



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 09:34 AM EDT

PDB ID : 5K9Q
Title : Crystal structure of multidonor HV1-18-class broadly neutralizing Influenza A antibody 16.a.26 in complex with A/Hong Kong/1-4-MA21-1/1968 (H3N2) Hemagglutinin
Authors : Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2016-06-01
Resolution : 2.50 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 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

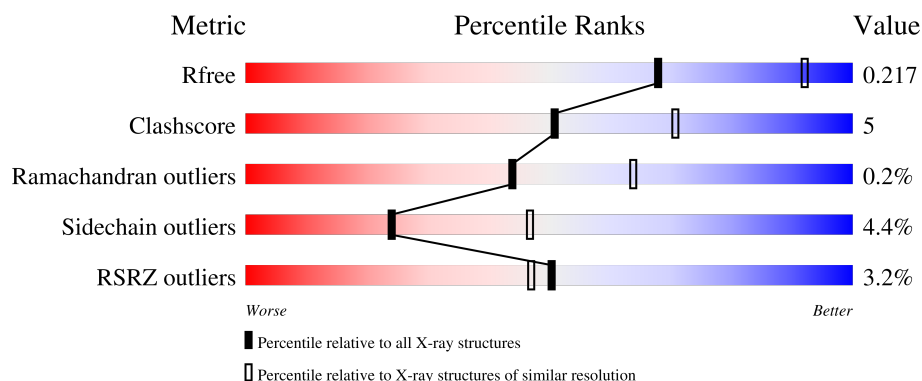
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	320	<div> <div>92%</div> <div>8%</div> </div>
1	C	320	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	E	320	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	M	320	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	320	 2% 89% 9% ..
1	Q	320	 % 89% 9% ..
2	B	170	 91% 8% .
2	D	170	 % 94% 5% .
2	F	170	 % 90% 9% .
2	N	170	 2% 85% 14% .
2	P	170	 2% 89% 6% .
2	R	170	 3% 91% 8% .
3	G	231	 12% 75% 21% .
3	H	231	 2% 77% 19% ..
3	J	231	 10% 82% 16% .
3	S	231	 7% 81% 18% .
3	U	231	 4% 86% 13% .
3	X	231	 4% 84% 15% .
4	I	214	 5% 85% 15% .
4	K	214	 % 81% 16% .
4	L	214	 2% 78% 19% .
4	T	214	 11% 82% 14% .
4	V	214	 % 85% 13% .
4	Y	214	 3% 86% 13% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45420 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2468	1544	433	478	13			
1	C	319	Total	C	N	O	S	0	0	0
			2467	1544	433	477	13			
1	E	318	Total	C	N	O	S	0	0	0
			2458	1538	431	476	13			
1	M	318	Total	C	N	O	S	0	0	0
			2458	1538	431	476	13			
1	O	318	Total	C	N	O	S	0	0	0
			2458	1538	431	476	13			
1	Q	318	Total	C	N	O	S	0	0	0
			2459	1540	431	475	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLU	GLY	conflict	UNP Q91MA7
A	327	ALA	GLN	conflict	UNP Q91MA7
C	218	GLU	GLY	conflict	UNP Q91MA7
C	327	ALA	GLN	conflict	UNP Q91MA7
E	218	GLU	GLY	conflict	UNP Q91MA7
E	327	ALA	GLN	conflict	UNP Q91MA7
M	218	GLU	GLY	conflict	UNP Q91MA7
M	327	ALA	GLN	conflict	UNP Q91MA7
O	218	GLU	GLY	conflict	UNP Q91MA7
O	327	ALA	GLN	conflict	UNP Q91MA7
Q	218	GLU	GLY	conflict	UNP Q91MA7
Q	327	ALA	GLN	conflict	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	0	0
			1366	845	241	274	6			
2	D	169	Total	C	N	O	S	0	0	0
			1377	854	242	275	6			
2	F	168	Total	C	N	O	S	0	0	0
			1371	848	242	275	6			
2	N	169	Total	C	N	O	S	0	0	0
			1368	846	240	276	6			
2	P	163	Total	C	N	O	S	0	0	0
			1340	829	236	269	6			
2	R	167	Total	C	N	O	S	0	0	0
			1362	843	240	273	6			

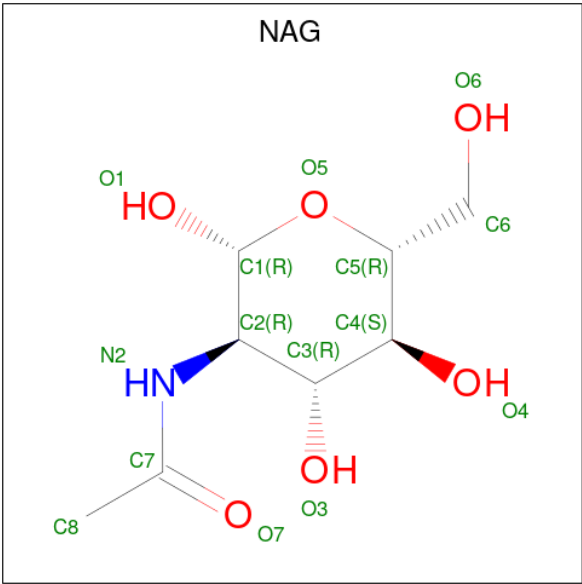
- Molecule 3 is a protein called 16.a.26 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	H	228	Total	C	N	O	S	0	0	0
			1707	1077	290	333	7			
3	J	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	S	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	U	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	X	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			

- Molecule 4 is a protein called 16.a.26 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	K	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	L	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	T	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	V	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	Y	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	N	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	R	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total	O	0	0
			173	173		
6	B	81	Total	O	0	0
			81	81		
6	C	156	Total	O	0	0
			156	156		
6	D	74	Total	O	0	0
			74	74		
6	E	110	Total	O	0	0
			110	110		
6	F	75	Total	O	0	0
			75	75		
6	G	29	Total	O	0	0
			29	29		
6	H	62	Total	O	0	0
			62	62		
6	I	34	Total	O	0	0
			34	34		
6	J	29	Total	O	0	0
			29	29		
6	K	30	Total	O	0	0
			30	30		
6	L	75	Total	O	0	0
			75	75		
6	M	126	Total	O	0	0
			126	126		
6	N	50	Total	O	0	0
			50	50		
6	O	96	Total	O	0	0
			96	96		
6	P	40	Total	O	0	0
			40	40		

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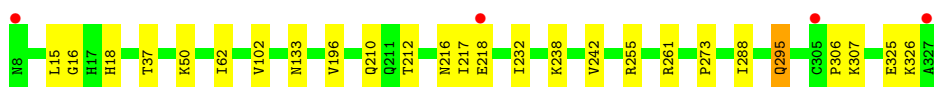
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	128	Total 128	O 128	0	0
6	R	51	Total 51	O 51	0	0
6	S	9	Total 9	O 9	0	0
6	T	19	Total 19	O 19	0	0
6	U	61	Total 61	O 61	0	0
6	V	55	Total 55	O 55	0	0
6	X	55	Total 55	O 55	0	0
6	Y	51	Total 51	O 51	0	0

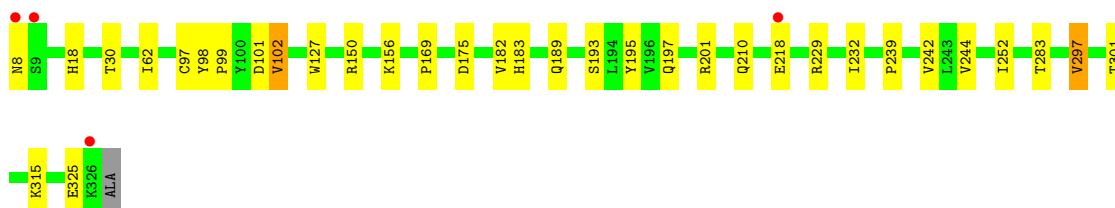
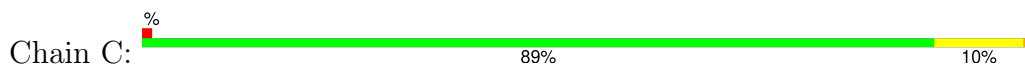
3 Residue-property plots [i](#)

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.

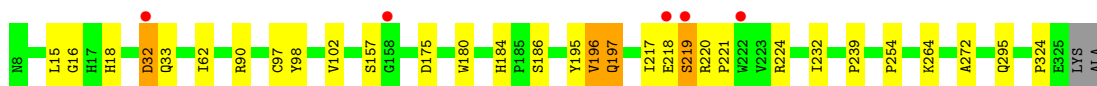
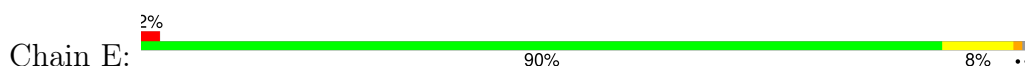
- Molecule 1: Hemagglutinin HA1



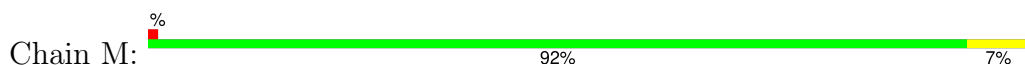
- Molecule 1: Hemagglutinin HA1



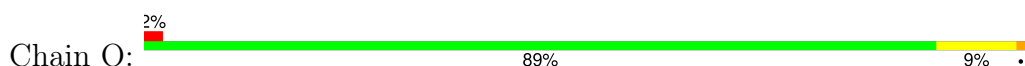
- Molecule 1: Hemagglutinin HA1

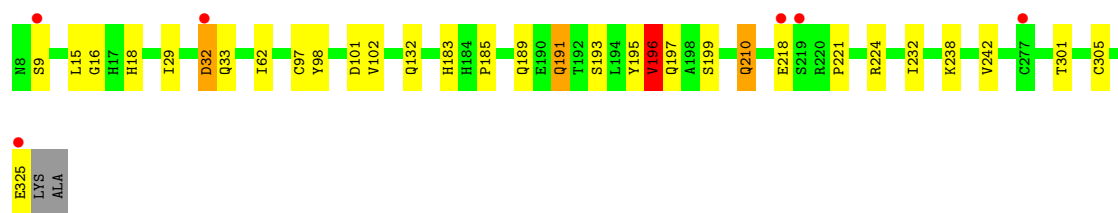


- Molecule 1: Hemagglutinin HA1

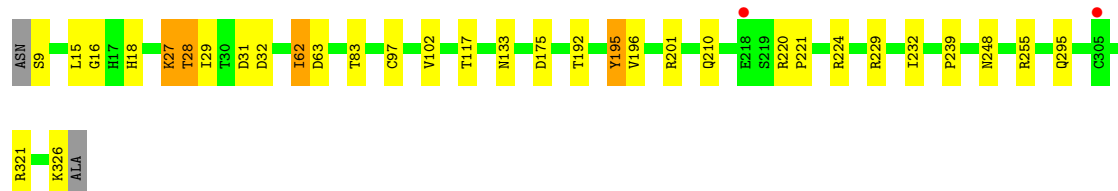
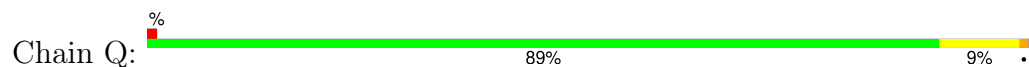


- Molecule 1: Hemagglutinin HA1





• Molecule 1: Hemagglutinin HA1



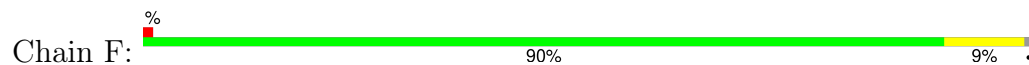
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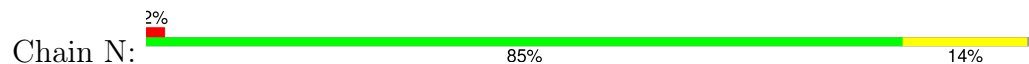
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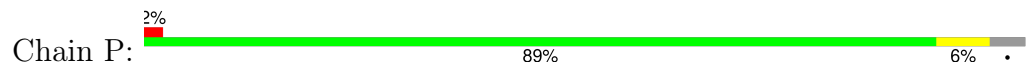
• Molecule 2: Hemagglutinin HA2



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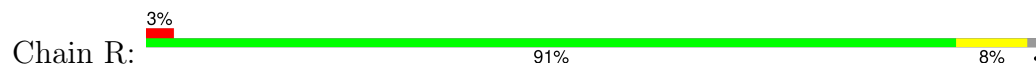


• Molecule 2: Hemagglutinin HA2

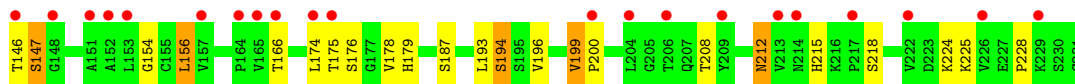
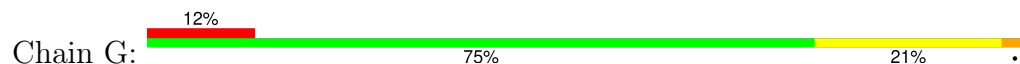




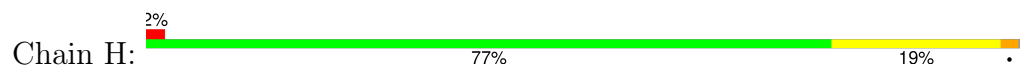
• Molecule 2: Hemagglutinin HA2



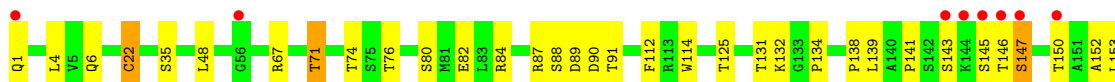
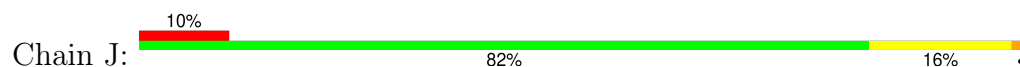
• Molecule 3: 16.a.26 Heavy chain



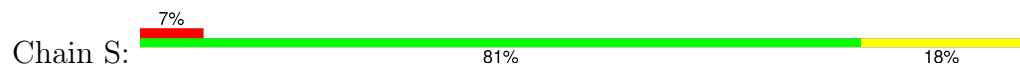
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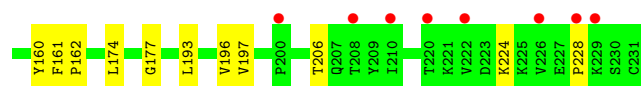


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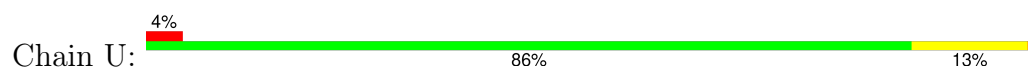


• Molecule 3: 16.a.26 Heavy chain

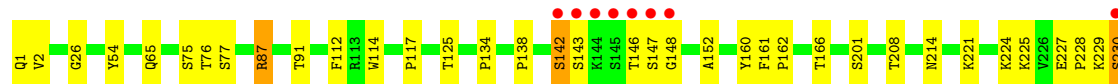
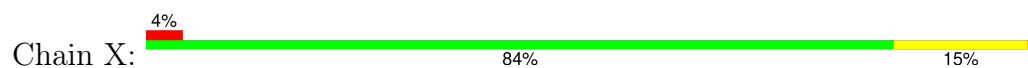




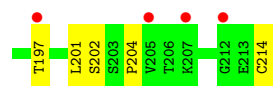
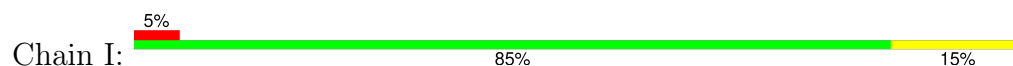
- Molecule 3: 16.a.26 Heavy chain



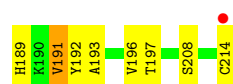
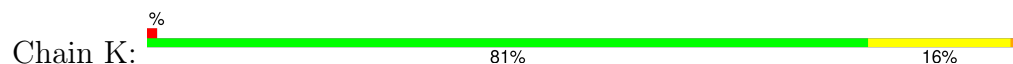
- Molecule 3: 16.a.26 Heavy chain



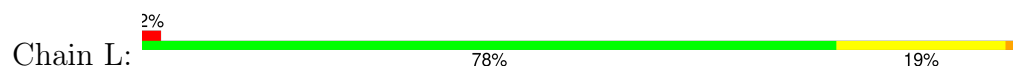
- Molecule 4: 16.a.26 Light chain

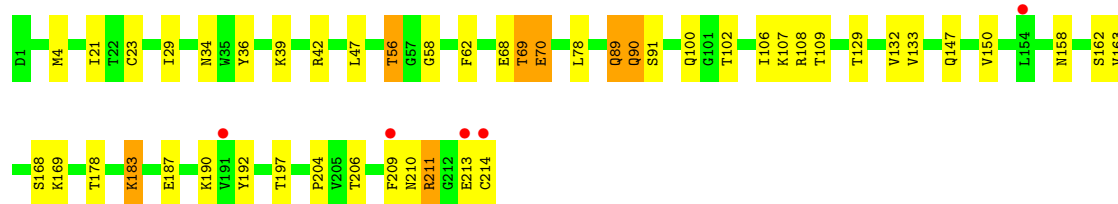


- Molecule 4: 16.a.26 Light chain

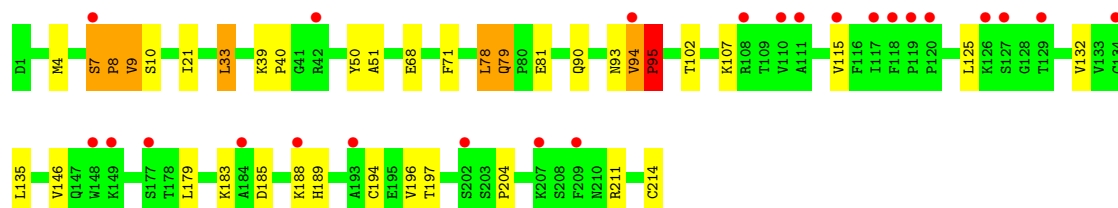
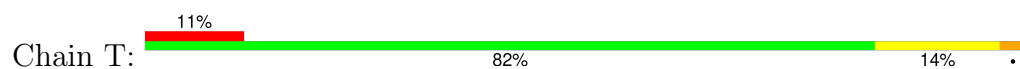


- Molecule 4: 16.a.26 Light chain

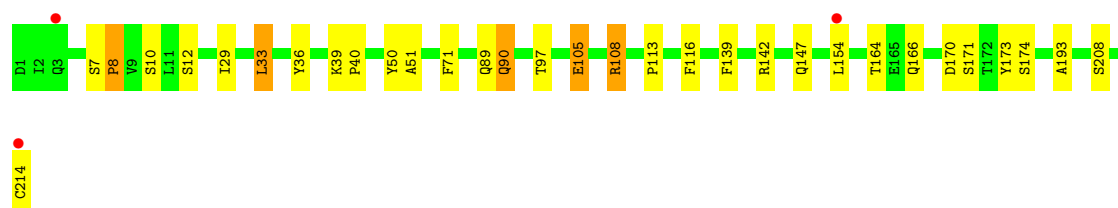
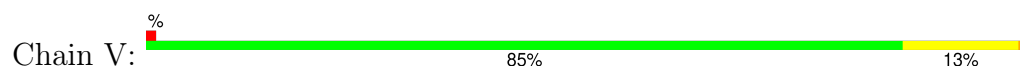




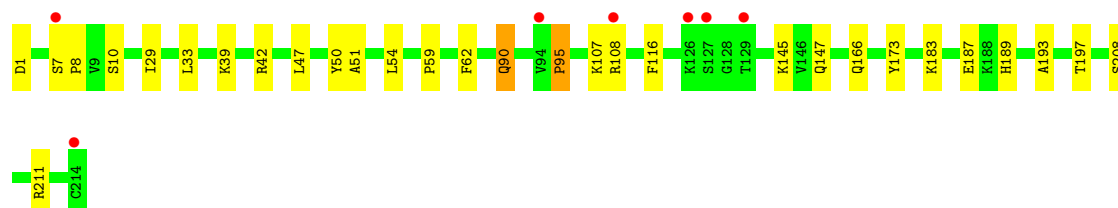
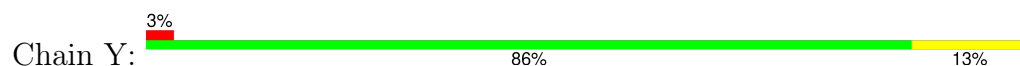
• Molecule 4: 16.a.26 Light chain



• Molecule 4: 16.a.26 Light chain



• Molecule 4: 16.a.26 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.81Å 233.91Å 302.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.50 49.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	82.5 (49.28-2.50) 82.5 (49.28-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.182 , 0.218 0.185 , 0.217	Depositor DCC
R_{free} test set	14775 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45420	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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	A	0.33	0/2524	0.49	0/3441
1	C	0.35	0/2523	0.47	0/3438
1	E	0.33	0/2514	0.47	0/3427
1	M	0.32	0/2514	0.48	0/3427
1	O	0.32	0/2514	0.47	0/3427
1	Q	0.32	0/2515	0.50	0/3427
2	B	0.28	0/1389	0.42	0/1867
2	D	0.33	0/1401	0.44	0/1883
2	F	0.35	0/1394	0.45	0/1874
2	N	0.33	0/1391	0.42	0/1870
2	P	0.28	0/1363	0.42	0/1832
2	R	0.28	0/1385	0.43	0/1862
3	G	0.33	0/1771	0.50	0/2411
3	H	0.32	0/1749	0.50	0/2381
3	J	0.29	0/1771	0.48	0/2411
3	S	0.30	0/1771	0.48	0/2411
3	U	0.31	0/1771	0.49	0/2411
3	X	0.34	0/1771	0.52	0/2411
4	I	0.34	0/1693	0.49	0/2294
4	K	0.39	1/1693 (0.1%)	0.54	1/2294 (0.0%)
4	L	0.35	0/1693	0.53	1/2294 (0.0%)
4	T	0.48	3/1693 (0.2%)	0.56	1/2294 (0.0%)
4	V	0.47	2/1693 (0.1%)	0.55	1/2294 (0.0%)
4	Y	0.51	2/1693 (0.1%)	0.56	1/2294 (0.0%)
All	All	0.35	8/44189 (0.0%)	0.49	5/59975 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	95	PRO	N-CD	5.64	1.55	1.47
4	T	95	PRO	N-CD	5.57	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	8	PRO	N-CD	5.55	1.55	1.47
4	Y	8	PRO	N-CD	5.45	1.55	1.47
4	V	8	PRO	N-CD	5.31	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	39	LYS	C-N-CD	5.95	140.89	128.40
4	Y	39	LYS	C-N-CD	5.92	140.82	128.40
4	T	39	LYS	C-N-CD	5.81	140.60	128.40
4	L	58	GLY	C-N-CD	5.67	140.31	128.40
4	V	39	LYS	C-N-CD	5.58	140.13	128.40

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	2468	0	2406	19	0
1	C	2467	0	2412	21	0
1	E	2458	0	2399	27	0
1	M	2458	0	2399	18	0
1	O	2458	0	2399	29	0
1	Q	2459	0	2406	35	0
2	B	1366	0	1282	15	0
2	D	1377	0	1291	8	0
2	F	1371	0	1287	15	0
2	N	1368	0	1278	17	0
2	P	1340	0	1255	13	0
2	R	1362	0	1279	16	0
3	G	1728	0	1705	36	0
3	H	1707	0	1681	23	1
3	J	1728	0	1705	20	0
3	S	1728	0	1705	43	0
3	U	1728	0	1705	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	1728	0	1705	31	2
4	I	1658	0	1609	14	0
4	K	1658	0	1609	12	1
4	L	1658	0	1609	26	0
4	T	1658	0	1611	25	0
4	V	1658	0	1609	19	0
4	Y	1658	0	1609	11	0
5	A	70	0	65	0	0
5	B	14	0	13	0	0
5	C	70	0	65	2	0
5	D	14	0	13	0	0
5	E	70	0	65	0	0
5	F	14	0	13	0	0
5	M	70	0	65	1	0
5	N	14	0	13	0	0
5	O	70	0	65	0	0
5	P	14	0	13	0	0
5	Q	70	0	65	0	0
5	R	14	0	13	0	0
6	A	173	0	0	2	0
6	B	81	0	0	1	0
6	C	156	0	0	3	0
6	D	74	0	0	0	0
6	E	110	0	0	3	0
6	F	75	0	0	2	0
6	G	29	0	0	1	0
6	H	62	0	0	2	0
6	I	34	0	0	0	0
6	J	29	0	0	0	0
6	K	30	0	0	1	0
6	L	75	0	0	3	0
6	M	126	0	0	2	0
6	N	50	0	0	1	0
6	O	96	0	0	2	0
6	P	40	0	0	0	0
6	Q	128	0	0	3	0
6	R	51	0	0	2	0
6	S	9	0	0	0	0
6	T	19	0	0	0	0
6	U	61	0	0	2	0
6	V	55	0	0	1	0
6	X	55	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Y	51	0	0	1	0
All	All	45420	0	42423	438	2

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.

The worst 5 of 438 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:S:146:THR:HG21	3:S:151:ALA:CA	1.48	1.43
3:S:146:THR:CG2	3:S:151:ALA:HA	1.52	1.38
3:S:146:THR:HG21	3:S:151:ALA:CB	1.54	1.36
3:J:147:SER:CB	3:J:150:THR:O	1.77	1.32
3:J:147:SER:HB2	3:J:150:THR:O	1.27	1.28

All (2) 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)
4:K:156:SER:OG	3:X:231:CYS:SG[1_455]	1.94	0.26
3:H:1:GLN:N	3:X:26:GLY:O[1_455]	2.15	0.05

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	318/320 (99%)	306 (96%)	11 (4%)	1 (0%)	37 56
1	C	317/320 (99%)	308 (97%)	8 (2%)	1 (0%)	37 56
1	E	316/320 (99%)	306 (97%)	9 (3%)	1 (0%)	37 56
1	M	316/320 (99%)	306 (97%)	9 (3%)	1 (0%)	37 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	316/320 (99%)	308 (98%)	6 (2%)	2 (1%)	22	39
1	Q	316/320 (99%)	307 (97%)	8 (2%)	1 (0%)	37	56
2	B	166/170 (98%)	160 (96%)	6 (4%)	0	100	100
2	D	167/170 (98%)	159 (95%)	8 (5%)	0	100	100
2	F	166/170 (98%)	160 (96%)	6 (4%)	0	100	100
2	N	167/170 (98%)	160 (96%)	7 (4%)	0	100	100
2	P	161/170 (95%)	155 (96%)	6 (4%)	0	100	100
2	R	165/170 (97%)	158 (96%)	7 (4%)	0	100	100
3	G	229/231 (99%)	218 (95%)	11 (5%)	0	100	100
3	H	224/231 (97%)	217 (97%)	6 (3%)	1 (0%)	30	49
3	J	229/231 (99%)	222 (97%)	7 (3%)	0	100	100
3	S	229/231 (99%)	218 (95%)	10 (4%)	1 (0%)	30	49
3	U	229/231 (99%)	219 (96%)	10 (4%)	0	100	100
3	X	229/231 (99%)	219 (96%)	10 (4%)	0	100	100
4	I	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
4	K	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	L	212/214 (99%)	208 (98%)	3 (1%)	1 (0%)	25	44
4	T	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	25	44
4	V	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	Y	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
All	All	5532/5610 (99%)	5346 (97%)	175 (3%)	11 (0%)	44	64

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	T	9	VAL
1	O	196	VAL
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE

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	281/282 (100%)	275 (98%)	6 (2%)	48	74
1	C	282/282 (100%)	275 (98%)	7 (2%)	42	69
1	E	281/282 (100%)	275 (98%)	6 (2%)	48	74
1	M	281/282 (100%)	280 (100%)	1 (0%)	89	96
1	O	281/282 (100%)	269 (96%)	12 (4%)	25	48
1	Q	281/282 (100%)	273 (97%)	8 (3%)	38	65
2	B	144/146 (99%)	143 (99%)	1 (1%)	81	93
2	D	145/146 (99%)	145 (100%)	0	100	100
2	F	145/146 (99%)	144 (99%)	1 (1%)	81	93
2	N	144/146 (99%)	142 (99%)	2 (1%)	62	83
2	P	143/146 (98%)	141 (99%)	2 (1%)	62	83
2	R	144/146 (99%)	141 (98%)	3 (2%)	48	74
3	G	194/194 (100%)	172 (89%)	22 (11%)	4	9
3	H	191/194 (98%)	175 (92%)	16 (8%)	9	19
3	J	194/194 (100%)	175 (90%)	19 (10%)	6	13
3	S	194/194 (100%)	183 (94%)	11 (6%)	17	35
3	U	194/194 (100%)	188 (97%)	6 (3%)	35	62
3	X	194/194 (100%)	187 (96%)	7 (4%)	30	56
4	I	189/189 (100%)	174 (92%)	15 (8%)	10	21
4	K	189/189 (100%)	169 (89%)	20 (11%)	5	11
4	L	189/189 (100%)	169 (89%)	20 (11%)	5	11
4	T	189/189 (100%)	179 (95%)	10 (5%)	19	38
4	V	189/189 (100%)	181 (96%)	8 (4%)	25	49
4	Y	189/189 (100%)	180 (95%)	9 (5%)	21	43
All	All	4847/4866 (100%)	4635 (96%)	212 (4%)	24	47

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	69	THR
1	O	197	GLN

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Mol	Chain	Res	Type
3	X	142	SER
4	L	91	SER
4	L	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	18	HIS
2	P	65	GLN
2	P	12	ASN
1	Q	18	HIS
1	E	33	GLN

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](#)

36 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	NAG	B	201	2	14,14,15	0.28	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	201	2	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	O	404	1	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	M	402	1	14,14,15	0.45	0	17,19,21	0.52	0
5	NAG	Q	402	1	14,14,15	0.36	0	17,19,21	0.49	0
5	NAG	C	405	1	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	R	201	2	14,14,15	0.17	0	17,19,21	0.53	0
5	NAG	E	404	1	14,14,15	0.35	0	17,19,21	0.37	0
5	NAG	A	402	1	14,14,15	0.35	0	17,19,21	0.41	0
5	NAG	Q	404	1	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	O	402	1	14,14,15	0.41	0	17,19,21	0.46	0
5	NAG	C	401	1	14,14,15	0.43	0	17,19,21	0.52	0
5	NAG	O	405	1	14,14,15	0.29	0	17,19,21	0.39	0
5	NAG	M	401	1	14,14,15	0.51	0	17,19,21	0.53	0
5	NAG	Q	403	1	14,14,15	0.17	0	17,19,21	0.42	0
5	NAG	F	201	2	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	E	402	1	14,14,15	0.32	0	17,19,21	0.37	0
5	NAG	Q	405	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	Q	401	1	14,14,15	0.34	0	17,19,21	0.36	0
5	NAG	O	403	1	14,14,15	0.21	0	17,19,21	0.54	0
5	NAG	A	404	1	14,14,15	0.49	0	17,19,21	0.69	1 (5%)
5	NAG	M	405	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	C	402	1	14,14,15	0.43	0	17,19,21	0.51	0
5	NAG	A	403	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	A	405	1	14,14,15	0.23	0	17,19,21	0.35	0
5	NAG	C	404	1	14,14,15	0.27	0	17,19,21	0.39	0
5	NAG	O	401	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	A	401	1	14,14,15	0.19	0	17,19,21	0.71	1 (5%)
5	NAG	M	404	1	14,14,15	0.29	0	17,19,21	0.37	0
5	NAG	N	201	2	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	C	403	1	14,14,15	1.28	1 (7%)	17,19,21	1.16	3 (17%)
5	NAG	E	403	1	14,14,15	0.18	0	17,19,21	0.43	0
5	NAG	E	401	1	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
5	NAG	P	201	2	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	M	403	1	14,14,15	0.95	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	E	405	1	14,14,15	0.24	0	17,19,21	0.47	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	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	404	1	-	0/6/23/26	0/1/1/1
5	NAG	M	402	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	405	1	-	0/6/23/26	0/1/1/1
5	NAG	R	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	402	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	404	1	-	0/6/23/26	0/1/1/1
5	NAG	O	402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
5	NAG	O	405	1	-	0/6/23/26	0/1/1/1
5	NAG	M	401	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	403	1	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	402	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	405	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	401	1	-	2/6/23/26	0/1/1/1
5	NAG	O	403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	404	1	-	2/6/23/26	0/1/1/1
5	NAG	M	405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	403	1	-	1/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	404	1	-	1/6/23/26	0/1/1/1
5	NAG	O	401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	M	404	1	-	2/6/23/26	0/1/1/1
5	NAG	N	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	403	1	-	2/6/23/26	0/1/1/1
5	NAG	E	403	1	-	2/6/23/26	0/1/1/1
5	NAG	E	401	1	-	1/6/23/26	0/1/1/1
5	NAG	P	201	2	-	0/6/23/26	0/1/1/1
5	NAG	M	403	1	-	1/6/23/26	0/1/1/1
5	NAG	E	405	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	403	NAG	C1-C2	4.30	1.58	1.52
5	M	403	NAG	O5-C1	3.28	1.49	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	403	NAG	C1-O5-C5	4.91	118.77	112.19
5	C	403	NAG	C1-O5-C5	2.87	116.03	112.19
5	A	404	NAG	C1-O5-C5	2.25	115.20	112.19
5	C	403	NAG	O5-C5-C4	-2.22	105.44	110.83
5	A	401	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	402	NAG	O5-C5-C6-O6
5	M	402	NAG	O5-C5-C6-O6
5	O	402	NAG	O5-C5-C6-O6
5	A	402	NAG	O5-C5-C6-O6
5	Q	401	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	405	NAG	1	0
5	M	401	NAG	1	0
5	C	403	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	320/320 (100%)	-0.45	4 (1%) 74 71	27, 38, 64, 116	0
1	C	319/320 (99%)	-0.36	4 (1%) 74 71	27, 43, 67, 109	1 (0%)
1	E	318/320 (99%)	-0.19	5 (1%) 70 67	33, 50, 79, 106	0
1	M	318/320 (99%)	-0.36	4 (1%) 74 71	30, 42, 72, 124	2 (0%)
1	O	318/320 (99%)	-0.12	6 (1%) 66 63	36, 53, 87, 134	1 (0%)
1	Q	318/320 (99%)	-0.36	2 (0%) 85 83	31, 44, 66, 102	2 (0%)
2	B	168/170 (98%)	-0.35	0 100 100	28, 45, 66, 161	2 (1%)
2	D	169/170 (99%)	-0.30	2 (1%) 76 73	28, 46, 71, 167	0
2	F	168/170 (98%)	-0.32	1 (0%) 85 83	31, 46, 65, 131	2 (1%)
2	N	169/170 (99%)	0.07	3 (1%) 67 64	32, 68, 105, 139	2 (1%)
2	P	163/170 (95%)	0.01	4 (2%) 58 55	31, 64, 101, 144	2 (1%)
2	R	167/170 (98%)	-0.06	5 (2%) 52 49	30, 55, 98, 114	0
3	G	231/231 (100%)	0.53	27 (11%) 10 10	34, 78, 164, 266	0
3	H	228/231 (98%)	-0.16	5 (2%) 62 59	28, 52, 86, 142	0
3	J	231/231 (100%)	0.44	22 (9%) 15 14	35, 77, 164, 268	1 (0%)
3	S	231/231 (100%)	0.77	16 (6%) 24 22	51, 94, 161, 280	0
3	U	231/231 (100%)	0.06	9 (3%) 44 40	32, 54, 88, 174	0
3	X	231/231 (100%)	-0.09	9 (3%) 44 40	35, 57, 98, 201	0
4	I	214/214 (100%)	0.43	10 (4%) 37 34	34, 74, 161, 216	1 (0%)
4	K	214/214 (100%)	0.28	3 (1%) 73 70	33, 79, 114, 174	0
4	L	214/214 (100%)	-0.01	5 (2%) 61 58	25, 51, 105, 158	0
4	T	214/214 (100%)	0.76	24 (11%) 11 11	24, 83, 169, 219	2 (0%)
4	V	214/214 (100%)	-0.08	3 (1%) 73 70	24, 50, 79, 152	0
4	Y	214/214 (100%)	0.01	7 (3%) 49 46	24, 56, 91, 118	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5582/5610 (99%)	-0.02	180 (3%)	50	47	24, 52, 125, 280	19 (0%)

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	146	THR	6.2
2	R	5	ALA	6.1
1	O	218	GLU	5.4
3	X	146	THR	5.3
3	H	146	THR	5.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	NAG	M	401	14/15	0.27	0.21	142,162,166,166	0
5	NAG	E	401	14/15	0.35	0.18	144,157,161,163	0
5	NAG	A	401	14/15	0.36	0.22	143,153,161,163	0
5	NAG	O	401	14/15	0.39	0.16	149,162,172,172	0
5	NAG	C	401	14/15	0.48	0.20	144,160,163,163	0
5	NAG	Q	401	14/15	0.57	0.20	138,157,160,161	0
5	NAG	O	404	14/15	0.69	0.18	93,109,116,121	0
5	NAG	M	403	14/15	0.72	0.18	95,104,111,111	0
5	NAG	Q	404	14/15	0.72	0.19	102,123,131,135	0
5	NAG	C	403	14/15	0.74	0.20	105,118,126,127	0
5	NAG	A	404	14/15	0.75	0.21	93,112,127,130	0
5	NAG	R	201	14/15	0.75	0.15	87,101,112,118	0
5	NAG	M	404	14/15	0.78	0.17	93,104,108,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	E	404	14/15	0.78	0.14	89,105,123,129	0
5	NAG	M	402	14/15	0.79	0.16	77,88,91,92	0
5	NAG	O	402	14/15	0.80	0.18	80,99,106,109	0
5	NAG	P	201	14/15	0.81	0.14	79,93,96,100	0
5	NAG	C	404	14/15	0.81	0.17	104,126,132,137	0
5	NAG	E	402	14/15	0.82	0.17	72,82,91,92	0
5	NAG	Q	402	14/15	0.82	0.18	81,93,105,110	0
5	NAG	Q	405	14/15	0.83	0.12	62,76,87,97	0
5	NAG	Q	403	14/15	0.83	0.17	86,95,107,113	0
5	NAG	A	402	14/15	0.84	0.16	76,87,92,97	0
5	NAG	N	201	14/15	0.84	0.12	83,94,99,105	0
5	NAG	A	403	14/15	0.84	0.15	78,94,104,106	0
5	NAG	C	402	14/15	0.85	0.14	65,77,83,93	0
5	NAG	A	405	14/15	0.86	0.11	56,67,76,83	0
5	NAG	B	201	14/15	0.87	0.12	52,62,73,85	0
5	NAG	M	405	14/15	0.88	0.11	59,72,86,86	0
5	NAG	C	405	14/15	0.88	0.12	64,69,85,86	0
5	NAG	D	201	14/15	0.89	0.10	52,67,75,78	0
5	NAG	E	405	14/15	0.90	0.10	49,62,70,76	0
5	NAG	O	405	14/15	0.92	0.10	59,75,87,88	0
5	NAG	F	201	14/15	0.92	0.08	48,66,72,75	0
5	NAG	O	403	14/15	0.92	0.09	53,62,70,72	0
5	NAG	E	403	14/15	0.92	0.10	57,72,79,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.