Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2023 – 01:53 AM JST

PDB ID	:	7FAH
Title	:	Immune complex of head region of CA09 HA and neutralizing antibody 12H5
Authors	:	Li, T.T.; Xue, W.H.; Gu, Y.; Li, S.W.
Deposited on	:	2021-07-06
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 (i)) were used in the production of this report:

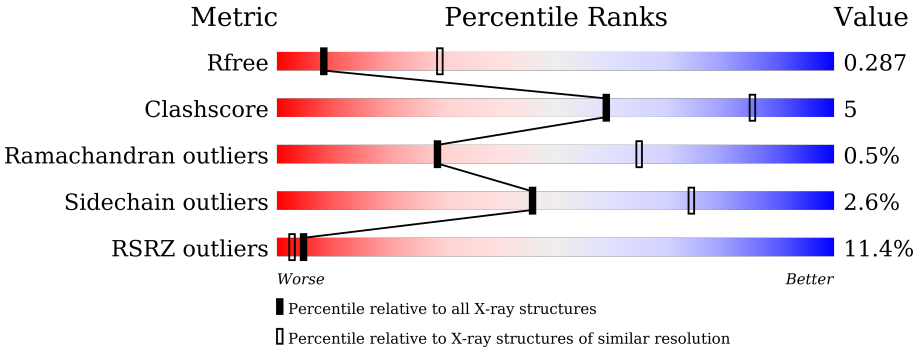
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	548	31% 8% 61%
1	B	548	30% 9% 61%
2	C	217	23% 89% 11%
2	H	217	10% 87% 12% •
3	D	218	24% 89% 9% •
3	L	218	10% 88% 11% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10066 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
			Total	C	N	O	S			
1	A	214	1705	1089	287	323	6	0	0	0
1	B	214	1705	1089	287	323	6	0	0	0

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP C3W5S1
A	511	SER	-	expression tag	UNP C3W5S1
A	512	GLY	-	expression tag	UNP C3W5S1
A	513	ARG	-	expression tag	UNP C3W5S1
A	514	LEU	-	expression tag	UNP C3W5S1
A	515	VAL	-	expression tag	UNP C3W5S1
A	516	PRO	-	expression tag	UNP C3W5S1
A	517	ARG	-	expression tag	UNP C3W5S1
A	518	GLY	-	expression tag	UNP C3W5S1
A	519	SER	-	expression tag	UNP C3W5S1
A	520	PRO	-	expression tag	UNP C3W5S1
A	521	GLY	-	expression tag	UNP C3W5S1
A	522	SER	-	expression tag	UNP C3W5S1
A	523	GLY	-	expression tag	UNP C3W5S1
A	524	TYR	-	expression tag	UNP C3W5S1
A	525	ILE	-	expression tag	UNP C3W5S1
A	526	PRO	-	expression tag	UNP C3W5S1
A	527	GLU	-	expression tag	UNP C3W5S1
A	528	ALA	-	expression tag	UNP C3W5S1
A	529	PRO	-	expression tag	UNP C3W5S1
A	530	ARG	-	expression tag	UNP C3W5S1
A	531	ASP	-	expression tag	UNP C3W5S1
A	532	GLY	-	expression tag	UNP C3W5S1
A	533	GLN	-	expression tag	UNP C3W5S1
A	534	ALA	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	TYR	-	expression tag	UNP C3W5S1
A	536	VAL	-	expression tag	UNP C3W5S1
A	537	ARG	-	expression tag	UNP C3W5S1
A	538	LYS	-	expression tag	UNP C3W5S1
A	539	ASP	-	expression tag	UNP C3W5S1
A	540	GLY	-	expression tag	UNP C3W5S1
A	541	GLU	-	expression tag	UNP C3W5S1
A	542	TRP	-	expression tag	UNP C3W5S1
A	543	VAL	-	expression tag	UNP C3W5S1
A	544	LEU	-	expression tag	UNP C3W5S1
A	545	LEU	-	expression tag	UNP C3W5S1
A	546	SER	-	expression tag	UNP C3W5S1
A	547	THR	-	expression tag	UNP C3W5S1
A	548	PHE	-	expression tag	UNP C3W5S1
A	549	LEU	-	expression tag	UNP C3W5S1
A	550	GLY	-	expression tag	UNP C3W5S1
A	551	HIS	-	expression tag	UNP C3W5S1
A	552	HIS	-	expression tag	UNP C3W5S1
A	553	HIS	-	expression tag	UNP C3W5S1
A	554	HIS	-	expression tag	UNP C3W5S1
A	555	HIS	-	expression tag	UNP C3W5S1
A	556	HIS	-	expression tag	UNP C3W5S1
B	9	MET	-	initiating methionine	UNP C3W5S1
B	511	SER	-	expression tag	UNP C3W5S1
B	512	GLY	-	expression tag	UNP C3W5S1
B	513	ARG	-	expression tag	UNP C3W5S1
B	514	LEU	-	expression tag	UNP C3W5S1
B	515	VAL	-	expression tag	UNP C3W5S1
B	516	PRO	-	expression tag	UNP C3W5S1
B	517	ARG	-	expression tag	UNP C3W5S1
B	518	GLY	-	expression tag	UNP C3W5S1
B	519	SER	-	expression tag	UNP C3W5S1
B	520	PRO	-	expression tag	UNP C3W5S1
B	521	GLY	-	expression tag	UNP C3W5S1
B	522	SER	-	expression tag	UNP C3W5S1
B	523	GLY	-	expression tag	UNP C3W5S1
B	524	TYR	-	expression tag	UNP C3W5S1
B	525	ILE	-	expression tag	UNP C3W5S1
B	526	PRO	-	expression tag	UNP C3W5S1
B	527	GLU	-	expression tag	UNP C3W5S1
B	528	ALA	-	expression tag	UNP C3W5S1
B	529	PRO	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	530	ARG	-	expression tag	UNP C3W5S1
B	531	ASP	-	expression tag	UNP C3W5S1
B	532	GLY	-	expression tag	UNP C3W5S1
B	533	GLN	-	expression tag	UNP C3W5S1
B	534	ALA	-	expression tag	UNP C3W5S1
B	535	TYR	-	expression tag	UNP C3W5S1
B	536	VAL	-	expression tag	UNP C3W5S1
B	537	ARG	-	expression tag	UNP C3W5S1
B	538	LYS	-	expression tag	UNP C3W5S1
B	539	ASP	-	expression tag	UNP C3W5S1
B	540	GLY	-	expression tag	UNP C3W5S1
B	541	GLU	-	expression tag	UNP C3W5S1
B	542	TRP	-	expression tag	UNP C3W5S1
B	543	VAL	-	expression tag	UNP C3W5S1
B	544	LEU	-	expression tag	UNP C3W5S1
B	545	LEU	-	expression tag	UNP C3W5S1
B	546	SER	-	expression tag	UNP C3W5S1
B	547	THR	-	expression tag	UNP C3W5S1
B	548	PHE	-	expression tag	UNP C3W5S1
B	549	LEU	-	expression tag	UNP C3W5S1
B	550	GLY	-	expression tag	UNP C3W5S1
B	551	HIS	-	expression tag	UNP C3W5S1
B	552	HIS	-	expression tag	UNP C3W5S1
B	553	HIS	-	expression tag	UNP C3W5S1
B	554	HIS	-	expression tag	UNP C3W5S1
B	555	HIS	-	expression tag	UNP C3W5S1
B	556	HIS	-	expression tag	UNP C3W5S1

- Molecule 2 is a protein called heavy chain of antibody 12H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1641	1039	275	318	9	0	0	0
			Total	C	N	O	S			
2	C	217	1641	1039	275	318	9	0	0	0

- Molecule 3 is a protein called Light chain of antibody 12H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	215	1661	1037	277	342	5	0	0	0

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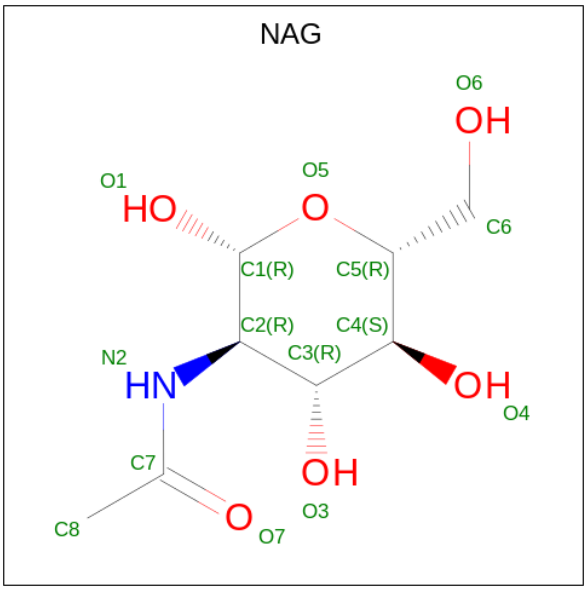
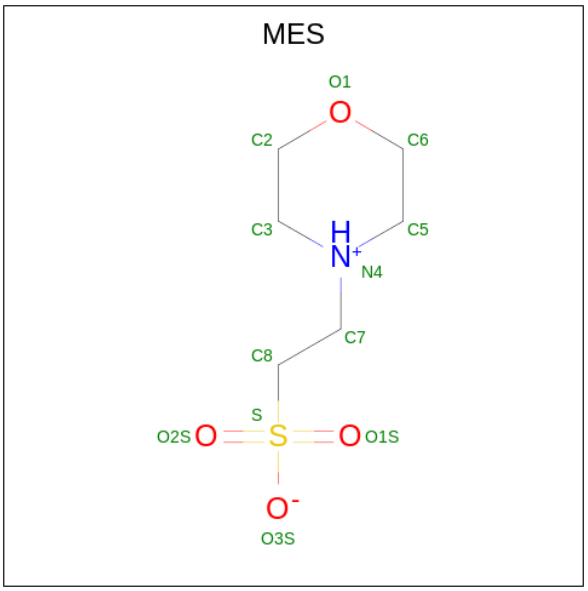
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	215	1661	1037	277	342	5	0	0	0

- 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	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



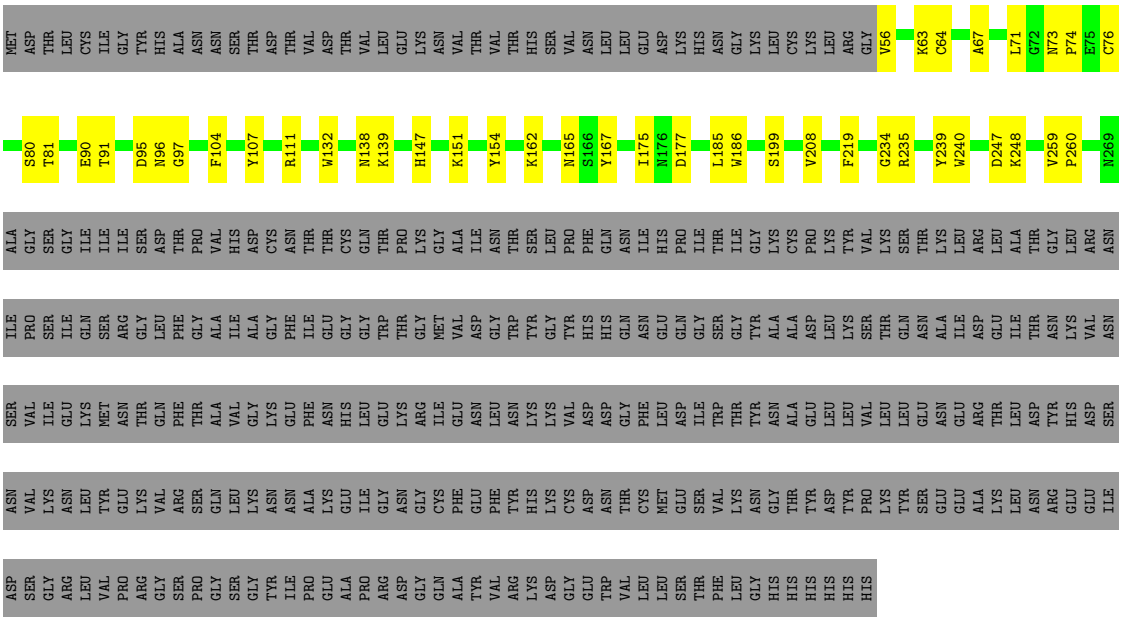
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	H	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	C	1	12	6	1	4	1	0	0

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.

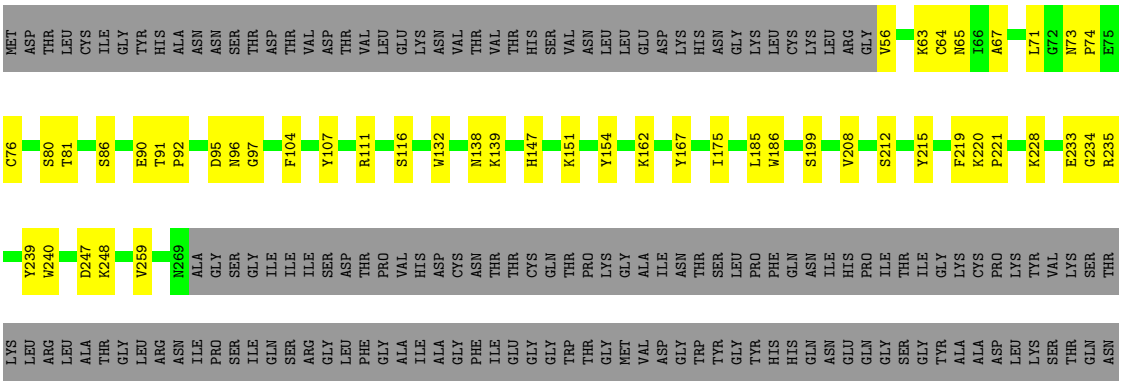
• Molecule 1: Hemagglutinin

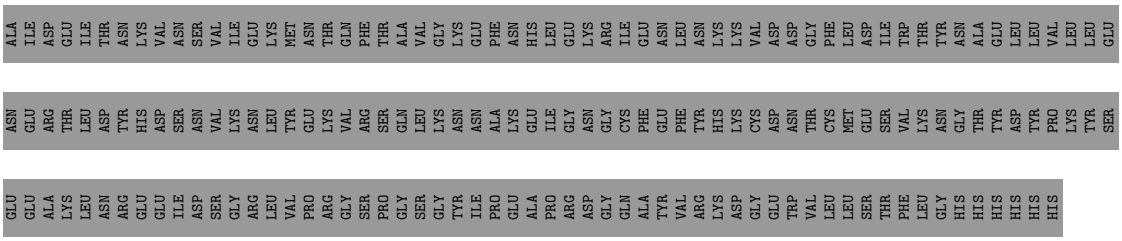
Chain A: 31% 8% 61%



• Molecule 1: Hemagglutinin

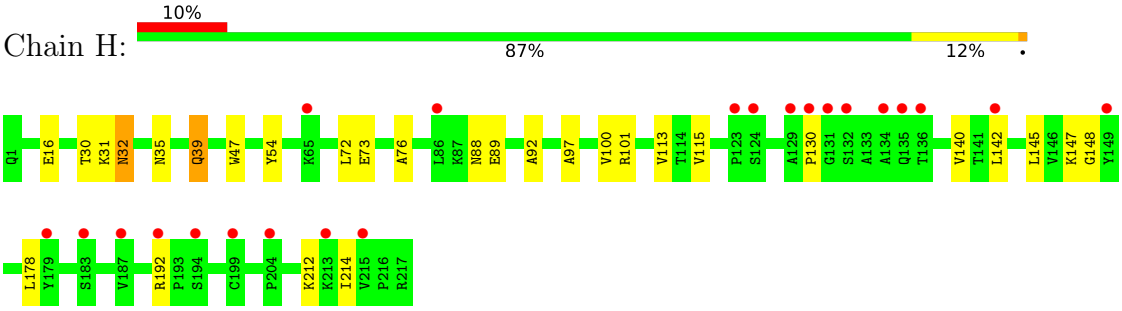
Chain B: 30% 9% 61%





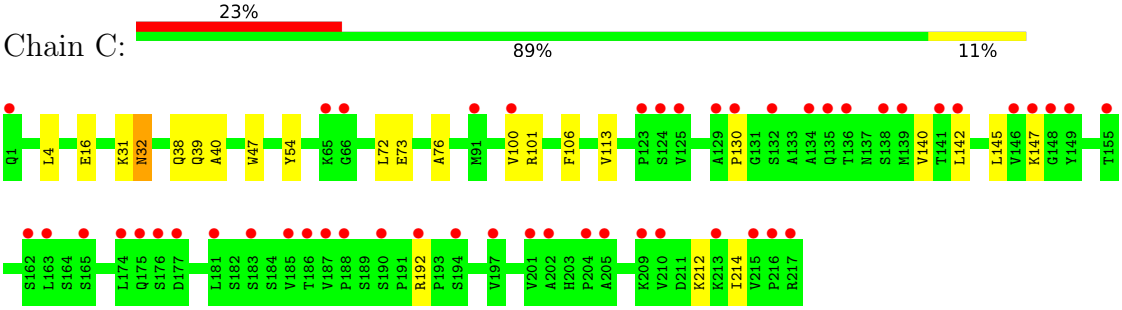
- Molecule 2: heavy chain of antibody 12H5

Chain H:



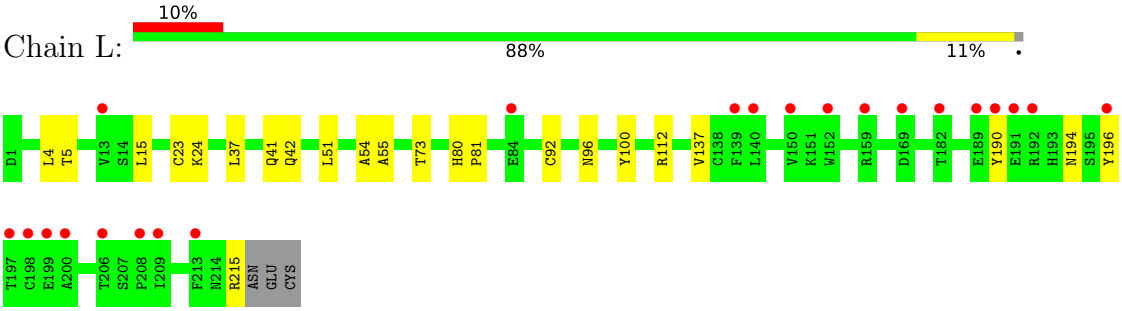
- Molecule 2: heavy chain of antibody 12H5

Chain C:



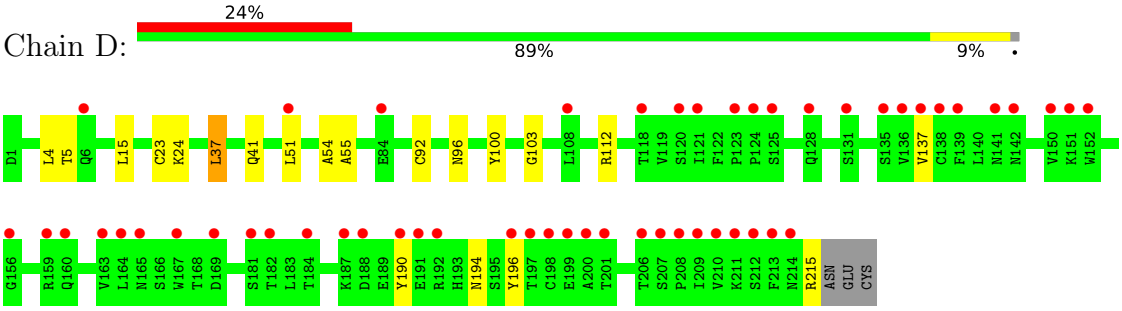
- Molecule 3: Light chain of antibody 12H5

Chain L:



- Molecule 3: Light chain of antibody 12H5

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.74Å 51.12Å 168.25Å 90.00° 106.90° 90.00°	Depositor
Resolution (Å)	38.61 – 3.15 38.61 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.61-3.15) 90.5 (38.61-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.266 , 0.289 0.266 , 0.287	Depositor DCC
R_{free} test set	1495 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 25.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.145 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10066	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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 (i)

5.1 Standard geometry (i)

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

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	0.28	0/1755	0.45	0/2383
1	B	0.28	0/1755	0.46	0/2383
2	C	0.27	0/1684	0.47	0/2298
2	H	0.27	0/1684	0.48	0/2298
3	D	0.25	0/1700	0.46	0/2312
3	L	0.25	0/1700	0.46	0/2312
All	All	0.27	0/10278	0.47	0/13986

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	1705	0	1639	22	0
1	B	1705	0	1639	23	0
2	C	1641	0	1614	13	0
2	H	1641	0	1614	16	0
3	D	1661	0	1577	12	0
3	L	1661	0	1577	13	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
5	C	12	0	13	1	0
5	H	12	0	13	0	0
All	All	10066	0	9712	92	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 5.

All (92) 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:88:ASN:ND2	2:H:115:VAL:O	2.13	0.81
1:B:95:ASP:O	1:B:97:GLY:N	2.15	0.79
2:H:39:GLN:OE1	3:L:42:GLN:NE2	2.20	0.74
1:B:90:GLU:OE1	1:B:111:ARG:NH2	2.19	0.74
1:B:162:LYS:NZ	1:B:199:SER:O	2.22	0.71
1:A:95:ASP:O	1:A:97:GLY:N	2.23	0.71
2:C:39:GLN:OE1	2:C:40:ALA:N	2.25	0.70
1:A:162:LYS:NZ	1:A:199:SER:O	2.27	0.67
3:L:194:ASN:ND2	3:L:215:ARG:O	2.32	0.63
1:A:90:GLU:OE1	1:A:111:ARG:NH2	2.32	0.63
3:D:194:ASN:ND2	3:D:215:ARG:O	2.37	0.58
3:L:54:ALA:N	3:L:55:ALA:HA	2.19	0.57
2:H:39:GLN:O	2:H:92:ALA:HB1	2.05	0.57
1:B:63:LYS:N	1:B:91:THR:OG1	2.39	0.56
1:B:73:ASN:ND2	1:B:76:CYS:SG	2.76	0.55
1:B:234:GLY:O	1:B:235:ARG:NH1	2.37	0.55
1:A:234:GLY:O	1:A:235:ARG:NH1	2.36	0.55
1:A:151:LYS:NZ	3:L:96:ASN:O	2.39	0.55
1:A:80:SER:O	1:A:81:THR:HG22	2.07	0.53
1:B:80:SER:O	1:B:81:THR:HG22	2.08	0.53
1:A:73:ASN:ND2	1:A:76:CYS:SG	2.77	0.52
1:B:151:LYS:NZ	3:D:96:ASN:O	2.42	0.52
2:C:31:LYS:O	2:C:32:ASN:ND2	2.35	0.52
1:A:247:ASP:OD1	1:A:248:LYS:N	2.43	0.51
3:D:54:ALA:N	3:D:55:ALA:HA	2.25	0.51
2:H:31:LYS:O	2:H:32:ASN:ND2	2.36	0.50
3:D:190:TYR:O	3:D:196:TYR:OH	2.28	0.50
3:L:190:TYR:O	3:L:196:TYR:OH	2.29	0.50
1:B:86:SER:O	1:B:116:SER:N	2.33	0.50
1:B:247:ASP:OD1	1:B:248:LYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:HB3	1:B:97:GLY:HA3	1.94	0.49
2:H:145:LEU:HD21	2:H:147:LYS:HB2	1.94	0.49
3:D:4:LEU:HD23	3:D:92:CYS:SG	2.54	0.48
2:C:145:LEU:HD21	2:C:147:LYS:HB2	1.96	0.48
3:L:4:LEU:HD23	3:L:92:CYS:SG	2.54	0.48
3:L:15:LEU:HD12	3:L:112:ARG:HD2	1.96	0.47
1:B:73:ASN:OD1	1:B:74:PRO:HD2	2.14	0.47
2:C:142:LEU:HG	2:C:192:ARG:CZ	2.44	0.47
2:H:35:ASN:N	2:H:97:ALA:O	2.41	0.47
2:C:140:VAL:O	2:C:192:ARG:NH2	2.47	0.47
2:H:73:GLU:O	2:H:76:ALA:O	2.32	0.47
2:H:140:VAL:O	2:H:192:ARG:NH2	2.48	0.47
3:L:5:THR:HG22	3:L:24:LYS:H	1.79	0.47
3:D:15:LEU:HD12	3:D:112:ARG:HD2	1.97	0.47
1:A:63:LYS:N	1:A:91:THR:OG1	2.48	0.47
2:H:142:LEU:HG	2:H:192:ARG:CZ	2.44	0.47
3:D:5:THR:HG22	3:D:24:LYS:H	1.80	0.47
1:A:67:ALA:HB3	1:A:97:GLY:HA3	1.98	0.46
1:A:175:ILE:HG22	1:A:175:ILE:O	2.16	0.46
1:A:73:ASN:OD1	1:A:74:PRO:HD2	2.15	0.46
1:B:175:ILE:HG22	1:B:175:ILE:O	2.15	0.46
2:C:100:VAL:HG13	2:C:101:ARG:N	2.32	0.45
1:A:177:ASP:OD1	1:A:177:ASP:N	2.49	0.45
2:C:73:GLU:O	2:C:76:ALA:O	2.34	0.45
1:A:186:TRP:CE2	1:A:239:TYR:HB2	2.52	0.45
2:C:145:LEU:HD12	3:D:137:VAL:HG21	1.98	0.45
1:A:185:LEU:HD23	1:A:240:TRP:HB3	1.98	0.45
2:H:100:VAL:HG13	2:H:101:ARG:N	2.32	0.44
1:B:208:VAL:HB	1:B:219:PHE:HB2	2.00	0.44
1:A:71:LEU:O	1:A:154:TYR:HB3	2.18	0.44
1:A:132:TRP:CH2	1:A:259:VAL:HG21	2.53	0.44
1:A:208:VAL:HB	1:A:219:PHE:HB2	2.01	0.43
3:D:37:LEU:HB3	3:D:55:ALA:HB2	1.99	0.43
2:H:47:TRP:CG	3:L:100:TYR:HB2	2.54	0.43
2:H:142:LEU:HD22	2:H:214:ILE:HG21	2.01	0.43
2:H:145:LEU:HD12	3:L:137:VAL:HG21	2.00	0.43
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.99	0.43
1:B:138:ASN:O	1:B:139:LYS:HB3	2.19	0.43
2:C:140:VAL:HB	2:C:192:ARG:NH1	2.33	0.43
1:A:138:ASN:O	1:A:139:LYS:HB3	2.19	0.42
1:A:165:ASN:O	1:A:165:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD23	1:B:240:TRP:HB3	2.02	0.42
2:H:30:THR:O	2:H:31:LYS:HB2	2.20	0.42
1:B:71:LEU:O	1:B:154:TYR:HB3	2.19	0.42
2:C:47:TRP:CG	3:D:100:TYR:HB2	2.55	0.42
2:C:142:LEU:HD22	2:C:214:ILE:HG21	2.01	0.41
3:D:92:CYS:O	3:D:103:GLY:N	2.52	0.41
1:B:228:LYS:HD2	1:B:233:GLU:HG3	2.02	0.41
2:H:140:VAL:HB	2:H:192:ARG:NH1	2.34	0.41
1:B:186:TRP:CE2	1:B:239:TYR:HB2	2.56	0.41
2:C:54:TYR:O	5:C:301:MES:H52	2.20	0.41
1:A:63:LYS:O	1:A:63:LYS:HG3	2.21	0.41
3:L:24:LYS:NZ	3:L:73:THR:OG1	2.54	0.41
1:B:220:LYS:HG3	1:B:221:PRO:HD2	2.03	0.41
1:B:132:TRP:CH2	1:B:259:VAL:HG21	2.56	0.41
3:D:41:GLN:HB2	3:D:51:LEU:HD11	2.03	0.41
3:L:80:HIS:HA	3:L:81:PRO:HA	1.97	0.41
1:A:259:VAL:HG22	1:A:260:PRO:HD2	2.03	0.40
2:H:148:GLY:HA2	2:H:178:LEU:HB3	2.03	0.40
2:C:4:LEU:HD12	2:C:106:PHE:O	2.21	0.40
1:B:65:ASN:HA	1:B:90:GLU:HB2	2.04	0.40
1:B:212:SER:N	1:B:215:TYR:O	2.53	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	212/548 (39%)	188 (89%)	23 (11%)	1 (0%)	29 65
1	B	212/548 (39%)	188 (89%)	22 (10%)	2 (1%)	17 53
2	C	215/217 (99%)	195 (91%)	19 (9%)	1 (0%)	29 65
2	H	215/217 (99%)	195 (91%)	18 (8%)	2 (1%)	17 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	213/218 (98%)	201 (94%)	12 (6%)	0	100	100
3	L	213/218 (98%)	201 (94%)	12 (6%)	0	100	100
All	All	1280/1966 (65%)	1168 (91%)	106 (8%)	6 (0%)	29	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	ASN
2	H	130	PRO
2	C	130	PRO
1	A	96	ASN
2	H	89	GLU
1	B	92	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	187/476 (39%)	181 (97%)	6 (3%)	39	70
1	B	187/476 (39%)	181 (97%)	6 (3%)	39	70
2	C	184/184 (100%)	178 (97%)	6 (3%)	38	69
2	H	184/184 (100%)	177 (96%)	7 (4%)	33	65
3	D	187/190 (98%)	185 (99%)	2 (1%)	73	88
3	L	187/190 (98%)	185 (99%)	2 (1%)	73	88
All	All	1116/1700 (66%)	1087 (97%)	29 (3%)	46	74

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	64	CYS
1	A	104	PHE
1	A	107	TYR

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Mol	Chain	Res	Type
1	A	147	HIS
1	A	167	TYR
2	H	16	GLU
2	H	32	ASN
2	H	39	GLN
2	H	54	TYR
2	H	72	LEU
2	H	113	VAL
2	H	212	LYS
3	L	23	CYS
3	L	37	LEU
1	B	56	VAL
1	B	64	CYS
1	B	104	PHE
1	B	107	TYR
1	B	147	HIS
1	B	167	TYR
2	C	16	GLU
2	C	32	ASN
2	C	38	GLN
2	C	72	LEU
2	C	113	VAL
2	C	212	LYS
3	D	23	CYS
3	D	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	B	147	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	$\#\|Z\| > 2$
5	MES	C	301	-	12,12,12	2.28	1 (8%)	14,16,16	1.54	3 (21%)
5	MES	H	301	-	12,12,12	2.29	1 (8%)	14,16,16	1.41	3 (21%)
4	NAG	A	601	1	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	B	601	1	14,14,15	0.42	0	17,19,21	0.45	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
5	MES	C	301	-	-	3/6/14/14	0/1/1/1
5	MES	H	301	-	-	3/6/14/14	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	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)
5	H	301	MES	C8-S	-7.68	1.66	1.77
5	C	301	MES	C8-S	-7.62	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	301	MES	C5-N4-C3	3.22	116.07	108.83
5	C	301	MES	C5-N4-C3	2.88	115.32	108.83
5	H	301	MES	O3S-S-C8	2.63	110.02	105.77
5	C	301	MES	O1S-S-C8	2.49	109.92	106.92
5	H	301	MES	O1S-S-C8	2.26	109.64	106.92
5	C	301	MES	O3S-S-C8	2.24	109.39	105.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	MES	C7-C8-S-O3S
5	C	301	MES	C7-C8-S-O3S
4	A	601	NAG	C1-C2-N2-C7
4	B	601	NAG	C1-C2-N2-C7
5	H	301	MES	C7-C8-S-O2S
5	C	301	MES	C7-C8-S-O1S
5	C	301	MES	C7-C8-S-O2S
4	A	601	NAG	C3-C2-N2-C7
4	B	601	NAG	C3-C2-N2-C7
5	H	301	MES	C7-C8-S-O1S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	MES	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 (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	A	214/548 (39%)	-0.02	0	100	100	28, 49, 73, 90	0
1	B	214/548 (39%)	0.02	0	100	100	31, 52, 77, 92	0
2	C	217/217 (100%)	1.20	50 (23%)	0	0	52, 115, 234, 248	0
2	H	217/217 (100%)	0.66	22 (10%)	7	3	51, 111, 197, 209	0
3	D	215/218 (98%)	1.30	53 (24%)	0	0	59, 153, 223, 236	0
3	L	215/218 (98%)	0.67	22 (10%)	6	3	57, 143, 184, 190	0
All	All	1292/1966 (65%)	0.64	147 (11%)	5	3	28, 90, 215, 248	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	142	LEU	16.5
2	H	135	GLN	13.7
2	H	134	ALA	9.7
3	D	160	GLN	9.1
3	D	150	VAL	8.6
3	D	198	CYS	8.4
3	L	206	THR	8.2
3	D	209	ILE	8.0
2	C	135	GLN	7.8
2	C	204	PRO	7.7
3	D	159	ARG	7.7
2	C	129	ALA	7.6
3	D	200	ALA	7.5
2	C	215	VAL	7.2
3	D	137	VAL	6.8
2	C	146	VAL	6.7
2	C	130	PRO	6.7
3	D	135	SER	6.7
2	C	155	THR	6.6

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Mol	Chain	Res	Type	RSRZ
2	C	123	PRO	6.3
2	C	136	THR	6.2
2	C	125	VAL	6.1
2	H	136	THR	6.0
3	D	181	SER	5.9
3	D	182	THR	5.7
2	H	142	LEU	5.5
3	D	124	PRO	5.5
3	D	199	GLU	5.1
3	D	131	SER	4.9
3	D	136	VAL	4.9
2	H	124	SER	4.7
2	C	181	LEU	4.6
2	C	210	VAL	4.6
3	D	191	GLU	4.6
3	L	198	CYS	4.5
3	D	213	PHE	4.5
3	D	208	PRO	4.5
3	L	213	PHE	4.5
3	D	6	GLN	4.4
2	C	205	ALA	4.4
2	C	209	LYS	4.3
3	D	121	ILE	4.3
2	H	123	PRO	4.2
3	D	165	ASN	4.1
3	D	196	TYR	3.9
2	C	162	SER	3.9
2	H	131	GLY	3.9
2	C	216	PRO	3.8
3	L	200	ALA	3.8
3	L	150	VAL	3.8
3	D	125	SER	3.8
2	C	124	SER	3.7
3	L	199	GLU	3.7
3	D	207	SER	3.7
3	D	151	LYS	3.7
3	D	188	ASP	3.6
2	C	194	SER	3.6
3	L	182	THR	3.6
3	D	84	GLU	3.6
3	L	192	ARG	3.5
2	C	183	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	201	VAL	3.4
3	L	139	PHE	3.3
3	D	197	THR	3.3
2	C	192	ARG	3.3
2	C	190	SER	3.3
2	H	204	PRO	3.3
3	D	206	THR	3.3
2	C	185	VAL	3.3
2	C	65	LYS	3.3
2	H	65	LYS	3.3
3	D	190	TYR	3.3
3	L	84	GLU	3.2
3	D	108	LEU	3.2
2	C	139	MET	3.2
2	H	129	ALA	3.2
3	D	120	SER	3.1
2	C	213	LYS	3.1
2	H	179	TYR	3.0
2	C	141	THR	3.0
2	C	149	TYR	3.0
3	D	164	LEU	3.0
3	L	191	GLU	3.0
2	C	132	SER	2.9
2	C	176	SER	2.9
3	L	196	TYR	2.9
3	D	139	PHE	2.9
2	H	149	TYR	2.9
2	C	202	ALA	2.9
3	D	201	THR	2.8
3	D	187	LYS	2.8
2	C	217	ARG	2.8
2	H	194	SER	2.8
3	D	152	TRP	2.7
2	H	199	CYS	2.7
2	C	134	ALA	2.7
2	H	187	VAL	2.7
3	D	192	ARG	2.7
3	D	51	LEU	2.7
2	C	163	LEU	2.6
3	D	184	THR	2.6
2	C	100	VAL	2.6
2	C	165	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	215	VAL	2.5
2	C	66	GLY	2.5
3	D	156	GLY	2.5
3	D	118	THR	2.5
2	H	183	SER	2.5
3	D	123	PRO	2.5
2	C	147	LYS	2.5
3	L	159	ARG	2.5
2	C	177	ASP	2.5
2	C	138	SER	2.4
2	C	174	LEU	2.4
3	L	189	GLU	2.4
3	L	140	LEU	2.4
3	D	167	TRP	2.3
3	D	138	CYS	2.3
3	D	214	ASN	2.3
3	D	211	LYS	2.3
2	C	175	GLN	2.3
3	D	163	VAL	2.3
2	H	86	LEU	2.2
3	D	169	ASP	2.2
3	L	190	TYR	2.2
3	L	152	TRP	2.2
2	H	192	ARG	2.2
2	C	188	PRO	2.2
2	C	186	THR	2.2
2	C	91	MET	2.1
2	C	1	GLN	2.1
2	C	187	VAL	2.1
3	L	197	THR	2.1
2	H	213	LYS	2.1
3	L	208	PRO	2.1
3	D	141	ASN	2.1
2	C	148	GLY	2.1
3	D	128	GLN	2.1
3	D	142	ASN	2.1
3	L	169	ASP	2.1
2	H	130	PRO	2.0
3	L	13	VAL	2.0
3	D	210	VAL	2.0
2	H	132	SER	2.0
2	C	197	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	212	SER	2.0
3	L	209	ILE	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, 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	601	14/15	0.74	0.30	99,99,99,99	0
4	NAG	B	601	14/15	0.75	0.33	96,96,96,96	0
5	MES	H	301	12/12	0.93	0.22	65,65,65,65	0
5	MES	C	301	12/12	0.93	0.24	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.