



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 07:50 PM EDT

PDB ID : 5CD5  
Title : Crystal structure of an immature VRC01-class antibody DRVIA7 from a Chinese donor bound to clade A/E HIV-1 gp120 core  
Authors : Kong, L.; Wilson, I.A.  
Deposited on : 2015-07-03  
Resolution : 3.40 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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-20027107

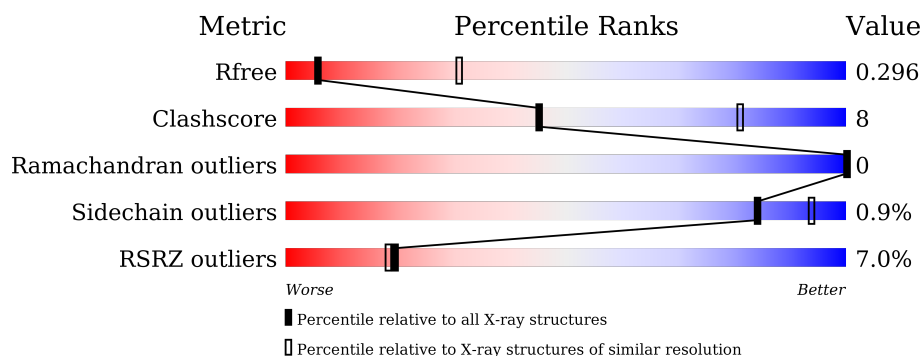
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	353	<div> <div>12%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
2	C	220	<div> <div>3%</div> <div>78%</div> <div>21%</div> </div>
3	D	210	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

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
4	NAG	A	505	-	-	-	X
4	NAG	A	506	-	-	-	X
4	NAG	A	513	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6215 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 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2685	1685	467	510	23	0	0	0

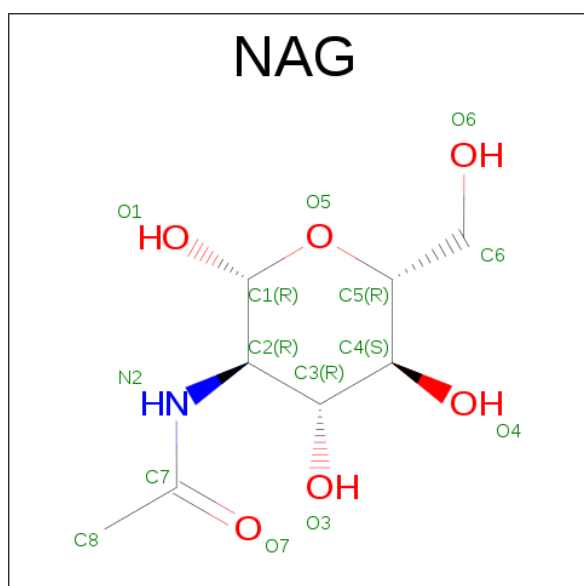
- Molecule 2 is a protein called DRVIA7 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	220	1690	1066	291	324	9	0	0	0

- Molecule 3 is a protein called DRVIA7 Fab Light Chain.

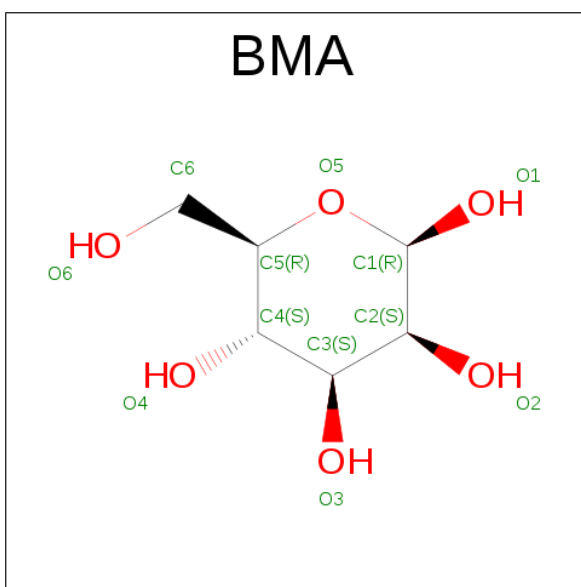
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	207	1611	1009	275	322	5	0	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



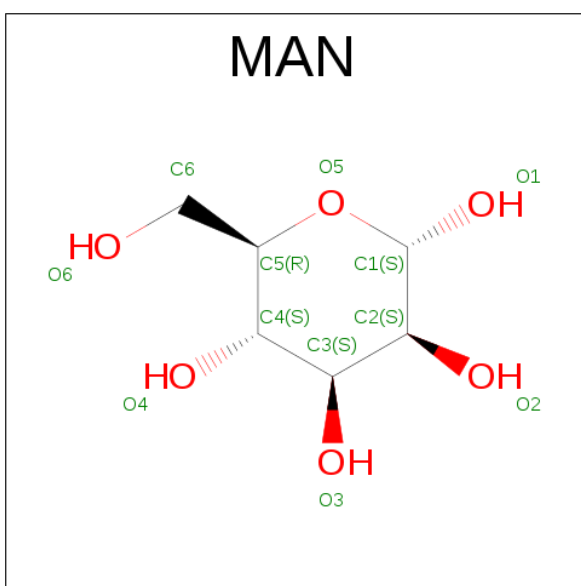
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1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

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

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

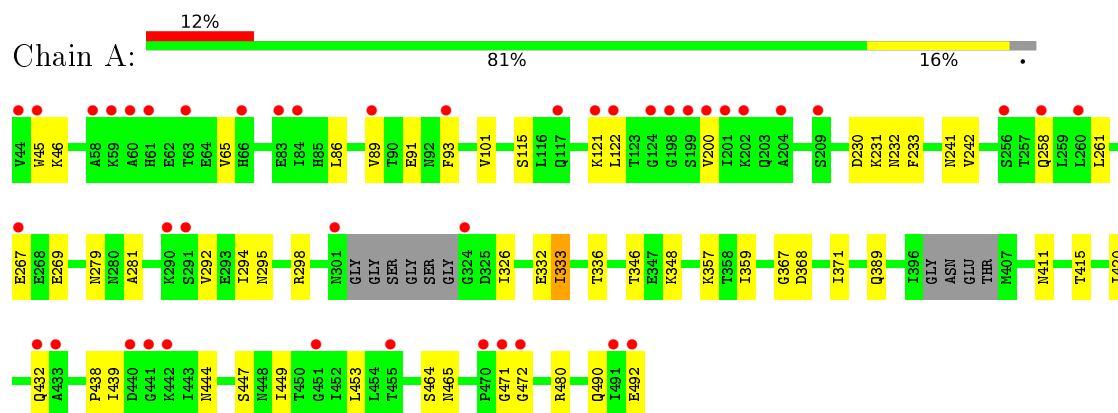


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

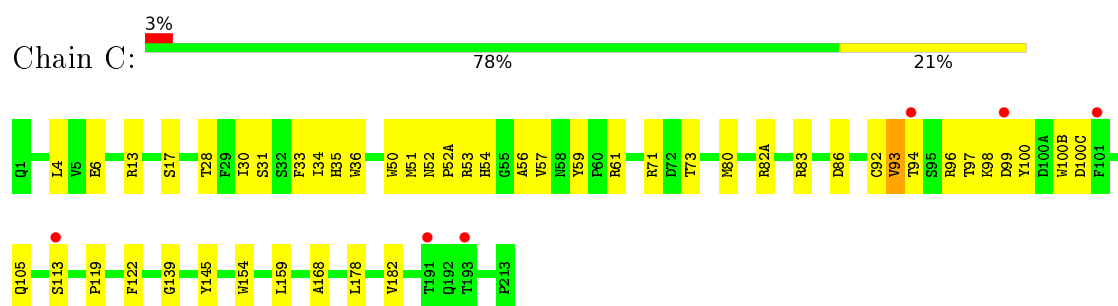
### 3 Residue-property plots [i](#)

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

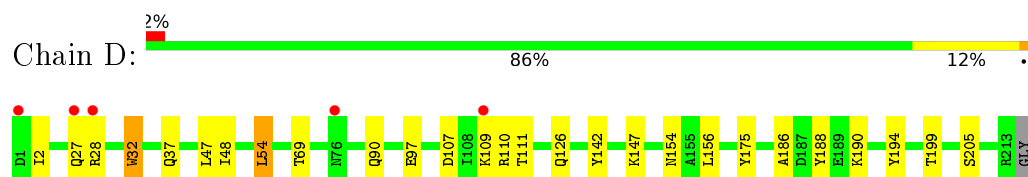
- Molecule 1: 93TH057 HIV-1 gp120 core



- Molecule 2: DRVIA7 Fab Heavy Chain



- Molecule 3: DRVIA7 Fab Light Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.33Å 72.33Å 338.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.97 – 3.40 28.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.97-3.40) 88.5 (28.97-3.39)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.253 , 0.306 0.266 , 0.296	Depositor DCC
$R_{free}$ test set	1170 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 13362 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: 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	0/2741	0.44	0/3719
2	C	0.25	0/1735	0.50	0/2363
3	D	0.23	0/1644	0.42	0/2231
All	All	0.23	0/6120	0.45	0/8313

There are no bond length outliers.

There are no bond angle outliers.

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	2685	0	2621	47	0
2	C	1690	0	1643	34	1
3	D	1611	0	1580	18	1
4	A	196	0	175	6	0
5	A	22	0	18	0	0
6	A	11	0	10	0	0
All	All	6215	0	6047	95	1

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 8.

All (95) 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:357:LYS:CE	1:A:464:SER:O	1.82	1.26
1:A:357:LYS:HE2	1:A:464:SER:O	1.38	1.19
1:A:357:LYS:HE3	1:A:464:SER:O	1.55	1.03
3:D:2:ILE:HG12	3:D:27:GLN:HB2	1.49	0.94
2:C:6:GLU:OE2	2:C:92:CYS:N	2.08	0.86
1:A:357:LYS:HE3	1:A:464:SER:C	1.97	0.83
1:A:357:LYS:CE	1:A:464:SER:C	2.51	0.76
1:A:357:LYS:HE3	1:A:464:SER:CA	2.18	0.73
3:D:2:ILE:HG12	3:D:27:GLN:CB	2.21	0.71
3:D:32:TRP:O	3:D:90:GLN:NE2	2.23	0.70
2:C:28:THR:O	2:C:31:SER:OG	2.11	0.68
1:A:368:ASP:OD2	2:C:71:ARG:NH1	2.28	0.66
3:D:2:ILE:O	3:D:97:GLU:HG3	1.97	0.64
1:A:230:ASP:HB2	1:A:233:PHE:HB2	1.80	0.64
1:A:346:THR:HG23	1:A:359:ILE:HB	1.80	0.63
2:C:34:ILE:HG12	2:C:94:THR:HG22	1.81	0.63
2:C:4:LEU:HD11	2:C:94:THR:HG23	1.81	0.62
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.81	0.62
1:A:357:LYS:HE3	1:A:464:SER:HA	1.81	0.61
1:A:101:VAL:HG21	1:A:480:ARG:HG3	1.83	0.60
1:A:46:LYS:HE3	1:A:492:GLU:OE2	2.01	0.60
2:C:30:ILE:HG23	2:C:53:ARG:HG2	1.82	0.60
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.85	0.59
1:A:447:SER:OG	4:A:503:NAG:N2	2.33	0.58
2:C:54:HIS:CD2	2:C:56:ALA:HB2	2.38	0.58
1:A:447:SER:HG	4:A:503:NAG:HN2	1.48	0.58
2:C:168:ALA:HA	2:C:178:LEU:HB3	1.85	0.58
1:A:298:ARG:NH2	1:A:439:ILE:O	2.36	0.58
1:A:465:ASN:HB2	2:C:61:ARG:NH2	2.18	0.58
3:D:28:ARG:HA	3:D:69:THR:HG22	1.86	0.57
3:D:110:ARG:HG2	3:D:111:THR:N	2.20	0.56
1:A:357:LYS:HB3	1:A:464:SER:O	2.05	0.56
2:C:71:ARG:NH2	2:C:73:THR:OG1	2.39	0.56
1:A:279:ASN:ND2	2:C:100(B):TRP:HE1	2.03	0.56
1:A:122:LEU:HD12	1:A:432:GLN:HB2	1.89	0.54
1:A:389:GLN:HG2	4:A:506:NAG:H81	1.90	0.54
1:A:294:ILE:N	1:A:447:SER:O	2.30	0.54
1:A:46:LYS:O	1:A:490:GLN:N	2.33	0.53
2:C:159:LEU:HD21	2:C:182:VAL:HG21	1.90	0.53
1:A:294:ILE:HG12	1:A:333:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:NH1	1:A:326:ILE:O	2.38	0.52
2:C:35:HIS:HB2	2:C:93:VAL:HG12	1.92	0.52
3:D:107:ASP:OD1	3:D:175:TYR:OH	2.22	0.52
2:C:17:SER:HB2	2:C:82(A):ARG:HG2	1.91	0.51
1:A:453:LEU:HD13	1:A:472:GLY:HA3	1.91	0.51
2:C:168:ALA:HB2	2:C:178:LEU:HD23	1.93	0.50
1:A:261:LEU:HD21	1:A:294:ILE:HD12	1.93	0.50
4:A:509:NAG:H61	4:A:510:NAG:HN2	1.76	0.50
2:C:36:TRP:CE2	2:C:80:MET:HB2	2.47	0.49
2:C:35:HIS:ND1	2:C:50:TRP:HB3	2.28	0.49
2:C:97:THR:HG21	2:C:100(C):ASP:OD2	2.14	0.48
3:D:110:ARG:NH1	3:D:111:THR:O	2.45	0.48
2:C:13:ARG:HG2	2:C:113:SER:HA	1.95	0.48
1:A:279:ASN:OD1	1:A:281:ALA:N	2.46	0.47
1:A:295:ASN:OD1	1:A:444:ASN:ND2	2.47	0.47
1:A:292:VAL:O	1:A:449:ILE:N	2.46	0.46
1:A:332:GLU:O	1:A:333:ILE:HD12	2.15	0.46
2:C:51:MET:SD	2:C:71:ARG:HB3	2.57	0.45
1:A:258:GLN:HG2	1:A:471:GLY:HA2	1.97	0.45
3:D:147:LYS:HB3	3:D:199:THR:HB	1.99	0.45
1:A:45:TRP:HZ2	1:A:89:VAL:HG11	1.80	0.45
2:C:139:GLY:HA2	2:C:154:TRP:CH2	2.52	0.45
1:A:91:GLU:HB2	1:A:242:VAL:HG21	1.98	0.45
1:A:367:GLY:HA3	1:A:371:ILE:HD11	1.98	0.45
2:C:83:ARG:N	2:C:86:ASP:OD2	2.43	0.45
3:D:2:ILE:HG12	3:D:27:GLN:CG	2.46	0.45
3:D:48:ILE:HD13	3:D:54:LEU:HA	1.98	0.44
1:A:45:TRP:CH2	1:A:86:LEU:HD13	2.51	0.44
1:A:389:GLN:NE2	1:A:415:THR:O	2.41	0.44
2:C:30:ILE:HG23	2:C:53:ARG:CG	2.48	0.44
3:D:188:TYR:O	3:D:194:TYR:OH	2.30	0.44
2:C:36:TRP:CH2	2:C:92:CYS:HB3	2.52	0.44
1:A:281:ALA:HB1	2:C:33:PHE:HE2	1.82	0.43
1:A:232:ASN:OD1	1:A:269:GLU:HB2	2.19	0.43
2:C:97:THR:OG1	2:C:100:TYR:HB3	2.18	0.43
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.54	0.43
2:C:122:PHE:CE2	3:D:126:GLN:HG3	2.53	0.43
3:D:109:LYS:HA	3:D:142:TYR:OH	2.19	0.43
1:A:420:ILE:HG21	1:A:438:PRO:HG3	2.00	0.42
1:A:241:ASN:HD21	4:A:502:NAG:C1	2.32	0.42
3:D:186:ALA:O	3:D:190:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:THR:OG1	1:A:411:ASN:HB3	2.20	0.42
2:C:54:HIS:HD2	2:C:56:ALA:HB2	1.80	0.42
1:A:231:LYS:HG2	1:A:267:GLU:OE1	2.21	0.41
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.88	0.41
1:A:65:VAL:HB	1:A:115:SER:HB3	2.01	0.41
3:D:2:ILE:CG1	3:D:27:GLN:HB2	2.36	0.41
2:C:96:ARG:HG3	2:C:97:THR:N	2.35	0.41
2:C:30:ILE:HG22	2:C:53:ARG:HE	1.86	0.41
2:C:57:VAL:HG11	2:C:59:TYR:CZ	2.56	0.41
1:A:389:GLN:HA	4:A:506:NAG:H81	2.02	0.41
2:C:98:LYS:O	2:C:99:ASP:HB2	2.20	0.41
3:D:110:ARG:HH11	3:D:110:ARG:HG2	1.85	0.40
1:A:121:LYS:O	1:A:200:VAL:HA	2.21	0.40
2:C:52:ASN:HA	2:C:52(A):PRO:HD3	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:GLN:O	3:D:205:SER:OG[5_755]	2.10	0.10

## 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	337/353 (96%)	327 (97%)	10 (3%)	0	100	100
2	C	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
3	D	205/210 (98%)	200 (98%)	5 (2%)	0	100	100
All	All	760/783 (97%)	742 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	306/311 (98%)	305 (100%)	1 (0%)	94	98
2	C	190/190 (100%)	189 (100%)	1 (0%)	92	96
3	D	183/185 (99%)	179 (98%)	4 (2%)	60	86
All	All	679/686 (99%)	673 (99%)	6 (1%)	84	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	ILE
2	C	93	VAL
3	D	32	TRP
3	D	54	LEU
3	D	154	ASN
3	D	156	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	54	HIS

### 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 ⓘ

17 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	501	1	14,14,15	1.13	0	15,19,21	1.37	2 (13%)
4	NAG	A	502	-	14,14,15	0.28	0	15,19,21	0.54	0
4	NAG	A	503	1	14,14,15	0.49	0	15,19,21	0.75	0
4	NAG	A	504	1	14,14,15	1.13	0	15,19,21	1.37	2 (13%)
4	NAG	A	505	1	14,14,15	0.57	0	15,19,21	0.92	0
4	NAG	A	506	1	14,14,15	0.44	0	15,19,21	1.60	4 (26%)
4	NAG	A	507	1,4	14,14,15	1.08	1 (7%)	15,19,21	1.71	3 (20%)
4	NAG	A	508	4	14,14,15	1.31	2 (14%)	15,19,21	3.22	6 (40%)
4	NAG	A	509	1,4	14,14,15	1.08	2 (14%)	15,19,21	1.72	3 (20%)
4	NAG	A	510	5,4	14,14,15	1.31	2 (14%)	15,19,21	3.21	6 (40%)
5	BMA	A	511	4,6	11,11,12	1.42	1 (9%)	15,15,17	3.29	11 (73%)
6	MAN	A	512	5	11,11,12	1.47	2 (18%)	15,15,17	1.01	2 (13%)
4	NAG	A	513	1,4	14,14,15	1.07	2 (14%)	15,19,21	1.72	3 (20%)
4	NAG	A	514	5,4	14,14,15	1.32	2 (14%)	15,19,21	3.21	6 (40%)
5	BMA	A	515	4	11,11,12	1.42	1 (9%)	15,15,17	3.29	10 (66%)
4	NAG	A	516	1,4	14,14,15	0.51	0	15,19,21	0.89	1 (6%)
4	NAG	A	517	4	14,14,15	1.31	3 (21%)	15,19,21	0.94	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	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	-	-	0/6/23/26	0/1/1/1
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	0/6/23/26	0/1/1/1
4	NAG	A	507	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	508	4	-	0/6/23/26	0/1/1/1
4	NAG	A	509	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	510	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	511	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	512	5	-	0/2/19/22	0/1/1/1
4	NAG	A	513	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	514	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	515	4	-	0/2/19/22	0/1/1/1
4	NAG	A	516	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	517	4	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	512	MAN	C2-C3	-3.44	1.47	1.52
4	A	508	NAG	C4-C5	-2.89	1.46	1.53
4	A	510	NAG	C4-C5	-2.87	1.46	1.53
4	A	514	NAG	C4-C5	-2.84	1.46	1.53
5	A	511	BMA	O5-C5	-2.83	1.37	1.43
5	A	515	BMA	O5-C5	-2.81	1.37	1.43
4	A	514	NAG	O4-C4	-2.32	1.37	1.43
4	A	508	NAG	O4-C4	-2.28	1.37	1.43
4	A	510	NAG	O4-C4	-2.24	1.37	1.43
4	A	513	NAG	O5-C1	-2.04	1.40	1.43
4	A	509	NAG	O5-C1	-2.03	1.40	1.43
4	A	517	NAG	O5-C1	2.02	1.47	1.43
4	A	517	NAG	O7-C7	2.09	1.28	1.23
4	A	513	NAG	O4-C4	2.12	1.48	1.43
4	A	517	NAG	C7-N2	2.12	1.42	1.34
4	A	507	NAG	O4-C4	2.15	1.48	1.43
4	A	509	NAG	O4-C4	2.15	1.48	1.43
6	A	512	MAN	O5-C1	2.60	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	508	NAG	C2-N2-C7	-8.74	111.73	123.11
4	A	510	NAG	C2-N2-C7	-8.71	111.78	123.11
4	A	514	NAG	C2-N2-C7	-8.70	111.79	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	515	BMA	C1-O5-C5	-6.29	102.89	112.14
5	A	511	BMA	C1-O5-C5	-6.29	102.89	112.14
5	A	515	BMA	C2-C3-C4	-5.40	101.64	111.05
5	A	511	BMA	C2-C3-C4	-5.38	101.67	111.05
4	A	509	NAG	C4-C3-C2	-4.52	104.32	111.34
4	A	507	NAG	C4-C3-C2	-4.50	104.36	111.34
4	A	513	NAG	C4-C3-C2	-4.49	104.37	111.34
4	A	506	NAG	C2-N2-C7	-3.40	118.68	123.11
5	A	511	BMA	O3-C3-C4	-3.25	103.02	110.36
4	A	513	NAG	C2-N2-C7	-3.25	118.88	123.11
4	A	514	NAG	O6-C6-C5	-3.24	100.49	111.30
4	A	508	NAG	O6-C6-C5	-3.23	100.50	111.30
5	A	515	BMA	O3-C3-C4	-3.23	103.08	110.36
4	A	504	NAG	C4-C3-C2	-3.22	106.34	111.34
4	A	510	NAG	O6-C6-C5	-3.21	100.57	111.30
4	A	510	NAG	O4-C4-C5	-3.21	100.76	109.23
4	A	508	NAG	O4-C4-C5	-3.21	100.76	109.23
4	A	509	NAG	C2-N2-C7	-3.21	118.93	123.11
4	A	501	NAG	C4-C3-C2	-3.21	106.36	111.34
4	A	514	NAG	O4-C4-C5	-3.20	100.78	109.23
4	A	507	NAG	C2-N2-C7	-3.20	118.94	123.11
4	A	504	NAG	C2-N2-C7	-3.10	119.07	123.11
4	A	501	NAG	C2-N2-C7	-3.07	119.11	123.11
5	A	511	BMA	O2-C2-C1	-2.96	103.31	109.23
5	A	515	BMA	O2-C2-C1	-2.94	103.35	109.23
5	A	515	BMA	O6-C6-C5	-2.67	102.37	111.30
5	A	511	BMA	O6-C6-C5	-2.66	102.42	111.30
4	A	510	NAG	O4-C4-C3	-2.33	105.10	110.36
4	A	508	NAG	O4-C4-C3	-2.31	105.15	110.36
4	A	514	NAG	O4-C4-C3	-2.29	105.19	110.36
6	A	512	MAN	O3-C3-C2	-2.28	105.83	110.01
5	A	511	BMA	C1-C2-C3	-2.27	106.80	109.55
5	A	515	BMA	C1-C2-C3	-2.26	106.81	109.55
5	A	511	BMA	O5-C5-C4	-2.06	106.72	110.13
4	A	514	NAG	O3-C3-C4	-2.04	105.75	110.36
4	A	510	NAG	O3-C3-C4	-2.04	105.77	110.36
4	A	508	NAG	O3-C3-C4	-2.03	105.77	110.36
4	A	516	NAG	O5-C5-C6	2.24	112.13	107.34
6	A	512	MAN	C1-C2-C3	2.26	112.30	109.55
5	A	511	BMA	C3-C4-C5	2.36	114.43	110.23
5	A	515	BMA	C3-C4-C5	2.37	114.45	110.23
4	A	509	NAG	C1-O5-C5	2.50	115.81	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	507	NAG	C1-O5-C5	2.52	115.84	112.14
4	A	506	NAG	C3-C4-C5	2.56	114.79	110.23
4	A	513	NAG	C1-O5-C5	2.56	115.91	112.14
4	A	506	NAG	C1-O5-C5	2.66	116.06	112.14
4	A	506	NAG	O5-C5-C4	2.87	114.89	110.13
5	A	515	BMA	O3-C3-C2	3.23	115.93	110.01
5	A	511	BMA	O3-C3-C2	3.27	116.01	110.01
5	A	515	BMA	O5-C1-C2	3.29	116.16	110.89
5	A	511	BMA	O5-C1-C2	3.30	116.17	110.89
5	A	511	BMA	O2-C2-C3	5.09	120.44	110.19
5	A	515	BMA	O2-C2-C3	5.13	120.51	110.19
4	A	508	NAG	O5-C5-C6	5.75	119.65	107.34
4	A	510	NAG	O5-C5-C6	5.76	119.67	107.34
4	A	514	NAG	O5-C5-C6	5.78	119.71	107.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	NAG	1	0
4	A	503	NAG	2	0
4	A	506	NAG	2	0
4	A	509	NAG	1	0
4	A	510	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	343/353 (97%)	0.77	43 (12%) 5 5	104, 166, 216, 276	0
2	C	220/220 (100%)	0.18	6 (2%) 58 53	78, 120, 156, 178	0
3	D	207/210 (98%)	0.20	5 (2%) 62 57	70, 117, 165, 198	0
All	All	770/783 (98%)	0.45	54 (7%) 19 18	70, 135, 203, 276	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	7.5
1	A	44	VAL	5.6
1	A	200	VAL	5.1
1	A	63	THR	4.7
1	A	324	GLY	4.7
3	D	27	GLN	4.7
1	A	440	ASP	4.5
3	D	1	ASP	4.4
1	A	45	TRP	4.3
1	A	59	LYS	4.3
1	A	89	VAL	4.2
1	A	60	ALA	4.2
1	A	199	SER	4.1
1	A	267	GLU	3.6
1	A	83	GLU	3.5
1	A	58	ALA	3.5
3	D	28	ARG	3.5
1	A	472	GLY	3.3
1	A	256	SER	3.3
1	A	492	GLU	3.3
1	A	202	LYS	3.2
1	A	290	LYS	3.1
1	A	117	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	76	ASN	3.1
1	A	61	HIS	3.1
1	A	124	GLY	3.0
1	A	432	GLN	3.0
1	A	301	ASN	3.0
1	A	491	ILE	3.0
1	A	433	ALA	3.0
1	A	258	GLN	2.9
1	A	451	GLY	2.7
1	A	291	SER	2.6
1	A	471	GLY	2.6
1	A	121	LYS	2.6
1	A	204	ALA	2.5
1	A	122	LEU	2.4
1	A	455	THR	2.4
1	A	260	LEU	2.4
1	A	442	LYS	2.4
1	A	84	ILE	2.3
1	A	93	PHE	2.3
1	A	201	ILE	2.3
1	A	441	GLY	2.3
2	C	113	SER	2.2
2	C	193	THR	2.1
3	D	109	LYS	2.1
2	C	99	ASP	2.1
2	C	101	PHE	2.1
1	A	209	SER	2.1
1	A	66	HIS	2.1
2	C	94	THR	2.1
1	A	470	PRO	2.1
2	C	191	THR	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 ⓘ

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	505	14/15	0.49	0.56	2.88	140,146,154,154	0
4	NAG	A	506	14/15	0.75	0.42	2.05	130,136,137,138	0
4	NAG	A	513	14/15	0.56	0.43	1.26	141,147,155,162	0
4	NAG	A	501	14/15	0.84	0.24	1.00	107,117,120,121	0
4	NAG	A	504	14/15	0.75	0.34	0.58	109,119,121,122	0
4	NAG	A	509	14/15	0.81	0.30	0.22	116,129,134,143	0
4	NAG	A	503	14/15	0.81	0.34	0.16	105,109,112,113	0
4	NAG	A	502	14/15	0.77	0.34	-0.05	172,173,174,175	0
5	BMA	A	511	11/12	0.59	0.37	-	177,181,185,186	0
4	NAG	A	508	14/15	0.72	0.34	-	141,148,150,150	0
5	BMA	A	515	11/12	0.79	0.49	-	179,181,181,181	0
4	NAG	A	510	14/15	0.91	0.37	-	153,160,165,172	0
4	NAG	A	514	14/15	0.75	0.63	-	169,175,176,178	0
4	NAG	A	516	14/15	0.74	0.44	-	125,134,138,139	0
4	NAG	A	517	14/15	0.68	0.57	-	196,199,199,199	0
6	MAN	A	512	11/12	0.44	0.50	-	189,190,190,190	0
4	NAG	A	507	14/15	0.88	0.32	-	109,120,123,132	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.