



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 08:35 PM EST

PDB ID : 5TIP
Title : The Structure of the Major Capsid protein of PBCV-1
Authors : Klose, T.; De Castro, C.; Speciale, I.; Molinaro, A.; Van Etten, J.L.; Rossmann, M.G.
Deposited on : 2016-10-03
Resolution : 2.00 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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

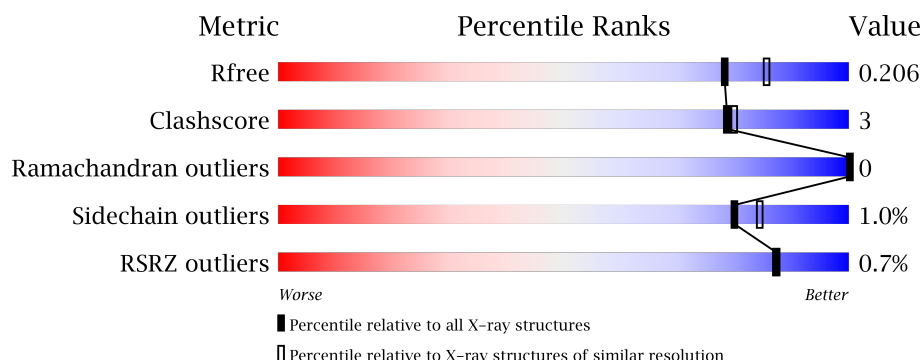
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	
1	B	436	
1	C	436	
1	D	436	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15788 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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3395	2156	576	655	8			
1	B	436	Total	C	N	O	S	0	0	0
			3395	2156	576	655	8			
1	C	436	Total	C	N	O	S	0	0	0
			3395	2156	576	655	8			
1	D	436	Total	C	N	O	S	0	0	0
			3395	2156	576	655	8			

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Hg	0	0
			1	1		
2	A	1	Total	Hg	0	0
			1	1		
2	D	1	Total	Hg	0	0
			1	1		
2	C	1	Total	Hg	0	0
			1	1		

- Molecule 3 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C₆H₁₂O₆).



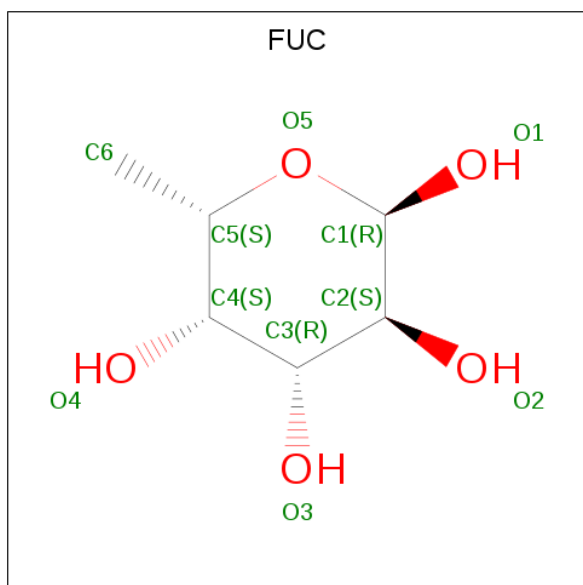
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



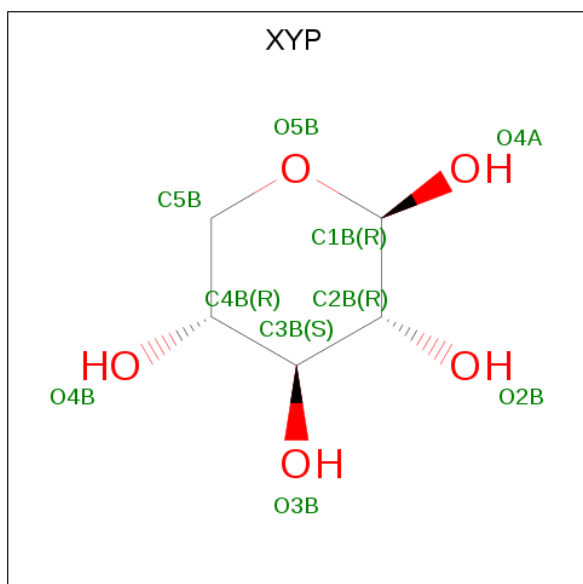
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



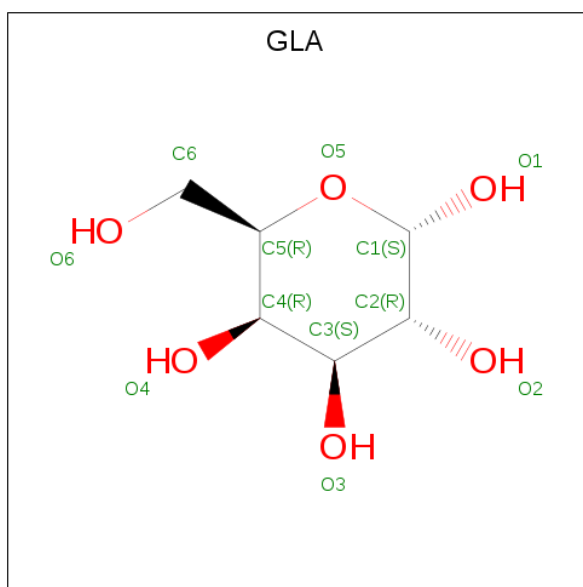
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	5	4		
5	A	1	Total	C	O	0	0
			9	5	4		
5	A	1	Total	C	O	0	0
			9	5	4		
5	A	1	Total	C	O	0	0
			9	5	4		
5	A	1	Total	C	O	0	0
			9	5	4		

Continued on next page...

Continued from previous page...

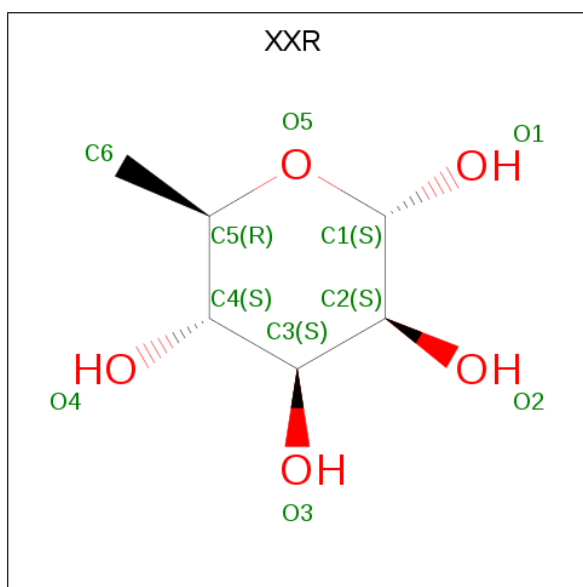
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	5	4		
5	B	1	Total	C	O	0	0
			9	5	4		
5	B	1	Total	C	O	0	0
			9	5	4		
5	B	1	Total	C	O	0	0
			9	5	4		
5	B	1	Total	C	O	0	0
			9	5	4		
5	B	1	Total	C	O	0	0
			9	5	4		
5	C	1	Total	C	O	0	0
			9	5	4		
5	C	1	Total	C	O	0	0
			9	5	4		
5	C	1	Total	C	O	0	0
			9	5	4		
5	C	1	Total	C	O	0	0
			9	5	4		
5	C	1	Total	C	O	0	0
			9	5	4		
5	C	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		

- Molecule 6 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula: C₆H₁₂O₆).



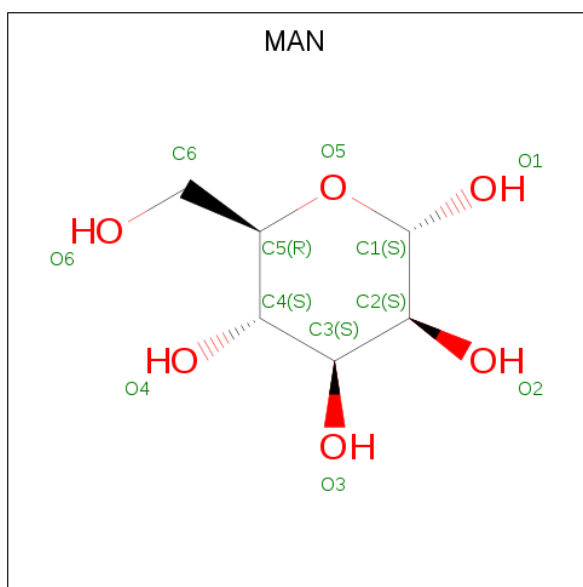
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6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

- Molecule 7 is 6-deoxy-alpha-D-mannopyranose (three-letter code: XXR) (formula: C₆H₁₂O₅).



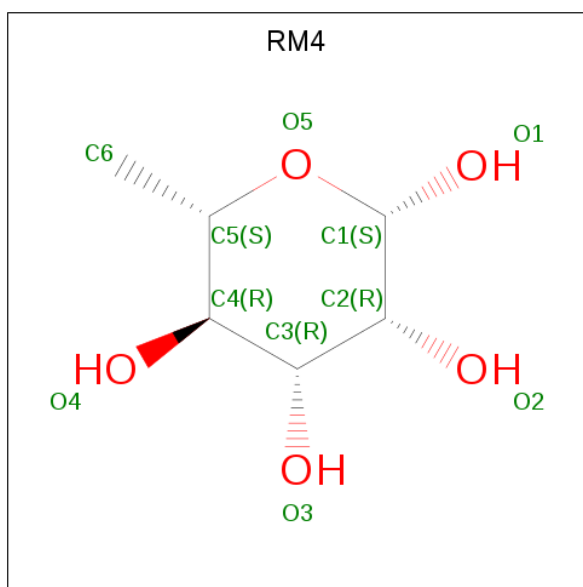
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



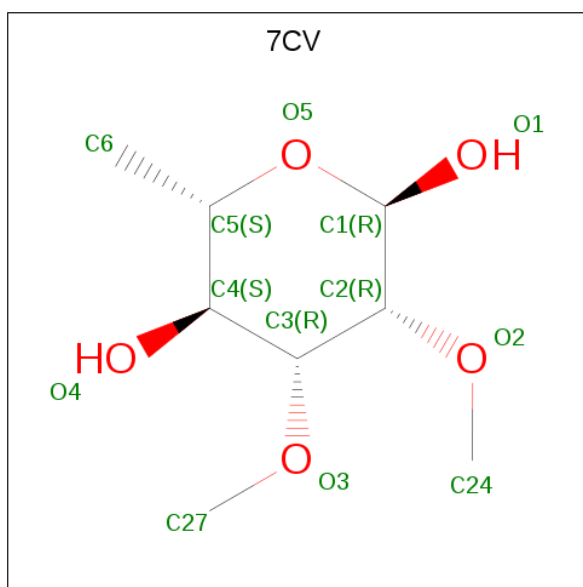
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8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

- Molecule 9 is 6-deoxy-beta-L-mannopyranose (three-letter code: RM4) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		
9	A	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		
9	C	1	Total	C	O	0	0
			10	6	4		
9	D	1	Total	C	O	0	0
			10	6	4		
9	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is 6-deoxy-2,3-di-O-methyl- α -L-mannopyranose (three-letter code: 7CV) (formula: $C_8H_{16}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			12	8	4		
10	A	1	Total	C	O	0	0
			12	8	4		
10	B	1	Total	C	O	0	0
			12	8	4		
10	C	1	Total	C	O	0	0
			12	8	4		
10	D	1	Total	C	O	0	0
			12	8	4		

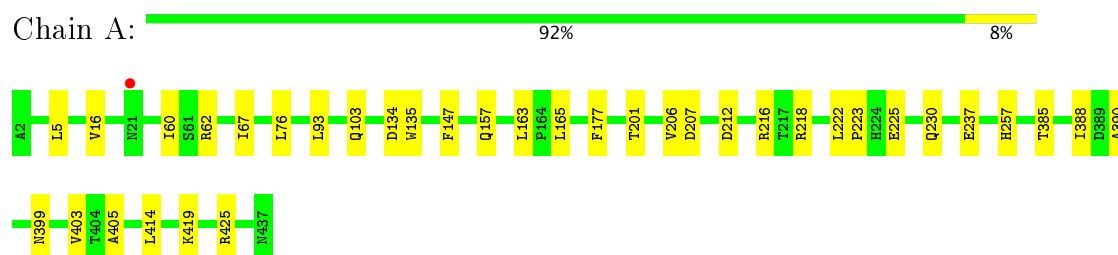
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	320	Total	O	0	0
			320	320		
11	B	288	Total	O	0	0
			288	288		
11	C	278	Total	O	0	0
			278	278		
11	D	273	Total	O	0	0
			273	273		

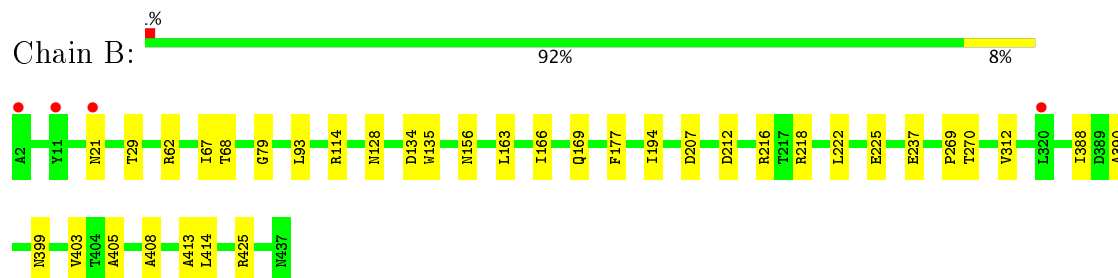
3 Residue-property plots [i](#)

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

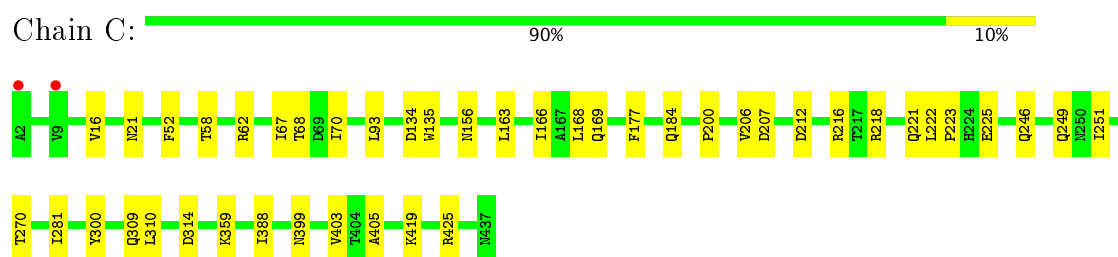
- Molecule 1: Major capsid protein



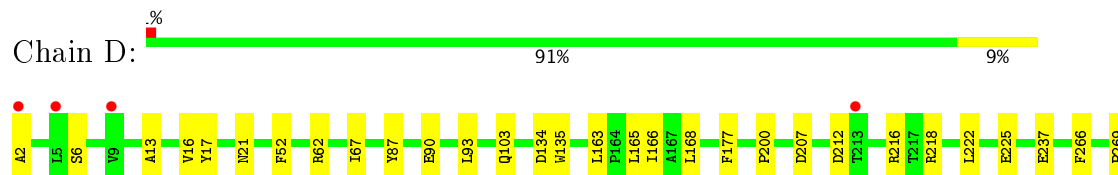
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	188.79Å 188.79Å 188.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.43 – 2.00 84.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (84.43-2.00) 92.5 (84.43-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.176 , 0.206 0.176 , 0.206	Depositor DCC
R_{free} test set	4090 reflections (2.94%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.278 for l,-k,h	Xtriage
Reported twinning fraction	0.696 for H, K, L 0.304 for L, -K, H	Depositor
Outliers	0 of 146411 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15788	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, XXR, BGC, RM4, 7CV, GLA, FUC, HG, 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	0.29	0/3473	0.46	0/4735
1	B	0.28	0/3473	0.46	0/4735
1	C	0.27	0/3473	0.46	0/4735
1	D	0.28	0/3473	0.47	0/4735
All	All	0.28	0/13892	0.46	0/18940

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	3395	0	3284	20	0
1	B	3395	0	3284	22	0
1	C	3395	0	3284	36	0
1	D	3395	0	3284	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	33	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	33	0	0
3	C	44	0	34	0	0
3	D	44	0	33	0	0
4	A	40	0	31	0	0
4	B	40	0	31	0	0
4	C	30	0	21	0	0
4	D	40	0	31	0	0
5	A	54	0	46	0	0
5	B	54	0	46	0	0
5	C	54	0	47	0	0
5	D	54	0	46	0	0
6	A	33	0	30	0	0
6	B	33	0	30	0	0
6	C	33	0	30	0	0
6	D	33	0	30	0	0
7	A	30	0	27	0	0
7	B	30	0	28	0	0
7	C	30	0	27	0	0
7	D	30	0	27	0	0
8	A	33	0	30	0	0
8	B	22	0	20	0	0
8	C	33	0	30	0	0
8	D	33	0	30	0	0
9	A	20	0	18	0	0
9	B	20	0	19	0	0
9	C	10	0	9	0	0
9	D	20	0	19	0	0
10	A	24	0	0	0	0
10	B	12	0	0	0	0
10	C	12	0	0	0	0
10	D	12	0	0	0	0
11	A	320	0	0	2	0
11	B	288	0	0	3	0
11	C	278	0	0	5	0
11	D	273	0	0	0	0
All	All	15788	0	13972	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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:D:62:ARG:NH2	1:D:165:LEU:O	2.00	0.95
1:A:62:ARG:NH2	1:A:165:LEU:O	2.11	0.84
1:B:312:VAL:CG1	1:B:408:ALA:HB1	2.08	0.83
1:A:257:HIS:HE1	11:A:722:HOH:O	1.65	0.77
1:A:16:VAL:HG13	1:B:218:ARG:HG2	1.69	0.75
1:C:251:ILE:HD11	11:C:621:HOH:O	1.87	0.73
1:B:312:VAL:HG12	1:B:408:ALA:HB1	1.71	0.72
1:D:2:ALA:HB3	1:D:6:SER:HB3	1.73	0.71
1:C:249:GLN:CD	11:C:621:HOH:O	2.30	0.69
1:C:221:GLN:OE1	1:D:13:ALA:HB1	1.94	0.68
1:C:218:ARG:HG2	1:D:16:VAL:HG13	1.76	0.67
1:C:62:ARG:NH2	1:C:168:LEU:O	2.30	0.64
1:B:270:THR:O	11:B:601:HOH:O	2.16	0.61
1:C:359:LYS:NZ	1:C:359:LYS:HB3	2.17	0.59
1:D:67:ILE:HD11	1:D:163:LEU:HD23	1.85	0.59
1:C:21:ASN:OD1	1:D:218:ARG:NH1	2.36	0.59
1:C:419:LYS:NZ	11:C:611:HOH:O	2.36	0.58
1:D:225:GLU:HG2	1:D:425:ARG:HG2	1.87	0.56
1:B:67:ILE:HD11	1:B:163:LEU:HD23	1.88	0.54
1:A:388:ILE:HD11	1:A:403:VAL:HG23	1.90	0.54
1:C:309:GLN:NE2	1:C:403:VAL:O	2.40	0.54
1:B:62:ARG:NH2	1:B:169:GLN:HA	2.24	0.52
1:A:237:GLU:HB2	1:A:414:LEU:HB3	1.92	0.52
1:C:281:ILE:HD11	1:C:310:LEU:HD11	1.91	0.52
1:D:62:ARG:NH2	1:D:168:LEU:O	2.43	0.51
1:B:225:GLU:HG2	1:B:425:ARG:HG2	1.91	0.51
1:A:230:GLN:O	1:A:419:LYS:HD2	2.10	0.51
1:B:169:GLN:O	1:B:169:GLN:HG3	2.09	0.50
1:A:390:ALA:HB2	1:A:405:ALA:HB1	1.94	0.50
1:C:270:THR:O	11:C:601:HOH:O	2.20	0.50
1:C:62:ARG:NH2	1:C:169:GLN:HA	2.28	0.49
1:C:221:GLN:OE1	1:D:13:ALA:O	2.31	0.49
1:C:218:ARG:HD3	1:D:21:ASN:OD1	2.12	0.49
1:D:388:ILE:HD11	1:D:403:VAL:HG23	1.94	0.49
1:C:52:PHE:CE2	1:C:200:PRO:HD3	2.48	0.49
1:C:67:ILE:HD11	1:C:163:LEU:HD23	1.94	0.49
1:D:269:PRO:HG3	1:D:413:ALA:HB2	1.94	0.48
1:C:249:GLN:NE2	11:C:621:HOH:O	2.45	0.48
1:C:93:LEU:HD11	1:C:177:PHE:HD1	1.79	0.48
1:D:212:ASP:O	1:D:216:ARG:HB2	2.13	0.47
1:B:68:THR:O	1:B:156:ASN:ND2	2.45	0.47
1:A:157:GLN:NE2	11:A:635:HOH:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD11	1:A:177:PHE:HD1	1.79	0.47
1:C:62:ARG:NH2	1:C:168:LEU:C	2.68	0.47
1:A:93:LEU:HD11	1:A:177:PHE:CD1	2.50	0.46
1:C:166:ILE:HD12	1:C:216:ARG:HG2	1.95	0.46
1:C:221:GLN:NE2	1:D:13:ALA:O	2.48	0.46
1:D:52:PHE:CE2	1:D:200:PRO:HD3	2.51	0.46
1:C:93:LEU:HD11	1:C:177:PHE:CD1	2.51	0.46
1:C:68:THR:O	1:C:156:ASN:ND2	2.47	0.46
1:C:184:GLN:HG2	1:C:300:TYR:CD1	2.51	0.45
1:C:388:ILE:HD11	1:C:403:VAL:HG23	1.98	0.45
1:D:166:ILE:HD12	1:D:216:ARG:HG2	1.99	0.45
1:C:218:ARG:HG2	1:D:16:VAL:CG1	2.46	0.45
1:B:388:ILE:HB	1:B:405:ALA:HA	1.99	0.45
1:C:70:ILE:HG12	1:C:206:VAL:HG22	1.98	0.44
1:C:246:GLN:NE2	1:C:314:ASP:OD2	2.49	0.44
1:B:79:GLY:HA3	1:B:194:ILE:HD13	1.98	0.44
1:C:388:ILE:HB	1:C:405:ALA:HA	1.99	0.44
1:B:212:ASP:O	1:B:216:ARG:HB2	2.17	0.44
1:B:269:PRO:HG3	1:B:413:ALA:HB2	2.00	0.44
1:A:67:ILE:HD11	1:A:163:LEU:HD23	2.00	0.44
1:B:114:ARG:NH1	11:B:640:HOH:O	2.51	0.44
1:C:16:VAL:HG13	1:D:218:ARG:HG2	2.00	0.44
1:D:93:LEU:HD11	1:D:177:PHE:HD1	1.83	0.44
1:D:266:PHE:CE1	1:D:414:LEU:HD13	2.53	0.44
1:A:60:ILE:HD12	1:A:206:VAL:HG21	2.00	0.43
1:D:134:ASP:OD1	1:D:135:TRP:N	2.50	0.43
1:B:166:ILE:HD12	1:B:216:ARG:HG2	2.00	0.43
1:B:388:ILE:HD11	1:B:403:VAL:HG23	2.00	0.43
1:A:103:GLN:HB3	1:D:103:GLN:HE22	1.83	0.43
1:D:390:ALA:HB2	1:D:405:ALA:HB1	2.01	0.43
1:B:128:ASN:ND2	11:B:644:HOH:O	2.52	0.43
1:C:134:ASP:OD1	1:C:135:TRP:N	2.51	0.43
1:D:62:ARG:NH2	1:D:168:LEU:C	2.72	0.42
1:D:237:GLU:HB2	1:D:414:LEU:HB3	2.01	0.42
1:C:212:ASP:O	1:C:216:ARG:HB2	2.19	0.42
1:A:76:LEU:HB2	1:A:147:PHE:HE2	1.84	0.42
1:B:93:LEU:HD11	1:B:177:PHE:HD1	1.84	0.42
1:D:385:THR:HB	1:D:403:VAL:HG12	2.02	0.42
1:C:222:LEU:HB3	1:C:223:PRO:HD2	2.00	0.42
1:A:134:ASP:OD1	1:A:135:TRP:N	2.53	0.41
1:A:225:GLU:HG2	1:A:425:ARG:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ALA:HB2	1:B:405:ALA:HB1	2.02	0.41
1:C:225:GLU:HG2	1:C:425:ARG:HG2	2.01	0.41
1:D:87:TYR:HB3	1:D:90:GLU:HB3	2.03	0.41
1:A:212:ASP:O	1:A:216:ARG:HB2	2.21	0.41
1:C:359:LYS:HZ3	1:C:359:LYS:HB3	1.83	0.41
1:C:222:LEU:HD22	1:D:17:TYR:CZ	2.55	0.41
1:B:134:ASP:OD1	1:B:135:TRP:N	2.51	0.41
1:D:317:LYS:HD3	1:D:328:THR:OG1	2.20	0.41
1:A:218:ARG:CZ	1:B:21:ASN:OD1	2.69	0.40
1:A:385:THR:HB	1:A:403:VAL:HG12	2.04	0.40
1:B:237:GLU:HB2	1:B:414:LEU:HB3	2.03	0.40
1:A:222:LEU:HB3	1:A:223:PRO:HD2	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	434/436 (100%)	421 (97%)	13 (3%)	0	100	100
1	B	434/436 (100%)	421 (97%)	13 (3%)	0	100	100
1	C	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
1	D	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
All	All	1736/1744 (100%)	1686 (97%)	50 (3%)	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	357/357 (100%)	353 (99%)	4 (1%)	78	82
1	B	357/357 (100%)	353 (99%)	4 (1%)	78	82
1	C	357/357 (100%)	354 (99%)	3 (1%)	85	88
1	D	357/357 (100%)	354 (99%)	3 (1%)	85	88
All	All	1428/1428 (100%)	1414 (99%)	14 (1%)	80	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	201	THR
1	A	207	ASP
1	A	399	ASN
1	B	29	THR
1	B	207	ASP
1	B	222	LEU
1	B	399	ASN
1	C	58	THR
1	C	207	ASP
1	C	399	ASN
1	D	207	ASP
1	D	222	LEU
1	D	399	ASN

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

Mol	Chain	Res	Type
1	A	103	GLN
1	B	128	ASN
1	C	256	ASN
1	D	103	GLN

5.3.3 RNA ⓘ

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](#)

Of 106 ligands modelled in this entry, 4 are monoatomic - leaving 102 for Mogul analysis.

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	$\# Z > 2$
3	BGC	A	502	1,5,4	11,11,12	0.21	0	13,15,17	0.85	0
4	FUC	A	503	3,5,7,6	9,10,11	0.35	0	13,14,16	0.74	0
5	XYP	A	504	9,4	9,9,10	0.20	0	10,12,14	0.40	0
5	XYP	A	505	3	9,9,10	0.19	0	10,12,14	0.68	0
6	GLA	A	506	4	11,11,12	0.23	0	13,15,17	0.66	0
7	XXR	A	507	8,4	9,10,11	0.17	0	13,14,16	0.42	0
8	MAN	A	508	7	11,11,12	0.28	0	13,15,17	0.69	0
9	RM4	A	509	10,5	9,10,11	0.28	0	13,14,16	0.52	0
10	7CV	A	510	9	11,12,13	0.70	0	15,16,18	0.25	0
3	BGC	A	511	1,5,4	11,11,12	0.40	0	13,15,17	0.82	0
4	FUC	A	512	3,5,7,6	9,10,11	0.28	0	13,14,16	0.77	0
5	XYP	A	513	9,4	9,9,10	0.20	0	10,12,14	0.41	0
5	XYP	A	514	3	9,9,10	0.20	0	10,12,14	0.42	0
6	GLA	A	515	4	11,11,12	0.23	0	13,15,17	0.50	0
7	XXR	A	516	8,4	9,10,11	0.20	0	13,14,16	0.37	0
8	MAN	A	517	7	11,11,12	0.27	0	13,15,17	0.58	0
9	RM4	A	518	10,5	9,10,11	0.29	0	13,14,16	0.52	0
10	7CV	A	519	9	11,12,13	0.69	0	15,16,18	0.27	0
3	BGC	A	520	1,5,4	11,11,12	0.22	0	13,15,17	0.72	0
4	FUC	A	521	3,5,7,6	9,10,11	0.29	0	13,14,16	0.61	0
5	XYP	A	522	4	9,9,10	0.22	0	10,12,14	0.41	0
5	XYP	A	523	3	9,9,10	0.20	0	10,12,14	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GLA	A	524	4	11,11,12	0.18	0	13,15,17	0.86	0
7	XXR	A	525	8,4	9,10,11	0.19	0	13,14,16	0.34	0
8	MAN	A	526	7	11,11,12	0.25	0	13,15,17	0.67	0
3	BGC	A	527	1,4	11,11,12	0.51	0	13,15,17	0.75	0
4	FUC	A	528	3	9,10,11	0.28	0	13,14,16	0.70	0
3	BGC	B	502	1,5,4	11,11,12	0.23	0	13,15,17	0.61	0
4	FUC	B	503	3,5,7,6	9,10,11	0.27	0	13,14,16	0.65	0
5	XYP	B	504	9,4	9,9,10	0.20	0	10,12,14	0.41	0
5	XYP	B	505	3	9,9,10	0.27	0	10,12,14	0.73	0
6	GLA	B	506	4	11,11,12	0.25	0	13,15,17	0.83	0
7	XXR	B	507	4	9,10,11	0.20	0	13,14,16	0.36	0
9	RM4	B	508	5	9,10,11	0.27	0	13,14,16	0.51	0
3	BGC	B	509	1,5,4	11,11,12	0.54	0	13,15,17	0.74	0
4	FUC	B	510	3,5,7,6	9,10,11	0.35	0	13,14,16	1.01	0
5	XYP	B	511	9,4	9,9,10	0.22	0	10,12,14	0.40	0
5	XYP	B	512	3	9,9,10	0.25	0	10,12,14	0.43	0
6	GLA	B	513	4	11,11,12	0.19	0	13,15,17	0.77	0
7	XXR	B	514	8,4	9,10,11	0.20	0	13,14,16	0.39	0
8	MAN	B	515	7	11,11,12	0.29	0	13,15,17	0.59	0
9	RM4	B	516	10,5	9,10,11	0.28	0	13,14,16	0.51	0
10	7CV	B	517	9	11,12,13	0.70	0	15,16,18	0.31	0
3	BGC	B	518	1,5,4	11,11,12	0.23	0	13,15,17	0.66	0
4	FUC	B	519	3,5,7,6	9,10,11	0.32	0	13,14,16	0.51	0
5	XYP	B	520	4	9,9,10	0.21	0	10,12,14	0.52	0
5	XYP	B	521	3	9,9,10	0.20	0	10,12,14	0.45	0
6	GLA	B	522	4	11,11,12	0.25	0	13,15,17	0.47	0
7	XXR	B	523	8,4	9,10,11	0.18	0	13,14,16	0.38	0
8	MAN	B	524	7	11,11,12	0.29	0	13,15,17	0.62	0
3	BGC	B	525	1,4	11,11,12	0.25	0	13,15,17	0.68	0
4	FUC	B	526	3	9,10,11	0.29	0	13,14,16	0.66	0
3	BGC	C	502	1,5,4	11,11,12	0.37	0	13,15,17	0.71	0
4	FUC	C	503	3,5,7,6	9,10,11	0.50	0	13,14,16	0.87	0
5	XYP	C	504	4	9,9,10	0.20	0	10,12,14	0.40	0
5	XYP	C	505	3	9,9,10	0.25	0	10,12,14	0.56	0
6	GLA	C	506	4	11,11,12	0.23	0	13,15,17	0.47	0
7	XXR	C	507	8,4	9,10,11	0.20	0	13,14,16	0.29	0
8	MAN	C	508	7	11,11,12	0.27	0	13,15,17	0.54	0
3	BGC	C	509	1,5,4	11,11,12	0.59	0	13,15,17	1.05	0
4	FUC	C	510	3,5,7,6	9,10,11	0.33	0	13,14,16	0.72	0
5	XYP	C	511	9,4	9,9,10	0.36	0	10,12,14	0.83	0
5	XYP	C	512	3	9,9,10	0.34	0	10,12,14	0.43	0
6	GLA	C	513	4	11,11,12	0.21	0	13,15,17	0.64	0
7	XXR	C	514	8,4	9,10,11	0.21	0	13,14,16	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	C	515	7	11,11,12	0.30	0	13,15,17	0.71	0
9	RM4	C	516	10,5	9,10,11	0.28	0	13,14,16	0.51	0
10	7CV	C	517	9	11,12,13	0.71	0	15,16,18	0.61	0
3	BGC	C	518	1,5,4	11,11,12	0.27	0	13,15,17	0.69	0
4	FUC	C	519	3,5,7,6	9,10,11	0.27	0	13,14,16	0.61	0
5	XYP	C	520	4	9,9,10	0.21	0	10,12,14	0.41	0
5	XYP	C	521	3	9,9,10	0.22	0	10,12,14	0.69	0
6	GLA	C	522	4	11,11,12	0.24	0	13,15,17	0.48	0
7	XXR	C	523	8,4	9,10,11	0.19	0	13,14,16	0.29	0
8	MAN	C	524	7	11,11,12	0.26	0	13,15,17	0.53	0
3	BGC	C	525	1	11,11,12	0.26	0	13,15,17	0.47	0
3	BGC	D	502	1,5,4	11,11,12	0.27	0	13,15,17	0.55	0
4	FUC	D	503	3,5,7,6	9,10,11	0.36	0	13,14,16	0.85	0
5	XYP	D	504	9,4	9,9,10	0.22	0	10,12,14	0.40	0
5	XYP	D	505	3	9,9,10	0.26	0	10,12,14	0.44	0
6	GLA	D	506	4	11,11,12	0.19	0	13,15,17	0.75	0
7	XXR	D	507	8,4	9,10,11	0.20	0	13,14,16	0.30	0
8	MAN	D	508	7	11,11,12	0.25	0	13,15,17	0.64	0
9	RM4	D	509	5	9,10,11	0.29	0	13,14,16	0.51	0
3	BGC	D	510	1,5,4	11,11,12	0.26	0	13,15,17	0.54	0
4	FUC	D	511	3,5,7,6	9,10,11	0.33	0	13,14,16	0.72	0
5	XYP	D	512	9,4	9,9,10	0.22	0	10,12,14	0.53	0
5	XYP	D	513	3	9,9,10	0.21	0	10,12,14	0.35	0
6	GLA	D	514	4	11,11,12	0.26	0	13,15,17	0.54	0
7	XXR	D	515	8,4	9,10,11	0.45	0	13,14,16	0.57	0
8	MAN	D	516	7	11,11,12	0.26	0	13,15,17	0.64	0
9	RM4	D	517	10,5	9,10,11	0.32	0	13,14,16	0.83	0
10	7CV	D	518	9	11,12,13	0.70	0	15,16,18	0.27	0
3	BGC	D	519	1,5,4	11,11,12	0.34	0	13,15,17	0.80	0
4	FUC	D	520	3,5,7,6	9,10,11	0.30	0	13,14,16	0.67	0
5	XYP	D	521	4	9,9,10	0.21	0	10,12,14	0.44	0
5	XYP	D	522	3	9,9,10	0.20	0	10,12,14	0.56	0
6	GLA	D	523	4	11,11,12	0.24	0	13,15,17	0.47	0
7	XXR	D	524	8,4	9,10,11	0.19	0	13,14,16	0.29	0
8	MAN	D	525	7	11,11,12	0.21	0	13,15,17	0.70	0
3	BGC	D	526	1,4	11,11,12	0.41	0	13,15,17	0.83	0
4	FUC	D	527	3	9,10,11	0.29	0	13,14,16	0.68	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
3	BGC	A	502	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	A	503	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	A	504	9,4	-	0/0/14/17	0/1/1/1
5	XYP	A	505	3	-	0/0/14/17	0/1/1/1
6	GLA	A	506	4	-	0/2/19/22	0/1/1/1
7	XXR	A	507	8,4	-	0/0/17/20	0/1/1/1
8	MAN	A	508	7	-	0/2/19/22	0/1/1/1
9	RM4	A	509	10,5	-	0/0/17/20	0/1/1/1
10	7CV	A	510	9	-	0/4/21/24	0/1/1/1
3	BGC	A	511	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	A	512	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	A	513	9,4	-	0/0/14/17	0/1/1/1
5	XYP	A	514	3	-	0/0/14/17	0/1/1/1
6	GLA	A	515	4	-	0/2/19/22	0/1/1/1
7	XXR	A	516	8,4	-	0/0/17/20	0/1/1/1
8	MAN	A	517	7	-	0/2/19/22	0/1/1/1
9	RM4	A	518	10,5	-	0/0/17/20	0/1/1/1
10	7CV	A	519	9	-	0/4/21/24	0/1/1/1
3	BGC	A	520	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	A	521	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	A	522	4	-	0/0/14/17	0/1/1/1
5	XYP	A	523	3	-	0/0/14/17	0/1/1/1
6	GLA	A	524	4	-	0/2/19/22	0/1/1/1
7	XXR	A	525	8,4	-	0/0/17/20	0/1/1/1
8	MAN	A	526	7	-	0/2/19/22	0/1/1/1
3	BGC	A	527	1,4	-	0/2/19/22	0/1/1/1
4	FUC	A	528	3	-	0/0/17/20	0/1/1/1
3	BGC	B	502	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	B	503	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	B	504	9,4	-	0/0/14/17	0/1/1/1
5	XYP	B	505	3	-	0/0/14/17	0/1/1/1
6	GLA	B	506	4	-	0/2/19/22	0/1/1/1
7	XXR	B	507	4	-	0/0/17/20	0/1/1/1
9	RM4	B	508	5	-	0/0/17/20	0/1/1/1
3	BGC	B	509	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	B	510	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	B	511	9,4	-	0/0/14/17	0/1/1/1
5	XYP	B	512	3	-	0/0/14/17	0/1/1/1
6	GLA	B	513	4	-	0/2/19/22	0/1/1/1
7	XXR	B	514	8,4	-	0/0/17/20	0/1/1/1
8	MAN	B	515	7	-	0/2/19/22	0/1/1/1
9	RM4	B	516	10,5	-	0/0/17/20	0/1/1/1
10	7CV	B	517	9	-	0/4/21/24	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	B	518	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	B	519	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	B	520	4	-	0/0/14/17	0/1/1/1
5	XYP	B	521	3	-	0/0/14/17	0/1/1/1
6	GLA	B	522	4	-	0/2/19/22	0/1/1/1
7	XXR	B	523	8,4	-	0/0/17/20	0/1/1/1
8	MAN	B	524	7	-	0/2/19/22	0/1/1/1
3	BGC	B	525	1,4	-	0/2/19/22	0/1/1/1
4	FUC	B	526	3	-	0/0/17/20	0/1/1/1
3	BGC	C	502	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	C	503	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	C	504	4	-	0/0/14/17	0/1/1/1
5	XYP	C	505	3	-	0/0/14/17	0/1/1/1
6	GLA	C	506	4	-	0/2/19/22	0/1/1/1
7	XXR	C	507	8,4	-	0/0/17/20	0/1/1/1
8	MAN	C	508	7	-	0/2/19/22	0/1/1/1
3	BGC	C	509	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	C	510	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	C	511	9,4	-	0/0/14/17	0/1/1/1
5	XYP	C	512	3	-	0/0/14/17	0/1/1/1
6	GLA	C	513	4	-	0/2/19/22	0/1/1/1
7	XXR	C	514	8,4	-	0/0/17/20	0/1/1/1
8	MAN	C	515	7	-	0/2/19/22	0/1/1/1
9	RM4	C	516	10,5	-	0/0/17/20	0/1/1/1
10	7CV	C	517	9	-	0/4/21/24	0/1/1/1
3	BGC	C	518	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	C	519	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	C	520	4	-	0/0/14/17	0/1/1/1
5	XYP	C	521	3	-	0/0/14/17	0/1/1/1
6	GLA	C	522	4	-	0/2/19/22	0/1/1/1
7	XXR	C	523	8,4	-	0/0/17/20	0/1/1/1
8	MAN	C	524	7	-	0/2/19/22	0/1/1/1
3	BGC	C	525	1	-	0/2/19/22	0/1/1/1
3	BGC	D	502	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	D	503	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	D	504	9,4	-	0/0/14/17	0/1/1/1
5	XYP	D	505	3	-	0/0/14/17	0/1/1/1
6	GLA	D	506	4	-	0/2/19/22	0/1/1/1
7	XXR	D	507	8,4	-	0/0/17/20	0/1/1/1
8	MAN	D	508	7	-	0/2/19/22	0/1/1/1
9	RM4	D	509	5	-	0/0/17/20	0/1/1/1
3	BGC	D	510	1,5,4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	D	511	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	D	512	9,4	-	0/0/14/17	0/1/1/1
5	XYP	D	513	3	-	0/0/14/17	0/1/1/1
6	GLA	D	514	4	-	0/2/19/22	0/1/1/1
7	XXR	D	515	8,4	-	0/0/17/20	0/1/1/1
8	MAN	D	516	7	-	0/2/19/22	0/1/1/1
9	RM4	D	517	10,5	-	0/0/17/20	0/1/1/1
10	7CV	D	518	9	-	0/4/21/24	0/1/1/1
3	BGC	D	519	1,5,4	-	0/2/19/22	0/1/1/1
4	FUC	D	520	3,5,7,6	-	0/0/17/20	0/1/1/1
5	XYP	D	521	4	-	0/0/14/17	0/1/1/1
5	XYP	D	522	3	-	0/0/14/17	0/1/1/1
6	GLA	D	523	4	-	0/2/19/22	0/1/1/1
7	XXR	D	524	8,4	-	0/0/17/20	0/1/1/1
8	MAN	D	525	7	-	0/2/19/22	0/1/1/1
3	BGC	D	526	1,4	-	0/2/19/22	0/1/1/1
4	FUC	D	527	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/436 (100%)	-0.33	1 (0%) 94 94	19, 30, 46, 73	0
1	B	436/436 (100%)	-0.23	4 (0%) 84 83	21, 34, 52, 122	0
1	C	436/436 (100%)	-0.25	2 (0%) 90 90	23, 35, 52, 94	0
1	D	436/436 (100%)	-0.23	5 (1%) 80 80	22, 34, 55, 85	0
All	All	1744/1744 (100%)	-0.26	12 (0%) 87 87	19, 34, 52, 122	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	4.4
1	B	21	ASN	4.3
1	D	2	ALA	3.8
1	D	437	ASN	3.3
1	D	9	VAL	3.2
1	C	2	ALA	3.2
1	B	320	LEU	2.8
1	D	5	LEU	2.8
1	C	9	VAL	2.6
1	D	213	THR	2.6
1	B	11	TYR	2.5
1	A	21	ASN	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GLA	D	514	11/12	0.92	0.12	1.47	34,37,39,42	0
6	GLA	B	513	11/12	0.90	0.12	1.11	32,33,35,38	0
6	GLA	C	513	11/12	0.91	0.12	0.96	32,35,38,38	0
2	HG	A	501	1/1	0.95	0.13	0.94	42,42,42,42	1
3	BGC	D	502	11/12	0.88	0.10	0.76	24,28,34,39	0
6	GLA	C	522	11/12	0.88	0.12	0.69	45,47,49,49	0
6	GLA	D	523	11/12	0.93	0.12	0.57	34,37,39,39	0
6	GLA	A	515	11/12	0.94	0.09	0.54	31,33,37,38	0
6	GLA	B	522	11/12	0.93	0.11	0.45	33,36,42,45	0
3	BGC	D	510	11/12	0.91	0.09	0.12	28,35,37,42	0
3	BGC	B	502	11/12	0.93	0.10	-0.04	27,34,40,41	0
3	BGC	A	520	11/12	0.92	0.10	-0.18	27,30,34,34	0
2	HG	D	501	1/1	0.91	0.12	-0.29	49,49,49,49	1
3	BGC	A	502	11/12	0.91	0.10	-0.29	25,29,34,37	0
6	GLA	A	524	11/12	0.94	0.09	-0.38	28,33,36,36	0
3	BGC	B	509	11/12	0.95	0.09	-0.69	26,30,34,34	0
3	BGC	C	502	11/12	0.89	0.10	-0.75	31,35,42,47	0
2	HG	B	501	1/1	0.94	0.08	-1.00	46,46,46,46	1
3	BGC	D	519	11/12	0.89	0.09	-1.19	32,38,40,43	0
2	HG	C	501	1/1	0.95	0.09	-1.27	45,45,45,45	1
3	BGC	A	511	11/12	0.94	0.08	-1.32	23,30,32,37	0
3	BGC	C	518	11/12	0.87	0.09	-1.48	30,36,39,42	0
3	BGC	C	509	11/12	0.93	0.08	-1.90	33,36,42,45	0
3	BGC	B	518	11/12	0.92	0.08	-2.19	27,32,36,40	0
4	FUC	C	503	10/11	0.86	0.10	-	48,51,58,60	0
9	RM4	D	517	10/11	0.94	0.10	-	43,46,48,52	0
8	MAN	C	508	11/12	0.72	0.20	-	70,71,75,76	0
4	FUC	A	528	10/11	0.75	0.19	-	70,74,78,83	0
3	BGC	B	525	11/12	0.83	0.16	-	45,54,62,64	0
5	XYP	A	522	9/10	0.90	0.14	-	47,51,53,56	0
5	XYP	B	521	9/10	0.84	0.13	-	39,40,42,43	0
9	RM4	A	509	10/11	0.89	0.18	-	59,64,69,70	0
4	FUC	B	503	10/11	0.90	0.10	-	40,44,52,58	0
4	FUC	B	526	10/11	0.67	0.21	-	62,68,70,71	0
7	XXR	A	507	10/11	0.89	0.11	-	38,44,46,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	7CV	A	510	12/13	0.81	0.16	-	57,60,62,64	0
5	XYP	D	512	9/10	0.95	0.10	-	33,35,39,41	0
9	RM4	D	509	10/11	0.85	0.26	-	84,90,93,97	0
8	MAN	A	508	11/12	0.86	0.15	-	54,59,61,61	0
8	MAN	A	517	11/12	0.85	0.12	-	38,43,45,49	0
5	XYP	C	504	9/10	0.76	0.16	-	62,63,65,67	0
3	BGC	A	527	11/12	0.86	0.12	-	43,51,57,63	0
5	XYP	D	522	9/10	0.80	0.15	-	41,48,51,52	0
3	BGC	C	525	11/12	0.83	0.18	-	48,57,65,66	0
5	XYP	A	513	9/10	0.93	0.10	-	26,28,32,36	0
7	XXR	C	514	10/11	0.91	0.11	-	42,44,46,49	0
7	XXR	A	525	10/11	0.89	0.10	-	50,54,62,64	0
4	FUC	B	510	10/11	0.96	0.07	-	29,31,35,37	0
5	XYP	A	505	9/10	0.91	0.11	-	31,33,37,38	0
6	GLA	D	506	11/12	0.86	0.12	-	40,42,46,47	0
6	GLA	B	506	11/12	0.90	0.12	-	35,40,46,47	0
5	XYP	D	505	9/10	0.91	0.09	-	32,36,40,42	0
7	XXR	B	514	10/11	0.90	0.10	-	38,42,43,47	0
9	RM4	B	516	10/11	0.88	0.15	-	48,52,53,54	0
7	XXR	D	507	10/11	0.91	0.14	-	53,56,60,61	0
8	MAN	B	515	11/12	0.82	0.11	-	40,51,58,61	0
7	XXR	C	507	10/11	0.83	0.14	-	62,64,67,69	0
5	XYP	B	511	9/10	0.95	0.09	-	29,33,39,42	0
5	XYP	B	520	9/10	0.77	0.14	-	58,61,62,62	0
5	XYP	D	521	9/10	0.86	0.13	-	47,49,52,53	0
5	XYP	B	505	9/10	0.87	0.13	-	38,40,45,45	0
10	7CV	A	519	12/13	0.88	0.13	-	31,38,40,41	0
5	XYP	D	513	9/10	0.89	0.13	-	45,49,51,52	0
5	XYP	A	504	9/10	0.83	0.11	-	41,44,50,56	0
5	XYP	C	511	9/10	0.89	0.10	-	33,38,43,46	0
4	FUC	A	521	10/11	0.89	0.12	-	34,39,45,45	0
5	XYP	C	505	9/10	0.87	0.11	-	36,39,41,43	0
5	XYP	C	521	9/10	0.81	0.13	-	43,44,45,46	0
7	XXR	B	507	10/11	0.87	0.12	-	41,44,46,47	0
5	XYP	D	504	9/10	0.66	0.16	-	64,68,74,79	0
8	MAN	D	516	11/12	0.89	0.12	-	48,53,57,61	0
10	7CV	C	517	12/13	0.86	0.13	-	51,55,61,62	0
5	XYP	C	512	9/10	0.86	0.11	-	50,55,56,58	0
4	FUC	C	510	10/11	0.94	0.07	-	33,35,38,38	0
5	XYP	A	523	9/10	0.88	0.12	-	36,37,40,40	0
4	FUC	A	503	10/11	0.92	0.10	-	35,40,41,45	0
4	FUC	B	519	10/11	0.89	0.10	-	36,42,48,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	XXR	D	515	10/11	0.94	0.10	-	39,44,49,49	0
4	FUC	A	512	10/11	0.93	0.09	-	25,27,28,32	0
5	XYP	A	514	9/10	0.90	0.11	-	34,38,43,45	0
4	FUC	D	511	10/11	0.95	0.08	-	33,35,38,41	0
9	RM4	C	516	10/11	0.88	0.14	-	46,49,52,53	0
9	RM4	A	518	10/11	0.91	0.10	-	38,41,43,46	0
10	7CV	B	517	12/13	0.86	0.15	-	40,48,53,54	0
3	BGC	D	526	11/12	0.81	0.12	-	41,54,57,67	0
5	XYP	B	512	9/10	0.91	0.10	-	38,40,43,44	0
4	FUC	D	520	10/11	0.89	0.09	-	38,40,41,47	0
4	FUC	D	503	10/11	0.90	0.09	-	40,45,52,59	0
8	MAN	A	526	11/12	0.74	0.16	-	69,73,78,79	0
8	MAN	C	524	11/12	0.84	0.15	-	66,70,73,74	0
7	XXR	B	523	10/11	0.85	0.13	-	55,60,62,65	0
8	MAN	B	524	11/12	0.72	0.16	-	71,77,82,83	0
6	GLA	C	506	11/12	0.87	0.14	-	44,45,48,51	0
6	GLA	A	506	11/12	0.94	0.11	-	31,32,37,42	0
8	MAN	D	508	11/12	0.83	0.18	-	66,69,72,73	0
9	RM4	B	508	10/11	0.69	0.24	-	70,73,76,79	0
4	FUC	C	519	10/11	0.92	0.09	-	42,46,51,51	0
5	XYP	B	504	9/10	0.74	0.13	-	62,65,67,67	0
8	MAN	C	515	11/12	0.84	0.12	-	49,56,59,60	0
5	XYP	C	520	9/10	0.89	0.14	-	56,60,62,62	0
8	MAN	D	525	11/12	0.83	0.15	-	75,77,80,83	0
7	XXR	A	516	10/11	0.96	0.09	-	31,36,39,41	0
10	7CV	D	518	12/13	0.95	0.10	-	41,46,49,50	0
7	XXR	D	524	10/11	0.86	0.15	-	49,59,66,69	0
7	XXR	C	523	10/11	0.87	0.14	-	55,59,61,63	0
4	FUC	D	527	10/11	0.66	0.24	-	77,85,88,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.