 2 is a protein called 19B3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1647	1025	278	339	5			
2	D	214	Total	C	N	O	S	0	0	0
			1630	1014	276	335	5			
2	F	214	Total	C	N	O	S	0	0	0
			1636	1018	276	337	5			
2	H	215	Total	C	N	O	S	0	0	0
			1638	1020	277	336	5			

- Molecule 3 is a protein called E2 AS412 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	0	0	0
			73	46	14	13			
3	J	10	Total	C	N	O	0	0	0
			82	51	16	15			
3	K	11	Total	C	N	O	0	0	0
			90	57	17	16			
3	L	12	Total	C	N	O	0	0	0
			98	61	19	18			

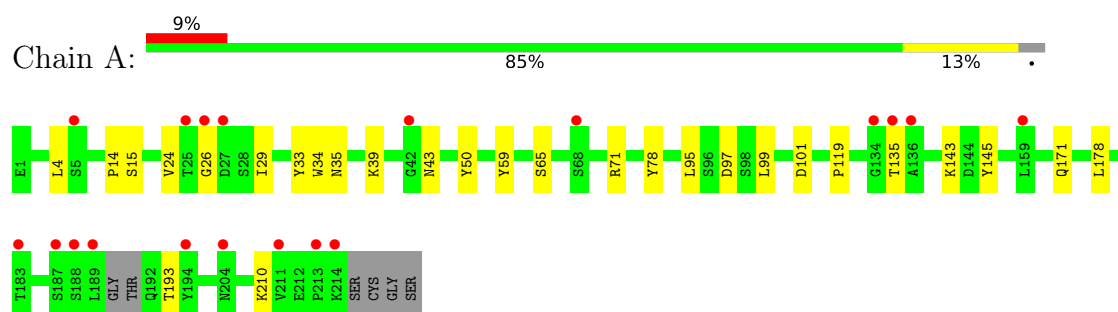
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	29	Total 29	O 29	0	0
4	C	24	Total 24	O 24	0	0
4	D	32	Total 32	O 32	0	0
4	E	26	Total 26	O 26	0	0
4	F	24	Total 24	O 24	0	0
4	G	34	Total 34	O 34	0	0
4	H	21	Total 21	O 21	0	0
4	I	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0
4	K	2	Total 2	O 2	0	0
4	L	2	Total 2	O 2	0	0

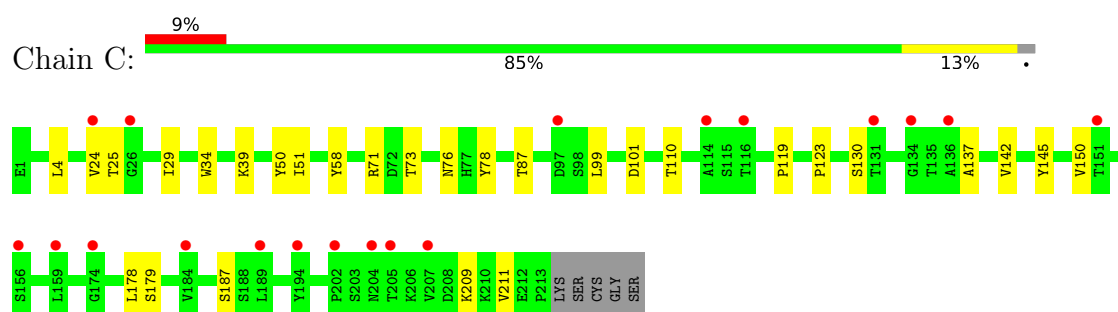
3 Residue-property plots [i](#)

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.

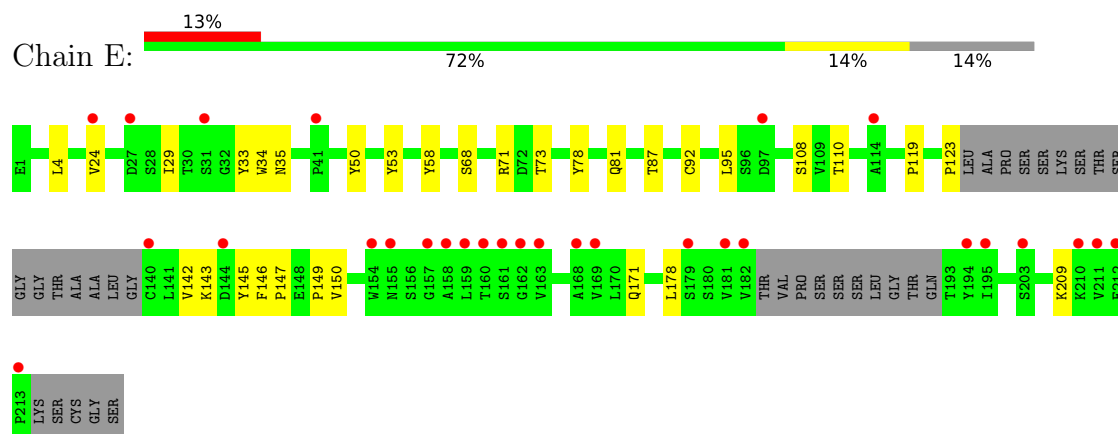
• Molecule 1: 19B3 Heavy Chain



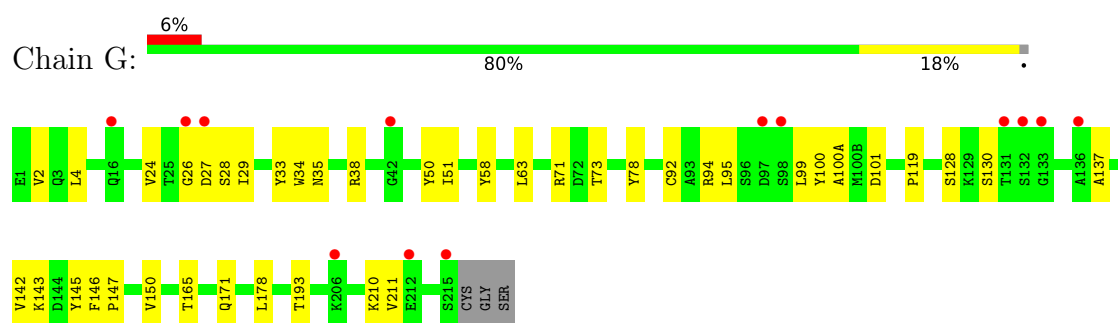
• Molecule 1: 19B3 Heavy Chain



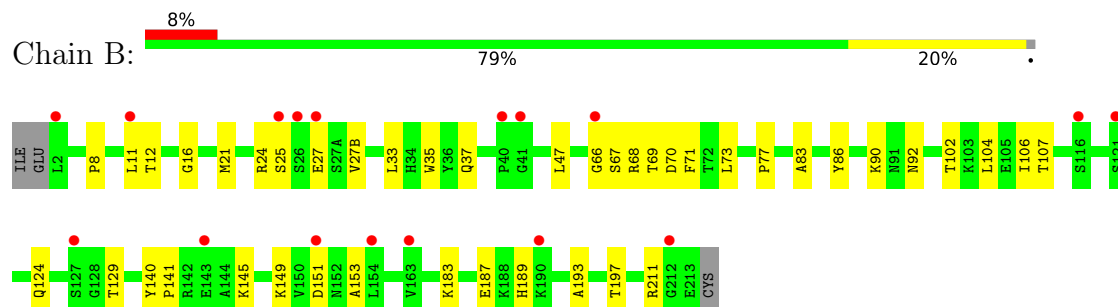
• Molecule 1: 19B3 Heavy Chain



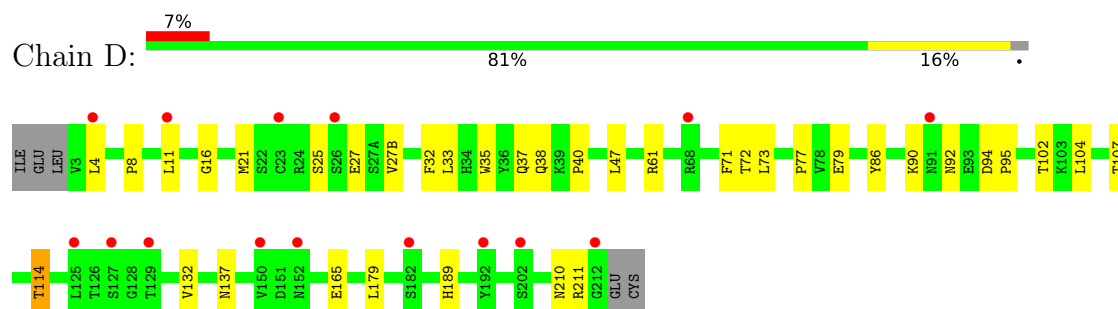
• Molecule 1: 19B3 Heavy Chain



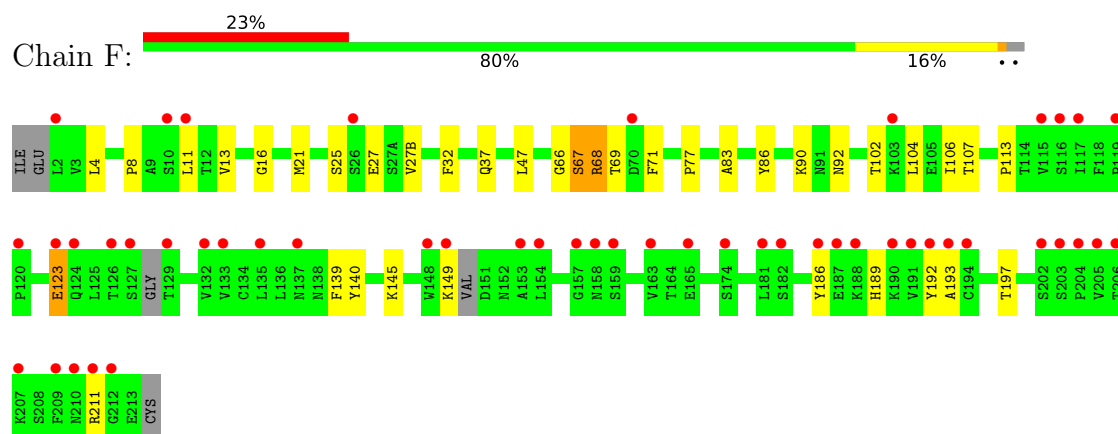
• Molecule 2: 19B3 Light Chain



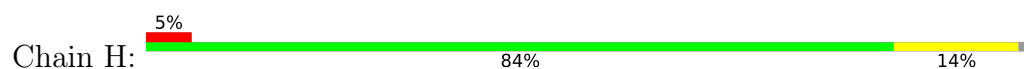
• Molecule 2: 19B3 Light Chain

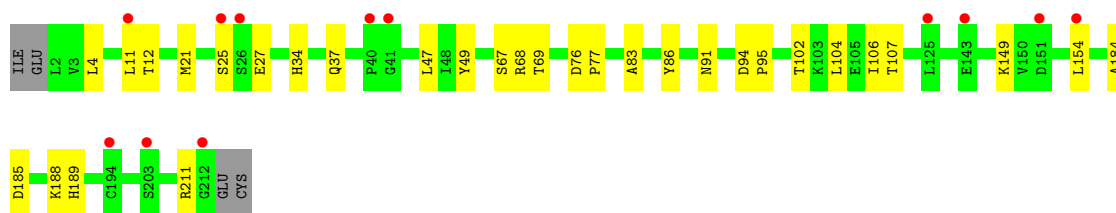


• Molecule 2: 19B3 Light Chain

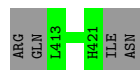


• Molecule 2: 19B3 Light Chain

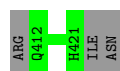
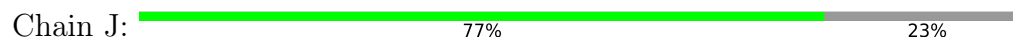




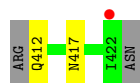
- Molecule 3: E2 AS412 peptide



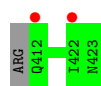
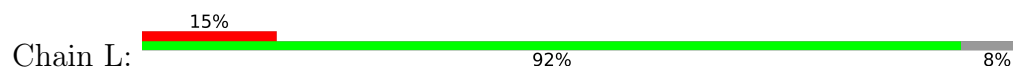
- Molecule 3: E2 AS412 peptide



- Molecule 3: E2 AS412 peptide



- Molecule 3: E2 AS412 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.70Å 55.60Å 155.26Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	29.82 – 2.70 29.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.82-2.70) 98.6 (29.82-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.265 , 0.290 0.265 , 0.289	Depositor DCC
R_{free} test set	3028 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13547	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6300e-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 [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	0.11	0/1684	0.32	0/2297
1	C	0.11	0/1687	0.32	0/2304
1	E	0.12	0/1519	0.33	0/2071
1	G	0.12	0/1702	0.34	0/2323
2	B	0.11	0/1683	0.35	0/2291
2	D	0.12	0/1666	0.36	0/2268
2	F	0.12	0/1670	0.35	0/2270
2	H	0.11	0/1674	0.34	0/2279
3	I	0.07	0/75	0.21	0/102
3	J	0.07	0/84	0.20	0/114
3	K	0.08	0/92	0.27	0/125
3	L	0.08	0/100	0.24	0/136
All	All	0.11	0/13636	0.34	0/18580

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	1644	0	1603	16	0
1	C	1646	0	1601	20	0
1	E	1482	0	1432	18	0
1	G	1661	0	1619	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1647	0	1584	24	0
2	D	1630	0	1567	22	0
2	F	1636	0	1570	23	0
2	H	1638	0	1578	21	0
3	I	73	0	65	0	0
3	J	82	0	73	0	0
3	K	90	0	84	1	0
3	L	98	0	90	0	0
4	A	23	0	0	0	0
4	B	29	0	0	0	0
4	C	24	0	0	1	0
4	D	32	0	0	1	0
4	E	26	0	0	0	0
4	F	24	0	0	0	0
4	G	34	0	0	1	0
4	H	21	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
All	All	13547	0	12866	164	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 (164) 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:2:VAL:HA	1:G:26:GLY:HA3	1.54	0.87
2:B:66:GLY:HA3	2:B:71:PHE:HA	1.63	0.78
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.75	0.69
2:D:40:PRO:HG2	2:D:165:GLU:HG3	1.75	0.69
1:C:29:ILE:HD11	1:C:73:THR:HA	1.77	0.66
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.78	0.65
1:A:39:LYS:NZ	1:A:43:ASN:OD1	2.30	0.65
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.79	0.64
1:C:130:SER:HB2	1:C:137:ALA:HB3	1.79	0.64
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.79	0.63
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.79	0.63
2:B:21:MET:HE1	2:B:86:TYR:HB2	1.81	0.63
2:B:24:ARG:NE	2:B:70:ASP:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:MET:HE1	2:H:86:TYR:HB2	1.81	0.62
2:F:21:MET:HE1	2:F:86:TYR:HB2	1.80	0.62
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.81	0.61
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.82	0.61
2:F:189:HIS:O	2:F:211:ARG:NH1	2.33	0.60
1:A:193:THR:HG23	1:A:210:LYS:HE3	1.84	0.60
1:A:143:LYS:NZ	1:A:171:GLN:OE1	2.34	0.60
2:D:21:MET:HG2	2:D:102:THR:HG21	1.83	0.60
2:B:11:LEU:HD23	2:B:104:LEU:HD13	1.84	0.59
2:H:189:HIS:O	2:H:211:ARG:NH1	2.35	0.59
1:C:71:ARG:HA	1:C:78:TYR:HA	1.86	0.58
1:G:99:LEU:HD12	1:G:101:ASP:HB3	1.84	0.58
2:D:11:LEU:HD23	2:D:104:LEU:HD13	1.86	0.58
1:E:143:LYS:NZ	1:E:171:GLN:OE1	2.38	0.57
1:G:29:ILE:HD11	1:G:73:THR:HA	1.86	0.57
2:H:11:LEU:HD23	2:H:104:LEU:HD13	1.86	0.56
2:F:27(B):VAL:HG12	2:F:90:LYS:HE2	1.85	0.56
2:B:21:MET:HG2	2:B:102:THR:HG21	1.87	0.56
2:D:8:PRO:HG3	2:D:11:LEU:HD13	1.88	0.56
2:F:83:ALA:HB2	2:F:106:ILE:HG12	1.87	0.56
1:G:4:LEU:HD22	1:G:24:VAL:HG12	1.88	0.56
2:D:210:ASN:ND2	4:D:306:HOH:O	2.39	0.56
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.88	0.55
1:G:143:LYS:NZ	1:G:171:GLN:OE1	2.39	0.55
2:F:11:LEU:HD23	2:F:104:LEU:HD13	1.89	0.55
2:D:21:MET:HE1	2:D:86:TYR:HB2	1.88	0.55
1:E:108:SER:HB3	1:E:149:PRO:HD3	1.88	0.55
1:A:71:ARG:HA	1:A:78:TYR:HA	1.89	0.55
1:C:142:VAL:HB	1:C:178:LEU:HG	1.89	0.54
1:G:142:VAL:HG11	1:G:150:VAL:HG11	1.90	0.54
2:H:83:ALA:HB2	2:H:106:ILE:HG12	1.89	0.54
2:F:16:GLY:HA2	2:F:77:PRO:HB2	1.90	0.54
2:B:189:HIS:O	2:B:211:ARG:NH1	2.41	0.54
2:D:189:HIS:O	2:D:211:ARG:NH1	2.41	0.54
2:H:25:SER:HB3	2:H:69:THR:HA	1.91	0.52
2:D:27(B):VAL:HG12	2:D:90:LYS:HE2	1.92	0.52
2:F:21:MET:HG2	2:F:102:THR:HG21	1.92	0.52
1:G:71:ARG:HA	1:G:78:TYR:HA	1.92	0.51
1:A:4:LEU:HD22	1:A:24:VAL:HG12	1.91	0.51
2:H:185:ASP:HA	2:H:188:LYS:HD3	1.92	0.51
1:C:4:LEU:HD22	1:C:24:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:PRO:HD3	1:E:209:LYS:HE2	1.93	0.50
1:E:68:SER:HB3	1:E:81:GLN:HB2	1.94	0.50
1:E:87:THR:HG23	1:E:110:THR:HA	1.93	0.50
1:A:33:TYR:HB2	1:A:95:LEU:HB3	1.94	0.50
1:G:100:TYR:O	2:H:91:ASN:ND2	2.45	0.50
2:H:149:LYS:HE2	2:H:154:LEU:HD12	1.93	0.50
2:F:32:PHE:HB2	2:F:92:ASN:HB3	1.94	0.49
2:H:25:SER:OG	2:H:27:GLU:O	2.23	0.49
2:D:32:PHE:HB2	2:D:92:ASN:HB3	1.94	0.49
1:E:4:LEU:HD22	1:E:24:VAL:HG12	1.95	0.49
2:F:186:TYR:O	2:F:192:TYR:OH	2.31	0.49
2:H:21:MET:HG2	2:H:102:THR:HG21	1.94	0.49
1:G:33:TYR:HB2	1:G:95:LEU:HB3	1.93	0.48
1:G:34:TRP:HB3	1:G:78:TYR:CZ	2.48	0.48
1:G:100(A):ALA:HB2	2:H:34:HIS:CE1	2.48	0.48
1:A:14:PRO:O	1:A:15:SER:OG	2.30	0.48
1:A:59:TYR:CE2	1:C:25:THR:HG21	2.49	0.48
1:G:24:VAL:HG21	1:G:29:ILE:HG23	1.96	0.48
2:B:16:GLY:HA2	2:B:77:PRO:HB2	1.96	0.47
1:E:53:TYR:O	1:E:71:ARG:NH2	2.44	0.47
1:G:50:TYR:CE2	1:G:58:TYR:HB3	2.48	0.47
2:H:25:SER:C	2:H:27:GLU:H	2.22	0.47
2:B:27(B):VAL:HG12	2:B:90:LYS:HE2	1.96	0.47
2:F:145:LYS:HB3	2:F:197:THR:HB	1.96	0.47
2:B:83:ALA:HB2	2:B:106:ILE:HG12	1.95	0.47
1:E:33:TYR:HB2	1:E:95:LEU:HB3	1.94	0.47
2:H:12:THR:HG22	2:H:107:THR:OG1	2.15	0.47
1:E:78:TYR:OH	1:E:92:CYS:HB2	2.15	0.46
2:B:145:LYS:HB3	2:B:197:THR:HB	1.97	0.46
1:C:39:LYS:HD2	2:D:38:GLN:NE2	2.31	0.46
2:D:61:ARG:CZ	2:D:79:GLU:HG3	2.45	0.46
2:D:114:THR:HG23	2:D:137:ASN:HB3	1.97	0.46
2:F:149:LYS:HB2	2:F:193:ALA:HB3	1.97	0.46
2:B:124:GLN:HG2	2:B:129:THR:O	2.16	0.46
2:B:12:THR:HG22	2:B:107:THR:OG1	2.15	0.45
2:D:4:LEU:HD23	2:D:25:SER:HA	1.98	0.45
2:F:66:GLY:HA3	2:F:71:PHE:CD2	2.52	0.45
1:G:130:SER:HB2	1:G:137:ALA:HB3	1.98	0.45
2:B:140:TYR:CG	2:B:141:PRO:HA	2.52	0.45
2:B:183:LYS:O	2:B:187:GLU:HG3	2.17	0.45
1:C:50:TYR:CE2	1:C:58:TYR:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:VAL:HG11	1:E:150:VAL:HG11	1.98	0.45
1:C:142:VAL:HG11	1:C:150:VAL:HG11	1.99	0.45
1:C:99:LEU:HD12	1:C:101:ASP:HB3	1.99	0.44
2:F:25:SER:C	2:F:27:GLU:H	2.24	0.44
2:D:33:LEU:HD13	2:D:71:PHE:CD1	2.53	0.44
1:A:35:ASN:OD1	1:A:50:TYR:HB3	2.17	0.44
1:C:34:TRP:HB3	1:C:78:TYR:CZ	2.53	0.44
1:C:51:ILE:HD13	1:C:71:ARG:HB3	1.99	0.44
2:F:25:SER:OG	2:F:27:GLU:O	2.26	0.44
1:G:27:ASP:OD1	1:G:28:SER:N	2.50	0.44
2:H:184:ALA:O	2:H:188:LYS:HG3	2.17	0.44
2:D:132:VAL:HB	2:D:179:LEU:HB3	1.99	0.44
2:F:11:LEU:HG	2:F:13:VAL:HG23	1.99	0.44
2:H:76:ASP:HA	2:H:77:PRO:HA	1.89	0.43
2:F:123:GLU:CD	2:F:123:GLU:H	2.26	0.43
1:C:145:TYR:OH	1:C:178:LEU:HD23	2.18	0.43
1:E:71:ARG:HA	1:E:78:TYR:HA	1.98	0.43
1:A:39:LYS:HZ1	1:A:43:ASN:HA	1.84	0.43
1:C:123:PRO:HD3	1:C:209:LYS:HE2	2.00	0.43
2:H:67:SER:O	2:H:69:THR:N	2.52	0.43
1:G:34:TRP:CZ3	1:G:94:ARG:HB2	2.54	0.43
1:E:34:TRP:HB3	1:E:78:TYR:CZ	2.54	0.43
2:B:67:SER:O	2:B:69:THR:N	2.51	0.42
2:B:151:ASP:OD2	2:B:189:HIS:ND1	2.36	0.42
2:F:25:SER:HB3	2:F:69:THR:HA	2.01	0.42
1:C:87:THR:HG23	1:C:110:THR:HA	2.00	0.42
1:A:99:LEU:HD12	1:A:101:ASP:HB3	2.02	0.42
2:B:149:LYS:HB2	2:B:193:ALA:HB3	2.02	0.42
1:A:24:VAL:HG21	1:A:29:ILE:HG23	2.02	0.42
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.54	0.42
2:B:25:SER:C	2:B:27:GLU:H	2.27	0.42
1:G:78:TYR:OH	1:G:92:CYS:HB2	2.19	0.42
1:G:165:THR:HG23	1:G:178:LEU:HD21	2.01	0.42
1:A:65:SER:HA	1:C:76:ASN:ND2	2.35	0.42
2:B:8:PRO:HG3	2:B:11:LEU:HD13	2.02	0.42
2:B:33:LEU:HD13	2:B:71:PHE:CD1	2.55	0.42
1:G:38:ARG:NH2	1:G:63:LEU:HD21	2.35	0.42
2:D:27(B):VAL:HA	2:D:92:ASN:ND2	2.34	0.42
2:F:107:THR:HA	2:F:140:TYR:OH	2.19	0.41
1:C:39:LYS:HD2	2:D:38:GLN:HE22	1.85	0.41
1:E:24:VAL:HG21	1:E:29:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HA	1:A:34:TRP:NE1	2.35	0.41
2:H:4:LEU:HD23	2:H:25:SER:HA	2.02	0.41
1:E:50:TYR:CE2	1:E:58:TYR:HB3	2.56	0.41
1:G:193:THR:HG23	1:G:210:LYS:HE3	2.03	0.41
2:D:35:TRP:CE2	2:D:73:LEU:HB2	2.56	0.41
2:F:4:LEU:HD11	2:F:90:LYS:HB3	2.02	0.41
1:G:128:SER:O	4:G:301:HOH:O	2.21	0.41
2:D:16:GLY:HA2	2:D:77:PRO:HB2	2.03	0.41
1:G:99:LEU:HD22	2:H:49:TYR:CG	2.55	0.41
1:G:146:PHE:HA	1:G:147:PRO:HA	1.84	0.41
2:H:94:ASP:HA	2:H:95:PRO:HA	1.88	0.41
1:A:35:ASN:HD21	1:A:95:LEU:HB2	1.85	0.41
2:B:27(B):VAL:HA	2:B:92:ASN:ND2	2.36	0.41
2:B:151:ASP:C	2:B:153:ALA:H	2.28	0.41
1:C:29:ILE:HA	1:C:34:TRP:NE1	2.35	0.41
2:F:67:SER:O	2:F:69:THR:N	2.54	0.41
1:G:35:ASN:OD1	1:G:50:TYR:HB3	2.21	0.41
1:E:146:PHE:HA	1:E:147:PRO:HA	1.84	0.40
2:D:25:SER:C	2:D:27:GLU:H	2.29	0.40
1:E:29:ILE:HD11	1:E:73:THR:HA	2.01	0.40
2:F:8:PRO:HG3	2:F:11:LEU:HD13	2.04	0.40
2:D:94:ASP:HA	2:D:95:PRO:HA	1.85	0.40
1:E:35:ASN:OD1	1:E:50:TYR:HB3	2.21	0.40
1:G:51:ILE:HD13	1:G:71:ARG:HB3	2.04	0.40
2:H:21:MET:HE3	2:H:102:THR:HB	2.04	0.40
3:K:412:GLN:N	3:K:412:GLN:OE1	2.54	0.40
1:C:187:SER:N	4:C:307:HOH:O	2.54	0.40
2:F:113:PRO:HB3	2:F:139:PHE:HB3	2.03	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	213/223 (96%)	208 (98%)	4 (2%)	1 (0%)	24	48
1	C	216/223 (97%)	211 (98%)	5 (2%)	0	100	100
1	E	186/223 (83%)	181 (97%)	5 (3%)	0	100	100
1	G	218/223 (98%)	214 (98%)	4 (2%)	0	100	100
2	B	214/219 (98%)	204 (95%)	9 (4%)	1 (0%)	24	48
2	D	212/219 (97%)	202 (95%)	10 (5%)	0	100	100
2	F	208/219 (95%)	201 (97%)	6 (3%)	1 (0%)	24	48
2	H	213/219 (97%)	204 (96%)	8 (4%)	1 (0%)	24	48
3	I	7/13 (54%)	7 (100%)	0	0	100	100
3	J	8/13 (62%)	8 (100%)	0	0	100	100
3	K	9/13 (69%)	9 (100%)	0	0	100	100
3	L	10/13 (77%)	10 (100%)	0	0	100	100
All	All	1714/1820 (94%)	1659 (97%)	51 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	68	ARG
2	F	68	ARG
2	H	68	ARG
1	A	26	GLY

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	192/196 (98%)	189 (98%)	3 (2%)	55	80
1	C	192/196 (98%)	190 (99%)	2 (1%)	68	86
1	E	173/196 (88%)	172 (99%)	1 (1%)	78	91
1	G	194/196 (99%)	193 (100%)	1 (0%)	81	92
2	B	187/190 (98%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	185/190 (97%)	182 (98%)	3 (2%)	55	80
2	F	186/190 (98%)	183 (98%)	3 (2%)	55	80
2	H	186/190 (98%)	186 (100%)	0	100	100
3	I	8/12 (67%)	8 (100%)	0	100	100
3	J	9/12 (75%)	9 (100%)	0	100	100
3	K	10/12 (83%)	9 (90%)	1 (10%)	7	19
3	L	11/12 (92%)	11 (100%)	0	100	100
All	All	1533/1592 (96%)	1519 (99%)	14 (1%)	70	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
1	A	135	THR
1	A	178	LEU
1	C	179	SER
1	C	211	VAL
2	D	72	THR
2	D	107	THR
2	D	114	THR
1	E	178	LEU
2	F	67	SER
2	F	68	ARG
2	F	123	GLU
1	G	211	VAL
3	K	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
2	B	38	GLN
2	B	53	ASN
1	C	57	ASN
1	C	105	GLN
2	D	199	GLN
1	E	57	ASN
2	F	137	ASN

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Mol	Chain	Res	Type
1	G	57	ASN
1	G	105	GLN
1	G	192	GLN
2	H	138	ASN
3	K	412	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	A	217/223 (97%)	0.86	19 (8%) 15 13	24, 39, 65, 77	0
1	C	218/223 (97%)	0.90	19 (8%) 16 13	23, 38, 63, 70	0
1	E	192/223 (86%)	1.20	29 (15%) 5 4	23, 38, 66, 75	0
1	G	220/223 (98%)	0.79	13 (5%) 28 25	22, 34, 52, 71	0
2	B	216/219 (98%)	0.78	17 (7%) 18 16	24, 35, 50, 58	0
2	D	214/219 (97%)	0.85	15 (7%) 22 19	21, 37, 51, 60	0
2	F	214/219 (97%)	1.33	50 (23%) 2 2	21, 44, 74, 86	0
2	H	215/219 (98%)	0.79	12 (5%) 30 26	24, 36, 54, 71	0
3	I	9/13 (69%)	0.62	0 100 100	34, 37, 41, 49	0
3	J	10/13 (76%)	0.78	0 100 100	36, 40, 47, 59	0
3	K	11/13 (84%)	1.12	1 (9%) 15 12	34, 39, 56, 57	0
3	L	12/13 (92%)	1.01	2 (16%) 4 3	34, 37, 54, 55	0
All	All	1748/1820 (96%)	0.93	177 (10%) 12 10	21, 37, 64, 86	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	194	TYR	4.6
2	H	212	GLY	4.5
1	E	155	ASN	4.2
1	E	211	VAL	4.2
1	E	27	ASP	3.9
2	F	116	SER	3.7
2	F	191	VAL	3.7
1	G	27	ASP	3.6
2	F	188	LYS	3.6
1	E	161	SER	3.6
1	G	42	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	182	VAL	3.5
1	E	97	ASP	3.5
2	F	157	GLY	3.5
2	F	211	ARG	3.5
2	F	126	THR	3.5
1	A	134	GLY	3.4
2	F	187	GLU	3.4
2	F	2	LEU	3.4
1	E	160	THR	3.4
2	B	127	SER	3.3
1	A	27	ASP	3.3
2	D	129	THR	3.3
2	F	210	ASN	3.3
1	G	98	SER	3.3
1	A	26	GLY	3.3
2	F	115	VAL	3.3
2	H	25	SER	3.2
2	B	41	GLY	3.2
2	F	153	ALA	3.2
1	A	189	LEU	3.2
1	A	187	SER	3.2
2	F	148	TRP	3.1
2	F	154	LEU	3.1
2	D	212	GLY	3.1
2	F	165	GLU	3.0
1	C	184	VAL	3.0
2	D	26	SER	3.0
1	E	213	PRO	3.0
1	C	174	GLY	3.0
2	F	181	LEU	3.0
2	B	40	PRO	3.0
1	A	214	LYS	3.0
2	B	2	LEU	2.9
1	A	194	TYR	2.9
1	C	136	ALA	2.9
2	F	205	VAL	2.9
1	A	188	SER	2.9
1	C	189	LEU	2.9
2	B	163	VAL	2.9
1	A	135	THR	2.9
1	C	205	THR	2.9
2	F	127	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	209	PHE	2.8
2	F	123	GLU	2.8
2	F	120	PRO	2.8
1	E	195	ILE	2.8
2	D	11	LEU	2.8
2	F	124	GLN	2.8
1	E	210	LYS	2.8
2	H	154	LEU	2.8
2	F	206	THR	2.8
1	C	24	VAL	2.8
2	F	10	SER	2.8
1	G	97	ASP	2.8
1	C	151	THR	2.8
2	F	193	ALA	2.8
2	D	127	SER	2.7
2	B	25	SER	2.7
1	A	159	LEU	2.6
1	E	154	TRP	2.6
2	D	150	VAL	2.6
2	F	133	VAL	2.6
2	F	212	GLY	2.6
2	F	70	ASP	2.6
2	F	135	LEU	2.6
2	D	152	ASN	2.6
2	H	40	PRO	2.6
1	E	157	GLY	2.6
2	B	212	GLY	2.6
2	F	132	VAL	2.6
2	F	192	TYR	2.5
1	C	207	VAL	2.5
1	E	163	VAL	2.5
1	A	136	ALA	2.5
2	B	27	GLU	2.5
2	F	204	PRO	2.5
1	A	183	THR	2.5
1	E	41	PRO	2.5
2	F	163	VAL	2.5
1	E	168	ALA	2.5
1	C	131	THR	2.5
2	F	149	LYS	2.5
2	F	158	ASN	2.5
1	C	159	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	26	SER	2.5
2	F	159	SER	2.5
1	C	134	GLY	2.5
1	C	202	PRO	2.5
2	F	129	THR	2.4
3	K	422	ILE	2.4
2	B	26	SER	2.4
1	C	26	GLY	2.4
2	H	26	SER	2.4
2	H	143	GLU	2.4
1	A	204	ASN	2.4
1	E	31	SER	2.4
1	G	133	GLY	2.4
1	A	211	VAL	2.4
2	D	192	TYR	2.4
2	D	4	LEU	2.4
3	L	422	ILE	2.4
1	E	140	CYS	2.4
2	B	190	LYS	2.4
1	G	26	GLY	2.4
1	E	169	VAL	2.4
1	C	194	TYR	2.3
2	B	143	GLU	2.3
1	E	144	ASP	2.3
2	H	151	ASP	2.3
2	F	194	CYS	2.3
2	H	194	CYS	2.3
1	C	116	THR	2.3
1	G	215	SER	2.3
2	B	121	SER	2.3
2	F	182	SER	2.3
1	E	159	LEU	2.3
2	D	125	LEU	2.3
1	A	5	SER	2.2
2	B	116	SER	2.2
1	E	203	SER	2.2
1	G	132	SER	2.2
2	H	41	GLY	2.2
2	B	11	LEU	2.2
2	B	154	LEU	2.2
1	E	181	VAL	2.2
1	A	42	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	151	ASP	2.2
1	E	212	GLU	2.2
2	D	23	CYS	2.2
1	C	204	ASN	2.2
2	F	186	TYR	2.2
1	E	24	VAL	2.2
2	H	203	SER	2.2
1	C	114	ALA	2.1
1	E	114	ALA	2.1
1	G	136	ALA	2.1
1	A	25	THR	2.1
1	E	162	GLY	2.1
2	D	182	SER	2.1
2	D	202	SER	2.1
2	F	203	SER	2.1
1	G	212	GLU	2.1
2	F	119	PRO	2.1
2	F	190	LYS	2.1
2	F	207	LYS	2.1
2	D	91	ASN	2.1
2	F	117	ILE	2.1
1	C	156	SER	2.1
2	D	68	ARG	2.1
1	G	131	THR	2.1
1	G	206	LYS	2.1
2	B	66	GLY	2.1
1	E	179	SER	2.1
2	F	11	LEU	2.1
2	F	137	ASN	2.1
1	E	158	ALA	2.0
2	H	11	LEU	2.0
1	C	97	ASP	2.0
2	F	103	LYS	2.0
1	A	68	SER	2.0
2	F	174	SER	2.0
2	F	202	SER	2.0
1	A	213	PRO	2.0
1	G	16	GLN	2.0
2	H	125	LEU	2.0
3	L	412	GLN	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.