



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:15 PM UTC

PDB ID : 7TE1 / pdb_00007te1
Title : SARS-CoV-2 Receptor Binding Domain in Complex with Ab17
Authors : Hauser, B.M.; Schmidt, A.G.
Deposited on : 2022-01-03
Resolution : 3.50 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

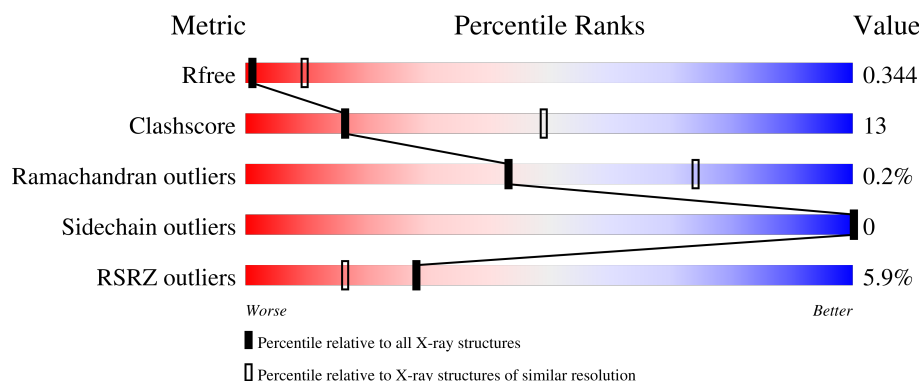
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



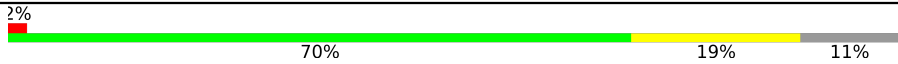
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	C	223	6% 71% 23% 6%
1	H	223	6% 66% 26% 8%
2	F	214	7% 75% 23% .
2	L	214	4% 67% 24% 8%
3	D	211	4% 67% 14% 19%

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Mol	Chain	Length	Quality of chain
3	E	211	 A horizontal bar chart showing the quality of chain E. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a large green segment labeled '70%', a yellow segment labeled '19%', and a small grey segment at the end labeled '11%'. The segments are separated by thin white lines.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9099 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 Ab17 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	209	Total	C	N	O	S	149	0	0
			1583	1010	250	315	8			
1	H	206	Total	C	N	O	S	135	0	0
			1570	999	249	314	8			

- Molecule 2 is a protein called Ab17 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	210	Total	C	N	O	S	259	0	0
			1605	1001	263	334	7			
2	L	196	Total	C	N	O	S	176	0	0
			1494	935	240	312	7			

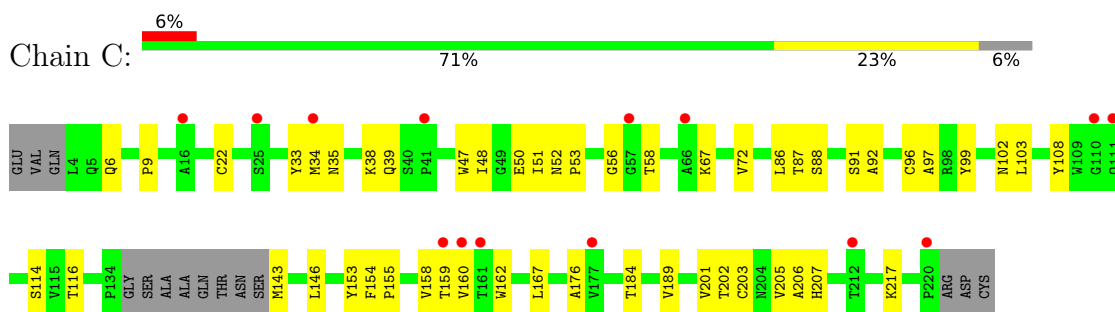
- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	170	Total	C	N	O	S	35	0	0
			1365	878	228	253	6			
3	E	187	Total	C	N	O	S	0	0	0
			1482	948	247	279	8			

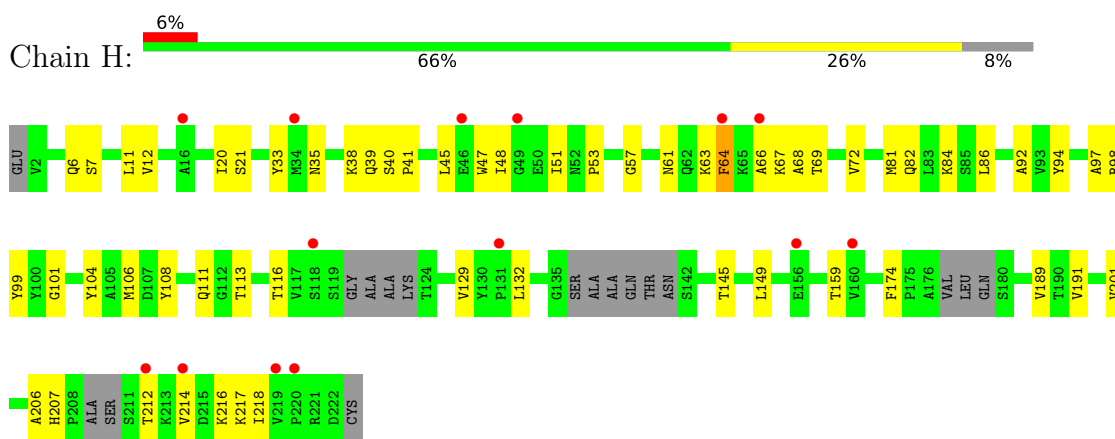
3 Residue-property plots [i](#)

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.

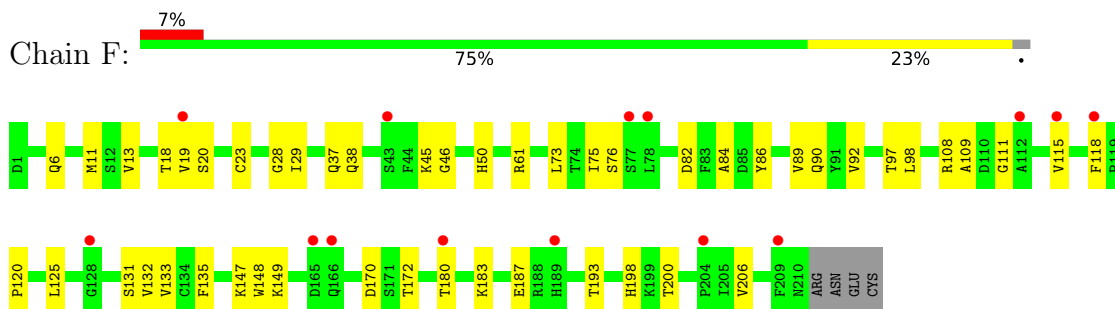
- Molecule 1: Ab17 heavy chain



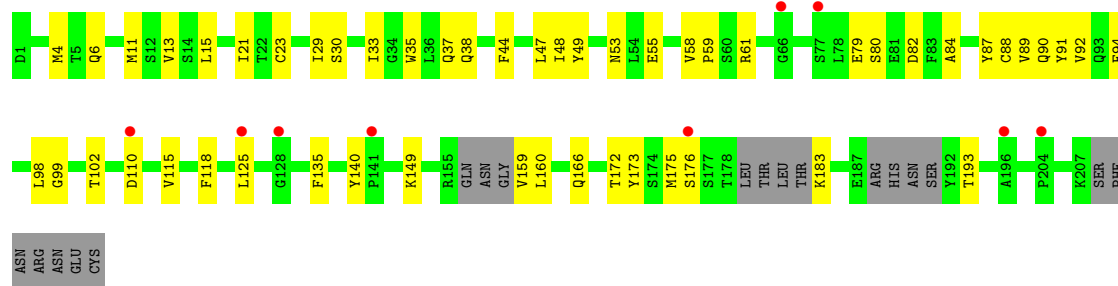
- Molecule 1: Ab17 chain



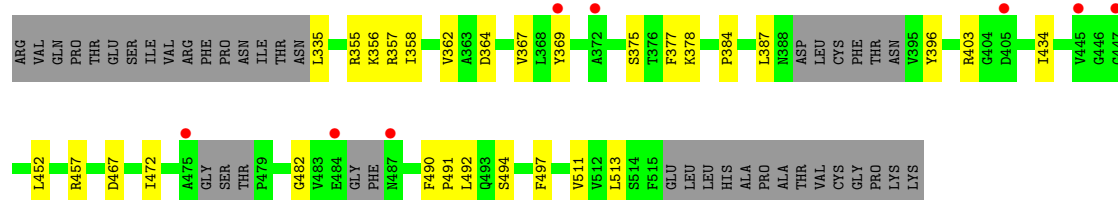
- Molecule 2: Ab17 light chain



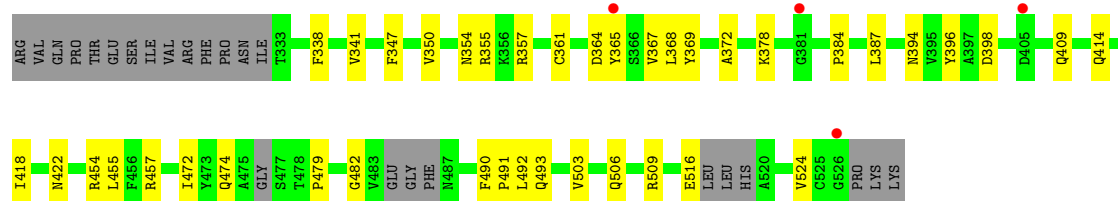
- Molecule 2: Ab17 light chain



• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.93Å 207.93Å 86.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.99 – 3.50 79.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.99-3.50) 96.3 (79.99-3.50)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.25 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.296 , 0.344 0.296 , 0.344	Depositor DCC
R_{free} test set	1206 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.9	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	0.85	EDS
Total number of atoms	9099	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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	C	0.14	0/1626	0.44	0/2223
1	H	0.14	0/1610	0.42	0/2196
2	F	0.13	0/1641	0.40	0/2226
2	L	0.14	0/1525	0.38	0/2064
3	D	0.17	0/1401	0.54	0/1899
3	E	0.17	0/1520	0.50	0/2065
All	All	0.15	0/9323	0.45	0/12673

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	C	1583	0	1547	41	0
1	H	1570	0	1522	49	0
2	F	1605	0	1527	38	0
2	L	1494	0	1420	45	0
3	D	1365	0	1297	29	0
3	E	1482	0	1400	34	0
All	All	9099	0	8713	212	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 13.

All (212) 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)
3:E:365:TYR:CG	3:E:387:LEU:HD11	2.17	0.80
1:C:159:THR:OG1	1:C:206:ALA:HB3	1.83	0.77
1:H:39:GLN:HB2	1:H:45:LEU:HD12	1.66	0.76
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.69	0.75
1:C:143:MET:HE3	2:L:59:PRO:HG3	1.69	0.74
3:D:491:PRO:HG2	3:D:492:LEU:HD12	1.71	0.73
1:H:33:TYR:HB2	1:H:99:TYR:HB3	1.71	0.72
3:E:409:GLN:HA	3:E:414:GLN:HG2	1.70	0.72
1:C:160:VAL:HG22	1:C:205:VAL:HG22	1.70	0.72
2:F:89:VAL:HG22	2:F:98:LEU:HG	1.72	0.72
2:F:125:LEU:HD11	2:F:183:LYS:HG3	1.72	0.71
1:C:158:VAL:HG12	1:C:207:HIS:ND1	2.07	0.69
2:F:45:LYS:NZ	2:F:46:GLY:O	2.26	0.68
1:C:103:LEU:HB3	2:F:50:HIS:HD2	1.59	0.68
1:H:38:LYS:NZ	1:H:94:TYR:OH	2.28	0.67
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.78	0.66
2:L:140:TYR:HB2	2:L:172:THR:HG22	1.76	0.66
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.77	0.65
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.78	0.64
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.31	0.62
3:E:387:LEU:C	3:E:387:LEU:HD12	2.25	0.62
1:C:35:ASN:HB2	1:C:97:ALA:HB3	1.81	0.62
3:E:365:TYR:CB	3:E:387:LEU:HD11	2.30	0.62
1:C:35:ASN:ND2	1:C:99:TYR:HB2	2.15	0.62
1:C:153:TYR:CZ	1:C:158:VAL:CG2	2.84	0.61
2:L:21:ILE:HG12	2:L:102:THR:HG21	1.83	0.61
3:E:472:ILE:HD12	3:E:472:ILE:H	1.66	0.61
3:E:354:ASN:O	3:E:398:ASP:HA	2.00	0.61
3:E:472:ILE:HD13	3:E:482:GLY:HA2	1.83	0.61
1:C:67:LYS:HZ3	1:C:87:THR:HG23	1.66	0.60
1:C:153:TYR:CE2	1:C:158:VAL:HG21	2.36	0.60
1:C:86:LEU:HD12	1:C:88:SER:H	1.66	0.60
2:F:170:ASP:HB3	2:F:172:THR:HG22	1.83	0.60
2:F:61:ARG:NH1	2:F:82:ASP:OD2	2.34	0.59
1:C:153:TYR:CZ	1:C:158:VAL:HG22	2.38	0.59
2:L:29:ILE:HG22	2:L:92:VAL:HG11	1.84	0.59
1:H:98:ARG:HE	1:H:108:TYR:HB2	1.66	0.59
1:C:91:SER:HB3	1:C:116:THR:HA	1.85	0.59
3:E:491:PRO:HG2	3:E:492:LEU:HD12	1.84	0.58
1:H:45:LEU:HD23	2:L:98:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLN:NE2	1:C:96:CYS:SG	2.73	0.58
1:C:33:TYR:HB2	1:C:99:TYR:HB3	1.85	0.57
1:H:7:SER:HB2	1:H:21:SER:H	1.69	0.57
3:D:355:ARG:HG3	3:D:355:ARG:HH11	1.71	0.56
3:D:384:PRO:HA	3:D:387:LEU:HG	1.88	0.56
1:C:158:VAL:O	1:C:158:VAL:HG23	2.05	0.56
2:L:89:VAL:HA	2:L:98:LEU:HA	1.88	0.55
3:E:387:LEU:HD12	3:E:387:LEU:O	2.05	0.55
3:D:377:PHE:CE1	3:D:434:ILE:HG12	2.41	0.55
2:L:4:MET:HB2	2:L:99:GLY:HA2	1.89	0.55
1:C:86:LEU:HD12	1:C:88:SER:N	2.22	0.55
1:H:48:ILE:HA	1:H:64:PHE:HZ	1.72	0.55
1:H:53:PRO:HA	1:H:72:VAL:HG21	1.89	0.54
3:D:472:ILE:HD12	3:D:472:ILE:H	1.71	0.54
1:H:207:HIS:HB3	1:H:212:THR:HB	1.88	0.54
1:H:45:LEU:HD22	2:L:87:TYR:CE2	2.43	0.54
1:H:132:LEU:HB3	2:L:118:PHE:CD2	2.43	0.54
3:E:384:PRO:HA	3:E:387:LEU:HD23	1.91	0.53
3:D:369:TYR:HE1	3:D:377:PHE:CZ	2.26	0.53
3:D:490:PHE:CD1	3:D:491:PRO:HD2	2.44	0.53
2:L:92:VAL:HG23	3:D:375:SER:O	2.08	0.52
2:F:18:THR:HA	2:F:75:ILE:O	2.08	0.52
1:H:145:THR:HG22	2:L:118:PHE:HZ	1.75	0.52
3:D:335:LEU:HD13	3:D:362:VAL:HG13	1.90	0.52
3:D:355:ARG:HH11	3:D:396:TYR:HB3	1.75	0.52
3:E:369:TYR:CE2	3:E:384:PRO:O	2.62	0.52
2:L:55:GLU:HB2	2:L:58:VAL:HG21	1.92	0.52
3:D:472:ILE:HD13	3:D:482:GLY:HA2	1.91	0.52
1:H:129:VAL:HG21	1:H:214:VAL:HG21	1.92	0.51
1:C:153:TYR:CZ	1:C:158:VAL:HG21	2.46	0.51
1:H:40:SER:OG	1:H:41:PRO:HD2	2.11	0.51
3:D:364:ASP:O	3:D:367:VAL:HG22	2.11	0.51
2:F:11:MET:HG3	2:F:13:VAL:HG13	1.93	0.51
2:L:149:LYS:HB2	2:L:193:THR:HB	1.93	0.51
2:F:38:GLN:O	2:F:84:ALA:HB1	2.10	0.50
1:H:51:ILE:HG13	1:H:57:GLY:O	2.11	0.50
1:C:52:ASN:O	1:C:56:GLY:HA3	2.11	0.50
2:L:175:MET:HG2	2:L:176:SER:N	2.27	0.49
2:L:33:ILE:HD11	2:L:88:CYS:HB2	1.93	0.49
3:D:452:LEU:HD13	3:D:494:SER:HB2	1.94	0.49
1:H:12:VAL:HG21	1:H:86:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:VAL:HG23	1:H:218:ILE:HB	1.95	0.49
2:F:108:ARG:HE	2:L:15:LEU:HD23	1.77	0.49
3:E:365:TYR:CD2	3:E:387:LEU:CD1	2.96	0.49
1:H:64:PHE:C	1:H:66:ALA:H	2.21	0.49
2:L:89:VAL:HG12	2:L:98:LEU:HA	1.95	0.48
1:C:146:LEU:HD12	1:C:201:VAL:HG21	1.95	0.48
2:F:108:ARG:HG2	2:F:109:ALA:N	2.28	0.48
2:L:11:MET:HG3	2:L:13:VAL:HG13	1.95	0.48
1:H:189:VAL:HG22	1:H:191:VAL:HG13	1.95	0.48
1:H:101:GLY:O	1:H:104:TYR:HB2	2.14	0.48
1:H:111:GLN:OE1	1:H:111:GLN:N	2.46	0.48
3:D:369:TYR:CE1	3:D:377:PHE:CZ	3.02	0.48
1:C:108:TYR:CE1	2:F:45:LYS:HE2	2.49	0.48
2:F:20:SER:HA	2:F:73:LEU:O	2.13	0.47
1:H:20:ILE:HD11	1:H:113:THR:HB	1.96	0.47
1:H:63:LYS:HG3	1:H:64:PHE:CD2	2.49	0.47
3:E:347:PHE:CD2	3:E:509:ARG:HD3	2.49	0.47
3:D:377:PHE:CD1	3:D:434:ILE:HG12	2.49	0.47
3:E:365:TYR:CG	3:E:387:LEU:CD1	2.95	0.47
1:H:68:ALA:HA	1:H:82:GLN:O	2.15	0.47
1:C:53:PRO:HA	1:C:72:VAL:HG21	1.97	0.47
1:H:35:ASN:HB2	1:H:97:ALA:HB3	1.96	0.47
1:C:22:CYS:SG	1:C:34:MET:HE1	2.55	0.47
1:H:159:THR:OG1	1:H:206:ALA:HB3	2.15	0.47
3:D:355:ARG:NH1	3:D:396:TYR:HB3	2.29	0.47
3:D:369:TYR:CE1	3:D:377:PHE:CE2	3.03	0.47
2:F:111:GLY:O	2:F:200:THR:HG21	2.16	0.46
2:F:125:LEU:HD12	2:F:125:LEU:HA	1.78	0.46
2:L:125:LEU:HB3	2:L:183:LYS:NZ	2.30	0.46
3:D:356:LYS:HG3	3:D:358:ILE:HD11	1.97	0.46
3:E:355:ARG:HE	3:E:396:TYR:HB3	1.81	0.46
3:E:357:ARG:HG2	3:E:396:TYR:HE1	1.80	0.46
3:D:369:TYR:HE1	3:D:377:PHE:CE2	2.34	0.46
1:H:47:TRP:CZ3	1:H:61:ASN:HB3	2.49	0.46
2:L:92:VAL:O	3:D:377:PHE:N	2.49	0.46
3:E:357:ARG:HG2	3:E:396:TYR:CE1	2.51	0.46
2:L:159:VAL:O	2:L:160:LEU:HD23	2.16	0.46
1:H:48:ILE:HA	1:H:64:PHE:CZ	2.50	0.46
1:C:67:LYS:NZ	1:C:87:THR:HA	2.30	0.46
2:L:4:MET:HE3	2:L:23:CYS:SG	2.56	0.46
3:E:503:VAL:HA	3:E:506:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:HIS:O	2:F:50:HIS:ND1	2.47	0.45
1:H:45:LEU:HB3	2:L:98:LEU:CD2	2.46	0.45
3:E:338:PHE:HA	3:E:341:VAL:HG12	1.98	0.45
1:H:45:LEU:HB3	2:L:98:LEU:HD21	1.98	0.45
3:D:403:ARG:HG2	3:D:497:PHE:HE1	1.80	0.45
1:C:51:ILE:HG13	1:C:58:THR:HG22	1.99	0.45
2:L:166:GLN:HG3	2:L:173:TYR:CE1	2.51	0.45
1:C:47:TRP:HZ2	1:C:50:GLU:HB2	1.80	0.45
2:F:6:GLN:HA	2:F:23:CYS:HA	1.99	0.45
2:L:59:PRO:HG2	2:L:61:ARG:NH2	2.31	0.45
1:H:132:LEU:HD11	1:H:149:LEU:HB2	1.99	0.45
2:F:115:VAL:HA	2:F:135:PHE:O	2.17	0.45
2:L:79:GLU:HG3	2:L:80:SER:H	1.82	0.45
2:L:38:GLN:O	2:L:84:ALA:HB1	2.17	0.45
1:C:35:ASN:HD21	1:C:99:TYR:HB2	1.80	0.44
2:L:94:PHE:CE2	3:D:378:LYS:HB3	2.53	0.44
2:F:90:GLN:HE21	2:F:97:THR:H	1.63	0.44
2:L:94:PHE:HE2	3:D:378:LYS:HB3	1.83	0.44
3:E:361:CYS:O	3:E:524:VAL:HA	2.16	0.44
3:E:364:ASP:O	3:E:367:VAL:HG12	2.17	0.44
1:H:97:ALA:HB1	1:H:106:MET:HB3	2.00	0.44
3:E:472:ILE:HD12	3:E:472:ILE:N	2.32	0.44
2:L:115:VAL:HA	2:L:135:PHE:O	2.17	0.44
3:E:365:TYR:CD2	3:E:387:LEU:HD11	2.52	0.44
1:C:102:ASN:OD1	3:E:378:LYS:HE2	2.18	0.44
2:L:6:GLN:HE21	2:L:102:THR:HB	1.83	0.43
3:E:367:VAL:HG13	3:E:368:LEU:HD12	2.00	0.43
3:E:454:ARG:HD3	3:E:457:ARG:HG3	1.99	0.43
2:F:198:HIS:ND1	2:F:200:THR:HG23	2.33	0.43
3:E:394:ASN:HB2	3:E:516:GLU:OE2	2.18	0.43
3:E:490:PHE:CD1	3:E:491:PRO:HD2	2.53	0.43
2:F:149:LYS:HB2	2:F:193:THR:HB	2.01	0.43
2:L:35:TRP:CH2	2:L:88:CYS:HB3	2.54	0.43
2:L:92:VAL:HG23	3:D:375:SER:C	2.44	0.43
2:F:131:SER:HA	2:F:180:THR:HA	2.00	0.43
1:H:20:ILE:HD11	1:H:113:THR:CB	2.48	0.43
1:H:106:MET:HG3	2:L:91:TYR:OH	2.18	0.43
2:F:193:THR:HG23	2:F:206:VAL:HB	2.00	0.43
1:H:20:ILE:HG22	1:H:81:MET:O	2.19	0.43
1:H:48:ILE:HD12	1:H:81:MET:HE1	2.00	0.43
2:L:90:GLN:OE1	2:L:92:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:VAL:HG11	2:F:19:VAL:HG11	2.00	0.42
2:F:18:THR:HG22	2:F:76:SER:HA	2.00	0.42
3:D:511:VAL:HG12	3:D:513:LEU:HD12	2.02	0.42
3:E:418:ILE:HA	3:E:422:ASN:HB2	1.99	0.42
1:H:6:GLN:H	1:H:111:GLN:HE22	1.67	0.42
3:D:355:ARG:HG3	3:D:355:ARG:NH1	2.34	0.42
3:E:455:LEU:HD12	3:E:493:GLN:HG3	2.02	0.42
3:D:457:ARG:NE	3:D:467:ASP:OD2	2.53	0.42
3:E:474:GLN:OE1	3:E:479:PRO:HA	2.20	0.42
1:C:167:LEU:HD13	1:C:189:VAL:HG21	2.02	0.42
2:F:147:LYS:HG2	2:F:148:TRP:N	2.34	0.42
1:H:45:LEU:HD11	2:L:44:PHE:CZ	2.54	0.42
1:C:108:TYR:HE1	2:F:45:LYS:HE2	1.85	0.42
1:C:153:TYR:CE1	1:C:158:VAL:HG13	2.55	0.42
2:F:118:PHE:HB2	2:F:133:VAL:O	2.20	0.42
1:C:154:PHE:HA	1:C:155:PRO:HA	1.74	0.42
1:H:174:PHE:CD2	2:L:176:SER:HB3	2.54	0.42
2:L:21:ILE:HG21	2:L:102:THR:HG21	2.01	0.42
1:C:153:TYR:OH	1:C:158:VAL:HG22	2.20	0.42
3:E:491:PRO:HG2	3:E:492:LEU:CD1	2.50	0.42
1:C:176:ALA:HA	1:C:184:THR:O	2.20	0.41
2:F:108:ARG:HG2	2:F:109:ALA:H	1.85	0.41
2:F:90:GLN:NE2	2:F:97:THR:H	2.18	0.41
2:F:183:LYS:HG2	2:F:187:GLU:OE1	2.20	0.41
2:F:45:LYS:HD2	2:F:45:LYS:HA	1.86	0.41
1:C:162:TRP:CH2	1:C:203:CYS:HB3	2.55	0.41
1:H:217:LYS:HE2	1:H:217:LYS:HB2	1.86	0.41
1:C:158:VAL:CG1	1:C:207:HIS:ND1	2.79	0.41
2:F:29:ILE:HG22	2:F:92:VAL:HG11	2.01	0.41
1:C:39:GLN:O	1:C:92:ALA:HB1	2.20	0.41
1:H:11:LEU:HD23	1:H:116:THR:OG1	2.21	0.41
1:H:48:ILE:HD13	1:H:64:PHE:CZ	2.56	0.41
2:F:118:PHE:HE2	2:F:135:PHE:CD2	2.38	0.41
1:H:39:GLN:O	1:H:92:ALA:HB1	2.21	0.41
1:H:64:PHE:HB2	1:H:67:LYS:HG2	2.01	0.41
1:H:86:LEU:HD12	1:H:86:LEU:HA	1.87	0.41
1:H:216:LYS:HA	1:H:216:LYS:HD2	1.74	0.41
3:E:350:VAL:HG22	3:E:422:ASN:HB3	2.03	0.41
1:C:202:THR:OG1	1:C:217:LYS:HD3	2.21	0.41
2:F:28:GLY:HA3	3:E:372:ALA:HB1	2.03	0.41
1:C:9:PRO:HB3	1:C:114:SER:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:GLN:HB2	2:F:86:TYR:CE1	2.57	0.40
3:D:356:LYS:HD2	3:D:357:ARG:N	2.36	0.40
1:H:69:THR:HG23	1:H:84:LYS:HE2	2.02	0.40
1:H:132:LEU:HB3	2:L:118:PHE:HD2	1.84	0.40
1:C:103:LEU:HB3	2:F:50:HIS:CD2	2.47	0.40
2:L:30:SER:HB3	3:D:375:SER:HA	2.03	0.40
2:L:49:TYR:O	2:L:53:ASN:HB2	2.21	0.40
1:H:51:ILE:HD13	1:H:72:VAL:HG13	2.03	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	C	205/223 (92%)	199 (97%)	6 (3%)	0	100	100
1	H	196/223 (88%)	185 (94%)	10 (5%)	1 (0%)	24	57
2	F	208/214 (97%)	195 (94%)	13 (6%)	0	100	100
2	L	188/214 (88%)	177 (94%)	10 (5%)	1 (0%)	24	57
3	D	162/211 (77%)	155 (96%)	7 (4%)	0	100	100
3	E	179/211 (85%)	170 (95%)	9 (5%)	0	100	100
All	All	1138/1296 (88%)	1081 (95%)	55 (5%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	64	PHE
2	L	110	ASP

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	C	181/192 (94%)	181 (100%)	0	100	100
1	H	181/192 (94%)	181 (100%)	0	100	100
2	F	185/189 (98%)	185 (100%)	0	100	100
2	L	172/189 (91%)	172 (100%)	0	100	100
3	D	148/184 (80%)	148 (100%)	0	100	100
3	E	162/184 (88%)	162 (100%)	0	100	100
All	All	1029/1130 (91%)	1029 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	GLN
1	C	204	ASN
2	F	198	HIS
2	L	161	ASN
3	D	501	ASN
3	E	388	ASN
3	E	409	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 [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(Å²)	Q<0.9
1	C	189/223 (84%)	0.92	14 (7%)	20	13	43, 101, 120, 138	4 (2%)
1	H	188/223 (84%)	0.77	14 (7%)	20	13	41, 95, 128, 137	3 (1%)
2	F	175/214 (81%)	0.66	14 (8%)	18	12	32, 81, 114, 124	1 (0%)
2	L	172/214 (80%)	0.66	9 (5%)	33	19	34, 80, 120, 135	1 (0%)
3	D	165/211 (78%)	0.48	8 (4%)	35	19	63, 87, 131, 145	0
3	E	187/211 (88%)	0.50	4 (2%)	63	38	74, 109, 143, 156	0
All	All	1076/1296 (83%)	0.67	63 (5%)	28	16	32, 92, 131, 156	9 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	VAL	8.8
1	C	177	VAL	8.1
1	H	220	PRO	6.9
1	H	160	VAL	5.3
1	C	220	PRO	5.2
2	F	77	SER	5.2
1	H	34	MET	4.9
2	L	77	SER	4.5
1	C	34	MET	4.5
1	C	16	ALA	4.1
3	E	365	TYR	3.8
1	C	41	PRO	3.7
2	L	128	GLY	3.7
1	H	16	ALA	3.5
3	E	381	GLY	3.4
1	C	212	THR	3.4
2	F	128	GLY	3.3
1	C	111	GLN	3.3
1	H	212	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	445	VAL	3.2
2	L	204	PRO	3.2
2	F	166	GLN	3.1
1	H	118	SER	3.1
1	C	110	GLY	3.1
3	E	405	ASP	2.9
3	D	372	ALA	2.9
2	F	43	SER	2.8
2	L	125	LEU	2.8
2	F	115	VAL	2.6
2	F	204	PRO	2.6
3	D	475	ALA	2.6
2	L	66	GLY	2.6
3	D	369	TYR	2.6
2	L	196	ALA	2.6
2	L	110	ASP	2.5
3	E	526	GLY	2.5
2	L	176	SER	2.4
1	H	66	ALA	2.4
2	F	165	ASP	2.4
2	F	112	ALA	2.3
3	D	484	GLU	2.3
3	D	405	ASP	2.3
1	C	25	SER	2.3
1	C	57	GLY	2.3
3	D	447	GLY	2.3
1	H	49	GLY	2.2
2	F	189	HIS	2.2
1	C	66	ALA	2.2
1	C	159	THR	2.2
1	H	156	GLU	2.1
3	D	487	ASN	2.1
2	F	78	LEU	2.1
1	H	219	VAL	2.1
1	C	161	THR	2.1
2	F	19	VAL	2.1
2	L	141	PRO	2.1
1	H	64	PHE	2.1
2	F	180	THR	2.1
2	F	118	PHE	2.1
2	F	209	PHE	2.1
1	H	214	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	131	PRO	2.0
1	H	46	GLU	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.