



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2018 – 12:42 AM EDT

PDB ID : 6B3M
Title : The crystal structure of a broadly-reactive human anti-hemagglutinin stalk antibody (70-1F02) in complex with H5 hemagglutinin
Authors : Shore, D.A.; Yang, H.; Stevens, J.
Deposited on : 2017-09-22
Resolution : 3.92 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

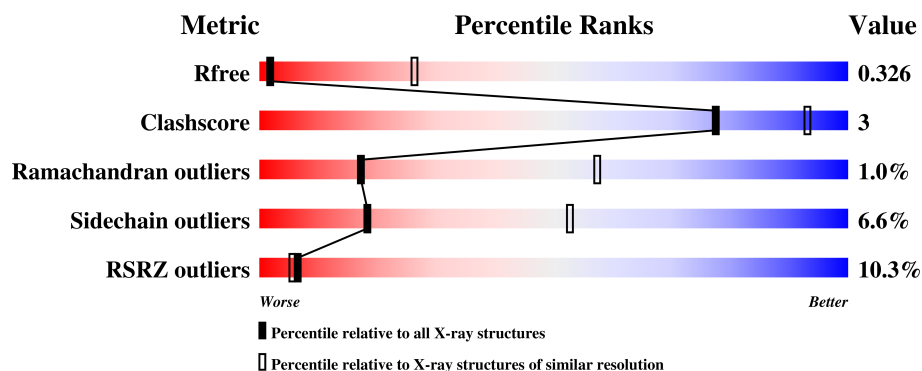
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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}	111664	1151 (4.24-3.60)
Clashscore	122126	1003 (4.22-3.62)
Ramachandran outliers	120053	1190 (4.24-3.60)
Sidechain outliers	120020	1181 (4.24-3.60)
RSRZ outliers	108989	1049 (4.24-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	330	<div> <div>6%</div> <div>82% 13% . .</div> </div>
1	E	330	<div> <div>6%</div> <div>83% 12% . .</div> </div>
1	G	330	<div> <div>2%</div> <div>84% 12% . .</div> </div>
1	K	330	<div> <div>2%</div> <div>82% 14% . .</div> </div>
1	Q	330	<div> <div>2%</div> <div>82% 13% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	330	
2	B	181	
2	F	181	
2	H	181	
2	L	181	
2	R	181	
2	T	181	
3	C	221	
3	I	221	
3	M	221	
3	O	221	
3	V	221	
3	Y	221	
4	D	215	
4	J	215	
4	N	215	
4	P	215	
4	U	215	
4	W	215	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	406	X	-	-	-
5	NAG	A	407	-	-	-	X
5	NAG	A	410	-	-	-	X
5	NAG	B	201	X	-	-	-
5	NAG	B	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	F	201	X	-	-	X
5	NAG	G	401	X	-	-	-
5	NAG	G	405	X	-	-	X
5	NAG	K	401	-	-	-	X
5	NAG	K	402	X	-	-	-
5	NAG	K	403	-	-	-	X
5	NAG	K	411	-	-	-	X
5	NAG	M	302	-	-	-	X
5	NAG	M	306	-	-	-	X
5	NAG	M	307	-	-	-	X
5	NAG	Q	401	-	-	-	X
5	NAG	Q	402	X	-	-	-
5	NAG	Q	403	-	-	-	X
5	NAG	Q	408	-	-	-	X
5	NAG	R	201	-	-	-	X
5	NAG	R	202	-	-	-	X
5	NAG	S	406	-	-	-	X
6	MAN	A	405	-	-	-	X
6	MAN	M	304	-	-	-	X
6	MAN	M	308	-	-	-	X
6	MAN	O	303	-	-	-	X
6	MAN	O	304	-	-	-	X
6	MAN	S	403	-	-	-	X
6	MAN	S	407	-	-	-	X
6	MAN	S	408	-	-	-	X
7	BMA	M	305	X	-	-	X
7	BMA	M	309	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 44024 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	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	E	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	G	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	K	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	Q	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	S	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	H	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	L	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	R	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	T	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	GLU	LYS	conflict	UNP A0A182DWE1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	147	GLU	LYS	conflict	UNP A0A182DWE1
H	147	GLU	LYS	conflict	UNP A0A182DWE1
L	147	GLU	LYS	conflict	UNP A0A182DWE1
R	147	GLU	LYS	conflict	UNP A0A182DWE1
T	147	GLU	LYS	conflict	UNP A0A182DWE1

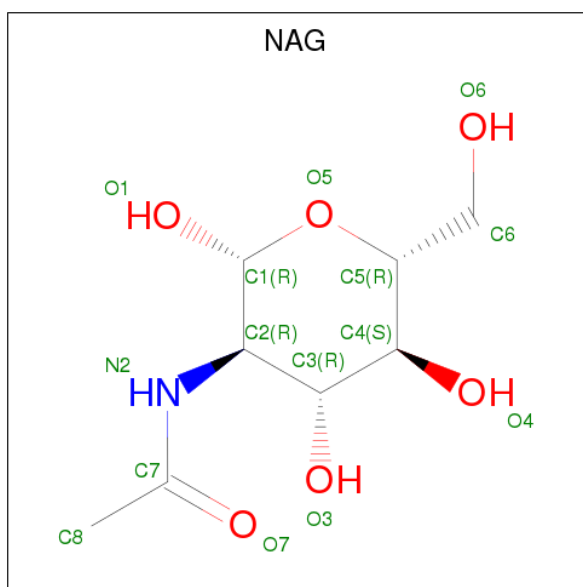
- Molecule 3 is a protein called 70-1F02 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	I	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	M	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	O	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	V	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	Y	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			

- Molecule 4 is a protein called 70-1F02 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	213	Total	C	N	O	S	0	0	0
			1626	1016	278	327	5			
4	U	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	J	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	D	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	W	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	N	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (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	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	B	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	G	1	Total	C	N	O	0	0
			14	8	1	5		

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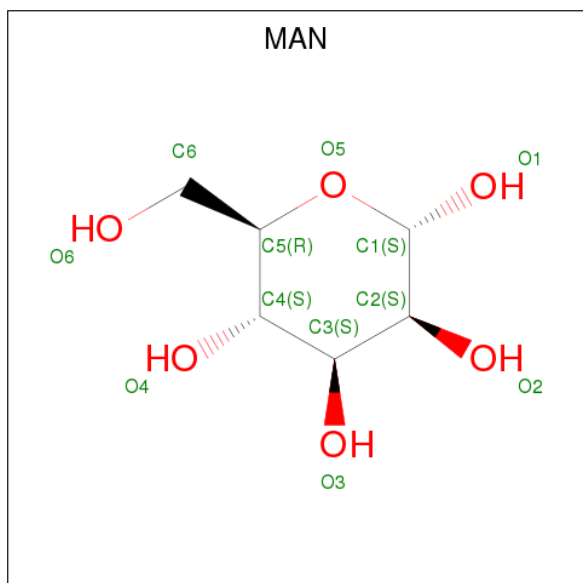
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1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

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



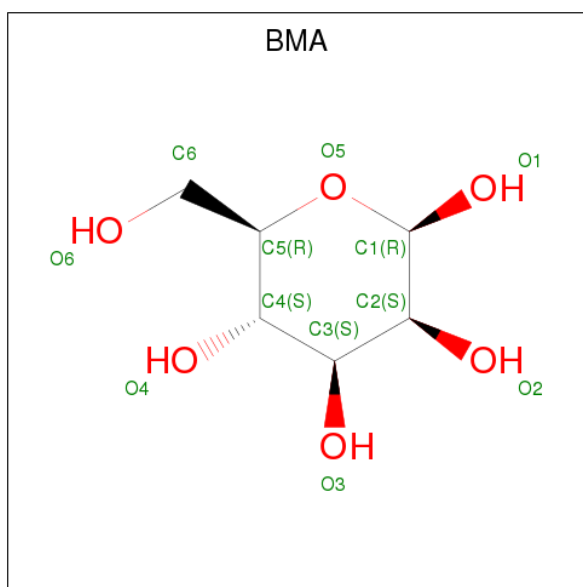
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

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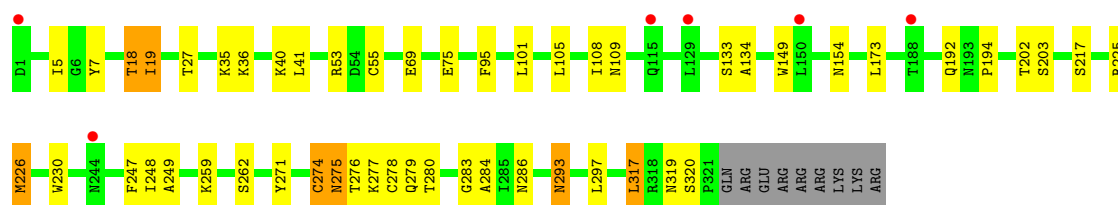
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	K	1	Total	C	O	0	0
			11	6	5		
6	K	1	Total	C	O	0	0
			11	6	5		
6	K	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	O	1	Total	C	O	0	0
			11	6	5		
6	O	1	Total	C	O	0	0
			11	6	5		
6	Q	1	Total	C	O	0	0
			11	6	5		
6	Q	1	Total	C	O	0	0
			11	6	5		
6	S	1	Total	C	O	0	0
			11	6	5		
6	S	1	Total	C	O	0	0
			11	6	5		
6	S	1	Total	C	O	0	0
			11	6	5		

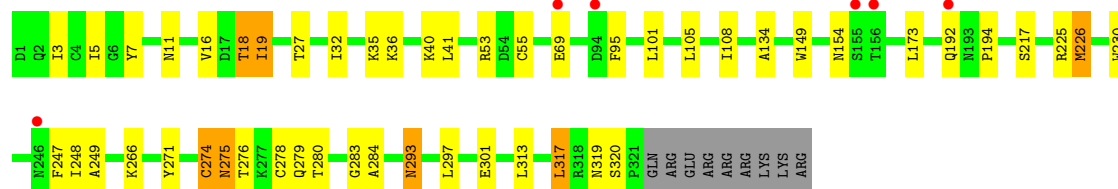
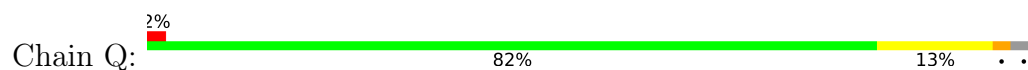
- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



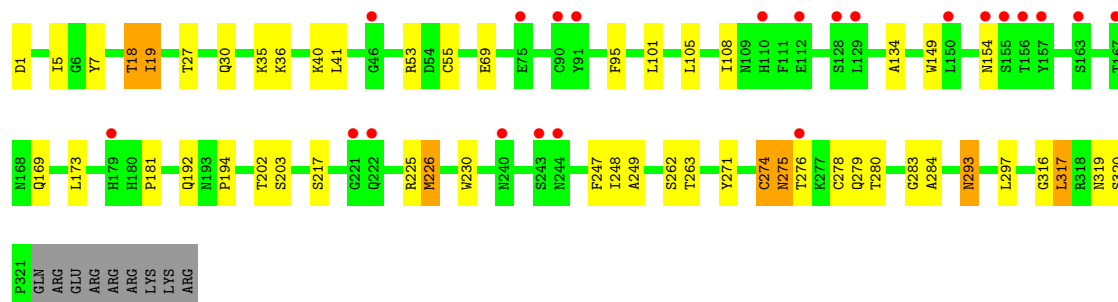
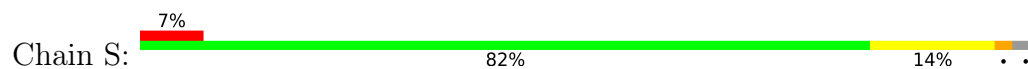
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	M	1	Total	C	O	0	0
			11	6	5		
7	M	1	Total	C	O	0	0
			11	6	5		
7	Q	1	Total	C	O	0	0
			11	6	5		



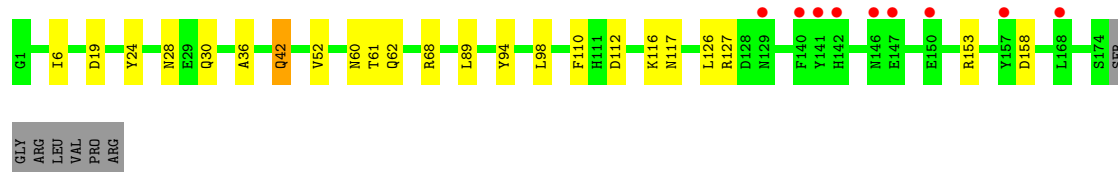
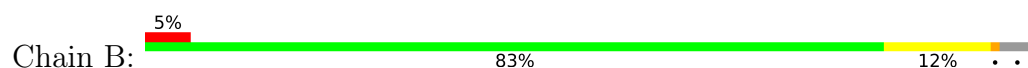
• Molecule 1: Hemagglutinin HA1



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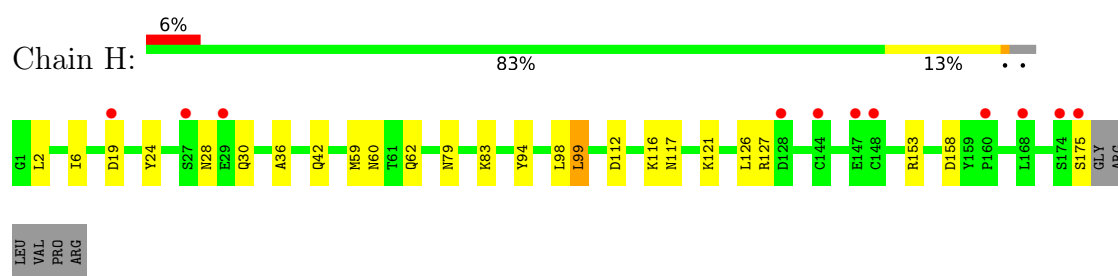
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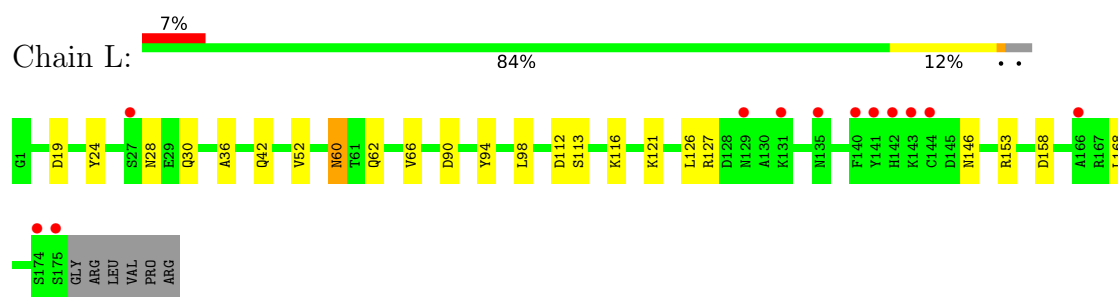
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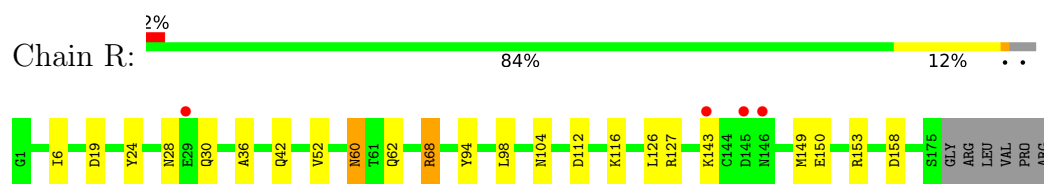
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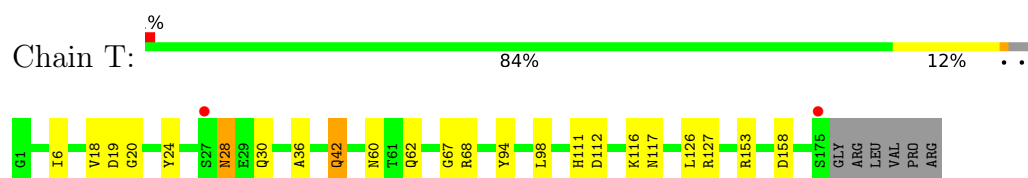
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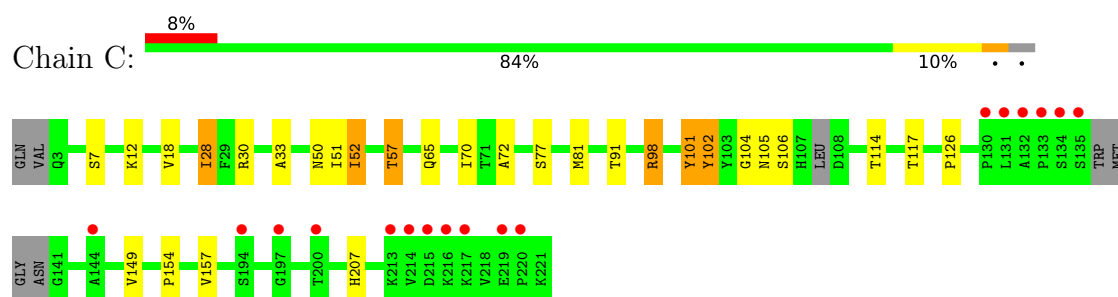
- Molecule 2: Hemagglutinin HA2



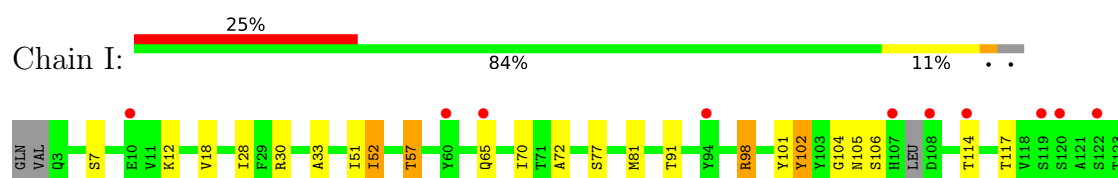
- Molecule 2: Hemagglutinin HA2

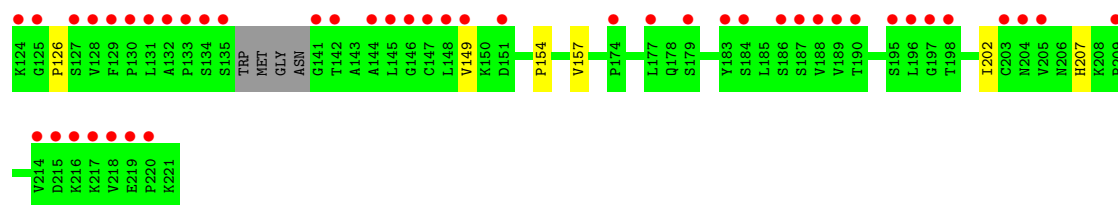


- Molecule 3: 70-1F02 Fab Heavy Chain

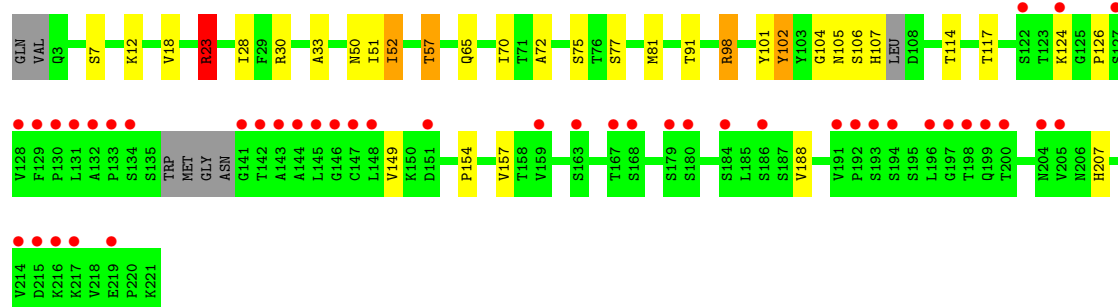
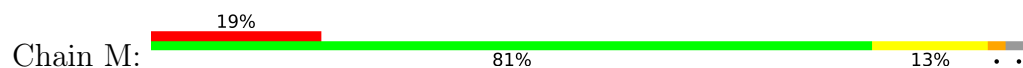


- Molecule 3: 70-1F02 Fab Heavy Chain

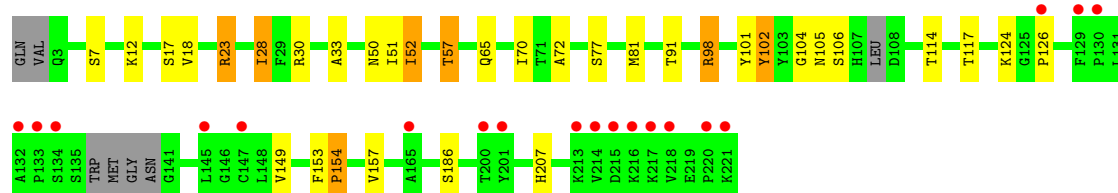
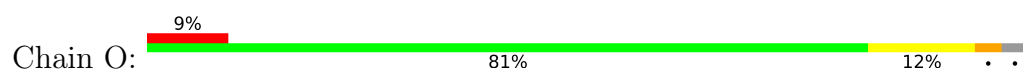




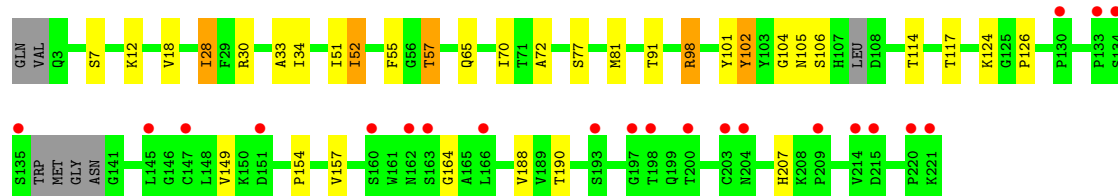
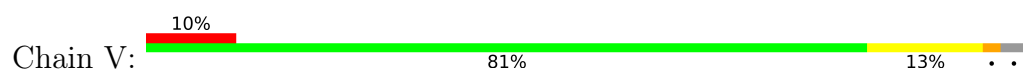
• Molecule 3: 70-1F02 Fab Heavy Chain



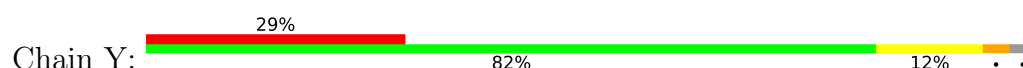
• Molecule 3: 70-1F02 Fab Heavy Chain

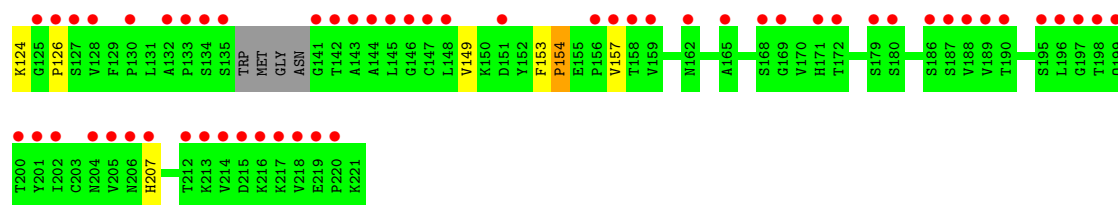


• Molecule 3: 70-1F02 Fab Heavy Chain



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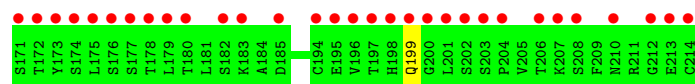
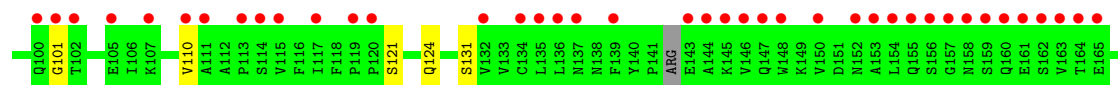
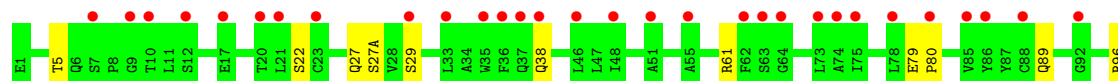
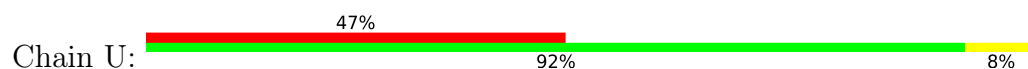




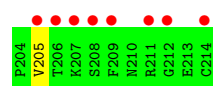
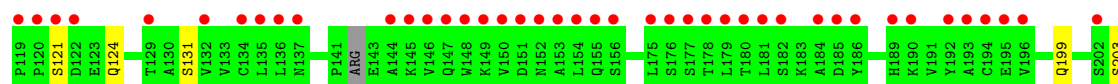
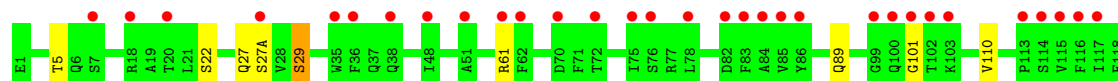
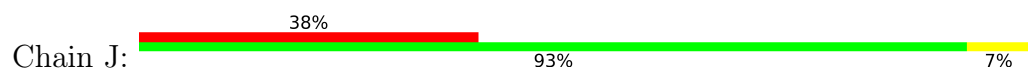
● Molecule 4: 70-1F02 Fab Light Chain



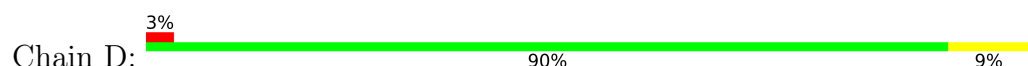
● Molecule 4: 70-1F02 Fab Light Chain



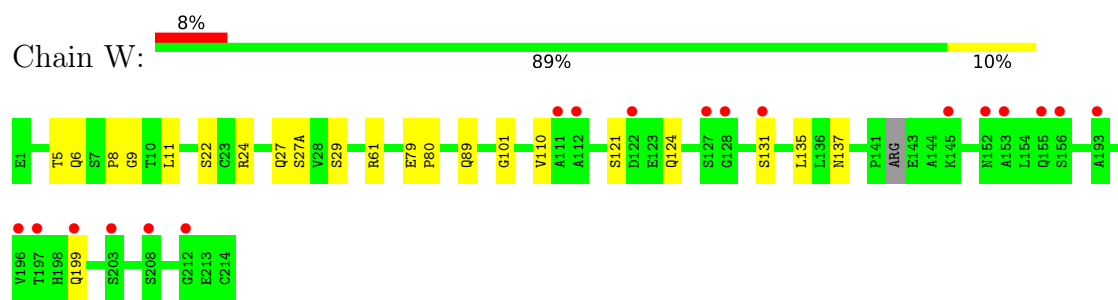
● Molecule 4: 70-1F02 Fab Light Chain



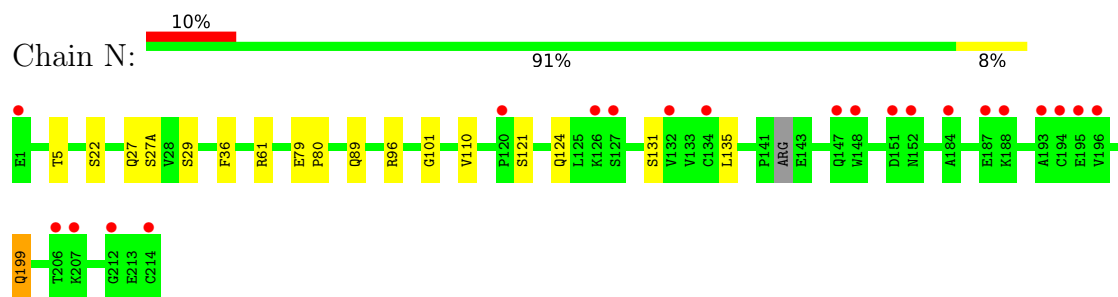
● Molecule 4: 70-1F02 Fab Light Chain



● Molecule 4: 70-1F02 Fab Light Chain



● Molecule 4: 70-1F02 Fab 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	174.58Å 205.37Å 222.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.92 49.49 – 3.92	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.01-3.92) 93.8 (49.49-3.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.286 , 0.329 0.285 , 0.326	Depositor DCC
R_{free} test set	3422 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	44024	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: BMA, NAG, MAN

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	0.56	0/2611	0.71	2/3546 (0.1%)
1	E	0.53	0/2611	0.69	1/3546 (0.0%)
1	G	0.55	0/2611	0.73	0/3546
1	K	0.53	0/2611	0.72	0/3546
1	Q	0.57	1/2611 (0.0%)	0.73	1/3546 (0.0%)
1	S	0.53	0/2611	0.70	0/3546
2	B	0.66	0/1439	0.72	0/1934
2	F	0.69	0/1443	0.75	0/1939
2	H	0.65	0/1443	0.73	0/1939
2	L	0.65	0/1443	0.71	0/1939
2	R	0.64	0/1443	0.72	1/1939 (0.1%)
2	T	0.67	0/1443	0.73	0/1939
3	C	0.57	0/1634	0.71	0/2224
3	I	0.52	0/1634	0.68	0/2224
3	M	0.61	2/1634 (0.1%)	0.84	5/2224 (0.2%)
3	O	0.58	0/1634	0.72	1/2224 (0.0%)
3	V	0.56	0/1634	0.70	0/2224
3	Y	0.53	0/1634	0.68	0/2224
4	D	0.50	0/1668	0.67	1/2261 (0.0%)
4	J	0.48	0/1668	0.64	0/2261
4	N	0.53	0/1668	0.66	0/2261
4	P	0.51	0/1659	0.68	0/2249
4	U	0.48	0/1668	0.63	0/2261
4	W	0.50	0/1668	0.65	0/2261
All	All	0.56	3/44123 (0.0%)	0.71	12/59803 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
2	R	0	1
2	T	0	1
3	M	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	23	ARG	CZ-NH1	-7.07	1.23	1.33
1	Q	301	GLU	CG-CD	5.63	1.60	1.51
3	M	23	ARG	CD-NE	5.06	1.55	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	23	ARG	NE-CZ-NH1	-20.07	110.26	120.30
3	O	23	ARG	NE-CZ-NH2	-7.31	116.65	120.30
4	D	45	ARG	NE-CZ-NH1	6.22	123.41	120.30
3	M	23	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
1	Q	266	LYS	CD-CE-NZ	5.66	124.72	111.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	68	ARG	Peptide
2	F	68	ARG	Peptide
3	M	23	ARG	Sidechain
2	R	68	ARG	Peptide
2	T	68	ARG	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2549	0	2493	19	0
1	E	2549	0	2493	16	0
1	G	2549	0	2493	15	0
1	K	2549	0	2494	22	0
1	Q	2549	0	2495	19	0
1	S	2549	0	2495	23	0
2	B	1412	0	1317	11	0
2	F	1416	0	1318	6	0
2	H	1416	0	1320	12	0
2	L	1416	0	1320	14	0
2	R	1416	0	1319	9	0
2	T	1416	0	1320	11	0
3	C	1596	0	1557	15	0
3	I	1596	0	1557	14	0
3	M	1596	0	1550	16	0
3	O	1596	0	1555	18	0
3	V	1596	0	1557	23	0
3	Y	1596	0	1556	16	0
4	D	1635	0	1582	6	0
4	J	1635	0	1582	7	0
4	N	1635	0	1582	7	0
4	P	1626	0	1573	5	0
4	U	1635	0	1582	6	0
4	W	1635	0	1582	13	0
5	A	98	0	86	3	0
5	B	28	0	25	0	0
5	E	42	0	38	0	0
5	F	14	0	13	0	0
5	G	84	0	76	0	0
5	K	112	0	100	2	0
5	M	56	0	48	0	0
5	O	28	0	24	2	0
5	Q	70	0	62	1	0
5	R	28	0	25	1	0
5	S	70	0	61	0	0
6	A	33	0	27	0	0
6	K	33	0	26	0	0
6	M	33	0	24	0	0
6	O	22	0	17	3	0
6	Q	22	0	17	0	0
6	S	44	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	11	0	10	0	0
7	M	22	0	16	1	0
7	Q	11	0	10	0	0
All	All	44024	0	42435	272	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 3.

The worst 5 of 272 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)
1:K:286:ASN:HD21	5:K:404:NAG:H2	1.36	0.90
1:S:169:GLN:NE2	4:J:203:SER:O	2.25	0.70
1:A:236:ASN:HA	5:A:406:NAG:H81	1.73	0.69
1:S:169:GLN:NE2	4:J:205:VAL:HG23	2.10	0.67
2:L:52:VAL:HG11	3:O:28:ILE:HG21	1.76	0.66

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	319/330 (97%)	282 (88%)	33 (10%)	4 (1%)	13	53
1	E	319/330 (97%)	283 (89%)	32 (10%)	4 (1%)	13	53
1	G	319/330 (97%)	283 (89%)	32 (10%)	4 (1%)	13	53
1	K	319/330 (97%)	283 (89%)	31 (10%)	5 (2%)	11	49
1	Q	319/330 (97%)	283 (89%)	33 (10%)	3 (1%)	19	59
1	S	319/330 (97%)	284 (89%)	31 (10%)	4 (1%)	13	53
2	B	172/181 (95%)	159 (92%)	12 (7%)	1 (1%)	27	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	27	67
2	H	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	27	67
2	L	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	27	67
2	R	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	27	67
2	T	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	27	67
3	C	210/221 (95%)	181 (86%)	26 (12%)	3 (1%)	12	51
3	I	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	12	51
3	M	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	12	51
3	O	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	12	51
3	V	210/221 (95%)	183 (87%)	24 (11%)	3 (1%)	12	51
3	Y	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	12	51
4	D	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	31	71
4	J	208/215 (97%)	198 (95%)	8 (4%)	2 (1%)	17	57
4	N	208/215 (97%)	199 (96%)	8 (4%)	1 (0%)	31	71
4	P	207/215 (96%)	198 (96%)	8 (4%)	1 (0%)	31	71
4	U	208/215 (97%)	199 (96%)	8 (4%)	1 (0%)	31	71
4	W	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	31	71
All	All	5458/5682 (96%)	4938 (90%)	465 (8%)	55 (1%)	17	57

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	GLN
3	I	65	GLN
3	M	65	GLN
3	O	65	GLN
3	V	65	GLN

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	289/298 (97%)	264 (91%)	25 (9%)	11	42
1	E	289/298 (97%)	264 (91%)	25 (9%)	11	42
1	G	289/298 (97%)	263 (91%)	26 (9%)	10	41
1	K	289/298 (97%)	263 (91%)	26 (9%)	10	41
1	Q	289/298 (97%)	264 (91%)	25 (9%)	11	42
1	S	289/298 (97%)	263 (91%)	26 (9%)	10	41
2	B	149/155 (96%)	139 (93%)	10 (7%)	18	52
2	F	149/155 (96%)	138 (93%)	11 (7%)	15	49
2	H	149/155 (96%)	137 (92%)	12 (8%)	13	46
2	L	149/155 (96%)	139 (93%)	10 (7%)	18	52
2	R	149/155 (96%)	139 (93%)	10 (7%)	18	52
2	T	149/155 (96%)	139 (93%)	10 (7%)	18	52
3	C	177/183 (97%)	168 (95%)	9 (5%)	26	60
3	I	177/183 (97%)	168 (95%)	9 (5%)	26	60
3	M	177/183 (97%)	165 (93%)	12 (7%)	17	52
3	O	177/183 (97%)	166 (94%)	11 (6%)	20	54
3	V	177/183 (97%)	167 (94%)	10 (6%)	23	58
3	Y	177/183 (97%)	167 (94%)	10 (6%)	23	58
4	D	183/185 (99%)	176 (96%)	7 (4%)	36	66
4	J	183/185 (99%)	177 (97%)	6 (3%)	41	70
4	N	183/185 (99%)	176 (96%)	7 (4%)	36	66
4	P	182/185 (98%)	176 (97%)	6 (3%)	41	70
4	U	183/185 (99%)	177 (97%)	6 (3%)	41	70
4	W	183/185 (99%)	177 (97%)	6 (3%)	41	70
All	All	4787/4926 (97%)	4472 (93%)	315 (7%)	18	53

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	271	TYR
3	O	51	ILE
4	J	29	SER
1	K	278	CYS
2	L	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	178	GLN
2	R	117	ASN
4	W	155	GLN
4	P	124	GLN
1	Q	11	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

66 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	A	401	1	14,14,15	1.64	3 (21%)	17,19,21	2.40	6 (35%)
5	NAG	A	402	1,5	14,14,15	0.96	1 (7%)	17,19,21	1.42	3 (17%)
5	NAG	A	403	5,6	14,14,15	0.77	0	17,19,21	2.13	6 (35%)
6	MAN	A	404	5,6	11,11,12	0.85	0	15,15,17	1.87	2 (13%)
6	MAN	A	405	6	11,11,12	0.72	0	15,15,17	1.98	6 (40%)
5	NAG	A	406	1,5	14,14,15	1.14	1 (7%)	17,19,21	2.60	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	407	5,6	14,14,15	0.66	0	17,19,21	1.13	1 (5%)
6	MAN	A	408	5	11,11,12	0.77	0	15,15,17	2.26	4 (26%)
5	NAG	A	409	1,5	14,14,15	0.79	0	17,19,21	0.93	0
5	NAG	A	410	5	14,14,15	0.88	0	17,19,21	1.67	4 (23%)
5	NAG	B	201	2,5	14,14,15	1.09	1 (7%)	17,19,21	1.27	1 (5%)
5	NAG	B	202	5	14,14,15	0.82	1 (7%)	17,19,21	1.41	4 (23%)
7	BMA	C	301	-	11,11,12	0.55	0	15,15,17	2.02	2 (13%)
5	NAG	E	401	1	14,14,15	0.91	1 (7%)	17,19,21	1.89	3 (17%)
5	NAG	E	402	1,5	14,14,15	0.51	0	17,19,21	2.08	4 (23%)
5	NAG	E	403	5	14,14,15	0.72	0	17,19,21	1.37	2 (11%)
5	NAG	F	201	2	14,14,15	1.08	1 (7%)	17,19,21	1.74	3 (17%)
5	NAG	G	401	1	14,14,15	0.82	0	17,19,21	1.07	1 (5%)
5	NAG	G	402	1	14,14,15	0.91	0	17,19,21	2.41	5 (29%)
5	NAG	G	403	1,5	14,14,15	1.33	2 (14%)	17,19,21	1.67	2 (11%)
5	NAG	G	404	5	14,14,15	0.69	0	17,19,21	1.34	2 (11%)
5	NAG	G	405	1,5	14,14,15	1.61	2 (14%)	17,19,21	1.86	4 (23%)
5	NAG	G	406	5	14,14,15	0.83	1 (7%)	17,19,21	2.05	5 (29%)
5	NAG	K	401	1	14,14,15	1.35	3 (21%)	17,19,21	1.93	5 (29%)
5	NAG	K	402	1,5	14,14,15	0.82	0	17,19,21	1.54	2 (11%)
5	NAG	K	403	5	14,14,15	0.44	0	17,19,21	1.42	3 (17%)
5	NAG	K	404	1,5	14,14,15	0.89	0	17,19,21	1.85	4 (23%)
5	NAG	K	405	5,6	14,14,15	0.47	0	17,19,21	1.95	6 (35%)
6	MAN	K	406	5,6	11,11,12	1.17	1 (9%)	15,15,17	2.42	6 (40%)
6	MAN	K	407	6	11,11,12	0.67	0	15,15,17	1.45	2 (13%)
6	MAN	K	408	6	11,11,12	1.11	2 (18%)	15,15,17	3.51	4 (26%)
5	NAG	K	409	1	14,14,15	0.83	0	17,19,21	1.83	3 (17%)
5	NAG	K	410	1,5	14,14,15	1.82	4 (28%)	17,19,21	1.97	4 (23%)
5	NAG	K	411	5	14,14,15	1.31	2 (14%)	17,19,21	1.94	3 (17%)
5	NAG	M	301	1,5	14,14,15	0.70	0	17,19,21	1.96	5 (29%)
5	NAG	M	302	5,6	14,14,15	0.62	0	17,19,21	1.88	4 (23%)
6	MAN	M	303	5,7,6	11,11,12	1.47	2 (18%)	15,15,17	2.54	6 (40%)
6	MAN	M	304	6	11,11,12	0.76	0	15,15,17	1.64	4 (26%)
7	BMA	M	305	6	11,11,12	2.07	3 (27%)	15,15,17	3.20	6 (40%)
5	NAG	M	306	1,5	14,14,15	1.76	4 (28%)	17,19,21	1.85	4 (23%)
5	NAG	M	307	5,6	14,14,15	0.64	0	17,19,21	1.70	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	M	308	5,7	11,11,12	0.96	0	15,15,17	3.08	7 (46%)
7	BMA	M	309	6	11,11,12	1.02	0	15,15,17	1.57	3 (20%)
5	NAG	O	301	1,5	14,14,15	0.67	0	17,19,21	2.92	8 (47%)
5	NAG	O	302	5,6	14,14,15	0.41	0	17,19,21	1.42	4 (23%)
6	MAN	O	303	5,6	11,11,12	1.43	3 (27%)	15,15,17	3.39	9 (60%)
6	MAN	O	304	6	11,11,12	1.12	2 (18%)	15,15,17	3.12	6 (40%)
5	NAG	Q	401	-	14,14,15	0.53	0	17,19,21	1.86	3 (17%)
5	NAG	Q	402	1,5	14,14,15	1.36	2 (14%)	17,19,21	2.19	4 (23%)
5	NAG	Q	403	5,6	14,14,15	0.85	0	17,19,21	1.87	4 (23%)
6	MAN	Q	404	5,7,6	11,11,12	1.45	2 (18%)	15,15,17	1.68	3 (20%)
6	MAN	Q	405	6	11,11,12	0.98	1 (9%)	15,15,17	2.06	5 (33%)
7	BMA	Q	406	6	11,11,12	0.40	0	15,15,17	0.90	0
5	NAG	Q	407	1,5	14,14,15	0.44	0	17,19,21	1.80	1 (5%)
5	NAG	Q	408	5	14,14,15	0.86	0	17,19,21	1.83	4 (23%)
5	NAG	R	201	2,5	14,14,15	0.81	0	17,19,21	2.00	6 (35%)
5	NAG	R	202	5	14,14,15	0.66	0	17,19,21	1.46	1 (5%)
5	NAG	S	401	1,5	14,14,15	1.47	2 (14%)	17,19,21	1.91	4 (23%)
5	NAG	S	402	5,6	14,14,15	0.79	0	17,19,21	1.66	4 (23%)
6	MAN	S	403	5,6	11,11,12	0.90	0	15,15,17	1.63	3 (20%)
6	MAN	S	404	6	11,11,12	0.79	0	15,15,17	2.47	2 (13%)
5	NAG	S	405	1,5	14,14,15	0.65	0	17,19,21	2.17	1 (5%)
5	NAG	S	406	5,6	14,14,15	0.75	0	17,19,21	1.26	3 (17%)
6	MAN	S	407	5,6	11,11,12	0.70	0	15,15,17	1.15	2 (13%)
6	MAN	S	408	6	11,11,12	0.40	0	15,15,17	1.03	2 (13%)
5	NAG	S	409	1	14,14,15	1.09	1 (7%)	17,19,21	1.46	2 (11%)

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	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	402	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	403	5,6	-	0/6/23/26	0/1/1/1
6	MAN	A	404	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	405	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	406	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	407	5,6	-	0/6/23/26	0/1/1/1
6	MAN	A	408	5	-	0/2/19/22	0/1/1/1
5	NAG	A	409	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	410	5	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	202	5	-	0/6/23/26	0/1/1/1
7	BMA	C	301	-	-	0/2/19/22	0/1/1/1
5	NAG	E	401	1	-	0/6/23/26	0/1/1/1
5	NAG	E	402	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	403	5	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	401	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	402	1	-	0/6/23/26	0/1/1/1
5	NAG	G	403	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	404	5	-	0/6/23/26	0/1/1/1
5	NAG	G	405	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	406	5	-	0/6/23/26	0/1/1/1
5	NAG	K	401	1	-	0/6/23/26	0/1/1/1
5	NAG	K	402	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	K	403	5	-	0/6/23/26	0/1/1/1
5	NAG	K	404	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	405	5,6	-	0/6/23/26	0/1/1/1
6	MAN	K	406	5,6	-	0/2/19/22	0/1/1/1
6	MAN	K	407	6	-	0/2/19/22	0/1/1/1
6	MAN	K	408	6	-	0/2/19/22	0/1/1/1
5	NAG	K	409	1	-	0/6/23/26	0/1/1/1
5	NAG	K	410	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	411	5	-	0/6/23/26	0/1/1/1
5	NAG	M	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	302	5,6	-	0/6/23/26	0/1/1/1
6	MAN	M	303	5,7,6	-	0/2/19/22	0/1/1/1
6	MAN	M	304	6	-	0/2/19/22	0/1/1/1
7	BMA	M	305	6	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	M	306	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	307	5,6	-	0/6/23/26	0/1/1/1
6	MAN	M	308	5,7	-	0/2/19/22	0/1/1/1
7	BMA	M	309	6	-	0/2/19/22	0/1/1/1
5	NAG	O	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	302	5,6	-	0/6/23/26	0/1/1/1
6	MAN	O	303	5,6	-	0/2/19/22	0/1/1/1
6	MAN	O	304	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Q	401	-	-	0/6/23/26	0/1/1/1
5	NAG	Q	402	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	Q	403	5,6	-	0/6/23/26	0/1/1/1
6	MAN	Q	404	5,7,6	-	0/2/19/22	0/1/1/1
6	MAN	Q	405	6	-	0/2/19/22	0/1/1/1
7	BMA	Q	406	6	-	0/2/19/22	0/1/1/1
5	NAG	Q	407	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	408	5	-	0/6/23/26	0/1/1/1
5	NAG	R	201	2,5	-	0/6/23/26	0/1/1/1
5	NAG	R	202	5	-	0/6/23/26	0/1/1/1
5	NAG	S	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	402	5,6	-	0/6/23/26	0/1/1/1
6	MAN	S	403	5,6	-	0/2/19/22	0/1/1/1
6	MAN	S	404	6	-	0/2/19/22	0/1/1/1
5	NAG	S	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	406	5,6	-	0/6/23/26	0/1/1/1
6	MAN	S	407	5,6	-	0/2/19/22	0/1/1/1
6	MAN	S	408	6	-	0/2/19/22	0/1/1/1
5	NAG	S	409	1	-	0/6/23/26	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	306	NAG	O5-C1	-4.90	1.35	1.43
5	K	410	NAG	O5-C1	-4.59	1.36	1.43
7	M	305	BMA	O5-C1	-4.30	1.36	1.43
5	S	401	NAG	O5-C1	-4.09	1.37	1.43
5	A	406	NAG	C2-N2	-2.77	1.41	1.46

The worst 5 of 243 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	408	MAN	C1-O5-C5	-12.19	95.41	112.19
7	M	305	BMA	C1-O5-C5	-7.69	101.61	112.19
5	A	406	NAG	C1-C2-N2	-7.28	98.05	110.49
5	M	306	NAG	O5-C1-C2	-5.04	104.57	111.52
6	O	303	MAN	C6-C5-C4	-5.01	101.16	112.99

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	201	NAG	C1

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Mol	Chain	Res	Type	Atom
7	M	305	BMA	C5
5	K	402	NAG	C1
5	G	405	NAG	C1
5	A	406	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	NAG	3	0
5	K	404	NAG	2	0
7	M	305	BMA	1	0
5	O	302	NAG	2	0
6	O	303	MAN	3	0
6	O	304	MAN	2	0
5	Q	401	NAG	1	0
5	R	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	P	1
4	J	1
4	D	1
4	W	1
4	N	1
4	U	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	27:GLN	C	27(A):SER	N	2.62
1	P	27:GLN	C	27(A):SER	N	2.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	27:GLN	C	27(A):SER	N	2.61
1	D	27:GLN	C	27(A):SER	N	2.61
1	W	27:GLN	C	27(A):SER	N	2.61

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	321/330 (97%)	0.41	20 (6%) 20 15	1, 43, 128, 182	0
1	E	321/330 (97%)	0.53	21 (6%) 19 13	1, 56, 147, 233	0
1	G	321/330 (97%)	0.24	6 (1%) 66 56	1, 38, 98, 145	0
1	K	321/330 (97%)	0.18	6 (1%) 66 56	1, 28, 91, 189	0
1	Q	321/330 (97%)	0.11	6 (1%) 66 56	1, 31, 107, 145	0
1	S	321/330 (97%)	0.52	22 (6%) 17 12	1, 52, 111, 147	0
2	B	174/181 (96%)	0.20	9 (5%) 27 22	1, 13, 112, 137	0
2	F	175/181 (96%)	-0.07	0 100 100	1, 10, 104, 172	0
2	H	175/181 (96%)	0.24	11 (6%) 20 14	1, 37, 138, 210	0
2	L	175/181 (96%)	0.25	12 (6%) 17 12	1, 27, 138, 185	0
2	R	175/181 (96%)	0.06	4 (2%) 60 49	1, 20, 112, 164	0
2	T	175/181 (96%)	0.08	2 (1%) 80 71	1, 13, 115, 164	0
3	C	214/221 (96%)	0.42	17 (7%) 12 10	1, 31, 145, 197	0
3	I	214/221 (96%)	1.47	55 (25%) 0 0	11, 115, 242, 317	0
3	M	214/221 (96%)	1.06	43 (20%) 1 1	1, 64, 214, 295	0
3	O	214/221 (96%)	0.51	19 (8%) 9 7	1, 37, 120, 166	0
3	V	214/221 (96%)	0.79	22 (10%) 6 5	1, 63, 144, 180	0
3	Y	214/221 (96%)	1.68	63 (29%) 0 0	1, 97, 270, 367	0
4	D	214/215 (99%)	0.40	7 (3%) 46 35	1, 48, 131, 162	0
4	J	214/215 (99%)	1.91	81 (37%) 0 0	59, 137, 196, 270	0
4	N	214/215 (99%)	0.68	21 (9%) 7 6	1, 40, 173, 230	0
4	P	213/215 (99%)	0.22	3 (1%) 75 65	1, 44, 83, 111	0
4	U	214/215 (99%)	2.37	101 (47%) 0 0	60, 167, 283, 360	0
4	W	214/215 (99%)	0.59	18 (8%) 11 9	1, 42, 149, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5542/5682 (97%)	0.61	569 (10%) 6 5	1, 48, 178, 367	0

The worst 5 of 569 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	214	VAL	12.0
4	U	136	LEU	11.3
3	I	134	SER	10.8
4	J	134	CYS	8.6
4	U	214	CYS	8.3

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 carbohydrates 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
6	MAN	S	408	11/12	0.25	0.42	144,166,175,180	0
7	BMA	M	305	11/12	0.30	0.58	141,159,196,214	0
6	MAN	S	407	11/12	0.41	0.43	192,209,219,224	0
6	MAN	O	303	11/12	0.43	0.49	112,143,181,190	0
5	NAG	A	407	14/15	0.45	0.41	119,137,149,152	0
5	NAG	Q	401	14/15	0.53	0.57	91,97,112,116	0
5	NAG	A	410	14/15	0.55	0.51	76,93,102,103	0
6	MAN	M	303	11/12	0.55	0.35	87,116,171,202	0
5	NAG	S	406	14/15	0.56	0.54	143,181,207,212	0
7	BMA	M	309	11/12	0.57	0.73	154,187,199,204	0
6	MAN	O	304	11/12	0.59	0.42	68,100,120,125	0
5	NAG	M	302	14/15	0.60	0.46	101,113,121,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	M	304	11/12	0.61	0.50	90,136,150,174	0
5	NAG	A	406	14/15	0.62	0.36	83,104,122,138	0
5	NAG	K	402	14/15	0.63	0.38	99,114,121,131	0
5	NAG	G	405	14/15	0.66	0.46	52,74,79,80	0
5	NAG	R	201	14/15	0.66	0.49	97,118,127,128	0
5	NAG	K	403	14/15	0.67	0.42	128,138,151,171	0
6	MAN	M	308	11/12	0.67	0.52	142,151,171,179	0
5	NAG	Q	408	14/15	0.67	0.50	68,77,89,91	0
5	NAG	K	411	14/15	0.70	0.49	59,75,80,80	0
6	MAN	A	408	11/12	0.72	0.30	97,107,115,117	0
5	NAG	F	201	14/15	0.73	0.46	65,85,92,97	0
5	NAG	Q	403	14/15	0.73	0.43	57,74,83,85	0
6	MAN	S	403	11/12	0.73	0.44	60,87,97,105	0
5	NAG	R	202	14/15	0.73	0.52	82,116,122,125	0
5	NAG	M	306	14/15	0.73	0.55	76,106,129,136	0
6	MAN	S	404	11/12	0.74	0.38	64,84,92,93	0
5	NAG	K	401	14/15	0.74	0.48	32,48,55,57	0
5	NAG	O	302	14/15	0.74	0.35	82,110,131,138	0
5	NAG	B	202	14/15	0.75	0.54	95,101,108,116	0
5	NAG	M	307	14/15	0.76	0.66	90,115,129,133	0
6	MAN	Q	404	11/12	0.76	0.34	54,74,80,84	0
5	NAG	A	403	14/15	0.77	0.38	30,71,85,86	0
5	NAG	G	402	14/15	0.77	0.35	25,35,39,40	0
5	NAG	A	409	14/15	0.77	0.34	20,42,61,73	0
6	MAN	A	405	11/12	0.78	0.48	66,73,88,95	0
5	NAG	S	405	14/15	0.79	0.34	75,81,101,134	0
5	NAG	A	401	14/15	0.80	0.35	34,44,48,50	0
5	NAG	G	406	14/15	0.80	0.34	53,63,69,70	0
5	NAG	B	201	14/15	0.80	0.41	58,72,83,93	0
5	NAG	A	402	14/15	0.80	0.44	38,48,59,61	0
5	NAG	O	301	14/15	0.81	0.37	69,83,93,97	0
6	MAN	K	407	11/12	0.81	0.30	76,83,96,104	0
5	NAG	Q	402	14/15	0.81	0.34	39,47,66,75	0
5	NAG	G	404	14/15	0.82	0.32	32,36,42,44	0
7	BMA	Q	406	11/12	0.82	0.35	74,80,92,98	0
5	NAG	G	401	14/15	0.82	0.31	41,63,75,78	0
5	NAG	S	409	14/15	0.82	0.32	18,23,28,31	0
5	NAG	K	409	14/15	0.83	0.34	16,21,39,42	0
6	MAN	Q	405	11/12	0.84	0.38	60,73,77,81	0
5	NAG	M	301	14/15	0.84	0.29	37,63,87,103	0
6	MAN	K	406	11/12	0.84	0.30	64,75,83,84	0
5	NAG	S	402	14/15	0.84	0.46	67,79,90,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	K	408	11/12	0.84	0.37	61,68,79,80	0
6	MAN	A	404	11/12	0.84	0.29	40,52,71,76	0
7	BMA	C	301	11/12	0.84	0.32	25,30,35,38	0
5	NAG	K	404	14/15	0.85	0.29	48,52,59,62	0
5	NAG	E	401	14/15	0.86	0.30	24,29,31,31	0
5	NAG	K	405	14/15	0.86	0.32	44,54,61,70	0
5	NAG	K	410	14/15	0.87	0.24	19,40,48,56	0
5	NAG	E	403	14/15	0.87	0.25	41,56,61,64	0
5	NAG	S	401	14/15	0.87	0.34	44,56,66,67	0
5	NAG	Q	407	14/15	0.89	0.28	21,28,35,50	0
5	NAG	E	402	14/15	0.89	0.25	32,40,43,47	0
5	NAG	G	403	14/15	0.93	0.23	20,29,33,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.