



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2017 – 02:03 PM EDT

PDB ID : 5KAQ  
Title : Crystal structure of broadly neutralizing Influenza A antibody 31.a.83 in complex with Hemagglutinin Hong Kong 1968.  
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 : 3.51 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

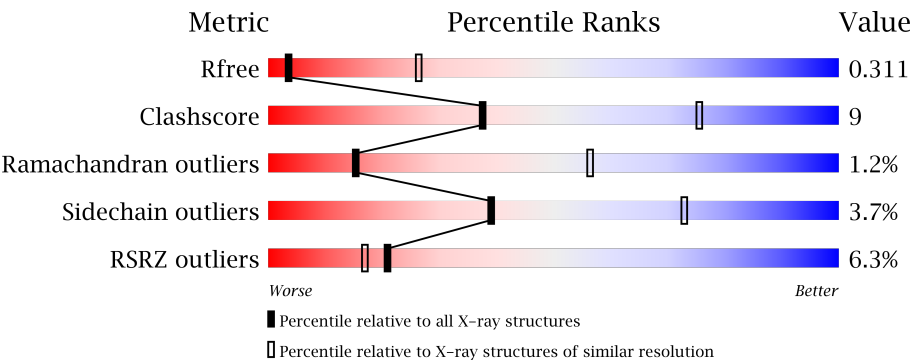
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 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.




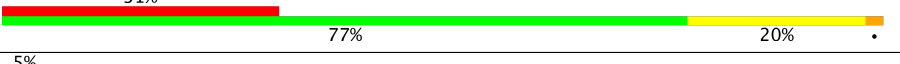


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
Ramachandran outliers	110173	1328 (3.64-3.40)
Sidechain outliers	110143	1329 (3.64-3.40)
RSRZ outliers	101464	1270 (3.64-3.40)

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  $\geq 3$ , 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	512	<div><div>0.1%</div><div><div>75%</div><div>19%</div><div>6%</div></div></div>
1	B	512	<div><div>2%</div><div><div>74%</div><div>18%</div><div>6%</div></div></div>
1	C	512	<div><div>4%</div><div><div>73%</div><div>20%</div><div>6%</div></div></div>
2	F	236	<div><div>10%</div><div><div>65%</div><div>29%</div><div>6%</div></div></div>
2	H	236	<div><div>7%</div><div><div>74%</div><div>23%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	Q	236	 6% 72% 25% ..
3	G	214	 31% 77% 20% .
3	L	214	 5% 78% 20% .
3	R	214	 3% 74% 24% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	1	0	0
			3786	2362	662	743	19			
1	C	482	Total	C	N	O	S	1	0	0
			3797	2368	666	744	19			
1	B	480	Total	C	N	O	S	0	0	0
			3788	2363	664	742	19			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	SER	-	expression tag	UNP E1AFM4
A	507	GLY	-	expression tag	UNP E1AFM4
A	508	ARG	-	expression tag	UNP E1AFM4
A	509	LEU	-	expression tag	UNP E1AFM4
A	510	VAL	-	expression tag	UNP E1AFM4
A	511	PRO	-	expression tag	UNP E1AFM4
A	512	ARG	-	expression tag	UNP E1AFM4
C	506	SER	-	expression tag	UNP E1AFM4
C	507	GLY	-	expression tag	UNP E1AFM4
C	508	ARG	-	expression tag	UNP E1AFM4
C	509	LEU	-	expression tag	UNP E1AFM4
C	510	VAL	-	expression tag	UNP E1AFM4
C	511	PRO	-	expression tag	UNP E1AFM4
C	512	ARG	-	expression tag	UNP E1AFM4
B	506	SER	-	expression tag	UNP E1AFM4
B	507	GLY	-	expression tag	UNP E1AFM4
B	508	ARG	-	expression tag	UNP E1AFM4
B	509	LEU	-	expression tag	UNP E1AFM4
B	510	VAL	-	expression tag	UNP E1AFM4
B	511	PRO	-	expression tag	UNP E1AFM4
B	512	ARG	-	expression tag	UNP E1AFM4

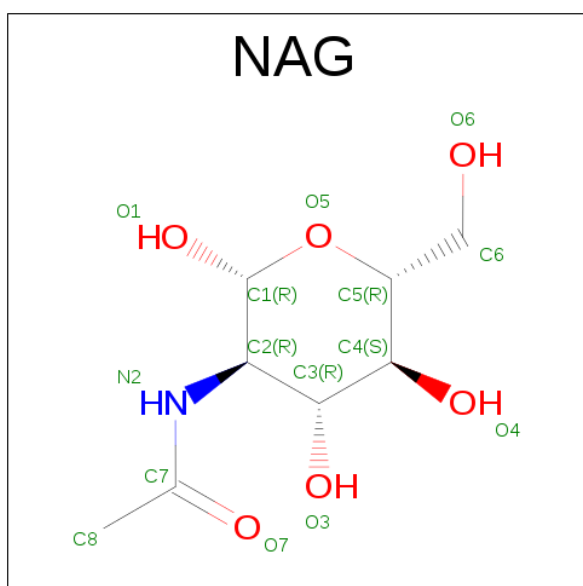
- Molecule 2 is a protein called ANTIBODY 31.A.83 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	232	Total	C	N	O	S	1	0	0
			1733	1093	285	347	8			
2	H	233	Total	C	N	O	S	0	0	0
			1742	1098	286	350	8			
2	Q	233	Total	C	N	O	S	0	0	0
			1742	1098	286	350	8			

- Molecule 3 is a protein called ANTIBODY 31.A.83 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	213	Total	C	N	O	S	0	0	0
			1642	1025	279	332	6			
3	L	213	Total	C	N	O	S	0	0	0
			1642	1025	279	332	6			
3	R	213	Total	C	N	O	S	0	0	0
			1642	1025	279	332	6			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (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	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		

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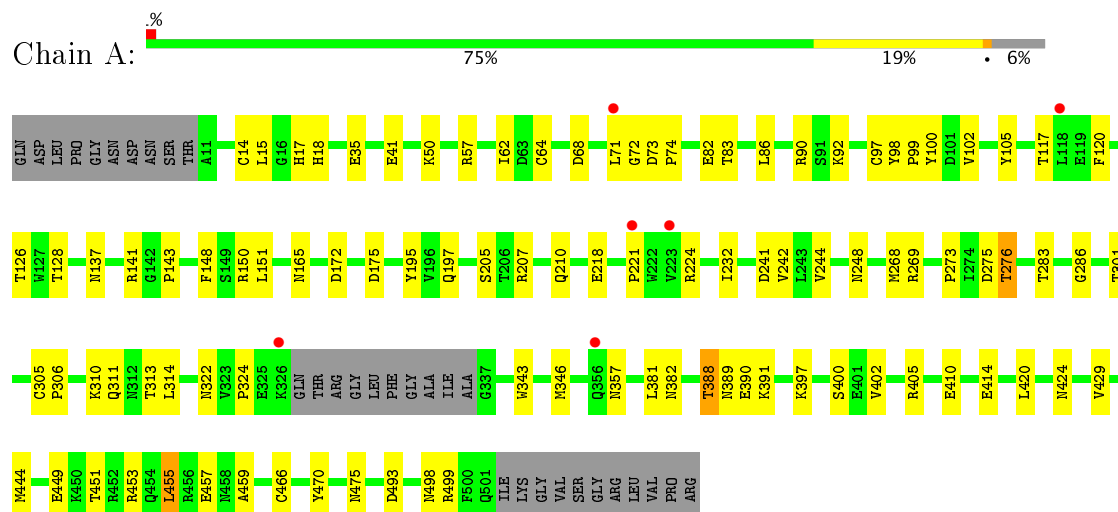
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
	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

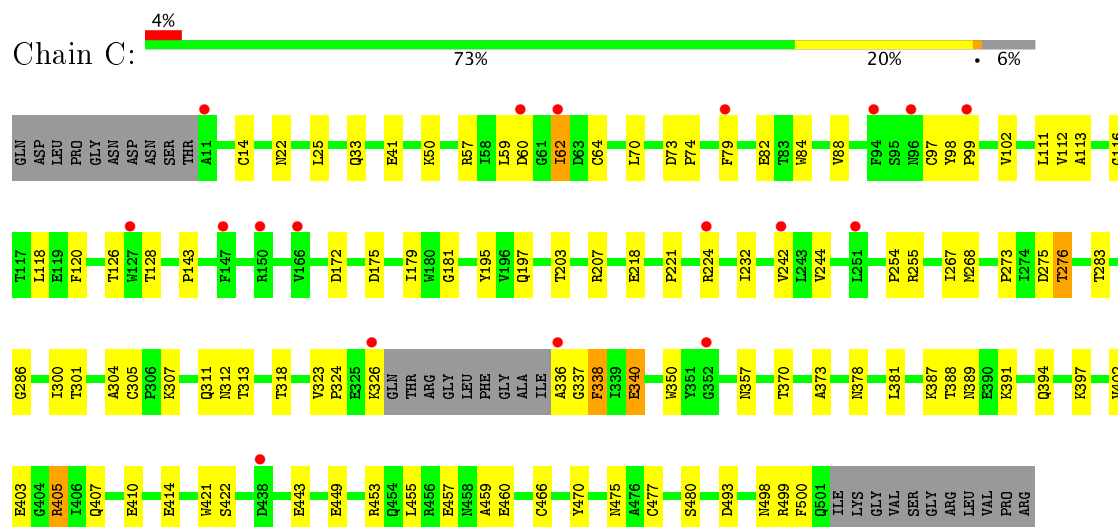
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

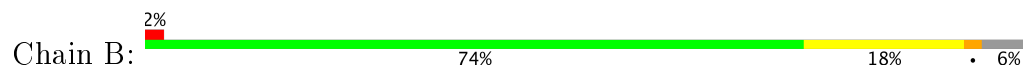
#### • Molecule 1: Hemagglutinin

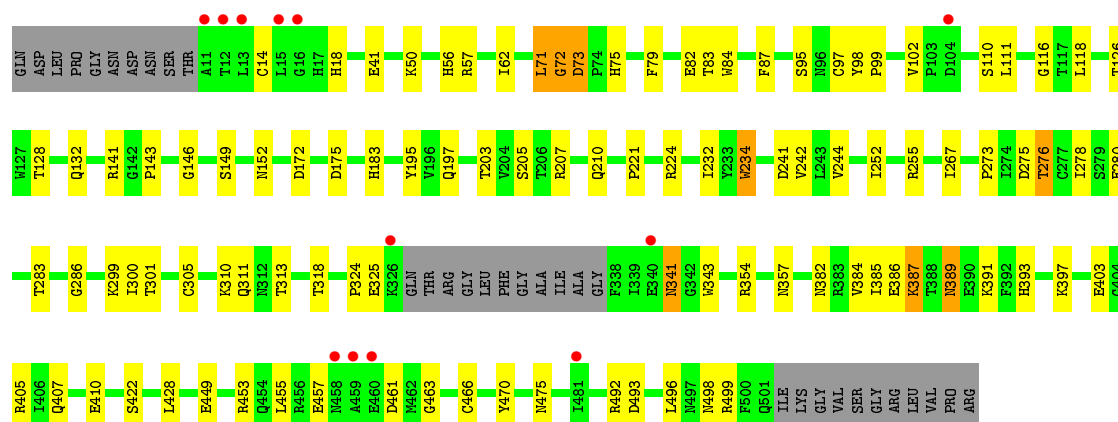


#### • Molecule 1: Hemagglutinin

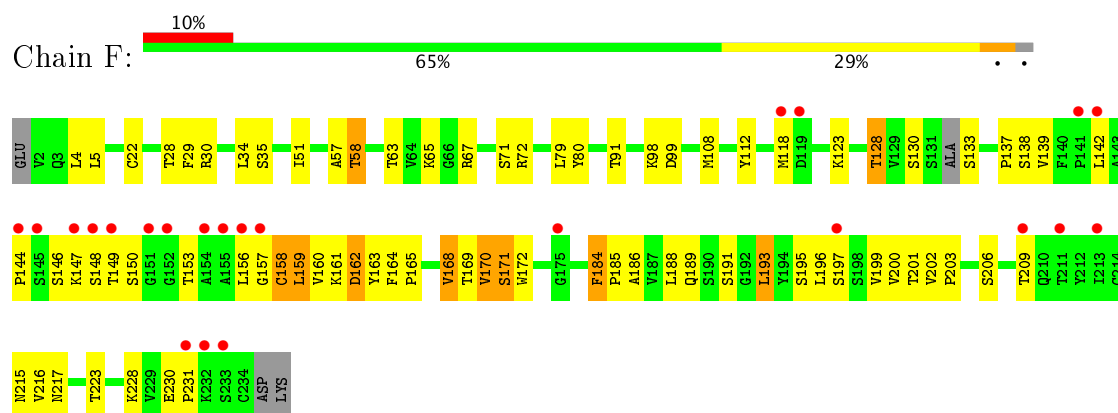


#### • Molecule 1: Hemagglutinin

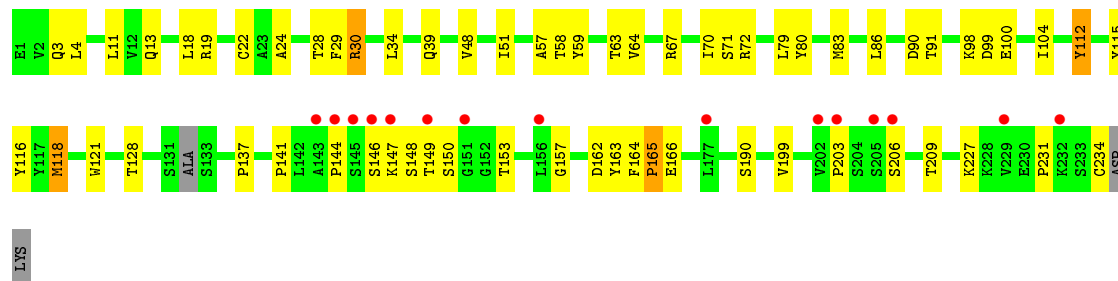
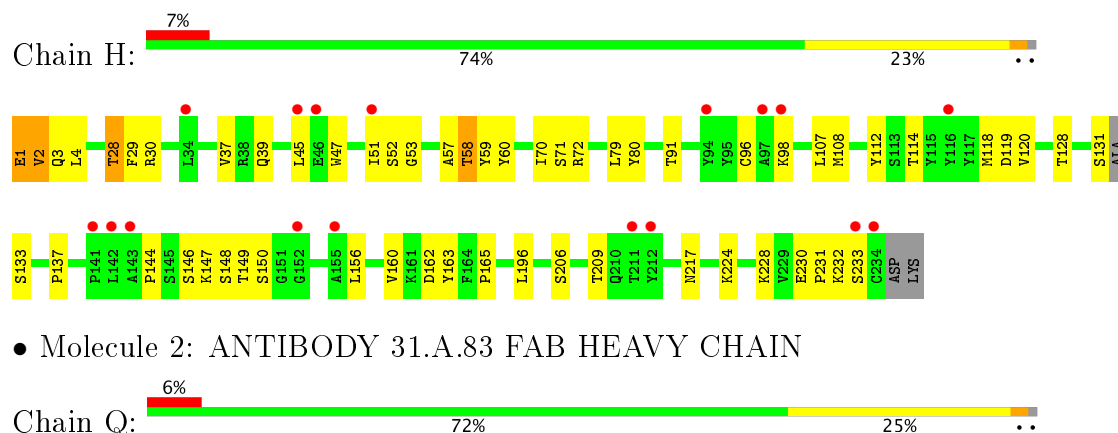




• Molecule 2: ANTIBODY 31.A.83 FAB HEAVY CHAIN

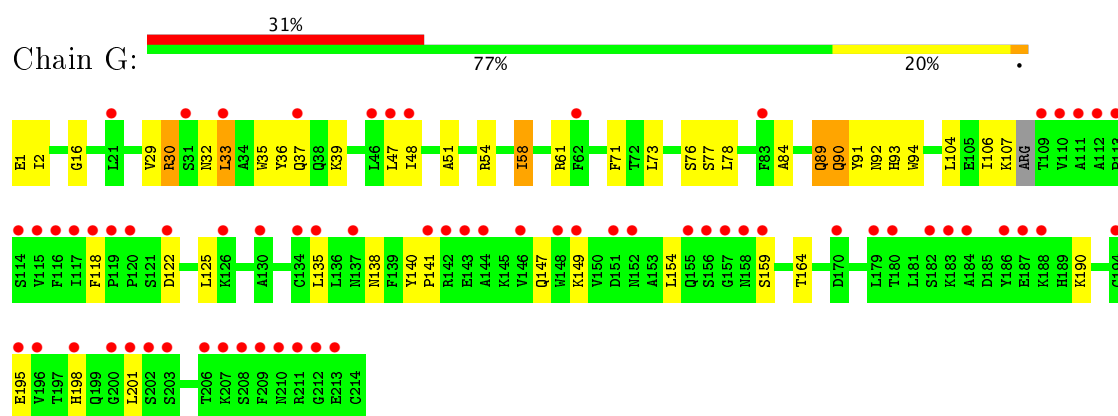


• Molecule 2: ANTIBODY 31.A.83 FAB HEAVY CHAIN

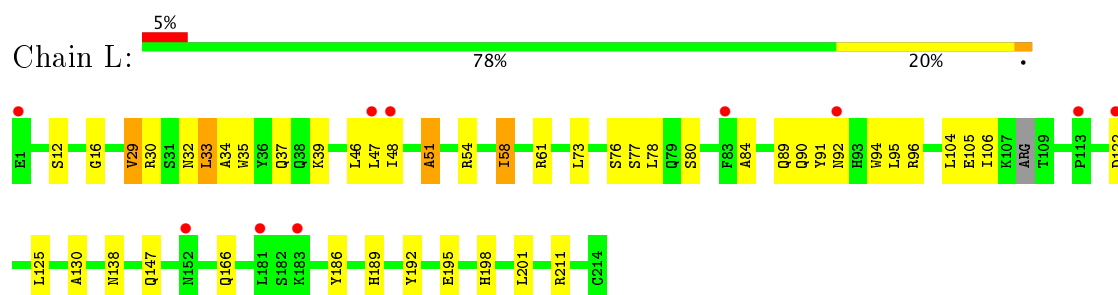


• Molecule 3: ANTIBODY 31.A.83 FAB LIGHT CHAIN

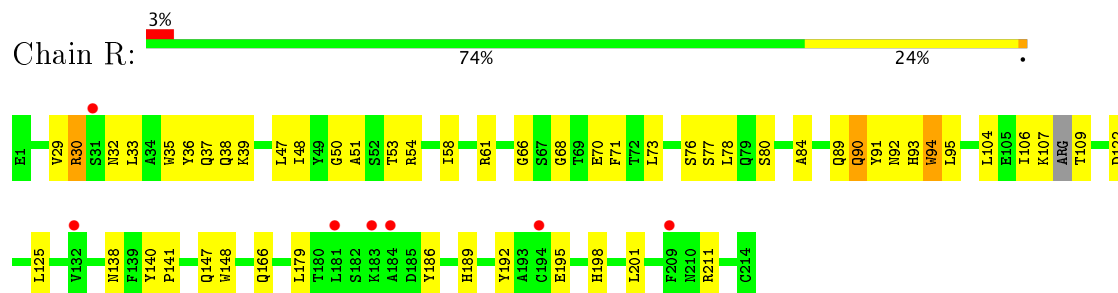




• Molecule 3: ANTIBODY 31.A.83 FAB LIGHT CHAIN



• Molecule 3: ANTIBODY 31.A.83 FAB LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.44Å 154.28Å 157.94Å 90.00° 116.86° 90.00°	Depositor
Resolution (Å)	41.88 – 3.51 48.86 – 3.51	Depositor EDS
% Data completeness (in resolution range)	78.9 (41.88-3.51) 78.9 (48.86-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.270 , 0.313 0.269 , 0.311	Depositor DCC
$R_{free}$ test set	2989 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.2	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 110.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	21766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.24	0/3865	0.42	0/5242
1	B	0.24	0/3867	0.41	0/5244
1	C	0.24	0/3876	0.41	0/5256
2	F	0.27	0/1776	0.48	0/2423
2	H	0.26	0/1784	0.46	0/2432
2	Q	0.26	0/1784	0.47	0/2432
3	G	0.24	0/1676	0.45	0/2274
3	L	0.25	0/1676	0.43	0/2274
3	R	0.24	0/1676	0.44	0/2274
All	All	0.25	0/21980	0.43	0/29851

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	Q	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Q	30	ARG	Peptide

## 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	3786	0	3637	60	0
1	B	3788	0	3645	65	0
1	C	3797	0	3654	65	0
2	F	1733	0	1684	46	0
2	H	1742	0	1692	40	0
2	Q	1742	0	1692	35	0
3	G	1642	0	1591	31	0
3	L	1642	0	1591	33	0
3	R	1642	0	1591	35	0
4	A	84	0	78	0	0
4	B	84	0	78	0	0
4	C	84	0	78	0	0
All	All	21766	0	21011	378	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 9.

All (378) 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:C:449:GLU:OE2	1:C:453:ARG:NH1	1.78	1.16
1:B:449:GLU:OE2	1:B:453:ARG:NH1	1.82	1.10
1:A:449:GLU:OE2	1:A:453:ARG:NH1	1.86	1.08
2:Q:98:LYS:NZ	2:Q:100:GLU:OE1	2.13	0.81
3:R:30:ARG:NH2	3:R:91:TYR:OH	2.15	0.79
1:C:57:ARG:HH12	1:C:59:LEU:HD13	1.49	0.78
3:L:189:HIS:O	3:L:211:ARG:NH1	2.16	0.77
1:B:234:TRP:H	1:B:234:TRP:HE3	1.32	0.76
3:R:30:ARG:HH21	3:R:91:TYR:HH	1.33	0.74
2:F:157:GLY:HA2	2:F:199:VAL:HG12	1.69	0.74
2:H:52:SER:HB3	2:H:112:TYR:HD1	1.52	0.74
3:L:32:ASN:HB3	3:L:91:TYR:HB3	1.69	0.73
2:F:153:THR:HG22	2:F:201:THR:HG22	1.70	0.72
1:C:387:LYS:O	1:C:389:ASN:N	2.21	0.71
1:A:306:PRO:HA	1:A:388:THR:HG21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PRO:HA	1:B:224:ARG:HH21	1.53	0.71
2:F:164:PHE:HB2	2:F:193:LEU:HB3	1.71	0.70
1:B:300:ILE:HG13	1:B:397:LYS:HD2	1.72	0.70
2:H:1:GLU:OE2	2:H:3:GLN:N	2.16	0.70
1:B:141:ARG:HG2	1:B:146:GLY:HA3	1.74	0.70
2:H:57:ALA:HA	2:H:58:THR:HG22	1.74	0.70
3:G:29:VAL:HG21	3:G:90:GLN:HB2	1.74	0.69
1:C:50:LYS:HG2	1:C:273:PRO:HG2	1.73	0.69
1:A:99:PRO:HA	1:A:224:ARG:HH21	1.57	0.69
3:R:29:VAL:HG21	3:R:90:GLN:HB2	1.75	0.68
1:A:72:GLY:O	1:A:141:ARG:NH2	2.25	0.68
2:F:186:ALA:HB2	2:F:196:LEU:HB2	1.75	0.68
3:G:92:ASN:O	3:G:93:HIS:ND1	2.27	0.68
3:L:106:ILE:HB	3:L:166:GLN:HE22	1.57	0.67
3:R:78:LEU:HD11	3:R:104:LEU:HD21	1.75	0.67
3:R:37:GLN:HB2	3:R:47:LEU:HD11	1.77	0.66
1:A:389:ASN:HB2	1:A:391:LYS:HE2	1.77	0.66
1:A:50:LYS:HG2	1:A:273:PRO:HG2	1.78	0.66
2:F:169:THR:HB	2:F:217:ASN:HB2	1.76	0.66
1:C:326:LYS:HD3	1:C:340:GLU:HG2	1.77	0.66
2:F:51:ILE:HA	2:F:57:ALA:HB3	1.79	0.65
1:A:420:LEU:O	1:A:424:ASN:ND2	2.30	0.65
1:A:405:ARG:NH2	1:C:410:GLU:OE2	2.26	0.65
1:C:318:THR:HG22	1:C:381:LEU:HD11	1.79	0.65
3:L:78:LEU:HD11	3:L:104:LEU:HD21	1.78	0.65
1:A:35:GLU:OE2	1:A:322:ASN:ND2	2.30	0.65
1:A:397:LYS:HG2	1:A:414:GLU:HG2	1.80	0.64
1:B:275:ASP:OD1	1:B:276:THR:N	2.30	0.64
2:H:28:THR:HG21	2:H:98:LYS:NZ	2.13	0.64
1:C:275:ASP:OD1	1:C:276:THR:N	2.31	0.64
2:Q:63:THR:O	2:Q:67:ARG:NH2	2.30	0.64
1:B:403:GLU:HB2	1:B:407:GLN:HB2	1.80	0.63
2:Q:51:ILE:HA	2:Q:57:ALA:HB3	1.79	0.63
1:A:15:LEU:HD11	1:A:451:THR:HG21	1.81	0.62
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.81	0.62
2:F:142:LEU:HD22	3:G:118:PHE:HB3	1.81	0.61
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.81	0.61
3:R:106:ILE:HB	3:R:166:GLN:HE22	1.65	0.61
3:G:78:LEU:HD11	3:G:104:LEU:HD21	1.81	0.61
1:A:68:ASP:OD1	1:A:100:TYR:OH	2.14	0.61
1:B:56:HIS:NE2	1:B:280:GLU:OE1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLY:HA3	1:B:149:SER:H	1.65	0.60
1:C:99:PRO:HA	1:C:224:ARG:HH21	1.66	0.60
2:F:139:VAL:HG22	2:F:160:VAL:HG22	1.84	0.60
2:F:130:SER:HB3	2:F:164:PHE:HZ	1.66	0.60
3:R:54:ARG:HB2	3:R:58:ILE:HD11	1.83	0.60
2:Q:91:THR:HG23	2:Q:128:THR:HA	1.82	0.59
2:F:30:ARG:NH1	2:F:72:ARG:HG3	2.16	0.59
2:F:200:VAL:HG22	2:F:201:THR:H	1.67	0.59
1:C:14:CYS:HA	1:C:466:CYS:HA	1.84	0.59
1:A:283:THR:OG1	1:A:286:GLY:O	2.20	0.59
1:B:50:LYS:HG2	1:B:273:PRO:HG2	1.84	0.58
2:F:184:PHE:HB2	2:F:196:LEU:HD11	1.83	0.58
1:A:14:CYS:HA	1:A:466:CYS:HA	1.84	0.58
1:C:402:VAL:HG11	1:B:111:LEU:HD13	1.84	0.58
2:Q:57:ALA:HA	2:Q:58:THR:OG1	2.04	0.58
2:F:137:PRO:HD2	2:F:223:THR:HB	1.87	0.57
2:H:71:SER:HB3	2:H:80:TYR:HB2	1.86	0.57
1:A:283:THR:HG22	1:A:301:THR:HG22	1.87	0.57
2:H:112:TYR:CE2	2:H:114:THR:HA	2.40	0.56
1:A:57:ARG:NH1	1:A:83:THR:O	2.37	0.56
2:F:130:SER:HB3	2:F:164:PHE:CZ	2.39	0.56
2:Q:30:ARG:NH1	2:Q:72:ARG:HG3	2.20	0.56
3:R:32:ASN:HA	3:R:50:GLY:HA2	1.87	0.56
2:F:57:ALA:HA	2:F:58:THR:OG1	2.05	0.56
3:L:198:HIS:HB3	3:L:201:LEU:HB2	1.87	0.56
1:B:183:HIS:HB2	1:B:252:ILE:HD11	1.87	0.56
2:F:202:VAL:HG12	2:F:203:PRO:HD2	1.87	0.56
3:R:36:TYR:HE2	3:R:89:GLN:HG2	1.70	0.55
2:F:148:SER:O	2:F:150:SER:N	2.40	0.55
2:F:162:ASP:H	2:F:195:SER:HB2	1.71	0.55
1:A:275:ASP:OD1	1:A:276:THR:N	2.40	0.55
3:R:39:LYS:HG3	3:R:84:ALA:HB2	1.89	0.55
1:A:455:LEU:HD13	1:A:459:ALA:HB3	1.87	0.55
1:A:148:PHE:HB2	1:A:151:LEU:HB2	1.89	0.55
1:B:14:CYS:HA	1:B:466:CYS:HA	1.89	0.55
2:H:4:LEU:HD23	2:H:98:LYS:HE2	1.89	0.55
1:C:311:GLN:HE22	1:C:422:SER:HB3	1.72	0.54
1:B:389:ASN:HB2	1:B:391:LYS:HE2	1.89	0.54
1:C:283:THR:HG22	1:C:301:THR:HG22	1.89	0.54
3:G:54:ARG:HB2	3:G:58:ILE:HD11	1.90	0.54
2:H:47:TRP:CD1	3:L:96:ARG:NH1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:OE1	1:A:499:ARG:NH1	2.33	0.54
2:H:1:GLU:OE2	2:H:3:GLN:HB2	2.08	0.54
2:H:28:THR:HG21	2:H:98:LYS:HZ1	1.72	0.54
1:B:384:VAL:HG23	1:B:428:LEU:HD21	1.90	0.53
1:B:384:VAL:HG13	1:B:385:ILE:HG23	1.89	0.53
1:B:71:LEU:HD11	1:B:232:ILE:HG13	1.91	0.53
2:H:91:THR:HG23	2:H:128:THR:HA	1.90	0.53
3:L:30:ARG:H	3:L:91:TYR:HE1	1.57	0.53
3:R:186:TYR:O	3:R:192:TYR:OH	2.25	0.53
3:R:68:GLY:O	3:R:70:GLU:N	2.40	0.53
1:A:381:LEU:HD21	2:Q:104:ILE:HG13	1.89	0.53
1:A:402:VAL:HG11	1:C:111:LEU:HD13	1.91	0.52
1:B:195:TYR:O	1:B:197:GLN:N	2.40	0.52
1:B:301:THR:HB	1:B:305:CYS:SG	2.49	0.52
1:B:457:GLU:HB3	1:B:499:ARG:NH1	2.24	0.52
1:C:41:GLU:OE2	1:C:313:THR:HA	2.10	0.52
1:B:357:ASN:ND2	1:B:475:ASN:OD1	2.40	0.52
2:Q:34:LEU:HD23	2:Q:98:LYS:HA	1.91	0.52
1:B:41:GLU:OE2	1:B:313:THR:HA	2.10	0.52
2:F:142:LEU:HD12	2:F:157:GLY:HA3	1.91	0.52
2:F:22:CYS:HB3	2:F:79:LEU:HB3	1.90	0.52
2:H:51:ILE:HG23	2:H:72:ARG:HH21	1.74	0.52
3:L:186:TYR:O	3:L:192:TYR:OH	2.27	0.52
1:A:410:GLU:OE2	1:B:405:ARG:NH2	2.43	0.52
3:L:48:ILE:HA	3:L:54:ARG:HA	1.91	0.52
1:A:195:TYR:O	1:A:197:GLN:N	2.41	0.51
1:B:283:THR:HG22	1:B:301:THR:HG22	1.92	0.51
2:Q:148:SER:O	2:Q:150:SER:N	2.42	0.51
1:C:195:TYR:O	1:C:197:GLN:N	2.42	0.51
3:L:39:LYS:HG3	3:L:84:ALA:HB2	1.93	0.51
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.41	0.51
3:L:147:GLN:HB2	3:L:195:GLU:HB3	1.91	0.51
2:H:112:TYR:HE2	2:H:114:THR:HA	1.75	0.51
1:A:301:THR:HB	1:A:305:CYS:SG	2.50	0.50
2:H:47:TRP:HZ3	3:L:95:LEU:HG	1.77	0.50
1:B:102:VAL:HG22	1:B:232:ILE:HB	1.93	0.50
1:B:387:LYS:HB2	3:L:30:ARG:HG2	1.94	0.50
2:H:148:SER:O	2:H:150:SER:N	2.45	0.50
1:C:457:GLU:HB3	1:C:499:ARG:HH12	1.77	0.50
1:B:110:SER:HG	1:B:393:HIS:HE2	1.58	0.50
1:C:357:ASN:ND2	1:C:475:ASN:OD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:HIS:HB3	3:G:201:LEU:HB2	1.94	0.50
3:R:147:GLN:HB2	3:R:195:GLU:HB3	1.94	0.50
1:B:283:THR:OG1	1:B:286:GLY:O	2.24	0.49
1:C:350:TRP:HB2	1:C:370:THR:HG23	1.93	0.49
1:C:457:GLU:HB3	1:C:499:ARG:NH1	2.26	0.49
2:F:71:SER:HB3	2:F:80:TYR:HB2	1.93	0.49
2:Q:157:GLY:HA3	2:Q:199:VAL:HG12	1.92	0.49
2:H:60:TYR:CE1	2:H:70:ILE:HD13	2.48	0.49
3:L:54:ARG:HB2	3:L:58:ILE:HD11	1.94	0.49
1:A:453:ARG:HE	1:B:463:GLY:HA2	1.77	0.49
1:A:86:LEU:HD21	1:A:268:MET:HE1	1.93	0.49
3:G:106:ILE:HG22	3:G:107:LYS:HG3	1.95	0.49
2:Q:4:LEU:HD13	2:Q:22:CYS:SG	2.52	0.49
3:R:147:GLN:O	3:R:195:GLU:N	2.46	0.49
1:B:110:SER:OG	1:B:393:HIS:NE2	2.42	0.49
3:R:33:LEU:HD13	3:R:71:PHE:CG	2.47	0.49
1:B:79:PHE:HA	1:B:82:GLU:HG3	1.95	0.49
3:L:33:LEU:HD12	3:L:51:ALA:HA	1.94	0.49
1:A:97:CYS:SG	1:A:98:TYR:N	2.83	0.49
1:C:323:VAL:HG21	1:C:336:ALA:HB2	1.94	0.49
2:F:5:LEU:HB3	2:F:123:LYS:HE3	1.95	0.49
2:F:206:SER:HA	2:F:209:THR:HG22	1.95	0.49
2:F:164:PHE:HD2	2:F:193:LEU:HA	1.77	0.49
1:B:311:GLN:HE22	1:B:422:SER:HB3	1.79	0.48
2:F:170:VAL:HG23	2:F:216:VAL:HG22	1.95	0.48
1:C:57:ARG:NH1	1:C:59:LEU:HD13	2.24	0.48
3:G:33:LEU:HD22	3:G:71:PHE:CD1	2.48	0.48
2:H:144:PRO:HD2	2:H:231:PRO:HA	1.94	0.48
2:H:217:ASN:HA	2:H:224:LYS:HG2	1.95	0.48
3:R:51:ALA:O	3:R:53:THR:N	2.45	0.48
1:B:84:TRP:HZ3	1:B:118:LEU:HG	1.79	0.48
2:Q:39:GLN:OE1	3:R:38:GLN:NE2	2.34	0.48
3:G:1:GLU:HB2	3:G:93:HIS:NE2	2.28	0.48
1:C:301:THR:HB	1:C:305:CYS:SG	2.53	0.48
1:C:300:ILE:HG13	1:C:397:LYS:HD3	1.95	0.48
1:B:97:CYS:SG	1:B:98:TYR:N	2.85	0.48
2:F:65:LYS:HZ1	3:G:94:TRP:HH2	1.61	0.48
2:Q:39:GLN:HG3	2:Q:39:GLN:O	2.13	0.48
1:C:113:ALA:HB1	1:C:267:ILE:HB	1.95	0.47
2:F:163:TYR:CZ	2:F:168:VAL:HG22	2.49	0.47
3:R:30:ARG:HD2	3:R:91:TYR:HH	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:SER:O	2:H:133:SER:N	2.47	0.47
2:H:206:SER:HA	2:H:209:THR:HG22	1.95	0.47
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.96	0.47
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.96	0.47
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.49	0.47
2:F:171:SER:O	2:F:215:ASN:N	2.46	0.47
3:G:93:HIS:O	3:G:93:HIS:CG	2.68	0.47
2:H:118:MET:HE3	3:L:96:ARG:NH1	2.30	0.47
2:Q:57:ALA:HB1	2:Q:58:THR:O	2.15	0.47
1:A:218:GLU:OE2	1:C:203:THR:OG1	2.27	0.47
1:A:310:LYS:HB2	1:A:310:LYS:NZ	2.30	0.47
1:C:338:PHE:HD1	1:C:338:PHE:H	1.63	0.47
3:G:147:GLN:HB2	3:G:195:GLU:HB3	1.97	0.47
3:R:198:HIS:HB3	3:R:201:LEU:HB2	1.97	0.47
2:Q:59:TYR:CE2	3:R:94:TRP:HB2	2.50	0.47
2:Q:141:PRO:HD3	2:Q:227:LYS:HG2	1.96	0.47
1:A:314:LEU:HB3	1:A:429:VAL:HG11	1.97	0.47
1:C:126:THR:HG22	1:C:128:THR:HG23	1.97	0.46
1:A:457:GLU:HG3	1:B:499:ARG:HH21	1.79	0.46
1:C:73:ASP:OD1	1:C:74:PRO:HD2	2.15	0.46
2:F:35:SER:OG	2:F:99:ASP:OD2	2.29	0.46
3:R:80:SER:HA	3:R:106:ILE:HG12	1.97	0.46
3:G:36:TYR:HE2	3:G:89:GLN:HG2	1.81	0.46
1:C:389:ASN:HB2	1:C:391:LYS:HE2	1.97	0.46
3:G:47:LEU:HB3	3:G:48:ILE:HD12	1.98	0.46
2:Q:153:THR:HA	2:Q:203:PRO:HA	1.96	0.46
1:B:84:TRP:CE2	1:B:116:GLY:HA2	2.51	0.46
3:R:122:ASP:HA	3:R:125:LEU:HD12	1.97	0.46
3:G:140:TYR:CG	3:G:141:PRO:HA	2.51	0.46
1:C:283:THR:OG1	1:C:286:GLY:O	2.27	0.46
2:F:199:VAL:HG21	3:G:135:LEU:HD13	1.98	0.46
1:B:449:GLU:OE2	1:B:453:ARG:HD2	2.15	0.45
2:Q:164:PHE:HA	2:Q:165:PRO:HA	1.74	0.45
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.97	0.45
3:L:12:SER:HA	3:L:105:GLU:HB2	1.99	0.45
2:F:91:THR:HG23	2:F:128:THR:HA	1.97	0.45
2:H:39:GLN:HB2	2:H:45:LEU:HD13	1.98	0.45
1:A:41:GLU:OE2	1:A:313:THR:HA	2.17	0.45
1:C:70:LEU:HD22	1:C:112:VAL:HG21	1.99	0.45
3:G:39:LYS:HG3	3:G:84:ALA:HB2	1.99	0.45
3:L:91:TYR:HB2	3:L:92:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:83:MET:HB3	2:Q:86:LEU:HD21	1.98	0.45
1:B:73:ASP:OD1	1:B:75:HIS:N	2.50	0.45
1:A:310:LYS:HB2	1:A:310:LYS:HZ2	1.81	0.45
2:Q:22:CYS:HB3	2:Q:79:LEU:HB3	1.99	0.45
1:A:449:GLU:OE2	1:A:453:ARG:HD2	2.17	0.45
1:B:87:PHE:HB3	1:B:267:ILE:HG13	1.98	0.45
1:B:343:TRP:CH2	1:B:354:ARG:NH1	2.85	0.45
2:F:162:ASP:HA	2:F:193:LEU:HD13	1.97	0.45
3:R:66:GLY:HA3	3:R:71:PHE:CD2	2.52	0.45
1:A:126:THR:HG22	1:A:128:THR:HG23	1.98	0.45
1:A:470:TYR:HB3	1:A:498:ASN:HB2	1.97	0.45
1:B:325:GLU:OE2	1:B:341:ASN:ND2	2.50	0.44
1:C:455:LEU:HD13	1:C:459:ALA:HB3	1.99	0.44
3:G:48:ILE:HA	3:G:54:ARG:HA	1.99	0.44
1:A:244:VAL:HG21	1:B:221:PRO:HG3	1.99	0.44
1:B:152:ASN:HB2	1:B:255:ARG:HG2	1.99	0.44
1:A:35:GLU:HG2	1:A:322:ASN:HB3	1.99	0.44
1:C:397:LYS:HG2	1:C:414:GLU:HG2	2.00	0.44
3:G:91:TYR:HB2	3:G:92:ASN:HB2	1.99	0.44
1:A:71:LEU:HB3	1:A:148:PHE:HD2	1.82	0.44
2:Q:118:MET:HG3	2:Q:121:TRP:CZ2	2.53	0.44
2:Q:146:SER:OG	2:Q:147:LYS:N	2.50	0.44
2:Q:51:ILE:HD13	2:Q:72:ARG:HB2	2.00	0.44
1:C:405:ARG:NH1	1:B:410:GLU:OE1	2.51	0.44
1:C:59:LEU:HA	1:C:59:LEU:HD12	1.91	0.44
2:H:228:LYS:HZ2	2:H:230:GLU:HB3	1.82	0.44
2:H:231:PRO:O	2:H:233:SER:N	2.51	0.44
2:H:30:ARG:NH1	2:H:72:ARG:HG3	2.32	0.44
2:Q:71:SER:HB3	2:Q:80:TYR:HB2	2.00	0.44
1:A:357:ASN:ND2	1:A:475:ASN:OD1	2.50	0.44
1:B:318:THR:HB	2:H:107:LEU:HD22	1.99	0.44
2:H:4:LEU:HD11	2:H:96:CYS:O	2.18	0.44
3:R:106:ILE:HG22	3:R:107:LYS:HG3	1.98	0.44
3:R:32:ASN:HB2	3:R:91:TYR:HB3	1.99	0.44
2:F:184:PHE:N	2:F:184:PHE:CD1	2.86	0.44
1:C:79:PHE:HA	1:C:82:GLU:HG3	1.99	0.43
2:H:1:GLU:OE2	2:H:2:VAL:N	2.51	0.43
1:A:314:LEU:HD22	1:A:429:VAL:HG21	2.00	0.43
1:C:218:GLU:HG3	1:B:203:THR:HG21	2.00	0.43
1:C:457:GLU:O	1:C:499:ARG:NH1	2.52	0.43
1:C:460:GLU:OE2	1:B:492:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:LEU:HD23	2:F:98:LYS:HA	2.00	0.43
2:H:47:TRP:CZ3	3:L:95:LEU:HG	2.53	0.43
1:B:241:ASP:OD1	1:B:242:VAL:N	2.50	0.43
2:H:137:PRO:HB3	2:H:163:TYR:HB3	2.01	0.43
2:Q:137:PRO:HB3	2:Q:163:TYR:HB3	2.01	0.43
1:A:74:PRO:HD3	1:A:97:CYS:HB2	2.00	0.43
3:G:149:LYS:HE2	3:G:154:LEU:HD11	2.00	0.43
2:H:228:LYS:NZ	2:H:230:GLU:HB3	2.33	0.43
3:R:35:TRP:CE3	3:R:73:LEU:HD22	2.53	0.43
1:C:22:ASN:N	1:C:22:ASN:OD1	2.52	0.43
1:C:207:ARG:HG3	1:C:242:VAL:HG12	1.99	0.43
3:L:47:LEU:HB3	3:L:48:ILE:HD12	2.01	0.43
1:A:90:ARG:HB3	1:A:92:LYS:HG2	2.00	0.43
1:C:403:GLU:HB2	1:C:407:GLN:HB2	2.00	0.43
2:F:164:PHE:HA	2:F:165:PRO:HA	1.72	0.43
2:Q:48:VAL:HG13	2:Q:64:VAL:HG21	2.01	0.43
3:R:189:HIS:O	3:R:211:ARG:NH1	2.51	0.43
3:R:61:ARG:HD2	3:R:77:SER:O	2.19	0.43
3:R:93:HIS:C	3:R:95:LEU:H	2.22	0.43
1:A:241:ASP:OD1	1:A:242:VAL:N	2.51	0.43
1:C:88:VAL:HA	1:C:268:MET:O	2.18	0.43
2:F:186:ALA:HB1	2:F:195:SER:H	1.83	0.43
1:C:470:TYR:HB3	1:C:498:ASN:HB2	2.01	0.43
1:C:500:PHE:HD1	1:B:496:LEU:HD13	1.83	0.43
1:A:205:SER:HA	1:A:210:GLN:HA	2.00	0.42
1:C:25:LEU:HD23	1:C:33:GLN:HB3	2.01	0.42
3:G:30:ARG:HD2	3:G:91:TYR:OH	2.19	0.42
3:L:80:SER:HA	3:L:106:ILE:HG12	2.01	0.42
1:C:394:GLN:CD	1:C:397:LYS:HZ1	2.22	0.42
3:G:33:LEU:HD13	3:G:71:PHE:CD2	2.54	0.42
3:R:48:ILE:HA	3:R:54:ARG:HA	2.01	0.42
1:A:71:LEU:HB3	1:A:148:PHE:CD2	2.54	0.42
2:F:200:VAL:HG22	2:F:201:THR:N	2.34	0.42
3:G:35:TRP:CE2	3:G:73:LEU:HB2	2.54	0.42
2:Q:206:SER:HA	2:Q:209:THR:HG22	2.00	0.42
1:A:197:GLN:HE21	1:A:248:ASN:HB2	1.83	0.42
1:A:207:ARG:HG3	1:A:242:VAL:HG12	2.01	0.42
1:B:310:LYS:NZ	1:B:310:LYS:HB2	2.34	0.42
1:C:179:ILE:O	1:C:254:PRO:HB3	2.19	0.42
1:A:499:ARG:HH21	1:C:457:GLU:HG3	1.85	0.42
2:H:59:TYR:HE2	2:H:112:TYR:CG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:92:ASN:N	3:L:92:ASN:OD1	2.52	0.42
1:A:221:PRO:HG3	1:C:244:VAL:HG21	2.01	0.42
2:F:146:SER:OG	2:F:147:LYS:N	2.51	0.42
3:G:61:ARG:HD2	3:G:77:SER:O	2.20	0.42
2:H:51:ILE:HG21	2:H:79:LEU:HD13	2.02	0.42
2:Q:112:TYR:HE1	2:Q:116:TYR:CD2	2.37	0.42
1:B:126:THR:HG22	1:B:128:THR:HG23	2.00	0.42
1:B:470:TYR:HB3	1:B:498:ASN:HB2	2.01	0.42
2:F:158:CYS:HB2	2:F:172:TRP:CZ2	2.55	0.42
3:G:122:ASP:HA	3:G:125:LEU:HD12	2.01	0.42
2:H:146:SER:OG	2:H:147:LYS:N	2.51	0.42
1:B:207:ARG:HG3	1:B:242:VAL:HG12	2.02	0.42
2:F:63:THR:O	2:F:67:ARG:NH2	2.53	0.42
3:G:2:ILE:HG22	3:G:93:HIS:CE1	2.55	0.42
1:A:17:HIS:HB3	1:A:444:MET:SD	2.60	0.42
2:F:159:LEU:HA	2:F:197:SER:HA	2.02	0.42
2:H:160:VAL:HB	2:H:196:LEU:HB3	2.02	0.42
1:B:387:LYS:HD3	3:L:30:ARG:HE	1.85	0.42
3:R:107:LYS:HD2	3:R:109:THR:N	2.35	0.42
1:B:341:ASN:N	1:B:341:ASN:OD1	2.51	0.42
1:C:60:ASP:HA	1:C:88:VAL:HG23	2.01	0.42
3:L:34:ALA:HB3	3:L:89:GLN:HG2	2.02	0.42
1:A:343:TRP:HB2	1:A:346:MET:HG3	2.02	0.42
1:A:382:ASN:HB2	2:Q:115:TYR:CE2	2.55	0.42
1:C:181:GLY:HA3	1:C:232:ILE:HD13	2.02	0.42
2:F:161:LYS:HA	2:F:195:SER:OG	2.19	0.42
2:F:188:LEU:HD12	2:F:189:GLN:O	2.20	0.42
1:C:378:ASN:HA	1:C:381:LEU:HB2	2.02	0.41
3:L:122:ASP:HA	3:L:125:LEU:HD12	2.01	0.41
2:Q:51:ILE:HB	2:Q:70:ILE:HD13	2.02	0.41
1:A:102:VAL:HB	1:A:105:TYR:HD1	1.86	0.41
1:C:499:ARG:NH2	1:B:457:GLU:OE1	2.53	0.41
3:L:16:GLY:H	3:L:78:LEU:HB3	1.84	0.41
3:L:61:ARG:HD2	3:L:77:SER:O	2.20	0.41
1:A:453:ARG:HG2	1:B:461:ASP:OD2	2.20	0.41
3:G:149:LYS:HD2	3:G:195:GLU:HB2	2.02	0.41
3:L:125:LEU:HD23	3:L:130:ALA:HB2	2.02	0.41
2:Q:24:ALA:HB3	2:Q:30:ARG:HD2	2.01	0.41
2:H:28:THR:HG21	2:H:98:LYS:HZ2	1.85	0.41
2:H:98:LYS:HG3	2:H:120:VAL:HB	2.01	0.41
3:L:30:ARG:N	3:L:91:TYR:HE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:140:TYR:CG	3:R:141:PRO:HA	2.55	0.41
1:B:205:SER:HA	1:B:210:GLN:HA	2.03	0.41
1:B:234:TRP:CE3	1:B:234:TRP:N	2.85	0.41
1:C:221:PRO:HG3	1:B:244:VAL:HG21	2.02	0.41
2:F:71:SER:O	2:F:79:LEU:HD12	2.20	0.41
2:Q:67:ARG:NH1	2:Q:90:ASP:OD2	2.54	0.41
3:L:35:TRP:CE3	3:L:73:LEU:HD22	2.56	0.41
3:R:92:ASN:OD1	3:R:92:ASN:N	2.52	0.41
1:B:57:ARG:NH1	1:B:83:THR:O	2.54	0.41
1:C:307:LYS:HD3	1:C:421:TRP:CE2	2.56	0.41
1:A:120:PHE:CD1	1:A:150:ARG:HD2	2.56	0.41
1:A:311:GLN:HG2	1:A:314:LEU:HD21	2.03	0.41
1:C:84:TRP:CZ3	1:C:118:LEU:HG	2.56	0.41
2:F:144:PRO:HD2	2:F:231:PRO:HA	2.02	0.41
1:B:95:SER:OG	1:B:224:ARG:NH1	2.54	0.41
1:B:382:ASN:O	1:B:386:GLU:HB2	2.21	0.41
3:G:16:GLY:H	3:G:78:LEU:HB3	1.86	0.41
1:B:132:GLN:O	1:B:152:ASN:ND2	2.54	0.40
1:C:120:PHE:HZ	1:C:255:ARG:HB2	1.86	0.40
1:C:373:ALA:HB2	1:C:443:GLU:HG3	2.03	0.40
2:F:228:LYS:HZ2	2:F:230:GLU:HB3	1.87	0.40
3:G:32:ASN:HB3	3:G:91:TYR:HB3	2.03	0.40
2:Q:144:PRO:HD2	2:Q:231:PRO:HA	2.02	0.40
2:Q:99:ASP:HB3	2:Q:116:TYR:HB3	2.04	0.40
3:R:148:TRP:CG	3:R:179:LEU:HD13	2.56	0.40
3:R:106:ILE:HD13	3:R:166:GLN:HE22	1.86	0.40
1:C:97:CYS:SG	1:C:98:TYR:N	2.89	0.40
1:B:457:GLU:HB3	1:B:499:ARG:HH12	1.86	0.40
1:C:62:ILE:H	1:C:62:ILE:HD13	1.86	0.40
3:G:35:TRP:CE3	3:G:73:LEU:HD22	2.57	0.40
2:H:57:ALA:HA	2:H:58:THR:CG2	2.49	0.40
2:H:119:ASP:HA	3:L:46:LEU:HD22	2.04	0.40
3:L:29:VAL:HG23	3:L:91:TYR:CD1	2.57	0.40
1:C:477:CYS:O	1:C:480:SER:OG	2.28	0.40
2:Q:11:LEU:HD12	2:Q:165:PRO:HG3	2.03	0.40

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	477/512 (93%)	453 (95%)	21 (4%)	3 (1%)	28	70
1	B	476/512 (93%)	450 (94%)	21 (4%)	5 (1%)	17	58
1	C	478/512 (93%)	450 (94%)	23 (5%)	5 (1%)	18	60
2	F	230/236 (98%)	209 (91%)	18 (8%)	3 (1%)	14	55
2	H	229/236 (97%)	209 (91%)	15 (7%)	5 (2%)	8	44
2	Q	229/236 (97%)	209 (91%)	17 (7%)	3 (1%)	14	55
3	G	209/214 (98%)	189 (90%)	17 (8%)	3 (1%)	13	53
3	L	209/214 (98%)	190 (91%)	15 (7%)	4 (2%)	9	46
3	R	209/214 (98%)	188 (90%)	18 (9%)	3 (1%)	13	53
All	All	2746/2886 (95%)	2547 (93%)	165 (6%)	34 (1%)	15	56

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	388	THR
3	L	94	TRP
3	R	94	TRP
1	A	62	ILE
1	C	337	GLY
1	B	387	LYS
2	H	232	LYS
3	L	76	SER
2	Q	149	THR
3	R	76	SER
1	C	304	ALA
2	F	133	SER
2	F	149	THR
3	G	76	SER
2	H	149	THR
3	L	51	ALA

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Mol	Chain	Res	Type
1	C	324	PRO
2	F	185	PRO
3	G	51	ALA
3	G	138	ASN
2	H	162	ASP
3	L	138	ASN
3	R	138	ASN
1	A	324	PRO
1	B	62	ILE
1	B	324	PRO
2	Q	162	ASP
1	C	143	PRO
1	B	143	PRO
2	H	53	GLY
1	A	143	PRO
1	B	72	GLY
2	H	165	PRO
2	Q	165	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	421/447 (94%)	406 (96%)	15 (4%)	40	74
1	B	422/447 (94%)	409 (97%)	13 (3%)	45	78
1	C	422/447 (94%)	412 (98%)	10 (2%)	54	82
2	F	195/198 (98%)	176 (90%)	19 (10%)	9	38
2	H	196/198 (99%)	189 (96%)	7 (4%)	40	74
2	Q	196/198 (99%)	185 (94%)	11 (6%)	25	62
3	G	186/187 (100%)	178 (96%)	8 (4%)	33	70
3	L	186/187 (100%)	182 (98%)	4 (2%)	57	83
3	R	186/187 (100%)	184 (99%)	2 (1%)	78	91
All	All	2410/2496 (97%)	2321 (96%)	89 (4%)	39	73

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	64	CYS
1	A	73	ASP
1	A	117	THR
1	A	137	ASN
1	A	165	ASN
1	A	172	ASP
1	A	175	ASP
1	A	269	ARG
1	A	276	THR
1	A	388	THR
1	A	390	GLU
1	A	400	SER
1	A	455	LEU
1	A	493	ASP
1	C	62	ILE
1	C	64	CYS
1	C	172	ASP
1	C	175	ASP
1	C	276	THR
1	C	312	ASN
1	C	338	PHE
1	C	340	GLU
1	C	405	ARG
1	C	493	ASP
2	F	4	LEU
2	F	28	THR
2	F	29	PHE
2	F	58	THR
2	F	108	MET
2	F	112	TYR
2	F	118	MET
2	F	128	THR
2	F	138	SER
2	F	156	LEU
2	F	158	CYS
2	F	159	LEU
2	F	162	ASP
2	F	168	VAL
2	F	170	VAL
2	F	171	SER
2	F	184	PHE

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Mol	Chain	Res	Type
2	F	191	SER
2	F	193	LEU
3	G	30	ARG
3	G	33	LEU
3	G	58	ILE
3	G	89	GLN
3	G	90	GLN
3	G	159	SER
3	G	164	THR
3	G	190	LYS
1	B	18	HIS
1	B	71	LEU
1	B	73	ASP
1	B	172	ASP
1	B	175	ASP
1	B	234	TRP
1	B	276	THR
1	B	278	ILE
1	B	299	LYS
1	B	341	ASN
1	B	389	ASN
1	B	455	LEU
1	B	493	ASP
2	H	1	GLU
2	H	2	VAL
2	H	28	THR
2	H	29	PHE
2	H	58	THR
2	H	108	MET
2	H	156	LEU
3	L	29	VAL
3	L	33	LEU
3	L	58	ILE
3	L	90	GLN
2	Q	3	GLN
2	Q	13	GLN
2	Q	18	LEU
2	Q	19	ARG
2	Q	28	THR
2	Q	29	PHE
2	Q	112	TYR
2	Q	118	MET

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Mol	Chain	Res	Type
2	Q	166	GLU
2	Q	190	SER
2	Q	234	CYS
3	R	30	ARG
3	R	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	382	ASN
3	L	166	GLN
3	R	166	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	601	1	14,14,15	0.60	1 (7%)	15,19,21	0.84	0
4	NAG	A	602	1	14,14,15	0.32	0	15,19,21	0.50	0
4	NAG	A	603	1	14,14,15	0.91	1 (7%)	15,19,21	1.36	1 (6%)
4	NAG	A	604	1	14,14,15	0.29	0	15,19,21	0.50	0
4	NAG	A	605	1	14,14,15	0.51	0	15,19,21	0.73	1 (6%)
4	NAG	A	606	1	14,14,15	0.28	0	15,19,21	0.44	0
4	NAG	B	601	1	14,14,15	0.36	0	15,19,21	0.53	0
4	NAG	B	602	1	14,14,15	0.32	0	15,19,21	0.52	0
4	NAG	B	603	1	14,14,15	0.23	0	15,19,21	0.49	0
4	NAG	B	604	1	14,14,15	0.24	0	15,19,21	0.48	0
4	NAG	B	605	1	14,14,15	0.26	0	15,19,21	0.49	0
4	NAG	B	606	1	14,14,15	0.25	0	15,19,21	0.49	0
4	NAG	C	601	-	14,14,15	0.21	0	15,19,21	0.46	0
4	NAG	C	602	1	14,14,15	0.33	0	15,19,21	0.57	0
4	NAG	C	603	1	14,14,15	0.30	0	15,19,21	0.49	0
4	NAG	C	604	1	14,14,15	0.26	0	15,19,21	0.50	0
4	NAG	C	605	1	14,14,15	0.27	0	15,19,21	0.49	0
4	NAG	C	606	1	14,14,15	0.24	0	15,19,21	0.50	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
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1	-	0/6/23/26	0/1/1/1
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
4	NAG	B	605	1	-	0/6/23/26	0/1/1/1
4	NAG	B	606	1	-	0/6/23/26	0/1/1/1
4	NAG	C	601	-	-	0/6/23/26	0/1/1/1
4	NAG	C	602	1	-	0/6/23/26	0/1/1/1
4	NAG	C	603	1	-	0/6/23/26	0/1/1/1
4	NAG	C	604	1	-	0/6/23/26	0/1/1/1
4	NAG	C	605	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	606	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)
4	A	601	NAG	O5-C1	-2.04	1.40	1.43
4	A	603	NAG	O5-C1	3.28	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	NAG	C1-O5-C5	2.42	115.50	112.17
4	A	603	NAG	C1-O5-C5	5.00	119.06	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	481/512 (93%)	0.11	6 (1%) 79 71	73, 139, 208, 368	3 (0%)
1	B	480/512 (93%)	0.15	12 (2%) 58 48	68, 150, 203, 287	0
1	C	482/512 (94%)	0.18	18 (3%) 42 35	87, 160, 221, 275	4 (0%)
2	F	232/236 (98%)	0.36	23 (9%) 8 8	87, 156, 332, 398	2 (0%)
2	H	233/236 (98%)	0.37	17 (7%) 16 14	122, 189, 276, 437	0
2	Q	233/236 (98%)	0.27	15 (6%) 20 16	75, 134, 278, 392	1 (0%)
3	G	213/214 (99%)	2.10	66 (30%) 0 0	97, 248, 529, 797	0
3	L	213/214 (99%)	0.47	10 (4%) 32 26	125, 191, 250, 306	1 (0%)
3	R	213/214 (99%)	0.18	7 (3%) 47 39	78, 157, 245, 295	0
All	All	2780/2886 (96%)	0.37	174 (6%) 21 17	68, 159, 296, 797	11 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	119	PRO	15.4
3	G	156	SER	14.5
3	G	157	GLY	13.4
3	G	117	ILE	12.7
3	G	198	HIS	12.1
3	G	141	PRO	11.4
3	G	137	ASN	11.0
3	G	115	VAL	10.3
3	G	144	ALA	10.2
3	G	109	THR	9.1
3	G	120	PRO	9.0
3	G	143	GLU	8.1
3	G	114	SER	8.0
3	G	186	TYR	7.6
3	G	116	PHE	7.6

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Mol	Chain	Res	Type	RSRZ
3	G	158	ASN	7.5
3	G	148	TRP	7.2
3	G	113	PRO	6.9
3	G	142	ARG	6.8
3	G	110	VAL	6.8
3	G	155	GLN	6.4
3	G	122	ASP	6.3
3	G	211	ARG	6.0
3	G	209	PHE	5.9
2	F	155	ALA	5.7
3	G	183	LYS	5.6
3	G	112	ALA	5.5
2	F	209	THR	5.5
3	G	212	GLY	5.4
3	G	201	LEU	5.2
2	F	148	SER	5.2
3	G	126	LYS	5.2
2	H	97	ALA	5.2
1	A	326	LYS	5.1
3	G	202	SER	5.1
3	G	37	GLN	5.0
3	G	210	ASN	4.8
3	L	1	GLU	4.8
2	F	156	LEU	4.7
2	Q	145	SER	4.6
2	Q	146	SER	4.5
2	F	154	ALA	4.5
3	G	184	ALA	4.5
3	G	207	LYS	4.5
1	B	458	ASN	4.4
2	F	211	THR	4.4
3	G	111	ALA	4.4
3	G	151	ASP	4.3
2	H	98	LYS	4.2
3	G	179	LEU	4.2
3	G	187	GLU	4.2
3	R	183	LYS	4.2
3	G	206	THR	4.1
3	G	135	LEU	4.1
3	G	130	ALA	4.0
3	L	122	ASP	4.0
2	F	145	SER	4.0

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Mol	Chain	Res	Type	RSRZ
3	G	118	PHE	3.8
2	Q	156	LEU	3.7
3	L	47	LEU	3.7
1	C	336	ALA	3.6
3	G	146	VAL	3.6
2	Q	205	SER	3.6
2	Q	147	LYS	3.6
3	L	183	LYS	3.5
2	Q	229	VAL	3.4
3	G	170	ASP	3.4
1	C	326	LYS	3.4
3	G	182	SER	3.4
3	G	194	CYS	3.2
2	F	151	GLY	3.2
2	H	51	ILE	3.2
3	R	184	ALA	3.2
2	F	149	THR	3.2
2	H	141	PRO	3.1
1	C	99	PRO	3.1
2	H	233	SER	3.1
1	B	15	LEU	3.1
2	H	211	THR	3.1
1	C	251	LEU	3.0
1	B	13	LEU	3.0
3	L	113	PRO	3.0
2	Q	206	SER	3.0
2	H	45	LEU	3.0
1	C	127	TRP	3.0
3	G	149	LYS	2.9
2	F	144	PRO	2.9
2	Q	232	LYS	2.9
3	L	152	ASN	2.9
3	G	159	SER	2.9
3	G	196	VAL	2.9
3	L	181	LEU	2.9
1	C	166	VAL	2.9
2	F	142	LEU	2.9
2	H	34	LEU	2.8
1	B	12	THR	2.8
2	F	141	PRO	2.8
1	B	11	ALA	2.8
2	Q	144	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	213	ILE	2.8
2	Q	151	GLY	2.8
2	H	94	TYR	2.8
2	Q	143	ALA	2.8
1	B	326	LYS	2.7
3	G	134	CYS	2.7
2	H	152	GLY	2.7
2	F	197	SER	2.7
2	F	152	GLY	2.7
2	F	175	GLY	2.7
3	G	31	SER	2.7
3	G	180	THR	2.7
3	G	33	LEU	2.7
3	G	47	LEU	2.7
2	Q	149	THR	2.7
2	Q	203	PRO	2.7
3	R	209	PHE	2.6
2	F	157	GLY	2.6
2	H	234	CYS	2.6
1	B	459	ALA	2.6
3	G	152	ASN	2.6
3	G	203	SER	2.6
3	G	188	LYS	2.5
3	G	46	LEU	2.5
1	C	242	VAL	2.5
2	H	212	TYR	2.5
1	C	150	ARG	2.4
1	B	340	GLU	2.4
2	F	118	MET	2.4
1	C	94	PHE	2.4
3	G	195	GLU	2.4
1	B	16	GLY	2.4
2	H	155	ALA	2.3
1	A	118	LEU	2.3
2	H	142	LEU	2.3
1	C	352	GLY	2.3
1	C	96	ASN	2.3
3	L	92	ASN	2.3
3	G	48	ILE	2.3
1	A	223	VAL	2.3
2	F	232	LYS	2.3
2	H	116	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	481	ILE	2.3
1	A	71	LEU	2.3
2	F	119	ASP	2.3
1	A	221	PRO	2.2
3	R	132	VAL	2.2
3	G	21	LEU	2.2
1	C	60	ASP	2.2
1	B	104	ASP	2.2
3	G	213	GLU	2.2
3	G	83	PHE	2.2
3	R	31	SER	2.2
1	C	224	ARG	2.2
1	C	62	ILE	2.2
2	Q	177	LEU	2.2
3	R	194	CYS	2.2
2	H	46	GLU	2.2
1	C	11	ALA	2.2
2	F	233	SER	2.2
3	G	62	PHE	2.1
1	C	147	PHE	2.1
3	G	208	SER	2.1
2	F	147	LYS	2.1
2	H	143	ALA	2.1
2	F	231	PRO	2.1
3	L	83	PHE	2.1
1	C	438	ASP	2.1
1	C	79	PHE	2.1
2	Q	202	VAL	2.1
3	L	48	ILE	2.1
1	B	460	GLU	2.1
3	R	181	LEU	2.0
3	G	200	GLY	2.0
1	A	356	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	605	14/15	0.65	0.29	0.46	186,198,199,200	0
4	NAG	C	606	14/15	0.80	0.22	-0.39	137,147,159,168	0
4	NAG	A	603	14/15	0.88	0.25	-0.68	137,150,157,165	0
4	NAG	A	602	14/15	0.92	0.20	-0.85	105,131,148,157	0
4	NAG	B	606	14/15	0.85	0.21	-0.85	136,152,170,178	0
4	NAG	B	603	14/15	0.83	0.18	-0.89	153,161,167,168	0
4	NAG	C	602	14/15	0.91	0.24	-0.92	125,145,176,179	0
4	NAG	B	602	14/15	0.88	0.20	-0.99	117,137,147,159	0
4	NAG	A	606	14/15	0.88	0.17	-1.11	132,150,158,158	0
4	NAG	A	604	14/15	0.88	0.30	-	133,144,153,155	0
4	NAG	B	601	14/15	0.82	0.43	-	198,209,219,222	0
4	NAG	C	604	14/15	0.88	0.16	-	147,159,166,176	0
4	NAG	A	601	14/15	0.84	0.24	-	204,213,226,229	0
4	NAG	C	601	14/15	0.50	0.66	-	254,256,258,258	0
4	NAG	B	604	14/15	0.82	0.32	-	154,165,185,188	0
4	NAG	B	605	14/15	0.84	0.18	-	154,169,175,179	0
4	NAG	C	603	14/15	0.88	0.16	-	165,174,183,187	0
4	NAG	C	605	14/15	0.90	0.36	-	173,187,203,215	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.