



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2021 – 04:19 PM EST

PDB ID : 7KFW
Title : Structural basis for a germline-biased antibody response to SARS-CoV-2 (RBD:C1A-B3 Fab)
Authors : Pan, J.; Abraham, J.; Clark, L.; Clark, S.
Deposited on : 2020-10-15
Resolution : 2.79 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

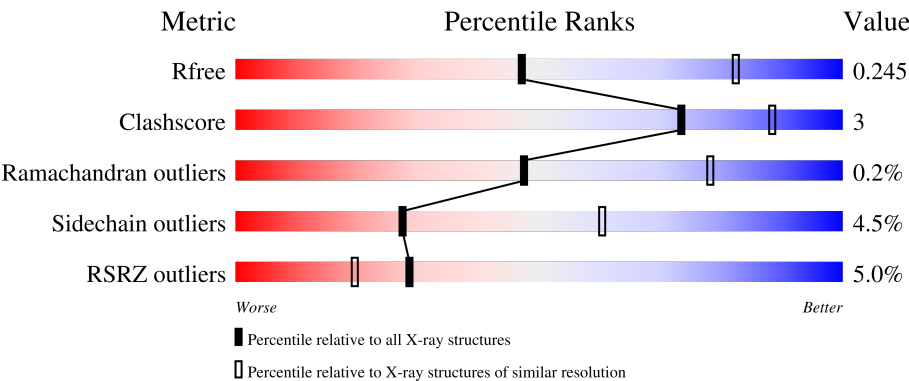
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	228	<div><div>6%</div><div><div></div><div>75%</div><div>9%</div><div>•</div><div>14%</div></div></div>
1	B	228	<div><div>7%</div><div><div></div><div>78%</div><div>7%</div><div>•</div><div>14%</div></div></div>
1	E	228	<div><div>16%</div><div><div></div><div>73%</div><div>12%</div><div>•</div><div>14%</div></div></div>
2	C	225	<div><div>•</div><div><div></div><div>89%</div><div>10%</div><div>•</div></div></div>
2	F	225	<div><div>7%</div><div><div></div><div>84%</div><div>13%</div><div>•</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
2	H	225	 90% 8%
3	D	214	 91% 9%
3	G	214	 90% 10%
3	L	214	 88% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	601[A]	-	-	-	X
4	NAG	E	601[B]	-	-	-	X
4	NAG	E	601[C]	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15119 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	5	0
			1584	1017	264	295	8			
1	B	195	Total	C	N	O	S	0	4	0
			1571	1005	264	294	8			
1	E	195	Total	C	N	O	S	6	5	0
			1587	1013	268	298	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	GLY	-	expression tag	UNP P0DTC2
A	315	SER	-	expression tag	UNP P0DTC2
A	316	GLY	-	expression tag	UNP P0DTC2
A	317	SER	-	expression tag	UNP P0DTC2
A	318	GLY	-	expression tag	UNP P0DTC2
B	314	GLY	-	expression tag	UNP P0DTC2
B	315	SER	-	expression tag	UNP P0DTC2
B	316	GLY	-	expression tag	UNP P0DTC2
B	317	SER	-	expression tag	UNP P0DTC2
B	318	GLY	-	expression tag	UNP P0DTC2
E	314	GLY	-	expression tag	UNP P0DTC2
E	315	SER	-	expression tag	UNP P0DTC2
E	316	GLY	-	expression tag	UNP P0DTC2
E	317	SER	-	expression tag	UNP P0DTC2
E	318	GLY	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called heavy chain of antibody C1A-B3 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	3	2	0
			1655	1041	279	329	6			

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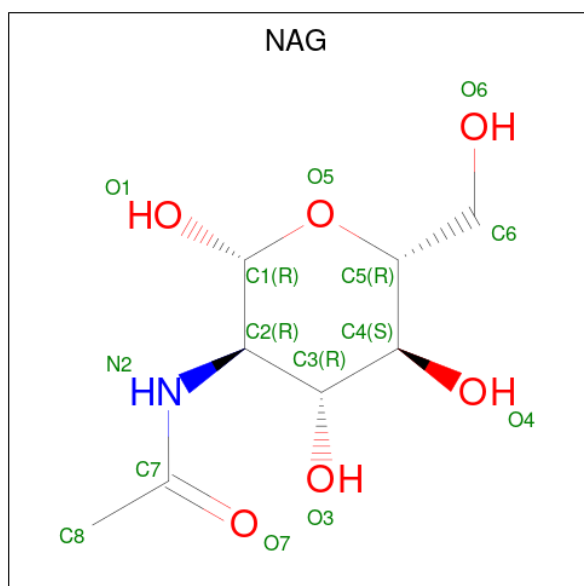
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	219	Total	C	N	O	S	3	2	0
			1636	1031	276	323	6			
2	H	222	Total	C	N	O	S	0	6	0
			1686	1059	286	335	6			

- Molecule 3 is a protein called light chain of antibody C1A-B3 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	4	2	0
			1639	1027	273	333	6			
3	G	214	Total	C	N	O	S	7	3	0
			1646	1031	274	335	6			
3	L	214	Total	C	N	O	S	4	3	0
			1645	1030	274	335	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	1
			42	24	3	15		

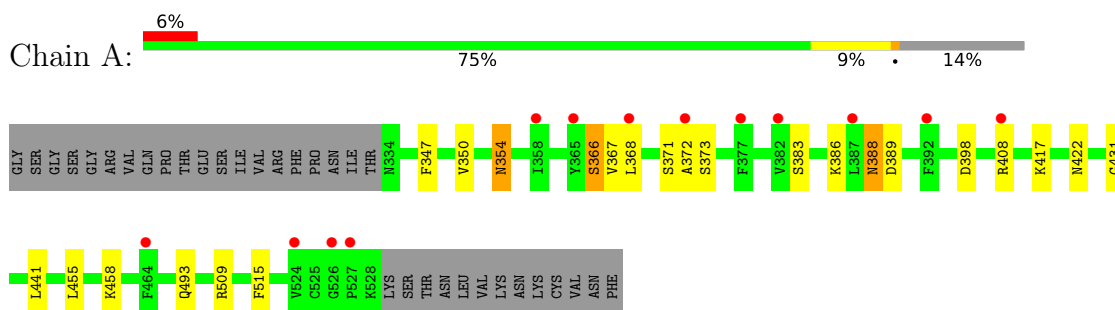
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total 40	O 40	0	0
5	B	31	Total 31	O 31	0	0
5	C	56	Total 56	O 56	0	0
5	D	66	Total 66	O 66	0	0
5	E	19	Total 19	O 19	0	0
5	F	19	Total 19	O 19	0	0
5	G	49	Total 49	O 49	0	0
5	H	62	Total 62	O 62	0	0
5	L	58	Total 58	O 58	0	0

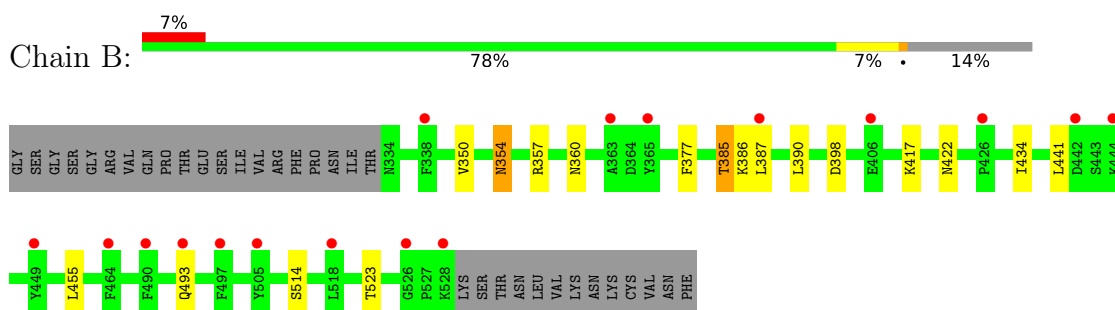
3 Residue-property plots [i](#)

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.

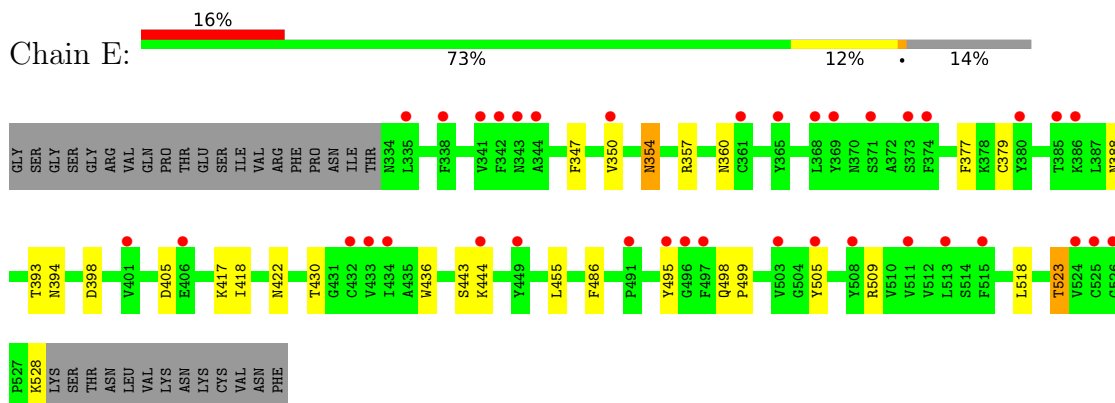
- Molecule 1: Spike glycoprotein



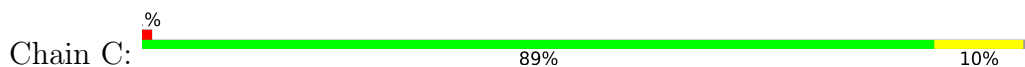
- Molecule 1: Spike glycoprotein

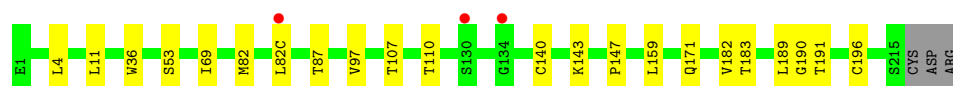


- Molecule 1: Spike glycoprotein

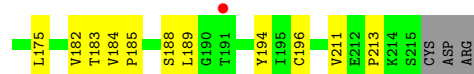
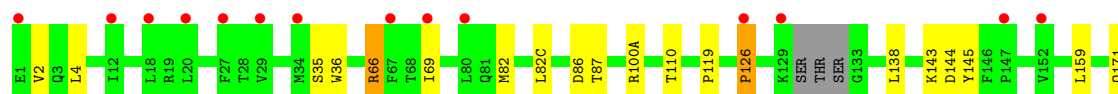
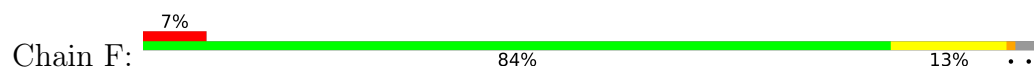


- Molecule 2: heavy chain of antibody C1A-B3 Fab

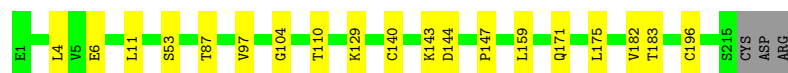
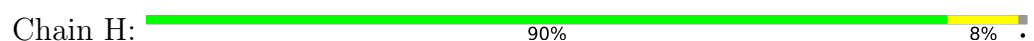




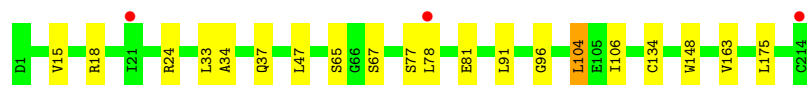
- Molecule 2: heavy chain of antibody C1A-B3 Fab



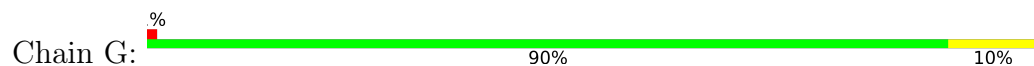
- Molecule 2: heavy chain of antibody C1A-B3 Fab



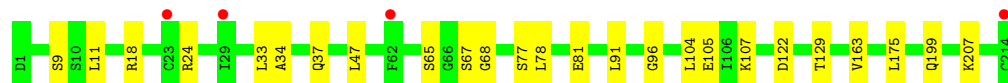
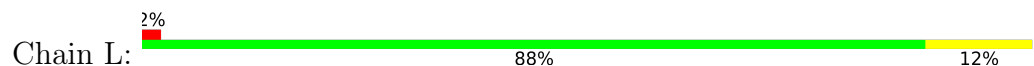
- Molecule 3: light chain of antibody C1A-B3 Fab



- Molecule 3: light chain of antibody C1A-B3 Fab



- Molecule 3: light chain of antibody C1A-B3 Fab



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.17Å 112.84Å 267.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	133.92 – 2.79 133.92 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (133.92-2.79) 99.0 (133.92-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.229 0.200 , 0.245	Depositor DCC
R_{free} test set	3092 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15119	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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](#)

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

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	0.41	0/1632	0.57	0/2218
1	B	0.41	0/1618	0.57	0/2200
1	E	0.34	0/1634	0.56	0/2222
2	C	0.42	0/1699	0.63	0/2313
2	F	0.39	0/1679	0.62	0/2284
2	H	0.43	0/1730	0.64	0/2355
3	D	0.42	0/1679	0.63	0/2280
3	G	0.41	0/1686	0.61	0/2290
3	L	0.44	0/1685	0.61	0/2288
All	All	0.41	0/15042	0.61	0/20450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1584	0	1507	10	0
1	B	1571	0	1490	9	0
1	E	1587	0	1499	16	0
2	C	1655	0	1624	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1636	0	1606	20	0
2	H	1686	0	1654	14	0
3	D	1639	0	1605	7	0
3	G	1646	0	1611	9	0
3	L	1645	0	1609	13	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	E	42	0	39	0	0
5	A	40	0	0	1	0
5	B	31	0	0	0	0
5	C	56	0	0	0	0
5	D	66	0	0	0	0
5	E	19	0	0	1	0
5	F	19	0	0	0	0
5	G	49	0	0	0	0
5	H	62	0	0	0	0
5	L	58	0	0	1	0
All	All	15119	0	14270	96	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 3.

All (96) 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:H:129:LYS:NZ	3:L:207:LYS:HZ2	1.76	0.82
2:H:129:LYS:NZ	3:L:207:LYS:NZ	2.28	0.80
2:F:36:TRP:CD1	2:F:69:ILE:HD12	2.20	0.77
2:F:126:PRO:HD2	2:F:213:PRO:HA	1.69	0.75
2:H:129:LYS:HZ1	3:L:207:LYS:NZ	1.86	0.73
2:C:190:GLY:HA3	3:G:20:THR:HB	1.71	0.71
1:E:436:TRP:HE1	1:E:509:ARG:HB2	1.57	0.69
1:E:436:TRP:NE1	1:E:509:ARG:HB2	2.07	0.67
2:H:129:LYS:HZ1	3:L:207:LYS:HZ2	1.42	0.66
2:F:184:VAL:HG21	2:F:194:TYR:OH	1.96	0.65
1:E:360:ASN:ND2	1:E:523:THR:OG1	2.30	0.64
2:F:184:VAL:CG2	2:F:185:PRO:HD2	2.28	0.64
2:C:11:LEU:HB2	2:C:147:PRO:HG3	1.78	0.64
3:L:78:LEU:HD11	3:L:104:LEU:HD21	1.79	0.64
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.79	0.63
2:F:36:TRP:HD1	2:F:69:ILE:HD12	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ARG:NH1	2:F:86:ASP:OD2	2.35	0.60
1:E:354:ASN:O	1:E:398:ASP:HA	2.05	0.57
2:H:129:LYS:HZ2	3:L:207:LYS:HZ2	1.50	0.56
2:F:184:VAL:HG23	2:F:185:PRO:HD2	1.87	0.56
1:A:354:ASN:O	1:A:398:ASP:HA	2.05	0.56
2:H:143:LYS:NZ	2:H:171:GLN:HE22	2.04	0.55
1:A:366:SER:H	1:A:388:ASN:ND2	2.04	0.54
1:E:388:ASN:ND2	1:E:528:LYS:NZ	2.54	0.54
1:B:354:ASN:O	1:B:398:ASP:HA	2.08	0.53
1:B:360:ASN:H	1:B:523:THR:HB	1.73	0.53
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.91	0.53
2:C:143:LYS:NZ	2:C:171:GLN:HE22	2.08	0.51
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.91	0.51
2:H:129:LYS:NZ	3:L:207:LYS:HZ3	2.09	0.51
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.93	0.51
1:B:387:LEU:HD12	1:B:390:LEU:HD12	1.92	0.51
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.12	0.50
2:F:119:PRO:HB3	2:F:145:TYR:HB3	1.94	0.50
2:F:143:LYS:NZ	2:F:171:GLN:HE22	2.09	0.49
1:E:486:PHE:HZ	2:F:2:VAL:HG21	1.78	0.49
1:A:417:LYS:HD3	1:A:455:LEU:HD12	1.94	0.49
1:A:455:LEU:HD22	1:A:493:GLN:HG3	1.94	0.49
2:F:159:LEU:HD21	2:F:182:VAL:HG21	1.95	0.49
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.94	0.49
2:C:191:THR:HA	3:G:11:LEU:HD11	1.95	0.49
2:C:97:VAL:HB	3:D:96:GLY:HA3	1.95	0.49
1:E:418:ILE:HA	1:E:422:ASN:HB2	1.94	0.49
2:C:159:LEU:HD21	2:C:182:VAL:HG21	1.95	0.48
3:L:34:ALA:HB2	3:L:91:LEU:HD11	1.95	0.48
2:F:138:LEU:HB2	2:F:211:VAL:HG11	1.95	0.48
1:B:385:THR:HB	1:B:386:LYS:HZ2	1.78	0.48
1:B:377:PHE:CE1	1:B:434:ILE:HG12	2.48	0.48
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.95	0.47
3:D:15:VAL:HG23	3:D:106:ILE:HG21	1.96	0.47
1:A:383:SER:HB2	1:A:386:LYS:HZ3	1.80	0.47
3:G:134:CYS:HB2	3:G:148:TRP:CH2	2.50	0.47
1:A:431:GLY:HA2	1:A:515:PHE:HD1	1.79	0.47
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.46
2:H:87:THR:HG23	2:H:110:THR:HA	1.97	0.46
1:B:455:LEU:HD22	1:B:493:GLN:HG3	1.97	0.46
3:D:78:LEU:HD11	3:D:104:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:THR:HB	1:B:386:LYS:NZ	2.31	0.46
1:E:417:LYS:HD3	1:E:455:LEU:HD12	1.98	0.45
1:B:417:LYS:HD3	1:B:455:LEU:HD12	1.97	0.45
2:F:87:THR:HG23	2:F:110:THR:HA	1.98	0.45
3:D:134:CYS:HB2	3:D:148:TRP:CZ2	2.52	0.45
3:D:34:ALA:HB2	3:D:91:LEU:HD11	1.98	0.45
2:F:184:VAL:HG22	2:F:188:SER:OG	2.17	0.45
1:A:347:PHE:CD2	1:A:509:ARG:HG2	2.52	0.44
2:C:87:THR:HG23	2:C:110:THR:HA	1.99	0.44
3:D:163[A]:VAL:HG22	3:D:175:LEU:HD12	1.99	0.44
3:G:34:ALA:HB2	3:G:91:LEU:HD11	1.98	0.44
1:A:383:SER:HB2	1:A:386:LYS:NZ	2.33	0.44
2:F:184:VAL:HG22	2:F:185:PRO:HD2	1.98	0.44
1:E:393:THR:HG21	1:E:518:LEU:HB2	1.99	0.44
3:L:163[A]:VAL:HG22	3:L:175:LEU:HD12	2.00	0.44
2:H:143:LYS:HZ3	2:H:171:GLN:HE22	1.67	0.43
1:E:388:ASN:CG	1:E:528:LYS:HZ2	2.22	0.43
3:L:199:GLN:HB2	5:L:302:HOH:O	2.19	0.42
1:A:458[B]:LYS:HG3	1:A:458[B]:LYS:H	1.61	0.42
3:G:78:LEU:HD21	3:G:104:LEU:HD21	2.02	0.42
3:G:163[A]:VAL:HG22	3:G:175:LEU:HD12	2.01	0.42
1:E:486:PHE:HZ	2:F:2:VAL:CG2	2.32	0.42
2:C:190:GLY:CA	3:G:20:THR:HB	2.44	0.42
2:F:143:LYS:HZ3	2:F:171:GLN:HE22	1.68	0.42
1:E:377:PHE:CE2	1:E:379:CYS:SG	3.13	0.41
5:A:704:HOH:O	3:L:68:GLY:HA2	2.20	0.41
2:C:143:LYS:HZ3	2:C:171:GLN:HE22	1.68	0.41
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	2.01	0.41
1:E:444:LYS:O	1:E:498:GLN:OE1	2.39	0.41
2:C:82:MET:HB3	2:C:82(C):LEU:HD21	2.02	0.41
1:E:499:PRO:HB3	5:E:719:HOH:O	2.21	0.41
2:F:36:TRP:CD1	2:F:69:ILE:CD1	2.99	0.41
2:H:144:ASP:HB3	2:H:175:LEU:HD13	2.02	0.41
2:H:11:LEU:HB2	2:H:147:PRO:HG3	2.03	0.41
3:G:134:CYS:HB2	3:G:148:TRP:CZ2	2.56	0.40
2:H:97:VAL:HB	3:L:96:GLY:HA3	2.03	0.40
2:C:36:TRP:HD1	2:C:69:ILE:HD12	1.86	0.40
2:F:144:ASP:HB3	2:F:175:LEU:HD13	2.04	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	198/228 (87%)	186 (94%)	10 (5%)	2 (1%)	15	44
1	B	197/228 (86%)	185 (94%)	12 (6%)	0	100	100
1	E	199/228 (87%)	175 (88%)	24 (12%)	0	100	100
2	C	222/225 (99%)	216 (97%)	6 (3%)	0	100	100
2	F	217/225 (96%)	210 (97%)	6 (3%)	1 (0%)	29	61
2	H	226/225 (100%)	215 (95%)	11 (5%)	0	100	100
3	D	214/214 (100%)	206 (96%)	8 (4%)	0	100	100
3	G	215/214 (100%)	210 (98%)	5 (2%)	0	100	100
3	L	215/214 (100%)	209 (97%)	6 (3%)	0	100	100
All	All	1903/2001 (95%)	1812 (95%)	88 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	ALA
1	A	373	SER
2	F	126	PRO

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	173/198 (87%)	164 (95%)	9 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	172/198 (87%)	166 (96%)	6 (4%)	36	70
1	E	174/198 (88%)	164 (94%)	10 (6%)	20	50
2	C	186/187 (100%)	179 (96%)	7 (4%)	33	67
2	F	183/187 (98%)	176 (96%)	7 (4%)	33	67
2	H	190/187 (102%)	183 (96%)	7 (4%)	34	68
3	D	188/186 (101%)	180 (96%)	8 (4%)	29	62
3	G	189/186 (102%)	180 (95%)	9 (5%)	25	58
3	L	189/186 (102%)	176 (93%)	13 (7%)	15	41
All	All	1644/1713 (96%)	1568 (95%)	76 (5%)	27	60

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	366	SER
1	A	367	VAL
1	A	368	LEU
1	A	371	SER
1	A	388	ASN
1	A	389	ASP
1	A	408	ARG
1	A	441	LEU
1	B	354	ASN
1	B	357	ARG
1	B	385	THR
1	B	441	LEU
1	B	514[A]	SER
1	B	514[B]	SER
2	C	4	LEU
2	C	53	SER
2	C	107	THR
2	C	140	CYS
2	C	183	THR
2	C	189	LEU
2	C	196	CYS
3	D	18	ARG
3	D	24	ARG
3	D	33	LEU
3	D	65	SER

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Mol	Chain	Res	Type
3	D	67	SER
3	D	77	SER
3	D	81	GLU
3	D	104	LEU
1	E	347	PHE
1	E	354	ASN
1	E	357	ARG
1	E	394	ASN
1	E	405	ASP
1	E	430	THR
1	E	443	SER
1	E	495	TYR
1	E	505	TYR
1	E	523	THR
2	F	4	LEU
2	F	35	SER
2	F	66	ARG
2	F	100(A)	ARG
2	F	183	THR
2	F	189	LEU
2	F	196	CYS
3	G	9	SER
3	G	24	ARG
3	G	33	LEU
3	G	65	SER
3	G	67	SER
3	G	77	SER
3	G	81	GLU
3	G	105	GLU
3	G	122	ASP
2	H	4	LEU
2	H	53[A]	SER
2	H	53[B]	SER
2	H	140	CYS
2	H	183[A]	THR
2	H	183[B]	THR
2	H	196	CYS
3	L	9	SER
3	L	11	LEU
3	L	18	ARG
3	L	24	ARG
3	L	33	LEU

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Mol	Chain	Res	Type
3	L	65	SER
3	L	67	SER
3	L	77	SER
3	L	81	GLU
3	L	105	GLU
3	L	107	LYS
3	L	122	ASP
3	L	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	388	ASN
2	C	171	GLN
2	C	199	ASN
3	D	155	GLN
3	D	210	ASN
1	E	360	ASN
1	E	394	ASN
1	E	437	ASN
1	E	448	ASN
1	E	450	ASN
1	E	498	GLN
2	F	171	GLN
3	G	155	GLN
2	H	171	GLN
2	H	199	ASN
3	L	155	GLN
3	L	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are 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	$\# Z > 2$
4	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.86	1 (5%)
4	NAG	B	601	1	14,14,15	0.33	0	17,19,21	1.02	2 (11%)
4	NAG	E	601[C]	1	14,14,15	0.25	0	17,19,21	0.90	1 (5%)
4	NAG	E	601[B]	1	14,14,15	0.30	0	17,19,21	1.04	2 (11%)
4	NAG	E	601[A]	1	14,14,15	0.32	0	17,19,21	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601[C]	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601[B]	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601[A]	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601[B]	NAG	C1-O5-C5	3.02	116.28	112.19
4	B	601	NAG	C1-O5-C5	3.01	116.27	112.19
4	E	601[B]	NAG	O5-C1-C2	2.72	115.58	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601[C]	NAG	C1-O5-C5	2.71	115.87	112.19
4	B	601	NAG	O5-C1-C2	2.34	114.98	111.29
4	A	601	NAG	C1-O5-C5	2.31	115.32	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6

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, 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	195/228 (85%)	0.87	13 (6%) 17 10	47, 80, 149, 180	0
1	B	195/228 (85%)	0.82	17 (8%) 10 5	49, 86, 140, 210	0
1	E	195/228 (85%)	1.22	37 (18%) 1 1	64, 132, 220, 264	0
2	C	222/225 (98%)	0.55	3 (1%) 75 70	44, 72, 117, 191	0
2	F	219/225 (97%)	0.76	15 (6%) 17 10	57, 93, 137, 212	0
2	H	222/225 (98%)	0.53	0 100 100	40, 68, 131, 236	0
3	D	214/214 (100%)	0.63	3 (1%) 75 70	47, 74, 107, 171	0
3	G	214/214 (100%)	0.49	3 (1%) 75 70	48, 75, 112, 167	0
3	L	214/214 (100%)	0.56	4 (1%) 66 59	46, 70, 109, 168	0
All	All	1890/2001 (94%)	0.70	95 (5%) 28 19	40, 79, 158, 264	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	214	CYS	11.9
3	L	214	CYS	7.9
1	A	387	LEU	7.5
1	E	497	PHE	5.7
1	E	365	TYR	5.7
1	E	342	PHE	5.5
1	E	373	SER	5.3
1	E	341	VAL	4.9
1	E	406	GLU	4.6
1	E	433	VAL	4.5
3	G	214	CYS	4.2
1	E	503	VAL	4.0
1	E	344	ALA	3.9
1	A	365	TYR	3.9
1	B	365	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	449	TYR	3.8
1	E	526	GLY	3.8
1	E	368	LEU	3.8
1	E	374	PHE	3.6
1	E	380	TYR	3.5
1	E	432	CYS	3.4
1	A	377	PHE	3.4
2	F	27	PHE	3.4
1	B	387	LEU	3.2
2	C	130	SER	3.2
2	F	191	THR	3.2
1	A	372	ALA	3.1
1	A	527	PRO	3.1
1	E	513	LEU	3.1
1	E	505	TYR	3.0
1	B	363	ALA	3.0
1	E	524	VAL	3.0
1	E	434	ILE	2.9
2	F	20	LEU	2.9
2	F	18	LEU	2.9
1	A	526	GLY	2.9
1	B	497	PHE	2.8
2	F	34	MET	2.8
1	E	371	SER	2.7
1	A	524	VAL	2.7
1	B	449	TYR	2.7
1	A	392	PHE	2.7
1	E	343[A]	ASN	2.7
3	L	23	CYS	2.7
1	E	401	VAL	2.6
1	E	495	TYR	2.6
1	E	515	PHE	2.6
1	E	338	PHE	2.6
3	D	21	ILE	2.6
1	E	386	LYS	2.6
1	B	338	PHE	2.6
1	E	525	CYS	2.5
1	A	368	LEU	2.5
2	F	29	VAL	2.5
2	F	152	VAL	2.5
2	F	1	GLU	2.5
1	B	505	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	369	TYR	2.5
1	A	358	ILE	2.5
1	B	490	PHE	2.4
1	E	335	LEU	2.4
3	D	78	LEU	2.4
1	E	496	GLY	2.4
1	E	511	VAL	2.4
1	B	493	GLN	2.3
1	B	444	LYS	2.3
3	L	29	ILE	2.3
3	L	62	PHE	2.3
2	C	82(C)	LEU	2.3
1	A	464	PHE	2.2
1	E	508	TYR	2.2
2	F	67	PHE	2.2
1	E	350	VAL	2.2
1	E	361	CYS	2.2
1	E	491	PRO	2.2
2	F	69	ILE	2.2
3	G	187	GLU	2.2
1	E	385	THR	2.2
2	C	134	GLY	2.2
2	F	126	PRO	2.2
1	B	528	LYS	2.1
1	B	406	GLU	2.1
1	E	444	LYS	2.1
1	B	426	PRO	2.1
1	B	442	ASP	2.1
2	F	129	LYS	2.1
3	G	179	LEU	2.1
1	B	464	PHE	2.1
2	F	147	PRO	2.1
1	B	526	GLY	2.1
1	A	382	VAL	2.1
1	B	518	LEU	2.0
1	A	408	ARG	2.0
2	F	12	ILE	2.0
2	F	80	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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(\AA^2)	Q<0.9
4	NAG	E	601[C]	14/15	0.45	0.60	40,40,41,41	14
4	NAG	E	601[B]	14/15	0.45	0.60	41,41,41,42	14
4	NAG	E	601[A]	14/15	0.45	0.60	142,142,142,142	14
4	NAG	B	601	14/15	0.73	0.38	158,159,159,159	0
4	NAG	A	601	14/15	0.92	0.15	119,119,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.