



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 08:12 PM JST

PDB ID : 6A67
Title : Crystal structure of influenza A virus H5 hemagglutinin globular head in complex with the Fab of antibody FLD21.140
Authors : Wang, P.; Zuo, Y.; Sun, J.; Zhang, L.; Wang, X.
Deposited on : 2018-06-26
Resolution : 2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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

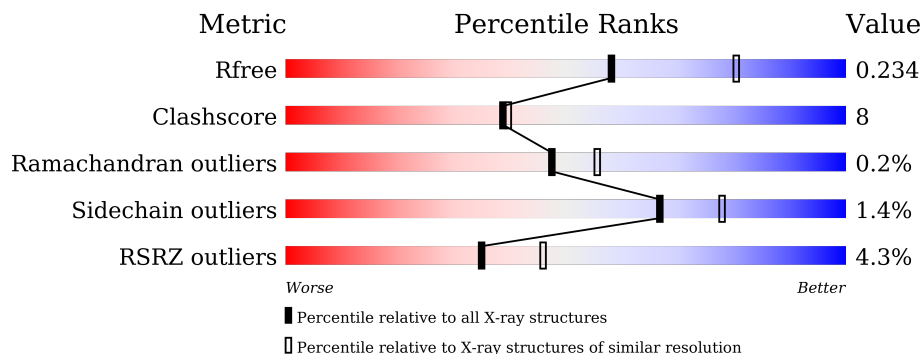
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	C	226	
1	H	226	
2	D	217	
2	L	217	
3	A	230	
3	B	230	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10252 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 FLD21.140 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	222	1661	1056	272	328	5	0	0	0
1	C	222	1661	1056	272	328	5	0	0	0

- Molecule 2 is a protein called FLD21.140 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1569	979	265	321	4	0	0	0
2	D	212	1569	979	265	321	4	0	0	0

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	204	1658	1060	285	307	6	0	1	0
3	A	205	1665	1065	286	308	6	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

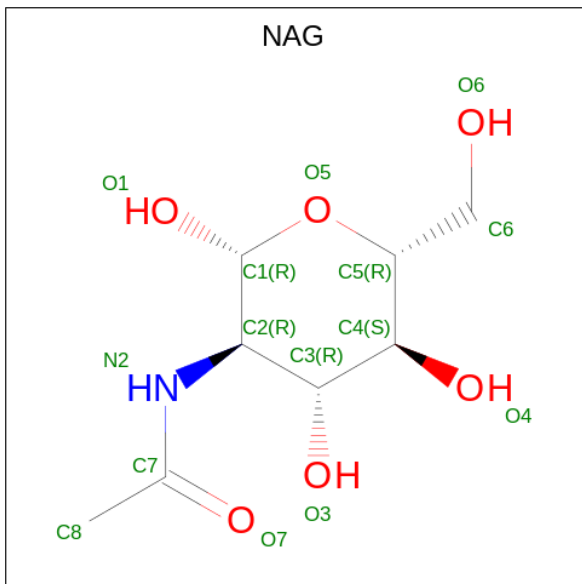
Chain	Residue	Modelled	Actual	Comment	Reference
B	269	HIS	-	expression tag	UNP Q6Q794
B	270	HIS	-	expression tag	UNP Q6Q794
B	271	HIS	-	expression tag	UNP Q6Q794
B	272	HIS	-	expression tag	UNP Q6Q794
B	273	HIS	-	expression tag	UNP Q6Q794
B	274	HIS	-	expression tag	UNP Q6Q794
A	269	HIS	-	expression tag	UNP Q6Q794
A	270	HIS	-	expression tag	UNP Q6Q794

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP Q6Q794
A	272	HIS	-	expression tag	UNP Q6Q794
A	273	HIS	-	expression tag	UNP Q6Q794
A	274	HIS	-	expression tag	UNP Q6Q794

- 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
			Total	C	N	O		
4	B	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	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	H	81	Total	O	0	0
			81	81		
5	L	59	Total	O	0	0
			59	59		
5	C	86	Total	O	0	0
			86	86		

Continued on next page...

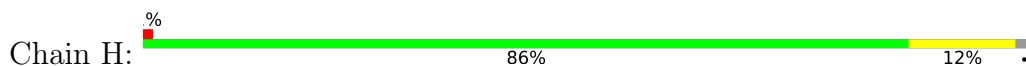
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	86	Total O 86 86	0	0
5	B	49	Total O 49 49	0	0
5	A	52	Total O 52 52	0	0

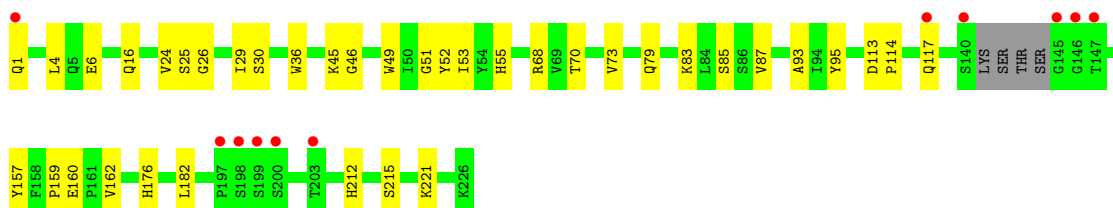
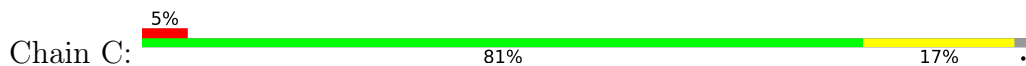
3 Residue-property plots [i](#)

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.

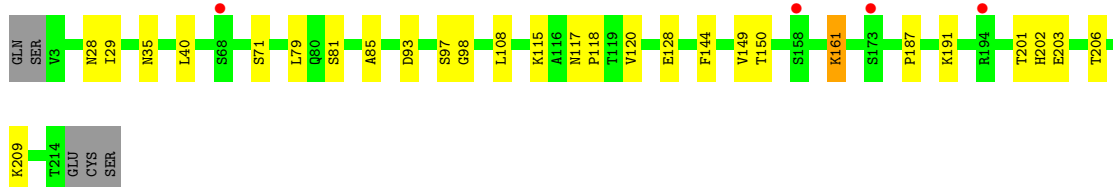
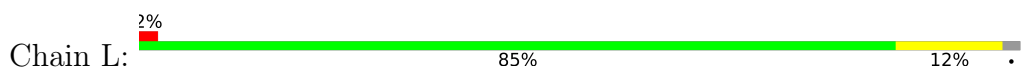
- Molecule 1: FLD21.140 Heavy Chain



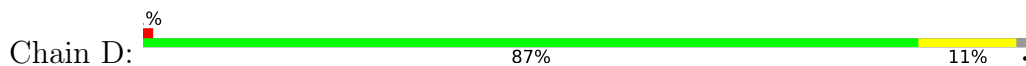
- Molecule 1: FLD21.140 Heavy Chain



- Molecule 2: FLD21.140 Light Chain

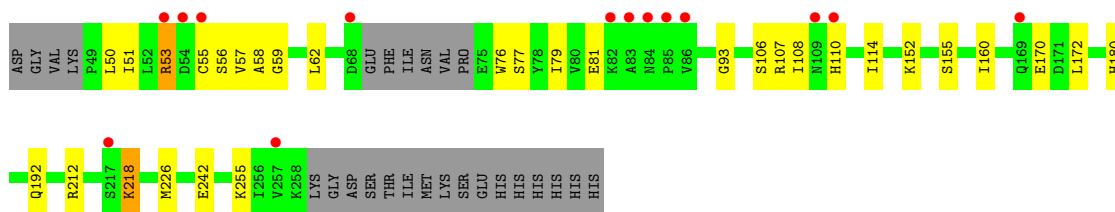


- Molecule 2: FLD21.140 Light Chain



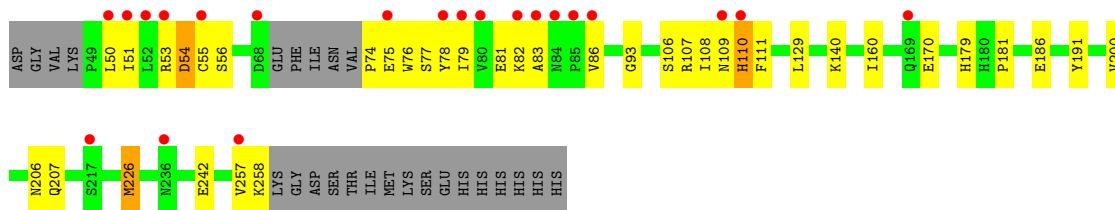
- Molecule 3: Hemagglutinin

Chain B: 6% 75% 13% 11%



• Molecule 3: Hemagglutinin

Chain A: 9% 73% 15% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.11Å 168.11Å 147.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.91 – 2.33 36.91 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.91-2.33) 99.5 (36.91-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.235 0.196 , 0.234	Depositor DCC
R_{free} test set	4414 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10252	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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	C	0.53	0/1706	0.69	0/2332
1	H	0.45	0/1706	0.65	0/2332
2	D	0.46	0/1608	0.65	0/2198
2	L	0.45	0/1608	0.63	0/2198
3	A	0.46	0/1714	0.67	0/2329
3	B	0.44	0/1706	0.65	0/2318
All	All	0.46	0/10048	0.66	0/13707

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	C	1661	0	1623	23	0
1	H	1661	0	1623	23	0
2	D	1569	0	1517	15	0
2	L	1569	0	1517	18	0
3	A	1665	0	1628	47	0
3	B	1658	0	1620	27	0
4	A	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	26	0	0
5	A	52	0	0	4	0
5	B	49	0	0	0	0
5	C	86	0	0	2	0
5	D	86	0	0	3	0
5	H	81	0	0	4	0
5	L	59	0	0	3	0
All	All	10252	0	9580	146	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 8.

All (146) 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:A:109:ASN:O	3:A:257:VAL:HG22	1.59	1.03
3:B:180:HIS:HD2	3:B:212:ARG:H	1.16	0.93
3:A:54:ASP:O	5:A:401:HOH:O	1.91	0.87
3:A:77:SER:O	3:A:107:ARG:N	2.07	0.87
3:B:152:LYS:HD2	3:B:192:GLN:HG2	1.56	0.86
2:D:13:THR:H	2:D:16:GLN:HE21	1.20	0.84
3:B:180:HIS:CD2	3:B:212:ARG:H	1.99	0.81
3:A:109:ASN:HB3	3:A:257:VAL:HG23	1.62	0.81
3:B:53:ARG:NH1	3:B:53:ARG:HB3	1.97	0.80
2:L:161:LYS:HD3	2:L:161:LYS:H	1.49	0.77
3:A:53:ARG:HH12	3:A:55:CYS:HB3	1.51	0.76
3:B:53:ARG:HB3	3:B:53:ARG:HH11	1.52	0.73
1:H:160:GLU:OE1	5:H:301:HOH:O	2.06	0.72
2:L:97:SER:OG	5:L:301:HOH:O	2.08	0.71
3:A:75:GLU:HG2	3:A:110:HIS:H	1.55	0.71
1:H:145:GLY:N	5:H:302:HOH:O	2.25	0.70
1:H:70:THR:HG23	1:H:83:LYS:HB2	1.76	0.67
1:C:159:PRO:O	1:C:212:HIS:HE1	1.78	0.67
3:B:51:ILE:HG23	3:B:79:ILE:HA	1.76	0.67
3:A:75:GLU:CG	3:A:110:HIS:H	2.08	0.66
3:A:53:ARG:NH1	3:A:55:CYS:HB3	2.10	0.66
3:B:53:ARG:HH11	3:B:53:ARG:CB	2.10	0.64
3:A:76:TRP:CZ2	3:A:108:ILE:HG12	2.33	0.64
3:A:110:HIS:HB2	3:A:257:VAL:CG2	2.27	0.64
2:D:13:THR:H	2:D:16:GLN:NE2	1.94	0.64
2:L:117:ASN:ND2	5:L:304:HOH:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:LYS:HD3	3:A:83:ALA:N	2.14	0.63
3:A:82:LYS:HD3	3:A:83:ALA:H	1.64	0.63
1:H:1:GLN:OE1	1:H:1:GLN:N	2.30	0.62
3:A:106:SER:O	3:A:258:LYS:NZ	2.33	0.62
3:A:109:ASN:O	3:A:110:HIS:O	2.18	0.61
3:A:109:ASN:C	3:A:257:VAL:HG22	2.21	0.61
3:A:109:ASN:O	3:A:257:VAL:CG2	2.42	0.61
1:C:30:SER:HA	1:C:55:HIS:CG	2.35	0.61
1:H:4:LEU:HD22	1:H:24:VAL:HG22	1.84	0.59
2:L:161:LYS:HD3	2:L:161:LYS:N	2.18	0.58
1:H:53:ILE:HD13	1:H:73:VAL:HG23	1.86	0.58
3:B:180:HIS:HD2	3:B:212:ARG:N	1.96	0.57
3:A:55:CYS:SG	3:A:56:SER:N	2.79	0.56
2:D:62:ARG:HH22	2:D:83:ASP:CG	2.09	0.56
1:H:111:GLY:H	2:L:35:ASN:HD21	1.52	0.55
3:B:155:SER:O	3:B:192:GLN:HG3	2.06	0.55
1:C:30:SER:HA	1:C:55:HIS:CD2	2.42	0.55
3:A:93:GLY:HA3	3:A:226:MET:O	2.06	0.55
1:H:110:GLU:HB2	2:L:35:ASN:HD21	1.72	0.55
3:A:76:TRP:CE2	3:A:108:ILE:HG12	2.43	0.54
3:A:110:HIS:HB2	3:A:257:VAL:HG21	1.90	0.54
3:B:93:GLY:HA3	3:B:226:MET:O	2.08	0.54
3:A:179:HIS:HB2	3:A:226:MET:HE2	1.90	0.54
3:B:76:TRP:CZ2	3:B:108:ILE:HG12	2.43	0.53
3:A:110:HIS:HB2	3:A:257:VAL:HG22	1.89	0.53
3:B:50:LEU:N	3:B:50:LEU:HD22	2.23	0.53
1:H:13:LYS:HB2	1:H:16:GLN:HG3	1.91	0.53
1:H:102:ASN:HD22	3:A:140:LYS:NZ	2.07	0.53
2:L:150:THR:HB	2:L:201:THR:OG1	2.08	0.52
2:L:187:PRO:O	2:L:191:LYS:HD2	2.09	0.52
1:C:212:HIS:HD2	1:C:215:SER:OG	1.94	0.51
1:H:213:LYS:NZ	5:H:303:HOH:O	2.28	0.51
1:C:70:THR:HG23	1:C:83:LYS:HB2	1.93	0.51
2:D:79:LEU:HD11	2:D:108:LEU:HD21	1.92	0.51
1:C:53:ILE:HD13	1:C:73:VAL:HG23	1.91	0.51
1:H:111:GLY:H	2:L:35:ASN:ND2	2.09	0.51
1:C:160:GLU:HG3	5:C:311:HOH:O	2.11	0.51
3:B:55:CYS:SG	3:B:56:SER:N	2.84	0.51
3:A:179:HIS:HD2	3:A:191:TYR:OH	1.93	0.50
3:A:75:GLU:OE2	3:A:110:HIS:CD2	2.64	0.50
1:H:11:LEU:HD11	1:H:124:SER:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:128:GLU:OE1	5:L:302:HOH:O	2.20	0.50
1:H:6:GLU:OE1	1:H:6:GLU:N	2.43	0.50
1:H:53:ILE:HG13	1:H:59:ALA:HB2	1.94	0.49
3:B:51:ILE:HG12	3:B:53:ARG:NH2	2.27	0.49
2:D:62:ARG:NH2	2:D:83:ASP:OD1	2.44	0.49
3:A:75:GLU:HG2	3:A:110:HIS:N	2.23	0.49
3:A:86:VAL:N	5:A:401:HOH:O	2.45	0.49
3:A:109:ASN:ND2	3:A:110:HIS:HD2	2.10	0.49
3:A:53:ARG:NH2	3:A:55:CYS:O	2.45	0.49
3:A:50:LEU:HD21	3:A:78:TYR:CE1	2.47	0.49
3:A:55:CYS:HA	5:A:401:HOH:O	2.11	0.49
1:H:102:ASN:HD22	3:A:140:LYS:HZ1	1.61	0.49
2:D:175:ASN:ND2	5:D:307:HOH:O	2.46	0.49
2:L:79:LEU:HD11	2:L:108:LEU:HD21	1.93	0.49
3:A:53:ARG:HH12	3:A:55:CYS:CB	2.22	0.48
1:H:162:VAL:HG22	1:H:190:LEU:HD21	1.96	0.48
3:A:181:PRO:HB3	3:A:186:GLU:HG2	1.95	0.48
1:C:4:LEU:HD22	1:C:24:VAL:HG22	1.95	0.48
3:B:114:ILE:HD11	3:B:172:LEU:HD21	1.96	0.47
3:B:106:SER:O	3:B:107:ARG:HG2	2.13	0.47
1:C:93:ALA:HB3	1:C:95:TYR:CE1	2.50	0.47
2:D:62:ARG:NH1	2:D:77:SER:O	2.43	0.47
3:A:74:PRO:O	3:A:75:GLU:HG3	2.15	0.47
1:C:6:GLU:OE1	1:C:6:GLU:N	2.38	0.46
2:L:40:LEU:HD23	2:L:85:ALA:HB2	1.96	0.46
1:H:54:TYR:CE1	3:A:129:LEU:HD21	2.51	0.46
1:H:49:TRP:CZ2	1:H:51:GLY:HA2	2.50	0.46
3:A:109:ASN:C	3:A:257:VAL:CG2	2.84	0.46
3:B:218:LYS:HE2	3:B:218:LYS:HB2	1.66	0.46
2:L:93:ASP:O	2:L:98:GLY:HA2	2.16	0.46
3:A:170:GLU:N	3:A:170:GLU:OE1	2.48	0.46
2:D:201:THR:HG22	2:D:206:THR:OG1	2.17	0.45
1:C:79:GLN:NE2	5:C:304:HOH:O	2.46	0.45
1:C:1:GLN:NE2	1:C:26:GLY:O	2.44	0.45
2:D:118:PRO:HB3	2:D:144:PHE:HB3	1.98	0.45
3:B:170:GLU:OE1	3:B:255:LYS:HD2	2.17	0.45
1:H:6:GLU:OE1	1:H:117:GLN:O	2.35	0.45
3:B:56:SER:OG	3:B:58:ALA:O	2.29	0.45
2:L:28:ASN:OD1	2:L:29:ILE:N	2.43	0.44
2:L:118:PRO:HB3	2:L:144:PHE:HB3	2.00	0.44
3:B:57:VAL:HG23	3:B:81:GLU:OE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ARG:HD2	1:C:85:SER:O	2.17	0.44
3:A:200:VAL:HB	3:A:207:GLN:HB2	2.00	0.44
3:A:53:ARG:CZ	3:A:53:ARG:HB2	2.46	0.44
3:B:160:ILE:O	3:B:242:GLU:HA	2.18	0.43
1:C:6:GLU:OE1	1:C:117:GLN:O	2.37	0.43
3:A:206:ASN:HB3	5:A:436:HOH:O	2.17	0.43
1:H:41:HIS:HD2	1:H:46:GLY:O	2.02	0.43
2:L:120:VAL:O	2:L:209:LYS:HE3	2.19	0.43
3:A:160:ILE:O	3:A:242:GLU:HA	2.19	0.43
1:C:221:LYS:HD2	1:C:221:LYS:HA	1.73	0.43
2:L:149:VAL:HG12	2:L:202:HIS:HB2	2.01	0.43
3:A:179:HIS:CD2	3:A:191:TYR:OH	2.72	0.43
3:B:76:TRP:CZ3	3:B:108:ILE:HD11	2.54	0.43
2:L:206:THR:CG2	1:C:182:LEU:HD21	2.49	0.42
3:B:53:ARG:NH1	3:B:53:ARG:CB	2.72	0.42
3:A:81:GLU:HG2	3:A:82:LYS:O	2.18	0.42
1:C:49:TRP:CZ2	1:C:51:GLY:HA2	2.54	0.42
3:B:50:LEU:HD13	3:B:77:SER:OG	2.19	0.42
2:D:3:VAL:N	5:D:314:HOH:O	2.52	0.42
1:C:29:ILE:HG12	1:C:36:TRP:CE2	2.55	0.42
2:D:197:SER:OG	2:D:210:THR:HG22	2.20	0.42
1:C:157:TYR:CE2	1:C:162:VAL:HG13	2.55	0.42
2:D:35:ASN:ND2	2:D:50:TYR:HA	2.34	0.42
2:D:125:PRO:HD3	2:D:137:LEU:CD2	2.50	0.42
2:D:155:ALA:HB2	2:D:196:TYR:CE2	2.55	0.42
3:A:53:ARG:HH12	3:A:55:CYS:C	2.23	0.41
3:A:51:ILE:CG2	3:A:79:ILE:HG12	2.51	0.41
3:A:108:ILE:HD13	3:A:111:PHE:HB2	2.03	0.41
1:H:162:VAL:CG2	1:H:190:LEU:HD21	2.49	0.41
1:C:113:ASP:HA	1:C:114:PRO:HA	1.95	0.41
1:C:29:ILE:O	1:C:30:SER:OG	2.22	0.41
3:B:59:GLY:HA2	3:B:62:LEU:HB2	2.02	0.41
1:H:117:GLN:HG2	5:H:343:HOH:O	2.20	0.40
1:C:45:LYS:HB3	1:C:46:GLY:H	1.76	0.40
1:C:16:GLN:O	1:C:87:VAL:HG22	2.22	0.40
3:B:53:ARG:CD	3:B:55:CYS:O	2.70	0.40
2:D:161:LYS:HG2	5:D:369:HOH:O	2.21	0.40
3:B:51:ILE:HD11	3:B:53:ARG:HH22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	218/226 (96%)	211 (97%)	7 (3%)	0	100	100
1	H	218/226 (96%)	212 (97%)	6 (3%)	0	100	100
2	D	210/217 (97%)	205 (98%)	5 (2%)	0	100	100
2	L	210/217 (97%)	205 (98%)	5 (2%)	0	100	100
3	A	202/230 (88%)	196 (97%)	5 (2%)	1 (0%)	29	31
3	B	201/230 (87%)	195 (97%)	5 (2%)	1 (0%)	29	31
All	All	1259/1346 (94%)	1224 (97%)	33 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	110	HIS
3	A	110	HIS

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	C	189/193 (98%)	186 (98%)	3 (2%)	62	74
1	H	189/193 (98%)	188 (100%)	1 (0%)	88	93
2	D	176/181 (97%)	174 (99%)	2 (1%)	73	83
2	L	176/181 (97%)	171 (97%)	5 (3%)	43	53
3	A	187/209 (90%)	185 (99%)	2 (1%)	73	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	186/209 (89%)	184 (99%)	2 (1%)	73	83
All	All	1103/1166 (95%)	1088 (99%)	15 (1%)	67	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	52	TYR
2	L	71	SER
2	L	81	SER
2	L	115	LYS
2	L	161	LYS
2	L	203	GLU
1	C	25	SER
1	C	52	TYR
1	C	176	HIS
2	D	71	SER
2	D	194	ARG
3	B	53	ARG
3	B	218	LYS
3	A	54	ASP
3	A	226	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	41	HIS
1	H	102	ASN
2	L	35	ASN
1	C	79	GLN
1	C	212	HIS
2	D	16	GLN
2	D	131	GLN
3	B	180	HIS
3	A	110	HIS
3	A	179	HIS

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](#)

4 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	302	3	14,14,15	0.60	0	17,19,21	0.64	1 (5%)
4	NAG	A	301	3	14,14,15	1.06	2 (14%)	17,19,21	0.74	0
4	NAG	B	301	3	14,14,15	0.42	0	17,19,21	0.52	0
4	NAG	B	302	3	14,14,15	0.49	0	17,19,21	0.73	1 (5%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	302	3	-	0/6/23/26	0/1/1/1
4	NAG	A	301	3	-	1/6/23/26	0/1/1/1
4	NAG	B	301	3	-	2/6/23/26	0/1/1/1
4	NAG	B	302	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	NAG	C1-C2	3.20	1.57	1.52
4	A	301	NAG	O5-C1	-2.17	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	NAG	C1-O5-C5	2.56	115.67	112.19
4	A	302	NAG	C1-O5-C5	2.23	115.21	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	NAG	C4-C5-C6-O6
4	B	302	NAG	C4-C5-C6-O6
4	B	301	NAG	O5-C5-C6-O6
4	B	302	NAG	O5-C5-C6-O6
4	A	301	NAG	C4-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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	C	222/226 (98%)	0.12	11 (4%) 28 39	29, 40, 66, 90	0
1	H	222/226 (98%)	-0.06	2 (0%) 84 89	28, 40, 70, 116	0
2	D	212/217 (97%)	-0.13	3 (1%) 75 82	30, 43, 70, 106	0
2	L	212/217 (97%)	-0.07	4 (1%) 66 75	30, 48, 85, 107	0
3	A	205/230 (89%)	0.29	21 (10%) 6 11	29, 47, 99, 129	0
3	B	204/230 (88%)	0.24	14 (6%) 16 24	30, 48, 94, 110	0
All	All	1277/1346 (94%)	0.06	55 (4%) 35 46	28, 44, 83, 129	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	GLY	13.2
1	C	146	GLY	6.4
3	B	86	VAL	5.7
3	B	84	ASN	4.7
3	A	51	ILE	4.6
3	A	80	VAL	4.6
3	A	86	VAL	4.4
3	B	83	ALA	4.4
3	A	52	LEU	4.2
3	A	110	HIS	3.9
3	A	68	ASP	3.8
3	A	84	ASN	3.7
3	A	85	PRO	3.6
1	C	140	SER	3.6
1	C	197	PRO	3.6
2	D	161	LYS	3.4
3	B	68	ASP	3.4
3	B	109	ASN	3.3
3	A	55	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	198	SER	3.2
3	A	75	GLU	3.2
3	A	53	ARG	3.1
3	B	55	CYS	3.1
1	C	199	SER	3.1
3	B	257	VAL	3.0
3	A	78	TYR	3.0
3	A	109	ASN	3.0
3	B	82	LYS	3.0
3	A	236	ASN	3.0
1	C	147	THR	2.9
3	B	85	PRO	2.9
1	C	1	GLN	2.8
3	B	110	HIS	2.8
3	A	50	LEU	2.7
3	A	83	ALA	2.7
1	C	203	THR	2.7
2	L	173	SER	2.6
1	H	140	SER	2.6
3	A	257	VAL	2.6
1	C	117	GLN	2.5
2	L	68	SER	2.5
3	A	82	LYS	2.5
1	H	1	GLN	2.5
3	A	79	ILE	2.4
2	D	158	SER	2.4
3	B	54	ASP	2.3
3	B	53	ARG	2.2
2	L	194	ARG	2.2
1	C	200	SER	2.2
3	A	217	SER	2.2
3	A	169	GLN	2.1
3	B	169	GLN	2.1
2	L	158	SER	2.1
2	D	117	ASN	2.1
3	B	217	SER	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(Å ²)	Q<0.9
4	NAG	A	301	14/15	0.73	0.23	83,94,103,109	0
4	NAG	B	302	14/15	0.85	0.28	67,76,86,87	0
4	NAG	B	301	14/15	0.85	0.34	84,96,110,111	0
4	NAG	A	302	14/15	0.89	0.22	58,81,89,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.