



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:12 PM UTC

PDB ID : 7SUE / pdb_00007sue
Title : Crystal Structure of Human Fab S24-188 in the complex with the N-terminal Domain of Nucleocapsid protein from SARS CoV-2
Authors : Kim, Y.; Maltseva, N.; Tesar, C.; Jedrzejczak, R.; Dugan, H.; Stamper, C.; Wilson, P.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2021-11-17
Resolution : 2.90 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

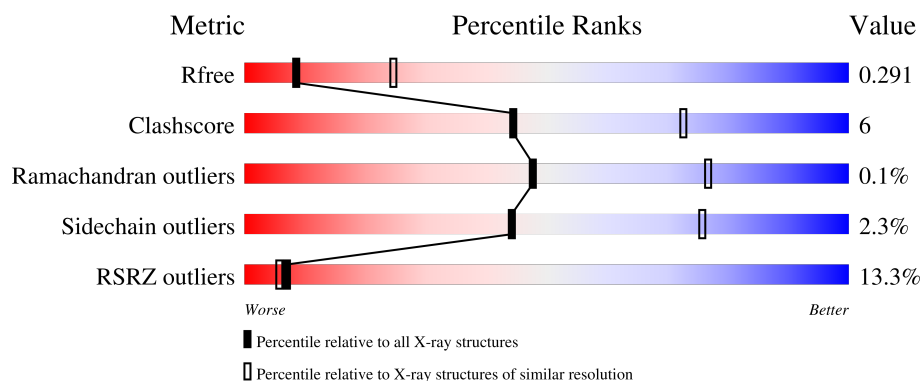
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	216	19% 84% 14% .
1	E	216	9% 38% 13% 50%
1	G	216	6% 44% 6% 50%
1	L	216	9% 84% 14% .
2	B	231	10% 87% 11% .

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Mol	Chain	Length	Quality of chain
2	F	231	9% 44% 12% 44%
2	H	231	10% 83% 15% ••
2	I	231	10% 44% 11% 45%
3	C	130	12% 76% 11% • 12%
3	D	130	11% 72% 17% 12%
3	J	130	9% 74% 13% • 12%
3	K	130	15% 72% 15% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13707 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 S24-188 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1577	984	263	325	5			
1	A	212	Total	C	N	O	S	0	0	0
			1577	984	263	325	5			
1	E	109	Total	C	N	O	S	0	0	0
			799	495	133	168	3			
1	G	109	Total	C	N	O	S	0	0	0
			799	495	133	168	3			

- Molecule 2 is a protein called S24-188 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1699	1076	283	331	9			
2	B	227	Total	C	N	O	S	0	0	0
			1699	1076	283	331	9			
2	F	129	Total	C	N	O	S	0	0	0
			995	630	167	192	6			
2	I	128	Total	C	N	O	S	0	0	0
			983	623	166	188	6			

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	115	Total	C	N	O	0	0	0
			896	571	156	169			
3	D	115	Total	C	N	O	0	0	0
			896	571	156	169			
3	J	114	Total	C	N	O	0	0	0
			891	567	158	166			
3	K	115	Total	C	N	O	0	0	0
			896	571	156	169			

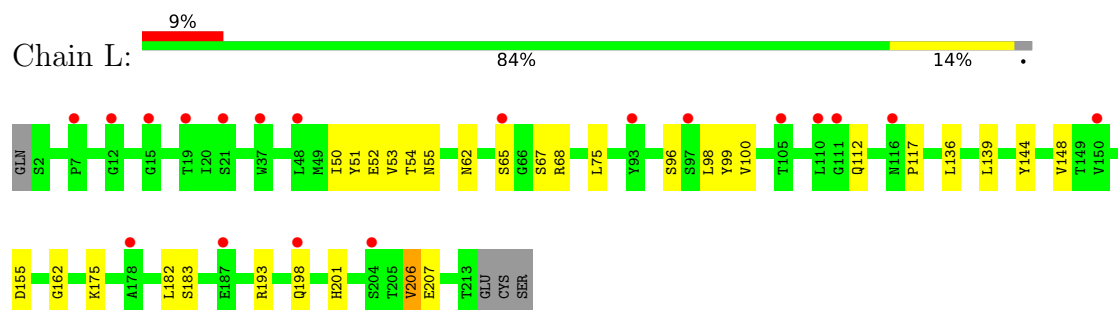
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	44	SER	-	expression tag	UNP P0DTC9
C	45	ASN	-	expression tag	UNP P0DTC9
C	46	MET	-	expression tag	UNP P0DTC9
D	44	SER	-	expression tag	UNP P0DTC9
D	45	ASN	-	expression tag	UNP P0DTC9
D	46	MET	-	expression tag	UNP P0DTC9
J	44	SER	-	expression tag	UNP P0DTC9
J	45	ASN	-	expression tag	UNP P0DTC9
J	46	MET	-	expression tag	UNP P0DTC9
K	44	SER	-	expression tag	UNP P0DTC9
K	45	ASN	-	expression tag	UNP P0DTC9
K	46	MET	-	expression tag	UNP P0DTC9

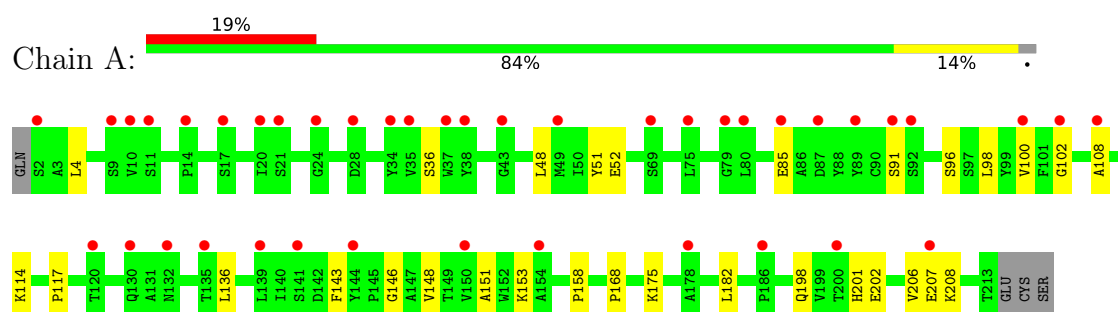
3 Residue-property plots [i](#)

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.

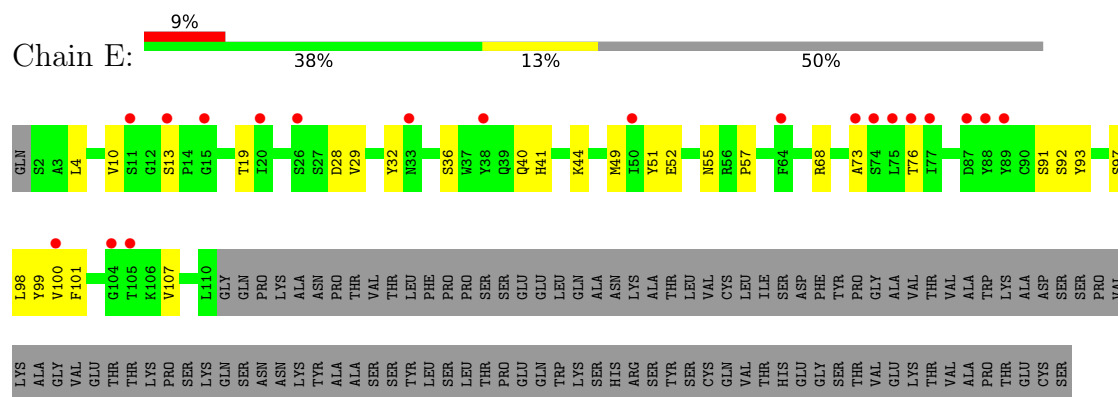
• Molecule 1: S24-188 Fab Light chain



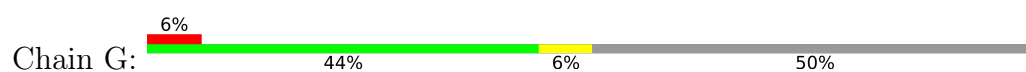
• Molecule 1: S24-188 Fab Light chain

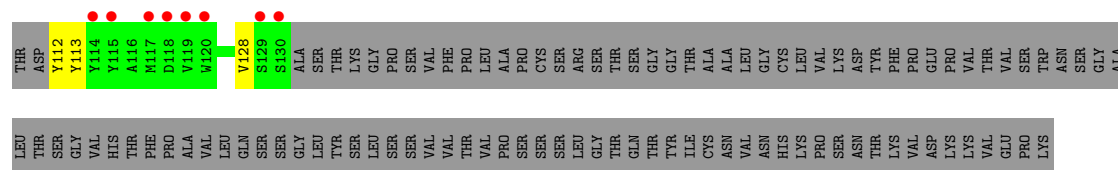


• Molecule 1: S24-188 Fab Light chain

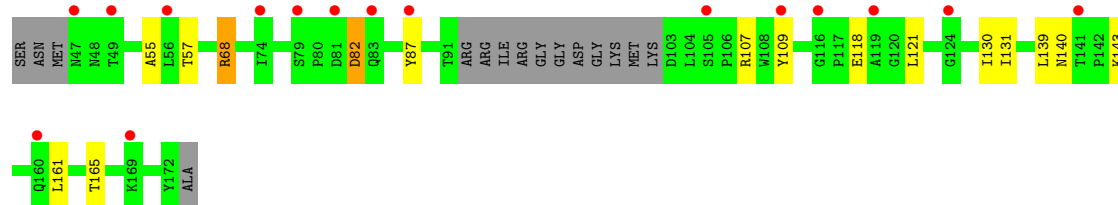
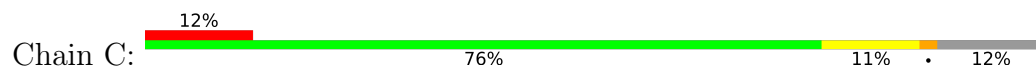


• Molecule 1: S24-188 Fab Light chain

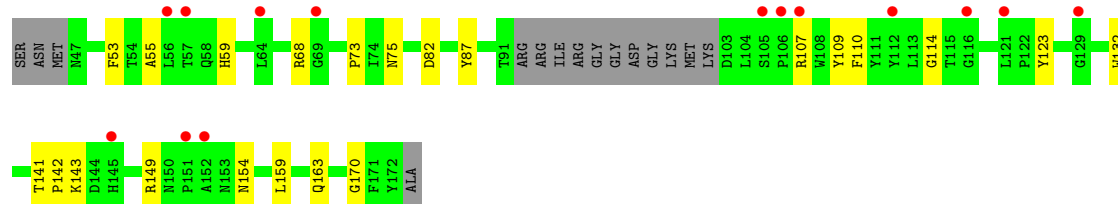
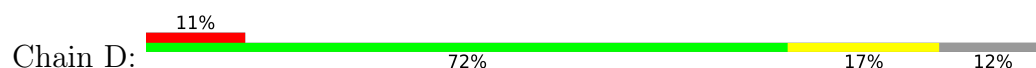




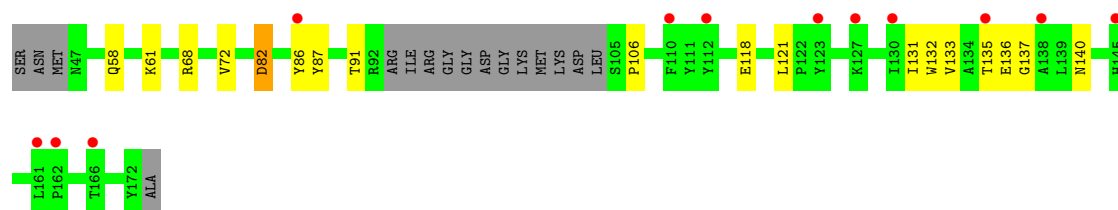
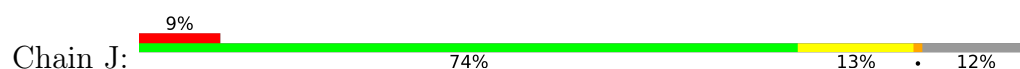
• Molecule 3: Nucleoprotein



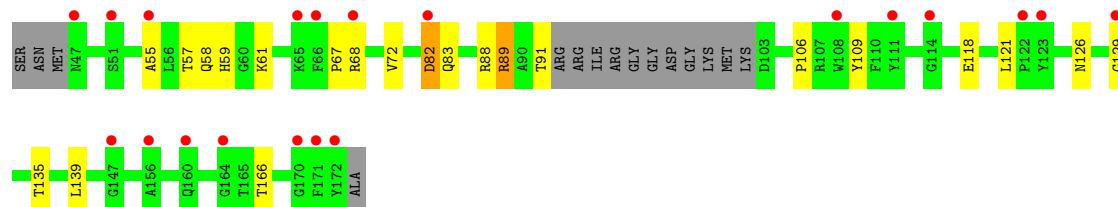
• Molecule 3: Nucleoprotein



• Molecule 3: Nucleoprotein



• Molecule 3: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.31Å 78.50Å 127.15Å 97.60° 89.96° 90.02°	Depositor
Resolution (Å)	39.20 – 2.90 39.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (39.20-2.90) 91.3 (39.20-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.262 , 0.292 0.262 , 0.291	Depositor DCC
R_{free} test set	2724 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 193.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	13707	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.14	0/1615	0.35	0/2205
1	E	0.09	0/816	0.31	0/1111
1	G	0.12	0/816	0.36	0/1111
1	L	0.13	0/1615	0.33	0/2205
2	B	0.09	0/1740	0.30	0/2366
2	F	0.12	0/1018	0.41	0/1379
2	H	0.16	0/1740	0.38	0/2366
2	I	0.23	0/1006	0.42	0/1361
3	C	0.09	0/923	0.35	0/1261
3	D	0.09	0/923	0.32	0/1261
3	J	0.09	0/918	0.32	0/1253
3	K	0.15	0/923	0.51	0/1261
All	All	0.13	0/14053	0.36	0/19140

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	1577	0	1519	18	0
1	E	799	0	755	19	0
1	G	799	0	755	12	0
1	L	1577	0	1519	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1699	0	1663	12	0
2	F	995	0	961	18	0
2	H	1699	0	1663	23	0
2	I	983	0	951	16	0
3	C	896	0	855	11	0
3	D	896	0	855	14	0
3	J	891	0	853	11	0
3	K	896	0	855	13	0
All	All	13707	0	13204	161	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 (161) 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:100:TRP:CD1	2:I:112:TYR:HH	2.17	0.63
3:K:72:VAL:HG11	3:K:83:GLN:HB3	1.81	0.61
2:H:6:GLN:H	2:H:122:GLN:HE22	1.49	0.59
2:I:41:PRO:HD3	2:I:92:ALA:HA	1.84	0.59
1:E:51:TYR:CZ	1:E:55:ASN:HB3	2.38	0.59
3:J:118:GLU:HB3	3:J:121:LEU:HD22	1.85	0.58
1:G:32:TYR:O	1:G:68:ARG:NH1	2.35	0.58
2:I:60:TYR:HE1	2:I:70:ILE:HG12	1.68	0.58
2:H:109:ARG:HD3	3:C:68:ARG:HD3	1.83	0.58
3:K:118:GLU:HB3	3:K:121:LEU:HD22	1.84	0.58
2:H:68:VAL:HG22	2:H:83:LEU:HD13	1.86	0.57
2:F:109:ARG:HD3	3:J:136:GLU:HG2	1.86	0.57
1:G:37:TRP:HB2	1:G:50:ILE:HB	1.87	0.57
3:K:58:GLN:HB3	3:K:106:PRO:HG2	1.85	0.56
2:H:48:MET:HG2	2:H:64:PHE:CE2	2.41	0.56
2:H:212:ILE:HG22	2:H:227:LYS:HA	1.87	0.56
3:K:57:THR:OG1	3:K:59:HIS:NE2	2.39	0.55
2:B:48:MET:HG2	2:B:64:PHE:CE2	2.42	0.55
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.88	0.55
3:K:89:ARG:HE	3:K:129:GLY:HA2	1.72	0.54
3:D:82:ASP:HA	3:D:143:LYS:HE3	1.88	0.54
2:B:176:LEU:HD21	2:B:199:VAL:HG11	1.90	0.54
1:G:68:ARG:HA	1:G:73:ALA:HA	1.89	0.53
1:G:49:MET:O	1:G:57:PRO:HD2	2.08	0.53
3:D:73:PRO:HB3	3:D:159:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:72:VAL:HG11	3:J:135:THR:HG23	1.90	0.53
1:A:136:LEU:HD12	1:A:182:LEU:HD23	1.89	0.53
3:C:118:GLU:HB3	3:C:121:LEU:HD22	1.90	0.53
3:K:88:ARG:HH12	3:K:91:THR:HB	1.74	0.53
3:D:141:THR:O	3:D:143:LYS:NZ	2.36	0.53
1:A:198:GLN:HG2	1:A:207:GLU:HG2	1.91	0.53
3:C:87:TYR:HB2	3:C:131:ILE:HG13	1.91	0.53
2:F:6:GLN:H	2:F:122:GLN:HE22	1.56	0.52
3:D:149:ARG:NH1	3:D:154:ASN:O	2.43	0.52
1:E:32:TYR:O	1:E:68:ARG:NH1	2.43	0.52
1:G:57:PRO:HB3	2:I:113:TYR:CE2	2.44	0.51
2:I:106:SER:HA	3:K:139:LEU:HA	1.92	0.51
2:H:107:TYR:OH	2:H:109:ARG:NH1	2.43	0.51
2:B:6:GLN:H	2:B:122:GLN:HE22	1.58	0.51
2:B:109:ARG:HD2	3:D:68:ARG:HB2	1.93	0.51
3:K:55:ALA:HB2	3:K:109:TYR:HE1	1.75	0.51
3:C:82:ASP:HA	3:C:143:LYS:HD2	1.92	0.51
2:B:97:ALA:HB1	2:B:117:MET:HB3	1.94	0.50
1:A:48:LEU:HD21	1:A:51:TYR:HB3	1.92	0.50
3:D:55:ALA:HB2	3:D:109:TYR:HE1	1.75	0.50
3:J:72:VAL:HG22	3:J:133:VAL:HB	1.94	0.50
2:H:182:THR:HA	2:H:197:SER:HA	1.94	0.50
3:D:55:ALA:HB1	3:D:107:ARG:HB3	1.92	0.49
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.47	0.49
2:F:107:TYR:HD2	3:J:137:GLY:H	1.60	0.49
3:K:67:PRO:HD2	3:K:166:THR:HG21	1.93	0.49
2:H:222:THR:HG23	1:A:208:LYS:HE2	1.93	0.49
1:L:50:ILE:HG22	1:L:52:GLU:O	2.13	0.48
1:G:51:TYR:CG	2:I:113:TYR:HD2	2.31	0.48
1:L:148:VAL:HG12	1:L:201:HIS:HB2	1.94	0.48
2:F:40:ALA:HB3	2:F:43:GLN:HB2	1.94	0.48
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.95	0.48
1:E:4:LEU:HD11	1:E:100:VAL:HG23	1.95	0.48
1:E:36:SER:HB2	1:E:91:SER:OG	2.14	0.48
2:I:102:PHE:HE1	2:I:107:TYR:HA	1.78	0.48
2:H:6:GLN:H	2:H:122:GLN:NE2	2.11	0.48
1:E:98:LEU:HD13	2:F:61:ALA:HA	1.94	0.48
2:F:33:ALA:O	2:F:99:GLY:N	2.46	0.48
2:I:29:PHE:HD2	2:I:74:LYS:HA	1.79	0.48
1:A:117:PRO:HA	1:A:143:PHE:HB3	1.95	0.48
1:E:28:ASP:O	1:E:92:SER:OG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:PRO:HB3	2:B:162:TYR:HB3	1.96	0.47
1:E:49:MET:O	1:E:57:PRO:HD2	2.14	0.47
1:L:162:GLY:O	1:L:183:SER:N	2.34	0.47
1:E:10:VAL:HG13	1:E:107:VAL:HG23	1.96	0.47
2:H:165:GLU:HB2	2:H:193:TYR:HE2	1.79	0.47
1:A:153:LYS:HD3	1:A:198:GLN:OE1	2.14	0.47
1:G:51:TYR:HD1	1:G:57:PRO:HD3	1.79	0.47
1:L:99:TYR:HB2	2:H:47:TRP:CG	2.50	0.47
1:A:114:LYS:NZ	1:A:202:GLU:OE1	2.43	0.47
1:A:153:LYS:HG2	1:A:158:PRO:HA	1.97	0.47
3:K:88:ARG:NH1	3:K:91:THR:HB	2.29	0.47
1:E:19:THR:HG22	1:E:76:THR:HG22	1.97	0.47
1:G:31:GLY:O	3:K:126:ASN:N	2.31	0.47
3:K:72:VAL:HG21	3:K:135:THR:HG23	1.96	0.46
3:C:57:THR:HG22	3:C:107:ARG:HG2	1.97	0.46
3:D:87:TYR:CE2	3:D:110:PHE:HB2	2.49	0.46
1:A:136:LEU:HB2	1:A:182:LEU:HB3	1.98	0.46
1:L:139:LEU:HB3	2:H:183:PHE:CZ	2.50	0.46
3:C:161:LEU:HB2	3:C:165:THR:HG21	1.97	0.46
3:D:53:PHE:HZ	3:D:75:ASN:HB2	1.81	0.45
1:E:51:TYR:CD2	1:E:52:GLU:HG2	2.51	0.45
1:L:98:LEU:HB2	2:H:47:TRP:CZ3	2.51	0.45
1:A:51:TYR:CD2	1:A:52:GLU:HG2	2.52	0.45
1:E:49:MET:N	1:E:49:MET:SD	2.89	0.45
2:H:165:GLU:HB2	2:H:193:TYR:CE2	2.52	0.45
3:D:59:HIS:N	3:D:170:GLY:O	2.49	0.45
2:H:106:SER:HA	3:C:139:LEU:HA	1.98	0.45
3:D:123:TYR:CE2	3:D:132:TRP:HB3	2.52	0.45
1:E:40:GLN:NE2	2:F:39:GLN:OE1	2.39	0.44
3:D:55:ALA:HB2	3:D:109:TYR:CE1	2.51	0.44
1:L:54:THR:HG22	1:L:67:SER:HA	1.98	0.44
2:F:50:ARG:HH21	2:F:59:ASN:CG	2.26	0.44
2:I:51:ILE:HD13	2:I:58:ALA:HB2	2.00	0.44
2:H:102:PHE:CE1	3:C:140:ASN:HB2	2.53	0.43
3:C:118:GLU:HG3	3:C:130:ILE:HD11	1.99	0.43
3:J:58:GLN:HB3	3:J:106:PRO:HG2	2.00	0.43
1:E:68:ARG:HA	1:E:73:ALA:HA	2.00	0.43
2:F:60:TYR:CE1	2:F:70:ILE:HG12	2.53	0.43
2:F:102:PHE:CE2	3:J:140:ASN:HB2	2.53	0.43
2:H:91:THR:HG23	2:H:127:THR:HA	1.98	0.43
2:I:68:VAL:HA	2:I:82:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:VAL:HG21	1:L:68:ARG:NH2	2.34	0.43
2:H:31:SER:H	2:H:54:ILE:HG21	1.83	0.43
2:F:19:LYS:HA	2:F:81:MET:O	2.18	0.43
2:F:111:ASP:OD1	3:J:68:ARG:NH1	2.52	0.43
1:A:198:GLN:HG2	1:A:207:GLU:CD	2.44	0.43
3:J:82:ASP:N	3:J:82:ASP:OD1	2.51	0.43
3:J:86:TYR:HB3	3:J:132:TRP:CE3	2.54	0.43
1:L:136:LEU:HD12	1:L:182:LEU:HD23	2.00	0.43
1:A:148:VAL:HG12	1:A:201:HIS:HB2	2.01	0.43
1:L:117:PRO:HG2	1:L:206:VAL:HG11	2.01	0.43
3:C:82:ASP:OD1	3:C:82:ASP:N	2.49	0.43
3:D:114:GLY:HA3	3:D:142:PRO:HB3	2.00	0.43
1:E:49:MET:HE2	1:E:49:MET:HB2	1.91	0.43
1:E:99:TYR:HB2	2:F:47:TRP:CD2	2.54	0.43
1:L:52:GLU:HB2	1:L:55:ASN:HB2	2.01	0.43
2:I:50:ARG:HH21	2:I:59:ASN:CG	2.25	0.43
3:K:82:ASP:OD1	3:K:82:ASP:N	2.50	0.43
2:H:136:PRO:HB3	2:H:162:TYR:HB3	2.00	0.42
1:L:65:SER:O	1:L:75:LEU:HD12	2.19	0.42
2:F:108:TYR:C	2:F:110:THR:H	2.27	0.42
1:A:36:SER:OG	1:A:91:SER:OG	2.36	0.42
3:J:87:TYR:HB2	3:J:131:ILE:HG13	2.02	0.42
1:L:51:TYR:CD2	2:H:113:TYR:CD1	3.07	0.42
1:L:112:GLN:HB3	1:L:144:TYR:CE2	2.55	0.42
2:B:139:PHE:HE2	2:B:160:LYS:HE2	1.85	0.42
1:G:6:GLN:HE21	1:G:22:CYS:HB2	1.84	0.42
1:G:51:TYR:CD2	2:I:113:TYR:HD2	2.38	0.42
1:L:198:GLN:HG2	1:L:207:GLU:HG2	2.02	0.41
2:H:97:ALA:HB1	2:H:117:MET:HB3	2.02	0.41
1:E:91:SER:HB3	1:E:101:PHE:CE1	2.54	0.41
1:E:93:TYR:CZ	1:E:97:SER:HA	2.55	0.41
2:I:109:ARG:HA	2:I:112:TYR:HB2	2.01	0.41
1:L:155:ASP:OD1	1:L:193:ARG:HB2	2.20	0.41
1:A:85:GLU:HG2	1:A:108:ALA:HA	2.01	0.41
1:A:151:ALA:HB3	1:A:198:GLN:HE21	1.85	0.41
1:E:41:HIS:HB2	1:E:44:LYS:HB3	2.02	0.41
3:D:163:GLN:OE1	3:D:163:GLN:N	2.40	0.41
1:G:51:TYR:CD2	1:G:52:GLU:HG2	2.55	0.41
2:F:28:THR:HB	2:F:98:ARG:HH12	1.85	0.41
2:I:86:LEU:HB3	2:I:128:VAL:HG21	2.02	0.41
1:A:146:GLY:O	1:A:168:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ASP:OD1	1:E:29:VAL:HG22	2.21	0.41
1:L:62:ASN:N	1:L:62:ASN:OD1	2.53	0.41
2:B:165:GLU:HG3	2:B:166:PRO:HA	2.02	0.41
2:F:50:ARG:HG2	2:F:51:ILE:N	2.36	0.41
2:H:176:LEU:HD21	2:H:199:VAL:HG21	2.03	0.41
3:C:55:ALA:HB2	3:C:109:TYR:HE1	1.86	0.41
1:A:4:LEU:HB2	1:A:102:GLY:HA2	2.03	0.40
2:F:109:ARG:O	2:F:109:ARG:HG2	2.20	0.40
2:H:213:CYS:SG	2:H:226:LYS:HB3	2.61	0.40
1:A:98:LEU:HB2	2:B:47:TRP:CZ3	2.56	0.40
2:F:60:TYR:HE1	2:F:70:ILE:HG12	1.85	0.40
2:B:201:VAL:HG22	2:B:202:PRO:HD2	2.02	0.40
1:G:40:GLN:NE2	2:I:39:GLN:OE1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	210/216 (97%)	206 (98%)	4 (2%)	0	100	100
1	E	107/216 (50%)	103 (96%)	4 (4%)	0	100	100
1	G	107/216 (50%)	103 (96%)	4 (4%)	0	100	100
1	L	210/216 (97%)	206 (98%)	4 (2%)	0	100	100
2	B	221/231 (96%)	216 (98%)	5 (2%)	0	100	100
2	F	125/231 (54%)	118 (94%)	7 (6%)	0	100	100
2	H	221/231 (96%)	217 (98%)	4 (2%)	0	100	100
2	I	124/231 (54%)	118 (95%)	6 (5%)	0	100	100
3	C	111/130 (85%)	109 (98%)	2 (2%)	0	100	100
3	D	111/130 (85%)	109 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	110/130 (85%)	109 (99%)	1 (1%)	0	100	100
3	K	111/130 (85%)	107 (96%)	3 (3%)	1 (1%)	14	41
All	All	1768/2308 (77%)	1721 (97%)	46 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	89	ARG

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	A	178/183 (97%)	174 (98%)	4 (2%)	45	77
1	E	89/183 (49%)	88 (99%)	1 (1%)	65	88
1	G	89/183 (49%)	89 (100%)	0	100	100
1	L	178/183 (97%)	174 (98%)	4 (2%)	45	77
2	B	188/192 (98%)	184 (98%)	4 (2%)	47	77
2	F	105/192 (55%)	102 (97%)	3 (3%)	37	71
2	H	188/192 (98%)	182 (97%)	6 (3%)	34	68
2	I	103/192 (54%)	99 (96%)	4 (4%)	28	63
3	C	92/103 (89%)	90 (98%)	2 (2%)	45	77
3	D	92/103 (89%)	92 (100%)	0	100	100
3	J	91/103 (88%)	88 (97%)	3 (3%)	33	67
3	K	92/103 (89%)	89 (97%)	3 (3%)	33	67
All	All	1485/1912 (78%)	1451 (98%)	34 (2%)	44	76

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	96	SER

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Mol	Chain	Res	Type
1	L	100	VAL
1	L	175	LYS
1	L	206	VAL
2	H	29	PHE
2	H	50	ARG
2	H	54	ILE
2	H	109	ARG
2	H	206	LEU
2	H	231	LYS
1	A	96	SER
1	A	100	VAL
1	A	175	LYS
1	A	206	VAL
2	B	29	PHE
2	B	50	ARG
2	B	54	ILE
2	B	206	LEU
3	C	68	ARG
3	C	82	ASP
1	E	13	SER
2	F	11	VAL
2	F	37	VAL
2	F	87	ARG
2	I	11	VAL
2	I	37	VAL
2	I	87	ARG
2	I	109	ARG
3	J	61	LYS
3	J	82	ASP
3	J	91	THR
3	K	61	LYS
3	K	68	ARG
3	K	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	40	GLN
2	H	39	GLN
1	G	6	GLN
3	J	126	ASN

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	212/216 (98%)	1.15	41 (19%) 3 2	88, 108, 126, 134	0
1	E	109/216 (50%)	1.14	20 (18%) 3 3	116, 135, 146, 152	0
1	G	109/216 (50%)	0.97	12 (11%) 10 9	125, 142, 156, 170	0
1	L	212/216 (98%)	0.98	19 (8%) 15 13	83, 107, 128, 147	0
2	B	227/231 (98%)	0.95	22 (9%) 13 11	87, 99, 122, 136	0
2	F	129/231 (55%)	1.06	20 (15%) 5 4	118, 139, 158, 167	0
2	H	227/231 (98%)	0.95	22 (9%) 13 11	83, 100, 117, 130	0
2	I	128/231 (55%)	1.05	23 (17%) 3 3	106, 141, 165, 178	0
3	C	115/130 (88%)	1.05	16 (13%) 6 5	94, 112, 147, 157	0
3	D	115/130 (88%)	0.88	14 (12%) 8 7	87, 96, 123, 150	0
3	J	114/130 (87%)	1.09	12 (10%) 11 10	115, 144, 166, 171	0
3	K	115/130 (88%)	1.17	20 (17%) 4 3	113, 140, 176, 197	0
All	All	1812/2308 (78%)	1.03	241 (13%) 7 6	83, 116, 154, 197	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	140	PRO	6.1
1	E	74	SER	5.9
3	K	55	ALA	5.5
1	L	111	GLY	5.0
1	G	2	SER	5.0
1	A	178	ALA	4.7
3	D	129	GLY	4.7
1	E	77	ILE	4.6
1	E	104	GLY	4.5
1	A	11	SER	4.5
1	A	75	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	19	THR	4.3
1	A	24	GLY	4.2
3	C	49	THR	4.1
2	B	174	GLY	4.0
1	L	65	SER	4.0
2	H	34	ILE	4.0
1	E	15	GLY	3.9
1	E	33	ASN	3.9
1	L	116	ASN	3.8
1	A	87	ASP	3.8
1	A	102	GLY	3.8
1	G	96	SER	3.8
1	A	20	ILE	3.8
1	L	7	PRO	3.7
1	A	10	VAL	3.7
2	B	183	PHE	3.7
3	J	112	TYR	3.7
2	F	94	TYR	3.6
2	I	11	VAL	3.6
1	G	49	MET	3.5
2	B	150	GLY	3.5
3	K	170	GLY	3.5
1	L	12	GLY	3.5
1	A	43	GLY	3.5
1	A	120	THR	3.4
2	B	99	GLY	3.4
2	H	173	SER	3.4
2	B	3	HIS	3.3
3	K	122	PRO	3.3
1	A	80	LEU	3.3
2	F	68	VAL	3.3
2	F	16	SER	3.3
1	E	100	VAL	3.3
3	K	82	ASP	3.2
1	L	110	LEU	3.2
2	B	211	TYR	3.2
2	B	154	ALA	3.2
1	A	186	PRO	3.2
3	J	161	LEU	3.1
2	H	47	TRP	3.1
2	I	118	ASP	3.1
2	B	1	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	69	THR	3.1
1	L	105	THR	3.1
3	K	123	TYR	3.0
2	B	131	ALA	3.0
3	C	81	ASP	3.0
1	A	79	GLY	3.0
3	D	116	GLY	3.0
2	B	186	VAL	3.0
2	B	106	SER	3.0
1	G	46	PRO	3.0
1	L	37	TRP	2.9
3	D	107	ARG	2.9
1	G	92	SER	2.9
2	I	130	SER	2.9
3	K	108	TRP	2.9
1	A	89	TYR	2.9
1	A	17	SER	2.9
1	A	69	SER	2.9
2	I	8	GLY	2.9
3	K	51	SER	2.9
1	A	135	THR	2.9
1	G	3	ALA	2.9
2	B	142	ALA	2.9
2	F	57	ILE	2.8
3	K	164	GLY	2.8
3	K	160	GLN	2.8
2	H	107	TYR	2.8
2	I	1	GLN	2.7
1	E	38	TYR	2.7
1	E	75	LEU	2.7
1	G	12	GLY	2.7
2	I	14	PRO	2.7
3	D	151	PRO	2.7
2	I	119	VAL	2.7
2	H	211	TYR	2.7
2	H	224	VAL	2.7
1	E	73	ALA	2.7
1	A	14	PRO	2.7
3	C	116	GLY	2.7
1	E	50	ILE	2.7
3	J	130	ILE	2.7
2	H	28	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	55	LEU	2.7
2	H	142	ALA	2.6
1	E	89	TYR	2.6
3	C	56	LEU	2.6
2	I	120	TRP	2.6
2	F	42	GLY	2.6
2	B	93	VAL	2.6
3	K	47	ASN	2.6
2	F	75	SER	2.6
3	J	127	LYS	2.6
3	C	74	ILE	2.6
1	E	87	ASP	2.6
1	A	9	SER	2.6
2	B	182	THR	2.6
1	A	130	GLN	2.6
2	B	116	ALA	2.6
3	K	171	PHE	2.6
2	I	46	GLU	2.5
2	I	71	THR	2.5
2	F	59	ASN	2.5
1	L	204	SER	2.5
3	J	162	PRO	2.5
1	A	100	VAL	2.5
3	J	86	TYR	2.5
1	L	198	GLN	2.5
1	E	105	THR	2.5
3	C	105	SER	2.5
3	C	124	GLY	2.5
3	D	69	GLY	2.5
1	L	150	VAL	2.5
1	A	150	VAL	2.5
3	C	109	TYR	2.5
2	H	124	THR	2.5
3	C	160	GLN	2.5
3	C	47	ASN	2.5
1	A	28	ASP	2.5
1	A	139	LEU	2.5
1	L	15	GLY	2.5
1	A	200	THR	2.5
3	D	56	LEU	2.4
1	E	11	SER	2.4
1	G	88	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	J	135	THR	2.4
2	F	55	LEU	2.4
1	A	2	SER	2.4
3	C	119	ALA	2.4
1	L	97	SER	2.4
2	B	132	SER	2.4
2	F	131	ALA	2.4
3	K	156	ALA	2.4
2	F	122	GLN	2.4
2	H	181	HIS	2.4
3	K	68	ARG	2.4
2	H	118	ASP	2.3
1	L	187	GLU	2.3
2	H	72	ALA	2.3
1	L	93	TYR	2.3
1	A	132	ASN	2.3
1	A	34	TYR	2.3
1	E	20	ILE	2.3
2	F	108	TYR	2.3
3	J	166	THR	2.3
1	A	35	VAL	2.3
1	G	107	VAL	2.3
2	I	97	ALA	2.3
2	I	117	MET	2.3
3	J	145	HIS	2.3
1	L	21	SER	2.3
3	K	111	TYR	2.3
3	K	65	LYS	2.3
1	A	92	SER	2.3
1	E	76	THR	2.3
3	C	141	THR	2.3
3	D	106	PRO	2.3
3	D	112	TYR	2.3
1	G	35	VAL	2.3
2	B	20	VAL	2.3
1	A	49	MET	2.2
1	E	13	SER	2.2
2	I	95	TYR	2.2
3	C	169	LYS	2.2
1	A	38	TYR	2.2
1	E	26	SER	2.2
3	J	123	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	K	172	TYR	2.2
2	B	66	GLY	2.2
2	H	139	PHE	2.2
2	H	57	ILE	2.2
2	F	109	ARG	2.2
2	F	28	THR	2.2
1	G	97	SER	2.2
2	I	108	TYR	2.2
2	I	129	SER	2.2
3	D	105	SER	2.2
3	D	121	LEU	2.2
1	A	108	ALA	2.2
1	A	207	GLU	2.2
3	J	138	ALA	2.2
2	B	28	THR	2.2
1	A	21	SER	2.2
1	A	91	SER	2.2
1	E	64	PHE	2.2
2	I	60	TYR	2.2
2	F	21	SER	2.2
3	J	110	PHE	2.2
3	D	57	THR	2.1
3	K	129	GLY	2.1
1	L	178	ALA	2.1
2	H	145	SER	2.1
3	C	83	GLN	2.1
1	E	88	TYR	2.1
1	A	141	SER	2.1
2	I	37	VAL	2.1
2	H	14	PRO	2.1
1	L	48	LEU	2.1
3	D	64	LEU	2.1
3	K	66	PHE	2.1
1	A	144	TYR	2.1
2	I	114	TYR	2.1
2	I	55	LEU	2.1
3	K	114	GLY	2.1
2	H	225	ASP	2.1
1	A	154	ALA	2.1
2	B	107	TYR	2.1
2	I	94	TYR	2.1
2	B	149	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	15	GLY	2.0
3	K	147	GLY	2.0
1	A	85	GLU	2.0
2	H	113	TYR	2.0
3	C	87	TYR	2.0
1	G	9	SER	2.0
2	H	68	VAL	2.0
2	F	20	VAL	2.0
2	F	88	SER	2.0
2	F	119	VAL	2.0
2	I	104	SER	2.0
3	C	79	SER	2.0
3	D	145	HIS	2.0
2	I	26	GLY	2.0
2	H	33	ALA	2.0
3	D	152	ALA	2.0
1	A	37	TRP	2.0
2	H	95	TYR	2.0
2	I	115	TYR	2.0
2	F	126	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.