



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:28 AM UTC

PDB ID : 8RRN / pdb_00008rrn
Title : Crystal structure of the SARS-CoV-2 S RBD in complex with pT1616 Fab
Authors : Hansen, G.; Krey, T.
Deposited on : 2024-01-23
Resolution : 3.11 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

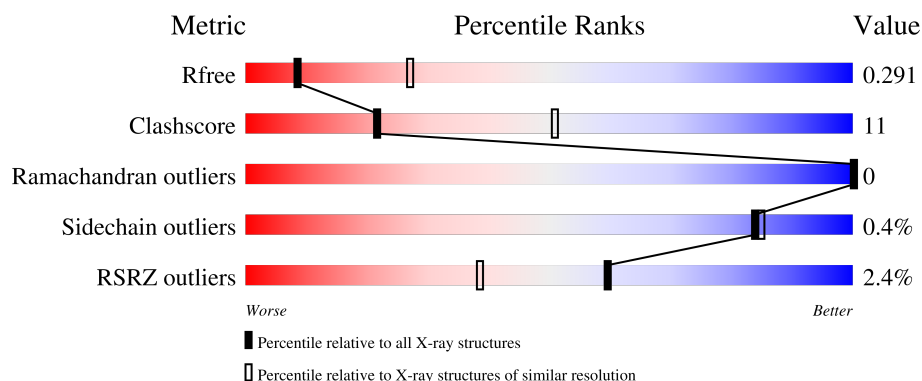
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	199	3% 76% 21% •
1	B	199	2% 78% 20% •
2	C	235	5% 73% 22% 5%
2	H	235	2% 66% 29% • 5%
3	D	217	2% 82% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	217	% 80% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18717 atoms, of which 9200 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	193	Total	C	H	N	O	S	0	0	0
			2975	981	1447	254	285	8			
1	B	195	Total	C	H	N	O	S	0	0	0
			3001	989	1457	257	290	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	ASP	-	expression tag	UNP P0DTC2
A	529	ASP	-	expression tag	UNP P0DTC2
A	530	ASP	-	expression tag	UNP P0DTC2
A	531	ASP	-	expression tag	UNP P0DTC2
A	532	LYS	-	expression tag	UNP P0DTC2
B	528	ASP	-	expression tag	UNP P0DTC2
B	529	ASP	-	expression tag	UNP P0DTC2
B	530	ASP	-	expression tag	UNP P0DTC2
B	531	ASP	-	expression tag	UNP P0DTC2
B	532	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called pT1616 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	224	Total	C	H	N	O	S	0	0	0
			3280	1040	1629	276	328	7			
2	C	223	Total	C	H	N	O	S	0	0	0
			3264	1035	1620	275	327	7			

- Molecule 3 is a protein called pT1616 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	213	Total	C	H	N	O	S	0	0	0
			3098	982	1523	266	323	4			

Continued on next page...

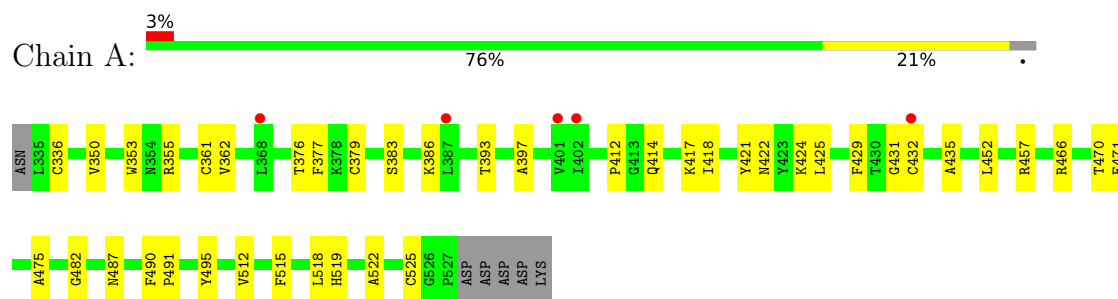
Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	213	Total	C	H	N	O	S	0	0	0
			3099	982	1524	266	323	4			

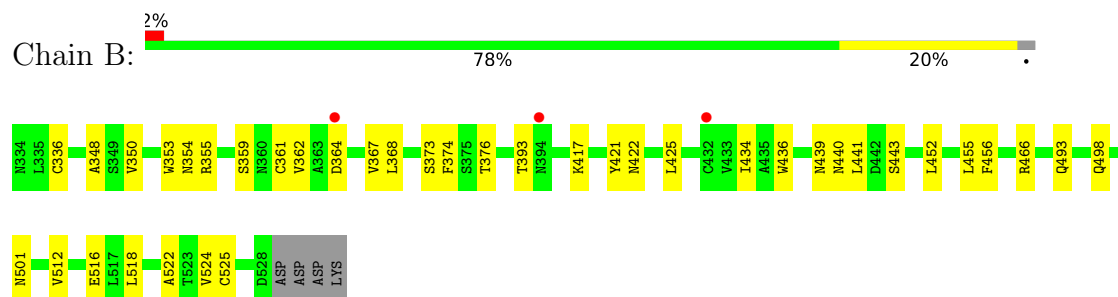
3 Residue-property plots [i](#)

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.

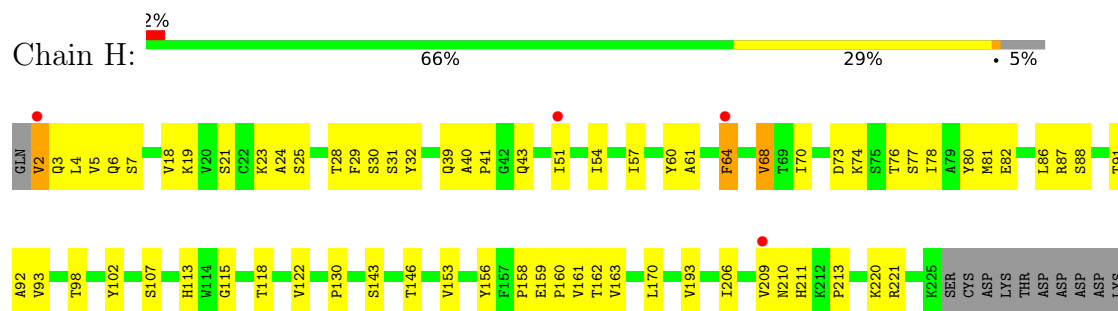
- Molecule 1: Spike protein S1



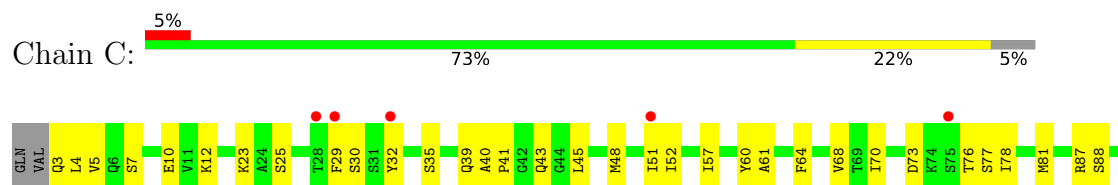
- Molecule 1: Spike protein S1

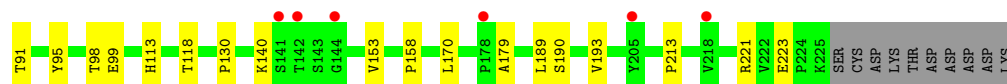


- Molecule 2: pT1616 Fab heavy chain

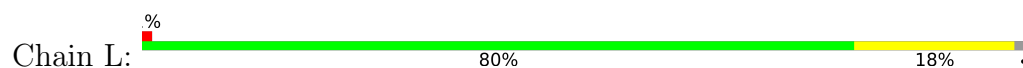


- Molecule 2: pT1616 Fab heavy chain

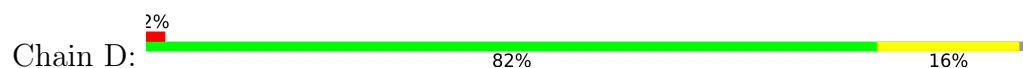




• Molecule 3: pT1616 Fab light chain



• Molecule 3: pT1616 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.10Å 59.06Å 152.03Å 90.00° 95.45° 90.00°	Depositor
Resolution (Å)	45.62 – 3.11 45.62 – 3.12	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.62-3.11) 99.6 (45.62-3.12)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.243 , 0.291 0.243 , 0.291	Depositor DCC
R_{free} test set	1388 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	96.6	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18717	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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	0.31	0/1572	0.43	0/2140
1	B	0.33	0/1588	0.44	0/2162
2	C	0.39	0/1682	0.56	1/2290 (0.0%)
2	H	0.36	0/1689	0.53	0/2300
3	D	0.31	0/1613	0.45	0/2206
3	L	0.32	0/1613	0.47	0/2206
All	All	0.34	0/9757	0.48	1/13304 (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	30	SER	N-CA-C	5.57	122.66	110.80

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	1528	1447	1447	26	0
1	B	1544	1457	1457	24	0
2	C	1644	1620	1620	42	0
2	H	1651	1629	1629	67	0
3	D	1575	1524	1523	22	0
3	L	1575	1523	1523	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9517	9200	9199	202	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 11.

All (202) 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:D:3:VAL:HA	3:D:101:LEU:HD21	1.55	0.87
2:H:3:GLN:O	2:H:4:LEU:HD23	1.73	0.87
3:D:20:ILE:HG21	3:D:106:THR:HG21	1.61	0.82
2:H:23:LYS:HG2	2:H:78:ILE:HD12	1.64	0.80
3:L:7:PRO:O	3:L:106:THR:HG22	1.80	0.80
2:H:51:ILE:HD11	2:H:70:ILE:HB	1.62	0.80
3:L:113:GLN:HG2	3:L:114:PRO:HD2	1.65	0.79
2:C:170:LEU:HD21	2:C:193:VAL:HG21	1.69	0.76
2:H:19:LYS:HD2	2:H:80:TYR:HB3	1.69	0.74
2:H:19:LYS:HE2	2:H:82:GLU:HB2	1.70	0.74
3:L:3:VAL:HA	3:L:101:LEU:HD21	1.70	0.73
2:H:5:VAL:HG22	2:H:23:LYS:HB2	1.70	0.73
3:L:6:GLN:NE2	3:L:90:CYS:SG	2.62	0.71
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.75	0.69
2:C:4:LEU:HA	2:C:25:SER:HB3	1.74	0.68
2:C:88:SER:O	2:C:91:THR:HG22	1.95	0.66
1:A:393:THR:HG21	1:A:518:LEU:HB3	1.77	0.66
3:L:113:GLN:HG2	3:L:114:PRO:CD	2.26	0.66
2:H:40:ALA:HB1	2:H:41:PRO:HD2	1.79	0.65
2:H:91:THR:HG22	2:H:122:VAL:H	1.60	0.65
1:B:455:LEU:HD22	1:B:493:GLN:HG3	1.80	0.64
1:A:470:THR:O	2:H:31:SER:HB3	1.98	0.63
2:H:170:LEU:HD21	2:H:193:VAL:HG21	1.79	0.63
2:H:158:PRO:HD2	2:H:213:PRO:CB	2.28	0.63
2:H:6:GLN:HA	2:H:21:SER:O	2.00	0.62
3:L:35:VAL:HG21	3:L:73:ALA:HB1	1.82	0.62
2:C:51:ILE:HD13	2:C:70:ILE:HG22	1.81	0.61
1:B:348:ALA:HB2	1:B:354:ASN:OD1	2.00	0.61
1:B:359:SER:HA	1:B:524:VAL:HG22	1.83	0.61
1:B:452:LEU:HD21	2:C:57:ILE:HD13	1.83	0.60
1:A:482:GLY:O	2:H:30:SER:HB2	2.02	0.59
3:L:6:GLN:OE1	3:L:106:THR:HG23	2.00	0.59
2:C:10:GLU:OE2	2:C:12:LYS:NZ	2.29	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:26:ASN:HA	3:L:30:GLY:HA3	1.84	0.59
2:H:220:LYS:NZ	3:L:128:GLU:OE1	2.30	0.58
2:H:3:GLN:HB3	2:H:113:HIS:HB3	1.85	0.58
2:C:130:PRO:HB2	2:C:153:VAL:HG13	1.84	0.58
2:H:4:LEU:HD11	2:H:98:THR:HG23	1.85	0.58
3:D:35:VAL:HG21	3:D:73:ALA:HB1	1.86	0.57
2:C:68:VAL:HG23	2:C:81:MET:HE3	1.86	0.57
1:A:518:LEU:HD23	1:A:519:HIS:C	2.29	0.57
2:C:190:SER:OG	3:D:182:TYR:OH	2.23	0.57
3:D:26:ASN:HA	3:D:30:GLY:HA3	1.86	0.57
2:C:158:PRO:HD2	2:C:213:PRO:CB	2.34	0.56
2:H:61:ALA:O	2:H:64:PHE:HB3	2.06	0.56
3:L:85:GLU:OE1	3:L:171:LYS:NZ	2.37	0.56
2:C:40:ALA:HB1	2:C:41:PRO:HD2	1.88	0.56
3:D:118:PRO:HB3	3:D:144:PHE:HB3	1.87	0.56
2:C:23:LYS:HG2	2:C:78:ILE:HG23	1.87	0.56
2:C:179:ALA:HB2	2:C:189:LEU:HB3	1.86	0.56
2:H:2:VAL:HG12	2:H:3:GLN:OE1	2.06	0.56
3:L:153:TRP:HB2	3:L:160:VAL:HG11	1.87	0.56
3:L:20:ILE:HG23	3:L:106:THR:HG21	1.86	0.56
1:A:353:TRP:O	1:A:466:ARG:NH1	2.40	0.55
2:H:60:TYR:HB2	2:H:64:PHE:CD1	2.41	0.55
2:H:64:PHE:CD2	2:H:68:VAL:HG13	2.41	0.55
2:H:40:ALA:HB3	2:H:43:GLN:HB3	1.89	0.55
2:C:68:VAL:CG2	2:C:81:MET:HE3	2.36	0.54
2:H:130:PRO:HB2	2:H:153:VAL:HG13	1.88	0.54
2:H:60:TYR:HB3	2:H:64:PHE:CG	2.42	0.54
1:A:490:PHE:CD1	2:H:54:ILE:HD12	2.43	0.54
1:A:518:LEU:HD23	1:A:519:HIS:N	2.22	0.53
3:L:6:GLN:NE2	3:L:90:CYS:H	2.06	0.53
2:C:130:PRO:CB	2:C:153:VAL:HG13	2.38	0.53
1:A:355:ARG:HA	1:A:397:ALA:O	2.08	0.53
2:H:163:VAL:HG22	2:H:209:VAL:HG22	1.90	0.53
2:C:23:LYS:HG2	2:C:78:ILE:HD12	1.90	0.53
2:H:5:VAL:CG2	2:H:23:LYS:HB2	2.37	0.53
2:H:158:PRO:HD2	2:H:213:PRO:HB2	1.90	0.53
2:H:87:ARG:HG3	2:H:88:SER:H	1.74	0.52
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.90	0.52
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.92	0.52
2:H:64:PHE:HD2	2:H:68:VAL:HG13	1.74	0.52
2:H:70:ILE:HG22	2:H:81:MET:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:O	1:B:374:PHE:HE2	1.92	0.52
1:B:336:CYS:HA	1:B:361:CYS:HB2	1.91	0.52
3:L:41:LEU:HD23	3:L:86:ALA:HB2	1.90	0.52
2:H:4:LEU:HD22	2:H:24:ALA:HA	1.93	0.51
2:C:52:ILE:HD12	2:C:57:ILE:HD12	1.93	0.51
2:H:156:TYR:CZ	2:H:161:VAL:HG11	2.46	0.51
1:B:393:THR:HA	1:B:522:ALA:HA	1.91	0.51
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.92	0.51
2:H:3:GLN:O	2:H:25:SER:HB3	2.11	0.50
3:L:113:GLN:OE1	3:L:145:TYR:CG	2.64	0.50
3:L:164:VAL:HG22	3:L:183:LEU:HD13	1.93	0.50
2:H:91:THR:CG2	2:H:122:VAL:H	2.22	0.50
2:C:76:THR:O	2:C:77:SER:HB3	2.11	0.50
3:D:149:VAL:HG13	3:D:200:VAL:HG13	1.93	0.50
1:A:418:ILE:HD11	1:A:495:TYR:OH	2.12	0.50
1:B:440:ASN:C	1:B:441:LEU:HD12	2.37	0.50
2:H:4:LEU:O	2:H:115:GLY:HA2	2.11	0.50
3:L:115:LYS:N	3:L:115:LYS:HD3	2.26	0.50
2:C:190:SER:HG	3:D:182:TYR:HH	1.51	0.50
2:C:32:TYR:HB3	2:C:99:GLU:O	2.11	0.50
2:H:60:TYR:CE2	2:H:70:ILE:HG12	2.47	0.50
3:D:20:ILE:CG2	3:D:106:THR:HG21	2.36	0.50
2:H:130:PRO:CB	2:H:153:VAL:HG13	2.42	0.49
3:D:154:LYS:HA	3:D:159:PRO:HA	1.93	0.49
1:B:355:ARG:O	3:D:95:SER:OG	2.29	0.49
2:H:156:TYR:HD2	2:H:211:HIS:HE2	1.61	0.49
2:H:51:ILE:HG12	2:H:70:ILE:HG13	1.94	0.49
2:H:76:THR:O	2:H:77:SER:HB3	2.12	0.49
3:L:149:VAL:HG12	3:L:202:HIS:HB2	1.95	0.49
2:C:3:GLN:HB3	2:C:113:HIS:HB3	1.95	0.49
2:C:73:ASP:HB2	2:C:76:THR:OG1	2.12	0.49
2:H:73:ASP:HB2	2:H:76:THR:OG1	2.13	0.48
1:A:376:THR:OG1	1:A:435:ALA:HB3	2.12	0.48
2:H:39:GLN:O	2:H:92:ALA:HB1	2.13	0.48
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.49	0.48
2:C:221:ARG:NH1	2:C:223:GLU:OE2	2.46	0.48
2:C:40:ALA:HB3	2:C:43:GLN:HB2	1.95	0.48
1:B:362:VAL:HA	1:B:525:CYS:O	2.13	0.48
3:D:88:TYR:HB2	3:D:106:THR:HG23	1.95	0.47
3:D:18:VAL:HG23	3:D:80:LEU:HD11	1.96	0.47
3:D:41:LEU:HD23	3:D:86:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD21	1:B:512:VAL:HG11	1.95	0.47
2:C:45:LEU:N	2:C:45:LEU:HD12	2.29	0.47
2:H:39:GLN:HB3	2:H:93:VAL:HG23	1.96	0.47
1:A:362:VAL:HA	1:A:525:CYS:O	2.15	0.46
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.46
3:D:141:ILE:HG22	3:D:144:PHE:CD2	2.51	0.46
3:D:153:TRP:HB2	3:D:160:VAL:CG2	2.45	0.46
1:B:373:SER:O	1:B:436:TRP:CB	2.63	0.46
2:H:7:SER:O	2:H:118:THR:HG22	2.15	0.46
1:A:336:CYS:HA	1:A:361:CYS:HB2	1.98	0.46
1:B:373:SER:O	1:B:436:TRP:HB3	2.16	0.46
3:L:20:ILE:HD13	3:L:106:THR:OG1	2.16	0.46
3:L:35:VAL:HG21	3:L:73:ALA:CB	2.45	0.46
2:C:158:PRO:HD2	2:C:213:PRO:HB2	1.96	0.46
2:H:158:PRO:HD2	2:H:213:PRO:HB3	1.96	0.45
1:B:353:TRP:O	1:B:466:ARG:NH1	2.49	0.45
2:H:60:TYR:HB2	2:H:64:PHE:CE1	2.52	0.45
3:L:145:TYR:HA	3:L:146:PRO:C	2.40	0.45
2:C:25:SER:C	2:C:29:PHE:HE1	2.24	0.45
3:L:30:GLY:HA2	3:L:71:THR:HG22	1.99	0.45
3:D:38:TYR:HE2	3:D:91:GLN:HB3	1.82	0.45
3:L:27:SER:HB2	3:L:94:ASP:OD1	2.17	0.45
1:A:383:SER:HB3	1:A:386:LYS:HB2	1.99	0.45
2:C:60:TYR:CE1	2:C:70:ILE:HD12	2.52	0.45
2:C:3:GLN:O	2:C:25:SER:C	2.60	0.45
1:B:417:LYS:O	1:B:421:TYR:HB2	2.17	0.45
2:H:23:LYS:HG2	2:H:78:ILE:HG23	1.99	0.45
2:H:77:SER:C	2:H:78:ILE:HD13	2.43	0.44
2:H:143:SER:HB3	2:H:146:THR:HB	1.98	0.44
2:H:162:THR:CG2	2:H:210:ASN:HB3	2.46	0.44
2:C:4:LEU:CA	2:C:25:SER:HB3	2.43	0.44
3:D:115:LYS:HG3	3:D:116:ALA:N	2.31	0.44
1:A:417:LYS:O	1:A:421:TYR:HB2	2.18	0.44
2:H:61:ALA:O	2:H:64:PHE:HD1	1.99	0.44
2:C:4:LEU:HD11	2:C:98:THR:HG23	1.99	0.44
3:L:6:GLN:HE22	3:L:90:CYS:N	2.16	0.44
3:L:113:GLN:OE1	3:L:145:TYR:CD1	2.71	0.44
2:C:35:SER:OG	2:C:99:GLU:OE2	2.35	0.44
1:B:498:GLN:HB3	1:B:501:ASN:ND2	2.32	0.44
1:B:376:THR:O	1:B:434:ILE:HA	2.17	0.44
2:H:29:PHE:CE1	2:H:74:LYS:HG3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ASN:O	1:B:443:SER:OG	2.30	0.43
2:H:102:TYR:CE2	2:H:107:SER:HA	2.53	0.43
2:C:61:ALA:HB3	2:C:64:PHE:HD1	1.83	0.43
1:B:364:ASP:O	1:B:367:VAL:HG22	2.18	0.43
3:D:171:LYS:HE2	3:D:177:TYR:OH	2.19	0.43
2:H:162:THR:O	2:H:209:VAL:HA	2.17	0.43
3:D:18:VAL:O	3:D:76:VAL:HA	2.18	0.43
1:A:471:GLU:O	1:A:491:PRO:HD3	2.18	0.43
2:H:41:PRO:HD3	2:H:91:THR:O	2.18	0.43
3:D:81:GLN:O	3:D:110:VAL:HG21	2.19	0.43
2:H:60:TYR:CB	2:H:64:PHE:CG	3.02	0.42
2:H:68:VAL:HA	2:H:82:GLU:O	2.19	0.42
2:H:159:GLU:N	2:H:160:PRO:CD	2.82	0.42
3:L:118:PRO:HB3	3:L:144:PHE:HB3	2.01	0.42
1:B:516:GLU:HG2	1:B:518:LEU:HG	2.00	0.42
2:H:28:THR:O	2:H:29:PHE:CG	2.73	0.42
2:C:221:ARG:CZ	2:C:223:GLU:OE2	2.68	0.42
1:A:412:PRO:HG3	1:A:429:PHE:HB3	2.00	0.42
2:C:7:SER:O	2:C:118:THR:HG22	2.20	0.42
2:H:206:ILE:HG12	2:H:221:ARG:HG2	2.01	0.42
3:L:153:TRP:CB	3:L:160:VAL:HG11	2.49	0.42
2:H:3:GLN:C	2:H:25:SER:HB3	2.45	0.42
1:B:455:LEU:HD23	1:B:456:PHE:CE2	2.55	0.41
2:H:32:TYR:CD1	2:H:98:THR:HB	2.56	0.41
2:C:48:MET:HG2	2:C:64:PHE:CE1	2.55	0.41
2:H:60:TYR:CD2	2:H:64:PHE:CE2	3.08	0.41
2:C:73:ASP:HB2	2:C:76:THR:HG1	1.83	0.41
1:A:377:PHE:CD1	1:A:377:PHE:C	2.99	0.41
1:A:452:LEU:HD21	2:H:57:ILE:HD13	2.03	0.41
2:H:19:LYS:HD3	2:H:81:MET:O	2.20	0.41
3:D:87:ASP:N	3:D:87:ASP:OD1	2.52	0.41
1:A:475:ALA:O	1:A:487:ASN:HB3	2.20	0.41
2:C:4:LEU:HD22	2:C:23:LYS:O	2.21	0.41
2:C:5:VAL:HG23	2:C:25:SER:HB2	2.03	0.41
1:A:379:CYS:HA	1:A:432:CYS:HA	2.03	0.41
2:C:140:LYS:N	2:C:140:LYS:HD2	2.36	0.41
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.57	0.40
1:B:440:ASN:OD1	1:B:440:ASN:N	2.52	0.40
2:H:5:VAL:O	2:H:5:VAL:HG23	2.20	0.40
2:C:39:GLN:HE21	2:C:95:TYR:HE2	1.68	0.40
3:L:36:HIS:ND1	3:L:51:TYR:HA	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:172:GLN:OE1	3:L:178:ALA:HB2	2.20	0.40
2:C:87:ARG:HA	2:C:87:ARG:HD2	1.86	0.40
3:L:88:TYR:O	3:L:105:GLY:HA2	2.21	0.40
1:A:414:GLN:O	1:A:424:LYS:NZ	2.54	0.40
1:B:498:GLN:HB3	1:B:501:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	191/199 (96%)	176 (92%)	15 (8%)	0	100	100
1	B	193/199 (97%)	177 (92%)	16 (8%)	0	100	100
2	C	221/235 (94%)	211 (96%)	10 (4%)	0	100	100
2	H	222/235 (94%)	209 (94%)	13 (6%)	0	100	100
3	D	211/217 (97%)	199 (94%)	12 (6%)	0	100	100
3	L	211/217 (97%)	201 (95%)	10 (5%)	0	100	100
All	All	1249/1302 (96%)	1173 (94%)	76 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/172 (96%)	166 (100%)	0	100	100
1	B	168/172 (98%)	168 (100%)	0	100	100
2	C	185/197 (94%)	185 (100%)	0	100	100
2	H	186/197 (94%)	183 (98%)	3 (2%)	55	73
3	D	177/181 (98%)	177 (100%)	0	100	100
3	L	177/181 (98%)	176 (99%)	1 (1%)	78	81
All	All	1059/1100 (96%)	1055 (100%)	4 (0%)	84	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	2	VAL
2	H	64	PHE
2	H	68	VAL
3	L	83	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	501	ASN
2	H	116	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 [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	193/199 (96%)	0.35	5 (2%)	57 36	74, 116, 158, 184	0
1	B	195/199 (97%)	0.22	3 (1%)	72 52	77, 110, 150, 175	0
2	C	223/235 (94%)	0.38	11 (4%)	35 18	69, 119, 181, 229	0
2	H	224/235 (95%)	0.29	4 (1%)	67 46	80, 117, 156, 208	0
3	D	213/217 (98%)	0.36	5 (2%)	61 39	80, 130, 173, 205	0
3	L	213/217 (98%)	0.25	2 (0%)	81 63	85, 114, 147, 171	0
All	All	1261/1302 (96%)	0.31	30 (2%)	59 38	69, 117, 165, 229	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	209	VAL	3.8
3	D	108	LEU	3.5
3	D	118	PRO	3.1
3	D	20	ILE	3.0
2	C	32	TYR	2.9
1	A	368	LEU	2.8
3	D	179	ALA	2.8
2	H	2	VAL	2.8
2	C	51	ILE	2.8
3	L	53	ASN	2.6
2	C	28	THR	2.6
1	A	432	CYS	2.5
1	B	432	CYS	2.5
3	L	49	LEU	2.4
2	C	141	SER	2.4
1	A	401	VAL	2.4
2	C	142	THR	2.3
2	C	218	VAL	2.3
2	C	29	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	144	GLY	2.3
1	B	394	ASN	2.3
1	A	387	LEU	2.2
2	C	75	SER	2.2
2	C	205	TYR	2.1
1	A	402	ILE	2.1
2	H	64	PHE	2.1
1	B	364	ASP	2.1
2	C	178	PRO	2.1
3	D	49	LEU	2.0
2	H	51	ILE	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.