



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 AM UTC

PDB ID : 7E7X / pdb_00007e7x
Title : SARS-CoV-2 Spike Protein N terminal domain in Complex with N11 Fab
Authors : Zhang, Z.; Shuo, D.; Xiao, J.
Deposited on : 2021-02-28
Resolution : 2.78 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

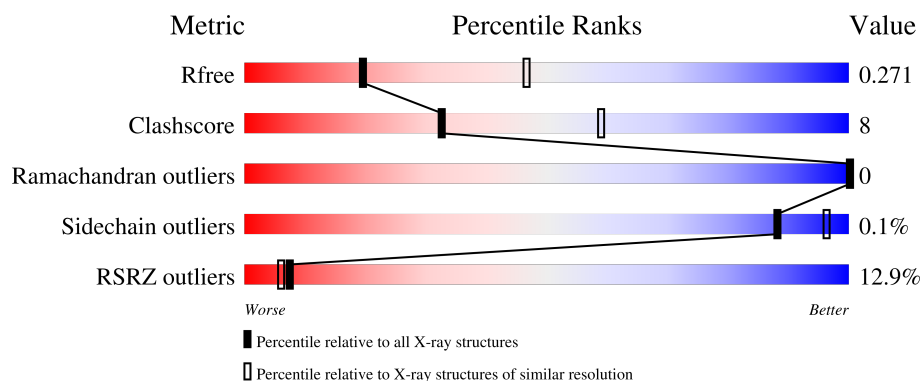
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	297	18% 60% 17% 23%
1	B	297	34% 50% 19% • 31%
2	H	234	2% 78% 12% 10%
2	M	234	% 75% 15% 10%
3	L	216	% 88% 10% •

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Mol	Chain	Length	Quality of chain
3	N	216	% 88% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9767 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1862	1212	301	344	5			
1	B	206	Total	C	N	O	S	0	0	0
			1675	1090	271	309	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	HIS	-	expression tag	UNP P0DTC2
A	305	HIS	-	expression tag	UNP P0DTC2
A	306	HIS	-	expression tag	UNP P0DTC2
A	307	HIS	-	expression tag	UNP P0DTC2
A	308	HIS	-	expression tag	UNP P0DTC2
A	309	HIS	-	expression tag	UNP P0DTC2
B	304	HIS	-	expression tag	UNP P0DTC2
B	305	HIS	-	expression tag	UNP P0DTC2
B	306	HIS	-	expression tag	UNP P0DTC2
B	307	HIS	-	expression tag	UNP P0DTC2
B	308	HIS	-	expression tag	UNP P0DTC2
B	309	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called N11 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1561	990	253	311	7			
2	M	211	Total	C	N	O	S	0	0	0
			1561	990	253	311	7			

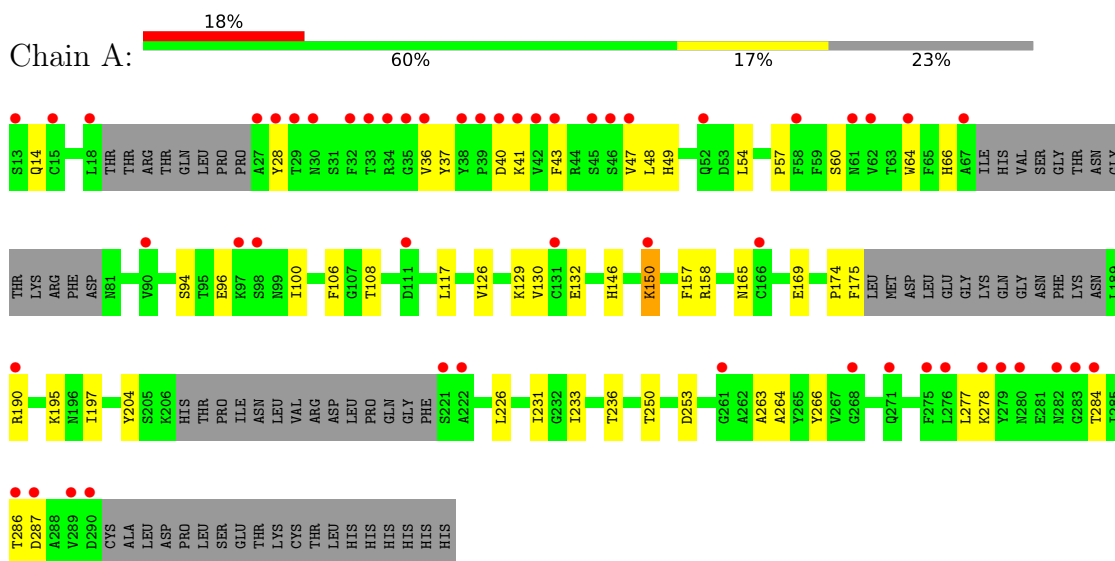
- Molecule 3 is a protein called N11 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1554	975	254	320	5			
3	N	211	Total	C	N	O	S	0	0	0
			1554	975	254	320	5			

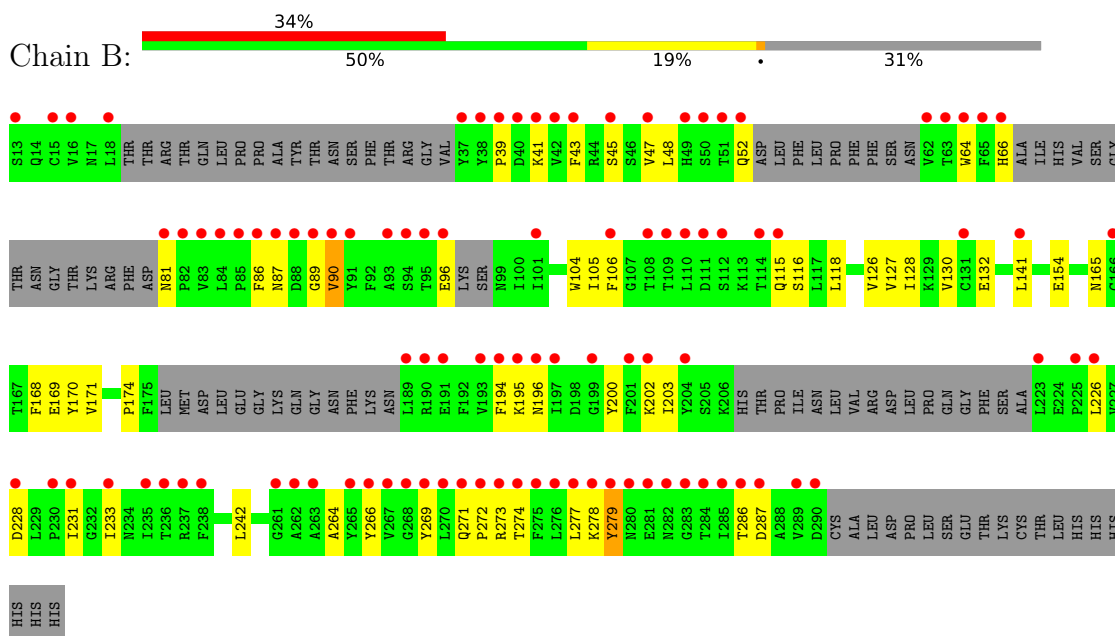
3 Residue-property plots

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.

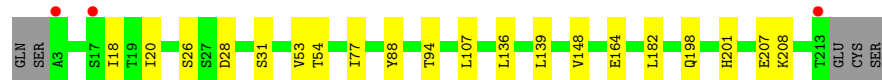
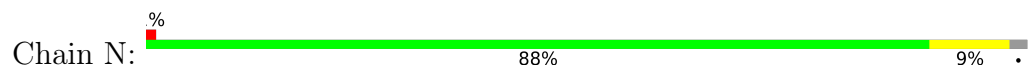
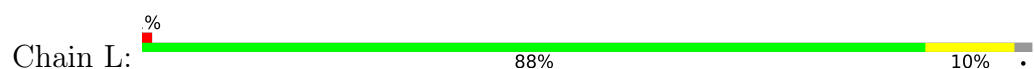
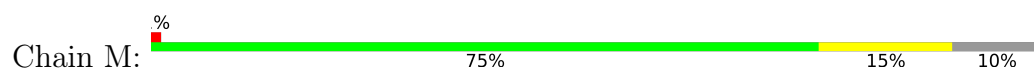
• Molecule 1: Spike protein S1



• Molecule 1: Spike protein S1



Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.42Å 113.28Å 210.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.47 – 2.78 19.47 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.47-2.78) 98.6 (19.47-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.248 , 0.279 (Not available) , 0.271	Depositor DCC
R_{free} test set	1988 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9767	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 48.34 % 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 8.7294e-05. 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

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	0.42	2/1914 (0.1%)	0.61	6/2602 (0.2%)
1	B	0.32	1/1719 (0.1%)	0.61	5/2334 (0.2%)
2	H	0.25	0/1599	0.53	3/2184 (0.1%)
2	M	0.37	1/1599 (0.1%)	0.59	4/2184 (0.2%)
3	L	0.25	0/1594	0.44	1/2180 (0.0%)
3	N	0.17	0/1594	0.40	0/2180
All	All	0.31	4/10019 (0.0%)	0.54	19/13664 (0.1%)

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	H	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	23	LYS	CE-NZ	10.17	1.79	1.49
1	A	150	LYS	CD-CE	9.57	1.81	1.52
1	A	150	LYS	CE-NZ	8.42	1.74	1.49
1	B	226	LEU	C-N	5.59	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	181	GLN	CA-CB-CG	8.28	130.66	114.10
2	M	62	GLN	CB-CG-CD	-7.84	99.27	112.60
1	B	195	LYS	CD-CE-NZ	-7.30	88.54	111.90
2	M	62	GLN	CA-CB-CG	7.11	128.32	114.10
2	M	23	LYS	CD-CE-NZ	-6.71	90.41	111.90
1	A	150	LYS	CB-CA-C	-6.66	101.21	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	LYS	CA-CB-CG	6.61	127.32	114.10
1	A	150	LYS	CA-C-N	-6.50	111.67	122.21
1	A	150	LYS	C-N-CA	-6.50	111.67	122.21
1	A	150	LYS	CG-CD-CE	-6.33	96.75	111.30
1	B	90	VAL	CG1-CB-CG2	5.83	123.63	110.80
2	M	62	GLN	CB-CA-C	-5.72	100.04	110.63
1	B	89	GLY	CA-C-N	-5.68	114.05	122.23
1	B	89	GLY	C-N-CA	-5.68	114.05	122.23
2	H	180	LEU	CA-C-N	-5.55	112.35	122.12
2	H	180	LEU	C-N-CA	-5.55	112.35	122.12
1	B	90	VAL	CA-CB-CG1	5.41	119.59	110.40
1	A	150	LYS	CD-CE-NZ	-5.41	94.60	111.90
3	L	44	LYS	CB-CA-C	5.20	120.45	109.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	181	GLN	Sidechain

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	1862	0	1782	39	0
1	B	1675	0	1603	43	1
2	H	1561	0	1518	18	0
2	M	1561	0	1518	27	0
3	L	1554	0	1484	17	0
3	N	1554	0	1484	16	0
All	All	9767	0	9389	151	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 8.

All (151) 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:A:150:LYS:CD	1:A:150:LYS:CE	1.81	1.57
1:A:150:LYS:CE	1:A:150:LYS:NZ	1.74	1.48
2:M:23:LYS:CE	2:M:23:LYS:NZ	1.79	1.41
1:A:150:LYS:CE	1:A:150:LYS:CG	2.44	0.95
2:M:23:LYS:NZ	2:M:23:LYS:CD	2.33	0.90
3:L:198:GLN:HG2	3:L:207:GLU:HG3	1.61	0.80
1:B:81:ASN:OD1	1:B:242:LEU:HD11	1.82	0.80
1:B:115:GLN:HG2	1:B:130:VAL:HG22	1.66	0.77
3:L:56:ARG:NH1	3:L:62:ASP:HA	2.01	0.74
1:A:57:PRO:HB2	1:A:60:SER:HB2	1.69	0.74
1:B:45:SER:HB2	1:B:279:TYR:CD2	2.23	0.74
1:A:150:LYS:CE	1:A:150:LYS:HG2	2.19	0.73
1:A:277:LEU:HD12	1:A:284:THR:HG21	1.70	0.71
1:B:128:ILE:HD12	1:B:170:TYR:HD2	1.54	0.71
1:B:48:LEU:HD12	1:B:278:LYS:HG2	1.73	0.70
2:M:27:TYR:HB2	2:M:32:ILE:HD11	1.72	0.70
3:L:136:LEU:HD12	3:L:182:LEU:HD23	1.74	0.68
3:N:136:LEU:HD12	3:N:182:LEU:HD23	1.75	0.68
1:B:90:VAL:HG23	1:B:194:PHE:HB2	1.76	0.67
1:B:86:PHE:CE1	1:B:90:VAL:HG22	2.29	0.66
3:N:20:ILE:HD11	3:N:107:LEU:HD12	1.77	0.66
2:H:27:TYR:HB2	2:H:32:ILE:HD11	1.78	0.65
3:L:20:ILE:HD11	3:L:107:LEU:HD12	1.78	0.65
1:B:130:VAL:HG12	1:B:168:PHE:HB3	1.77	0.65
1:A:150:LYS:CD	1:A:150:LYS:NZ	2.61	0.64
1:A:100:ILE:HD13	1:A:263:ALA:HB2	1.81	0.63
1:A:157:PHE:O	1:A:158:ARG:HB2	1.97	0.63
3:L:56:ARG:HH12	3:L:62:ASP:HB3	1.64	0.62
1:B:141:LEU:HD21	1:B:154:GLU:HG2	1.80	0.62
3:N:28:ASP:HB3	3:N:94:THR:HG22	1.82	0.62
1:A:286:THR:HG22	1:A:287:ASP:H	1.65	0.61
1:A:37:TYR:OH	1:A:54:LEU:O	2.17	0.61
1:B:242:LEU:HD12	1:B:242:LEU:N	2.16	0.60
1:B:66:HIS:HB3	1:B:264:ALA:HA	1.83	0.60
2:M:191:VAL:HG21	3:N:139:LEU:HD13	1.84	0.60
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.86	0.58
2:M:23:LYS:NZ	2:M:23:LYS:CG	2.66	0.58
3:L:56:ARG:HH12	3:L:62:ASP:CB	2.17	0.58
1:B:286:THR:HG22	1:B:287:ASP:H	1.69	0.56
1:B:130:VAL:CG1	1:B:168:PHE:HB3	2.34	0.56
1:A:28:TYR:HB2	1:A:64:TRP:HD1	1.70	0.55
2:H:191:VAL:HG21	3:L:139:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:HG22	1:B:48:LEU:H	1.71	0.55
2:H:179:VAL:HG21	3:L:164:GLU:HB3	1.88	0.55
1:B:271:GLN:HB3	1:B:273:ARG:HG3	1.89	0.55
3:L:50:ILE:HD13	3:L:56:ARG:HG2	1.90	0.54
1:A:47:VAL:HG22	1:A:48:LEU:H	1.72	0.54
2:H:89:GLU:OE1	2:H:89:GLU:N	2.37	0.53
2:M:29:LEU:HD23	2:M:72:GLU:HG2	1.89	0.53
1:A:126:VAL:HB	1:A:174:PRO:HA	1.92	0.52
1:A:41:LYS:HD3	1:A:43:PHE:HE1	1.75	0.52
2:M:179:VAL:HG21	3:N:164:GLU:HB3	1.91	0.52
1:A:146:HIS:CE1	2:H:30:ILE:HD11	2.45	0.52
1:A:195:LYS:HE2	1:A:197:ILE:HD13	1.92	0.52
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.18	0.51
1:B:202:LYS:HA	1:B:228:ASP:HB3	1.93	0.51
1:B:52:GLN:NE2	1:B:272:PRO:O	2.43	0.51
1:B:126:VAL:HB	1:B:174:PRO:HA	1.94	0.50
3:N:88:TYR:CE1	3:N:107:LEU:HD13	2.46	0.50
3:N:18:ILE:CD1	3:N:107:LEU:HD11	2.42	0.50
3:N:148:VAL:HG12	3:N:201:HIS:HB2	1.94	0.49
1:B:231:ILE:HG22	1:B:233:ILE:HG22	1.95	0.49
1:B:86:PHE:CE1	1:B:90:VAL:CG2	2.96	0.49
1:B:228:ASP:N	1:B:228:ASP:OD1	2.46	0.48
3:N:53:VAL:HG12	3:N:54:THR:HG23	1.94	0.48
2:M:91:THR:HG23	2:M:120:THR:HA	1.94	0.48
1:A:94:SER:OG	1:A:96:GLU:HG2	2.14	0.48
1:A:278:LYS:HD2	1:A:286:THR:HB	1.96	0.48
2:M:36:TRP:HB2	2:M:70:MET:HE2	1.96	0.48
2:M:81:MET:HE2	2:M:81:MET:HB3	1.79	0.47
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.13	0.47
1:B:127:VAL:HG22	1:B:171:VAL:HG22	1.95	0.47
1:B:115:GLN:HG2	1:B:130:VAL:CG2	2.42	0.47
3:L:170:LYS:HG3	3:L:176:TYR:CZ	2.50	0.47
1:B:132:GLU:HG3	1:B:165:ASN:HB2	1.96	0.47
1:B:279:TYR:CD1	1:B:279:TYR:N	2.83	0.47
2:M:23:LYS:CD	2:M:23:LYS:HZ2	2.22	0.47
1:A:41:LYS:HD3	1:A:43:PHE:CE1	2.49	0.47
3:L:185:THR:OG1	3:L:188:GLN:HG3	2.15	0.47
1:B:104:TRP:HB2	1:B:106:PHE:CE1	2.49	0.47
1:A:36:VAL:HG21	1:A:287:ASP:OD2	2.14	0.47
2:H:33:SER:OG	2:H:51:PHE:HB3	2.15	0.46
2:H:107:THR:HG22	3:L:52:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HG22	1:B:118:LEU:HD13	1.97	0.46
1:A:132:GLU:HG3	1:A:165:ASN:HB2	1.98	0.46
3:L:56:ARG:NH1	3:L:62:ASP:CA	2.75	0.46
1:A:129:LYS:HD3	1:A:169:GLU:OE2	2.15	0.46
2:H:36:TRP:HB2	2:H:70:MET:HE2	1.97	0.46
1:A:40:ASP:OD1	1:A:204:TYR:OH	2.28	0.46
2:M:129:PRO:HB3	2:M:155:TYR:HB3	1.97	0.45
2:M:169:LEU:HD21	2:M:192:VAL:HG21	1.97	0.45
1:A:96:GLU:OE2	1:A:264:ALA:N	2.47	0.45
2:M:35:HIS:HB2	2:M:97:ALA:HB3	1.99	0.45
1:B:116:SER:O	1:B:130:VAL:HA	2.16	0.45
1:A:175:PHE:CD1	1:A:226:LEU:HD21	2.51	0.45
1:B:87:ASN:OD1	1:B:269:TYR:CG	2.70	0.45
1:B:242:LEU:HD12	1:B:242:LEU:H	1.81	0.45
3:N:26:SER:O	3:N:31:SER:OG	2.34	0.45
3:L:18:ILE:HD11	3:L:107:LEU:HD11	1.97	0.45
2:M:33:SER:OG	2:M:51:PHE:HB3	2.16	0.45
2:M:37:VAL:HG22	2:M:95:TYR:HB2	1.99	0.45
1:B:86:PHE:HE1	1:B:90:VAL:CG2	2.30	0.44
2:H:169:LEU:HD21	2:H:192:VAL:HG21	1.99	0.44
2:M:35:HIS:ND1	2:M:50:GLY:HA3	2.33	0.44
2:M:52:ASP:HB3	2:M:55:ALA:HB3	2.01	0.43
1:A:14:GLN:HB3	1:A:158:ARG:HD2	1.99	0.43
1:B:194:PHE:CD1	1:B:203:ILE:HG12	2.54	0.43
1:A:108:THR:HG22	1:A:236:THR:HG23	2.00	0.43
1:B:279:TYR:N	1:B:279:TYR:HD1	2.16	0.43
3:L:68:LYS:HG2	3:L:69:SER:N	2.32	0.43
2:M:160:VAL:HG12	2:M:210:HIS:CD2	2.53	0.43
3:N:136:LEU:HB2	3:N:182:LEU:HB3	2.01	0.43
1:A:41:LYS:HB3	1:A:43:PHE:CD1	2.53	0.43
2:M:10:GLU:HB3	2:M:12:LYS:HE2	2.01	0.43
3:N:198:GLN:HE21	3:N:207:GLU:HG3	1.84	0.43
1:A:43:PHE:HZ	1:A:49:HIS:ND1	2.16	0.42
2:H:35:HIS:HB2	2:H:97:ALA:HB3	2.01	0.42
2:H:91:THR:HG23	2:H:120:THR:HA	2.01	0.42
3:N:18:ILE:HD12	3:N:107:LEU:HD11	2.00	0.42
3:L:56:ARG:NH1	3:L:62:ASP:CB	2.82	0.42
2:M:192:VAL:HG22	2:M:194:VAL:HG13	2.02	0.42
1:B:66:HIS:HB3	1:B:264:ALA:CA	2.46	0.42
1:A:64:TRP:CE3	1:A:266:TYR:CE1	3.07	0.42
1:B:277:LEU:HB3	1:B:279:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HB3	1:A:43:PHE:HD1	1.84	0.42
1:B:128:ILE:O	1:B:169:GLU:HA	2.20	0.42
1:B:39:PRO:C	1:B:41:LYS:H	2.28	0.42
2:H:16:ALA:O	2:H:86:LEU:HG	2.19	0.41
1:B:41:LYS:HB3	1:B:43:PHE:CD1	2.55	0.41
2:M:194:VAL:HG11	2:M:204:TYR:CE1	2.56	0.41
2:H:35:HIS:ND1	2:H:50:GLY:HA3	2.34	0.41
2:H:214:ASN:HB2	2:M:220:LYS:HB3	2.02	0.41
3:L:88:TYR:CE1	3:L:107:LEU:HD13	2.54	0.41
3:N:18:ILE:HD11	3:N:77:ILE:HD12	2.01	0.41
2:M:36:TRP:HB3	2:M:48:MET:HE3	2.02	0.41
3:N:208:LYS:HD3	3:N:208:LYS:HA	1.96	0.41
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.02	0.41
2:H:217:VAL:HG22	2:M:217:VAL:HG22	2.01	0.41
1:B:64:TRP:CE3	1:B:266:TYR:CE2	3.08	0.41
1:A:175:PHE:O	1:A:190:ARG:NH2	2.46	0.41
1:B:278:LYS:HD2	1:B:286:THR:HB	2.03	0.41
2:H:81:MET:HE2	2:H:81:MET:HB3	1.85	0.41
1:A:64:TRP:NE1	1:A:66:HIS:CE1	2.90	0.40
2:H:194:VAL:HG11	2:H:204:TYR:CE1	2.56	0.40
1:A:233:ILE:HD12	1:A:233:ILE:HA	1.92	0.40
1:B:196:ASN:HA	1:B:200:TYR:O	2.21	0.40
1:B:96:GLU:CD	1:B:264:ALA:H	2.30	0.40
1:A:250:THR:OG1	1:A:253:ASP:OD1	2.40	0.40
2:H:91:THR:HA	2:H:119:VAL:O	2.22	0.40
2:M:27:TYR:HB2	2:M:32:ILE:CD1	2.49	0.40
2:M:191:VAL:CG2	3:N:139:LEU:HD13	2.51	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)
1:B:200:TYR:OH	1:B:228:ASP:OD1[2_655]	2.18	0.02

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	220/297 (74%)	204 (93%)	16 (7%)	0	100	100
1	B	192/297 (65%)	177 (92%)	15 (8%)	0	100	100
2	H	207/234 (88%)	198 (96%)	9 (4%)	0	100	100
2	M	207/234 (88%)	199 (96%)	8 (4%)	0	100	100
3	L	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
3	N	209/216 (97%)	201 (96%)	8 (4%)	0	100	100
All	All	1244/1494 (83%)	1181 (95%)	63 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	206/267 (77%)	206 (100%)	0	100	100
1	B	186/267 (70%)	185 (100%)	1 (0%)	81	92
2	H	172/196 (88%)	172 (100%)	0	100	100
2	M	172/196 (88%)	172 (100%)	0	100	100
3	L	173/183 (94%)	173 (100%)	0	100	100
3	N	173/183 (94%)	173 (100%)	0	100	100
All	All	1082/1292 (84%)	1081 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	279	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	146	HIS
1	A	165	ASN
2	H	174	HIS
2	H	202	GLN
3	L	192	HIS
1	B	14	GLN
1	B	66	HIS
1	B	115	GLN
1	B	165	ASN
1	B	196	ASN
2	M	115	GLN
2	M	174	HIS
2	M	202	GLN
3	N	112	GLN
3	N	198	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	230/297 (77%)	1.21	52 (22%) 2 1	46, 68, 96, 117	0
1	B	206/297 (69%)	2.10	100 (48%) 0 0	58, 84, 111, 126	0
2	H	211/234 (90%)	0.16	5 (2%) 59 52	35, 49, 65, 74	0
2	M	211/234 (90%)	0.20	3 (1%) 73 67	37, 52, 70, 77	0
3	L	211/216 (97%)	-0.06	2 (0%) 81 76	31, 43, 58, 66	0
3	N	211/216 (97%)	0.05	3 (1%) 73 67	37, 48, 60, 68	0
All	All	1280/1494 (85%)	0.61	165 (12%) 7 6	31, 54, 96, 126	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	GLY	7.6
1	B	287	ASP	6.5
1	B	89	GLY	6.3
1	B	278	LYS	6.0
1	A	32	PHE	5.6
1	B	45	SER	5.4
1	B	284	THR	5.4
1	B	279	TYR	5.1
1	B	40	ASP	5.1
1	B	90	VAL	5.0
1	B	42	VAL	4.9
1	B	277	LEU	4.8
1	A	28	TYR	4.8
1	B	280	ASN	4.6
1	B	62	VAL	4.6
1	B	37	TYR	4.5
1	B	204	TYR	4.5
1	A	35	GLY	4.3
1	B	195	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	SER	4.2
1	B	193	VAL	4.2
1	A	29	THR	4.2
1	B	223	LEU	4.1
1	B	88	ASP	4.1
1	B	266	TYR	3.9
1	B	49	HIS	3.9
1	B	82	PRO	3.9
1	B	270	LEU	3.8
1	B	85	PRO	3.8
1	A	284	THR	3.7
1	B	276	LEU	3.7
1	A	45	SER	3.7
1	A	97	LYS	3.7
1	A	33	THR	3.7
1	A	268	GLY	3.6
1	B	271	GLN	3.6
1	A	27	ALA	3.6
1	A	279	TYR	3.6
1	B	91	TYR	3.6
1	A	47	VAL	3.5
1	B	286	THR	3.4
1	B	190	ARG	3.4
1	B	95	THR	3.4
1	B	66	HIS	3.4
1	A	98	SER	3.4
1	B	272	PRO	3.4
1	B	289	VAL	3.4
1	A	275	PHE	3.3
1	B	290	ASP	3.3
1	A	290	ASP	3.3
1	A	276	LEU	3.2
1	B	275	PHE	3.2
1	A	150	LYS	3.2
1	A	278	LYS	3.2
1	B	39	PRO	3.2
1	B	283	GLY	3.2
1	B	15	CYS	3.2
1	B	51	THR	3.2
1	B	13	SER	3.2
1	B	238	PHE	3.2
1	A	36	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	13	SER	3.1
1	B	50	SER	3.1
1	B	228	ASP	3.1
1	B	94	SER	3.1
1	A	289	VAL	3.1
1	B	191	GLU	3.0
1	B	109	THR	3.0
1	B	231	ILE	3.0
1	A	282	ASN	3.0
1	B	108	THR	3.0
1	A	39	PRO	3.0
1	A	61	ASN	3.0
1	A	286	THR	3.0
3	N	3	ALA	3.0
1	B	64	TRP	3.0
1	B	269	TYR	3.0
3	L	213	THR	2.9
1	A	43	PHE	2.9
1	A	62	VAL	2.9
1	B	273	ARG	2.9
1	A	40	ASP	2.9
2	H	181	GLN	2.9
1	A	34	ARG	2.9
1	B	285	ILE	2.8
1	B	282	ASN	2.8
1	B	16	VAL	2.8
1	B	93	ALA	2.8
1	B	86	PHE	2.8
1	B	189	LEU	2.8
1	B	233	ILE	2.7
1	B	262	ALA	2.7
1	B	267	VAL	2.7
1	B	196	ASN	2.7
1	B	237	ARG	2.7
1	B	274	THR	2.7
1	B	87	ASN	2.6
1	B	65	PHE	2.6
1	B	110	LEU	2.6
2	H	114	GLY	2.6
1	A	222	ALA	2.6
1	B	81	ASN	2.6
1	B	38	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	86	LEU	2.6
1	B	194	PHE	2.6
1	B	115	GLN	2.6
1	A	58	PHE	2.5
1	B	43	PHE	2.5
3	L	3	ALA	2.5
3	N	213	THR	2.5
1	B	281	GLU	2.5
1	B	201	PHE	2.5
1	B	111	ASP	2.5
1	B	235	ILE	2.5
1	A	283	GLY	2.5
1	B	63	THR	2.5
2	M	114	GLY	2.5
1	A	287	ASP	2.4
1	B	226	LEU	2.4
1	A	111	ASP	2.4
1	B	131	CYS	2.4
1	B	101	ILE	2.3
1	B	197	ILE	2.3
1	B	166	CYS	2.3
1	A	18	LEU	2.3
1	A	280	ASN	2.3
1	B	83	VAL	2.3
1	B	84	LEU	2.3
1	B	263	ALA	2.2
1	B	96	GLU	2.2
1	B	265	TYR	2.2
1	A	271	GLN	2.2
1	B	112	SER	2.2
1	A	41	LYS	2.2
1	A	15	CYS	2.2
1	B	114	THR	2.2
1	A	30	ASN	2.2
1	B	230	PRO	2.2
2	M	86	LEU	2.2
2	M	144	GLY	2.2
1	A	67	ALA	2.2
1	B	225	PRO	2.2
1	A	52	GLN	2.2
1	B	41	LYS	2.2
1	A	190	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	CYS	2.1
1	B	141	LEU	2.1
1	B	47	VAL	2.1
1	B	199	GLY	2.1
1	A	90	VAL	2.1
1	A	46	SER	2.1
1	B	52	GLN	2.1
1	B	18	LEU	2.1
1	A	166	CYS	2.1
1	B	261	GLY	2.1
1	B	106	PHE	2.1
2	H	10	GLU	2.1
1	A	64	TRP	2.1
1	B	236	THR	2.1
2	H	32	ILE	2.1
3	N	17	SER	2.0
1	A	38	TYR	2.0
1	B	202	LYS	2.0
1	A	261	GLY	2.0
1	A	42	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.