



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 7FAH / pdb_00007fah
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

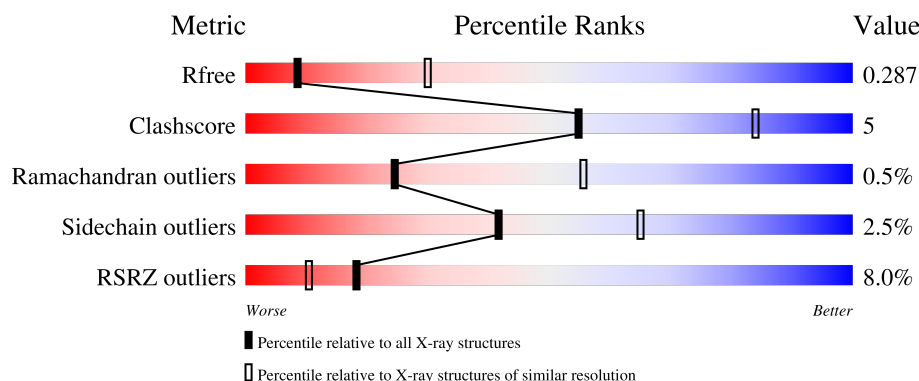
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 $\leq 5\%$. 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	548	32% 7% 61%
1	B	548	% 31% 8% 61%
2	C	217	14% 88% 12%
2	H	217	6% 87% 12% .
3	D	218	15% 88% 10% ..

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Mol	Chain	Length	Quality of chain
3	L	218	9% 88% 11%

2 Entry composition

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
1	A	214	Total	C	N	O	S	0	0	0
			1705	1089	287	323	6			
1	B	214	Total	C	N	O	S	0	0	0
			1705	1089	287	323	6			

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
2	H	217	Total	C	N	O	S	0	0	0
			1641	1039	275	318	9			
2	C	217	Total	C	N	O	S	0	0	0
			1641	1039	275	318	9			

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

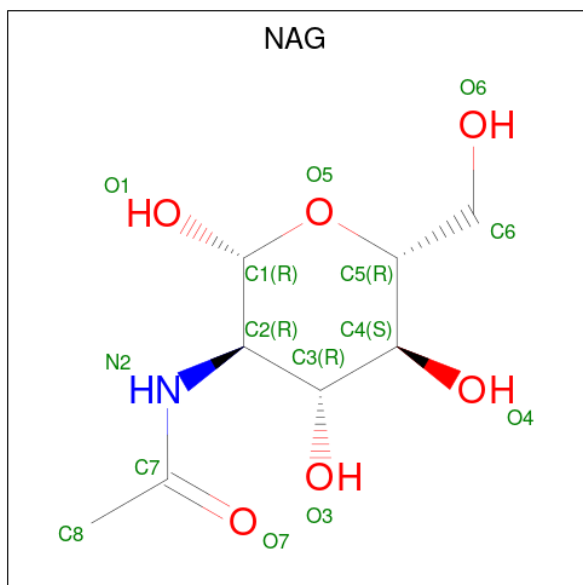
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1661	1037	277	342	5			

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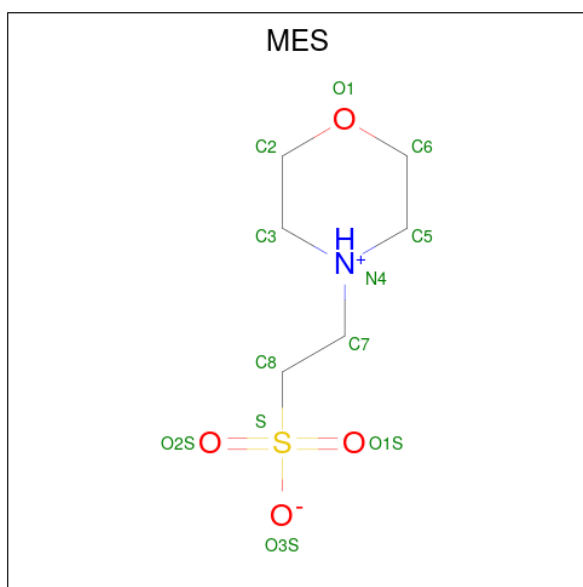
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	215	Total	C	N	O	S	0	0	0
			1661	1037	277	342	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

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

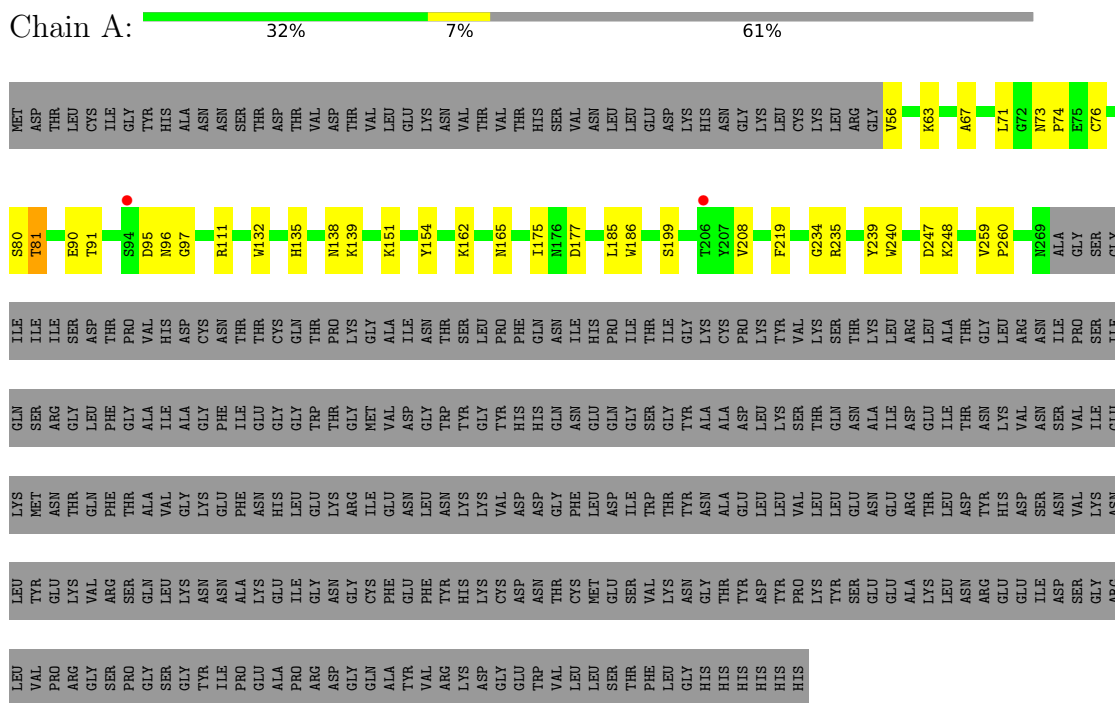


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

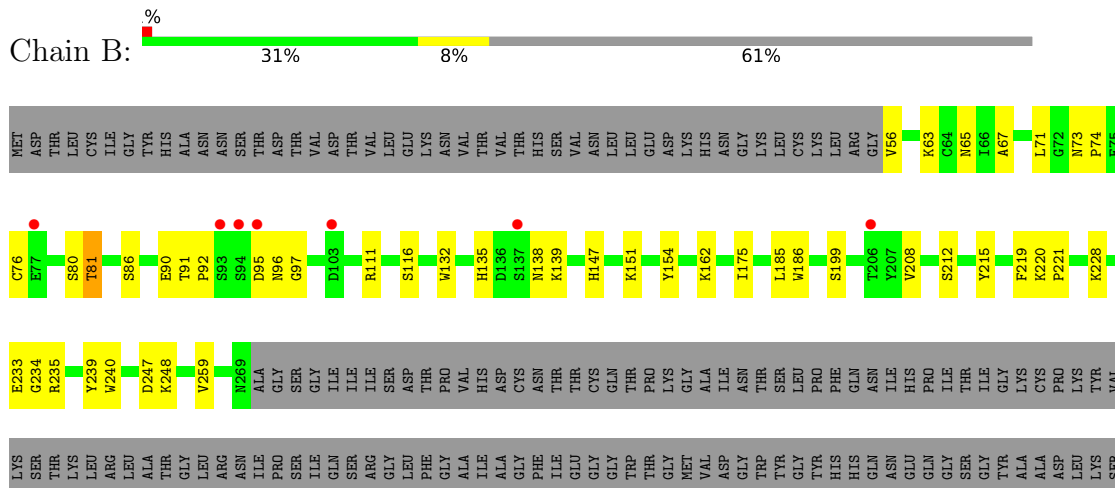
3 Residue-property plots

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



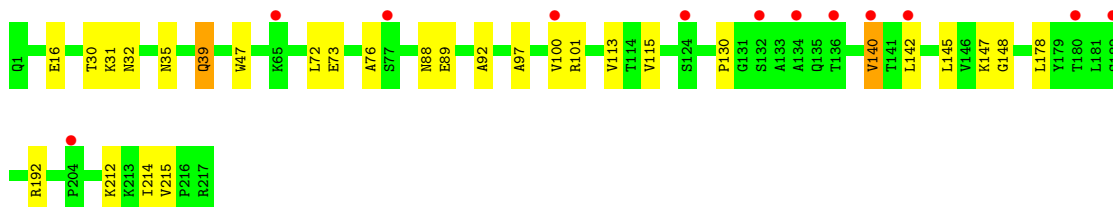
- Molecule 1: Hemagglutinin



THR	GLN	ASN	ALA	ILE	ASP	GLU	GLU	THR	THR	ASN	LYS	VAL	ASN	SER	VAL	GLY	LYS	LEU	MET	ASN	THR	GLN	PHE	THR	ALA	VAL	GLY	GLY	ASN	LYS	GLY	ASN	GLY	PHE	ASN	ASN	HIS	LEU	LEU	LYS	LYS	VAL	VAL	ASP	ASP	GLY	PHE	LEU	ASP	ILE	THR	THR	TYR	ASN	ALA	GLU	LEU	LEU				
LEU	LEU	ASN	GLU	ARG	THR	THR	LEU	ASP	THR	HIS	HIS	ASP	SER	ASN	VAL	GLY	ASN	LEU	TYR	GLU	LYS	VAL	ARG	SER	GLN	LEU	LYS	ASN	ASN	ALA	LYS	GLU	ILE	GLY	ASN	GLY	CYS	PHE	GLU	PHE	THR	TYR	HIS	LYS	CYS	ASN	ASP	THR	CYS	MET	GLU	SER	SER	VAL	LYS	ASN	GLY	THR	TYR	ASP	TYR	PRO
LYS	TYR	SER	GLU	ALA	LYS	LYS	LEU	ARG	GLU	GLU	GLU	GLY	ARG	ASP	GLY	GLY	LEU	VAL	PRO	ARG	GLY	GLY	SER	SER	GLY	GLY	ILE	ASN	PRO	GLU	ALA	PRO	ARG	GLY	GLY	GLN	ALA	TYR	VAL	ARG	TYR	ASN	LYS	ASP	GLY	GLU	THR	VAL	LEU	SER	THR	THR	LEU	GLY	HIS	HIS	HIS	HIS	HIS			

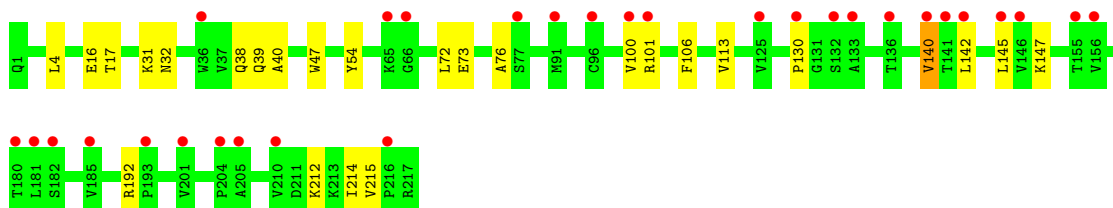
• Molecule 2: heavy chain of antibody 12H5

Chain H: 



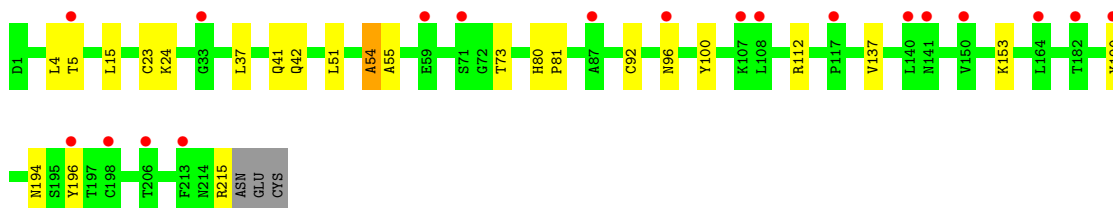
• Molecule 2: heavy chain of antibody 12H5

Chain C: 



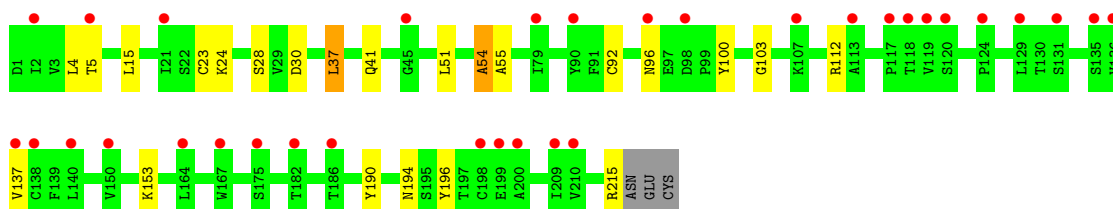
• Molecule 3: Light chain of antibody 12H5

Chain L: 



• Molecule 3: Light chain of antibody 12H5

Chain D: 



4 Data and refinement statistics

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) 98.6 (38.61-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.266 , 0.289 0.264 , 0.287	Depositor DCC
R_{free} test set	1495 reflections (4.81%)	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 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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, 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	0.15	0/1755	0.35	0/2383
1	B	0.15	0/1755	0.36	0/2383
2	C	0.14	0/1684	0.33	0/2298
2	H	0.14	0/1684	0.35	0/2298
3	D	0.12	0/1700	0.36	1/2312 (0.0%)
3	L	0.13	0/1700	0.34	1/2312 (0.0%)
All	All	0.14	0/10278	0.35	2/13986 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	54	ALA	N-CA-C	6.99	121.29	111.92
3	L	54	ALA	N-CA-C	6.56	120.70	111.92

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	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1641	0	1614	16	0
3	D	1661	0	1577	13	0
3	L	1661	0	1577	13	0
4	A	14	0	13	0	0
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	94	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 (94) 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
3:D:28:SER:OG	3:D:30:ASP:OD1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:B:175:ILE:HG22	1:B:175:ILE:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:54:TYR:CD2	2:C:54:TYR:C	2.99	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%)	24	55
1	B	212/548 (39%)	188 (89%)	22 (10%)	2 (1%)	14	43
2	C	215/217 (99%)	195 (91%)	19 (9%)	1 (0%)	24	55
2	H	215/217 (99%)	195 (91%)	18 (8%)	2 (1%)	14	43
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%)	24	55

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 ⓘ

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%)	184 (98%)	3 (2%)	55	71
1	B	187/476 (39%)	183 (98%)	4 (2%)	47	67
2	C	184/184 (100%)	176 (96%)	8 (4%)	26	54
2	H	184/184 (100%)	177 (96%)	7 (4%)	29	58
3	D	187/190 (98%)	184 (98%)	3 (2%)	55	71
3	L	187/190 (98%)	184 (98%)	3 (2%)	55	71
All	All	1116/1700 (66%)	1088 (98%)	28 (2%)	42	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	81	THR
1	A	135	HIS
2	H	16	GLU
2	H	39	GLN
2	H	72	LEU
2	H	113	VAL
2	H	140	VAL
2	H	212	LYS
2	H	215	VAL
3	L	23	CYS
3	L	37	LEU
3	L	153	LYS
1	B	56	VAL
1	B	81	THR
1	B	135	HIS
1	B	147	HIS
2	C	16	GLU
2	C	17	THR
2	C	38	GLN
2	C	72	LEU
2	C	113	VAL
2	C	140	VAL
2	C	212	LYS
2	C	215	VAL
3	D	23	CYS
3	D	37	LEU
3	D	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	165	ASN
1	A	237	ASN
2	H	82	GLN
3	L	149	ASN
3	L	165	ASN
3	L	214	ASN
1	B	138	ASN
1	B	147	HIS
2	C	82	GLN
3	D	165	ASN

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Mol	Chain	Res	Type
3	D	214	ASN

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 oligosaccharides 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	601	1	14,14,15	0.35	0	17,19,21	0.46	0
4	NAG	B	601	1	14,14,15	0.44	0	17,19,21	0.46	0
5	MES	C	301	-	12,12,12	2.33	1 (8%)	15,16,16	1.42	2 (13%)
5	MES	H	301	-	12,12,12	2.34	1 (8%)	15,16,16	1.29	2 (13%)

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	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1	-	1/6/23/26	0/1/1/1
5	MES	C	301	-	-	3/6/14/14	0/1/1/1
5	MES	H	301	-	-	3/6/14/14	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	-7.85	1.66	1.77
5	C	301	MES	C8-S	-7.79	1.66	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	MES	C5-N4-C3	3.36	116.07	108.84
5	C	301	MES	C5-N4-C3	3.01	115.32	108.84
5	C	301	MES	O1S-S-C8	2.11	109.92	106.73
5	H	301	MES	O3S-S-C8	2.05	110.02	106.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	214/548 (39%)	0.31	2 (0%) 81 64	28, 49, 73, 90	0
1	B	214/548 (39%)	0.39	7 (3%) 49 29	31, 52, 77, 92	0
2	C	217/217 (100%)	1.11	30 (13%) 6 4	52, 115, 234, 248	0
2	H	217/217 (100%)	0.82	12 (5%) 30 17	51, 111, 197, 209	0
3	D	215/218 (98%)	1.11	33 (15%) 5 3	59, 153, 223, 236	0
3	L	215/218 (98%)	0.89	19 (8%) 15 9	57, 143, 184, 190	0
All	All	1292/1966 (65%)	0.77	103 (7%) 18 10	28, 90, 215, 248	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	100	VAL	4.9
3	D	182	THR	4.7
2	C	142	LEU	4.5
2	C	146	VAL	4.0
3	D	198	CYS	3.9
3	L	182	THR	3.9
2	C	182	SER	3.8
3	D	117	PRO	3.6
3	D	150	VAL	3.5
2	H	180	THR	3.4
1	B	137	SER	3.4
2	H	100	VAL	3.4
1	B	94	SER	3.3
3	D	209	ILE	3.3
3	L	5	THR	3.3
2	C	204	PRO	3.2
2	C	155	THR	3.1
3	D	5	THR	3.1
3	D	200	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	145	LEU	3.0
3	L	96	ASN	3.0
3	D	136	VAL	3.0
3	D	135	SER	3.0
3	D	45	GLY	2.9
3	D	137	VAL	2.9
3	D	79	ILE	2.9
3	D	119	VAL	2.8
2	H	182	SER	2.8
2	C	132	SER	2.8
3	L	164	LEU	2.8
1	A	206	THR	2.8
3	L	140	LEU	2.8
2	H	142	LEU	2.7
3	L	196	TYR	2.7
3	L	198	CYS	2.7
3	D	167	TRP	2.7
3	L	107	LYS	2.7
3	D	96	ASN	2.7
2	C	65	LYS	2.6
2	C	66	GLY	2.6
2	C	36	TRP	2.6
2	C	136	THR	2.6
2	H	132	SER	2.6
3	D	120	SER	2.6
3	D	131	SER	2.6
2	C	201	VAL	2.6
1	B	206	THR	2.6
3	L	213	PHE	2.5
3	L	71	SER	2.5
3	D	164	LEU	2.5
2	H	140	VAL	2.5
2	H	134	ALA	2.5
2	C	205	ALA	2.5
3	D	124	PRO	2.5
1	B	93	SER	2.5
3	D	138	CYS	2.4
3	L	206	THR	2.4
3	L	150	VAL	2.4
3	L	108	LEU	2.4
2	C	125	VAL	2.4
2	C	96	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	204	PRO	2.4
2	C	156	VAL	2.4
3	D	2	ILE	2.4
2	C	77	SER	2.4
2	C	193	PRO	2.4
1	B	95	ASP	2.3
3	D	90	TYR	2.3
3	L	117	PRO	2.3
2	C	141	THR	2.3
2	C	181	LEU	2.3
3	L	141	ASN	2.3
3	D	113	ALA	2.3
2	H	136	THR	2.3
2	C	180	THR	2.3
2	C	140	VAL	2.3
3	D	129	LEU	2.2
2	C	101	ARG	2.2
3	D	199	GLU	2.2
2	H	65	LYS	2.2
2	C	133	ALA	2.2
3	D	186	THR	2.2
2	C	91	MET	2.2
2	C	185	VAL	2.1
1	B	77	GLU	2.1
3	D	210	VAL	2.1
2	H	77	SER	2.1
2	C	130	PRO	2.1
3	D	107	LYS	2.1
3	D	140	LEU	2.1
3	L	87	ALA	2.1
1	B	103	ASP	2.1
3	D	98	ASP	2.1
2	C	216	PRO	2.1
2	C	210	VAL	2.1
3	D	21	ILE	2.1
3	D	118	THR	2.1
1	A	94	SER	2.0
2	H	124	SER	2.0
3	D	175	SER	2.0
3	L	33	GLY	2.0
3	L	190	TYR	2.0
3	L	59	GLU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	NAG	B	601	14/15	0.51	0.18	96,96,96,96	0
4	NAG	A	601	14/15	0.52	0.17	99,99,99,99	0
5	MES	C	301	12/12	0.80	0.16	68,68,68,68	0
5	MES	H	301	12/12	0.84	0.17	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.