



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 06:30 AM EDT

PDB ID : 3BGF
Title : X-ray crystal structure of the SARS coronavirus spike receptor binding domain
in complex with F26G19 Fab
Authors : Pak, J.E.; Rini, J.M.
Deposited on : unknown
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

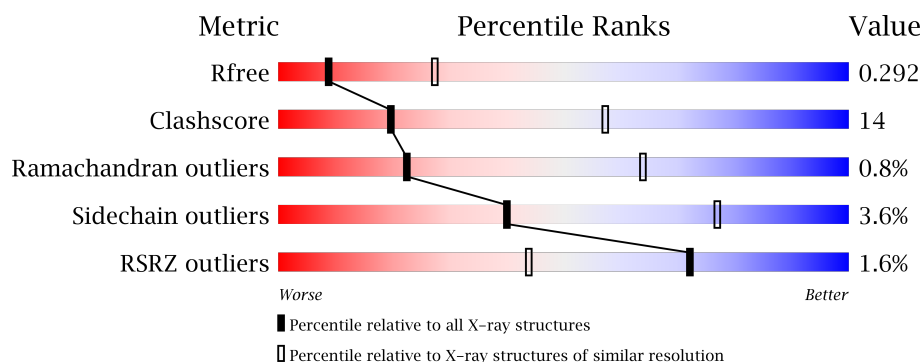
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	193	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 64%, yellow 25%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 1% 64% 25% 8% </div> </div>
1	S	193	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 70%, yellow 20%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 4% 70% 20% 7% </div> </div>
2	C	212	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 68%, yellow 28%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 1% 68% 28% 3% </div> </div>
2	L	212	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 73%, yellow 26%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 73% 26% 1% </div> </div>
3	B	220	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 77%, yellow 20%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 3% 77% 20% 1% </div> </div>

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Mol	Chain	Length	Quality of chain
3	H	220	 A horizontal bar chart showing the quality of chain H. The bar is divided into two segments: a green segment on the left representing 65% and a yellow segment on the right representing 32%. At the far right end of the bar, there are two small grey squares followed by two dots (..).

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9417 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	S	179	Total	C	N	O	S	0	0	0
			1440	933	234	265	8			
1	A	178	Total	C	N	O	S	0	0	0
			1429	925	232	264	8			

- Molecule 2 is a protein called F26G19 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1649	1028	274	341	6			
2	C	210	Total	C	N	O	S	0	0	0
			1629	1018	268	337	6			

- Molecule 3 is a protein called F26G19 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1632	1031	267	326	8			
3	B	216	Total	C	N	O	S	0	0	0
			1632	1031	267	326	8			

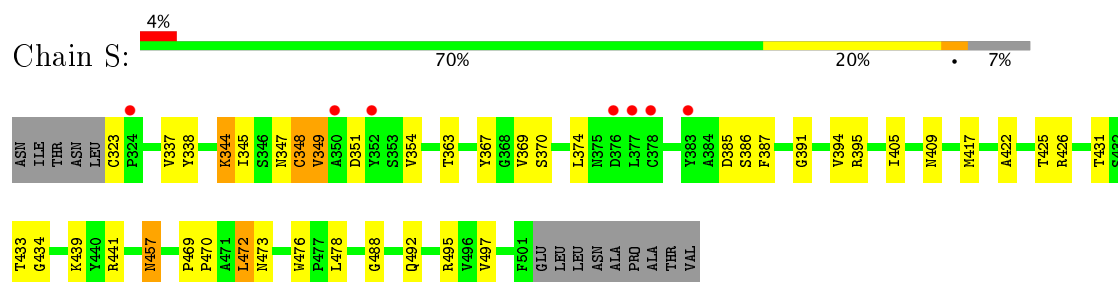
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		

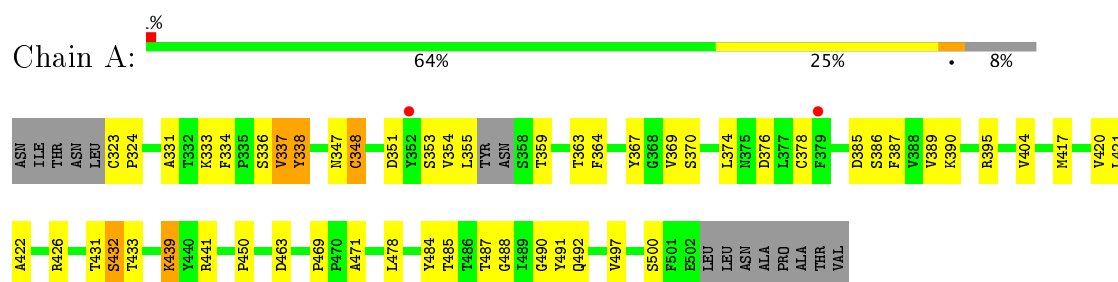
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

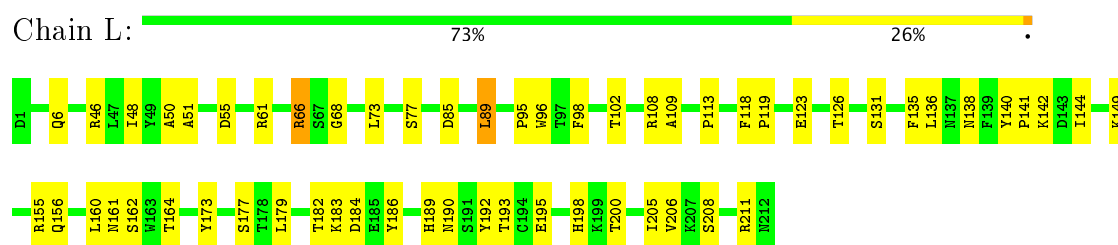
• Molecule 1: Spike protein S1



• Molecule 1: Spike protein S1

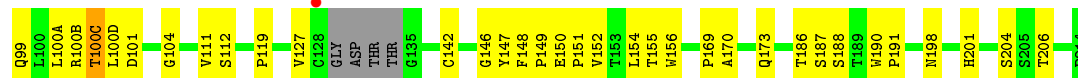
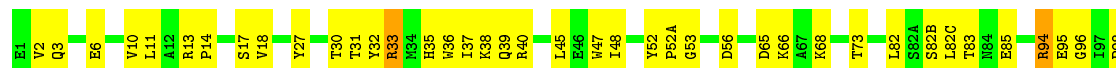


• Molecule 2: F26G19 Fab

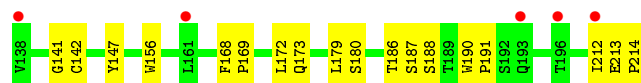
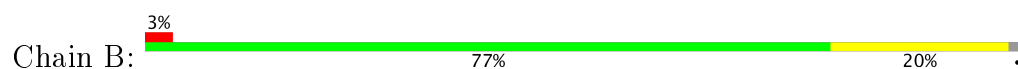




• Molecule 3: F26G19 Fab



• Molecule 3: F26G19 Fab



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	183.69 Å 73.36 Å 110.78 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 47.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-3.00) 98.7 (47.43-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.01 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.286 0.242 , 0.292	Depositor DCC
R_{free} test set	1495 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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	0.38	0/1474	0.55	0/2008
1	S	0.36	0/1487	0.51	0/2028
2	C	0.33	0/1664	0.56	1/2256 (0.0%)
2	L	0.36	0/1685	0.56	0/2284
3	B	0.36	0/1671	0.56	0/2281
3	H	0.41	0/1671	0.59	0/2281
All	All	0.37	0/9652	0.56	1/13138 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	89	LEU	CA-CB-CG	5.40	127.71	115.30

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	1429	0	1352	49	0
1	S	1440	0	1362	37	0
2	C	1629	0	1563	59	0
2	L	1649	0	1583	49	0
3	B	1632	0	1606	29	0
3	H	1632	0	1606	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
4	H	2	0	0	1	0
4	L	1	0	0	0	0
All	All	9417	0	9072	264	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 14.

All (264) 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:L:66:ARG:HH11	2:L:66:ARG:CG	1.73	1.02
1:S:472:LEU:H	1:S:472:LEU:HD12	1.29	0.93
1:S:425:THR:HG21	1:S:495:ARG:HG3	1.51	0.91
1:A:359:THR:HG23	3:B:30:THR:HG21	1.52	0.90
2:L:66:ARG:HH11	2:L:66:ARG:HG2	1.37	0.86
2:C:66:ARG:CG	2:C:66:ARG:HH11	1.87	0.86
2:C:32:TYR:HB2	2:C:92:VAL:HG22	1.57	0.85
1:S:369:VAL:HG12	1:S:370:SER:H	1.43	0.84
2:C:144:ILE:HG22	2:C:145:ASN:N	1.94	0.80
1:A:369:VAL:HG23	1:A:417:MET:HG3	1.64	0.80
2:C:112:ALA:HA	2:C:200:THR:HG21	1.63	0.80
1:A:390:LYS:HG3	1:A:491:TYR:HA	1.64	0.77
1:A:432:SER:HA	1:A:485:THR:HG22	1.67	0.77
3:H:150:GLU:OE1	3:H:170:ALA:HB3	1.85	0.77
3:H:100(C):THR:O	3:H:100(D):LEU:HB2	1.84	0.74
2:C:54:LEU:HD11	2:C:58:VAL:HB	1.71	0.72
2:C:32:TYR:HB2	2:C:92:VAL:CG2	2.18	0.72
2:L:198:HIS:HD2	2:L:200:THR:CG2	2.03	0.72
2:L:66:ARG:NH1	2:L:68:GLY:O	2.22	0.72
3:B:38:LYS:HB2	3:B:48:ILE:HD11	1.71	0.72
3:H:10:VAL:HG11	3:H:18:VAL:HG21	1.73	0.71
2:L:66:ARG:HG3	2:L:66:ARG:HH11	1.54	0.70
2:C:144:ILE:CG2	2:C:145:ASN:N	2.55	0.69
2:C:198:HIS:HD2	2:C:200:THR:CG2	2.05	0.69
2:C:198:HIS:HD2	2:C:200:THR:HG22	1.58	0.69
1:A:431:THR:HG22	1:A:433:THR:H	1.59	0.68
1:S:391:GLY:O	1:S:394:VAL:HG23	1.93	0.68
1:A:369:VAL:HG12	1:A:370:SER:N	2.08	0.68
1:S:431:THR:HG22	1:S:433:THR:H	1.58	0.68
2:C:66:ARG:HG2	2:C:66:ARG:HH11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:470:PRO:HB3	1:A:404:VAL:HG22	1.77	0.67
3:H:100(B):ARG:NH1	4:H:216:HOH:O	2.25	0.67
3:B:96:GLY:H	3:B:100(C):THR:HG22	1.60	0.66
1:S:405:ILE:HA	1:S:409:ASN:HD22	1.60	0.66
3:H:30:THR:HG23	3:H:53:GLY:HA2	1.77	0.66
2:C:33:LEU:HD13	2:C:71:TYR:CG	2.30	0.66
1:A:338:TYR:HE2	1:A:439:LYS:HG3	1.60	0.65
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.78	0.65
1:S:472:LEU:H	1:S:472:LEU:CD1	2.09	0.65
2:L:198:HIS:CD2	2:L:200:THR:HB	2.31	0.65
2:C:32:TYR:CB	2:C:92:VAL:HG22	2.27	0.64
2:L:108:ARG:NH1	2:L:109:ALA:O	2.29	0.64
1:A:441:ARG:HA	1:A:478:LEU:HD23	1.80	0.64
2:C:66:ARG:HG3	2:C:66:ARG:HH11	1.60	0.63
1:S:363:THR:HB	1:S:422:ALA:HB3	1.81	0.63
2:L:198:HIS:CD2	2:L:200:THR:CG2	2.82	0.62
2:C:14:SER:O	2:C:17:GLU:HB2	1.99	0.62
1:S:472:LEU:O	1:S:473:ASN:HB2	2.00	0.62
3:H:40:ARG:HH12	3:H:85:GLU:HA	1.64	0.61
2:L:136:LEU:N	2:L:136:LEU:HD12	2.15	0.61
2:C:37:GLN:OE1	2:C:45:LYS:HE2	2.01	0.61
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.83	0.61
2:C:89:LEU:HG	2:C:98:PHE:CE1	2.36	0.60
2:L:66:ARG:NH1	2:L:66:ARG:CG	2.45	0.60
2:C:144:ILE:CG2	2:C:145:ASN:H	2.13	0.60
2:C:160:LEU:HD13	3:B:173:GLN:OE1	2.00	0.60
3:H:40:ARG:NH1	3:H:85:GLU:HA	2.17	0.60
3:B:119:PRO:HB3	3:B:147:TYR:HB3	1.83	0.60
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.84	0.60
1:A:363:THR:HB	1:A:422:ALA:HB3	1.83	0.59
2:C:123:GLU:N	2:C:123:GLU:OE2	2.28	0.59
2:C:198:HIS:CD2	2:C:200:THR:HG22	2.37	0.59
3:H:94:ARG:NH1	3:H:101:ASP:OD1	2.35	0.59
2:C:187:GLU:HG2	2:C:211:ARG:HH12	1.66	0.59
2:C:131:SER:HA	2:C:179:LEU:O	2.02	0.59
3:H:95:GLU:HA	3:H:100(C):THR:HB	1.84	0.59
1:S:472:LEU:N	1:S:472:LEU:HD12	2.11	0.59
2:L:192:TYR:O	2:L:208:SER:HB2	2.03	0.59
3:H:150:GLU:OE2	3:H:151:PRO:HA	2.02	0.59
1:A:337:VAL:CG1	1:A:389:VAL:HG12	2.32	0.58
1:S:425:THR:CG2	1:S:495:ARG:HG3	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:94:ARG:NH1	3:B:101:ASP:OD1	2.36	0.58
1:S:425:THR:HG21	1:S:495:ARG:CG	2.31	0.58
2:L:135:PHE:C	2:L:136:LEU:HD12	2.24	0.58
3:H:2:VAL:HG12	3:H:3:GLN:N	2.19	0.58
2:L:198:HIS:CD2	2:L:200:THR:HG22	2.40	0.57
2:L:66:ARG:HG2	2:L:66:ARG:NH1	2.12	0.57
2:L:182:THR:HG22	2:L:184:ASP:H	1.70	0.56
1:S:348:CYS:SG	1:S:349:VAL:N	2.79	0.56
1:S:323:CYS:SG	1:S:345:ILE:HG23	2.45	0.56
1:S:338:TYR:CE2	1:S:439:LYS:HG3	2.41	0.55
1:A:337:VAL:HG11	1:A:389:VAL:HG12	1.87	0.55
1:A:338:TYR:CE2	1:A:439:LYS:HG3	2.39	0.55
2:C:61:ARG:NH2	2:C:82:ASP:OD1	2.38	0.55
1:A:369:VAL:CG1	1:A:370:SER:N	2.70	0.55
1:S:431:THR:HG22	1:S:433:THR:N	2.21	0.55
2:L:131:SER:HA	2:L:179:LEU:O	2.07	0.54
3:H:14:PRO:HA	3:H:82(C):LEU:O	2.08	0.53
2:L:155:ARG:HD3	2:L:156:GLN:H	1.73	0.53
3:H:190:TRP:CG	3:H:191:PRO:HA	2.43	0.53
3:B:100(D):LEU:HD12	3:B:103:TRP:CZ2	2.42	0.53
3:B:12:ALA:O	3:B:111:VAL:HA	2.08	0.53
1:S:351:ASP:O	1:S:354:VAL:HG22	2.09	0.53
3:H:155:THR:OG1	3:H:198:ASN:HB2	2.08	0.53
1:A:432:SER:HA	1:A:485:THR:CG2	2.35	0.52
2:L:149:LYS:HB2	2:L:193:THR:HB	1.90	0.52
1:S:369:VAL:HG22	1:S:417:MET:HG3	1.91	0.52
2:L:95:PRO:HB3	3:H:47:TRP:CZ3	2.44	0.52
1:A:469:PRO:HA	1:A:471:ALA:H	1.74	0.52
3:H:17:SER:HA	3:H:82:LEU:O	2.10	0.52
3:H:99:GLN:O	3:H:100(C):THR:HG23	2.10	0.52
3:H:152:VAL:CG1	3:H:201:HIS:HD2	2.23	0.52
1:S:426:ARG:NH1	3:H:56:ASP:OD2	2.40	0.52
3:H:154:LEU:HD23	3:H:154:LEU:C	2.29	0.51
2:C:35:TRP:CZ3	2:C:88:CYS:HB3	2.45	0.51
2:L:140:TYR:CG	2:L:141:PRO:HA	2.44	0.51
1:S:347:ASN:O	1:S:348:CYS:HB3	2.10	0.51
3:H:6:GLU:OE1	3:H:104:GLY:HA3	2.11	0.51
3:B:142:CYS:HB2	3:B:156:TRP:CH2	2.45	0.51
2:C:175:MET:CA	3:B:168:PHE:HE1	2.23	0.51
3:H:36:TRP:C	3:H:37:ILE:HD12	2.31	0.51
1:A:395:ARG:C	1:A:395:ARG:HD2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:LEU:HD11	2:C:86:TYR:CE2	2.46	0.51
3:B:190:TRP:CD1	3:B:191:PRO:HA	2.46	0.50
2:C:66:ARG:NH1	2:C:68:GLY:O	2.44	0.50
1:S:385:ASP:O	1:S:497:VAL:HA	2.11	0.50
3:H:100(C):THR:OG1	3:H:100(D):LEU:HD23	2.10	0.50
1:A:369:VAL:HG12	1:A:370:SER:H	1.76	0.50
2:C:192:TYR:O	2:C:208:SER:HB2	2.11	0.50
2:C:11:LEU:HD23	2:C:12:SER:N	2.27	0.50
3:H:13:ARG:HA	3:H:112:SER:O	2.11	0.50
3:H:30:THR:HG23	3:H:53:GLY:CA	2.41	0.50
1:A:390:LYS:CG	1:A:490:GLY:O	2.60	0.50
1:A:351:ASP:C	1:A:353:SER:H	2.14	0.49
2:C:161:ASN:HD22	2:C:177:SER:HA	1.77	0.49
3:H:32:TYR:CE1	3:H:96:GLY:HA3	2.46	0.49
2:C:89:LEU:HB3	2:C:98:PHE:CD1	2.48	0.49
2:L:198:HIS:CD2	2:L:200:THR:CB	2.96	0.49
3:B:179:LEU:HD23	3:B:179:LEU:C	2.32	0.49
1:S:351:ASP:N	1:S:351:ASP:OD2	2.43	0.49
1:S:431:THR:HG22	1:S:434:GLY:H	1.78	0.49
2:L:89:LEU:HG	2:L:98:PHE:CE1	2.47	0.49
2:C:47:LEU:HD11	2:C:86:TYR:HE2	1.77	0.49
3:B:10:VAL:HG11	3:B:18:VAL:HG21	1.94	0.49
1:S:386:SER:O	1:S:387:PHE:HB3	2.13	0.49
2:C:134:CYS:HB2	2:C:148:TRP:CH2	2.48	0.49
2:L:113:PRO:HG2	2:L:205:ILE:HD12	1.95	0.49
3:H:98:PRO:HG2	3:H:100(A):LEU:HG	1.96	0.48
2:C:195:GLU:HG2	2:C:206:VAL:HG22	1.95	0.48
1:S:338:TYR:HE2	1:S:439:LYS:HG3	1.77	0.48
3:B:21:SER:HB3	3:B:79:TYR:CE2	2.49	0.48
3:H:40:ARG:HG2	3:H:40:ARG:HH11	1.79	0.48
1:S:344:LYS:O	1:S:344:LYS:HD3	2.14	0.48
1:A:488:GLY:O	1:A:492:GLN:HG3	2.14	0.48
2:C:112:ALA:CA	2:C:200:THR:HG21	2.39	0.48
2:C:133:VAL:HG22	2:C:178:THR:HG23	1.95	0.48
2:C:66:ARG:HG2	2:C:66:ARG:NH1	2.26	0.48
3:H:94:ARG:HD3	3:H:101:ASP:OD2	2.13	0.48
1:S:441:ARG:HA	1:S:478:LEU:HD23	1.96	0.48
1:A:333:LYS:HE2	1:A:333:LYS:HB3	1.59	0.47
1:A:355:LEU:HD22	1:A:421:LEU:HD21	1.95	0.47
3:B:124:LEU:HB2	3:B:141:GLY:CA	2.45	0.47
1:A:353:SER:C	1:A:355:LEU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:ARG:CZ	3:H:52:TYR:HB2	2.44	0.47
2:C:155:ARG:HD3	2:C:156:GLN:H	1.80	0.47
2:L:95:PRO:CB	3:H:47:TRP:CE3	2.98	0.47
2:L:160:LEU:HD13	3:H:173:GLN:CD	2.36	0.47
1:A:369:VAL:CG1	1:A:370:SER:H	2.27	0.47
3:B:179:LEU:HD23	3:B:180:SER:N	2.30	0.47
3:H:31:THR:HG22	3:H:31:THR:O	2.15	0.47
2:L:164:THR:HG22	3:H:169:PRO:HD3	1.97	0.47
1:A:386:SER:O	1:A:387:PHE:HB3	2.15	0.47
2:L:142:LYS:HB3	2:L:173:TYR:CD1	2.49	0.47
1:A:421:LEU:N	1:A:421:LEU:HD12	2.31	0.46
3:B:212:ILE:HD12	3:B:212:ILE:N	2.30	0.46
2:L:160:LEU:HD13	3:H:173:GLN:NE2	2.30	0.46
1:A:426:ARG:NH1	1:A:485:THR:O	2.34	0.46
3:H:33:ARG:HG2	3:H:52:TYR:HD1	1.80	0.46
1:S:344:LYS:O	1:S:345:ILE:HD12	2.16	0.46
1:A:374:LEU:C	1:A:376:ASP:H	2.19	0.46
1:A:469:PRO:HA	1:A:471:ALA:N	2.29	0.46
2:C:147:LYS:N	2:C:147:LYS:HD2	2.30	0.46
2:C:147:LYS:HE3	2:C:197:THR:OG1	2.15	0.46
1:S:469:PRO:HG3	1:S:476:TRP:CZ2	2.50	0.46
2:C:186:TYR:HA	2:C:192:TYR:OH	2.16	0.46
1:A:336:SER:HB3	1:A:439:LYS:O	2.16	0.45
1:S:369:VAL:HG12	1:S:370:SER:N	2.21	0.45
1:A:390:LYS:CG	1:A:491:TYR:HA	2.40	0.45
2:C:175:MET:HA	3:B:168:PHE:HE1	1.81	0.45
3:H:10:VAL:CG1	3:H:18:VAL:HG21	2.46	0.45
2:L:50:ALA:O	2:L:51:ALA:HB3	2.16	0.45
2:C:183:LYS:HE2	2:C:187:GLU:OE2	2.17	0.45
2:L:142:LYS:HB3	2:L:173:TYR:CE1	2.52	0.45
2:C:12:SER:HG	2:C:105:GLU:CD	2.20	0.45
1:A:323:CYS:HB2	1:A:348:CYS:HB2	1.50	0.45
3:B:94:ARG:HH11	3:B:101:ASP:CG	2.20	0.45
3:B:96:GLY:N	3:B:100(C):THR:HG22	2.28	0.45
2:C:110:ASP:OD1	2:C:110:ASP:N	2.50	0.45
1:A:420:VAL:C	1:A:421:LEU:HD12	2.38	0.44
2:L:89:LEU:HB3	2:L:98:PHE:CD1	2.52	0.44
1:A:347:ASN:O	1:A:348:CYS:HB3	2.16	0.44
2:C:54:LEU:CD1	2:C:58:VAL:HB	2.45	0.44
2:C:35:TRP:CE3	2:C:88:CYS:HB3	2.53	0.44
2:L:161:ASN:HD22	2:L:177:SER:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:CYS:HA	1:A:324:PRO:HD2	1.87	0.44
2:L:155:ARG:HD3	2:L:156:GLN:N	2.32	0.44
1:A:367:TYR:C	1:A:369:VAL:H	2.21	0.44
3:B:100(C):THR:O	3:B:100(D):LEU:HB2	2.17	0.44
3:H:150:GLU:OE1	3:H:170:ALA:CB	2.63	0.44
2:C:198:HIS:HD2	2:C:200:THR:CB	2.31	0.43
2:C:32:TYR:CG	2:C:92:VAL:HG22	2.53	0.43
2:L:189:HIS:O	2:L:211:ARG:HD3	2.17	0.43
1:A:354:VAL:O	1:A:354:VAL:HG12	2.18	0.43
1:A:337:VAL:HG13	1:A:389:VAL:HG12	2.00	0.43
1:A:337:VAL:HG23	1:A:338:TYR:H	1.83	0.43
2:C:6:GLN:NE2	2:C:101:GLY:HA2	2.33	0.43
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.82	0.43
2:L:66:ARG:HG3	2:L:66:ARG:NH1	2.21	0.43
3:H:2:VAL:HG13	3:H:27:TYR:CD1	2.53	0.43
1:A:431:THR:HG22	1:A:433:THR:N	2.30	0.43
1:A:337:VAL:CG1	1:A:389:VAL:CG1	2.97	0.43
2:C:135:PHE:C	2:C:136:LEU:HD12	2.39	0.43
2:C:198:HIS:CD2	2:C:200:THR:H	2.37	0.43
2:C:66:ARG:CG	2:C:66:ARG:NH1	2.58	0.43
3:H:204:SER:O	3:H:206:THR:HG23	2.18	0.43
3:H:38:LYS:HB2	3:H:48:ILE:HD11	2.01	0.43
1:S:470:PRO:HB3	1:A:404:VAL:CG2	2.47	0.42
3:H:148:PHE:HA	3:H:149:PRO:HA	1.80	0.42
1:A:351:ASP:O	1:A:354:VAL:HG23	2.18	0.42
3:H:190:TRP:CD1	3:H:191:PRO:HA	2.54	0.42
2:L:190:ASN:OD1	2:L:211:ARG:HB2	2.18	0.42
2:L:95:PRO:HB3	3:H:47:TRP:CE3	2.54	0.42
3:B:95:GLU:HG3	3:B:100(C):THR:HG21	2.02	0.42
1:A:385:ASP:O	1:A:497:VAL:HA	2.20	0.42
3:H:142:CYS:HB2	3:H:156:TRP:CH2	2.54	0.42
2:L:96:TRP:CZ2	3:H:35:HIS:CE1	3.08	0.42
1:A:484:TYR:HB2	1:A:487:THR:HG23	2.01	0.42
1:S:488:GLY:O	1:S:492:GLN:HG3	2.19	0.42
2:C:18:ARG:HG3	2:C:76:SER:HA	2.01	0.42
3:H:83:THR:O	3:H:111:VAL:HG21	2.20	0.42
3:B:186:THR:O	3:B:188:SER:N	2.52	0.42
3:B:213:GLU:HA	3:B:214:PRO:HD3	1.78	0.42
2:C:198:HIS:CD2	2:C:200:THR:HB	2.55	0.42
2:L:108:ARG:HG3	2:L:109:ALA:O	2.19	0.42
1:A:331:ALA:HB3	1:A:334:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:140:TYR:CG	2:C:141:PRO:HA	2.55	0.41
3:H:101:ASP:N	3:H:101:ASP:OD2	2.52	0.41
1:S:441:ARG:HH22	1:S:457:ASN:H	1.66	0.41
1:A:355:LEU:HD13	1:A:364:PHE:CE1	2.56	0.41
3:B:16:ALA:O	3:B:82(C):LEU:HG	2.20	0.41
2:C:164:THR:HG22	3:B:169:PRO:HD3	2.03	0.41
3:B:24:ALA:HB1	3:B:27:TYR:CE1	2.56	0.41
3:H:154:LEU:HD23	3:H:155:THR:N	2.35	0.41
2:L:162:SER:OG	3:H:169:PRO:HD2	2.21	0.41
2:L:161:ASN:ND2	2:L:177:SER:OG	2.53	0.41
2:L:48:ILE:HD13	2:L:73:LEU:CD1	2.51	0.41
3:B:190:TRP:CG	3:B:191:PRO:HA	2.55	0.41
3:H:2:VAL:CG1	3:H:3:GLN:N	2.81	0.41
1:S:367:TYR:O	1:S:417:MET:HA	2.21	0.41
3:B:52:TYR:O	3:B:55:SER:N	2.54	0.41
2:L:6:GLN:NE2	2:L:102:THR:OG1	2.48	0.41
1:S:431:THR:CG2	1:S:433:THR:H	2.31	0.41
3:H:186:THR:O	3:H:188:SER:N	2.53	0.41
3:H:52(A):PRO:O	3:H:53:GLY:C	2.58	0.41
1:A:331:ALA:HB3	1:A:334:PHE:HE1	1.86	0.41
2:C:198:HIS:HD2	2:C:200:THR:HB	1.86	0.41
2:L:46:ARG:HD2	2:L:55:ASP:OD2	2.21	0.40
2:L:61:ARG:HD2	2:L:77:SER:O	2.20	0.40
2:C:138:ASN:ND2	2:C:172:THR:OG1	2.46	0.40
3:H:68:LYS:HE2	3:H:68:LYS:HB2	1.74	0.40
2:L:123:GLU:O	2:L:126:THR:HB	2.22	0.40
2:L:186:TYR:HA	2:L:192:TYR:OH	2.21	0.40
3:H:2:VAL:HG13	3:H:27:TYR:HD1	1.86	0.40
1:S:337:VAL:HA	1:S:387:PHE:HB2	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	A	174/193 (90%)	157 (90%)	15 (9%)	2 (1%)	17	56
1	S	177/193 (92%)	158 (89%)	18 (10%)	1 (1%)	28	70
2	C	206/212 (97%)	193 (94%)	12 (6%)	1 (0%)	32	74
2	L	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	32	74
3	B	212/220 (96%)	197 (93%)	13 (6%)	2 (1%)	20	62
3	H	212/220 (96%)	193 (91%)	16 (8%)	3 (1%)	13	49
All	All	1191/1250 (95%)	1097 (92%)	84 (7%)	10 (1%)	22	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	127	VAL
3	B	127	VAL
1	S	348	CYS
1	A	348	CYS
3	H	187	SER
3	B	187	SER
2	L	138	ASN
2	C	138	ASN
1	A	450	PRO
3	H	146	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/169 (92%)	149 (96%)	7 (4%)	32	71
1	S	157/169 (93%)	151 (96%)	6 (4%)	38	75
2	C	187/189 (99%)	180 (96%)	7 (4%)	39	76
2	L	189/189 (100%)	184 (97%)	5 (3%)	51	83
3	B	187/190 (98%)	182 (97%)	5 (3%)	50	82
3	H	187/190 (98%)	179 (96%)	8 (4%)	33	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1063/1096 (97%)	1025 (96%)	38 (4%)	40 77

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	344	LYS
1	S	349	VAL
1	S	374	LEU
1	S	395	ARG
1	S	457	ASN
1	S	472	LEU
1	A	337	VAL
1	A	338	TYR
1	A	378	CYS
1	A	432	SER
1	A	439	LYS
1	A	463	ASP
1	A	500	SER
2	L	66	ARG
2	L	85	ASP
2	L	89	LEU
2	L	144	ILE
2	L	183	LYS
3	H	11	LEU
3	H	33	ARG
3	H	65	ASP
3	H	66	LYS
3	H	73	THR
3	H	82(B)	SER
3	H	94	ARG
3	H	100(C)	THR
2	C	22	THR
2	C	66	ARG
2	C	89	LEU
2	C	105	GLU
2	C	110	ASP
2	C	147	LYS
2	C	184	ASP
3	B	33	ARG
3	B	58	THR
3	B	61	GLN
3	B	94	ARG

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Mol	Chain	Res	Type
3	B	172	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	457	ASN
1	A	457	ASN
2	L	161	ASN
2	L	198	HIS
2	L	210	ASN
3	H	3	GLN
3	H	61	GLN
3	H	193	GLN
2	C	124	GLN
2	C	161	ASN
2	C	198	HIS
2	C	210	ASN
3	B	43	GLN
3	B	61	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	178/193 (92%)	0.10	2 (1%) 80 55	24, 44, 83, 92	0
1	S	179/193 (92%)	0.19	7 (3%) 40 16	24, 44, 83, 93	0
2	C	210/212 (99%)	0.28	3 (1%) 75 49	26, 50, 74, 83	0
2	L	212/212 (100%)	0.05	0 100 100	26, 50, 74, 83	0
3	B	216/220 (98%)	0.07	6 (2%) 53 25	24, 38, 62, 67	0
3	H	216/220 (98%)	-0.10	1 (0%) 90 74	24, 38, 62, 67	0
All	All	1211/1250 (96%)	0.10	19 (1%) 72 44	24, 44, 75, 93	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	324	PRO	3.3
1	S	350	ALA	3.1
1	S	352	TYR	3.0
3	B	193	GLN	2.7
3	B	196	THR	2.6
1	S	377	LEU	2.6
3	B	138	VAL	2.5
1	A	379	PHE	2.4
3	B	161	LEU	2.4
1	S	378	CYS	2.4
1	S	383	TYR	2.3
3	B	128	CYS	2.2
3	H	128	CYS	2.2
1	A	352	TYR	2.1
2	C	145	ASN	2.1
2	C	152	GLY	2.1
1	S	376	ASP	2.1
3	B	212	ILE	2.0
2	C	197	THR	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 carbohydrates 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.