Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 10:50 PM EDT

PDB ID	:	7LK9
Title	:	Crystal structure of SARS-CoV-2 RBD-targeting antibody COV107-23 HC + COVD21-C8 LC
Authors	:	Yuan, M.; Zhu, X.; Wilson, I.A.; Wu, N.C.
Deposited on	:	2021-02-01
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

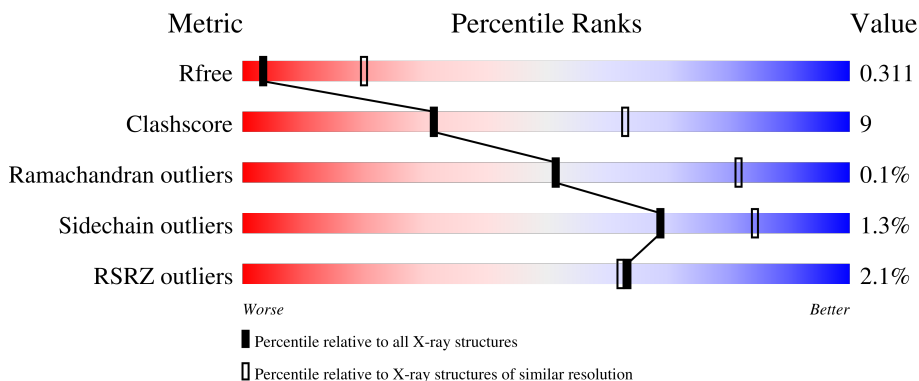|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.40 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.
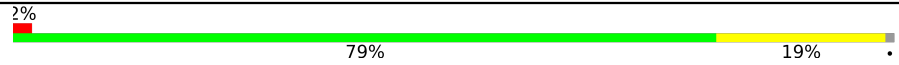
Metric	Percentile Ranks	Value
Rfree		0.311
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		1.3%
RSRZ outliers		2.1%

Worse .... *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	220	73% ... 24% ...
1	C	220	76% ... 21% ...
1	H	220	76% ... 21% ...
1	M	220	73% ... 24% ...
2	B	216	75% ... 24% ...

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Mol	Chain	Length	Quality of chain
2	D	216	
2	L	216	
2	N	216	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 12881 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 COV107-23 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1589	1004	265	314	6			
1	A	214	Total	C	N	O	S	0	0	0
			1589	1004	265	314	6			
1	C	214	Total	C	N	O	S	0	0	0
			1589	1004	265	314	6			
1	M	214	Total	C	N	O	S	0	0	0
			1589	1004	265	314	6			

- Molecule 2 is a protein called COVD21-C8 light chain.

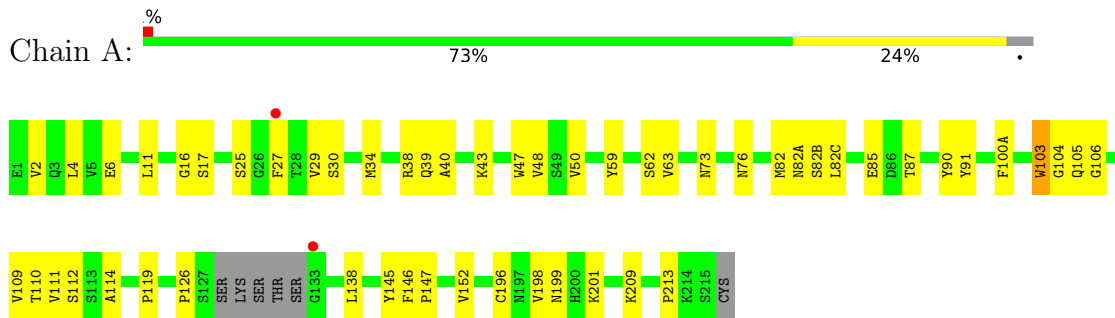| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1640	1023	280	333	4			
2	B	214	Total	C	N	O	S	0	0	0
			1640	1023	280	333	4			
2	D	214	Total	C	N	O	S	0	0	0
			1640	1023	280	333	4			
2	N	209	Total	C	N	O	S	0	0	0
			1605	1003	272	326	4			

3 Residue-property plots ⓘ

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.
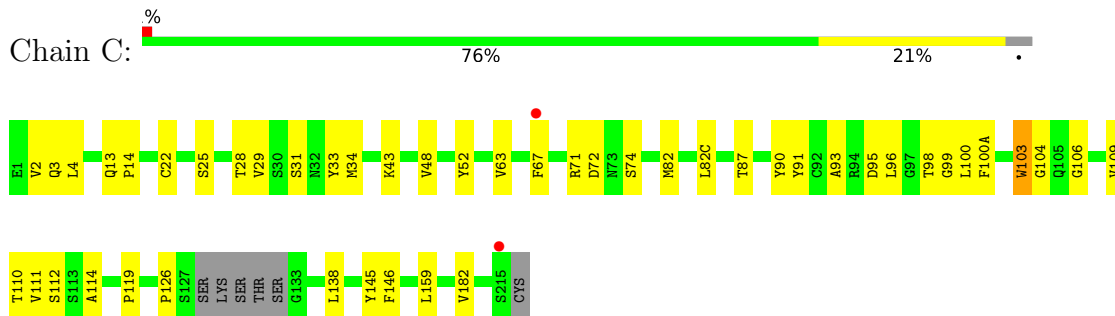
- Molecule 1: COV107-23 heavy chain

Chain H:

76% 21%

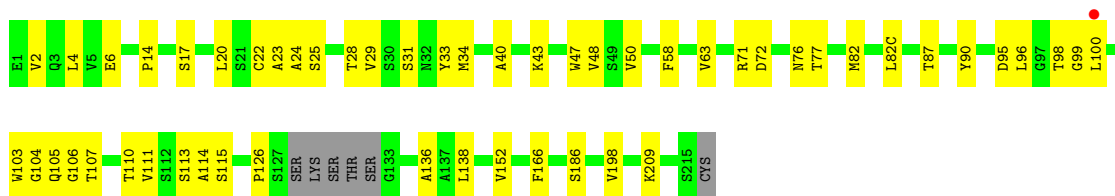- Molecule 1: COV107-23 heavy chain

Chain A:

%

73% 24%

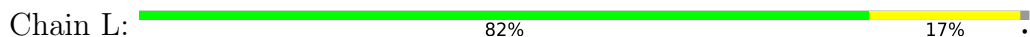- Molecule 1: COV107-23 heavy chain

Chain C:

%

76% 21%

- Molecule 1: COV107-23 heavy chain

Chain M:

73% 24%

E1 V2 Q3 L4 V5 E6 P14 S17 L20 S21 C22 A23 A24 S25 T28 V29 S30 S31 N32 Y33 M34 A40 K43 W47 V48 S49 V50 F58 V63 R71 D72 N76 T77 M82 L82C T87 Y90 D95 L96 G97 T98 G99 L100

W103 G104 Q105 G106 T107 T110 V111 S112 S113 A114 S115 P126 S127 SER LYS SER THR SER G133 A136 A137 L138 V152 F166 S186 V198 K209 S215 CYS

• Molecule 2: COVD21-C8 light chain

Chain L:

E1 Q6 S7 P8 P15 A19 T20 L21 S29 S30 S31 Y32 L33 Y36 Q37 Q38 L47 G50 F71 I75 S76 R77 A84 Q100 G101 T102 E105 I106 K107 P120 Q124 G128 T129 A130 N138 F139 Y140 K145 V146 Q147 Q166

T172 V191 K207 E213 CYS SER

• Molecule 2: COVD21-C8 light chain

Chain B:

E1 I2 P15 G16 A19 T20 L21 Q27 S29 S30 S31 Y32 L33 Q37 Q38 R45 L46 L47 R54 A55 T56 G57 I58 F71 T72 L73 I74 I75 S76 R77 A84 C88 Q89 Q90 Y91 P95 R96 G99 Q100 G101 T102 E105 I106 K107 R108 F118

P119 P120 Q124 G128 T129 A130 V133 R142 K145 K149 V163 L175 Y186 K190 V191 Y192 A193 T197 T206 N210 E213 CYS SER

• Molecule 2: COVD21-C8 light chain

Chain D:

E1 I2 Q6 S7 P8 P15 A19 T20 L21 R24 Q27 S29 Y32 L33 Y36 Q37 R45 L46 L47 A51 G57 D60 R61 G66 T69 D70 F71 L78 D82 Q89 Q90 Y91 R96 Q100 G101 T102 E105 I106 F118
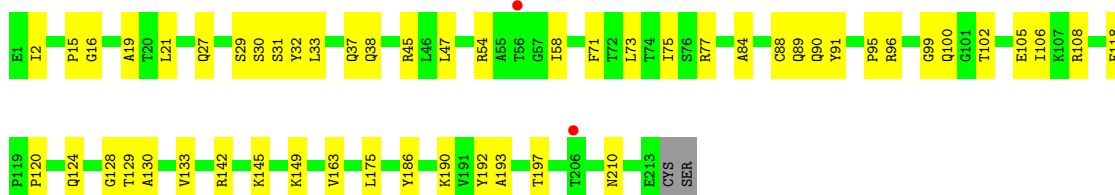
P119 P120 Q124 T129 A130 S131 V132 V133 N138 R142 T172 L179 F209 E213 CYS SER

• Molecule 2: COVD21-C8 light chain

Chain N:

E1 I2 V3 L4 T5 Q6 S7 PRO GLY T10 P15 GLY GLU ARG A19 T20 L21 S22 C23 S26 Q27 S27A V28 S29 Y32 L33 A34 W35 Y36 Q37 Q38 K39 R45 L46 L47 A51 P59 D60 R61 F62 G66 F71 T72 L73 T74 I75 L78 E79 P80 E81 D82

F83 A84 Y87 C88 Q89 Q90 Y91 S94 P95 R96 Q100 G101 T102 K103 K107 P113 F118 P119 P120 Q124 T129 A130 V133 N138 F139 Y140 P141 R142 K149 S156 T172 S176 E195 E213 CYS SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.30Å　　78.38Å　　91.63Å 100.12°　　112.09°　　92.80°	Depositor
Resolution (Å)	40.19　–　3.40 40.19　–　3.40	Depositor EDS
% Data completeness (in resolution range)	88.3 (40.19-3.40) 75.8 (40.19-3.40)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.60 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.276　,　0.311 0.276　,　0.311	Depositor DCC
R_{free} test set	1087 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	1.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , -2.6	EDS
L-test for twinning[2]	$<|L|> = 0.39, <L^2> = 0.22$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	12881	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	A	0.26	0/1625	0.50	0/2212
1	C	0.25	0/1625	0.48	0/2212
1	H	0.26	0/1625	0.48	0/2212
1	M	0.25	0/1625	0.48	0/2212
2	B	0.26	0/1675	0.47	0/2273
2	D	0.25	0/1675	0.45	0/2273
2	L	0.27	0/1675	0.49	0/2273
2	N	0.26	0/1637	0.52	0/2219
All	All	0.26	0/13162	0.48	0/17886

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	79	GLU	Peptide

5.2 Too-close contacts ⓘ

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	1589	0	1559	35	0
1	C	1589	0	1559	30	0
1	H	1589	0	1559	27	1
1	M	1589	0	1559	30	1
2	B	1640	0	1595	36	1
2	D	1640	0	1595	27	0
2	L	1640	0	1595	28	1
2	N	1605	0	1561	39	0
All	All	12881	0	12582	230	2

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 9.

All (230) 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:C:99:GLY:HA3	2:D:91:TYR:HB2	1.58	0.85
1:A:82(A):ASN:ND2	1:C:71:ARG:O	2.09	0.85
1:M:82(C):LEU:HB3	1:M:111:VAL:HG21	1.59	0.83
1:H:33:TYR:HB2	1:H:95:ASP:HB2	1.61	0.82
2:D:27:GLN:NE2	2:N:27(A):SER:O	2.17	0.77
1:C:98:THR:O	2:D:96:ARG:NH1	2.19	0.76
1:M:29:VAL:HG13	1:M:34:MET:HG3	1.66	0.76
2:L:77:ARG:NH1	2:B:128:GLY:HA2	2.01	0.75
1:H:90:TYR:O	1:H:106:GLY:HA2	1.87	0.73
1:A:82(C):LEU:HB3	1:A:111:VAL:HG11	1.74	0.69
1:A:112:SER:HB2	1:A:146:PHE:HZ	1.57	0.68
1:M:98:THR:O	2:N:96:ARG:NH1	2.28	0.67
2:N:10:THR:HG23	2:N:103:LYS:HB3	1.76	0.67
1:A:90:TYR:O	1:A:106:GLY:HA2	1.95	0.65
2:B:54:ARG:NH2	2:B:58:ILE:O	2.30	0.65
2:N:39:LYS:HG2	2:N:84:ALA:HB2	1.79	0.65
2:N:19:ALA:HB3	2:N:75:ILE:HB	1.80	0.64
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.79	0.64
1:H:126:PRO:HG3	1:H:138:LEU:HB3	1.80	0.64
1:M:14:PRO:HD3	1:M:113:SER:HB3	1.80	0.63
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.81	0.63
1:A:2:VAL:HA	1:A:25:SER:O	1.97	0.63
1:A:48:VAL:HG13	1:A:63:VAL:HG11	1.81	0.62
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:33:LEU:HB3	2:N:51:ALA:HB2	1.82	0.61
2:L:107:LYS:HA	2:L:140:TYR:OH	2.00	0.61
1:C:87:THR:HG23	1:C:110:THR:HA	1.82	0.61
1:C:13:GLN:HG3	1:C:14:PRO:HD2	1.83	0.61
1:M:33:TYR:HB2	1:M:95:ASP:HB2	1.82	0.61
2:L:120:PRO:HG3	2:L:130:ALA:HB1	1.82	0.61
1:H:17:SER:HA	1:H:82:MET:O	2.02	0.60
1:A:29:VAL:HG13	1:A:34:MET:HG3	1.82	0.60
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.82	0.60
2:N:138:ASN:HA	2:N:172:THR:HB	1.83	0.60
1:M:90:TYR:O	1:M:106:GLY:HA2	2.01	0.59
1:A:82(B):SER:OG	1:C:71:ARG:NH2	2.35	0.59
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.85	0.59
1:M:28:THR:OG1	1:M:31:SER:OG	2.20	0.59
2:B:33:LEU:HA	2:B:89:GLN:O	2.02	0.59
1:C:90:TYR:O	1:C:106:GLY:HA2	2.02	0.59
2:D:33:LEU:HB3	2:D:51:ALA:HB2	1.85	0.58
1:M:126:PRO:HG3	1:M:138:LEU:HB3	1.84	0.58
1:M:4:LEU:HB2	1:M:104:GLY:HA2	1.86	0.58
1:H:133:GLY:HA3	1:A:62:SER:HB3	1.84	0.58
1:H:29:VAL:HG13	1:H:34:MET:HG3	1.85	0.57
1:C:3:GLN:HB3	1:C:25:SER:HB2	1.87	0.57
1:C:28:THR:HG1	1:C:31:SER:HG	1.37	0.57
2:L:15:PRO:HD3	2:L:106:ILE:HG23	1.87	0.57
1:A:17:SER:HA	1:A:82:MET:O	2.05	0.57
1:C:82:MET:HE2	1:C:82(C):LEU:HD11	1.87	0.56
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.86	0.56
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.88	0.56
1:C:82(C):LEU:HB3	1:C:111:VAL:HG11	1.88	0.56
2:N:62:PHE:CE1	2:N:75:ILE:HG23	2.40	0.56
1:A:114:ALA:HB3	1:A:146:PHE:CE1	2.40	0.56
2:B:91:TYR:HA	2:B:96:ARG:HG2	1.87	0.56
1:M:23:ALA:HA	1:M:77:THR:HG22	1.89	0.55
2:N:36:TYR:HE1	2:N:89:GLN:HB3	1.72	0.55
2:B:32:TYR:O	2:B:90:GLN:HA	2.07	0.55
2:N:38:GLN:O	2:N:84:ALA:HB1	2.05	0.55
1:M:99:GLY:HA3	2:N:91:TYR:HB2	1.88	0.55
1:A:100(A):PHE:HE1	2:B:89:GLN:HE22	1.54	0.54
2:B:16:GLY:HA2	2:B:77:ARG:HE	1.73	0.53
1:H:28:THR:OG1	1:H:31:SER:OG	2.27	0.53
1:M:17:SER:HA	1:M:82:MET:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:ARG:NH2	1:H:73:ASN:HD21	2.07	0.53
1:H:96:LEU:O	1:H:100:LEU:HB2	2.08	0.53
1:M:40:ALA:HB3	1:M:43:LYS:HB3	1.89	0.53
2:B:29:SER:HB3	2:B:32:TYR:CD2	2.44	0.53
1:C:4:LEU:HB2	1:C:104:GLY:HA2	1.91	0.53
2:D:138:ASN:HA	2:D:172:THR:HB	1.91	0.53
2:L:191:VAL:HG21	1:C:52:TYR:HE2	1.74	0.52
1:A:11:LEU:HD22	1:A:147:PRO:HG3	1.92	0.52
2:B:2:ILE:HG23	2:B:27:GLN:H	1.74	0.52
1:M:2:VAL:HA	1:M:25:SER:O	2.09	0.52
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.91	0.52
2:L:29:SER:HB3	2:L:32:TYR:HD2	1.74	0.52
1:A:40:ALA:HB3	1:A:43:LYS:HB3	1.92	0.52
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.91	0.51
1:M:29:VAL:HG23	1:M:76:ASN:HB2	1.92	0.51
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.91	0.51
2:L:77:ARG:HH11	2:B:128:GLY:HA2	1.72	0.51
1:C:126:PRO:HG3	1:C:138:LEU:HB3	1.92	0.51
2:L:31:SER:HA	2:L:50:GLY:HA2	1.92	0.51
1:A:16:GLY:HA2	1:C:74:SER:OG	2.11	0.51
1:A:87:THR:HA	1:A:109:VAL:O	2.11	0.51
1:A:4:LEU:HD21	1:A:27:PHE:HE1	1.76	0.50
2:N:29:SER:HB3	2:N:32:TYR:HD2	1.77	0.50
1:H:39:GLN:NE2	2:L:38:GLN:OE1	2.42	0.50
1:A:59:TYR:HB3	1:A:63:VAL:HG23	1.92	0.50
1:A:39:GLN:NE2	2:B:38:GLN:OE1	2.38	0.50
2:D:120:PRO:HG3	2:D:130:ALA:HB1	1.94	0.50
1:H:114:ALA:HB3	1:H:146:PHE:CE1	2.47	0.50
2:N:21:LEU:HD22	2:N:102:THR:HG21	1.93	0.50
2:B:29:SER:O	2:B:31:SER:N	2.45	0.49
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.46	0.49
1:M:96:LEU:O	1:M:100:LEU:HB2	2.13	0.49
1:H:11:LEU:HD22	1:H:147:PRO:HG3	1.94	0.49
2:B:15:PRO:HD3	2:B:106:ILE:HG23	1.93	0.49
1:A:38:ARG:NH1	1:A:85:GLU:OE1	2.46	0.49
2:L:29:SER:HB3	2:L:32:TYR:CD2	2.48	0.48
2:N:32:TYR:HA	2:N:91:TYR:CE2	2.48	0.48
1:M:82:MET:HE2	1:M:82(C):LEU:HD11	1.95	0.48
2:N:4:LEU:HD11	2:N:90:GLN:H	1.78	0.48
2:N:45:ARG:HE	2:N:59:PRO:HG3	1.77	0.48
2:B:21:LEU:HD22	2:B:102:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:SER:HB3	2:B:32:TYR:HD2	1.78	0.48
2:D:6:GLN:H	2:D:100:GLN:HE22	1.59	0.48
1:M:114:ALA:O	1:M:115:SER:OG	2.28	0.48
2:D:19:ALA:HB2	2:D:78:LEU:HD11	1.94	0.48
1:M:6:GLU:H	1:M:105:GLN:HE22	1.62	0.48
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.48	0.48
2:N:29:SER:HB3	2:N:32:TYR:CD2	2.48	0.48
1:C:48:VAL:HG13	1:C:63:VAL:HG21	1.96	0.47
2:B:145:LYS:HB3	2:B:197:THR:HB	1.95	0.47
1:C:29:VAL:HG13	1:C:34:MET:HG3	1.96	0.47
1:C:91:TYR:HB3	1:C:103:TRP:HD1	1.78	0.47
2:D:29:SER:HB3	2:D:32:TYR:CD2	2.49	0.47
1:M:87:THR:HG23	1:M:110:THR:HA	1.96	0.47
2:D:124:GLN:HG2	2:D:129:THR:O	2.14	0.47
2:N:107:LYS:HA	2:N:140:TYR:OH	2.15	0.47
1:H:209:LYS:HD2	2:N:156:SER:HB3	1.97	0.47
1:H:103:TRP:HH2	2:L:36:TYR:CD2	2.32	0.47
1:M:152:VAL:HG22	1:M:198:VAL:HG22	1.97	0.47
2:L:38:GLN:O	2:L:84:ALA:HB1	2.16	0.46
2:L:19:ALA:HB3	2:L:75:ILE:HB	1.96	0.46
2:B:90:GLN:NE2	2:B:95:PRO:O	2.47	0.46
2:B:45:ARG:HH11	2:B:58:ILE:HD13	1.80	0.46
2:D:15:PRO:HD3	2:D:106:ILE:HG23	1.97	0.46
2:B:118:PHE:HB2	2:B:133:VAL:HB	1.97	0.46
1:C:96:LEU:O	1:C:100:LEU:HB2	2.15	0.46
2:N:118:PHE:HB2	2:N:133:VAL:HB	1.98	0.46
2:N:113:PRO:HB3	2:N:139:PHE:HB3	1.97	0.46
2:B:16:GLY:HA2	2:B:77:ARG:NE	2.30	0.46
1:A:199:ASN:ND2	1:A:201:LYS:HG3	2.31	0.46
1:A:91:TYR:HB3	1:A:103:TRP:HD1	1.81	0.45
2:B:37:GLN:O	2:B:45:ARG:N	2.49	0.45
2:D:37:GLN:O	2:D:45:ARG:N	2.49	0.45
1:A:6:GLU:H	1:A:105:GLN:HE22	1.62	0.45
1:H:71:ARG:HH21	1:H:73:ASN:HD21	1.62	0.45
2:B:88:CYS:O	2:B:99:GLY:N	2.46	0.45
1:M:47:TRP:HZ2	1:M:50:VAL:HG12	1.81	0.45
2:L:138:ASN:HA	2:L:172:THR:HB	1.99	0.45
2:L:77:ARG:CZ	2:B:128:GLY:HA2	2.46	0.45
1:A:17:SER:OG	1:C:72:ASP:OD1	2.31	0.45
1:M:50:VAL:HG12	1:M:58:PHE:HB2	1.98	0.45
2:N:2:ILE:HD12	2:N:90:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:THR:HA	1:H:109:VAL:O	2.17	0.45
1:H:152:VAL:HG22	1:H:198:VAL:HG22	1.97	0.45
1:H:48:VAL:HG13	1:H:63:VAL:HG11	1.98	0.44
2:L:6:GLN:H	2:L:100:GLN:HE22	1.64	0.44
2:N:120:PRO:HG3	2:N:130:ALA:HB1	1.98	0.44
1:H:136:ALA:HB2	1:H:186:SER:HB3	1.98	0.44
2:N:79:GLU:HB3	2:N:80:PRO:HD2	2.00	0.44
2:L:145:LYS:HE3	2:L:147:GLN:NE2	2.33	0.44
2:L:105:GLU:OE1	2:L:166:GLN:NE2	2.46	0.44
2:D:142:ARG:O	2:D:142:ARG:NH1	2.51	0.44
2:N:149:LYS:NZ	2:N:195:GLU:OE1	2.34	0.44
2:B:21:LEU:HD12	2:B:73:LEU:HD23	2.00	0.44
2:B:124:GLN:HG2	2:B:129:THR:O	2.17	0.44
2:D:119:PRO:HB3	2:D:209:PHE:CE1	2.53	0.43
2:N:33:LEU:HD22	2:N:71:PHE:CG	2.53	0.43
1:M:136:ALA:HB2	1:M:186:SER:HB3	2.00	0.43
2:N:32:TYR:HA	2:N:91:TYR:CZ	2.53	0.43
2:N:2:ILE:HG21	2:N:28:VAL:HG22	2.01	0.43
1:C:87:THR:HA	1:C:109:VAL:O	2.19	0.43
1:M:48:VAL:HG13	1:M:63:VAL:HG21	2.00	0.43
2:D:36:TYR:HE1	2:D:89:GLN:HB3	1.82	0.43
2:D:89:GLN:HE21	2:D:96:ARG:HB3	1.83	0.43
2:D:118:PHE:HB2	2:D:133:VAL:HB	1.99	0.43
2:D:21:LEU:HD22	2:D:102:THR:HG21	2.00	0.43
2:N:124:GLN:HG2	2:N:129:THR:O	2.19	0.43
2:B:33:LEU:HD22	2:B:71:PHE:CD1	2.54	0.42
1:H:19:ARG:NH1	1:H:79:TYR:CG	2.87	0.42
1:A:39:GLN:OE1	2:B:38:GLN:NE2	2.44	0.42
2:B:186:TYR:HA	2:B:192:TYR:OH	2.20	0.42
2:N:61:ARG:NH1	2:N:82:ASP:OD2	2.53	0.42
2:L:21:LEU:HD22	2:L:102:THR:HG21	2.01	0.42
2:L:7:SER:HA	2:L:8:PRO:HA	1.84	0.42
1:A:4:LEU:HB2	1:A:104:GLY:HA2	2.01	0.42
1:C:93:ALA:HB3	1:C:100(A):PHE:HD2	1.84	0.42
2:D:32:TYR:O	2:D:90:GLN:HA	2.19	0.42
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.02	0.42
1:A:126:PRO:HD2	1:A:213:PRO:HA	2.02	0.42
1:C:112:SER:HG	1:C:146:PHE:HZ	1.65	0.42
1:M:4:LEU:HD23	1:M:24:ALA:HA	2.02	0.42
2:N:142:ARG:O	2:N:142:ARG:NH1	2.52	0.42
1:H:67:PHE:HA	1:H:81:GLN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:TRP:HZ2	1:H:50:VAL:HG12	1.84	0.42
1:H:189:LEU:HD23	1:H:189:LEU:HA	1.93	0.42
1:H:40:ALA:HB3	1:H:43:LYS:HB3	2.01	0.42
2:L:107:LYS:HA	2:L:140:TYR:CZ	2.55	0.42
2:B:33:LEU:HD21	2:B:88:CYS:HB2	2.02	0.42
1:A:87:THR:HG23	1:A:110:THR:HA	2.01	0.41
2:B:149:LYS:HB2	2:B:193:ALA:HB3	2.02	0.41
2:N:28:VAL:HG12	2:N:32:TYR:HB2	2.00	0.41
1:A:47:TRP:HZ2	1:A:50:VAL:HG12	1.84	0.41
1:C:33:TYR:HB2	1:C:95:ASP:HB2	2.01	0.41
1:C:114:ALA:HB3	1:C:146:PHE:CE1	2.55	0.41
1:M:99:GLY:HA3	2:N:91:TYR:CD2	2.55	0.41
2:N:6:GLN:H	2:N:100:GLN:HE22	1.68	0.41
2:N:6:GLN:H	2:N:100:GLN:NE2	2.18	0.41
2:L:6:GLN:HB3	2:L:102:THR:OG1	2.21	0.41
2:L:124:GLN:HG2	2:L:129:THR:O	2.21	0.41
1:M:47:TRP:HE1	1:M:50:VAL:HB	1.85	0.41
1:A:146:PHE:HA	1:A:147:PRO:HA	1.89	0.41
2:D:6:GLN:H	2:D:100:GLN:NE2	2.19	0.41
2:D:7:SER:HA	2:D:8:PRO:HA	1.85	0.41
2:D:61:ARG:NE	2:D:82:ASP:OD2	2.54	0.41
1:M:20:LEU:HG	1:M:107:THR:HG21	2.01	0.41
1:H:59:TYR:HB3	1:H:63:VAL:HG23	2.02	0.41
2:B:38:GLN:O	2:B:84:ALA:HB1	2.21	0.41
1:C:159:LEU:HD21	1:C:182:VAL:HG21	2.03	0.41
2:N:35:TRP:CE3	2:N:73:LEU:HD22	2.55	0.41
2:D:66:GLY:HA3	2:D:71:PHE:HA	2.03	0.41
1:H:43:LYS:HA	1:H:43:LYS:HD2	1.92	0.40
2:L:6:GLN:H	2:L:100:GLN:NE2	2.18	0.40
1:C:67:PHE:CZ	1:C:82:MET:HE3	2.56	0.40
2:N:4:LEU:HD11	2:N:90:GLN:N	2.35	0.40
1:C:2:VAL:HA	1:C:25:SER:O	2.21	0.40
1:C:43:LYS:HA	1:C:43:LYS:HD2	1.90	0.40
1:A:199:ASN:HD21	1:A:201:LYS:HG3	1.85	0.40
2:D:24:ARG:HA	2:D:69:THR:O	2.22	0.40
2:D:131:SER:HA	2:D:179:LEU:O	2.22	0.40
2:L:33:LEU:HD22	2:L:71:PHE:CD1	2.57	0.40
2:L:207:LYS:HD2	2:L:207:LYS:HA	1.93	0.40
1:A:30:SER:HB3	1:A:73:ASN:CG	2.41	0.40
2:B:19:ALA:HB3	2:B:75:ILE:HB	2.04	0.40
2:B:190:LYS:HE3	2:B:210:ASN:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:PHE:CE1	2:N:176:SER:HB3	2.57	0.40

All (2) 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)
2:L:128:GLY:O	2:B:77:ARG:NH2[1_655]	2.10	0.10
1:H:17:SER:OG	1:M:72:ASP:OD1[1_656]	2.15	0.05

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	210/220 (96%)	201 (96%)	9 (4%)	0	100	100
1	C	210/220 (96%)	200 (95%)	10 (5%)	0	100	100
1	H	210/220 (96%)	200 (95%)	10 (5%)	0	100	100
1	M	210/220 (96%)	200 (95%)	10 (5%)	0	100	100
2	B	212/216 (98%)	201 (95%)	10 (5%)	1 (0%)	29	61
2	D	212/216 (98%)	203 (96%)	9 (4%)	0	100	100
2	L	212/216 (98%)	204 (96%)	8 (4%)	0	100	100
2	N	203/216 (94%)	189 (93%)	14 (7%)	0	100	100
All	All	1679/1744 (96%)	1598 (95%)	80 (5%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	SER

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	178/184 (97%)	174 (98%)	4 (2%)	52	75
1	C	178/184 (97%)	176 (99%)	2 (1%)	73	86
1	H	178/184 (97%)	176 (99%)	2 (1%)	73	86
1	M	178/184 (97%)	174 (98%)	4 (2%)	52	75
2	B	185/187 (99%)	181 (98%)	4 (2%)	52	75
2	D	185/187 (99%)	183 (99%)	2 (1%)	73	86
2	L	185/187 (99%)	185 (100%)	0	100	100
2	N	182/187 (97%)	181 (100%)	1 (0%)	88	94
All	All	1449/1484 (98%)	1430 (99%)	19 (1%)	69	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	76	ASN
1	H	85	GLU
1	A	76	ASN
1	A	103	TRP
1	A	196	CYS
1	A	209	LYS
2	B	100	GLN
2	B	105	GLU
2	B	108	ARG
2	B	142	ARG
1	C	22	CYS
1	C	103	TRP
2	D	105	GLU
2	D	142	ARG
1	M	22	CYS
1	M	71	ARG
1	M	103	TRP
1	M	209	LYS
2	N	142	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	73	ASN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	214/220 (97%)	0.14	2 (0%)	84	83	39, 57, 80, 93	0
1	C	214/220 (97%)	0.16	2 (0%)	84	83	45, 60, 75, 89	0
1	H	214/220 (97%)	0.09	1 (0%)	91	90	38, 53, 75, 98	0
1	M	214/220 (97%)	0.02	1 (0%)	91	90	43, 54, 75, 94	0
2	B	214/216 (99%)	0.09	2 (0%)	84	83	43, 59, 82, 89	0
2	D	214/216 (99%)	0.16	4 (1%)	66	65	42, 63, 95, 121	0
2	L	214/216 (99%)	0.08	1 (0%)	91	90	38, 58, 86, 105	0
2	N	209/216 (96%)	0.55	22 (10%)	6	7	42, 75, 133, 148	0
All	All	1707/1744 (97%)	0.16	35 (2%)	63	62	38, 58, 94, 148	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	4	LEU	5.9
2	L	1	GLU	4.9
2	N	71	PHE	4.9
2	N	34	ALA	4.5
2	N	23	CYS	4.3
2	D	60	ASP	4.2
2	N	100	GLN	4.2
1	C	215	SER	3.9
2	N	3	VAL	3.6
2	N	1	GLU	3.5
2	N	94	SER	3.4
2	N	75	ILE	3.3
2	N	47	LEU	3.2
2	N	7	SER	3.2
2	N	26	SER	3.2
2	D	57	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	N	66	GLY	2.9
2	N	27	GLN	2.8
1	M	100	LEU	2.8
1	A	27	PHE	2.7
1	H	191	THR	2.4
2	N	5	THR	2.3
2	N	36	TYR	2.2
2	N	78	LEU	2.2
1	C	67	PHE	2.2
2	N	27(A)	SER	2.2
2	N	62	PHE	2.2
2	D	27	GLN	2.2
2	N	87	TYR	2.1
2	N	6	GLN	2.1
2	N	46	LEU	2.1
2	B	56	THR	2.1
2	D	2	ILE	2.1
1	A	133	GLY	2.1
2	B	206	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.