



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2021 – 06:08 PM EST

PDB ID : 6WEQ
Title : DENV1 NS1 in complex with neutralizing 2B7 Fab fragment
Authors : Akey, D.L.; Smith, J.L.
Deposited on : 2020-04-02
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

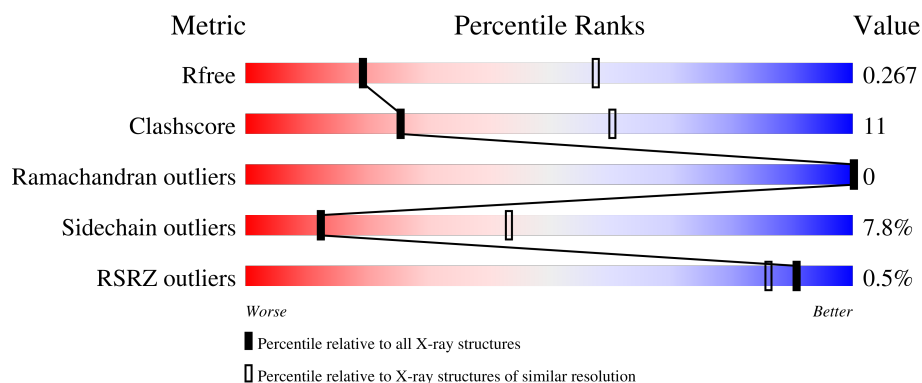
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	376	 61% 27% • 10%
1	B	376	 60% 28% • 10%
1	C	376	 64% 24% • 10%
1	D	376	 62% 26% • 10%
2	E	268	 60% 18% • 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	268	<div><div></div><div>56%22%21%</div></div>
2	I	268	<div><div>%</div><div>56%21%21%</div></div>
2	K	268	<div><div></div><div>55%23%21%</div></div>
3	F	238	<div><div>%</div><div>63%24%10%</div></div>
3	H	238	<div><div></div><div>66%23%10%</div></div>
3	J	238	<div><div>2%</div><div>66%22%10%</div></div>
3	L	238	<div><div>%</div><div>66%22%10%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24057 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2720	1725	469	506	20			
1	B	340	Total	C	N	O	S	0	0	0
			2720	1725	469	506	20			
1	C	340	Total	C	N	O	S	0	0	0
			2720	1725	469	506	20			
1	D	340	Total	C	N	O	S	0	0	0
			2720	1725	469	506	20			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	ALA	-	expression tag	UNP Q9J7C6
A	-22	HIS	-	expression tag	UNP Q9J7C6
A	-21	HIS	-	expression tag	UNP Q9J7C6
A	-20	HIS	-	expression tag	UNP Q9J7C6
A	-19	HIS	-	expression tag	UNP Q9J7C6
A	-18	HIS	-	expression tag	UNP Q9J7C6
A	-17	HIS	-	expression tag	UNP Q9J7C6
A	-16	SER	-	expression tag	UNP Q9J7C6
A	-15	SER	-	expression tag	UNP Q9J7C6
A	-14	GLY	-	expression tag	UNP Q9J7C6
A	-13	VAL	-	expression tag	UNP Q9J7C6
A	-12	ASP	-	expression tag	UNP Q9J7C6
A	-11	LEU	-	expression tag	UNP Q9J7C6
A	-10	GLY	-	expression tag	UNP Q9J7C6
A	-9	THR	-	expression tag	UNP Q9J7C6
A	-8	GLU	-	expression tag	UNP Q9J7C6
A	-7	ASN	-	expression tag	UNP Q9J7C6
A	-6	LEU	-	expression tag	UNP Q9J7C6
A	-5	TYR	-	expression tag	UNP Q9J7C6
A	-4	PHE	-	expression tag	UNP Q9J7C6
A	-3	GLN	-	expression tag	UNP Q9J7C6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9J7C6
A	-1	ASN	-	expression tag	UNP Q9J7C6
B	-23	ALA	-	expression tag	UNP Q9J7C6
B	-22	HIS	-	expression tag	UNP Q9J7C6
B	-21	HIS	-	expression tag	UNP Q9J7C6
B	-20	HIS	-	expression tag	UNP Q9J7C6
B	-19	HIS	-	expression tag	UNP Q9J7C6
B	-18	HIS	-	expression tag	UNP Q9J7C6
B	-17	HIS	-	expression tag	UNP Q9J7C6
B	-16	SER	-	expression tag	UNP Q9J7C6
B	-15	SER	-	expression tag	UNP Q9J7C6
B	-14	GLY	-	expression tag	UNP Q9J7C6
B	-13	VAL	-	expression tag	UNP Q9J7C6
B	-12	ASP	-	expression tag	UNP Q9J7C6
B	-11	LEU	-	expression tag	UNP Q9J7C6
B	-10	GLY	-	expression tag	UNP Q9J7C6
B	-9	THR	-	expression tag	UNP Q9J7C6
B	-8	GLU	-	expression tag	UNP Q9J7C6
B	-7	ASN	-	expression tag	UNP Q9J7C6
B	-6	LEU	-	expression tag	UNP Q9J7C6
B	-5	TYR	-	expression tag	UNP Q9J7C6
B	-4	PHE	-	expression tag	UNP Q9J7C6
B	-3	GLN	-	expression tag	UNP Q9J7C6
B	-2	SER	-	expression tag	UNP Q9J7C6
B	-1	ASN	-	expression tag	UNP Q9J7C6
C	-23	ALA	-	expression tag	UNP Q9J7C6
C	-22	HIS	-	expression tag	UNP Q9J7C6
C	-21	HIS	-	expression tag	UNP Q9J7C6
C	-20	HIS	-	expression tag	UNP Q9J7C6
C	-19	HIS	-	expression tag	UNP Q9J7C6
C	-18	HIS	-	expression tag	UNP Q9J7C6
C	-17	HIS	-	expression tag	UNP Q9J7C6
C	-16	SER	-	expression tag	UNP Q9J7C6
C	-15	SER	-	expression tag	UNP Q9J7C6
C	-14	GLY	-	expression tag	UNP Q9J7C6
C	-13	VAL	-	expression tag	UNP Q9J7C6
C	-12	ASP	-	expression tag	UNP Q9J7C6
C	-11	LEU	-	expression tag	UNP Q9J7C6
C	-10	GLY	-	expression tag	UNP Q9J7C6
C	-9	THR	-	expression tag	UNP Q9J7C6
C	-8	GLU	-	expression tag	UNP Q9J7C6
C	-7	ASN	-	expression tag	UNP Q9J7C6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	expression tag	UNP Q9J7C6
C	-5	TYR	-	expression tag	UNP Q9J7C6
C	-4	PHE	-	expression tag	UNP Q9J7C6
C	-3	GLN	-	expression tag	UNP Q9J7C6
C	-2	SER	-	expression tag	UNP Q9J7C6
C	-1	ASN	-	expression tag	UNP Q9J7C6
D	-23	ALA	-	expression tag	UNP Q9J7C6
D	-22	HIS	-	expression tag	UNP Q9J7C6
D	-21	HIS	-	expression tag	UNP Q9J7C6
D	-20	HIS	-	expression tag	UNP Q9J7C6
D	-19	HIS	-	expression tag	UNP Q9J7C6
D	-18	HIS	-	expression tag	UNP Q9J7C6
D	-17	HIS	-	expression tag	UNP Q9J7C6
D	-16	SER	-	expression tag	UNP Q9J7C6
D	-15	SER	-	expression tag	UNP Q9J7C6
D	-14	GLY	-	expression tag	UNP Q9J7C6
D	-13	VAL	-	expression tag	UNP Q9J7C6
D	-12	ASP	-	expression tag	UNP Q9J7C6
D	-11	LEU	-	expression tag	UNP Q9J7C6
D	-10	GLY	-	expression tag	UNP Q9J7C6
D	-9	THR	-	expression tag	UNP Q9J7C6
D	-8	GLU	-	expression tag	UNP Q9J7C6
D	-7	ASN	-	expression tag	UNP Q9J7C6
D	-6	LEU	-	expression tag	UNP Q9J7C6
D	-5	TYR	-	expression tag	UNP Q9J7C6
D	-4	PHE	-	expression tag	UNP Q9J7C6
D	-3	GLN	-	expression tag	UNP Q9J7C6
D	-2	SER	-	expression tag	UNP Q9J7C6
D	-1	ASN	-	expression tag	UNP Q9J7C6

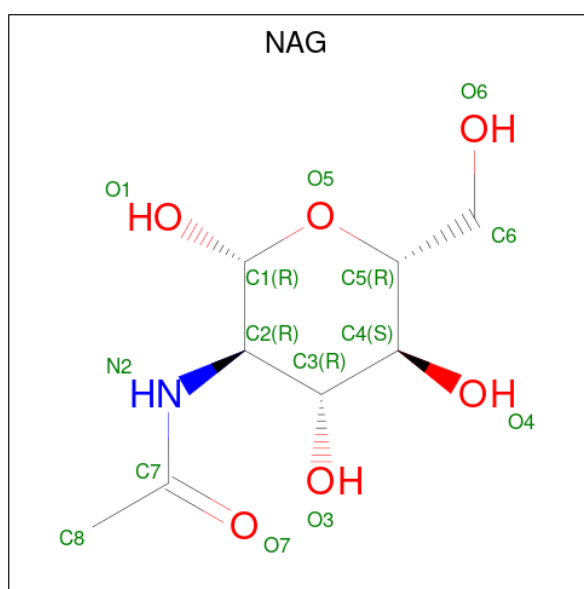
- Molecule 2 is a protein called 2B7 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	214	Total	C	N	O	S	0	0	0
			1607	1013	257	324	13			
2	G	213	Total	C	N	O	S	0	0	0
			1603	1011	256	323	13			
2	I	213	Total	C	N	O	S	0	0	0
			1603	1011	256	323	13			
2	K	213	Total	C	N	O	S	0	0	0
			1603	1011	256	323	13			

- Molecule 3 is a protein called 2B7 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	215	Total	C	N	O	S	0	0	0
			1661	1035	281	339	6			
3	H	215	Total	C	N	O	S	0	0	0
			1661	1035	281	339	6			
3	J	215	Total	C	N	O	S	0	0	0
			1661	1035	281	339	6			
3	L	215	Total	C	N	O	S	0	0	0
			1661	1035	281	339	6			

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



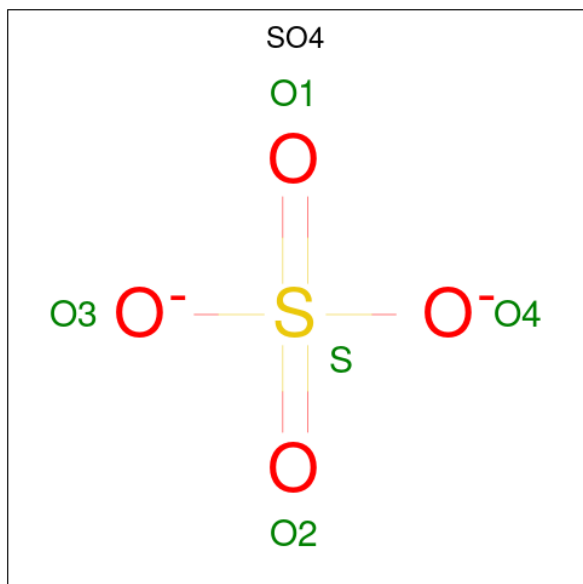
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

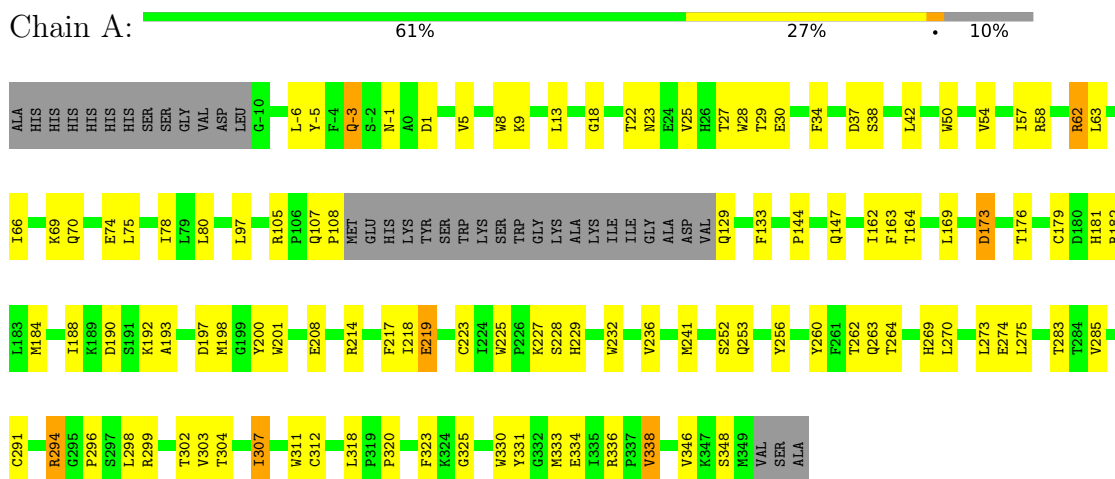


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

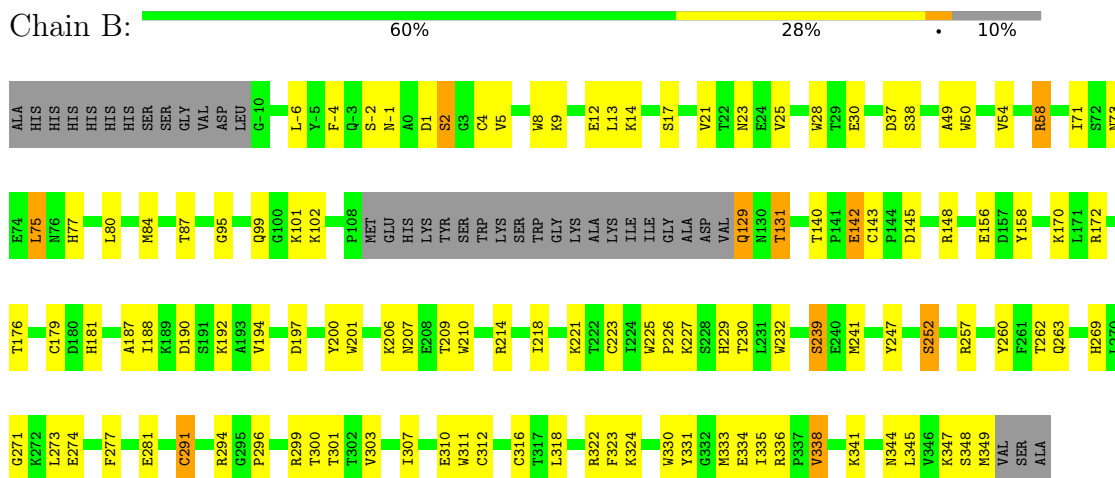
3 Residue-property plots [i](#)

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: Non-structural protein 1

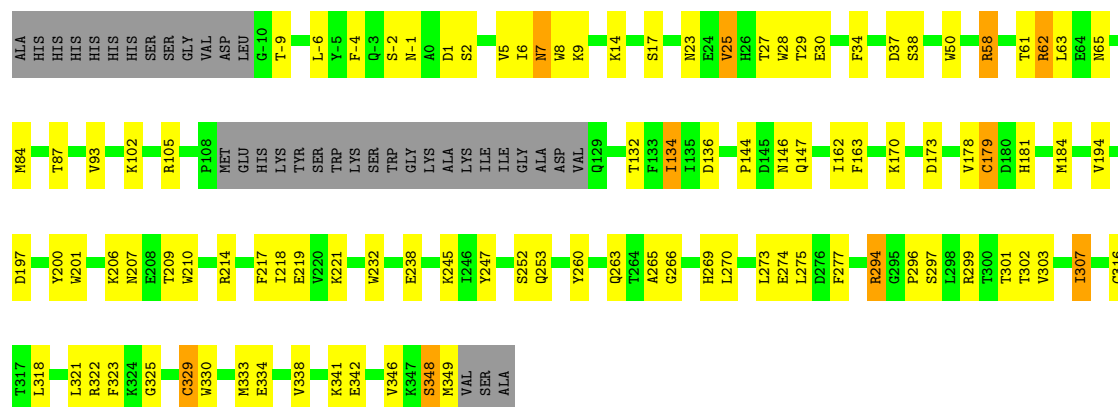


• Molecule 1: Non-structural protein 1



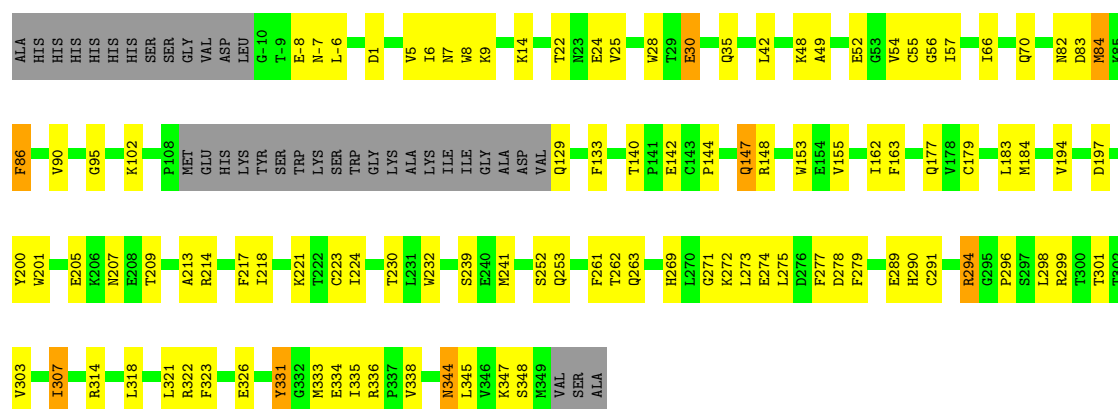
• Molecule 1: Non-structural protein 1





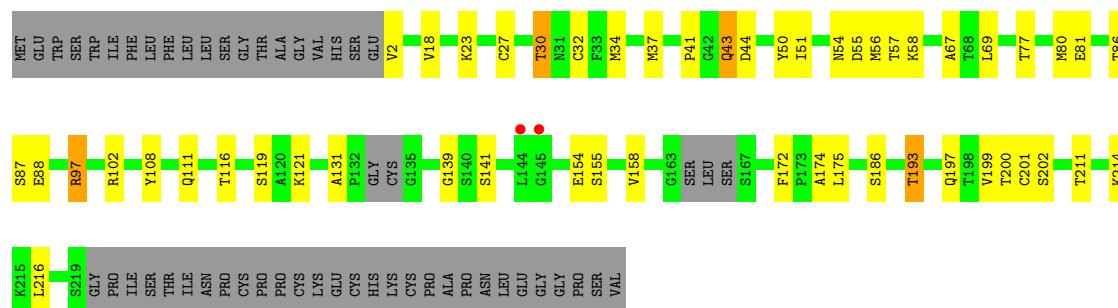
• Molecule 1: Non-structural protein 1

Chain D: 62% 26% 10%



• Molecule 2: 2B7 Fab fragment heavy chain

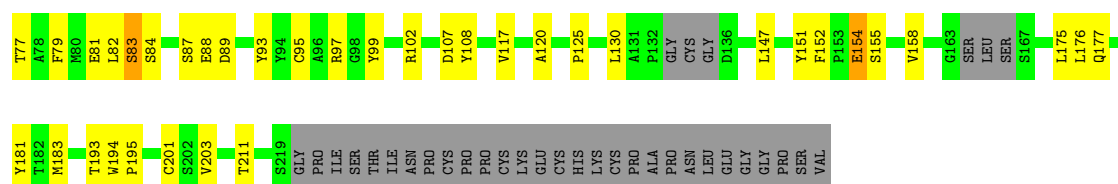
Chain E: 60% 18% 20%



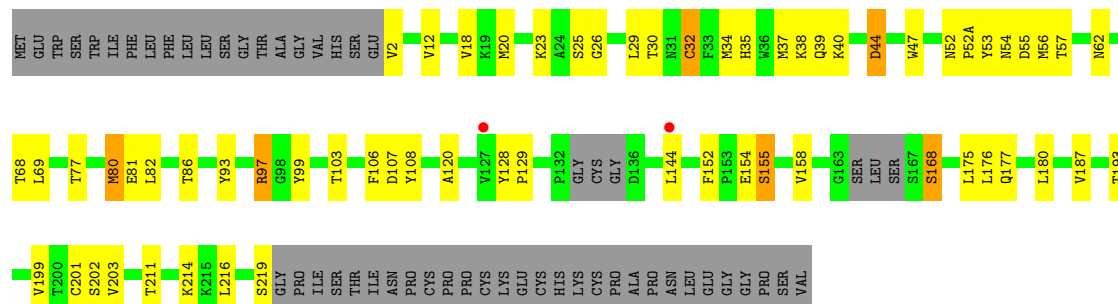
• Molecule 2: 2B7 Fab fragment heavy chain

Chain G: 56% 22% 21%

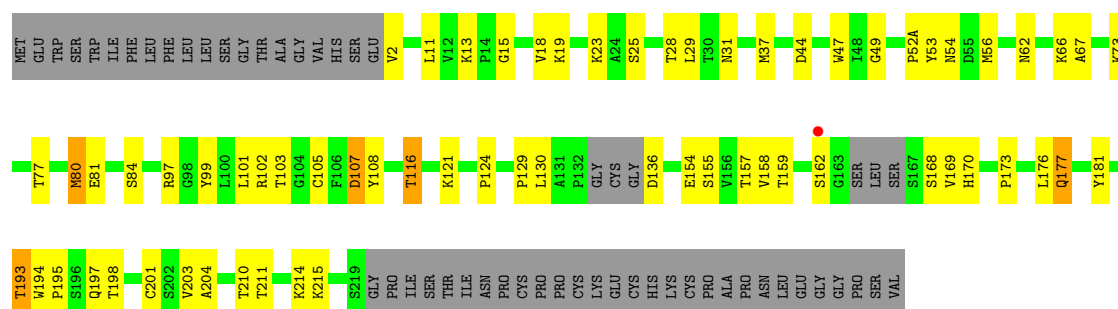




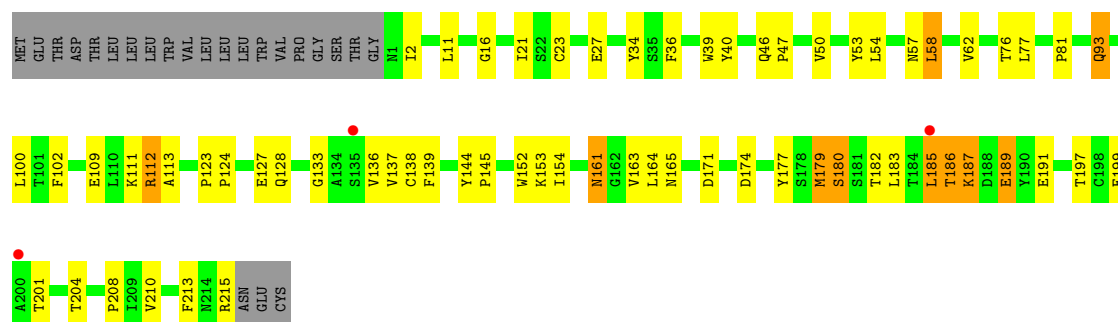
- Molecule 2: 2B7 Fab fragment heavy chain



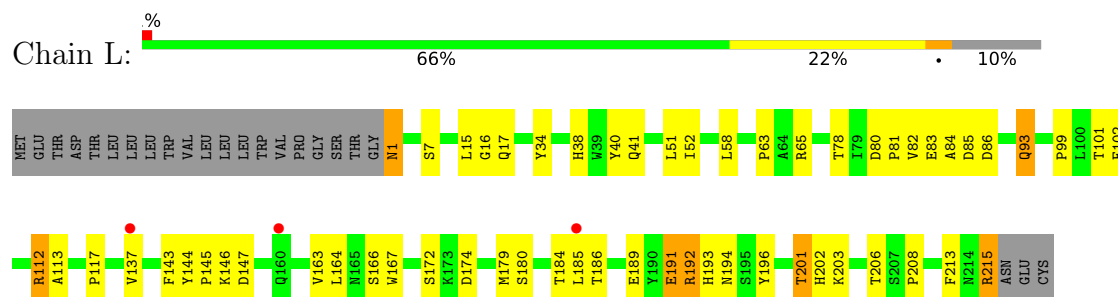
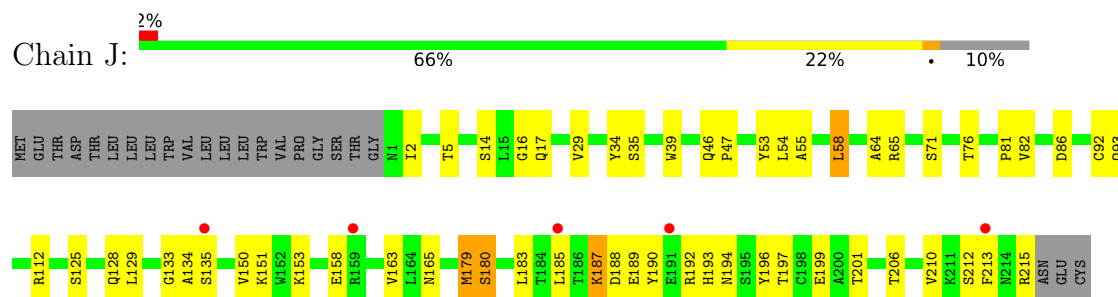
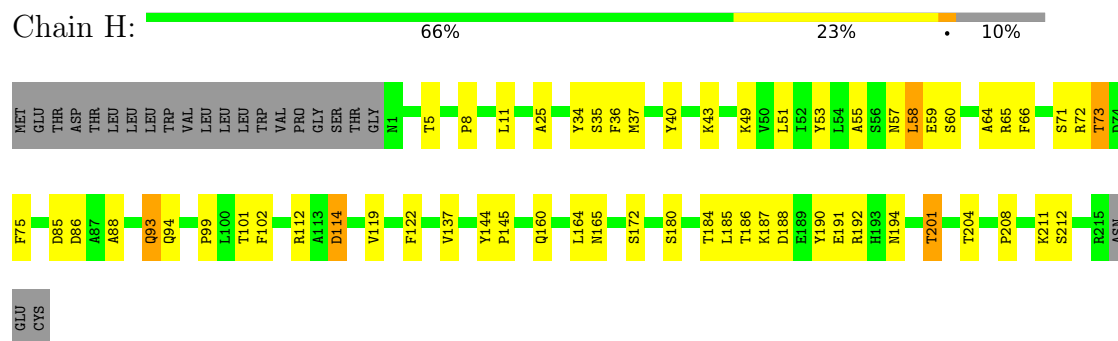
- Molecule 2: 2B7 Fab fragment heavy chain



- Molecule 3: 2B7 Fab fragment light chain



- Molecule 3: 2B7 Fab fragment light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 329.71Å 86.72Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20 48.17 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.17-3.20) 82.9 (48.17-3.01)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.207 , 0.261 0.216 , 0.267	Depositor DCC
R_{free} test set	3089 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.118 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24057	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, SO4

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	0.64	0/2791	0.73	1/3783 (0.0%)
1	B	0.68	2/2791 (0.1%)	0.77	3/3783 (0.1%)
1	C	0.64	0/2791	0.72	1/3783 (0.0%)
1	D	0.64	1/2791 (0.0%)	0.75	2/3783 (0.1%)
2	E	0.48	0/1647	0.67	1/2244 (0.0%)
2	G	0.48	1/1643 (0.1%)	0.66	0/2239
2	I	0.53	1/1643 (0.1%)	0.66	0/2239
2	K	0.46	0/1643	0.65	0/2239
3	F	0.44	0/1699	0.67	2/2312 (0.1%)
3	H	0.48	0/1699	0.65	0/2312
3	J	0.46	0/1699	0.67	0/2312
3	L	0.44	0/1699	0.63	0/2312
All	All	0.56	5/24536 (0.0%)	0.70	10/33341 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	291	CYS	CB-SG	-9.45	1.66	1.82
1	B	312	CYS	CB-SG	-6.86	1.70	1.82
2	I	32	CYS	CB-SG	-5.26	1.73	1.81
1	B	4	CYS	CB-SG	-5.14	1.73	1.81
2	G	95	CYS	CB-SG	-5.12	1.73	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	CYS	CA-CB-SG	-12.27	91.91	114.00
1	B	291	CYS	CA-CB-SG	-9.22	97.41	114.00
1	A	223	CYS	CA-CB-SG	-6.88	101.61	114.00
1	D	223	CYS	CA-CB-SG	-6.78	101.80	114.00
1	B	223	CYS	CA-CB-SG	-6.75	101.86	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2720	0	2630	72	0
1	B	2720	0	2630	65	1
1	C	2720	0	2630	62	0
1	D	2720	0	2630	70	1
2	E	1607	0	1557	30	0
2	G	1603	0	1552	36	0
2	I	1603	0	1552	37	0
2	K	1603	0	1552	39	0
3	F	1661	0	1590	38	0
3	H	1661	0	1590	30	0
3	J	1661	0	1590	34	0
3	L	1661	0	1590	33	0
4	A	28	0	26	2	0
4	B	28	0	26	1	0
4	C	28	0	26	3	0
4	D	28	0	26	0	0
5	C	5	0	0	0	0
All	All	24057	0	23197	501	1

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 11.

The worst 5 of 501 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:J:129:LEU:HA	3:J:187:LYS:HE2	1.49	0.95
1:B:341:LYS:HG3	1:B:345:LEU:HD12	1.54	0.90
3:L:1:ASN:HB3	3:L:99:PRO:HD2	1.53	0.90
1:A:62:ARG:HD2	1:A:219:GLU:HB3	1.55	0.89
2:I:54:ASN:HB3	2:I:56:MET:HG3	1.55	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:SER:OG	1:D:239:SER:OG[1_554]	2.08	0.12

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	336/376 (89%)	313 (93%)	23 (7%)	0	100	100
1	B	336/376 (89%)	314 (94%)	22 (6%)	0	100	100
1	C	336/376 (89%)	314 (94%)	22 (6%)	0	100	100
1	D	336/376 (89%)	314 (94%)	22 (6%)	0	100	100
2	E	208/268 (78%)	194 (93%)	14 (7%)	0	100	100
2	G	207/268 (77%)	196 (95%)	11 (5%)	0	100	100
2	I	207/268 (77%)	198 (96%)	9 (4%)	0	100	100
2	K	207/268 (77%)	197 (95%)	10 (5%)	0	100	100
3	F	213/238 (90%)	204 (96%)	9 (4%)	0	100	100
3	H	213/238 (90%)	201 (94%)	12 (6%)	0	100	100
3	J	213/238 (90%)	203 (95%)	10 (5%)	0	100	100
3	L	213/238 (90%)	202 (95%)	11 (5%)	0	100	100
All	All	3025/3528 (86%)	2850 (94%)	175 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	297/326 (91%)	277 (93%)	20 (7%)	16	50
1	B	297/326 (91%)	271 (91%)	26 (9%)	10	36
1	C	297/326 (91%)	272 (92%)	25 (8%)	11	39
1	D	297/326 (91%)	275 (93%)	22 (7%)	13	46
2	E	187/233 (80%)	174 (93%)	13 (7%)	15	48
2	G	187/233 (80%)	175 (94%)	12 (6%)	17	52
2	I	187/233 (80%)	172 (92%)	15 (8%)	12	42
2	K	187/233 (80%)	176 (94%)	11 (6%)	19	54
3	F	188/209 (90%)	174 (93%)	14 (7%)	13	46
3	H	188/209 (90%)	171 (91%)	17 (9%)	9	34
3	J	188/209 (90%)	172 (92%)	16 (8%)	10	38
3	L	188/209 (90%)	170 (90%)	18 (10%)	8	32
All	All	2688/3072 (88%)	2479 (92%)	209 (8%)	12	43

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	34	MET
3	F	186	THR
3	L	58	LEU
2	E	44	ASP
3	F	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	43	GLN
2	G	3	GLN
3	L	41	GLN
2	E	170	HIS
2	G	111	GLN

5.3.3 RNA ⓘ

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](#)

9 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	D	401	1	14,14,15	0.91	2 (14%)	17,19,21	0.52	0
4	NAG	A	401	1	14,14,15	0.83	1 (7%)	17,19,21	0.56	0
4	NAG	C	401	1	14,14,15	0.87	1 (7%)	17,19,21	0.76	0
4	NAG	D	402	1	14,14,15	0.48	0	17,19,21	1.21	1 (5%)
4	NAG	B	402	1	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
5	SO4	C	403	-	4,4,4	0.41	0	6,6,6	0.62	0
4	NAG	A	402	1	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	C	402	1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
4	NAG	B	401	1	14,14,15	0.69	0	17,19,21	1.06	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	402	1	-	4/6/23/26	0/1/1/1
4	NAG	B	402	1	-	4/6/23/26	0/1/1/1
4	NAG	A	402	1	-	4/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	401	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	NAG	C1-C2	2.95	1.56	1.52
4	A	401	NAG	C1-C2	2.72	1.56	1.52
4	A	402	NAG	O5-C1	2.54	1.47	1.43
4	D	401	NAG	C1-C2	2.48	1.56	1.52
4	D	401	NAG	O5-C1	2.06	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	NAG	C1-O5-C5	4.17	117.84	112.19
4	C	402	NAG	C1-O5-C5	3.29	116.64	112.19
4	A	402	NAG	C1-O5-C5	3.23	116.57	112.19
4	B	401	NAG	C2-N2-C7	2.64	126.66	122.90
4	B	402	NAG	C1-O5-C5	2.38	115.42	112.19

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	NAG	O5-C5-C6-O6
4	D	402	NAG	O5-C5-C6-O6
4	B	402	NAG	O5-C5-C6-O6
4	A	402	NAG	C4-C5-C6-O6
4	B	401	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	NAG	1	0
4	C	401	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	NAG	1	0
4	C	402	NAG	2	0
4	B	401	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 [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	340/376 (90%)	-0.46	0 100 100	52, 79, 109, 125	0
1	B	340/376 (90%)	-0.42	0 100 100	51, 71, 99, 114	0
1	C	340/376 (90%)	-0.47	0 100 100	53, 76, 105, 121	0
1	D	340/376 (90%)	-0.38	0 100 100	51, 77, 116, 142	0
2	E	214/268 (79%)	-0.44	2 (0%) 84 75	77, 96, 142, 156	0
2	G	213/268 (79%)	-0.45	0 100 100	74, 99, 142, 162	0
2	I	213/268 (79%)	-0.36	2 (0%) 84 75	72, 90, 148, 162	0
2	K	213/268 (79%)	-0.44	1 (0%) 91 86	75, 101, 140, 156	0
3	F	215/238 (90%)	-0.22	3 (1%) 75 63	75, 112, 156, 165	0
3	H	215/238 (90%)	-0.47	0 100 100	69, 106, 129, 140	0
3	J	215/238 (90%)	-0.26	5 (2%) 60 47	71, 106, 171, 185	0
3	L	215/238 (90%)	-0.41	3 (1%) 75 63	76, 108, 140, 148	0
All	All	3073/3528 (87%)	-0.40	16 (0%) 91 86	51, 88, 143, 185	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	144	LEU	3.8
2	E	144	LEU	3.4
3	J	159	ARG	3.4
3	J	135	SER	3.1
3	L	185	LEU	3.1

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	401	14/15	0.88	0.12	102,112,121,125	0
4	NAG	C	401	14/15	0.88	0.13	100,108,114,118	0
4	NAG	B	402	14/15	0.88	0.19	102,102,102,102	0
4	NAG	C	402	14/15	0.88	0.26	101,101,101,101	0
4	NAG	D	401	14/15	0.89	0.14	119,129,139,143	0
4	NAG	A	402	14/15	0.91	0.21	102,102,102,102	0
4	NAG	D	402	14/15	0.91	0.13	102,102,102,102	0
4	NAG	B	401	14/15	0.91	0.12	90,97,102,105	0
5	SO4	C	403	5/5	0.92	0.14	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.