



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:36 AM JST

PDB ID : 7CHF
Title : Crystal structure of the SARS-CoV-2 RBD in complex with BD-604 Fab and BD-368-2 Fab
Authors : Xiao, J.; Zhu, Q.
Deposited on : 2020-07-05
Resolution : 2.67 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

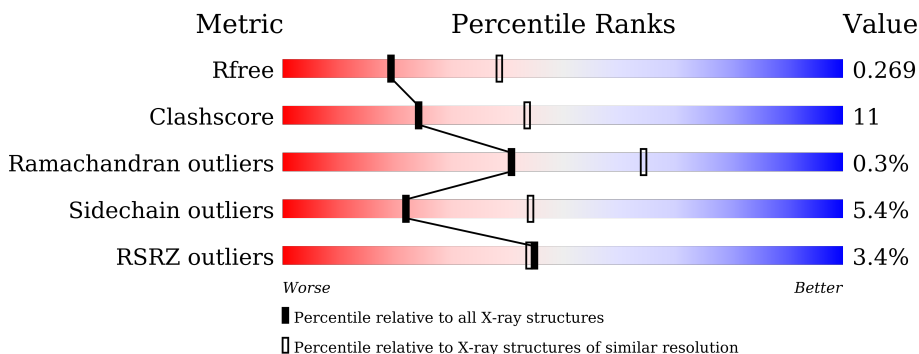
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	H	222	 79% 16% 5%
2	L	214	 81% 16% ..
3	R	223	 8% 60% 23% . 15%
4	A	230	 2% 73% 19% 5% ..
5	B	219	 6% 79% 16% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8008 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 BD-604 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	210	1556	983	259	307	7	0	0	0

- Molecule 2 is a protein called BD-604 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	211	1615	1012	270	329	4	0	0	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	R	189	1498	958	249	283	8	0	0	0

- Molecule 4 is a protein called BD-368-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	226	1680	1058	286	330	6	0	0	0

- Molecule 5 is a protein called BD-368-2 Fab light chain.

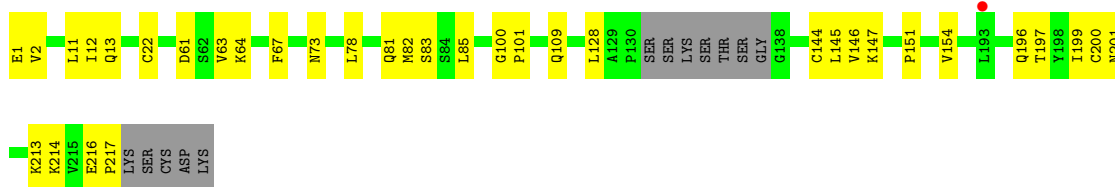
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	216	1659	1038	281	334	6	0	0	0

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.

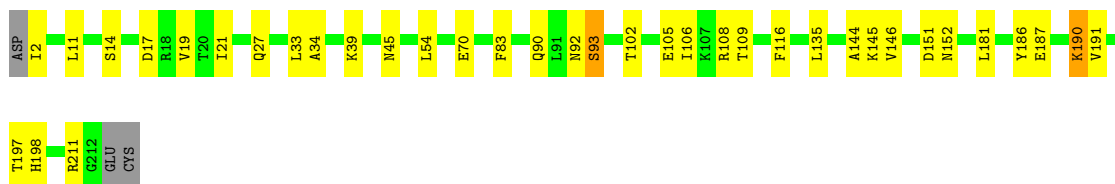
- Molecule 1: BD-604 Fab heavy chain

Chain H: 79% 16% 5%



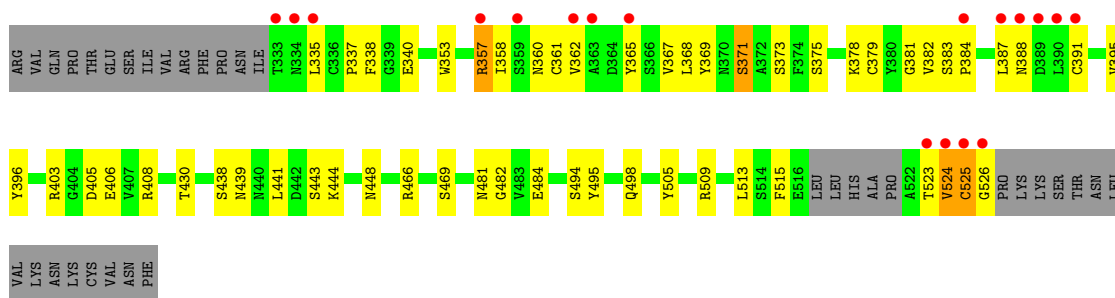
- Molecule 2: BD-604 Fab light chain

Chain L: 81% 16% ..



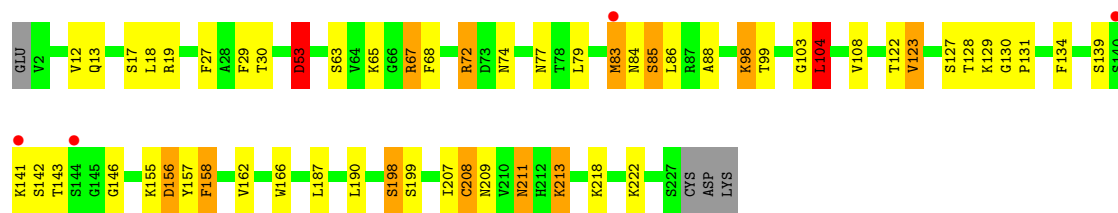
- Molecule 3: Spike protein S1

Chain R: 8% 60% 23% 15%

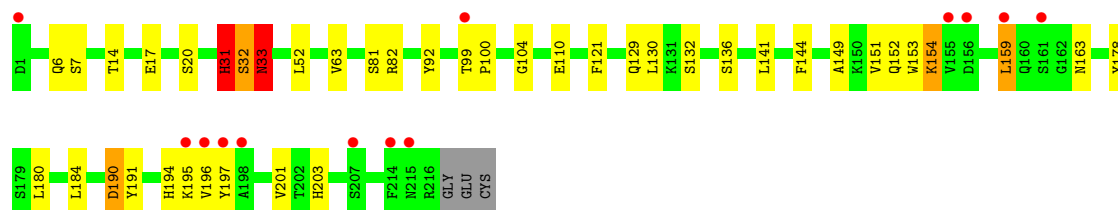
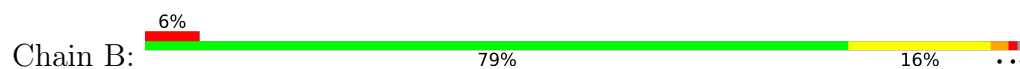


- Molecule 4: BD-368-2 Fab heavy chain

Chain A: 2% 73% 19% 5% ..



● Molecule 5: BD-368-2 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.85Å 116.22Å 115.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.87 – 2.67 50.08 – 2.67	Depositor EDS
% Data completeness (in resolution range)	96.0 (45.87-2.67) 92.6 (50.08-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.220 , 0.270 0.221 , 0.269	Depositor DCC
R_{free} test set	1868 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -h,l,k	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8008	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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	H	0.60	0/1591	0.70	0/2169
2	L	0.63	0/1648	0.73	1/2238 (0.0%)
3	R	0.68	2/1538 (0.1%)	0.84	3/2090 (0.1%)
4	A	0.77	4/1720 (0.2%)	0.89	3/2341 (0.1%)
5	B	0.54	1/1695 (0.1%)	0.72	2/2303 (0.1%)
All	All	0.65	7/8192 (0.1%)	0.78	9/11141 (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
4	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	213	LYS	C-N	8.67	1.50	1.34
3	R	498	GLN	C-N	8.28	1.50	1.34
4	A	130	GLY	C-N	7.99	1.49	1.34
4	A	158	PHE	C-N	7.86	1.49	1.34
5	B	32	SER	CA-CB	-6.56	1.43	1.52
3	R	406	GLU	CD-OE1	-5.45	1.19	1.25
4	A	103	GLY	C-O	-5.32	1.15	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	357	ARG	NE-CZ-NH1	-13.31	113.64	120.30
2	L	151	ASP	CB-CA-C	8.30	126.99	110.40
4	A	53	ASP	CB-CA-C	-7.08	96.25	110.40
5	B	33	ASN	CB-CA-C	-6.94	96.53	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	104	LEU	N-CA-C	-5.58	95.93	111.00
4	A	83	MET	CA-CB-CG	5.34	122.37	113.30
3	R	495	TYR	CB-CA-C	-5.33	99.73	110.40
3	R	357	ARG	NE-CZ-NH2	5.12	122.86	120.30
5	B	32	SER	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	53	ASP	Mainchain

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	H	1556	0	1534	25	0
2	L	1615	0	1573	29	0
3	R	1498	0	1413	47	1
4	A	1680	0	1642	48	2
5	B	1659	0	1618	29	1
All	All	8008	0	7780	173	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (173) 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)
4:A:68:PHE:CE1	4:A:83:MET:HB3	1.50	1.44
4:A:68:PHE:HE1	4:A:83:MET:CB	1.39	1.34
2:L:187:GLU:HA	2:L:211:ARG:HH11	1.06	1.15
3:R:369:TYR:CE2	3:R:384:PRO:HG3	1.87	1.09
4:A:72:ARG:NH1	4:A:74:ASN:OD1	1.90	1.04
2:L:187:GLU:O	2:L:211:ARG:NH1	1.93	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:187:GLU:CA	2:L:211:ARG:HH11	1.77	0.96
3:R:391:CYS:SG	3:R:525:CYS:HB3	2.09	0.92
4:A:68:PHE:CE1	4:A:83:MET:CB	2.29	0.91
2:L:187:GLU:HA	2:L:211:ARG:NH1	1.85	0.90
3:R:382:VAL:HG12	3:R:383:SER:H	1.37	0.89
3:R:391:CYS:SG	3:R:525:CYS:CB	2.62	0.88
1:H:196:GLN:OE1	1:H:197:THR:N	2.07	0.87
4:A:68:PHE:HE1	4:A:83:MET:HB3	0.69	0.86
3:R:391:CYS:HA	3:R:525:CYS:HB3	1.57	0.84
2:L:187:GLU:C	2:L:211:ARG:NH1	2.33	0.82
3:R:335:LEU:HD12	3:R:335:LEU:O	1.80	0.81
2:L:187:GLU:CA	2:L:211:ARG:NH1	2.39	0.81
3:R:337:PRO:HB2	3:R:340:GLU:HG3	1.62	0.81
5:B:141:LEU:HD11	5:B:201:VAL:HG11	1.64	0.79
3:R:369:TYR:HE2	3:R:384:PRO:HG3	1.41	0.78
5:B:99:THR:HG23	5:B:100:PRO:HD3	1.65	0.78
4:A:30:THR:HG22	4:A:74:ASN:HB3	1.67	0.77
3:R:391:CYS:HG	3:R:525:CYS:HG	1.31	0.76
4:A:68:PHE:CD1	4:A:83:MET:HA	2.22	0.75
4:A:72:ARG:HH12	4:A:74:ASN:ND2	1.85	0.75
3:R:371:SER:OG	3:R:373:SER:OG	2.03	0.75
1:H:196:GLN:OE1	1:H:197:THR:O	2.06	0.74
4:A:72:ARG:CZ	4:A:74:ASN:OD1	2.37	0.72
4:A:72:ARG:HH12	4:A:74:ASN:HD21	1.37	0.72
3:R:369:TYR:CD2	3:R:384:PRO:HG3	2.25	0.71
3:R:391:CYS:HG	3:R:525:CYS:CB	2.02	0.71
3:R:391:CYS:CA	3:R:525:CYS:HB3	2.21	0.70
3:R:482:GLY:O	4:A:104:LEU:O	2.10	0.68
5:B:151:VAL:HG12	5:B:201:VAL:HG22	1.76	0.68
4:A:207:ILE:HG12	4:A:222:LYS:HG2	1.76	0.67
3:R:388:ASN:O	3:R:526:GLY:HA3	1.94	0.67
4:A:68:PHE:HD1	4:A:83:MET:HA	1.60	0.65
3:R:369:TYR:CE2	3:R:384:PRO:CG	2.74	0.65
5:B:152:GLN:HG2	5:B:159:LEU:HD11	1.77	0.65
3:R:369:TYR:HD2	3:R:384:PRO:CB	2.09	0.65
3:R:395:VAL:HG22	3:R:515:PHE:HD1	1.62	0.65
2:L:21:ILE:HD12	2:L:102:THR:HG21	1.78	0.64
1:H:61:ASP:HA	1:H:64:LYS:HD3	1.79	0.64
3:R:369:TYR:CD2	3:R:384:PRO:CB	2.79	0.64
3:R:369:TYR:CD2	3:R:384:PRO:CG	2.80	0.64
3:R:361:CYS:O	3:R:524:VAL:HA	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:ILE:HD11	2:L:27:GLN:CB	2.29	0.63
4:A:72:ARG:HH12	4:A:74:ASN:CG	2.01	0.63
4:A:157:TYR:CE1	4:A:162:VAL:HG23	2.33	0.62
4:A:18:LEU:HD12	4:A:19:ARG:H	1.65	0.62
1:H:128:LEU:HD11	1:H:145:LEU:HB2	1.84	0.60
5:B:14:THR:HB	5:B:17:GLU:HG3	1.83	0.60
3:R:381:GLY:HA3	3:R:430:THR:HG23	1.83	0.60
4:A:68:PHE:HE1	4:A:83:MET:HB2	1.58	0.59
4:A:72:ARG:NH1	4:A:74:ASN:CG	2.55	0.59
3:R:360:ASN:H	3:R:523:THR:HB	1.68	0.58
4:A:72:ARG:HB3	4:A:79:LEU:HD12	1.84	0.58
1:H:1:GLU:HG3	1:H:2:VAL:HG23	1.85	0.58
3:R:357:ARG:HG3	3:R:396:TYR:CE1	2.40	0.57
1:H:199:ILE:HD13	1:H:214:LYS:N	2.20	0.57
1:H:216:GLU:HG2	1:H:217:PRO:HD2	1.87	0.56
2:L:144:ALA:HB2	2:L:198:HIS:HD2	1.70	0.56
1:H:199:ILE:HD13	1:H:213:LYS:C	2.25	0.56
5:B:163:ASN:HB2	5:B:184:LEU:HD12	1.88	0.56
5:B:52:LEU:HA	5:B:63:VAL:HG21	1.88	0.56
5:B:153:TRP:CD1	5:B:184:LEU:HD13	2.40	0.56
3:R:338:PHE:HE1	3:R:358:ILE:HD13	1.71	0.56
3:R:395:VAL:HG22	3:R:515:PHE:CD1	2.40	0.56
3:R:365:TYR:HB2	3:R:388:ASN:HB3	1.88	0.55
4:A:157:TYR:CE1	4:A:162:VAL:CG2	2.89	0.55
2:L:2:ILE:HD11	2:L:27:GLN:HB2	1.90	0.54
1:H:146:VAL:HG11	1:H:154:VAL:HG11	1.90	0.54
3:R:438:SER:HB3	3:R:509:ARG:HG3	1.90	0.54
5:B:144:PHE:HZ	5:B:180:LEU:HD23	1.72	0.54
2:L:2:ILE:HD11	2:L:27:GLN:HB3	1.89	0.54
2:L:181:LEU:CD1	2:L:186:TYR:HB2	2.38	0.54
5:B:32:SER:O	5:B:32:SER:OG	2.25	0.53
5:B:6:GLN:HE22	5:B:92:TYR:HA	1.73	0.53
4:A:68:PHE:CE1	4:A:83:MET:CA	2.92	0.53
3:R:382:VAL:HG12	3:R:383:SER:N	2.16	0.52
3:R:403:ARG:HG2	3:R:505:TYR:HA	1.91	0.52
3:R:338:PHE:CD2	3:R:368:LEU:HD11	2.45	0.52
4:A:128:THR:HA	4:A:158:PHE:O	2.09	0.52
3:R:391:CYS:CB	3:R:525:CYS:HB3	2.40	0.51
4:A:67:ARG:O	4:A:84:ASN:ND2	2.43	0.51
2:L:181:LEU:HD13	2:L:186:TYR:HB2	1.91	0.51
1:H:109:GLN:OE1	1:H:109:GLN:N	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:144:PHE:CZ	5:B:180:LEU:HD23	2.45	0.51
4:A:211:ASN:HB2	4:A:218:LYS:NZ	2.26	0.51
2:L:14:SER:N	2:L:17:ASP:OD2	2.39	0.51
4:A:139:SER:HB3	5:B:121:PHE:HD2	1.75	0.51
3:R:382:VAL:CG1	3:R:383:SER:H	2.18	0.51
3:R:387:LEU:HD21	3:R:515:PHE:CE2	2.46	0.50
1:H:214:LYS:NZ	1:H:216:GLU:HB2	2.27	0.50
4:A:131:PRO:HB3	4:A:157:TYR:HB3	1.92	0.50
2:L:2:ILE:CD1	2:L:27:GLN:HB2	2.42	0.50
2:L:145:LYS:HD2	2:L:146:VAL:H	1.77	0.50
1:H:13:GLN:H	1:H:13:GLN:CD	2.15	0.50
5:B:191:TYR:O	5:B:197:TYR:OH	2.30	0.50
5:B:195:LYS:HG3	5:B:196:VAL:N	2.26	0.49
2:L:108:ARG:HG2	2:L:109:THR:N	2.27	0.49
2:L:190:LYS:HG3	2:L:191:VAL:HG23	1.94	0.49
2:L:145:LYS:HD2	2:L:146:VAL:N	2.28	0.49
1:H:199:ILE:HD11	1:H:214:LYS:HB2	1.93	0.49
5:B:141:LEU:HB2	5:B:180:LEU:HG	1.94	0.49
3:R:369:TYR:O	3:R:369:TYR:CD1	2.66	0.48
5:B:163:ASN:HB2	5:B:184:LEU:CD1	2.44	0.48
1:H:63:VAL:HG13	1:H:67:PHE:CG	2.49	0.48
4:A:88:ALA:HA	4:A:123:VAL:HG12	1.95	0.47
3:R:369:TYR:O	3:R:369:TYR:HD1	1.96	0.47
3:R:441:LEU:HD12	3:R:441:LEU:H	1.79	0.47
4:A:127:SER:O	4:A:158:PHE:HD1	1.97	0.47
2:L:105:GLU:HG2	2:L:106:ILE:N	2.30	0.46
3:R:358:ILE:HD12	3:R:395:VAL:HG12	1.98	0.46
3:R:369:TYR:HD2	3:R:384:PRO:HB3	1.79	0.46
1:H:11:LEU:HD22	1:H:151:PRO:HD3	1.98	0.46
4:A:166:TRP:CZ3	4:A:208:CYS:HB3	2.51	0.46
1:H:12:ILE:HG21	1:H:85:LEU:HD13	1.98	0.45
2:L:116:PHE:HD2	2:L:135:LEU:HD23	1.81	0.45
1:H:101:PRO:HG3	2:L:92:ASN:HD21	1.81	0.45
4:A:146:GLY:C	4:A:198:SER:HB2	2.37	0.45
5:B:31:HIS:ND1	5:B:31:HIS:C	2.70	0.45
5:B:152:GLN:CG	5:B:159:LEU:HD11	2.47	0.45
3:R:353:TRP:O	3:R:466:ARG:HD2	2.17	0.45
4:A:30:THR:HA	4:A:72:ARG:HH22	1.80	0.45
3:R:378:LYS:HD3	3:R:379:CYS:H	1.82	0.45
4:A:68:PHE:CE1	4:A:83:MET:HA	2.51	0.45
4:A:18:LEU:O	4:A:83:MET:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:11:LEU:HD21	2:L:19:VAL:HG13	1.97	0.44
5:B:136:SER:HA	5:B:184:LEU:O	2.17	0.44
2:L:144:ALA:HB1	2:L:197:THR:O	2.17	0.44
5:B:190:ASP:O	5:B:194:HIS:ND1	2.49	0.44
4:A:68:PHE:CE1	4:A:83:MET:HB2	2.41	0.44
5:B:6:GLN:HE21	5:B:104:GLY:HA3	1.83	0.44
1:H:22:CYS:HB3	1:H:78:LEU:HB3	1.99	0.44
1:H:100:GLY:HA3	1:H:101:PRO:HD3	1.85	0.44
4:A:72:ARG:NH1	4:A:74:ASN:ND2	2.60	0.44
1:H:199:ILE:HD13	1:H:214:LYS:CA	2.48	0.43
1:H:63:VAL:HG13	1:H:67:PHE:HB2	2.00	0.43
4:A:72:ARG:NH1	4:A:74:ASN:HD21	2.12	0.43
5:B:110:GLU:OE2	5:B:178:TYR:OH	2.33	0.43
4:A:156:ASP:HB3	4:A:187:LEU:HD12	2.00	0.43
1:H:67:PHE:HA	1:H:81:GLN:O	2.19	0.43
4:A:142:SER:OG	4:A:143:THR:N	2.52	0.43
2:L:54:LEU:HD12	2:L:54:LEU:HA	1.73	0.42
5:B:154:LYS:HB3	5:B:154:LYS:HE2	1.73	0.42
4:A:157:TYR:OH	4:A:190:LEU:HD23	2.19	0.42
4:A:166:TRP:CH2	4:A:208:CYS:HB3	2.53	0.42
1:H:82:MET:HE2	1:H:85:LEU:HD21	2.02	0.42
3:R:387:LEU:HD21	3:R:515:PHE:CZ	2.54	0.42
4:A:134:PHE:CE2	5:B:129:GLN:HG3	2.55	0.42
3:R:444:LYS:HB2	3:R:448:ASN:HB2	2.02	0.42
4:A:85:SER:O	4:A:85:SER:OG	2.29	0.42
1:H:63:VAL:CG1	1:H:67:PHE:HB2	2.50	0.42
4:A:29:PHE:CE2	4:A:77:ASN:HA	2.55	0.42
2:L:90:GLN:CD	2:L:93:SER:HB2	2.40	0.41
3:R:369:TYR:CD2	3:R:384:PRO:HB2	2.55	0.41
4:A:68:PHE:CD1	4:A:83:MET:CA	2.99	0.41
3:R:481:ASN:HB3	5:B:33:ASN:HB2	2.01	0.41
5:B:130:LEU:C	5:B:132:SER:H	2.23	0.41
2:L:33:LEU:HD13	2:L:34:ALA:N	2.36	0.41
4:A:99:THR:HG21	4:A:108:VAL:O	2.21	0.41
5:B:153:TRP:CG	5:B:184:LEU:HD13	2.55	0.41
5:B:149:ALA:HB2	5:B:203:HIS:HD2	1.85	0.41
4:A:86:LEU:HD23	4:A:86:LEU:HA	1.85	0.40
2:L:211:ARG:HE	2:L:211:ARG:HB3	1.65	0.40
3:R:396:TYR:O	3:R:513:LEU:HA	2.21	0.40
3:R:439:ASN:O	3:R:443:SER:HB3	2.21	0.40
4:A:27:PHE:CE2	4:A:98:LYS:HD2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:156:ASP:HB3	4:A:187:LEU:CD1	2.50	0.40
1:H:199:ILE:HG22	1:H:201:ASN:ND2	2.36	0.40
2:L:39:LYS:HE3	2:L:83:PHE:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:84:ASN:OD1	5:B:82:ARG:NH1[4_555]	1.39	0.81
3:R:375:SER:OG	4:A:199:SER:OG[3_645]	2.01	0.19

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	H	206/222 (93%)	199 (97%)	7 (3%)	0	100	100
2	L	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
3	R	185/223 (83%)	171 (92%)	14 (8%)	0	100	100
4	A	224/230 (97%)	201 (90%)	22 (10%)	1 (0%)	34	58
5	B	214/219 (98%)	203 (95%)	9 (4%)	2 (1%)	17	37
All	All	1038/1108 (94%)	973 (94%)	62 (6%)	3 (0%)	41	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	33	ASN
5	B	31	HIS
4	A	156	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	H	175/186 (94%)	170 (97%)	5 (3%)	42	69
2	L	184/187 (98%)	179 (97%)	5 (3%)	44	71
3	R	163/196 (83%)	153 (94%)	10 (6%)	18	38
4	A	184/188 (98%)	163 (89%)	21 (11%)	5	12
5	B	190/192 (99%)	183 (96%)	7 (4%)	34	60
All	All	896/949 (94%)	848 (95%)	48 (5%)	22	44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	73	ASN
1	H	83	SER
1	H	144	CYS
1	H	147	LYS
1	H	200	CYS
2	L	45	ASN
2	L	70	GLU
2	L	93	SER
2	L	152	ASN
2	L	190	LYS
3	R	362	VAL
3	R	367	VAL
3	R	371	SER
3	R	405	ASP
3	R	408	ARG
3	R	469	SER
3	R	484	GLU
3	R	494	SER
3	R	524	VAL
3	R	525	CYS
4	A	12	VAL
4	A	13	GLN
4	A	17	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	53	ASP
4	A	63	SER
4	A	65	LYS
4	A	67	ARG
4	A	72	ARG
4	A	85	SER
4	A	98	LYS
4	A	104	LEU
4	A	122	THR
4	A	123	VAL
4	A	129	LYS
4	A	141	LYS
4	A	155	LYS
4	A	198	SER
4	A	208	CYS
4	A	209	ASN
4	A	211	ASN
4	A	213	LYS
5	B	7	SER
5	B	20	SER
5	B	31	HIS
5	B	81	SER
5	B	154	LYS
5	B	159	LEU
5	B	190	ASP

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

Mol	Chain	Res	Type
2	L	92	ASN
3	R	360	ASN
3	R	498	GLN
4	A	35	ASN
4	A	211	ASN
4	A	216	ASN
5	B	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
1	H	210/222 (94%)	-0.04	1 (0%) 91 92	19, 40, 59, 74	0
2	L	211/214 (98%)	-0.12	0 100 100	15, 33, 54, 67	0
3	R	189/223 (84%)	0.41	18 (9%) 8 6	16, 36, 89, 113	0
4	A	226/230 (98%)	0.09	4 (1%) 68 69	20, 42, 73, 86	0
5	B	216/219 (98%)	0.27	13 (6%) 21 20	15, 39, 72, 77	0
All	All	1052/1108 (94%)	0.11	36 (3%) 45 44	15, 38, 74, 113	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	333	THR	8.5
3	R	387	LEU	4.5
5	B	196	VAL	4.5
3	R	526	GLY	4.4
3	R	365	TYR	4.3
4	A	140	SER	4.3
3	R	525	CYS	3.9
3	R	335	LEU	3.4
3	R	389	ASP	3.4
5	B	197	TYR	3.3
4	A	144	SER	3.3
5	B	195	LYS	3.3
4	A	83	MET	3.2
3	R	357	ARG	3.1
3	R	524	VAL	3.0
5	B	214	PHE	2.8
4	A	141	LYS	2.8
5	B	198	ALA	2.7
5	B	155	VAL	2.6
3	R	359	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	R	523	THR	2.6
3	R	391	CYS	2.6
3	R	388	ASN	2.5
5	B	156	ASP	2.5
3	R	362	VAL	2.5
5	B	159	LEU	2.5
3	R	334	ASN	2.5
5	B	99	THR	2.5
5	B	207	SER	2.5
5	B	215	ASN	2.5
1	H	193	LEU	2.4
3	R	390	LEU	2.3
3	R	363	ALA	2.2
3	R	384	PRO	2.2
5	B	161	SER	2.2
5	B	1	ASP	2.2

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 monosaccharides 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.