



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:48 PM GMT

PDB ID : 1M3Y
Title : The Structure of Major Capsid protein of a large, lipid containing, DNA virus
Authors : Nandhagopal, N.; Simpson, A.A.; Gurnon, J.R.; Yan, X.; Baker, T.S.; Graves, M.V.; Van Etten, J.L.; Rossmann, M.G.
Deposited on : 2002-07-01
Resolution : 2.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

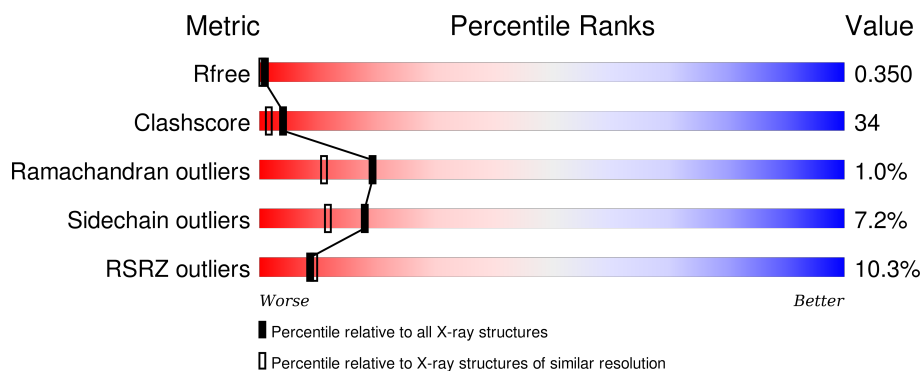
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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	413	<div> <div>9%</div> <div>53%</div> <div>42%</div> <div>5%</div> </div>
1	B	413	<div> <div>9%</div> <div>56%</div> <div>39%</div> <div>5%</div> </div>
1	C	413	<div> <div>10%</div> <div>55%</div> <div>39%</div> <div>6%</div> </div>
1	D	413	<div> <div>12%</div> <div>55%</div> <div>40%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	A	438	-	-	X	X
2	NDG	A	442	-	-	X	X
2	NDG	B	538	-	-	X	X
2	NDG	B	542	-	-	-	X
2	NDG	C	638	-	-	X	X
2	NDG	C	642	-	-	X	-
2	NDG	D	738	-	-	X	X
2	NDG	D	742	-	-	X	X
3	MAN	A	439	-	-	X	-
3	MAN	B	539	-	-	X	-
3	MAN	D	739	-	-	X	-
4	NAG	A	440	-	-	X	-
4	NAG	B	540	-	-	X	-
4	NAG	C	640	-	-	X	-
4	NAG	D	740	-	-	X	-
5	HG	C	644	-	-	-	X
5	HG	D	744	-	-	-	X

2 Entry composition [i](#)

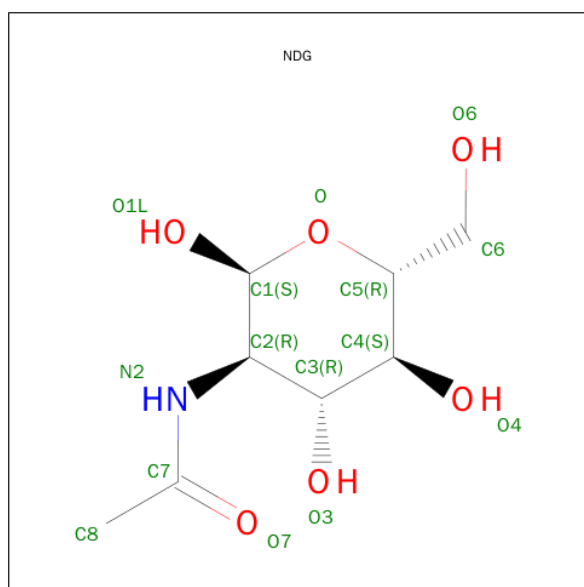
There are 6 unique types of molecules in this entry. The entry contains 13261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 The Major capsid protein of PBCV-1, Vp54.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			
1	B	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			
1	C	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			
1	D	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



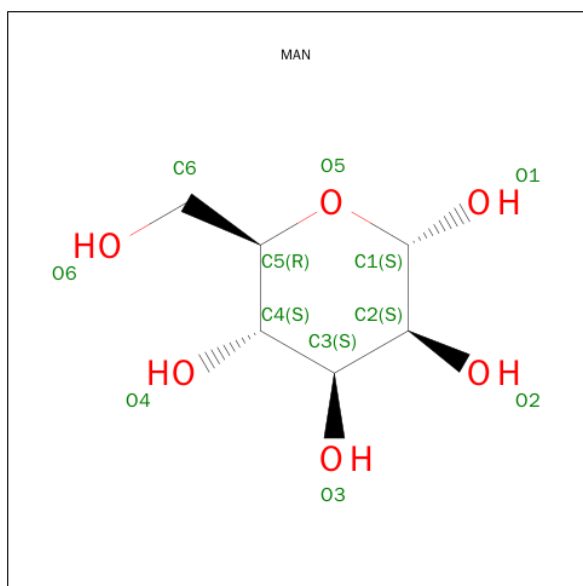
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	C	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Hg	0	0
			2	2		
5	A	2	Total	Hg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total 2	Hg 2	0	0
5	C	2	Total 2	Hg 2	0	0

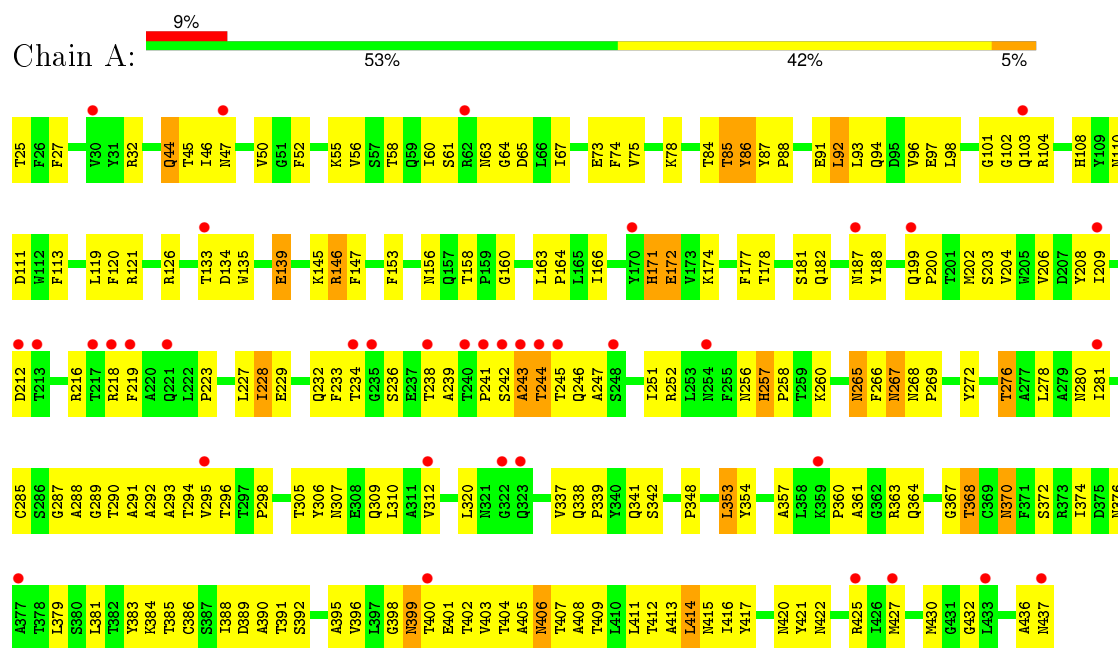
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total 24	O 24	0	0
6	B	9	Total 9	O 9	0	0
6	C	8	Total 8	O 8	0	0
6	D	12	Total 12	O 12	0	0

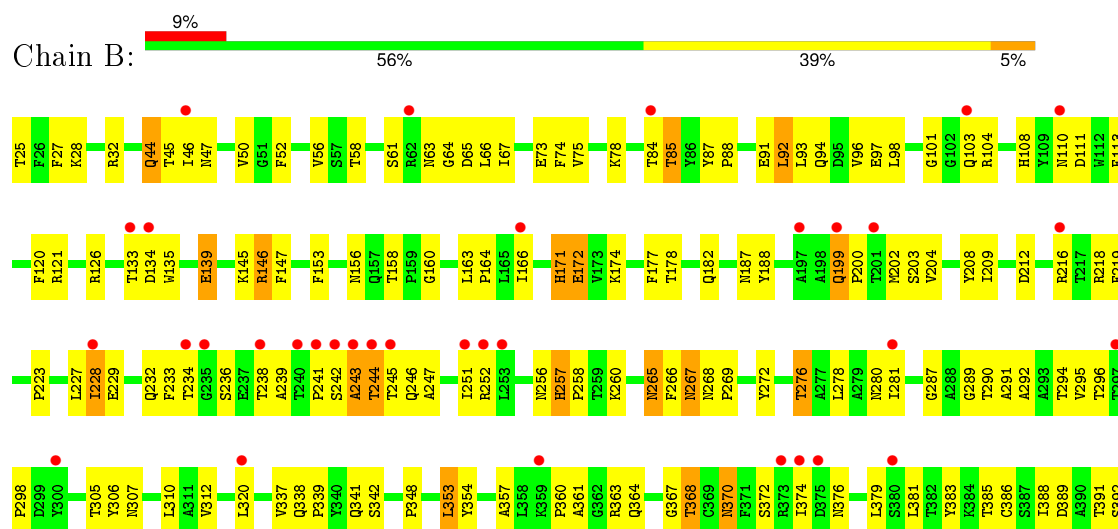
3 Residue-property plots

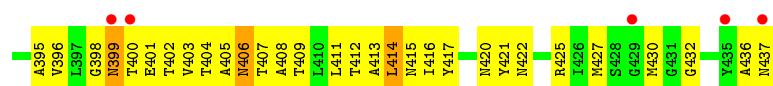
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: The Major capsid protein of PBCV-1, Vp54

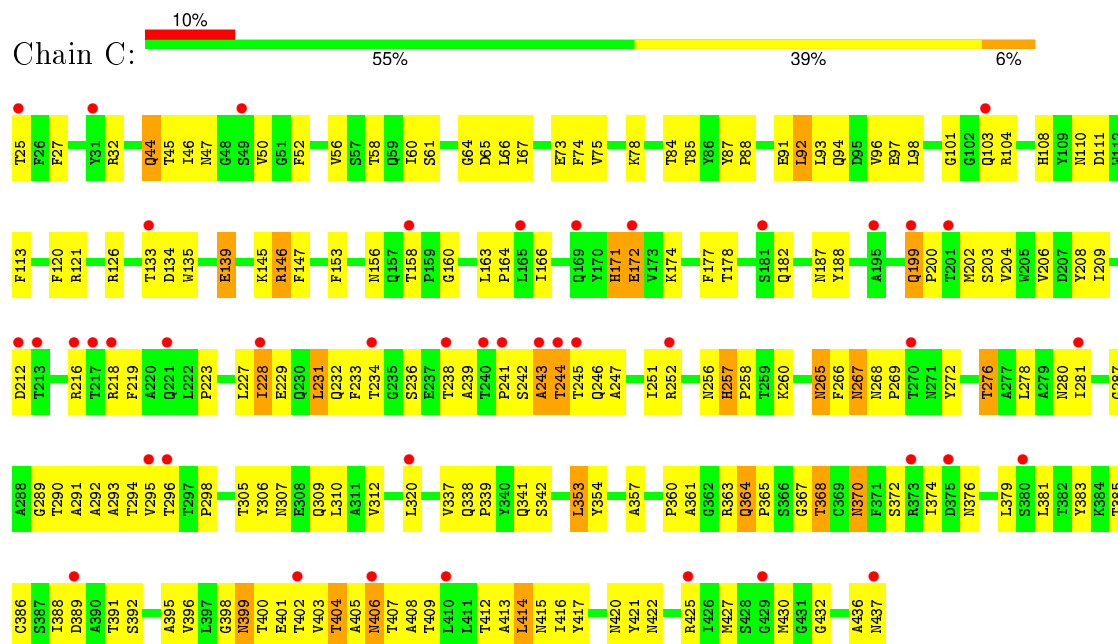


- Molecule 1: The Major capsid protein of PBCV-1, Vp54

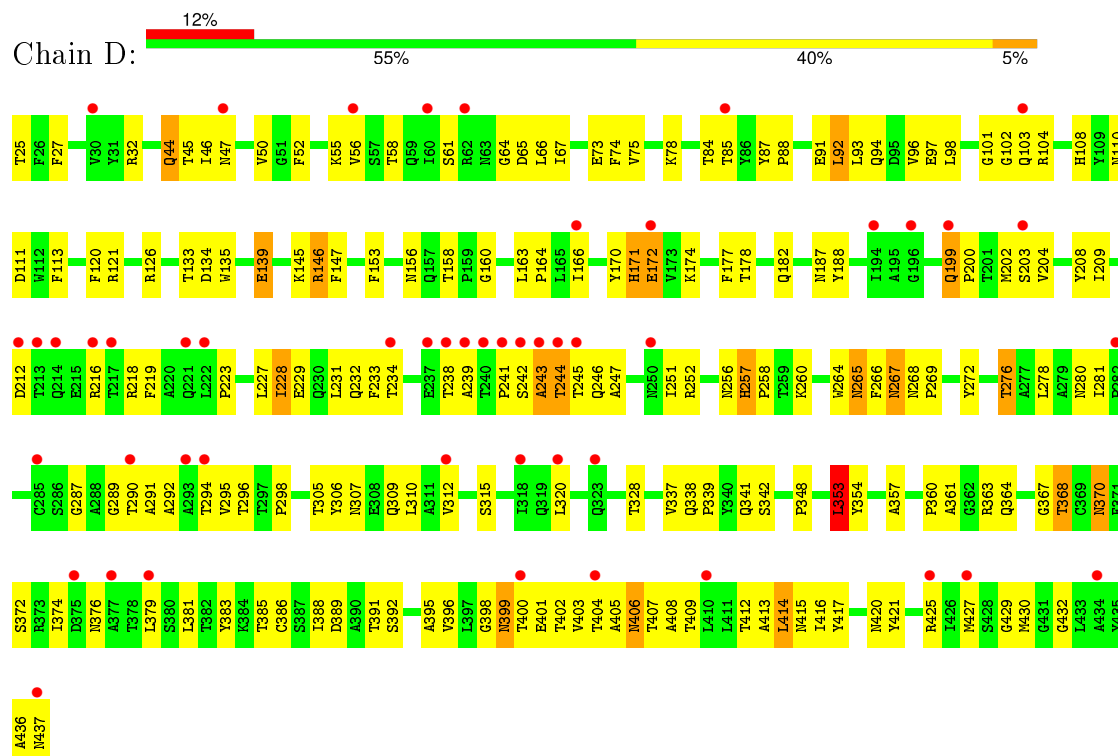




• Molecule 1: The Major capsid protein of PBCV-1, Vp54



• Molecule 1: The Major capsid protein of PBCV-1, Vp54



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)	92.4 (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	CNS 1.0	Depositor
R, R_{free}	0.342 , 0.352 0.342 , 0.350	Depositor DCC
R_{free} test set	4095 reflections (3.03%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.9	EDS
Estimated twinning fraction	0.278 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 146411 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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, 0.375 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: HG, NAG, NDG, 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	0.44	3/3306 (0.1%)	0.68	4/4506 (0.1%)
1	B	0.40	0/3306	0.65	1/4506 (0.0%)
1	C	0.39	0/3306	0.64	1/4506 (0.0%)
1	D	0.39	0/3306	0.65	1/4506 (0.0%)
All	All	0.41	3/13224 (0.0%)	0.66	7/18024 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	LEU	CG-CD2	-7.86	1.22	1.51
1	A	86	TYR	CE1-CZ	6.26	1.46	1.38
1	A	86	TYR	CD1-CE1	-5.79	1.30	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TYR	CG-CD1-CE1	-9.57	113.64	121.30
1	A	119	LEU	CB-CG-CD2	-7.96	97.46	111.00
1	C	353	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	86	TYR	CE1-CZ-CE2	-5.71	110.66	119.80
1	A	353	LEU	CA-CB-CG	5.66	128.31	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3231	0	3128	221	0
1	B	3231	0	3128	208	0
1	C	3231	0	3128	204	0
1	D	3231	0	3128	220	0
2	A	30	0	30	22	0
2	B	30	0	30	18	0
2	C	30	0	30	22	0
2	D	30	0	30	24	0
3	A	24	0	24	10	0
3	B	24	0	24	11	0
3	C	24	0	24	9	0
3	D	24	0	24	11	0
4	A	15	0	15	15	0
4	B	15	0	15	14	0
4	C	15	0	15	14	0
4	D	15	0	15	16	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	1	0
6	A	24	0	0	4	0
6	B	9	0	0	1	0
6	C	8	0	0	1	0
6	D	12	0	0	1	0
All	All	13261	0	12788	887	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 34.

The worst 5 of 887 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)
2:C:638:NDG:H4	3:C:639:MAN:O2	1.45	1.16
2:B:538:NDG:H4	3:B:539:MAN:O2	1.45	1.14
2:D:738:NDG:H4	3:D:739:MAN:O2	1.50	1.11
2:A:438:NDG:H4	3:A:439:MAN:O2	1.49	1.09
2:B:538:NDG:C4	3:B:539:MAN:O2	2.07	1.03

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	411/413 (100%)	375 (91%)	32 (8%)	4 (1%)	19	11
1	B	411/413 (100%)	377 (92%)	30 (7%)	4 (1%)	19	11
1	C	411/413 (100%)	378 (92%)	29 (7%)	4 (1%)	19	11
1	D	411/413 (100%)	378 (92%)	29 (7%)	4 (1%)	19	11
All	All	1644/1652 (100%)	1508 (92%)	120 (7%)	16 (1%)	19	11

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	THR
1	B	244	THR
1	C	244	THR
1	D	244	THR
1	A	272	TYR

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	341/341 (100%)	318 (93%)	23 (7%)	20	14
1	B	341/341 (100%)	317 (93%)	24 (7%)	19	12
1	C	341/341 (100%)	315 (92%)	26 (8%)	16	10
1	D	341/341 (100%)	316 (93%)	25 (7%)	17	11
All	All	1364/1364 (100%)	1266 (93%)	98 (7%)	18	12

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	406	ASN
1	C	171	HIS
1	D	364	GLN
1	B	409	THR
1	C	92	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	323	GLN
1	C	156	ASN
1	D	280	ASN
1	B	370	ASN
1	C	43	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](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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$
2	NDG	A	438	-	15,15,15	1.45	2 (13%)	17,21,21	1.30	2 (11%)
3	MAN	A	439	-	12,12,12	1.58	4 (33%)	17,17,17	1.80	5 (29%)
4	NAG	A	440	-	15,15,15	0.78	0	17,21,21	0.84	0
3	MAN	A	441	-	12,12,12	0.70	0	17,17,17	0.40	0
2	NDG	A	442	-	15,15,15	1.30	2 (13%)	17,21,21	0.77	0
2	NDG	B	538	-	15,15,15	1.18	2 (13%)	17,21,21	1.25	2 (11%)
3	MAN	B	539	-	12,12,12	1.31	0	17,17,17	1.68	4 (23%)
4	NAG	B	540	-	15,15,15	1.00	1 (6%)	17,21,21	0.81	0
3	MAN	B	541	-	12,12,12	0.86	0	17,17,17	0.45	0
2	NDG	B	542	-	15,15,15	1.34	1 (6%)	17,21,21	0.70	0
2	NDG	C	638	-	15,15,15	1.65	3 (20%)	17,21,21	1.33	2 (11%)
3	MAN	C	639	-	12,12,12	1.52	3 (25%)	17,17,17	1.88	5 (29%)
4	NAG	C	640	-	15,15,15	0.97	0	17,21,21	0.80	0
3	MAN	C	641	-	12,12,12	0.70	0	17,17,17	0.47	0
2	NDG	C	642	-	15,15,15	1.46	3 (20%)	17,21,21	0.65	0
2	NDG	D	738	-	15,15,15	1.47	2 (13%)	17,21,21	1.29	2 (11%)
3	MAN	D	739	-	12,12,12	1.55	3 (25%)	17,17,17	1.82	4 (23%)
4	NAG	D	740	-	15,15,15	1.08	1 (6%)	17,21,21	0.87	0
3	MAN	D	741	-	12,12,12	0.71	0	17,17,17	0.45	0
2	NDG	D	742	-	15,15,15	1.38	3 (20%)	17,21,21	0.65	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
2	NDG	A	438	-	-	0/6/26/26	0/1/1/1
3	MAN	A	439	-	-	0/2/22/22	0/1/1/1
4	NAG	A	440	-	-	2/6/26/26	0/1/1/1
3	MAN	A	441	-	-	0/2/22/22	0/1/1/1
2	NDG	A	442	-	-	0/6/26/26	0/1/1/1
2	NDG	B	538	-	-	0/6/26/26	0/1/1/1
3	MAN	B	539	-	-	0/2/22/22	0/1/1/1
4	NAG	B	540	-	-	2/6/26/26	0/1/1/1
3	MAN	B	541	-	-	0/2/22/22	0/1/1/1
2	NDG	B	542	-	-	0/6/26/26	0/1/1/1
2	NDG	C	638	-	-	0/6/26/26	0/1/1/1
3	MAN	C	639	-	-	0/2/22/22	0/1/1/1
4	NAG	C	640	-	-	2/6/26/26	0/1/1/1
3	MAN	C	641	-	-	0/2/22/22	0/1/1/1
2	NDG	C	642	-	-	0/6/26/26	0/1/1/1
2	NDG	D	738	-	-	0/6/26/26	0/1/1/1
3	MAN	D	739	-	-	0/2/22/22	0/1/1/1
4	NAG	D	740	-	-	2/6/26/26	0/1/1/1
3	MAN	D	741	-	-	0/2/22/22	0/1/1/1
2	NDG	D	742	-	-	0/6/26/26	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	638	NDG	C3-C2	2.00	1.57	1.53
2	C	642	NDG	O7-C7	2.04	1.27	1.23
2	D	742	NDG	C3-C2	2.12	1.57	1.53
2	B	538	NDG	C8-C7	2.14	1.54	1.50
3	D	739	MAN	O5-C5	2.16	1.49	1.44

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	739	MAN	C3-C4-C5	-4.31	102.68	110.20
3	C	639	MAN	C3-C4-C5	-4.05	103.14	110.20
3	A	439	MAN	C3-C4-C5	-3.93	103.34	110.20
3	B	539	MAN	C3-C4-C5	-3.80	103.58	110.20
3	A	439	MAN	O2-C2-C1	-3.56	101.98	109.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	640	NAG	C8-C7-N2-C2
4	B	540	NAG	C8-C7-N2-C2
4	A	440	NAG	C8-C7-N2-C2
4	D	740	NAG	C8-C7-N2-C2
4	D	740	NAG	O7-C7-N2-C2

There are no ring outliers.

20 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	438	NDG	15	0
3	A	439	MAN	6	0
4	A	440	NAG	15	0
3	A	441	MAN	4	0
2	A	442	NDG	7	0
2	B	538	NDG	12	0
3	B	539	MAN	7	0
4	B	540	NAG	14	0
3	B	541	MAN	4	0
2	B	542	NDG	6	0
2	C	638	NDG	15	0
3	C	639	MAN	5	0
4	C	640	NAG	14	0
3	C	641	MAN	4	0
2	C	642	NDG	7	0
2	D	738	NDG	16	0
3	D	739	MAN	7	0
4	D	740	NAG	16	0
3	D	741	MAN	4	0
2	D	742	NDG	8	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, 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	413/413 (100%)	0.89	38 (9%)	11 12	22, 34, 47, 61	0
1	B	413/413 (100%)	0.83	39 (9%)	11 11	22, 34, 47, 61	0
1	C	413/413 (100%)	0.85	43 (10%)	8 9	22, 34, 47, 61	0
1	D	413/413 (100%)	0.95	50 (12%)	6 6	22, 34, 47, 61	0
All	All	1652/1652 (100%)	0.88	170 (10%)	9 9	22, 34, 48, 61	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	THR	9.1
1	A	234	THR	9.1
1	B	234	THR	8.2
1	C	244	THR	8.0
1	D	323	GLN	7.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	NDG	D	742	15/15	0.67	0.27	7.75	18,24,34,35	0
2	NDG	B	538	15/15	0.57	0.28	4.91	18,24,34,35	0
5	HG	C	644	1/1	0.89	0.48	4.36	67,67,67,67	0
2	NDG	D	738	15/15	0.54	0.29	3.70	18,24,34,35	0
2	NDG	C	638	15/15	0.64	0.25	3.54	18,24,34,35	0
2	NDG	B	542	15/15	0.68	0.25	3.21	18,24,34,35	0
2	NDG	A	442	15/15	0.68	0.29	2.87	18,24,34,35	0
5	HG	D	744	1/1	0.89	0.45	2.45	67,67,67,67	0
2	NDG	A	438	15/15	0.67	0.21	2.17	18,24,34,35	0
2	NDG	C	642	15/15	0.61	0.32	1.94	18,24,34,35	0
5	HG	A	444	1/1	0.88	0.37	1.74	67,67,67,67	0
4	NAG	C	640	15/15	0.69	0.24	1.30	18,24,34,35	0
4	NAG	A	440	15/15	0.79	0.21	0.92	18,24,34,35	0
4	NAG	D	740	15/15	0.77	0.21	0.87	18,24,34,35	0
5	HG	B	544	1/1	0.93	0.35	0.87	67,67,67,67	0
4	NAG	B	540	15/15	0.80	0.15	-0.65	18,24,34,35	0
5	HG	B	543	1/1	0.97	0.12	-1.25	55,55,55,55	0
5	HG	D	743	1/1	0.97	0.06	-2.91	55,55,55,55	0
5	HG	C	643	1/1	0.98	0.05	-3.67	55,55,55,55	0
5	HG	A	443	1/1	0.96	0.06	-5.32	55,55,55,55	0
3	MAN	C	639	12/12	0.67	0.27	-	15,19,24,34	0
3	MAN	B	541	12/12	0.61	0.26	-	19,24,34,35	0
3	MAN	D	741	12/12	0.74	0.23	-	19,24,34,35	0
3	MAN	A	441	12/12	0.66	0.25	-	19,24,34,35	0
3	MAN	B	539	12/12	0.54	0.34	-	15,19,24,34	0
3	MAN	D	739	12/12	0.56	0.25	-	15,19,24,34	0
3	MAN	A	439	12/12	0.48	0.29	-	15,19,24,34	0
3	MAN	C	641	12/12	0.64	0.32	-	19,24,34,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.