



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:23 PM GMT

PDB ID : 5C7K  
Title : Crystal structure BG505 SOSIP gp140 HIV-1 Env trimer bound to broadly neutralizing antibodies PGT128 and 8ANC195  
Authors : Kong, L.; Stanfield, R.L.; Wilson, I.A.  
Deposited on : 2015-06-24  
Resolution : 4.60 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

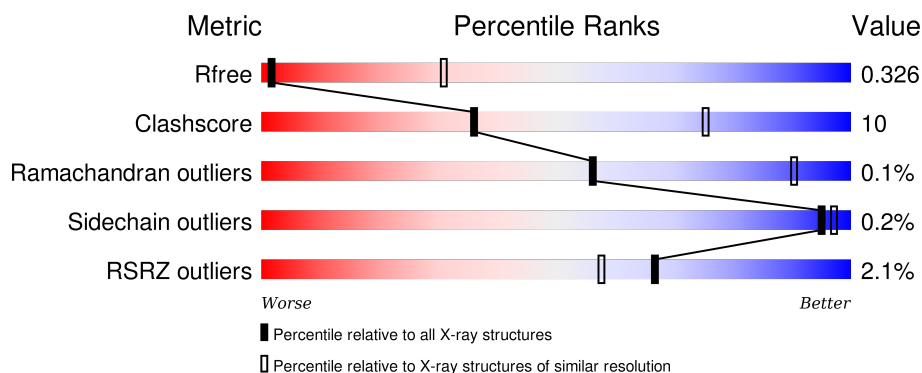
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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  $\geq 3$ , 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	239	<div> <div>5%</div> <div>72% 25%</div> </div>
2	B	211	<div> <div>6%</div> <div>73% 23%</div> </div>
3	C	487	<div> <div>%</div> <div>69% 23% 8%</div> </div>
4	D	153	<div> <div>61% 19% 20%</div> </div>
5	E	238	<div> <div>%</div> <div>73% 21% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	215	 79%20%

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
7	NAG	C	601	-	-	-	X
7	NAG	C	605	-	-	-	X
7	NAG	C	621	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12092 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 Antibody Fab PGT128 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1735	1105	292	332	6			

- Molecule 2 is a protein called Antibody Fab PGT128 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1514	950	254	306	4			

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	450	Total	C	N	O	S	0	0	0
			3544	2224	628	664	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	508	SER	ARG	engineered mutation	UNP Q2N0S6
C	511	SER	-	expression tag	UNP Q2N0S6
C	512	GLY	-	expression tag	UNP Q2N0S6
C	513	HIS	-	expression tag	UNP Q2N0S6
C	514	HIS	-	expression tag	UNP Q2N0S6
C	515	HIS	-	expression tag	UNP Q2N0S6
C	516	HIS	-	expression tag	UNP Q2N0S6
C	517	HIS	-	expression tag	UNP Q2N0S6
C	518	HIS	-	expression tag	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	122	Total	C	N	O	S	0	0	0
			978	618	169	185	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	559	PRO	ILE	engineered mutation	UNP Q2N0S6
D	605	CYS	THR	engineered mutation	UNP Q2N0S6

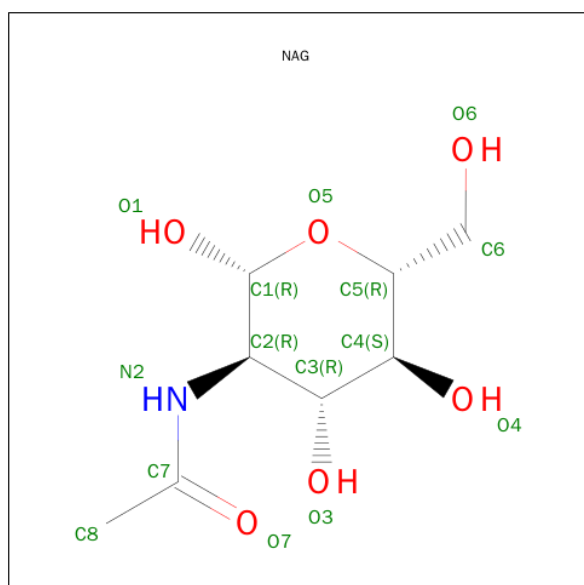
- Molecule 5 is a protein called Antibody Fab 8ANC195 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	224	Total	C	N	O	S	0	0	0
			1686	1072	284	325	5			

- Molecule 6 is a protein called Antibody Fab 8ANC195 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	212	Total	C	N	O	S	0	0	0
			1626	1018	279	324	5			

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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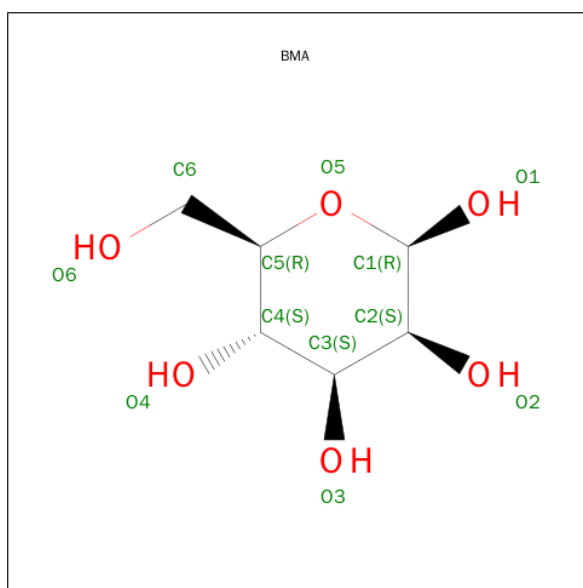
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1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

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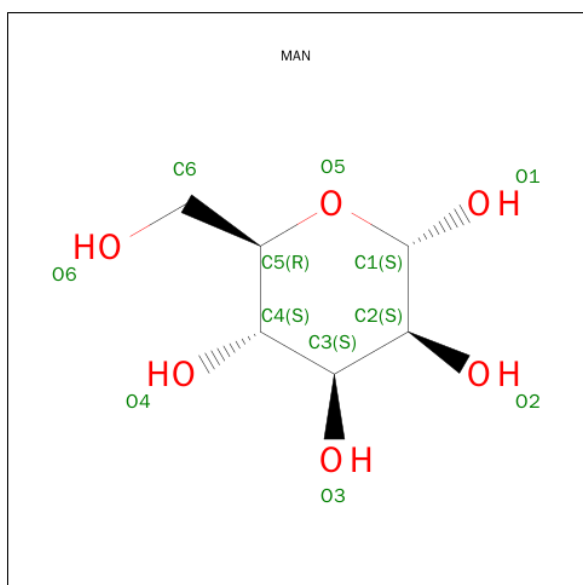
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1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

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 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
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		

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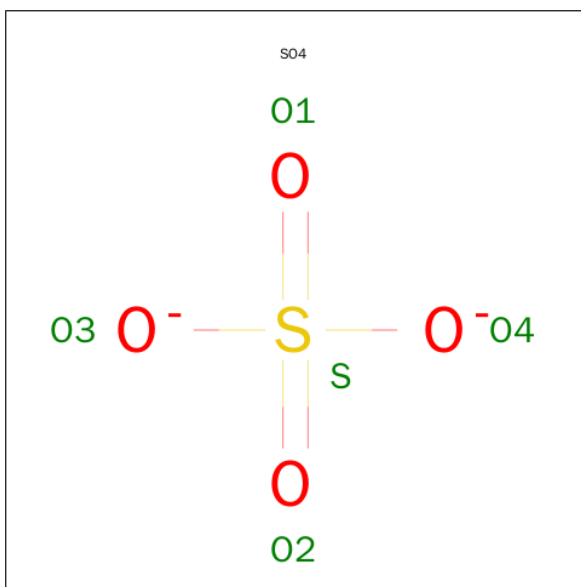
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

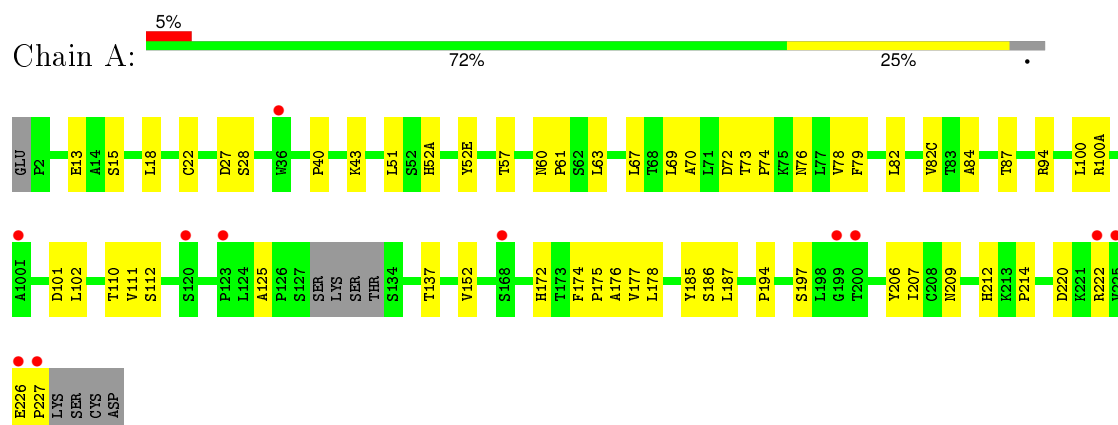


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

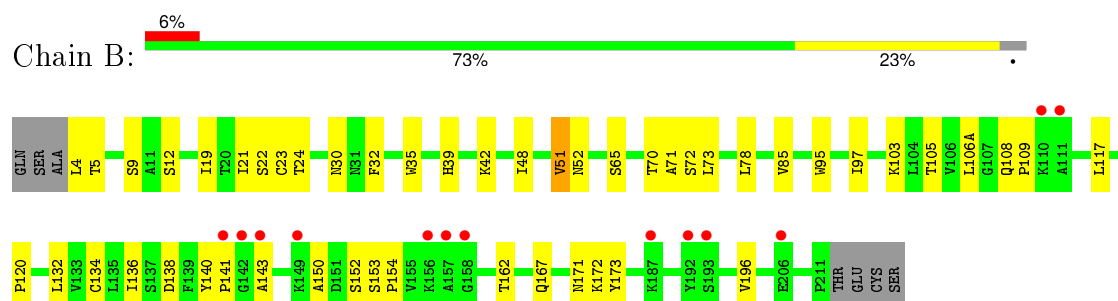
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

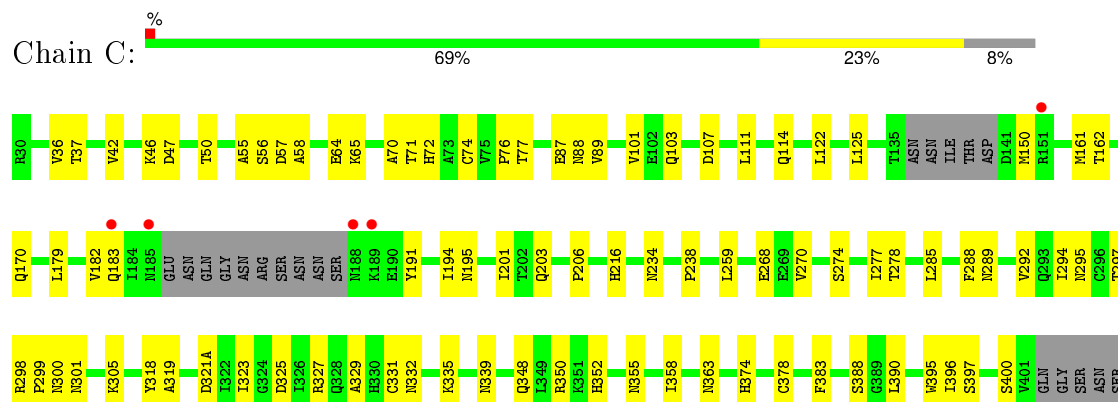
#### • Molecule 1: Antibody Fab PGT128 heavy chain

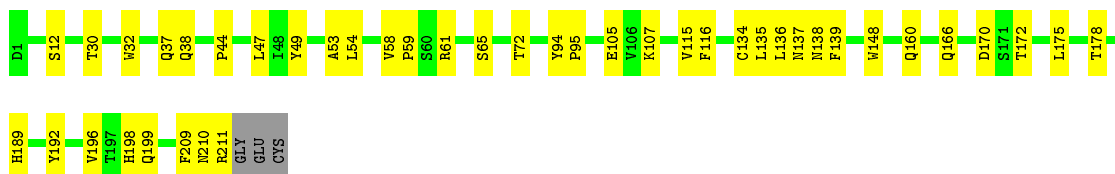
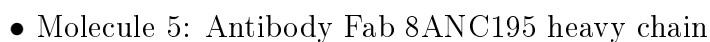


#### • Molecule 2: Antibody Fab PGT128 light chain



#### • Molecule 3: Envelope glycoprotein gp120





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.13Å 261.13Å 261.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.68 – 4.60 47.68 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.68-4.60) 99.8 (47.68-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.289 , 0.295 0.324 , 0.326	Depositor DCC
$R_{free}$ test set	1637 reflections (10.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	157.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 113.6	EDS
Estimated twinning fraction	0.046 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 16539 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	12092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.23	0/1786	0.44	0/2449
2	B	0.23	0/1552	0.53	1/2121 (0.0%)
3	C	0.25	0/3617	0.48	0/4908
4	D	0.26	0/995	0.51	0/1349
5	E	0.24	0/1730	0.45	0/2361
6	F	0.24	0/1661	0.45	0/2256
All	All	0.24	0/11341	0.48	1/15444 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	GLN	C-N-CD	-11.29	95.77	120.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1690	38	0
2	B	1514	0	1473	31	0
3	C	3544	0	3480	84	0
4	D	978	0	959	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1686	0	1658	36	0
6	F	1626	0	1581	27	0
7	C	392	0	344	16	0
7	D	56	0	50	3	0
7	E	28	0	24	0	0
8	C	88	0	71	0	0
8	D	11	0	8	2	0
8	E	11	0	8	0	0
9	C	275	0	234	5	0
9	D	55	0	47	0	0
9	E	88	0	72	1	0
10	C	5	0	0	0	0
All	All	12092	0	11699	229	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 10.

The worst 5 of 229 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)
5:E:61:HIS:HA	5:E:64:ARG:HG3	1.59	0.84
3:C:502:LYS:HG2	3:C:503:ARG:H	1.45	0.81
7:C:610:NAG:H61	7:C:611:NAG:HN2	1.45	0.81
3:C:396:ILE:HG22	3:C:397:SER:H	1.50	0.76
3:C:58:ALA:HB2	3:C:76:PRO:HB3	1.70	0.74

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	226/239 (95%)	212 (94%)	14 (6%)	0	100	100
2	B	202/211 (96%)	193 (96%)	7 (4%)	2 (1%)	19	65
3	C	442/487 (91%)	418 (95%)	24 (5%)	0	100	100
4	D	118/153 (77%)	110 (93%)	8 (7%)	0	100	100
5	E	218/238 (92%)	210 (96%)	8 (4%)	0	100	100
6	F	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
All	All	1416/1543 (92%)	1348 (95%)	66 (5%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	109	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	194/203 (96%)	194 (100%)	0	100	100
2	B	171/177 (97%)	171 (100%)	0	100	100
3	C	401/433 (93%)	399 (100%)	2 (0%)	92	96
4	D	106/129 (82%)	106 (100%)	0	100	100
5	E	192/204 (94%)	192 (100%)	0	100	100
6	F	180/182 (99%)	180 (100%)	0	100	100
All	All	1244/1328 (94%)	1242 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	234	ASN
3	C	339	ASN

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

Mol	Chain	Res	Type
3	C	195	ASN
4	D	575	GLN
5	E	39	GLN
6	F	38	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](#)

83 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	$\# Z  > 2$
7	NAG	C	601	3	14,14,15	0.34	0	15,19,21	0.54	0
7	NAG	C	602	3,7	14,14,15	0.28	0	15,19,21	0.54	0
7	NAG	C	603	7	14,14,15	0.19	0	15,19,21	0.28	0
7	NAG	C	604	3	14,14,15	0.28	0	15,19,21	0.37	0
7	NAG	C	605	3,7	14,14,15	0.23	0	15,19,21	0.33	0
7	NAG	C	606	7	14,14,15	0.24	0	15,19,21	0.32	0
7	NAG	C	607	3	14,14,15	0.34	0	15,19,21	0.47	0
7	NAG	C	608	3,7	14,14,15	0.21	0	15,19,21	1.04	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	C	609	7	14,14,15	0.23	0	15,19,21	0.27	0
7	NAG	C	610	3,7	14,14,15	0.27	0	15,19,21	0.45	0
7	NAG	C	611	7	14,14,15	0.27	0	15,19,21	0.23	0
7	NAG	C	612	3,7	14,14,15	0.59	0	15,19,21	0.42	0
7	NAG	C	613	8,7	14,14,15	0.56	0	15,19,21	0.44	0
8	BMA	C	614	9,7	11,11,12	0.53	0	15,15,17	0.71	0
9	MAN	C	615	9,8	11,11,12	0.67	0	15,15,17	1.06	1 (6%)
9	MAN	C	616	9	11,11,12	0.55	0	15,15,17	1.00	1 (6%)
9	MAN	C	617	9	11,11,12	0.52	0	15,15,17	1.07	2 (13%)
9	MAN	C	618	9,8	11,11,12	0.86	0	15,15,17	0.90	1 (6%)
9	MAN	C	619	9	11,11,12	0.76	1 (9%)	15,15,17	1.40	2 (13%)
9	MAN	C	620	9	11,11,12	0.62	0	15,15,17	1.00	2 (13%)
7	NAG	C	621	3	14,14,15	0.34	0	15,19,21	0.25	0
7	NAG	C	622	3,7	14,14,15	0.24	0	15,19,21	0.38	0
7	NAG	C	623	8,7	14,14,15	0.23	0	15,19,21	0.28	0
9	MAN	C	624	9	11,11,12	0.65	0	15,15,17	1.22	2 (13%)
9	MAN	C	625	9	11,11,12	0.67	0	15,15,17	0.89	1 (6%)
8	BMA	C	626	9,7	11,11,12	0.79	0	15,15,17	0.88	0
9	MAN	C	627	9,8	11,11,12	0.70	0	15,15,17	1.11	2 (13%)
9	MAN	C	628	9,8	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
9	MAN	C	629	9	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
9	MAN	C	630	9	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
9	MAN	C	631	9	11,11,12	0.78	0	15,15,17	0.95	1 (6%)
7	NAG	C	632	3,7	14,14,15	0.51	0	15,19,21	0.56	0
7	NAG	C	633	8,7	14,14,15	0.18	0	15,19,21	0.66	0
8	BMA	C	634	9,7	11,11,12	0.82	0	15,15,17	1.07	0
9	MAN	C	635	9,8	11,11,12	0.69	0	15,15,17	0.94	2 (13%)
9	MAN	C	636	9	11,11,12	0.65	0	15,15,17	0.95	1 (6%)
9	MAN	C	637	9	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
9	MAN	C	638	9,8	11,11,12	0.75	0	15,15,17	1.29	2 (13%)
9	MAN	C	639	9	11,11,12	0.57	0	15,15,17	1.09	2 (13%)
9	MAN	C	640	9	11,11,12	0.57	0	15,15,17	1.11	2 (13%)
7	NAG	C	641	3,7	14,14,15	0.29	0	15,19,21	0.42	0
7	NAG	C	642	8,7	14,14,15	0.39	0	15,19,21	0.45	0
8	BMA	C	643	9,7	11,11,12	0.64	0	15,15,17	1.00	1 (6%)
9	MAN	C	644	8	11,11,12	0.72	1 (9%)	15,15,17	1.15	2 (13%)
9	MAN	C	645	9,8	11,11,12	0.66	0	15,15,17	1.27	1 (6%)
9	MAN	C	646	9	11,11,12	0.50	0	15,15,17	1.11	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	C	647	9	11,11,12	0.62	0	15,15,17	1.23	2 (13%)
7	NAG	C	648	3,7	14,14,15	0.47	0	15,19,21	0.37	0
7	NAG	C	649	8,7	14,14,15	0.24	0	15,19,21	0.55	0
8	BMA	C	650	9,7	11,11,12	0.65	0	15,15,17	1.25	1 (6%)
9	MAN	C	651	9,8	11,11,12	0.59	0	15,15,17	1.30	2 (13%)
9	MAN	C	652	9	11,11,12	0.22	0	15,15,17	0.52	0
7	NAG	C	653	3,7	14,14,15	0.40	0	15,19,21	0.29	0
7	NAG	C	654	8,7	14,14,15	0.26	0	15,19,21	0.59	0
8	BMA	C	655	7	11,11,12	0.62	0	15,15,17	0.77	0
10	SO4	C	656	3	4,4,4	0.24	0	6,6,6	0.06	0
7	NAG	C	657	3,7	14,14,15	0.31	0	15,19,21	0.43	0
7	NAG	C	658	8,7	14,14,15	0.37	0	15,19,21	0.59	0
8	BMA	C	659	7	11,11,12	0.64	0	15,15,17	0.78	0
7	NAG	C	660	3,7	14,14,15	0.29	0	15,19,21	0.65	0
7	NAG	C	661	8,7	14,14,15	0.22	0	15,19,21	0.63	1 (6%)
8	BMA	C	662	7	11,11,12	0.61	0	15,15,17	0.74	0
7	NAG	D	701	4,7	14,14,15	0.23	0	15,19,21	0.32	0
7	NAG	D	702	8,7	14,14,15	0.40	0	15,19,21	1.43	2 (13%)
8	BMA	D	703	9,7	11,11,12	0.72	0	15,15,17	1.01	0
9	MAN	D	704	9,8	11,11,12	1.54	3 (27%)	15,15,17	1.33	2 (13%)
9	MAN	D	705	9	11,11,12	0.58	0	15,15,17	0.96	2 (13%)
9	MAN	D	706	9	11,11,12	0.61	0	15,15,17	0.96	1 (6%)
9	MAN	D	707	9	11,11,12	0.63	0	15,15,17	1.15	2 (13%)
9	MAN	D	708	8	11,11,12	0.57	0	15,15,17	1.05	2 (13%)
7	NAG	D	709	4	14,14,15	0.21	0	15,19,21	0.32	0
7	NAG	D	710	4	14,14,15	0.31	0	15,19,21	0.57	0
7	NAG	E	301	3,7	14,14,15	0.18	0	15,19,21	0.28	0
7	NAG	E	302	8,7	14,14,15	0.37	0	15,19,21	0.38	0
8	BMA	E	303	9,7	11,11,12	0.50	0	15,15,17	0.70	0
9	MAN	E	304	9,8	11,11,12	0.48	0	15,15,17	1.07	2 (13%)
9	MAN	E	305	9	11,11,12	0.72	0	15,15,17	1.07	0
9	MAN	E	306	9	11,11,12	0.53	0	15,15,17	0.97	2 (13%)
9	MAN	E	307	9,8	11,11,12	0.56	0	15,15,17	1.13	2 (13%)
9	MAN	E	308	9	11,11,12	0.61	0	15,15,17	1.16	2 (13%)
9	MAN	E	309	9	11,11,12	0.81	0	15,15,17	1.41	3 (20%)
9	MAN	E	310	9,5	11,11,12	0.64	0	15,15,17	0.94	2 (13%)
9	MAN	E	311	9	11,11,12	0.56	0	15,15,17	1.01	2 (13%)

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
7	NAG	C	601	3	-	0/6/23/26	0/1/1/1
7	NAG	C	602	3,7	-	1/6/23/26	0/1/1/1
7	NAG	C	603	7	-	0/6/23/26	0/1/1/1
7	NAG	C	604	3	-	0/6/23/26	0/1/1/1
7	NAG	C	605	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	606	7	-	0/6/23/26	0/1/1/1
7	NAG	C	607	3	-	0/6/23/26	0/1/1/1
7	NAG	C	608	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	609	7	-	0/6/23/26	0/1/1/1
7	NAG	C	610	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	611	7	-	0/6/23/26	0/1/1/1
7	NAG	C	612	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	613	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	614	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	615	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	616	9	-	0/2/19/22	0/1/1/1
9	MAN	C	617	9	-	0/2/19/22	0/1/1/1
9	MAN	C	618	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	619	9	-	0/2/19/22	0/1/1/1
9	MAN	C	620	9	-	0/2/19/22	0/1/1/1
7	NAG	C	621	3	-	0/6/23/26	0/1/1/1
7	NAG	C	622	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	623	8,7	-	0/6/23/26	0/1/1/1
9	MAN	C	624	9	-	0/2/19/22	0/1/1/1
9	MAN	C	625	9	-	0/2/19/22	0/1/1/1
8	BMA	C	626	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	627	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	628	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	629	9	-	0/2/19/22	0/1/1/1
9	MAN	C	630	9	-	0/2/19/22	0/1/1/1
9	MAN	C	631	9	-	0/2/19/22	0/1/1/1
7	NAG	C	632	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	633	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	634	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	635	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	636	9	-	0/2/19/22	0/1/1/1
9	MAN	C	637	9	-	0/2/19/22	0/1/1/1
9	MAN	C	638	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	639	9	-	0/2/19/22	0/1/1/1
9	MAN	C	640	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	641	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	642	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	643	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	644	8	-	0/2/19/22	0/1/1/1
9	MAN	C	645	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	646	9	-	0/2/19/22	0/1/1/1
9	MAN	C	647	9	-	0/2/19/22	0/1/1/1
7	NAG	C	648	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	649	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	650	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	651	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	652	9	-	0/2/19/22	0/1/1/1
7	NAG	C	653	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	654	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	655	7	-	0/2/19/22	0/1/1/1
10	SO4	C	656	3	-	0/0/0/0	0/0/0/0
7	NAG	C	657	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	658	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	659	7	-	0/2/19/22	0/1/1/1
7	NAG	C	660	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	661	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	662	7	-	0/2/19/22	0/1/1/1
7	NAG	D	701	4,7	-	0/6/23/26	0/1/1/1
7	NAG	D	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	703	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	704	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	705	9	-	0/2/19/22	0/1/1/1
9	MAN	D	706	9	-	0/2/19/22	0/1/1/1
9	MAN	D	707	9	-	0/2/19/22	0/1/1/1
9	MAN	D	708	8	-	0/2/19/22	0/1/1/1
7	NAG	D	709	4	-	0/6/23/26	0/1/1/1
7	NAG	D	710	4	-	0/6/23/26	0/1/1/1
7	NAG	E	301	3,7	-	0/6/23/26	0/1/1/1
7	NAG	E	302	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	303	9,7	-	0/2/19/22	0/1/1/1
9	MAN	E	304	9,8	-	0/2/19/22	0/1/1/1
9	MAN	E	305	9	-	0/2/19/22	0/1/1/1
9	MAN	E	306	9	-	0/2/19/22	0/1/1/1
9	MAN	E	307	9,8	-	0/2/19/22	0/1/1/1
9	MAN	E	308	9	-	0/2/19/22	0/1/1/1
9	MAN	E	309	9	-	0/2/19/22	0/1/1/1
9	MAN	E	310	9,5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	E	311	9	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	619	MAN	C1-C2	2.06	1.57	1.52
9	C	644	MAN	C1-C2	2.13	1.57	1.52
9	D	704	MAN	C1-C2	2.48	1.58	1.52
9	D	704	MAN	O2-C2	2.59	1.49	1.43
9	D	704	MAN	C2-C3	3.26	1.56	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	309	MAN	O2-C2-C3	-3.30	103.54	110.19
9	C	630	MAN	O2-C2-C3	-3.13	103.88	110.19
9	C	624	MAN	O2-C2-C3	-3.01	104.13	110.19
8	C	643	BMA	C1-C2-C3	-2.82	106.13	109.55
9	E	309	MAN	C1-C2-C3	-2.52	106.50	109.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	602	NAG	O7-C7-N2-C2

There are no ring outliers.

21 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	602	NAG	4	0
7	C	607	NAG	1	0
7	C	609	NAG	1	0
7	C	610	NAG	2	0
7	C	611	NAG	1	0
7	C	613	NAG	1	0
9	C	616	MAN	1	0
9	C	631	MAN	1	0
7	C	632	NAG	1	0
7	C	633	NAG	1	0
9	C	637	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	641	NAG	3	0
7	C	642	NAG	2	0
9	C	645	MAN	1	0
9	C	646	MAN	1	0
9	C	647	MAN	1	0
7	C	654	NAG	1	0
7	C	660	NAG	3	0
7	D	702	NAG	3	0
8	D	703	BMA	2	0
9	E	310	MAN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	230/239 (96%)	0.25	11 (4%) 34 27	183, 200, 258, 262	0
2	B	204/211 (96%)	0.48	13 (6%) 23 17	186, 226, 250, 255	0
3	C	450/487 (92%)	-0.10	5 (1%) 82 76	126, 172, 188, 203	0
4	D	122/153 (79%)	-0.25	0 100 100	128, 139, 177, 187	0
5	E	224/238 (94%)	-0.08	2 (0%) 85 80	136, 154, 186, 196	0
6	F	212/215 (98%)	-0.08	0 100 100	136, 157, 189, 192	0
All	All	1442/1543 (93%)	0.03	31 (2%) 67 58	126, 177, 247, 262	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	ALA	5.7
1	A	200	THR	5.2
2	B	142	GLY	4.6
2	B	141	PRO	4.2
2	B	158	GLY	4.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
7	NAG	C	601	14/15	0.70	0.47	6.62	144,144,144,144	0
7	NAG	E	301	14/15	0.87	0.37	1.61	144,144,144,144	0
7	NAG	C	605	14/15	0.66	0.52	1.58	196,196,196,196	0
9	MAN	E	308	11/12	0.83	0.36	1.33	147,147,147,147	0
9	MAN	E	305	11/12	0.88	0.26	0.41	148,148,148,148	0
7	NAG	C	621	14/15	0.57	0.67	0.34	198,198,198,198	0
7	NAG	C	604	14/15	0.77	0.37	0.30	184,184,184,184	0
7	NAG	D	701	14/15	0.90	0.31	0.25	144,144,144,144	0
9	MAN	C	631	11/12	0.86	0.33	0.25	184,184,184,184	0
7	NAG	C	632	14/15	0.87	0.29	0.06	184,184,184,184	0
9	MAN	E	306	11/12	0.87	0.28	0.03	151,151,151,151	0
7	NAG	D	702	14/15	0.87	0.32	-0.08	155,155,155,155	0
9	MAN	C	630	11/12	0.74	0.28	-0.41	183,183,183,183	0
7	NAG	C	613	14/15	0.91	0.29	-0.46	159,159,159,159	0
7	NAG	C	612	14/15	0.94	0.22	-0.52	154,154,154,154	0
9	MAN	E	310	11/12	0.79	0.29	-0.58	151,151,151,151	0
7	NAG	C	648	14/15	0.81	0.28	-0.63	187,187,187,187	0
7	NAG	C	622	14/15	0.86	0.27	-0.63	180,180,180,180	0
9	MAN	C	645	11/12	0.85	0.30	-0.64	190,190,190,190	0
7	NAG	C	641	14/15	0.95	0.24	-0.64	173,173,173,173	0
7	NAG	C	607	14/15	0.90	0.21	-0.83	177,177,177,177	0
7	NAG	C	633	14/15	0.94	0.22	-1.82	186,186,186,186	0
9	MAN	C	625	11/12	0.95	0.11	-2.30	182,182,182,182	0
7	NAG	C	654	14/15	0.83	0.43	-	194,194,194,194	0
7	NAG	C	602	14/15	0.89	0.20	-	187,187,187,187	0
7	NAG	C	609	14/15	0.80	0.48	-	191,191,191,191	0
8	BMA	C	659	11/12	0.53	0.59	-	211,211,211,211	0
7	NAG	C	603	14/15	0.75	0.41	-	192,192,192,192	0
9	MAN	C	635	11/12	0.81	0.18	-	192,192,192,192	0
9	MAN	E	311	11/12	0.83	0.36	-	159,159,159,159	0
8	BMA	C	650	11/12	0.70	0.37	-	217,217,217,217	0
9	MAN	C	637	11/12	0.81	0.44	-	200,200,200,200	0
9	MAN	C	639	11/12	0.88	0.33	-	199,199,199,199	0
9	MAN	C	615	11/12	0.93	0.32	-	179,179,179,179	0
9	MAN	D	708	11/12	0.78	0.29	-	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	C	651	11/12	0.74	0.37	-	221,221,221,221	0
9	MAN	C	617	11/12	0.80	0.43	-	196,196,196,196	0
7	NAG	E	302	14/15	0.90	0.31	-	144,144,144,144	0
8	BMA	E	303	11/12	0.92	0.33	-	146,146,146,146	0
7	NAG	C	623	14/15	0.78	0.31	-	183,183,183,183	0
7	NAG	C	608	14/15	0.90	0.35	-	186,186,186,186	0
8	BMA	D	703	11/12	0.82	0.24	-	168,168,168,168	0
9	MAN	D	707	11/12	0.61	0.72	-	199,199,199,199	0
9	MAN	C	636	11/12	0.85	0.29	-	193,193,193,193	0
9	MAN	D	704	11/12	0.80	0.41	-	180,180,180,180	0
8	BMA	C	614	11/12	0.91	0.30	-	169,169,169,169	0
7	NAG	C	653	14/15	0.88	0.30	-	186,186,186,186	0
9	MAN	C	627	11/12	0.93	0.19	-	181,181,181,181	0
9	MAN	C	619	11/12	0.83	0.34	-	184,184,184,184	0
9	MAN	D	705	11/12	0.76	0.45	-	190,190,190,190	0
9	MAN	C	640	11/12	0.84	0.33	-	202,202,202,202	0
7	NAG	D	710	14/15	0.91	0.23	-	145,145,145,145	0
9	MAN	C	624	11/12	0.95	0.17	-	180,180,180,180	0
7	NAG	D	709	14/15	0.79	0.37	-	143,143,143,143	0
7	NAG	C	660	14/15	0.66	0.60	-	198,198,198,198	0
9	MAN	C	652	11/12	0.62	0.50	-	225,225,225,225	0
9	MAN	E	304	11/12	0.91	0.26	-	147,147,147,147	0
7	NAG	C	661	14/15	0.79	0.49	-	211,211,211,211	0
7	NAG	C	649	14/15	0.78	0.30	-	204,204,204,204	0
9	MAN	C	644	11/12	0.72	0.35	-	193,193,193,193	0
9	MAN	C	638	11/12	0.80	0.25	-	194,194,194,194	0
9	MAN	C	616	11/12	0.88	0.33	-	188,188,188,188	0
8	BMA	C	626	11/12	0.91	0.19	-	182,182,182,182	0
10	SO4	C	656	5/5	0.67	0.39	-	171,171,171,171	0
9	MAN	C	646	11/12	0.89	0.40	-	192,192,192,192	0
7	NAG	C	657	14/15	0.80	0.56	-	197,197,197,197	0
9	MAN	E	307	11/12	0.92	0.32	-	147,147,147,147	0
7	NAG	C	606	14/15	0.68	0.49	-	199,199,199,199	0
9	MAN	C	647	11/12	0.83	0.47	-	191,191,191,191	0
7	NAG	C	658	14/15	0.79	0.50	-	206,206,206,206	0
9	MAN	C	628	11/12	0.90	0.18	-	184,184,184,184	0
9	MAN	C	629	11/12	0.95	0.15	-	186,186,186,186	0
8	BMA	C	662	11/12	0.68	0.47	-	222,222,222,222	0
9	MAN	C	618	11/12	0.85	0.19	-	180,180,180,180	0
7	NAG	C	642	14/15	0.91	0.24	-	180,180,180,180	0
8	BMA	C	643	11/12	0.83	0.22	-	188,188,188,188	0
8	BMA	C	634	11/12	0.89	0.20	-	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	D	706	11/12	0.73	0.43	-	189,189,189,189	0
7	NAG	C	611	14/15	0.73	0.56	-	194,194,194,194	0
9	MAN	E	309	11/12	0.94	0.26	-	154,154,154,154	0
9	MAN	C	620	11/12	0.84	0.36	-	186,186,186,186	0
7	NAG	C	610	14/15	0.80	0.25	-	182,182,182,182	0
8	BMA	C	655	11/12	0.76	0.41	-	198,198,198,198	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.