Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 09:35 PM EDT

PDB ID	:	7LKA
Title	:	Crystal structure of SARS-CoV-2 RBD-targeting antibody COV107-23
Authors	:	Yuan, M.; Zhu, X.; Wilson, I.A.; Wu, N.C.
Deposited on	:	2021-02-02
Resolution	:	1.98 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 (i) 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 (1)) were used in the production of this report:

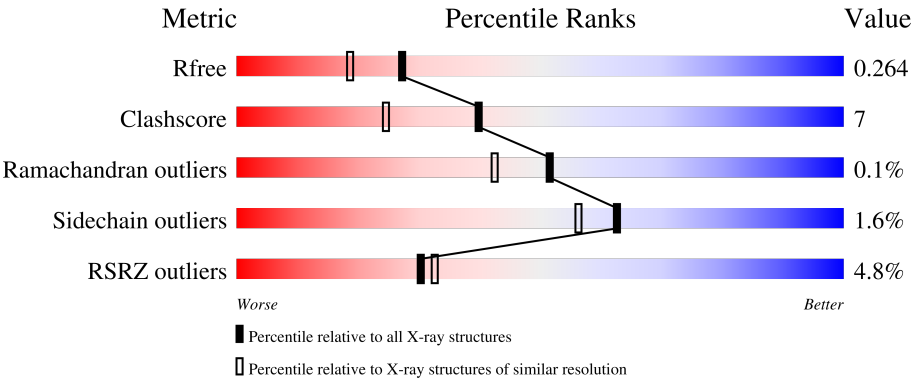
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	220	7% 80% 16% ·
1	C	220	3% 91% 9%
1	E	220	3% 86% 12% ·
1	H	220	3% 82% 16% ·
2	B	216	4% 81% 18% ·

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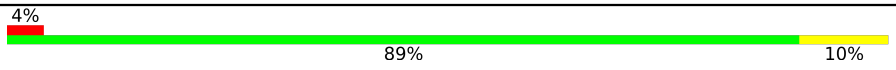
Mol	Chain	Length	Quality of chain
2	D	216	
2	F	216	
2	L	216	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14051 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.

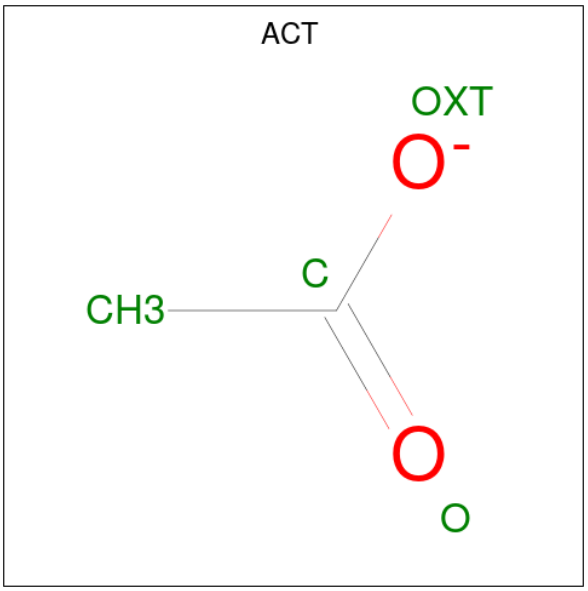
- Molecule 1 is a protein called COV107-23 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	0	0
			1599	1009	267	317	6			
1	A	211	Total	C	N	O	S	0	0	0
			1565	990	261	308	6			
1	C	219	Total	C	N	O	S	0	0	0
			1620	1021	271	321	7			
1	E	217	Total	C	N	O	S	0	0	0
			1608	1015	269	318	6			

- Molecule 2 is a protein called COV107-23 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1626	1023	270	329	4			
2	B	213	Total	C	N	O	S	0	0	0
			1626	1023	270	329	4			
2	D	215	Total	C	N	O	S	0	0	0
			1641	1031	272	333	5			
2	F	214	Total	C	N	O	S	0	0	0
			1633	1027	271	330	5			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

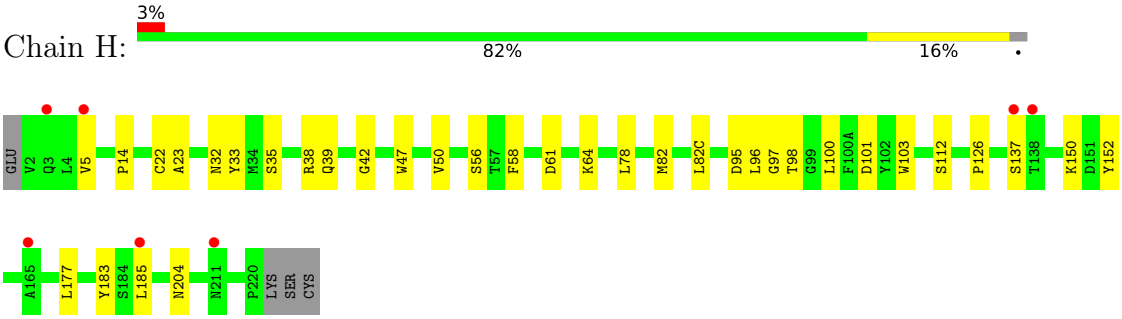
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	138	Total O 138 138	0	0
4	L	135	Total O 135 135	0	0
4	A	133	Total O 133 133	0	0
4	B	110	Total O 110 110	0	0
4	C	207	Total O 207 207	0	0
4	D	162	Total O 162 162	0	0
4	E	133	Total O 133 133	0	0
4	F	111	Total O 111 111	0	0

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.

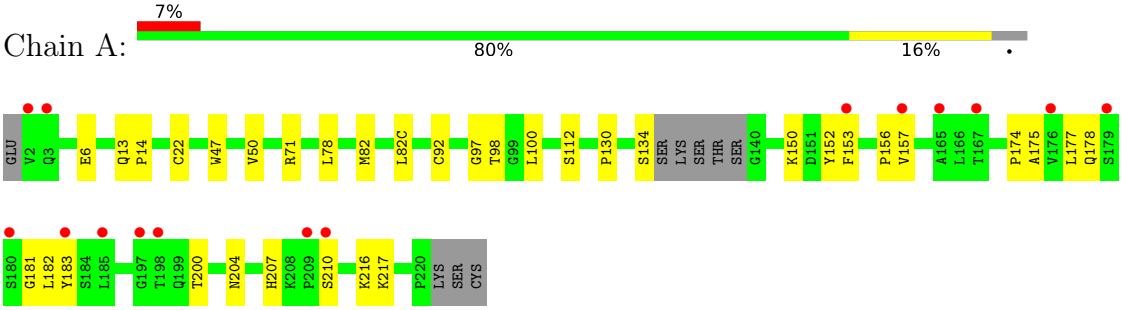
• Molecule 1: COV107-23 heavy chain

Chain H:



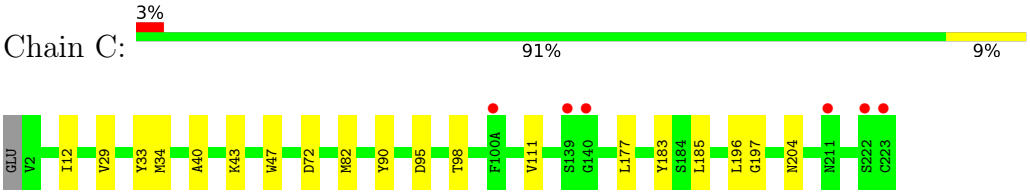
• Molecule 1: COV107-23 heavy chain

Chain A:



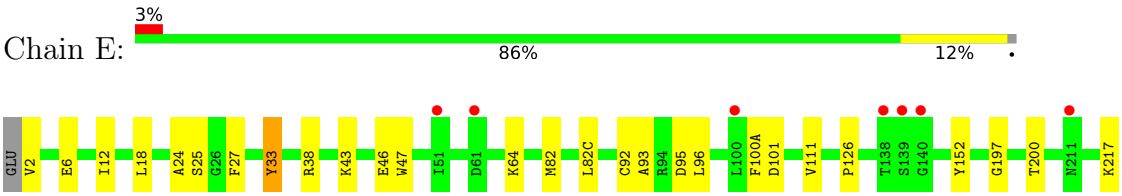
• Molecule 1: COV107-23 heavy chain

Chain C:



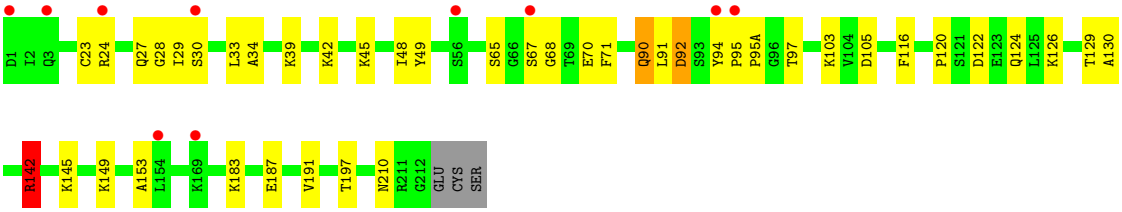
• Molecule 1: COV107-23 heavy chain

Chain E:



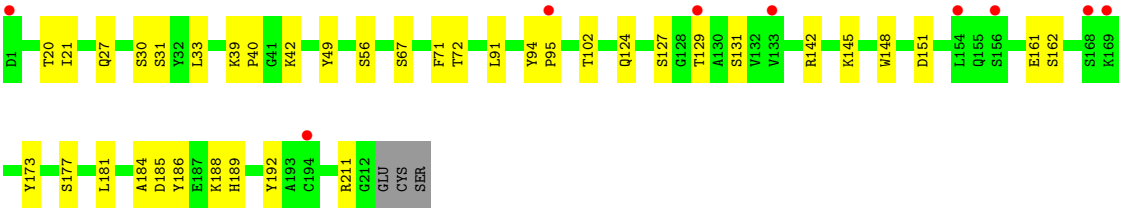
• Molecule 2: COV107-23 light chain

Chain L:



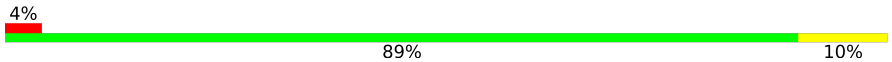
• Molecule 2: COV107-23 light chain

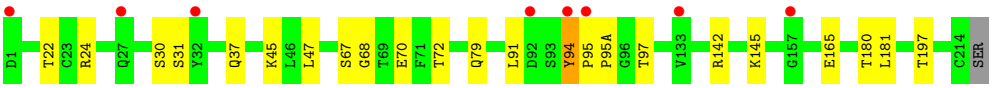
Chain B:



• Molecule 2: COV107-23 light chain

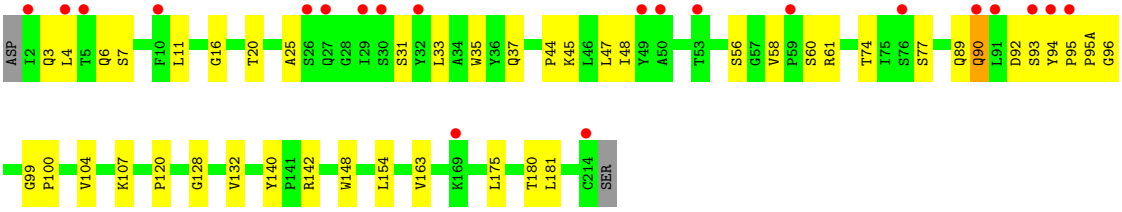
Chain D:





• Molecule 2: COV107-23 light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.42Å 74.80Å 172.68Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	31.00 – 1.98 31.01 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.9 (31.00-1.98) 93.9 (31.01-1.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.215 , 0.264 0.215 , 0.264	Depositor DCC
R_{free} test set	6632 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14051	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0916e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.56	0/1601	0.71	0/2181
1	C	0.58	0/1657	0.70	1/2256 (0.0%)
1	E	0.52	0/1645	0.66	0/2240
1	H	0.51	0/1636	0.68	1/2229 (0.0%)
2	B	0.52	0/1663	0.68	0/2261
2	D	0.55	0/1678	0.70	0/2281
2	F	0.50	0/1670	0.63	0/2270
2	L	0.53	0/1663	0.68	1/2261 (0.0%)
All	All	0.53	0/13213	0.68	3/17979 (0.0%)

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
1	C	0	1
1	E	0	1
1	H	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	L	0	2
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	196	LEU	C-N-CA	-5.96	109.79	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	185	LEU	CA-CB-CG	5.75	128.51	115.30
2	L	142	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	94	TYR	Peptide
1	C	197	GLY	Peptide
2	D	94	TYR	Peptide
1	E	197	GLY	Peptide
2	F	94	TYR	Peptide
1	H	32	ASN	Peptide
2	L	29	ILE	Peptide
2	L	94	TYR	Peptide

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	1565	0	1532	31	0
1	C	1620	0	1590	13	0
1	E	1608	0	1581	23	0
1	H	1599	0	1568	22	0
2	B	1626	0	1587	42	0
2	D	1641	0	1597	16	0
2	F	1633	0	1591	28	0
2	L	1626	0	1587	30	0
3	C	4	0	3	0	0
4	A	133	0	0	12	0
4	B	110	0	0	5	0
4	C	207	0	0	2	1
4	D	162	0	0	4	0
4	E	133	0	0	6	0
4	F	111	0	0	6	0
4	H	138	0	0	5	1
4	L	135	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14051	0	12636	186	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 7.

All (186) 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:B:124:GLN:HG2	2:B:129:THR:OG1	1.64	0.97
1:E:64:LYS:NZ	4:E:301:HOH:O	1.96	0.97
2:B:124:GLN:HE22	2:B:131:SER:N	1.68	0.91
2:L:45:LYS:NZ	4:L:301:HOH:O	2.08	0.86
2:F:3:GLN:NE2	4:F:302:HOH:O	2.09	0.84
2:F:6:GLN:HE21	2:F:99:GLY:HA3	1.42	0.83
2:L:24:ARG:HG2	2:L:70:GLU:HG2	1.62	0.82
1:E:12:ILE:HD11	1:E:18:LEU:HD22	1.62	0.82
2:F:61:ARG:NH1	4:F:303:HOH:O	2.13	0.81
2:B:185:ASP:HA	2:B:188:LYS:HE2	1.62	0.80
2:B:124:GLN:HE22	2:B:131:SER:H	1.25	0.79
2:B:27:GLN:OE1	4:B:301:HOH:O	1.99	0.79
1:H:64:LYS:NZ	4:H:301:HOH:O	2.16	0.78
1:A:152:TYR:O	4:A:301:HOH:O	2.01	0.77
2:B:124:GLN:NE2	2:B:131:SER:H	1.83	0.77
2:F:47:LEU:O	4:F:301:HOH:O	2.03	0.76
2:B:42:LYS:NZ	4:B:304:HOH:O	2.17	0.76
2:B:124:GLN:OE1	4:B:302:HOH:O	2.02	0.75
1:E:2:VAL:N	4:E:304:HOH:O	2.20	0.72
2:B:181:LEU:O	4:B:303:HOH:O	2.09	0.70
1:E:95:ASP:O	4:E:302:HOH:O	2.09	0.68
2:D:165:GLU:OE2	4:D:301:HOH:O	2.11	0.67
2:B:124:GLN:HG2	2:B:129:THR:HG1	1.60	0.67
1:A:177:LEU:HB2	1:A:183:TYR:CE1	2.30	0.66
2:B:161:GLU:HG2	2:B:177:SER:HB2	1.78	0.66
2:D:24:ARG:HG2	2:D:70:GLU:HG2	1.76	0.66
1:A:134:SER:O	4:A:302:HOH:O	2.14	0.66
1:A:177:LEU:HD11	1:A:181:GLY:HA2	1.77	0.66
2:B:184:ALA:O	2:B:188:LYS:HG3	1.97	0.65
2:F:6:GLN:HG3	2:F:100:PRO:HD2	1.80	0.64
2:F:95:PRO:O	2:F:96:GLY:N	2.31	0.64
2:L:142:ARG:HB2	2:L:142:ARG:NH1	2.13	0.63
1:C:72:ASP:OD2	4:C:401:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:VAL:HG23	1:H:23:ALA:HB3	1.80	0.61
2:B:124:GLN:NE2	2:B:131:SER:N	2.40	0.61
2:D:30:SER:HA	2:D:68:GLY:H	1.64	0.61
1:H:38:ARG:O	4:H:302:HOH:O	2.16	0.60
2:F:128:GLY:O	4:F:304:HOH:O	2.16	0.60
2:B:151:ASP:OD2	2:B:189:HIS:HB3	2.03	0.59
2:L:183:LYS:O	2:L:187:GLU:HG2	2.02	0.59
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.84	0.58
2:F:180:THR:O	2:F:181:LEU:HD23	2.02	0.58
1:A:200:THR:CG2	1:A:217:LYS:HE3	2.34	0.58
2:D:79:GLN:NE2	4:D:305:HOH:O	2.31	0.58
1:H:97:GLY:O	1:H:98:THR:HG22	2.04	0.57
1:H:50:VAL:HG12	2:L:95:PRO:HG3	1.87	0.57
1:A:97:GLY:O	1:A:98:THR:HG22	2.05	0.57
2:L:124:GLN:HG2	2:L:129:THR:O	2.05	0.56
1:H:150:LYS:NZ	4:H:312:HOH:O	2.37	0.56
2:F:20:THR:HG22	2:F:74:THR:HG23	1.87	0.56
1:C:47:TRP:HB3	2:D:95:PRO:O	2.06	0.56
2:L:30:SER:HA	2:L:68:GLY:H	1.71	0.56
1:C:29:VAL:HG13	1:C:34:MET:HG3	1.88	0.56
1:H:33:TYR:HB2	1:H:95:ASP:O	2.07	0.55
1:E:25:SER:OG	4:E:303:HOH:O	2.18	0.55
1:A:183:TYR:N	4:A:301:HOH:O	2.31	0.54
2:L:23:CYS:O	2:L:24:ARG:HG3	2.08	0.54
2:B:186:TYR:CE2	2:B:211:ARG:HG3	2.43	0.54
2:L:142:ARG:HB2	2:L:142:ARG:HH11	1.72	0.53
1:A:174:PRO:HD2	2:B:162:SER:OG	2.09	0.53
2:B:145:LYS:HG2	4:B:338:HOH:O	2.08	0.53
1:E:33:TYR:N	1:E:33:TYR:HD2	2.07	0.53
2:F:33:LEU:HD12	2:F:89:GLN:O	2.09	0.52
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.91	0.52
4:A:411:HOH:O	2:B:129:THR:HG21	2.08	0.52
1:A:130:PRO:HD3	1:A:216:LYS:HE3	1.90	0.52
2:B:20:THR:HG23	2:B:72:THR:HG23	1.91	0.52
1:A:200:THR:HG23	1:A:217:LYS:CE	2.39	0.52
1:E:43:LYS:HB3	4:E:351:HOH:O	2.08	0.52
2:B:21:ILE:HG21	2:B:102:THR:HG21	1.92	0.52
2:B:181:LEU:HB3	2:B:185:ASP:HB2	1.91	0.52
1:A:200:THR:HG23	1:A:217:LYS:HE3	1.90	0.52
2:B:181:LEU:HD11	2:B:192:TYR:HE1	1.75	0.52
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:TYR:N	1:E:33:TYR:CD2	2.77	0.51
1:E:2:VAL:N	4:E:310:HOH:O	2.42	0.51
2:B:124:GLN:O	2:B:127:SER:HB3	2.10	0.51
1:E:47:TRP:CD2	2:F:95:PRO:HA	2.46	0.51
2:F:90:GLN:OE1	2:F:92:ASP:HB3	2.11	0.51
1:H:82:MET:HE2	1:H:82(C):LEU:HD21	1.92	0.51
2:F:163:VAL:HG22	2:F:175:LEU:HD12	1.93	0.50
2:B:186:TYR:O	2:B:211:ARG:HD2	2.12	0.50
1:H:98:THR:HG23	2:L:91:LEU:HB3	1.94	0.49
2:B:39:LYS:HB2	2:B:42:LYS:HD3	1.93	0.49
2:L:67:SER:HA	2:L:71:PHE:CE2	2.46	0.49
2:F:60:SER:N	4:F:313:HOH:O	2.46	0.49
1:A:150:LYS:HD3	4:A:411:HOH:O	2.11	0.49
1:E:12:ILE:O	1:E:111:VAL:HA	2.13	0.49
2:F:16:GLY:HA2	2:F:77:SER:OG	2.13	0.49
1:A:50:VAL:HG12	2:B:95:PRO:HG3	1.93	0.49
2:L:142:ARG:HH11	2:L:142:ARG:CB	2.26	0.48
2:D:95:PRO:N	2:D:95(A):PRO:HD2	2.29	0.48
1:H:39:GLN:HA	4:H:302:HOH:O	2.13	0.48
1:E:24:ALA:HB1	1:E:27:PHE:CE1	2.49	0.48
2:B:185:ASP:CA	2:B:188:LYS:HE2	2.40	0.48
1:C:177:LEU:HD13	1:C:183:TYR:CZ	2.49	0.48
2:F:95:PRO:O	2:F:95(A):PRO:C	2.52	0.48
2:F:148:TRP:O	2:F:154:LEU:HD12	2.13	0.48
1:E:47:TRP:HB3	2:F:95:PRO:O	2.14	0.48
1:A:47:TRP:CE3	2:B:95:PRO:HA	2.49	0.48
1:C:12:ILE:O	1:C:111:VAL:HA	2.14	0.48
1:C:40:ALA:HB3	1:C:43:LYS:HD2	1.96	0.47
1:A:175:ALA:N	4:A:303:HOH:O	2.28	0.47
1:H:177:LEU:HD13	1:H:183:TYR:CZ	2.49	0.47
2:L:30:SER:O	2:L:67:SER:HB2	2.15	0.47
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.95	0.47
2:L:34:ALA:HA	2:L:48:ILE:O	2.15	0.47
1:E:96:LEU:HD11	1:E:101:ASP:CG	2.34	0.47
2:D:97:THR:HG23	4:D:447:HOH:O	2.15	0.47
2:D:22:THR:HG22	2:D:72:THR:HG22	1.96	0.47
2:B:124:GLN:HE22	2:B:131:SER:CB	2.28	0.47
1:H:98:THR:HA	2:L:92:ASP:O	2.15	0.47
1:C:43:LYS:HB3	4:C:456:HOH:O	2.15	0.46
2:L:90:GLN:O	2:L:90:GLN:HG3	2.14	0.46
1:C:82:MET:HE3	1:C:90:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:ARG:CZ	2:F:163:VAL:HG21	2.45	0.46
1:H:103:TRP:HB2	4:L:301:HOH:O	2.15	0.46
1:E:6:GLU:HG2	1:E:92:CYS:SG	2.55	0.46
1:A:153:PHE:HD1	4:A:301:HOH:O	1.99	0.46
2:B:30:SER:O	2:B:67:SER:HB2	2.16	0.46
2:B:40:PRO:O	2:B:42:LYS:HD2	2.16	0.45
2:B:21:ILE:HD12	2:B:102:THR:HB	1.97	0.45
1:A:82:MET:HE2	1:A:82(C):LEU:HD21	1.98	0.45
2:B:148:TRP:HE1	2:B:177:SER:HG	1.62	0.45
2:B:124:GLN:HE22	2:B:131:SER:HB2	1.81	0.45
1:H:42:GLY:N	4:H:311:HOH:O	2.36	0.45
2:B:142:ARG:HB3	2:B:173:TYR:CE2	2.52	0.44
1:A:13:GLN:HG3	1:A:14:PRO:HD2	1.99	0.44
2:F:107:LYS:HA	2:F:140:TYR:OH	2.16	0.44
1:H:22:CYS:HB3	1:H:78:LEU:HB3	1.99	0.44
2:L:191:VAL:HG22	2:L:210:ASN:OD1	2.18	0.44
1:E:82:MET:HE2	1:E:82(C):LEU:HD21	1.99	0.44
1:H:100:LEU:HD11	2:L:49:TYR:HB3	2.00	0.44
2:D:45:LYS:NZ	4:D:320:HOH:O	2.50	0.44
2:D:94:TYR:HA	2:D:95:PRO:HD3	1.83	0.44
1:A:14:PRO:HD3	1:A:112:SER:C	2.38	0.44
2:L:27:GLN:HG3	2:L:28:GLY:N	2.33	0.43
2:L:103:LYS:NZ	4:L:308:HOH:O	2.48	0.43
1:E:38:ARG:NH1	1:E:46:GLU:OE2	2.49	0.43
2:B:181:LEU:CD1	2:B:192:TYR:HE1	2.32	0.43
2:F:44:PRO:O	2:F:45:LYS:HD3	2.18	0.43
1:A:71:ARG:NH2	4:A:307:HOH:O	2.34	0.43
2:L:90:GLN:HG2	2:L:97:THR:HB	2.00	0.43
1:E:96:LEU:HD11	1:E:101:ASP:OD2	2.17	0.43
2:F:47:LEU:O	2:F:48:ILE:HD13	2.18	0.43
2:L:71:PHE:HB3	4:L:371:HOH:O	2.19	0.43
1:A:47:TRP:CE3	2:B:95:PRO:O	2.71	0.43
1:A:182:LEU:HA	4:A:301:HOH:O	2.18	0.43
1:E:126:PRO:HB3	1:E:152:TYR:HB3	2.01	0.43
1:A:22:CYS:HB3	1:A:78:LEU:HB3	2.01	0.42
4:A:352:HOH:O	2:B:95:PRO:HD2	2.19	0.42
2:L:122:ASP:O	2:L:126:LYS:HG3	2.18	0.42
1:H:47:TRP:CE3	2:L:95:PRO:HA	2.54	0.42
2:F:58:VAL:HG21	4:F:301:HOH:O	2.19	0.42
1:A:100:LEU:HD11	2:B:49:TYR:HB3	2.00	0.42
1:A:177:LEU:HD12	1:A:178:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:SER:HA	2:B:71:PHE:CE2	2.53	0.42
1:C:47:TRP:CD2	2:D:95:PRO:HA	2.55	0.42
1:A:200:THR:HG21	1:A:217:LYS:HE3	1.99	0.42
2:D:180:THR:O	2:D:181:LEU:HD23	2.18	0.42
2:F:35:TRP:HB2	2:F:48:ILE:HB	2.00	0.42
2:B:186:TYR:HA	2:B:192:TYR:OH	2.19	0.41
1:C:33:TYR:HB2	1:C:95:ASP:O	2.19	0.41
1:A:6:GLU:HG2	1:A:92:CYS:SG	2.60	0.41
1:C:185:LEU:C	1:C:185:LEU:HD12	2.41	0.41
1:E:2:VAL:HA	1:E:25:SER:O	2.21	0.41
1:H:137:SER:HA	2:L:116:PHE:HD1	1.84	0.41
2:L:145:LYS:HB3	2:L:197:THR:HB	2.02	0.41
1:E:200:THR:HG23	1:E:217:LYS:HE3	2.03	0.41
1:H:58:PHE:O	2:L:95:PRO:HG2	2.20	0.41
2:L:120:PRO:HG3	2:L:130:ALA:HB1	2.02	0.41
1:H:14:PRO:HD3	1:H:112:SER:C	2.41	0.41
2:L:149:LYS:HA	2:L:153:ALA:O	2.21	0.41
1:A:207:HIS:O	1:A:210:SER:HB2	2.21	0.41
2:D:145:LYS:HB3	2:D:197:THR:HB	2.03	0.41
1:E:93:ALA:HB1	1:E:100(A):PHE:HB3	2.02	0.41
1:H:96:LEU:HD11	1:H:101:ASP:OD2	2.21	0.40
2:L:39:LYS:HB2	2:L:42:LYS:HD3	2.04	0.40
1:A:157:VAL:HG22	4:A:311:HOH:O	2.21	0.40
1:C:98:THR:HG22	2:D:91:LEU:C	2.41	0.40
2:F:4:LEU:HD12	2:F:25:ALA:HA	2.02	0.40
1:A:98:THR:HG23	2:B:91:LEU:HB3	2.03	0.40
1:A:156:PRO:HG2	4:A:361:HOH:O	2.20	0.40
1:C:47:TRP:O	2:D:95:PRO:O	2.40	0.40
2:F:11:LEU:O	2:F:104:VAL:HA	2.22	0.40
1:E:18:LEU:HD12	1:E:18:LEU:HA	1.91	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:H:310:HOH:O	4:H:310:HOH:O[2_656]	2.03	0.17
4:C:481:HOH:O	4:C:583:HOH:O[2_555]	2.14	0.06

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	207/220 (94%)	200 (97%)	7 (3%)	0	100	100
1	C	217/220 (99%)	211 (97%)	6 (3%)	0	100	100
1	E	215/220 (98%)	206 (96%)	9 (4%)	0	100	100
1	H	214/220 (97%)	209 (98%)	5 (2%)	0	100	100
2	B	211/216 (98%)	200 (95%)	11 (5%)	0	100	100
2	D	213/216 (99%)	201 (94%)	12 (6%)	0	100	100
2	F	212/216 (98%)	199 (94%)	13 (6%)	0	100	100
2	L	211/216 (98%)	200 (95%)	10 (5%)	1 (0%)	29	16
All	All	1700/1744 (98%)	1626 (96%)	73 (4%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95(A)	PRO

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	175/184 (95%)	174 (99%)	1 (1%)	86	85
1	C	183/184 (100%)	182 (100%)	1 (0%)	88	87
1	E	181/184 (98%)	180 (99%)	1 (1%)	86	85
1	H	180/184 (98%)	176 (98%)	4 (2%)	52	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	185/188 (98%)	182 (98%)	3 (2%)	62	56
2	D	187/188 (100%)	184 (98%)	3 (2%)	62	56
2	F	186/188 (99%)	181 (97%)	5 (3%)	44	35
2	L	185/188 (98%)	179 (97%)	6 (3%)	39	28
All	All	1462/1488 (98%)	1438 (98%)	24 (2%)	62	56

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	SER
1	H	56	SER
1	H	61	ASP
1	H	204	ASN
2	L	33	LEU
2	L	65	SER
2	L	90	GLN
2	L	92	ASP
2	L	105	ASP
2	L	142	ARG
1	A	204	ASN
2	B	31	SER
2	B	33	LEU
2	B	56	SER
1	C	204	ASN
2	D	31	SER
2	D	67	SER
2	D	142	ARG
1	E	33	TYR
2	F	7	SER
2	F	31	SER
2	F	56	SER
2	F	90	GLN
2	F	93	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	211	ASN
1	A	199	GLN
2	B	3	GLN

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Mol	Chain	Res	Type
2	B	124	GLN
2	F	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACT	C	301	-	3,3,3	2.37	1 (33%)	3,3,3	1.19	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	ACT	CH3-C	3.61	1.64	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	211/220 (95%)	0.36	15 (7%)	16	17	20, 37, 55, 67	0
1	C	219/220 (99%)	0.09	6 (2%)	54	56	19, 26, 45, 93	0
1	E	217/220 (98%)	0.27	7 (3%)	47	50	21, 35, 57, 82	0
1	H	216/220 (98%)	0.16	7 (3%)	47	50	21, 34, 51, 62	0
2	B	213/216 (98%)	0.32	9 (4%)	36	38	23, 40, 62, 82	0
2	D	215/216 (99%)	0.12	8 (3%)	41	44	20, 34, 54, 89	0
2	F	214/216 (99%)	0.63	21 (9%)	7	8	22, 44, 77, 91	0
2	L	213/216 (98%)	0.20	10 (4%)	31	33	20, 37, 56, 87	0
All	All	1718/1744 (98%)	0.27	83 (4%)	30	32	19, 35, 63, 93	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	CYS	6.8
2	F	93	SER	5.8
2	D	1	ASP	5.7
2	F	30	SER	5.4
2	B	1	ASP	4.6
2	F	94	TYR	4.6
1	A	209	PRO	4.3
2	F	95	PRO	4.1
1	H	137	SER	4.0
2	D	95	PRO	3.8
1	C	222	SER	3.8
2	L	95	PRO	3.6
2	F	27	GLN	3.6
2	L	1	ASP	3.6
2	D	94	TYR	3.5
2	F	91	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	3.3
2	F	29	ILE	3.3
1	C	211	ASN	3.3
2	B	168	SER	3.3
1	E	139	SER	3.3
2	B	129	THR	3.3
2	F	2	ILE	3.2
2	B	156	SER	3.2
2	D	27	GLN	3.1
1	A	185	LEU	3.1
1	C	140	GLY	3.1
2	F	10	PHE	3.1
1	E	211	ASN	3.0
2	F	32	TYR	3.0
2	L	24	ARG	3.0
1	A	153	PHE	2.9
2	L	56	SER	2.9
2	D	157	GLY	2.8
2	F	26	SER	2.8
1	A	3	GLN	2.7
1	H	3	GLN	2.6
2	B	154	LEU	2.6
2	F	214	CYS	2.6
2	F	4	LEU	2.6
2	D	32	TYR	2.6
2	F	5	THR	2.6
1	H	5	VAL	2.6
2	B	169	LYS	2.5
1	C	139	SER	2.5
1	H	165	ALA	2.5
2	F	59	PRO	2.5
1	A	179	SER	2.5
2	F	49	TYR	2.5
2	L	67	SER	2.5
1	E	51	ILE	2.4
1	A	210	SER	2.4
2	D	133	VAL	2.4
2	D	92	ASP	2.3
1	E	100	LEU	2.3
2	L	154	LEU	2.3
2	B	133	VAL	2.2
2	F	169	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	30	SER	2.2
2	F	50	ALA	2.2
1	A	2	VAL	2.2
1	A	197	GLY	2.2
1	E	140	GLY	2.2
1	A	180	SER	2.2
2	L	169	LYS	2.2
2	L	3	GLN	2.2
2	B	194	CYS	2.2
1	A	176	VAL	2.2
2	F	90	GLN	2.2
1	H	138	THR	2.1
1	A	183	TYR	2.1
1	E	138	THR	2.1
2	L	94	TYR	2.1
1	A	165	ALA	2.1
1	H	185	LEU	2.1
2	F	76	SER	2.1
1	H	211	ASN	2.1
1	A	198	THR	2.1
1	E	61	ASP	2.1
1	A	157	VAL	2.0
2	F	53	THR	2.0
1	C	100(A)	PHE	2.0
1	A	167	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	C	301	4/4	0.74	0.14	22,42,43,49	0

6.5 Other polymers (i)

There are no such residues in this entry.