



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:23 PM GMT

PDB ID : 4XHJ  
Title : gHgL of Varicella-zoster virus in complex with human neutralizing antibodies.  
Authors : Xing, Y.  
Deposited on : 2015-01-05  
Resolution : 3.16 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

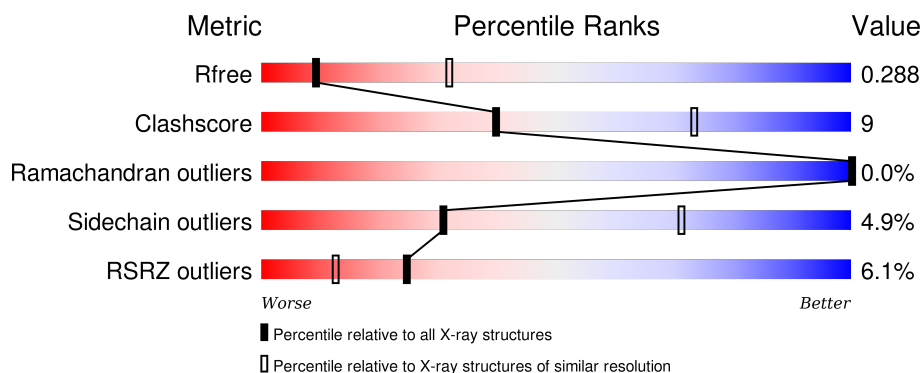
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	833	<div> <div>5%</div> <div>63% 22% 12%</div> </div>
1	E	833	<div> <div>5%</div> <div>63% 21% 15%</div> </div>
2	B	138	<div> <div>3%</div> <div>73% 20% 6%</div> </div>
2	F	138	<div> <div>2%</div> <div>69% 22% 6%</div> </div>
3	C	215	<div> <div>13%</div> <div>79% 17% 4%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	G	215	
4	D	282	
4	H	282	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19505 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5610	3602	936	1047	25			
1	E	705	Total	C	N	O	S	0	0	0
			5452	3508	906	1015	23			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	796	GLY	-	expression tag	UNP Q775J3
A	797	SER	-	expression tag	UNP Q775J3
A	798	GLU	-	expression tag	UNP Q775J3
A	799	ASN	-	expression tag	UNP Q775J3
A	800	LEU	-	expression tag	UNP Q775J3
A	801	TYR	-	expression tag	UNP Q775J3
A	802	PHE	-	expression tag	UNP Q775J3
A	803	GLN	-	expression tag	UNP Q775J3
A	804	GLY	-	expression tag	UNP Q775J3
A	805	SER	-	expression tag	UNP Q775J3
A	806	TRP	-	expression tag	UNP Q775J3
A	807	SER	-	expression tag	UNP Q775J3
A	808	HIS	-	expression tag	UNP Q775J3
A	809	PRO	-	expression tag	UNP Q775J3
A	810	GLN	-	expression tag	UNP Q775J3
A	811	PHE	-	expression tag	UNP Q775J3
A	812	GLU	-	expression tag	UNP Q775J3
A	813	LYS	-	expression tag	UNP Q775J3
A	814	GLY	-	expression tag	UNP Q775J3
A	815	GLY	-	expression tag	UNP Q775J3
A	816	GLY	-	expression tag	UNP Q775J3
A	817	SER	-	expression tag	UNP Q775J3
A	818	GLY	-	expression tag	UNP Q775J3
A	819	GLY	-	expression tag	UNP Q775J3
A	820	GLY	-	expression tag	UNP Q775J3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	821	SER	-	expression tag	UNP Q775J3
A	822	GLY	-	expression tag	UNP Q775J3
A	823	GLY	-	expression tag	UNP Q775J3
A	824	GLY	-	expression tag	UNP Q775J3
A	825	SER	-	expression tag	UNP Q775J3
A	826	TRP	-	expression tag	UNP Q775J3
A	827	SER	-	expression tag	UNP Q775J3
A	828	HIS	-	expression tag	UNP Q775J3
A	829	PRO	-	expression tag	UNP Q775J3
A	830	GLN	-	expression tag	UNP Q775J3
A	831	PHE	-	expression tag	UNP Q775J3
A	832	GLU	-	expression tag	UNP Q775J3
A	833	LYS	-	expression tag	UNP Q775J3
E	796	GLY	-	expression tag	UNP Q775J3
E	797	SER	-	expression tag	UNP Q775J3
E	798	GLU	-	expression tag	UNP Q775J3
E	799	ASN	-	expression tag	UNP Q775J3
E	800	LEU	-	expression tag	UNP Q775J3
E	801	TYR	-	expression tag	UNP Q775J3
E	802	PHE	-	expression tag	UNP Q775J3
E	803	GLN	-	expression tag	UNP Q775J3
E	804	GLY	-	expression tag	UNP Q775J3
E	805	SER	-	expression tag	UNP Q775J3
E	806	TRP	-	expression tag	UNP Q775J3
E	807	SER	-	expression tag	UNP Q775J3
E	808	HIS	-	expression tag	UNP Q775J3
E	809	PRO	-	expression tag	UNP Q775J3
E	810	GLN	-	expression tag	UNP Q775J3
E	811	PHE	-	expression tag	UNP Q775J3
E	812	GLU	-	expression tag	UNP Q775J3
E	813	LYS	-	expression tag	UNP Q775J3
E	814	GLY	-	expression tag	UNP Q775J3
E	815	GLY	-	expression tag	UNP Q775J3
E	816	GLY	-	expression tag	UNP Q775J3
E	817	SER	-	expression tag	UNP Q775J3
E	818	GLY	-	expression tag	UNP Q775J3
E	819	GLY	-	expression tag	UNP Q775J3
E	820	GLY	-	expression tag	UNP Q775J3
E	821	SER	-	expression tag	UNP Q775J3
E	822	GLY	-	expression tag	UNP Q775J3
E	823	GLY	-	expression tag	UNP Q775J3
E	824	GLY	-	expression tag	UNP Q775J3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	825	SER	-	expression tag	UNP Q775J3
E	826	TRP	-	expression tag	UNP Q775J3
E	827	SER	-	expression tag	UNP Q775J3
E	828	HIS	-	expression tag	UNP Q775J3
E	829	PRO	-	expression tag	UNP Q775J3
E	830	GLN	-	expression tag	UNP Q775J3
E	831	PHE	-	expression tag	UNP Q775J3
E	832	GLU	-	expression tag	UNP Q775J3
E	833	LYS	-	expression tag	UNP Q775J3

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1007	647	163	192	5			
2	F	130	Total	C	N	O	S	0	0	0
			997	641	161	190	5			

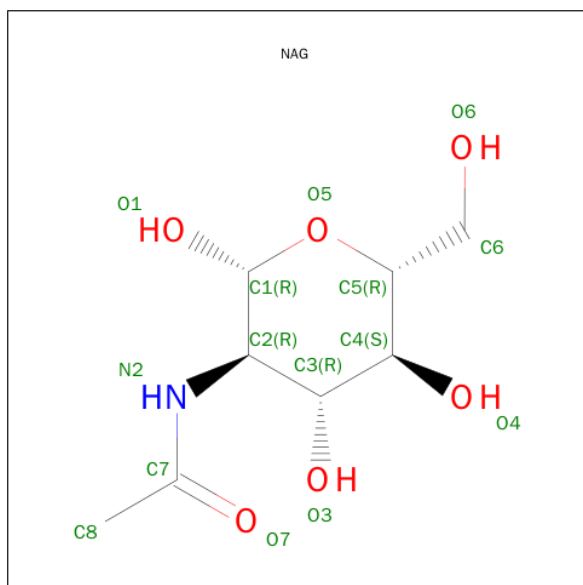
- Molecule 3 is a protein called Fab-RC light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1569	984	265	315	5			
3	G	196	Total	C	N	O	S	0	0	0
			1481	936	247	293	5			

- Molecule 4 is a protein called Fab-RC heavy chain.

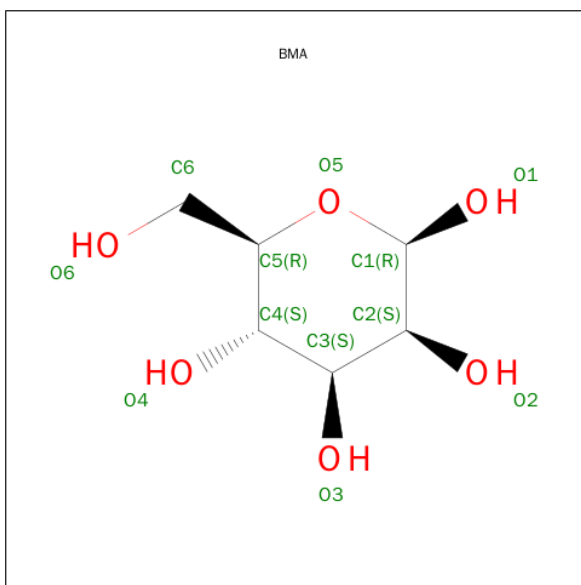
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	207	Total	C	N	O	S	0	0	0
			1569	992	265	299	13			
4	H	206	Total	C	N	O	S	0	0	0
			1561	988	264	296	13			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



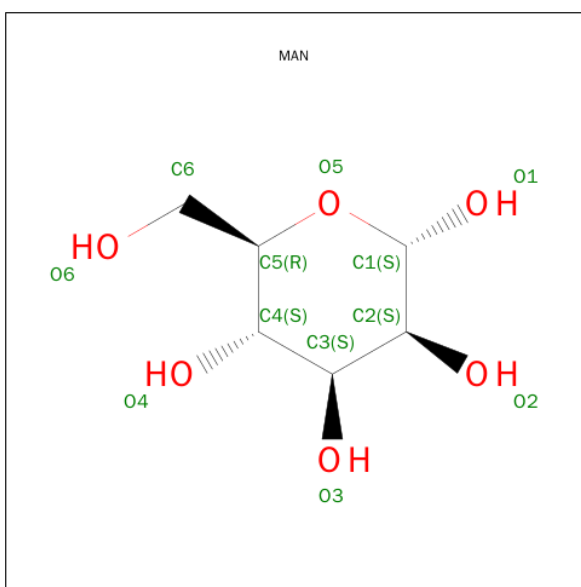
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



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

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

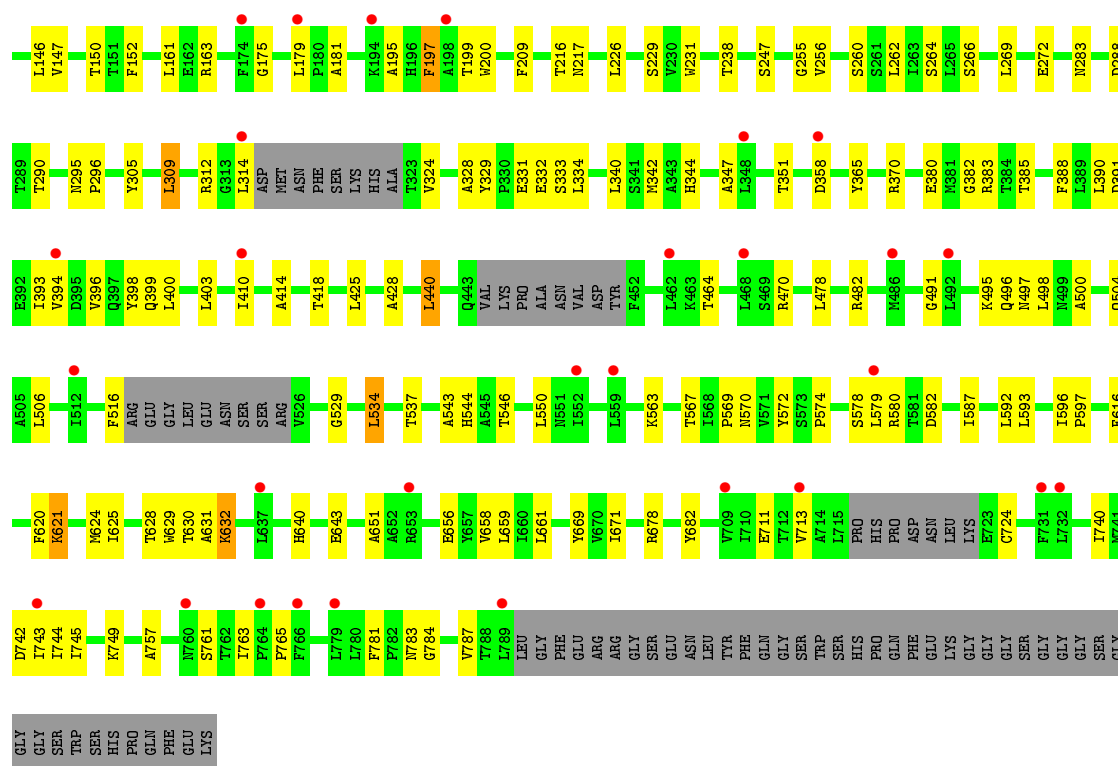
*Continued on next page...*



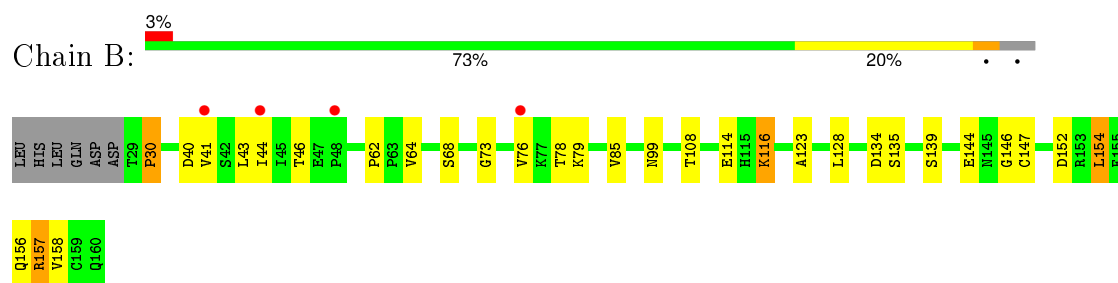
*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		

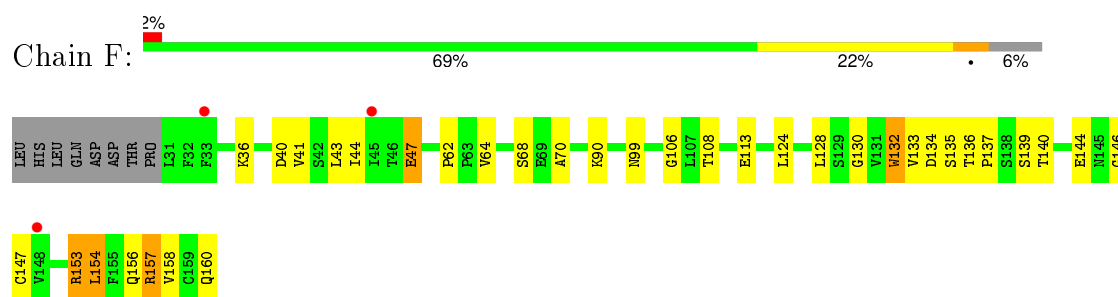




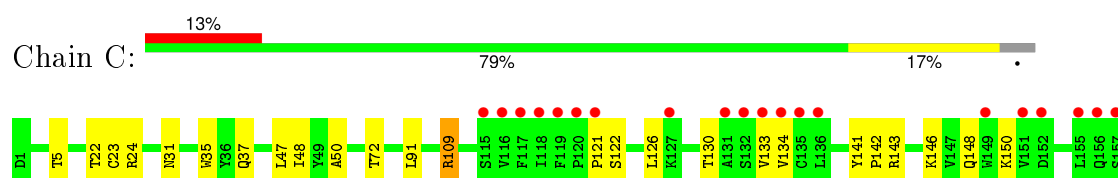
- Molecule 2: Envelope glycoprotein L

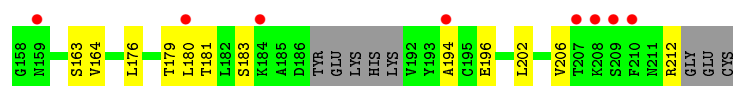


- Molecule 2: Envelope glycoprotein L

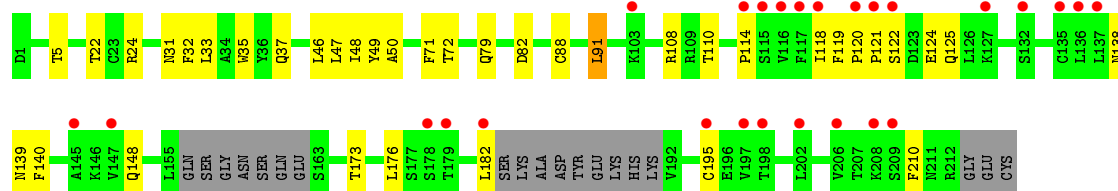
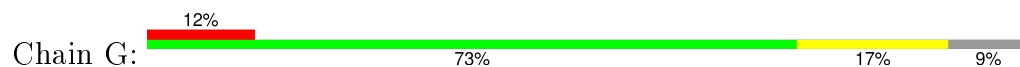


- Molecule 3: Fab-RC light chain

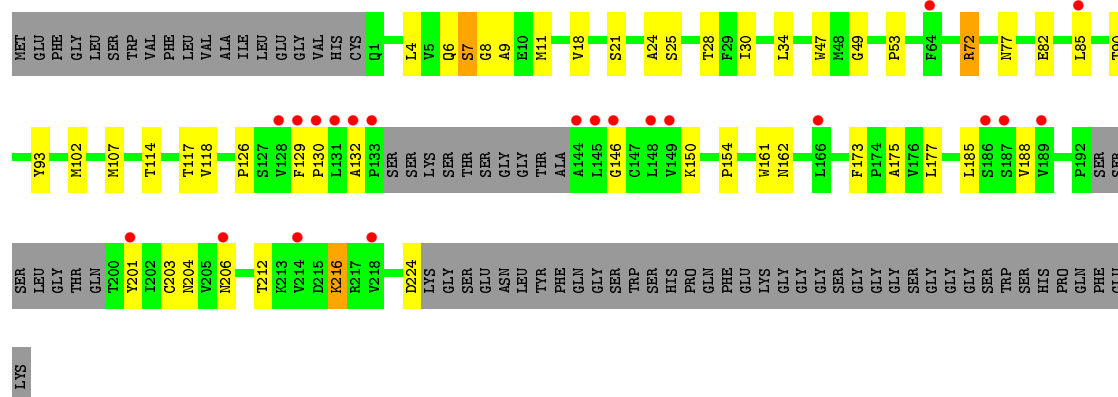




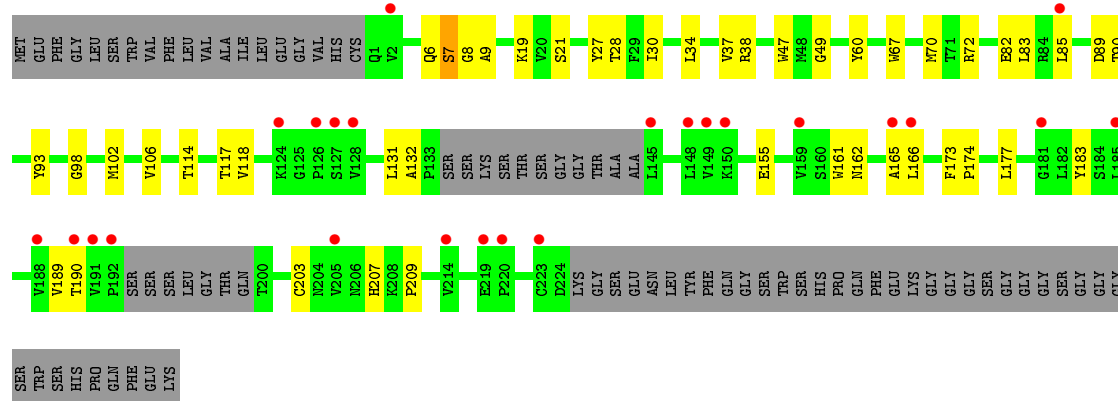
• Molecule 3: Fab-RC light chain



• Molecule 4: Fab-RC heavy chain



• Molecule 4: Fab-RC heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.00Å 147.00Å 198.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 3.16 41.10 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.10-3.16) 99.7 (41.10-3.16)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.236 , 0.278 0.244 , 0.288	Depositor DCC
$R_{free}$ test set	3636 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.8	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.7	EDS
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72015 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.25	0/5749	0.47	0/7854
1	E	0.23	0/5582	0.45	0/7619
2	B	0.26	0/1034	0.53	1/1416 (0.1%)
2	F	0.23	0/1024	0.51	0/1402
3	C	0.24	0/1600	0.46	0/2173
3	G	0.24	0/1511	0.46	0/2055
4	D	0.23	0/1608	0.47	0/2191
4	H	0.23	0/1600	0.46	0/2180
All	All	0.24	0/19708	0.47	1/26890 (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
4	D	0	1
4	H	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	PRO	N-CA-CB	5.89	110.36	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	7	SER	Peptide
4	H	7	SER	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	5610	0	5452	119	0
1	E	5452	0	5349	109	0
2	B	1007	0	972	22	0
2	F	997	0	969	29	0
3	C	1569	0	1527	20	0
3	G	1481	0	1440	22	0
4	D	1569	0	1517	27	0
4	H	1561	0	1510	27	0
5	A	56	0	50	1	0
5	B	28	0	24	1	0
5	E	70	0	63	0	0
5	F	28	0	24	0	0
6	A	11	0	10	0	0
6	B	11	0	8	0	0
6	F	11	0	8	0	0
7	B	22	0	20	0	0
7	F	22	0	20	0	0
All	All	19505	0	18963	338	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 (338) 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:A:98:LYS:HD2	2:B:68:SER:HB3	1.57	0.86
1:E:175:GLY:HA3	1:E:333:SER:HA	1.63	0.79
1:E:73:LYS:O	1:E:98:LYS:NZ	2.17	0.78
3:G:5:THR:HB	3:G:24:ARG:HB2	1.69	0.75
1:E:757:ALA:HB3	1:E:761:SER:HB3	1.68	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:GLU:HB3	1:E:64:LYS:HB2	1.68	0.74
1:E:161:LEU:HB3	1:E:324:VAL:HG12	1.73	0.70
1:E:394:VAL:HG11	1:E:464:THR:HG22	1.74	0.70
3:C:202:LEU:HD13	3:C:206:VAL:HG22	1.74	0.69
1:A:175:GLY:HA3	1:A:333:SER:HA	1.72	0.69
1:A:537:THR:HA	1:A:578:SER:HB2	1.75	0.68
1:E:98:LYS:HD2	2:F:68:SER:HB3	1.75	0.68
1:A:134:ASP:OD1	5:B:800:NAG:H82	1.94	0.68
1:A:163:ARG:NH2	1:A:331:GLU:OE2	2.27	0.67
1:E:579:LEU:HA	1:E:631:ALA:HB2	1.76	0.67
3:C:5:THR:HB	3:C:24:ARG:HB2	1.77	0.66
1:A:73:LYS:O	1:A:98:LYS:NZ	2.27	0.66
1:A:757:ALA:HB3	1:A:761:SER:HB3	1.76	0.66
2:F:144:GLU:O	2:F:157:ARG:NH2	2.29	0.66
1:E:163:ARG:NH2	1:E:331:GLU:OE2	2.28	0.66
1:A:342:MET:HB2	1:A:370:ARG:HD2	1.77	0.65
1:E:129:ASP:OD2	1:E:135:SER:OG	2.13	0.65
1:A:579:LEU:HA	1:A:631:ALA:HB2	1.78	0.65
4:D:175:ALA:HA	4:D:185:LEU:HB3	1.79	0.65
1:A:266:SER:HA	2:B:146:GLY:HA2	1.79	0.65
1:E:580:ARG:HG2	1:E:659:LEU:HD12	1.79	0.64
1:A:763:ILE:HG22	1:A:765:PRO:HD2	1.79	0.64
1:A:394:VAL:HG11	1:A:464:THR:HG22	1.77	0.64
1:E:763:ILE:HG22	1:E:765:PRO:HD2	1.80	0.63
3:C:122:SER:O	3:C:126:LEU:N	2.30	0.63
1:E:593:LEU:HD11	1:E:616:PHE:HD1	1.63	0.63
2:F:134:ASP:O	4:H:28:THR:OG1	2.18	0.62
1:A:649:ASP:OD2	1:A:678:ARG:NH1	2.32	0.62
1:A:238:THR:H	1:A:255:GLY:HA2	1.64	0.62
4:H:6:GLN:NE2	4:H:93:TYR:O	2.28	0.61
4:D:53:PRO:O	4:D:72:ARG:NH1	2.33	0.61
1:A:580:ARG:HG2	1:A:659:LEU:HD12	1.83	0.61
1:A:143:THR:O	2:B:99:ASN:ND2	2.29	0.61
1:A:75:VAL:HG23	1:A:98:LYS:HZ1	1.65	0.61
2:F:130:GLY:O	2:F:133:VAL:HG23	2.01	0.61
1:A:129:ASP:OD2	1:A:135:SER:OG	2.19	0.60
1:E:342:MET:HB2	1:E:370:ARG:HD2	1.84	0.60
1:E:534:LEU:HD22	1:E:745:ILE:HD11	1.84	0.60
1:E:724:CYS:HB2	1:E:749:LYS:HE2	1.83	0.60
1:A:226:LEU:O	1:A:229:SER:OG	2.18	0.60
3:G:48:ILE:HG22	3:G:50:ALA:O	2.02	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:GLN:NE2	1:E:570:ASN:OD1	2.36	0.59
1:A:529:GLY:HA3	1:A:640:HIS:CD2	2.38	0.59
1:A:671:ILE:HG21	1:A:740:ILE:HD11	1.84	0.59
4:H:90:THR:HG23	4:H:117:THR:HA	1.85	0.59
2:B:108:THR:HG22	2:B:128:LEU:HD13	1.83	0.59
4:D:11:MET:HB2	4:D:154:PRO:HG3	1.83	0.59
4:H:85:LEU:HD13	4:H:118:VAL:HG22	1.82	0.59
1:E:628:THR:HA	1:E:632:LYS:HB2	1.83	0.59
1:A:161:LEU:HB3	1:A:324:VAL:HG12	1.85	0.58
1:A:534:LEU:HD22	1:A:745:ILE:HD11	1.86	0.58
2:F:40:ASP:HB2	2:F:43:LEU:HG	1.86	0.57
1:E:70:ASN:HB2	2:F:90:LYS:HD2	1.85	0.57
1:E:37:LEU:HD12	1:E:60:GLU:HG2	1.86	0.57
1:E:537:THR:HA	1:E:578:SER:HB2	1.85	0.57
1:E:179:LEU:O	1:E:181:ALA:N	2.37	0.57
3:G:108:ARG:NH2	3:G:110:THR:OG1	2.37	0.57
1:E:238:THR:H	1:E:255:GLY:HA2	1.70	0.57
1:A:313:GLY:HA2	1:A:317:ASN:HB2	1.87	0.57
3:C:130:THR:HG22	3:C:183:SER:HA	1.86	0.57
1:A:567:THR:HG22	1:A:570:ASN:HB2	1.86	0.57
1:A:68:TRP:CD1	2:B:41:VAL:HB	2.40	0.56
1:E:582:ASP:HB3	1:E:658:VAL:HG13	1.86	0.56
1:A:178:LEU:HD11	1:A:338:TYR:HA	1.87	0.56
2:F:108:THR:HG22	2:F:128:LEU:HD13	1.87	0.56
4:D:146:GLY:HA3	4:D:188:VAL:HA	1.87	0.56
1:A:715:LEU:HD13	1:A:756:ALA:HA	1.88	0.56
3:C:134:VAL:HG12	3:C:179:THR:HG23	1.88	0.56
1:E:226:LEU:N	1:E:272:GLU:OE1	2.37	0.56
1:A:179:LEU:O	1:A:181:ALA:N	2.39	0.56
1:A:724:CYS:HB2	1:A:749:LYS:HE2	1.87	0.56
1:A:226:LEU:HD13	1:A:262:LEU:HD11	1.87	0.55
4:D:85:LEU:HD13	4:D:118:VAL:HG22	1.89	0.55
1:A:486:MET:O	1:A:490:LYS:HG3	2.07	0.55
1:E:197:PHE:HD2	1:E:390:LEU:HD21	1.71	0.55
1:E:266:SER:HA	2:F:146:GLY:HA2	1.88	0.55
3:C:133:VAL:O	3:C:180:LEU:HB3	2.08	0.54
1:E:713:VAL:HG22	1:E:787:VAL:HG11	1.89	0.54
2:B:79:LYS:NZ	2:B:134:ASP:OD2	2.39	0.54
1:E:671:ILE:HG21	1:E:740:ILE:HD11	1.88	0.54
1:A:195:ALA:HB2	1:A:209:PHE:CD1	2.43	0.54
1:A:68:TRP:HZ3	1:A:93:LEU:HD22	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:GLY:HA2	4:D:161:TRP:CH2	2.42	0.54
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.88	0.54
1:E:624:MET:O	1:E:628:THR:HG22	2.09	0.53
4:H:207:HIS:CD2	4:H:209:PRO:HD2	2.43	0.53
1:E:264:SER:HB2	2:F:147:CYS:HA	1.90	0.53
1:A:393:ILE:HD11	1:A:428:ALA:HB2	1.90	0.53
1:A:618:ALA:O	1:A:622:THR:HG22	2.08	0.53
1:A:504:GLN:NE2	1:A:570:ASN:OD1	2.42	0.53
1:E:529:GLY:HA3	1:E:640:HIS:CD2	2.43	0.53
1:A:264:SER:HB2	2:B:147:CYS:HA	1.91	0.53
1:E:543:ALA:O	1:E:546:THR:OG1	2.25	0.53
1:A:765:PRO:HA	1:A:771:HIS:NE2	2.23	0.53
4:D:4:LEU:HD23	4:D:24:ALA:HA	1.91	0.53
1:E:179:LEU:HB2	1:E:563:LYS:HD3	1.91	0.52
1:A:197:PHE:HD2	1:A:390:LEU:HD21	1.73	0.52
1:E:49:LYS:HZ3	1:E:68:TRP:HZ2	1.55	0.52
1:E:247:SER:H	1:E:414:ALA:HB2	1.75	0.52
1:A:220:LEU:HD11	1:A:234:ARG:HB3	1.90	0.52
2:B:134:ASP:O	4:D:28:THR:OG1	2.28	0.52
2:F:133:VAL:HG12	4:H:27:TYR:HB2	1.92	0.52
4:D:130:PRO:HD3	4:D:216:LYS:HD3	1.91	0.52
1:A:661:LEU:HB2	1:A:669:TYR:HB2	1.91	0.52
2:F:62:PRO:HB2	2:F:64:VAL:HG12	1.92	0.52
2:F:36:LYS:NZ	2:F:47:GLU:OE1	2.42	0.52
1:A:214:ILE:O	1:A:218:SER:OG	2.27	0.52
1:A:646:THR:HG21	1:A:700:LYS:HA	1.92	0.52
1:A:68:TRP:HD1	2:B:41:VAL:HB	1.75	0.51
3:C:212:ARG:NH2	4:D:224:ASP:H	2.09	0.51
1:E:143:THR:O	2:F:99:ASN:ND2	2.37	0.51
1:E:682:TYR:OH	1:E:784:GLY:O	2.19	0.51
2:B:40:ASP:HB2	2:B:43:LEU:HG	1.91	0.51
1:A:647:CYS:C	1:A:649:ASP:H	2.14	0.51
1:A:226:LEU:N	1:A:272:GLU:OE1	2.41	0.51
1:A:646:THR:OG1	1:A:678:ARG:NH2	2.41	0.51
1:E:393:ILE:HD11	1:E:428:ALA:HB2	1.91	0.51
1:E:661:LEU:HD21	1:E:743:ILE:HG21	1.93	0.51
1:A:725:LEU:HG	5:A:904:NAG:H83	1.92	0.50
1:A:500:ALA:O	1:A:504:GLN:HG3	2.12	0.50
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.93	0.50
1:E:195:ALA:HB2	1:E:209:PHE:CD1	2.46	0.50
1:A:305:TYR:OH	1:A:380:GLU:HG2	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:THR:HA	1:A:632:LYS:HB2	1.93	0.50
4:H:161:TRP:CZ3	4:H:203:CYS:HB3	2.47	0.50
1:E:269:LEU:O	1:E:365:TYR:OH	2.23	0.50
1:A:595:ALA:O	1:A:598:THR:OG1	2.24	0.50
3:G:91:LEU:HD21	4:H:106:VAL:HG22	1.93	0.50
1:E:147:VAL:O	2:F:139:SER:OG	2.30	0.49
1:E:620:PHE:HD2	1:E:621:LYS:HE2	1.77	0.49
1:A:121:PHE:HE2	1:A:383:ARG:HH12	1.60	0.49
2:B:144:GLU:O	2:B:157:ARG:NH2	2.43	0.49
1:A:651:ALA:HB1	1:A:656:GLU:HB2	1.94	0.49
1:A:686:ASP:OD1	1:A:686:ASP:N	2.35	0.49
3:C:48:ILE:HG22	3:C:50:ALA:O	2.11	0.49
1:A:147:VAL:O	2:B:139:SER:OG	2.29	0.49
1:E:340:LEU:HD13	1:E:399:GLN:HG3	1.95	0.49
1:A:260:SER:OG	1:A:272:GLU:OE2	2.30	0.49
4:H:155:GLU:HG2	4:H:183:TYR:CD1	2.48	0.49
1:A:74:HIS:ND1	1:A:97:PRO:HA	2.28	0.49
1:A:247:SER:H	1:A:414:ALA:HB2	1.78	0.48
1:A:180:PRO:HB2	1:A:337:ARG:HH12	1.77	0.48
1:E:651:ALA:HB1	1:E:656:GLU:HB2	1.95	0.48
4:H:166:LEU:HD13	4:H:189:VAL:HG21	1.96	0.48
1:A:344:HIS:CD2	1:A:403:LEU:HD21	2.48	0.48
1:E:68:TRP:CD1	2:F:41:VAL:HB	2.48	0.48
1:A:124:HIS:HB3	1:A:236:TRP:CG	2.49	0.48
4:D:9:ALA:HA	4:D:114:THR:HG23	1.96	0.48
1:E:256:VAL:HG13	1:E:383:ARG:HH11	1.78	0.48
4:D:129:PHE:HE2	4:D:150:LYS:HE2	1.79	0.48
4:H:6:GLN:HA	4:H:21:SER:O	2.14	0.48
1:E:347:ALA:O	1:E:351:THR:HG23	2.13	0.48
3:C:179:THR:HG22	3:C:181:THR:HG23	1.96	0.48
2:F:154:LEU:HG	2:F:154:LEU:H	1.35	0.48
1:E:226:LEU:HD13	1:E:262:LEU:HD11	1.96	0.47
4:D:7:SER:HA	4:D:8:GLY:HA2	1.58	0.47
1:A:146:LEU:HD23	1:A:150:THR:HG22	1.96	0.47
1:E:312:ARG:NH2	2:F:140:THR:O	2.47	0.47
1:A:80:VAL:HA	1:A:91:VAL:HG12	1.96	0.47
1:E:669:TYR:OH	1:E:781:PHE:O	2.21	0.47
3:G:119:PHE:HB3	4:H:131:LEU:HB3	1.95	0.47
3:G:138:ASN:ND2	3:G:139:ASN:OD1	2.47	0.47
1:A:318:PHE:CD1	1:A:322:ALA:HB3	2.49	0.47
1:E:329:TYR:CE2	1:E:370:ARG:HG2	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG22	1:A:410:ILE:HD13	1.97	0.47
1:E:506:LEU:HD21	1:E:574:PRO:HG3	1.95	0.47
4:D:6:GLN:NE2	4:D:93:TYR:O	2.37	0.47
4:D:162:ASN:O	4:D:204:ASN:ND2	2.47	0.47
3:G:114:PRO:HB3	3:G:140:PHE:HB3	1.97	0.47
1:E:546:THR:HA	1:E:592:LEU:HD13	1.97	0.47
3:G:32:PHE:HB3	3:G:91:LEU:HB3	1.96	0.47
1:E:260:SER:OG	1:E:272:GLU:OE2	2.33	0.47
2:B:156:GLN:HG2	2:B:158:VAL:HG23	1.96	0.47
4:H:162:ASN:HB2	4:H:165:ALA:HB3	1.97	0.47
3:C:148:GLN:HB2	3:C:196:GLU:HB3	1.97	0.47
1:E:497:ASN:OD1	1:E:498:LEU:N	2.45	0.47
1:A:425:LEU:HB2	1:A:428:ALA:HB3	1.97	0.46
1:E:351:THR:HG22	1:E:410:ILE:HD13	1.95	0.46
3:C:150:LYS:HG2	3:C:194:ALA:HB3	1.97	0.46
1:E:305:TYR:OH	1:E:380:GLU:HG2	2.15	0.46
4:D:6:GLN:HA	4:D:21:SER:O	2.14	0.46
1:A:582:ASP:HB3	1:A:658:VAL:CG1	2.45	0.46
1:A:238:THR:O	1:A:426:ILE:HG12	2.16	0.46
1:A:544:HIS:NE2	1:A:574:PRO:HD2	2.30	0.46
1:E:132:PHE:CE1	2:F:106:GLY:HA3	2.51	0.46
1:A:497:ASN:OD1	1:A:498:LEU:N	2.45	0.46
4:H:7:SER:HA	4:H:8:GLY:HA2	1.59	0.46
4:H:60:TYR:HE1	4:H:70:MET:HG3	1.80	0.46
3:G:79:GLN:HB2	3:G:82:ASP:OD1	2.16	0.46
1:A:347:ALA:O	1:A:351:THR:HG23	2.16	0.45
1:A:142:THR:OG1	2:B:154:LEU:HD13	2.16	0.45
4:D:130:PRO:HG3	4:D:216:LYS:HB3	1.98	0.45
1:A:216:THR:OG1	1:A:217:ASN:N	2.49	0.45
1:A:371:ILE:HD11	1:A:403:LEU:HB3	1.98	0.45
4:H:37:VAL:HG22	4:H:47:TRP:HA	1.98	0.45
3:G:120:PRO:HB3	3:G:210:PHE:CE1	2.50	0.45
1:E:382:GLY:HA3	1:E:388:PHE:CZ	2.51	0.45
1:E:75:VAL:HG23	1:E:98:LYS:NZ	2.31	0.45
1:E:400:LEU:HD12	1:E:400:LEU:HA	1.80	0.45
4:D:90:THR:HG23	4:D:117:THR:HA	1.98	0.45
3:C:109:ARG:HD2	3:C:109:ARG:H	1.81	0.45
1:E:75:VAL:HG23	1:E:98:LYS:HZ1	1.81	0.45
1:A:643:GLU:HA	1:A:646:THR:HG23	1.98	0.45
1:E:96:PHE:CG	2:F:124:LEU:HD11	2.52	0.45
1:E:100:LEU:HA	1:E:100:LEU:HD12	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:742:ASP:HB3	1:E:744:ILE:HD13	1.99	0.45
1:E:396:VAL:O	1:E:400:LEU:HB2	2.17	0.44
1:A:396:VAL:O	1:A:400:LEU:HB2	2.17	0.44
2:F:133:VAL:HG12	4:H:27:TYR:CB	2.48	0.44
1:A:582:ASP:HB3	1:A:658:VAL:HG13	1.97	0.44
1:A:409:ARG:NH2	1:A:628:THR:O	2.51	0.44
4:H:38:ARG:HH12	4:H:89:ASP:HA	1.82	0.44
1:E:70:ASN:OD1	1:E:71:ASP:N	2.51	0.44
1:E:54:TYR:HA	1:E:55:PRO:HD2	1.84	0.44
1:A:351:THR:HG21	1:A:629:TRP:CZ3	2.53	0.44
2:F:156:GLN:HG2	2:F:158:VAL:HG23	1.99	0.44
1:A:605:VAL:O	1:A:609:GLN:HG2	2.17	0.44
3:G:46:LEU:HD21	3:G:49:TYR:HB3	2.00	0.44
3:G:118:ILE:HD12	3:G:195:CYS:HB2	2.00	0.43
3:C:141:TYR:CG	3:C:142:PRO:HA	2.53	0.43
1:E:67:HIS:ND1	1:E:67:HIS:O	2.51	0.43
1:E:783:ASN:N	1:E:783:ASN:OD1	2.49	0.43
1:A:256:VAL:HG13	1:A:383:ARG:HH11	1.82	0.43
1:A:577:GLY:HA2	1:A:630:THR:HG21	2.00	0.43
2:B:154:LEU:HG	2:B:154:LEU:H	1.32	0.43
2:F:134:ASP:HA	4:H:27:TYR:HA	2.00	0.43
1:E:290:THR:HB	3:G:49:TYR:OH	2.19	0.43
4:H:9:ALA:HA	4:H:114:THR:HG23	2.00	0.43
1:A:550:LEU:HD12	1:A:550:LEU:HA	1.85	0.43
2:F:132:TRP:HB3	2:F:135:SER:OG	2.18	0.43
3:C:121:PRO:HG2	4:D:132:ALA:H	1.84	0.43
1:E:587:ILE:H	1:E:587:ILE:HD12	1.84	0.43
1:A:75:VAL:HG13	2:B:73:GLY:HA2	2.00	0.43
1:A:329:TYR:CE2	1:A:370:ARG:HG2	2.54	0.43
1:E:328:ALA:O	1:E:332:GLU:HG3	2.19	0.43
1:A:592:LEU:HD23	1:A:619:ALA:HB1	2.01	0.43
1:E:491:GLY:O	1:E:495:LYS:HG2	2.18	0.42
2:B:62:PRO:HB2	2:B:64:VAL:HG12	2.01	0.42
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.54	0.42
1:E:146:LEU:HD23	1:E:150:THR:HG22	2.00	0.42
1:A:581:THR:OG1	1:A:658:VAL:HA	2.19	0.42
1:A:713:VAL:HG22	1:A:787:VAL:HG11	2.00	0.42
1:A:560:ASN:HB3	1:A:564:HIS:ND1	2.35	0.42
1:A:102:SER:O	2:B:116:LYS:NZ	2.43	0.42
4:H:98:GLY:HA2	4:H:106:VAL:O	2.19	0.42
1:E:567:THR:OG1	1:E:569:PRO:HD2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:TRP:CZ3	4:D:203:CYS:HB3	2.54	0.42
1:E:142:THR:OG1	2:F:154:LEU:HD13	2.20	0.42
4:D:18:VAL:O	4:D:82:GLU:HA	2.19	0.42
1:E:80:VAL:HA	1:E:91:VAL:HG12	2.01	0.42
4:D:24:ALA:HB3	4:D:77:ASN:HB3	2.02	0.42
1:A:180:PRO:O	1:A:337:ARG:NH1	2.46	0.42
1:A:351:THR:HG21	1:A:629:TRP:HZ3	1.85	0.42
1:A:68:TRP:CZ3	1:A:93:LEU:HD22	2.54	0.42
1:A:485:ILE:HG23	1:A:539:MET:HE1	2.02	0.42
1:E:309:LEU:HD13	1:E:314:LEU:HD21	2.01	0.42
1:E:470:ARG:HD2	1:E:470:ARG:HA	1.90	0.42
1:A:154:PRO:HD3	1:A:312:ARG:NH2	2.35	0.42
1:E:60:GLU:HG3	1:E:61:GLU:N	2.35	0.42
1:E:659:LEU:HB3	1:E:671:ILE:HG13	2.01	0.42
1:E:332:GLU:OE2	1:E:370:ARG:NH2	2.53	0.42
1:E:425:LEU:HB2	1:E:428:ALA:HB3	2.01	0.42
1:E:569:PRO:HA	1:E:572:TYR:HB2	2.00	0.42
4:D:126:PRO:HD2	4:D:212:THR:HG21	2.02	0.42
1:E:344:HIS:CD2	1:E:403:LEU:HD21	2.55	0.42
1:A:231:TRP:HD1	1:A:283:ASN:HB3	1.85	0.42
4:D:173:PHE:HE1	4:D:188:VAL:HG22	1.85	0.42
1:A:550:LEU:HB3	1:A:599:ARG:NH1	2.34	0.42
1:E:593:LEU:HD21	1:E:616:PHE:HA	2.02	0.42
3:G:121:PRO:HG2	4:H:132:ALA:HB3	2.02	0.41
1:E:200:TRP:CE2	1:E:440:LEU:HD22	2.55	0.41
1:E:580:ARG:NH2	1:E:582:ASP:OD2	2.37	0.41
1:E:68:TRP:CZ3	1:E:93:LEU:HD13	2.55	0.41
2:B:78:THR:O	2:B:135:SER:HB3	2.20	0.41
1:A:76:PHE:CE1	2:B:73:GLY:HA3	2.54	0.41
3:C:163:SER:OG	4:D:173:PHE:HB3	2.21	0.41
3:G:139:ASN:HA	3:G:173:THR:HB	2.01	0.41
3:C:150:LYS:HD3	3:C:150:LYS:HA	1.86	0.41
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.55	0.41
1:A:241:VAL:HB	1:A:252:VAL:HB	2.03	0.41
1:A:432:GLN:O	1:A:436:GLU:HG3	2.20	0.41
1:E:295:ASN:HA	1:E:296:PRO:HD2	1.84	0.41
1:E:500:ALA:O	1:E:504:GLN:HG3	2.20	0.41
1:E:544:HIS:NE2	1:E:574:PRO:HD2	2.36	0.41
2:B:76:VAL:HG22	2:B:85:VAL:HG22	2.02	0.41
1:E:596:ILE:N	1:E:597:PRO:HD2	2.35	0.41
1:A:295:ASN:HA	1:A:296:PRO:HD2	1.87	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ARG:NH2	1:A:738:GLY:O	2.54	0.41
1:A:328:ALA:O	1:A:332:GLU:HG3	2.20	0.41
4:H:67:TRP:O	4:H:83:LEU:HD12	2.20	0.41
1:E:351:THR:HG21	1:E:629:TRP:CZ3	2.56	0.41
1:A:560:ASN:HA	1:A:561:PRO:HD2	1.91	0.41
1:A:369:ALA:O	1:A:373:THR:HG23	2.20	0.41
1:A:132:PHE:HB2	1:A:137:PHE:HA	2.03	0.41
1:A:75:VAL:HG23	1:A:98:LYS:NZ	2.33	0.41
1:A:393:ILE:HD12	1:A:393:ILE:HA	1.87	0.41
3:G:35:TRP:CZ3	3:G:88:CYS:HB3	2.56	0.41
1:E:74:HIS:ND1	1:E:97:PRO:HA	2.35	0.41
1:A:299:PRO:HD2	1:A:307:VAL:O	2.21	0.41
1:E:37:LEU:HD22	1:E:53:PHE:HB2	2.03	0.41
1:E:625:ILE:O	1:E:629:TRP:HB2	2.21	0.41
4:D:47:TRP:CZ2	4:D:49:GLY:HA2	2.55	0.41
1:A:538:SER:HB2	1:A:745:ILE:HG13	2.03	0.41
2:F:64:VAL:HG21	2:F:70:ALA:HB2	2.03	0.41
3:G:182:LEU:HA	3:G:182:LEU:HD23	1.92	0.41
1:E:231:TRP:HD1	1:E:283:ASN:HB3	1.86	0.41
4:H:19:LYS:HE2	4:H:82:GLU:OE2	2.21	0.41
1:A:38:LEU:HD13	2:B:123:ALA:HB1	2.02	0.41
1:A:763:ILE:HA	1:A:764:PRO:HD2	1.97	0.41
1:A:318:PHE:HB3	1:A:320:LYS:O	2.21	0.41
3:G:120:PRO:HD2	3:G:121:PRO:HD3	2.02	0.41
1:A:200:TRP:CE2	1:A:440:LEU:HD22	2.56	0.41
1:E:216:THR:OG1	1:E:217:ASN:N	2.53	0.41
4:H:177:LEU:H	4:H:177:LEU:HD12	1.86	0.41
1:A:583:LEU:HA	1:A:583:LEU:HD13	1.74	0.41
3:C:143:ARG:NH2	3:C:164:VAL:HG21	2.37	0.40
3:C:146:LYS:HA	3:C:146:LYS:HD2	1.87	0.40
1:E:478:LEU:O	1:E:482:ARG:HG3	2.22	0.40
1:E:130:VAL:HG21	2:F:113:GLU:OE2	2.21	0.40
2:F:153:ARG:HH11	2:F:153:ARG:HB3	1.86	0.40
1:E:39:ARG:O	1:E:93:LEU:N	2.52	0.40
1:E:121:PHE:HE2	1:E:383:ARG:HH12	1.69	0.40
1:E:152:PHE:CZ	1:E:229:SER:HB2	2.56	0.40
1:E:418:THR:HB	2:F:160:GLN:NE2	2.36	0.40
1:A:430:PRO:HB3	1:A:468:LEU:HD12	2.04	0.40
4:D:24:ALA:O	4:D:25:SER:OG	2.38	0.40
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.56	0.40
4:H:173:PHE:HA	4:H:174:PRO:HD3	1.98	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:LEU:HD12	1:E:179:LEU:HA	1.86	0.40
1:A:601:GLY:O	1:A:605:VAL:HG23	2.21	0.40
2:F:136:THR:HA	2:F:137:PRO:HD3	1.88	0.40
3:G:124:GLU:OE1	3:G:124:GLU:N	2.52	0.40
3:G:122:SER:HB3	3:G:125:GLN:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	721/833 (87%)	687 (95%)	34 (5%)	0	100	100
1	E	691/833 (83%)	660 (96%)	31 (4%)	0	100	100
2	B	130/138 (94%)	119 (92%)	10 (8%)	1 (1%)	24	67
2	F	128/138 (93%)	115 (90%)	13 (10%)	0	100	100
3	C	203/215 (94%)	196 (97%)	7 (3%)	0	100	100
3	G	190/215 (88%)	182 (96%)	8 (4%)	0	100	100
4	D	201/282 (71%)	192 (96%)	9 (4%)	0	100	100
4	H	200/282 (71%)	192 (96%)	8 (4%)	0	100	100
All	All	2464/2936 (84%)	2343 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	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	604/717 (84%)	568 (94%)	36 (6%)	24	63
1	E	591/717 (82%)	564 (95%)	27 (5%)	33	73
2	B	111/121 (92%)	104 (94%)	7 (6%)	22	61
2	F	111/121 (92%)	105 (95%)	6 (5%)	27	67
3	C	176/187 (94%)	170 (97%)	6 (3%)	44	80
3	G	165/187 (88%)	159 (96%)	6 (4%)	42	78
4	D	173/233 (74%)	164 (95%)	9 (5%)	29	68
4	H	172/233 (74%)	167 (97%)	5 (3%)	50	83
All	All	2103/2516 (84%)	2001 (95%)	102 (5%)	31	71

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	53	PHE
1	A	54	TYR
1	A	93	LEU
1	A	94	VAL
1	A	98	LYS
1	A	99	TYR
1	A	100	LEU
1	A	123	SER
1	A	134	ASP
1	A	197	PHE
1	A	229	SER
1	A	288	ASP
1	A	309	LEU
1	A	385	THR
1	A	398	TYR
1	A	440	LEU
1	A	456	ASP
1	A	496	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	512	ILE
1	A	516	PHE
1	A	534	LEU
1	A	550	LEU
1	A	567	THR
1	A	571	VAL
1	A	576	MET
1	A	583	LEU
1	A	621	LYS
1	A	622	THR
1	A	632	LYS
1	A	643	GLU
1	A	664	VAL
1	A	674	ASN
1	A	678	ARG
1	A	701	ASP
1	A	788	THR
2	B	44	ILE
2	B	46	THR
2	B	114	GLU
2	B	116	LYS
2	B	152	ASP
2	B	154	LEU
2	B	157	ARG
3	C	22	THR
3	C	31	ASN
3	C	72	THR
3	C	91	LEU
3	C	109	ARG
3	C	176	LEU
4	D	30	ILE
4	D	34	LEU
4	D	72	ARG
4	D	102	MET
4	D	107	MET
4	D	177	LEU
4	D	201	TYR
4	D	206	ASN
4	D	216	LYS
1	E	50	LEU
1	E	67	HIS
1	E	94	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	98	LYS
1	E	100	LEU
1	E	123	SER
1	E	134	ASP
1	E	197	PHE
1	E	199	THR
1	E	288	ASP
1	E	309	LEU
1	E	334	LEU
1	E	358	ASP
1	E	385	THR
1	E	391	ASP
1	E	398	TYR
1	E	440	LEU
1	E	496	GLN
1	E	516	PHE
1	E	534	LEU
1	E	550	LEU
1	E	621	LYS
1	E	630	THR
1	E	632	LYS
1	E	643	GLU
1	E	678	ARG
1	E	711	GLU
2	F	44	ILE
2	F	47	GLU
2	F	132	TRP
2	F	153	ARG
2	F	154	LEU
2	F	157	ARG
3	G	22	THR
3	G	31	ASN
3	G	72	THR
3	G	91	LEU
3	G	148	GLN
3	G	176	LEU
4	H	30	ILE
4	H	34	LEU
4	H	72	ARG
4	H	102	MET
4	H	190	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 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 ⓘ

20 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	901	1	14,14,15	0.46	0	15,19,21	0.83	0
5	NAG	A	902	1	14,14,15	0.46	0	15,19,21	1.13	1 (6%)
5	NAG	A	903	1,5	14,14,15	0.57	0	15,19,21	0.89	0
5	NAG	A	904	5,6	14,14,15	0.43	0	15,19,21	0.97	0
6	BMA	A	905	5	11,11,12	0.71	0	14,15,17	0.67	0
5	NAG	B	800	2,5	14,14,15	0.94	1 (7%)	15,19,21	0.96	2 (13%)
5	NAG	B	801	5,6	14,14,15	0.55	0	15,19,21	0.71	0
6	BMA	B	802	5,7	11,11,12	1.01	1 (9%)	14,15,17	1.39	2 (14%)
7	MAN	B	803	6	11,11,12	0.67	0	14,15,17	0.94	1 (7%)
7	MAN	B	804	6	11,11,12	0.63	0	14,15,17	0.58	0
5	NAG	E	901	1,5	14,14,15	0.64	0	15,19,21	0.99	0
5	NAG	E	902	5	14,14,15	0.58	0	15,19,21	0.90	1 (6%)
5	NAG	E	903	1,5	14,14,15	0.45	0	15,19,21	0.91	1 (6%)
5	NAG	E	904	5	14,14,15	0.58	0	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	905	1	14,14,15	0.29	0	15,19,21	0.77	1 (6%)
5	NAG	F	800	2,5	14,14,15	0.51	0	15,19,21	0.79	0
5	NAG	F	801	5,6	14,14,15	0.57	0	15,19,21	0.94	1 (6%)
6	BMA	F	802	5,7	11,11,12	1.20	0	14,15,17	1.01	1 (7%)
7	MAN	F	803	6	11,11,12	0.58	0	14,15,17	1.01	1 (7%)
7	MAN	F	804	6	11,11,12	0.50	0	14,15,17	1.03	1 (7%)

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	901	1	-	0/6/23/26	0/1/1/1
5	NAG	A	902	1	-	0/6/23/26	0/1/1/1
5	NAG	A	903	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	904	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	905	5	-	0/2/19/22	0/1/1/1
5	NAG	B	800	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	801	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	802	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	803	6	-	0/2/19/22	0/1/1/1
7	MAN	B	804	6	-	0/2/19/22	0/1/1/1
5	NAG	E	901	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	902	5	-	0/6/23/26	0/1/1/1
5	NAG	E	903	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	904	5	-	0/6/23/26	0/1/1/1
5	NAG	E	905	1	-	0/6/23/26	0/1/1/1
5	NAG	F	800	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	801	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	802	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	803	6	-	0/2/19/22	0/1/1/1
7	MAN	F	804	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	800	NAG	O5-C1	-3.21	1.38	1.43
6	B	802	BMA	O5-C1	-2.31	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	803	MAN	O5-C1-C2	-2.21	107.28	110.86
5	B	800	NAG	O4-C4-C5	-2.16	103.52	109.24
5	B	800	NAG	C1-O5-C5	2.02	114.81	112.25
6	F	802	BMA	C3-C4-C5	2.15	113.95	110.20
7	F	803	MAN	C1-O5-C5	2.20	115.03	112.25
5	E	903	NAG	C1-O5-C5	2.28	115.14	112.25
5	E	902	NAG	C1-O5-C5	2.37	115.25	112.25
5	F	801	NAG	C4-C3-C2	2.56	115.21	111.23
5	E	905	NAG	C1-O5-C5	2.58	115.53	112.25
6	B	802	BMA	C1-C2-C3	2.63	112.66	109.54
6	B	802	BMA	C2-C3-C4	2.66	115.57	111.04
7	F	804	MAN	C1-O5-C5	3.08	116.16	112.25
5	A	902	NAG	C1-O5-C5	3.24	116.36	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	NAG	1	0
5	B	800	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, 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	729/833 (87%)	0.21	9 (1%) 81 69	25, 58, 145, 178	0
1	E	705/833 (84%)	0.35	38 (5%) 29 15	55, 112, 159, 213	0
2	B	132/138 (95%)	0.18	4 (3%) 54 37	53, 94, 138, 198	0
2	F	130/138 (94%)	0.07	3 (2%) 64 47	67, 93, 118, 140	0
3	C	207/215 (96%)	0.71	28 (13%) 4 2	52, 99, 201, 212	0
3	G	196/215 (91%)	0.63	26 (13%) 4 2	58, 94, 211, 221	0
4	D	207/282 (73%)	0.42	21 (10%) 9 4	52, 116, 184, 201	0
4	H	206/282 (73%)	0.55	24 (11%) 6 3	68, 126, 196, 205	0
All	All	2512/2936 (85%)	0.36	153 (6%) 25 12	25, 96, 182, 221	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	120	PRO	12.4
3	C	119	PHE	11.4
3	G	136	LEU	9.8
4	D	145	LEU	8.6
3	G	117	PHE	8.1
3	G	145	ALA	7.7
4	D	133	PRO	7.5
4	D	130	PRO	7.4
3	G	116	VAL	7.1
3	C	118	ILE	7.0
4	D	131	LEU	6.9
1	E	68	TRP	6.8
3	C	152	ASP	6.8
3	G	197	VAL	6.6
3	C	156	GLN	6.3
3	C	149	TRP	6.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	H	192	PRO	6.3
3	G	135	CYS	6.1
4	H	145	LEU	5.8
4	H	166	LEU	5.7
3	C	132	SER	5.7
4	D	132	ALA	5.7
3	G	198	THR	5.6
1	E	174	PHE	5.6
4	D	144	ALA	5.5
3	G	208	LYS	5.4
1	E	50	LEU	5.4
4	D	148	LEU	5.3
3	C	133	VAL	5.2
1	E	314	LEU	5.2
4	H	191	VAL	4.9
3	C	134	VAL	4.7
4	D	129	PHE	4.7
1	E	49	LYS	4.7
4	H	128	VAL	4.7
3	C	136	LEU	4.7
3	G	121	PRO	4.6
3	G	195	CYS	4.5
3	G	118	ILE	4.4
3	G	132	SER	4.4
3	G	137	LEU	4.4
1	A	41	TYR	4.2
4	H	127	SER	4.2
1	A	101	LEU	4.2
3	C	127	LYS	4.0
3	C	184	LYS	3.9
3	C	155	LEU	3.9
1	E	653	ARG	3.8
4	D	128	VAL	3.8
3	G	120	PRO	3.8
1	E	89	GLY	3.8
4	H	214	VAL	3.8
3	C	209	SER	3.7
4	H	148	LEU	3.6
3	C	151	VAL	3.6
3	C	117	PHE	3.6
1	E	358	ASP	3.6
4	H	165	ALA	3.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	121	PRO	3.6
4	D	201	TYR	3.5
4	H	149	VAL	3.5
2	F	45	ILE	3.4
3	C	135	CYS	3.4
4	H	124	LYS	3.4
4	H	190	THR	3.3
3	G	182	LEU	3.3
1	E	462	LEU	3.3
3	G	122	SER	3.3
4	H	159	VAL	3.2
1	E	85	THR	3.2
1	E	468	LEU	3.2
3	G	178	SER	3.2
3	C	116	VAL	3.1
3	C	194	ALA	3.1
1	E	579	LEU	3.1
4	H	185	LEU	3.1
3	C	210	PHE	3.0
4	D	149	VAL	3.0
4	D	214	VAL	3.0
4	H	223	CYS	3.0
4	D	146	GLY	3.0
1	E	779	LEU	2.9
4	H	126	PRO	2.9
3	G	115	SER	2.9
1	A	100	LEU	2.9
3	G	206	VAL	2.9
3	G	147	VAL	2.9
1	E	789	LEU	2.9
4	H	85	LEU	2.9
1	E	65	SER	2.8
4	D	189	VAL	2.8
3	C	131	ALA	2.8
3	C	180	LEU	2.7
3	C	159	ASN	2.7
4	D	85	LEU	2.7
1	E	713	VAL	2.7
4	H	205	VAL	2.7
1	A	53	PHE	2.6
4	H	219	GLU	2.6
3	C	208	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	H	2	VAL	2.6
1	E	59	ASP	2.6
1	E	743	ILE	2.6
3	G	209	SER	2.6
1	E	760	ASN	2.6
3	G	114	PRO	2.6
1	A	68	TRP	2.5
4	D	166	LEU	2.5
1	E	41	TYR	2.4
3	C	157	SER	2.4
1	E	194	LYS	2.4
2	F	33	PHE	2.4
2	B	41	VAL	2.4
1	E	410	ILE	2.4
4	D	186	SER	2.3
4	D	187	SER	2.3
1	E	43	ASP	2.3
4	H	220	PRO	2.3
4	H	181	GLY	2.3
3	G	103	LYS	2.3
3	G	179	THR	2.3
1	E	731	PHE	2.3
1	E	512	ILE	2.2
1	E	709	VAL	2.2
3	C	207	THR	2.2
4	D	206	ASN	2.2
3	G	202	LEU	2.2
2	F	148	VAL	2.2
1	E	559	LEU	2.2
1	A	470	ARG	2.2
1	A	96	PHE	2.2
1	E	198	ALA	2.2
1	E	348	LEU	2.2
2	B	48	PRO	2.2
4	D	64	PHE	2.2
1	E	179	LEU	2.1
4	D	218	VAL	2.1
1	E	766	PHE	2.1
3	C	115	SER	2.1
1	A	512	ILE	2.1
1	E	394	VAL	2.1
1	A	203	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	492	LEU	2.1
1	E	486	MET	2.1
1	E	552	ILE	2.1
1	E	637	LEU	2.1
4	H	188	VAL	2.1
4	H	150	LYS	2.0
3	G	127	LYS	2.0
1	E	764	PRO	2.0
2	B	44	ILE	2.0
1	E	732	LEU	2.0
2	B	76	VAL	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
5	NAG	B	800	14/15	0.88	0.26	0.33	181,206,217,218	0
5	NAG	E	903	14/15	0.76	0.22	0.29	139,150,156,157	0
5	NAG	A	902	14/15	0.83	0.21	-0.41	20,63,79,79	0
5	NAG	F	800	14/15	0.93	0.13	-0.93	95,104,111,111	0
5	NAG	A	903	14/15	0.97	0.16	-	78,95,114,115	0
5	NAG	F	801	14/15	0.90	0.24	-	86,112,133,133	0
7	MAN	B	803	11/12	0.88	0.15	-	140,150,161,166	0
6	BMA	F	802	11/12	0.88	0.12	-	118,127,138,151	0
5	NAG	E	905	14/15	0.64	0.35	-	197,219,232,234	0
5	NAG	E	901	14/15	0.82	0.22	-	125,141,149,152	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MAN	B	804	11/12	0.71	0.24	-	138,153,163,169	0
7	MAN	F	804	11/12	0.89	0.17	-	101,131,141,149	0
5	NAG	A	901	14/15	0.83	0.20	-	125,133,142,148	0
5	NAG	E	902	14/15	0.85	0.23	-	133,145,153,157	0
6	BMA	B	802	11/12	0.80	0.14	-	131,144,153,158	0
7	MAN	F	803	11/12	0.93	0.09	-	120,138,144,146	0
5	NAG	A	904	14/15	0.85	0.29	-	104,130,144,148	0
6	BMA	A	905	11/12	0.80	0.20	-	136,150,161,163	0
5	NAG	E	904	14/15	0.85	0.23	-	132,150,160,160	0
5	NAG	B	801	14/15	0.94	0.15	-	119,134,149,160	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.