Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 07:40 PM JST

PDB ID	:	6A4K
Title	:	Human antibody 32D6 Fab in complex with H1N1 influenza A virus HA1
Authors	:	Lee, C.C.; Ko, T.P.; Lin, L.L.; Wang, A.H.J.
Deposited on	:	2018-06-20
Resolution	:	3.15 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:

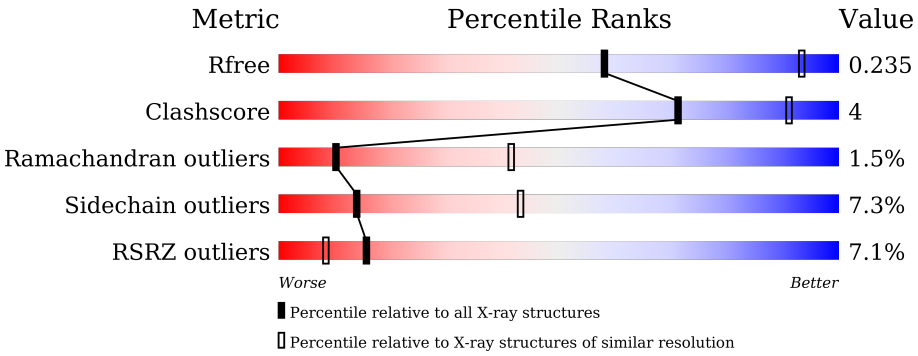
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	235	84% 10% • 5%
1	B	235	5% 82% 9% • 6%
1	C	235	% 83% 11% • 5%
1	D	235	4% 81% 10% • 6%
2	H	238	6% 86% 10% • •
2	I	238	18% 77% 19% • •

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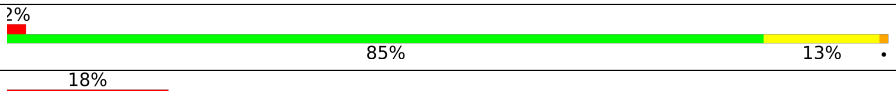
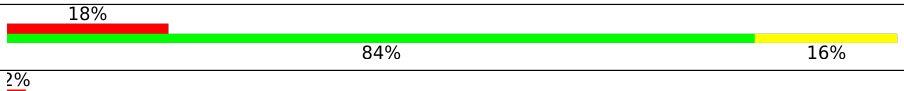
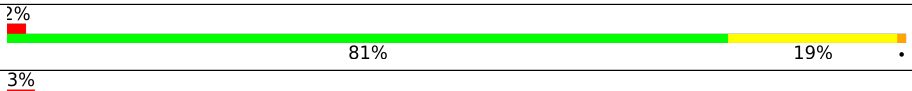
Mol	Chain	Length	Quality of chain
2	J	238	
2	K	238	
3	L	216	
3	M	216	
3	N	216	
3	O	216	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20618 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1760	1123	296	335	6			
1	B	221	Total	C	N	O	S	0	0	0
			1745	1114	294	331	6			
1	C	223	Total	C	N	O	S	0	0	0
			1760	1123	296	335	6			
1	D	221	Total	C	N	O	S	0	0	0
			1745	1114	294	331	6			

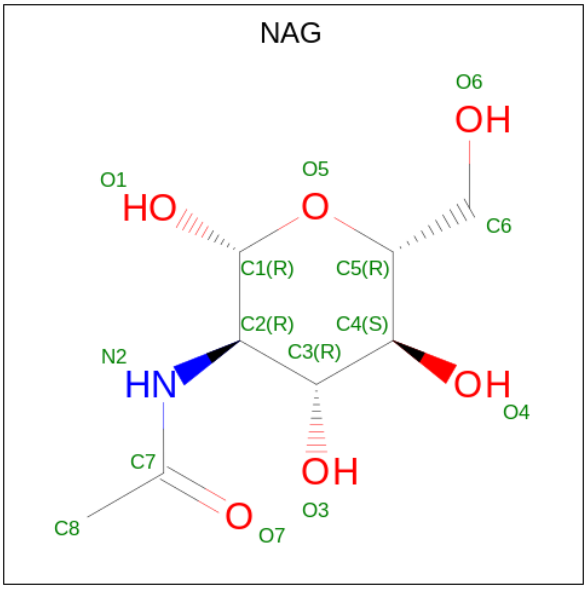
- Molecule 2 is a protein called immunoglobulin Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	I	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	J	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	K	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	M	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	N	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	O	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			

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

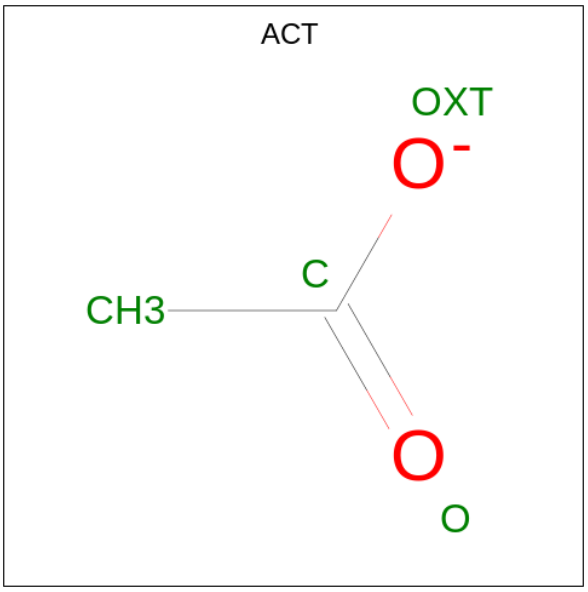


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	O	1	Total Ca 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	28	Total O 28 28	0	0
7	H	17	Total O 17 17	0	0
7	L	29	Total O 29 29	0	0
7	B	15	Total O 15 15	0	0
7	I	6	Total O 6 6	0	0
7	M	5	Total O 5 5	0	0
7	C	24	Total O 24 24	0	0
7	N	7	Total O 7 7	0	0
7	D	31	Total O 31 31	0	0
7	K	12	Total O 12 12	0	0

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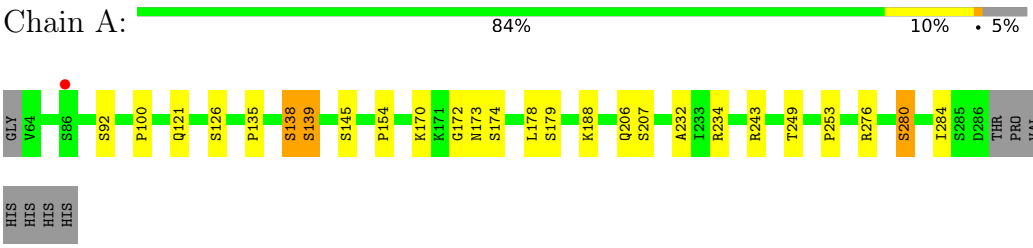
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	O	21	Total O 21 21	0	0

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.

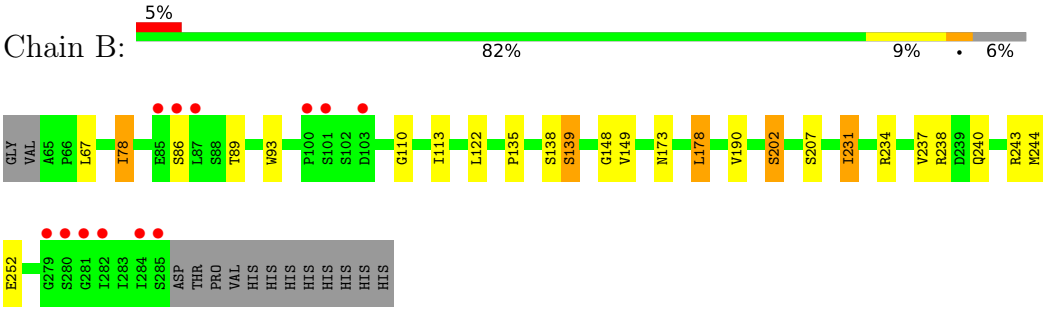
• Molecule 1: Hemagglutinin

Chain A:



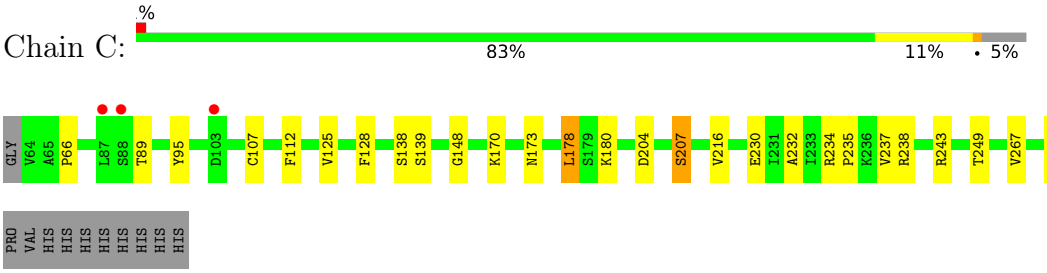
• Molecule 1: Hemagglutinin

Chain B:



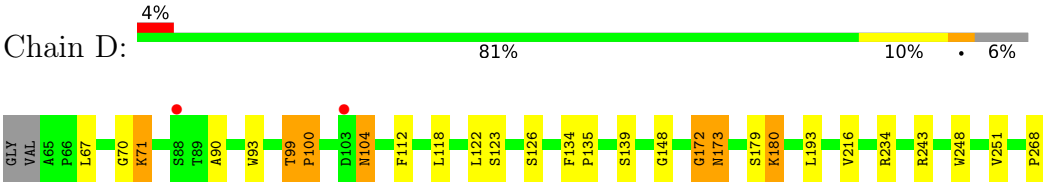
• Molecule 1: Hemagglutinin

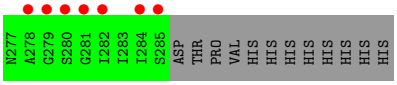
Chain C:



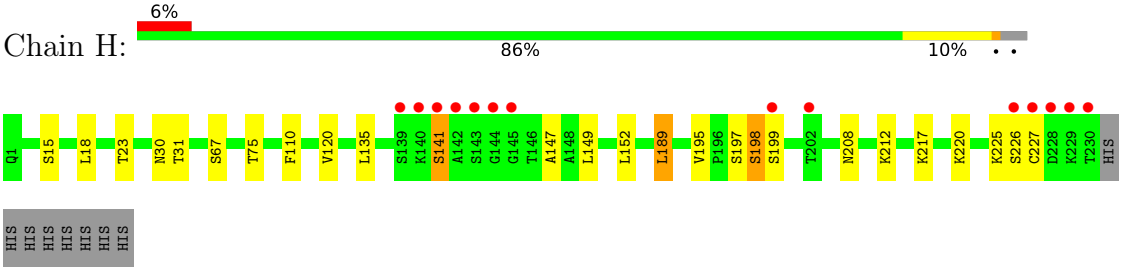
• Molecule 1: Hemagglutinin

Chain D:

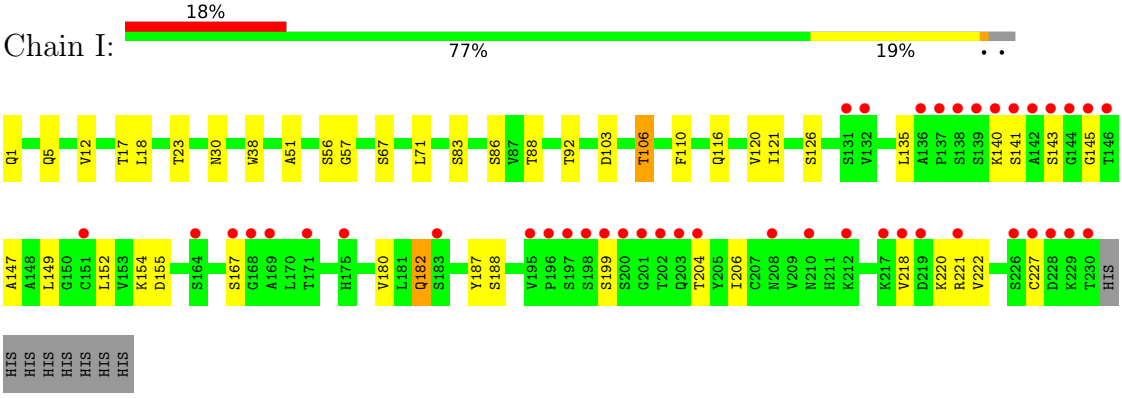




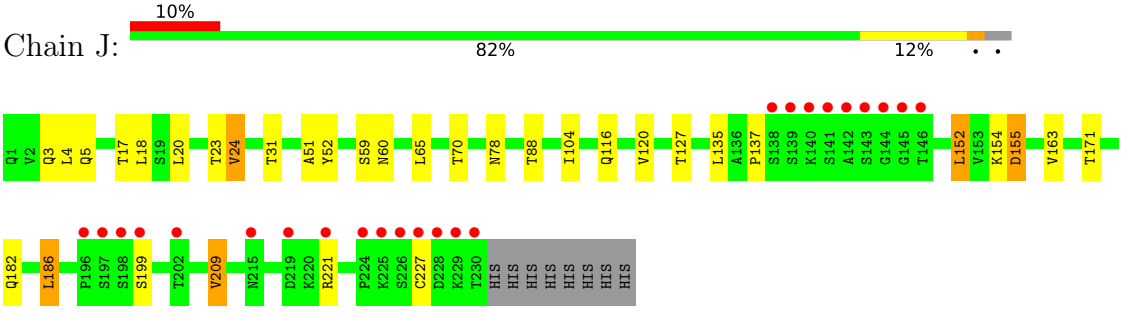
• Molecule 2: immunoglobulin Fab heavy chain



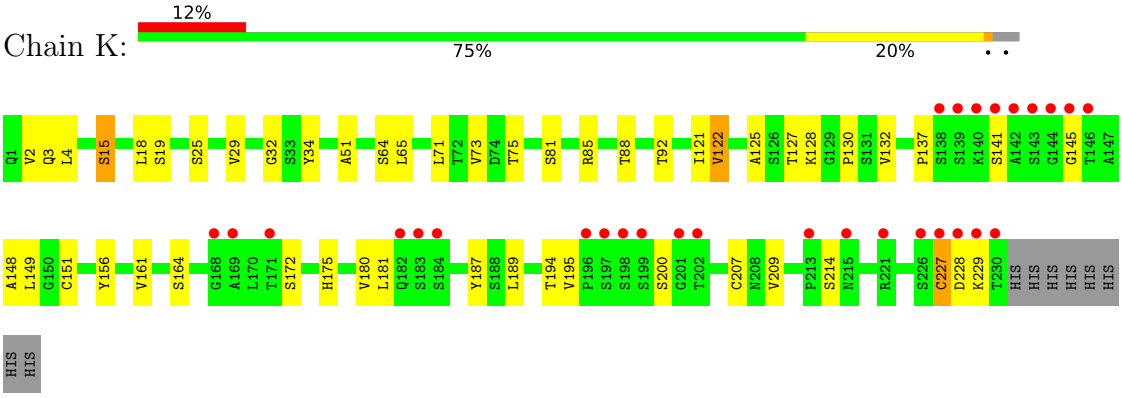
• Molecule 2: immunoglobulin Fab heavy chain



• Molecule 2: immunoglobulin Fab heavy chain

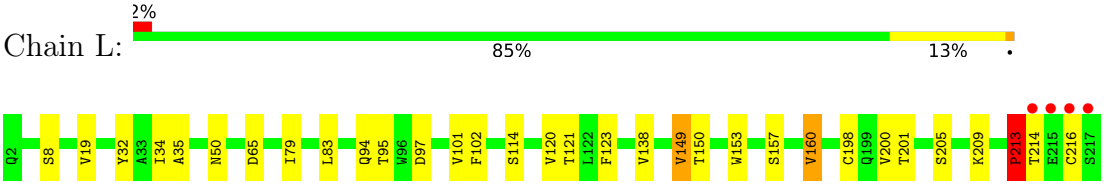


• Molecule 2: immunoglobulin Fab heavy chain



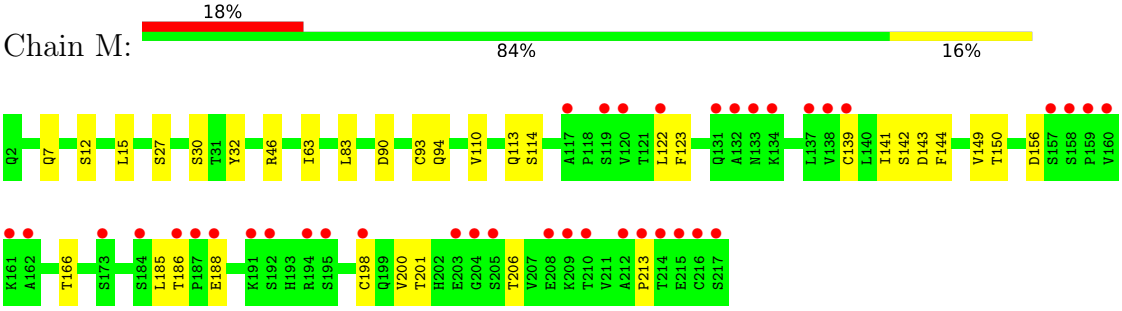
• Molecule 3: immunoglobulin Fab light chain

Chain L:



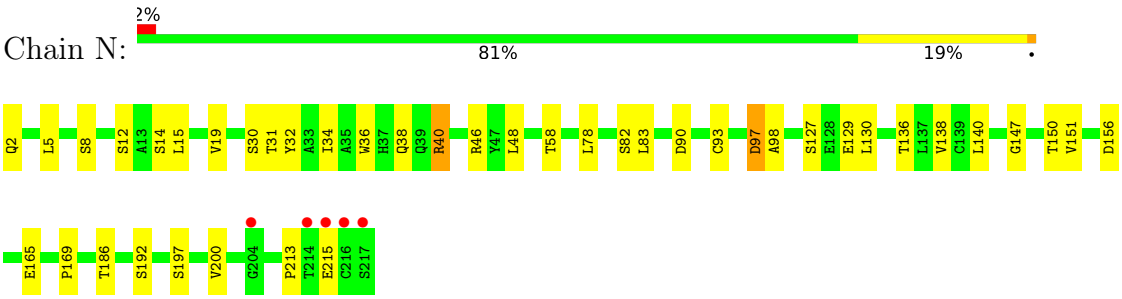
• Molecule 3: immunoglobulin Fab light chain

Chain M:



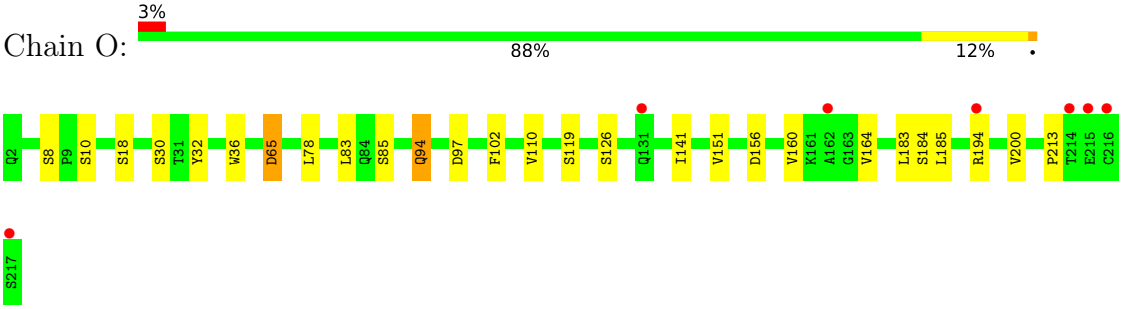
• Molecule 3: immunoglobulin Fab light chain

Chain N:



• Molecule 3: immunoglobulin Fab light chain

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	181.74Å 181.74Å 248.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15 19.91 – 3.15	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-3.15) 94.8 (19.91-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.175 , 0.233 0.178 , 0.235	Depositor DCC
R_{free} test set	3830 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20618	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, NAG, CA

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	0.54	0/1810	0.74	0/2457
1	B	0.51	0/1795	0.72	0/2436
1	C	0.52	0/1810	0.74	0/2457
1	D	0.53	0/1795	0.74	1/2436 (0.0%)
2	H	0.53	0/1766	0.77	1/2414 (0.0%)
2	I	0.54	0/1766	0.73	0/2414
2	J	0.51	0/1766	0.69	0/2414
2	K	0.55	0/1766	0.74	0/2414
3	L	0.54	0/1651	0.78	0/2246
3	M	0.54	0/1651	0.73	0/2246
3	N	0.51	0/1651	0.72	1/2246 (0.0%)
3	O	0.55	0/1651	0.75	0/2246
All	All	0.53	0/20878	0.74	3/28426 (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	A	0	1
1	C	0	1
1	D	0	1
2	H	0	1
3	L	0	1
3	N	0	1
All	All	0	6

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	D	173	ASN	N-CA-CB	-5.33	101.01	110.60
3	N	40	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	H	189	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	SER	Peptide
1	C	89	THR	Peptide
1	D	172	GLY	Peptide
2	H	198	SER	Peptide
3	L	213	PRO	Peptide
3	N	215	GLU	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	1760	0	1696	8	0
1	B	1745	0	1683	12	0
1	C	1760	0	1696	9	0
1	D	1745	0	1683	15	0
2	H	1722	0	1687	8	0
2	I	1722	0	1687	18	0
2	J	1722	0	1687	12	0
2	K	1722	0	1687	18	0
3	L	1614	0	1553	13	0
3	M	1614	0	1553	14	0
3	N	1614	0	1553	14	0
3	O	1614	0	1553	9	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	O	1	0	0	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	A	28	0	0	0	0
7	B	15	0	0	1	0
7	C	24	0	0	0	0
7	D	31	0	0	0	0
7	H	17	0	0	1	0
7	I	6	0	0	0	0
7	K	12	0	0	0	0
7	L	29	0	0	1	0
7	M	5	0	0	0	0
7	N	7	0	0	1	0
7	O	21	0	0	0	0
All	All	20618	0	19776	142	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 4.

All (142) 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:M:7:GLN:NE2	3:M:93:CYS:SG	2.48	0.87
3:M:7:GLN:HE22	3:M:93:CYS:H	1.31	0.78
2:I:218:VAL:HG12	2:I:220:LYS:HG2	1.73	0.71
3:O:151:VAL:HG12	3:O:200:VAL:HG12	1.72	0.70
2:H:110:PHE:HA	3:L:94:GLN:HE22	1.59	0.67
2:H:18:LEU:HD13	2:H:120:VAL:HG11	1.76	0.67
1:C:173:ASN:HB2	3:N:32:TYR:HA	1.76	0.66
3:M:7:GLN:HE22	3:M:93:CYS:N	1.95	0.64
1:C:230:GLU:O	1:C:234:ARG:NH2	2.29	0.64
2:H:30:ASN:HD21	2:H:75:THR:HG23	1.63	0.64
1:B:234:ARG:HD3	1:B:243:ARG:HG3	1.80	0.64
2:I:110:PHE:HA	3:M:94:GLN:HE22	1.63	0.63
1:B:190:VAL:HG13	1:B:251:VAL:HG13	1.79	0.63
1:B:78:ILE:HD13	1:B:122:LEU:HD11	1.79	0.63
2:I:5:GLN:NE2	2:I:116:GLN:HE22	1.98	0.61
3:M:7:GLN:NE2	3:M:93:CYS:H	1.98	0.61
3:N:2:GLN:HE22	3:N:97:ASP:HB3	1.64	0.61
1:A:170:LYS:HE2	1:A:207:SER:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:138:VAL:HG12	3:N:140:LEU:HD11	1.83	0.60
2:K:132:VAL:HG21	2:K:209:VAL:HG11	1.86	0.58
1:C:235:PRO:O	1:C:243:ARG:NH2	2.37	0.57
2:K:92:THR:HG23	2:K:121:ILE:HA	1.85	0.57
3:O:141:ILE:HG12	3:O:200:VAL:HG11	1.87	0.57
2:I:149:LEU:HD13	2:I:222:VAL:HG11	1.88	0.55
1:A:173:ASN:HB2	3:L:32:TYR:HA	1.88	0.55
2:H:18:LEU:HD12	7:H:302:HOH:O	2.07	0.55
2:I:5:GLN:HE21	2:I:116:GLN:HE22	1.53	0.55
1:B:173:ASN:HB2	3:M:32:TYR:HA	1.88	0.54
2:I:141:SER:HB3	2:I:147:ALA:HA	1.89	0.54
1:D:99:THR:HG22	1:D:100:PRO:HD2	1.91	0.53
2:I:18:LEU:HD12	2:I:120:VAL:HG11	1.91	0.53
2:K:148:ALA:HB2	2:K:194:THR:HG22	1.90	0.53
2:I:135:LEU:HD11	2:I:152:LEU:HB2	1.91	0.52
2:H:135:LEU:HD11	2:H:152:LEU:HB2	1.91	0.52
2:K:180:VAL:O	2:K:187:TYR:HA	2.09	0.52
2:I:92:THR:HG23	2:I:121:ILE:HA	1.91	0.51
2:K:3:GLN:O	2:K:4:LEU:HD23	2.10	0.51
1:C:232:ALA:O	1:C:234:ARG:NH1	2.43	0.51
2:I:206:ILE:HG22	2:I:221:ARG:HB2	1.92	0.51
3:N:151:VAL:HG12	3:N:200:VAL:HG12	1.92	0.51
3:N:2:GLN:NE2	3:N:2:GLN:HA	2.25	0.51
3:L:120:VAL:HG23	3:L:209:LYS:HG3	1.93	0.50
1:D:71:LYS:HE2	1:D:99:THR:HG21	1.93	0.50
1:B:178:LEU:HD12	1:B:178:LEU:C	2.32	0.50
1:A:121:GLN:HE22	1:A:276:ARG:HH11	1.59	0.50
1:A:135:PRO:O	1:A:139:SER:OG	2.30	0.50
2:J:155:ASP:HB3	2:J:186:LEU:HD12	1.94	0.49
2:K:64:SER:C	2:K:65:LEU:HD12	2.33	0.49
1:A:188:LYS:O	1:A:253:PRO:HG3	2.13	0.49
3:M:200:VAL:O	3:M:200:VAL:HG23	2.12	0.49
3:M:122:LEU:HD22	3:M:198:CYS:HB2	1.95	0.49
1:B:135:PRO:O	1:B:139:SER:OG	2.31	0.49
2:I:51:ALA:HB3	2:I:71:LEU:HD11	1.94	0.48
2:K:181:LEU:HD13	2:K:187:TYR:CE2	2.49	0.48
2:H:30:ASN:ND2	2:H:75:THR:HG23	2.28	0.48
2:H:135:LEU:HB3	3:L:123:PHE:CD1	2.48	0.48
2:J:5:GLN:HG3	2:J:116:GLN:HE21	1.78	0.48
2:K:161:VAL:CG2	2:K:189:LEU:HD22	2.44	0.48
2:K:227:CYS:SG	2:K:228:ASP:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LEU:HD13	1:D:90:ALA:CB	2.45	0.47
1:A:232:ALA:O	1:A:234:ARG:NH1	2.48	0.47
3:N:5:LEU:HD13	3:N:93:CYS:SG	2.54	0.47
1:D:234:ARG:HG3	1:D:243:ARG:HG3	1.96	0.47
1:B:238:ARG:O	1:B:240:GLN:HG2	2.15	0.47
1:D:104:ASN:HD22	1:D:104:ASN:N	2.11	0.47
3:N:138:VAL:HG12	3:N:140:LEU:CD1	2.44	0.46
2:K:127:THR:HG21	2:K:214:SER:HA	1.97	0.46
1:C:178:LEU:C	1:C:178:LEU:HD12	2.36	0.46
1:B:110:GLY:HA3	1:B:244:MET:O	2.16	0.46
2:I:135:LEU:HD23	3:M:123:PHE:CG	2.51	0.46
1:D:118:LEU:HD13	1:D:248:TRP:CD2	2.51	0.46
2:K:88:THR:O	2:K:122:VAL:HG11	2.15	0.46
3:O:194:ARG:O	3:O:213:PRO:HD2	2.15	0.46
3:N:19:VAL:CG2	3:N:83:LEU:HD22	2.46	0.45
3:N:38:GLN:HB2	3:N:48:LEU:HD11	1.98	0.45
1:D:122:LEU:HD23	1:D:274:MET:HE3	1.98	0.45
1:A:234:ARG:HD3	1:A:243:ARG:HG3	1.98	0.45
3:L:94:GLN:HB3	3:L:102:PHE:CD1	2.51	0.45
2:I:18:LEU:CD1	2:I:120:VAL:HG11	2.46	0.45
2:J:52:TYR:CE2	2:J:60:ASN:HB3	2.52	0.45
3:N:147:GLY:O	3:N:169:PRO:HG2	2.16	0.45
2:K:51:ALA:HB3	2:K:71:LEU:HD11	1.97	0.45
3:L:149:VAL:HG22	3:L:200:VAL:HG13	2.00	0.44
3:M:83:LEU:HD21	3:M:110:VAL:CG1	2.47	0.44
1:C:170:LYS:HE2	1:C:207:SER:O	2.16	0.44
3:N:2:GLN:HE22	3:N:98:ALA:H	1.65	0.44
2:J:3:GLN:C	2:J:4:LEU:HD12	2.38	0.44
2:I:182:GLN:NE2	2:I:188:SER:OG	2.51	0.44
3:L:214:THR:HA	7:L:308:HOH:O	2.18	0.44
1:D:135:PRO:O	1:D:139:SER:OG	2.34	0.44
3:M:46:ARG:HE	3:M:63:ILE:HD11	1.82	0.44
2:J:135:LEU:HD11	2:J:152:LEU:HB3	2.00	0.44
3:O:94:GLN:HB3	3:O:102:PHE:CD1	2.53	0.44
2:I:180:VAL:O	2:I:187:TYR:HA	2.18	0.43
2:J:163:VAL:HG22	2:J:209:VAL:HG23	1.99	0.43
1:D:122:LEU:HD23	1:D:274:MET:CE	2.47	0.43
1:B:67:LEU:HD12	1:B:93:TRP:CD2	2.52	0.43
2:J:65:LEU:HD12	2:J:65:LEU:N	2.33	0.43
3:O:36:TRP:CE2	3:O:78:LEU:HB2	2.53	0.43
2:H:141:SER:HB3	2:H:147:ALA:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:153:TRP:HB2	3:L:160:VAL:HG22	2.00	0.43
2:I:38:TRP:CD1	2:I:71:LEU:HD21	2.52	0.43
2:K:18:LEU:HD12	2:K:19:SER:N	2.34	0.43
2:I:103:ASP:CG	2:I:106:THR:HG22	2.39	0.43
2:J:24:VAL:O	2:J:78:ASN:ND2	2.52	0.43
2:J:155:ASP:OD1	2:J:182:GLN:NE2	2.50	0.43
3:N:129:GLU:OE1	3:N:136:THR:N	2.51	0.43
1:A:154:PRO:HD2	4:A:501:NAG:H83	2.00	0.43
2:I:5:GLN:HE21	2:I:116:GLN:NE2	2.17	0.43
3:M:201:THR:HG22	3:M:206:THR:OG1	2.19	0.42
2:K:65:LEU:HD12	2:K:65:LEU:N	2.34	0.42
3:N:36:TRP:CE2	3:N:78:LEU:HB2	2.55	0.42
1:D:134:PHE:CE1	1:D:180:LYS:HG2	2.55	0.42
3:L:19:VAL:CG2	3:L:83:LEU:HD13	2.50	0.42
2:K:130:PRO:HB3	2:K:156:TYR:HB3	2.01	0.42
3:O:164:VAL:HG22	3:O:183:LEU:HD13	2.02	0.42
3:L:35:ALA:HA	3:L:50:ASN:HA	2.02	0.41
1:B:113:ILE:HG13	1:B:247:TYR:CE2	2.55	0.41
1:C:125:VAL:HG11	1:C:128:PHE:HB2	2.02	0.41
3:L:79:ILE:HD12	3:L:79:ILE:N	2.34	0.41
1:B:202:SER:HA	1:B:231:ILE:HD12	2.03	0.41
1:B:252:GLU:HA	7:B:610:HOH:O	2.20	0.41
3:M:15:LEU:HD11	3:M:113:GLN:HG2	2.02	0.41
1:D:67:LEU:HD22	1:D:93:TRP:CD2	2.54	0.41
3:L:19:VAL:HG21	3:L:83:LEU:HD13	2.03	0.41
3:O:83:LEU:HD21	3:O:110:VAL:HG22	2.02	0.41
3:O:151:VAL:CG1	3:O:200:VAL:HG12	2.48	0.41
3:L:34:ILE:HG22	3:L:95:THR:HB	2.03	0.41
2:J:18:LEU:HD11	2:J:20:LEU:CD1	2.51	0.41
1:D:193:LEU:O	1:D:268:PRO:HB3	2.21	0.41
1:C:107:CYS:O	1:C:238:ARG:HD2	2.21	0.41
1:D:173:ASN:HB2	3:O:32:TYR:HA	2.03	0.41
2:J:18:LEU:HD11	2:J:20:LEU:HD11	2.02	0.41
2:K:29:VAL:HG11	2:K:73:VAL:CG1	2.50	0.41
3:M:141:ILE:HD11	3:M:200:VAL:HG11	2.03	0.41
1:C:66:PRO:HB3	1:C:95:TYR:CZ	2.56	0.40
1:D:123:SER:HG	1:D:276:ARG:HH12	1.68	0.40
2:K:32:GLY:HA3	2:K:34:TYR:CE2	2.56	0.40
1:D:70:GLY:O	1:D:99:THR:OG1	2.39	0.40
2:J:18:LEU:HD13	2:J:120:VAL:HG11	2.04	0.40
3:N:12:SER:N	7:N:301:HOH:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:127:THR:HG22	2:K:128:LYS:N	2.37	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	221/235 (94%)	202 (91%)	16 (7%)	3 (1%)	11	43
1	B	219/235 (93%)	197 (90%)	19 (9%)	3 (1%)	11	43
1	C	221/235 (94%)	203 (92%)	17 (8%)	1 (0%)	29	65
1	D	219/235 (93%)	201 (92%)	15 (7%)	3 (1%)	11	43
2	H	228/238 (96%)	200 (88%)	23 (10%)	5 (2%)	6	32
2	I	228/238 (96%)	198 (87%)	26 (11%)	4 (2%)	8	37
2	J	228/238 (96%)	203 (89%)	20 (9%)	5 (2%)	6	32
2	K	228/238 (96%)	197 (86%)	25 (11%)	6 (3%)	5	28
3	L	214/216 (99%)	200 (94%)	12 (6%)	2 (1%)	17	53
3	M	214/216 (99%)	193 (90%)	19 (9%)	2 (1%)	17	53
3	N	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	11	43
3	O	214/216 (99%)	204 (95%)	7 (3%)	3 (1%)	11	43
All	All	2648/2756 (96%)	2399 (91%)	209 (8%)	40 (2%)	10	41

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	15	SER
2	H	225	LYS
2	H	227	CYS

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Mol	Chain	Res	Type
3	L	213	PRO
1	B	86	SER
2	I	57	GLY
2	J	227	CYS
3	O	65	ASP
1	B	89	THR
2	I	56	SER
2	I	145	GLY
1	D	148	GLY
2	K	15	SER
2	K	137	PRO
2	K	145	GLY
1	A	138	SER
1	B	148	GLY
2	I	143	SER
3	M	156	ASP
3	M	213	PRO
2	J	155	ASP
2	J	199	SER
2	K	125	ALA
3	O	97	ASP
3	O	156	ASP
2	H	197	SER
2	H	226	SER
3	L	97	ASP
3	N	156	ASP
1	D	100	PRO
2	J	51	ALA
2	J	137	PRO
3	N	97	ASP
2	K	229	LYS
1	C	148	GLY
1	D	172	GLY
1	A	100	PRO
3	N	213	PRO
1	A	172	GLY
2	K	2	VAL

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	192/203 (95%)	180 (94%)	12 (6%)	18 49
1	B	190/203 (94%)	180 (95%)	10 (5%)	22 55
1	C	192/203 (95%)	180 (94%)	12 (6%)	18 49
1	D	190/203 (94%)	180 (95%)	10 (5%)	22 55
2	H	199/207 (96%)	186 (94%)	13 (6%)	17 48
2	I	199/207 (96%)	180 (90%)	19 (10%)	8 30
2	J	199/207 (96%)	184 (92%)	15 (8%)	13 42
2	K	199/207 (96%)	183 (92%)	16 (8%)	12 39
3	L	180/180 (100%)	165 (92%)	15 (8%)	11 37
3	M	180/180 (100%)	165 (92%)	15 (8%)	11 37
3	N	180/180 (100%)	162 (90%)	18 (10%)	7 28
3	O	180/180 (100%)	168 (93%)	12 (7%)	16 47
All	All	2280/2360 (97%)	2113 (93%)	167 (7%)	14 43

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	126	SER
1	A	138	SER
1	A	139	SER
1	A	145	SER
1	A	174	SER
1	A	178	LEU
1	A	179	SER
1	A	206	GLN
1	A	249	THR
1	A	280	SER
1	A	284	ILE
2	H	23	THR
2	H	31	THR
2	H	67	SER
2	H	141	SER
2	H	149	LEU
2	H	189	LEU

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Mol	Chain	Res	Type
2	H	195	VAL
2	H	198	SER
2	H	199	SER
2	H	208	ASN
2	H	212	LYS
2	H	217	LYS
2	H	220	LYS
3	L	8	SER
3	L	65	ASP
3	L	101	VAL
3	L	114	SER
3	L	121	THR
3	L	138	VAL
3	L	149	VAL
3	L	150	THR
3	L	157	SER
3	L	160	VAL
3	L	198	CYS
3	L	201	THR
3	L	205	SER
3	L	213	PRO
3	L	216	CYS
1	B	78	ILE
1	B	138	SER
1	B	139	SER
1	B	149	VAL
1	B	178	LEU
1	B	202	SER
1	B	207	SER
1	B	231	ILE
1	B	237	VAL
1	B	251	VAL
2	I	1	GLN
2	I	12	VAL
2	I	17	THR
2	I	23	THR
2	I	30	ASN
2	I	67	SER
2	I	83	SER
2	I	86	SER
2	I	88	THR
2	I	106	THR

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Mol	Chain	Res	Type
2	I	126	SER
2	I	140	LYS
2	I	154	LYS
2	I	155	ASP
2	I	167	SER
2	I	182	GLN
2	I	199	SER
2	I	204	THR
2	I	227	CYS
3	M	12	SER
3	M	27	SER
3	M	30	SER
3	M	90	ASP
3	M	114	SER
3	M	139	CYS
3	M	142	SER
3	M	143	ASP
3	M	144	PHE
3	M	149	VAL
3	M	150	THR
3	M	166	THR
3	M	185	LEU
3	M	186	THR
3	M	188	GLU
1	C	112	PHE
1	C	138	SER
1	C	139	SER
1	C	178	LEU
1	C	180	LYS
1	C	204	ASP
1	C	207	SER
1	C	216	VAL
1	C	237	VAL
1	C	249	THR
1	C	267	VAL
1	C	282	ILE
2	J	17	THR
2	J	23	THR
2	J	24	VAL
2	J	31	THR
2	J	59	SER
2	J	70	THR

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Mol	Chain	Res	Type
2	J	88	THR
2	J	104	ILE
2	J	127	THR
2	J	152	LEU
2	J	154	LYS
2	J	171	THR
2	J	186	LEU
2	J	209	VAL
2	J	221	ARG
3	N	8	SER
3	N	14	SER
3	N	15	LEU
3	N	30	SER
3	N	31	THR
3	N	34	ILE
3	N	40	ARG
3	N	46	ARG
3	N	58	THR
3	N	82	SER
3	N	90	ASP
3	N	127	SER
3	N	130	LEU
3	N	150	THR
3	N	165	GLU
3	N	186	THR
3	N	192	SER
3	N	197	SER
1	D	71	LYS
1	D	99	THR
1	D	104	ASN
1	D	112	PHE
1	D	126	SER
1	D	179	SER
1	D	180	LYS
1	D	216	VAL
1	D	251	VAL
1	D	275	GLU
2	K	15	SER
2	K	25	SER
2	K	75	THR
2	K	81	SER
2	K	85	ARG

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Mol	Chain	Res	Type
2	K	122	VAL
2	K	141	SER
2	K	149	LEU
2	K	151	CYS
2	K	164	SER
2	K	172	SER
2	K	175	HIS
2	K	195	VAL
2	K	200	SER
2	K	207	CYS
2	K	227	CYS
3	O	8	SER
3	O	10	SER
3	O	18	SER
3	O	30	SER
3	O	65	ASP
3	O	85	SER
3	O	94	GLN
3	O	119	SER
3	O	126	SER
3	O	160	VAL
3	O	184	SER
3	O	185	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
3	L	84	GLN
3	L	94	GLN
1	B	121	GLN
2	I	5	GLN
2	I	182	GLN
2	I	208	ASN
3	M	94	GLN
3	M	113	GLN
1	C	121	GLN
2	J	116	GLN
2	J	166	ASN
3	N	2	GLN
1	D	173	ASN
2	K	30	ASN

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Mol	Chain	Res	Type
3	O	84	GLN
3	O	133	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
6	ACT	D	503	-	3,3,3	0.75	0	3,3,3	0.79	0
4	NAG	A	501	1	14,14,15	0.57	0	17,19,21	1.96	2 (11%)
4	NAG	D	501	1	14,14,15	0.58	0	17,19,21	1.31	2 (11%)
4	NAG	C	501	1	14,14,15	0.57	0	17,19,21	1.06	1 (5%)
4	NAG	B	501	1	14,14,15	0.91	0	17,19,21	1.73	4 (23%)
6	ACT	B	503	-	3,3,3	0.78	0	3,3,3	0.87	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	C	501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	NAG	C1-O5-C5	7.21	121.97	112.19
4	B	501	NAG	C2-N2-C7	3.55	127.96	122.90
4	C	501	NAG	C1-O5-C5	2.82	116.02	112.19
4	B	501	NAG	C1-O5-C5	2.67	115.82	112.19
4	D	501	NAG	O5-C5-C6	2.64	111.35	107.20
4	B	501	NAG	C1-C2-N2	2.41	114.61	110.49
4	D	501	NAG	C2-N2-C7	2.34	126.23	122.90
4	A	501	NAG	O7-C7-C8	-2.12	118.12	122.06
4	B	501	NAG	O5-C5-C6	2.08	110.46	107.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C4-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6
4	C	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	1	0

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	223/235 (94%)	-0.53	1 (0%) 92 89	34, 55, 110, 171	0
1	B	221/235 (94%)	-0.18	12 (5%) 25 13	42, 72, 155, 183	0
1	C	223/235 (94%)	-0.49	3 (1%) 77 66	40, 62, 112, 169	0
1	D	221/235 (94%)	-0.37	9 (4%) 37 22	33, 60, 136, 196	0
2	H	230/238 (96%)	-0.21	14 (6%) 21 11	33, 67, 150, 226	0
2	I	230/238 (96%)	0.62	43 (18%) 1 0	43, 76, 223, 261	0
2	J	230/238 (96%)	0.24	24 (10%) 6 3	46, 95, 186, 200	0
2	K	230/238 (96%)	0.19	29 (12%) 3 2	33, 86, 182, 212	0
3	L	216/216 (100%)	-0.58	4 (1%) 66 53	32, 56, 88, 202	0
3	M	216/216 (100%)	0.53	39 (18%) 1 1	43, 81, 219, 268	0
3	N	216/216 (100%)	-0.12	5 (2%) 60 46	43, 95, 145, 197	0
3	O	216/216 (100%)	-0.20	7 (3%) 47 30	30, 65, 155, 191	0
All	All	2672/2756 (96%)	-0.09	190 (7%) 16 8	30, 69, 183, 268	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	282	ILE	11.8
2	H	227	CYS	10.7
1	D	281	GLY	9.9
2	I	196	PRO	9.2
3	M	216	CYS	7.6
3	M	214	THR	7.3
2	J	227	CYS	7.1
2	I	137	PRO	7.0
3	N	214	THR	7.0
2	K	230	THR	6.9
3	O	214	THR	6.9

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Mol	Chain	Res	Type	RSRZ
3	L	216	CYS	6.9
2	I	195	VAL	6.8
2	I	138	SER	6.8
3	O	216	CYS	6.8
2	J	230	THR	6.8
2	H	230	THR	6.7
1	B	282	ILE	6.4
3	M	215	GLU	6.3
2	I	139	SER	6.3
2	I	164	SER	6.2
2	K	199	SER	6.2
2	K	227	CYS	6.0
2	I	228	ASP	6.0
2	J	228	ASP	5.9
1	B	279	GLY	5.8
2	J	143	SER	5.8
1	B	281	GLY	5.8
2	H	141	SER	5.7
3	M	188	GLU	5.6
1	B	280	SER	5.6
2	K	142	ALA	5.6
2	I	168	GLY	5.6
1	B	285	SER	5.4
2	J	139	SER	5.3
2	K	145	GLY	5.3
2	I	227	CYS	5.2
2	H	142	ALA	5.1
3	M	217	SER	5.1
3	N	215	GLU	5.0
1	B	284	ILE	4.9
2	I	208	ASN	4.9
3	M	132	ALA	4.9
2	K	143	SER	4.8
2	J	144	GLY	4.8
2	J	142	ALA	4.8
2	I	198	SER	4.8
2	I	136	ALA	4.8
3	O	217	SER	4.7
2	K	229	LYS	4.7
2	I	218	VAL	4.7
2	K	141	SER	4.7
2	K	228	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
3	M	204	GLY	4.7
2	J	202	THR	4.6
1	D	285	SER	4.6
2	I	144	GLY	4.6
2	J	224	PRO	4.6
2	K	139	SER	4.6
2	J	138	SER	4.5
2	I	143	SER	4.5
3	M	212	ALA	4.5
3	M	213	PRO	4.5
2	K	144	GLY	4.5
3	M	205	SER	4.4
2	I	204	THR	4.4
1	D	280	SER	4.4
3	O	215	GLU	4.4
2	I	142	ALA	4.3
2	K	202	THR	4.3
2	I	200	SER	4.3
2	I	146	THR	4.3
3	M	210	THR	4.3
2	I	141	SER	4.3
2	I	201	GLY	4.2
3	N	217	SER	4.2
3	M	161	LYS	4.1
2	H	199	SER	4.1
2	I	131	SER	4.0
2	K	146	THR	4.0
3	M	195	SER	3.9
2	H	140	LYS	3.9
2	I	219	ASP	3.9
2	I	202	THR	3.8
3	N	216	CYS	3.8
2	J	229	LYS	3.7
2	I	145	GLY	3.7
3	O	131	GLN	3.7
3	L	214	THR	3.6
2	J	199	SER	3.6
2	J	141	SER	3.6
2	H	229	LYS	3.5
2	H	139	SER	3.5
1	D	279	GLY	3.5
3	M	157	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	144	GLY	3.5
2	I	167	SER	3.4
2	K	138	SER	3.4
3	O	194	ARG	3.4
2	I	229	LYS	3.4
1	D	284	ILE	3.3
2	J	145	GLY	3.3
2	I	203	GLN	3.3
2	K	201	GLY	3.3
2	I	212	LYS	3.2
2	J	196	PRO	3.2
2	H	202	THR	3.2
3	M	192	SER	3.2
2	J	226	SER	3.1
3	M	137	LEU	3.1
2	I	199	SER	3.1
2	H	143	SER	3.1
2	I	210	ASN	3.1
2	I	171	THR	3.0
3	M	122	LEU	3.0
2	J	198	SER	3.0
2	I	217	LYS	3.0
3	M	173	SER	3.0
2	I	230	THR	3.0
3	M	134	LYS	3.0
1	C	103	ASP	2.9
1	D	278	ALA	2.9
3	M	186	THR	2.9
2	K	171	THR	2.9
1	C	88	SER	2.8
2	K	198	SER	2.8
3	M	209	LYS	2.8
2	I	169	ALA	2.8
3	M	160	VAL	2.8
2	K	221	ARG	2.8
3	M	158	SER	2.7
3	M	198	CYS	2.7
3	M	162	ALA	2.7
2	I	151	CYS	2.6
1	B	87	LEU	2.6
2	I	221	ARG	2.6
3	L	217	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	228	ASP	2.6
2	K	168	GLY	2.6
3	M	194	ARG	2.6
3	M	139	CYS	2.6
2	K	196	PRO	2.6
2	K	226	SER	2.5
3	M	208	GLU	2.5
2	H	226	SER	2.5
2	J	140	LYS	2.5
2	I	183	SER	2.5
3	M	133	ASN	2.5
3	O	162	ALA	2.5
2	K	140	LYS	2.5
1	A	86	SER	2.5
2	J	197	SER	2.4
2	K	184	SER	2.4
1	B	100	PRO	2.4
1	B	101	SER	2.4
1	B	86	SER	2.4
3	M	203	GLU	2.4
1	D	88	SER	2.4
3	M	120	VAL	2.4
2	K	197	SER	2.3
3	M	119	SER	2.3
2	I	226	SER	2.3
2	I	132	VAL	2.3
2	J	146	THR	2.3
2	K	183	SER	2.3
3	M	138	VAL	2.2
3	L	215	GLU	2.2
2	J	215	ASN	2.2
2	I	140	LYS	2.2
2	K	169	ALA	2.2
2	K	215	ASN	2.2
1	B	85	GLU	2.2
2	H	145	GLY	2.2
2	J	225	LYS	2.1
3	M	159	PRO	2.1
2	K	213	PRO	2.1
3	M	184	SER	2.1
3	N	204	GLY	2.1
1	D	103	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	187	PRO	2.1
1	B	103	ASP	2.1
3	M	117	ALA	2.1
2	J	221	ARG	2.1
1	C	87	LEU	2.1
2	K	182	GLN	2.0
3	M	191	LYS	2.0
2	I	175	HIS	2.0
2	I	197	SER	2.0
3	M	131	GLN	2.0
2	J	219	ASP	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
4	NAG	B	501	14/15	0.83	0.31	97,120,125,127	0
4	NAG	D	501	14/15	0.86	0.31	116,127,130,132	0
4	NAG	C	501	14/15	0.88	0.27	111,122,127,129	0
4	NAG	A	501	14/15	0.88	0.29	80,103,112,117	0
6	ACT	B	503	4/4	0.92	0.25	58,60,63,66	0
6	ACT	D	503	4/4	0.93	0.20	51,51,57,58	0
5	CA	O	301	1/1	0.97	0.46	122,122,122,122	1
5	CA	A	502	1/1	0.98	0.09	69,69,69,69	0
5	CA	B	502	1/1	0.98	0.06	72,72,72,72	0
5	CA	C	502	1/1	0.98	0.07	71,71,71,71	0
5	CA	D	502	1/1	0.99	0.04	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.