



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:18 AM BST

PDB ID : 6P8M
Title : Crystal Structure of Antibody P-p3b3 A60C Heavy Chain in Complex with
426c HIV-1 gp120 core G459C
Authors : Weidle, C.; Pancera, M.
Deposited on : 2019-06-07
Resolution : 3.59 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

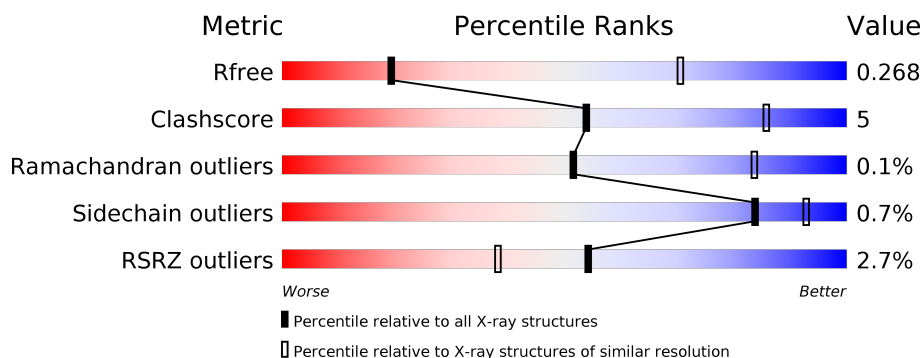
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 respectively. 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	C	347	<div> <div style="width: 84%;"></div> <div style="width: 12%;"></div> <div style="width: 4%;"></div> </div>
2	H	233	<div> <div style="width: 6%;"></div> <div style="width: 82%;"></div> <div style="width: 11%;"></div> <div style="width: 7%;"></div> </div>
3	L	216	<div> <div style="width: 2%;"></div> <div style="width: 81%;"></div> <div style="width: 13%;"></div> <div style="width: 6%;"></div> </div>
4	A	5	<div> <div style="width: 40%;"></div> <div style="width: 60%;"></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
5	NAG	C	1401	-	-	-	X
5	NAG	C	1417	-	-	-	X
6	NH4	C	1403	-	-	-	X
7	EDO	C	1405	-	-	-	X
9	NA	H	302	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 11337 atoms, of which 5469 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 Gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	333	Total	C	H	N	O	S	0	0	0
			4960	1597	2410	438	492	23			

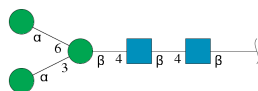
- Molecule 2 is a protein called P-p3b3 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	216	Total	C	H	N	O	S	0	0	0
			3212	1032	1575	283	314	8			

- Molecule 3 is a protein called P-p3b3 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	204	Total	C	H	N	O	S	0	0	0
			2706	900	1255	246	299	6			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



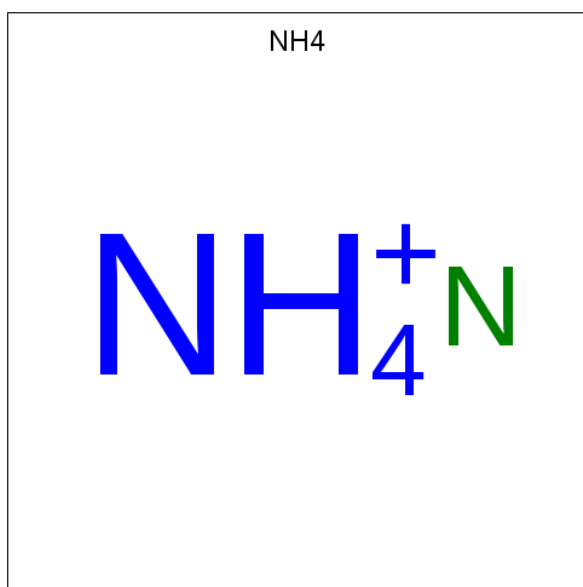
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	5	Total	C	H	N	O		0	0	0
			117	34	56	2	25				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



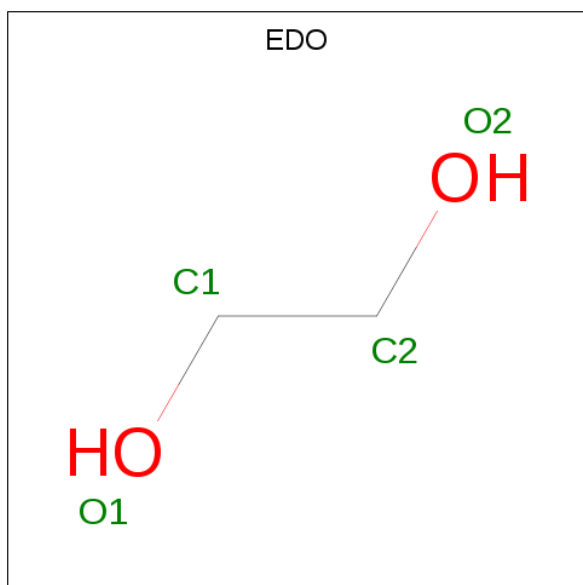
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



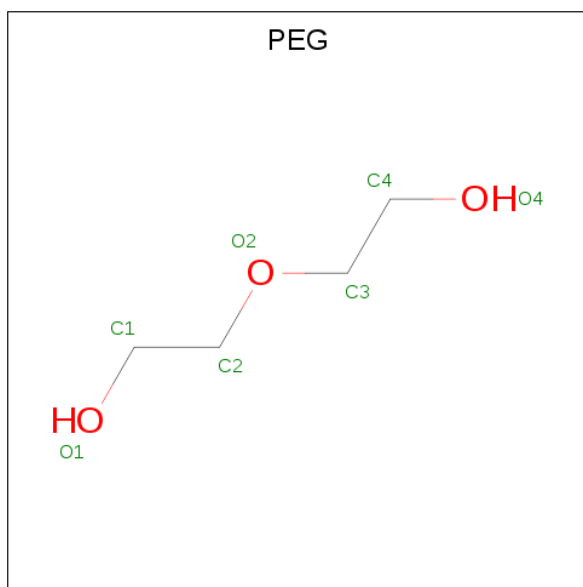
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	H	N	0	0
			5	4	1		
6	C	1	Total	H	N	0	0
			5	4	1		
6	C	1	Total	H	N	0	0
			5	4	1		
6	L	1	Total	H	N	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	H	O	0	0
			17	4	10	3		
8	H	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	Na	0	0
			1	1		
9	C	3	Total	Na	0	0
			3	3		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	Cl	0	0
			1	1		

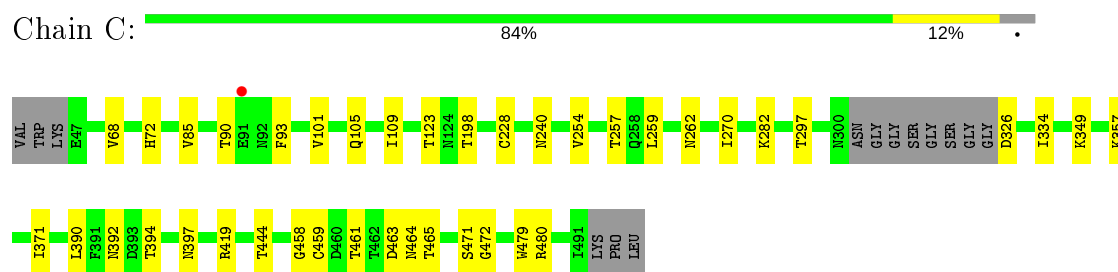
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	7	Total 7	O 7	0	0
11	L	5	Total 5	O 5	0	0

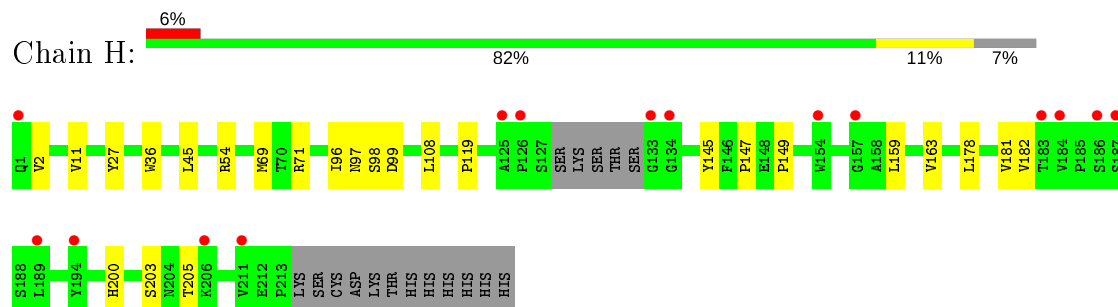
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

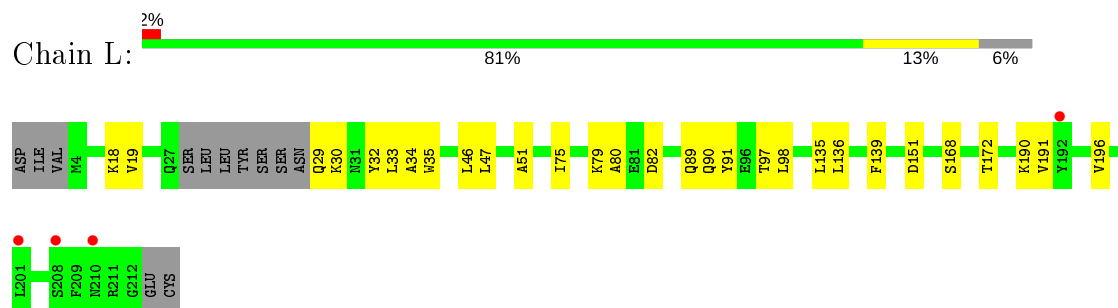
• Molecule 1: Gp120



• Molecule 2: P-p3b3 Heavy Chain



• Molecule 3: P-p3b3 Light Chain



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BM/3
MAIN4
MAIN5

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.80Å 176.75Å 108.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.59 50.09 – 3.59	Depositor EDS
% Data completeness (in resolution range)	68.7 (50.00-3.59) 68.8 (50.09-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472)	Depositor
R, R_{free}	0.232 , 0.268 0.232 , 0.268	Depositor DCC
R_{free} test set	571 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 98.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11337	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, NA, EDO, NH4, PEG, 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	C	0.25	0/2602	0.47	0/3542
2	H	0.29	0/1679	0.51	0/2289
3	L	0.25	0/1480	0.44	0/2024
All	All	0.26	0/5761	0.48	0/7855

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

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	C	2550	2410	2422	22	0
2	H	1637	1575	1585	19	0
3	L	1451	1255	1281	19	0
4	A	61	56	52	3	0
5	C	126	125	117	3	0
6	C	3	12	0	0	0
6	L	1	4	0	0	0
7	C	8	12	12	0	0
8	C	7	10	10	0	0
8	H	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	3	0	0	0	0
9	H	1	0	0	0	0
10	C	1	0	0	0	0
11	C	7	0	0	0	0
11	L	5	0	0	0	0
All	All	5868	5469	5489	60	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 5.

All (60) 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)
3:L:19:VAL:HG22	3:L:75:ILE:HB	1.53	0.89
1:C:461:THR:HG21	1:C:465:THR:H	1.46	0.79
5:C:1419:NAG:O3	5:C:1419:NAG:O7	2.04	0.74
4:A:1:NAG:O3	4:A:2:NAG:O5	2.06	0.72
1:C:68:VAL:O	1:C:72:HIS:ND1	2.26	0.68
2:H:96:ILE:HD12	2:H:97:ASN:HB2	1.79	0.65
3:L:33:LEU:HD12	3:L:89:GLN:O	1.98	0.64
1:C:105:GLN:O	1:C:109:ILE:HD13	1.99	0.62
3:L:80:ALA:HB1	3:L:168:SER:O	2.00	0.62
1:C:101:VAL:HG13	1:C:479:TRP:HB2	1.83	0.61
3:L:32:TYR:O	3:L:90:GLN:NE2	2.32	0.60
1:C:461:THR:HG22	1:C:463:ASP:H	1.66	0.60
1:C:101:VAL:HG21	1:C:480:ARG:HG2	1.85	0.58
3:L:136:LEU:HD21	3:L:196:VAL:HG21	1.86	0.57
2:H:159:LEU:HD21	2:H:182:VAL:HG11	1.87	0.57
2:H:159:LEU:CD2	2:H:182:VAL:HG11	2.35	0.56
1:C:392:ASN:OD1	1:C:394:THR:N	2.34	0.56
1:C:270:ILE:O	1:C:349:LYS:HE2	2.06	0.55
2:H:45:LEU:HB2	3:L:98:LEU:HD22	1.89	0.55
2:H:203:SER:OG	2:H:205:THR:HG23	2.08	0.54
1:C:297:THR:HG22	1:C:444:THR:HG23	1.89	0.53
3:L:18:LYS:HA	3:L:75:ILE:O	2.10	0.52
1:C:326:ASP:OD2	1:C:419:ARG:NH2	2.38	0.52
1:C:371:ILE:HG21	2:H:54:ARG:HG2	1.92	0.51
1:C:90:THR:HG22	1:C:240:ASN:HA	1.93	0.51
2:H:181:VAL:HG21	3:L:135:LEU:CD2	2.41	0.50
2:H:108:LEU:HD23	2:H:149:PRO:HG3	1.93	0.49
2:H:145:TYR:OH	2:H:178:LEU:HD23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:HIS:HB3	2:H:205:THR:OG1	2.13	0.48
3:L:97:THR:C	3:L:98:LEU:HD12	2.33	0.48
1:C:257:THR:O	1:C:259:LEU:N	2.45	0.48
1:C:282:LYS:NZ	2:H:99:ASP:O	2.25	0.48
4:A:2:NAG:O3	4:A:3:BMA:O5	2.20	0.47
1:C:357:LYS:HD3	1:C:464:ASN:OD1	2.14	0.47
3:L:35:TRP:O	3:L:46:LEU:HD12	2.15	0.47
2:H:2:VAL:HG13	2:H:27:TYR:CD1	2.51	0.46
3:L:33:LEU:HD12	3:L:34:ALA:H	1.81	0.46
3:L:30:LYS:HD3	3:L:30:LYS:HA	1.68	0.46
2:H:181:VAL:HG21	3:L:135:LEU:HD22	1.96	0.46
3:L:139:PHE:N	3:L:172:THR:OG1	2.48	0.46
3:L:151:ASP:HA	3:L:191:VAL:HB	1.98	0.46
3:L:136:LEU:HD21	3:L:196:VAL:CG2	2.45	0.46
3:L:89:GLN:NE2	3:L:91:TYR:O	2.41	0.45
1:C:85:VAL:HG21	5:C:1419:NAG:C8	2.47	0.45
2:H:97:ASN:OD1	2:H:98:SER:N	2.42	0.45
2:H:11:VAL:CG2	2:H:147:PRO:HG3	2.47	0.44
1:C:471:SER:OG	1:C:472:GLY:N	2.51	0.43
2:H:36:TRP:CD1	2:H:69:MET:SD	3.12	0.43
5:C:1419:NAG:C7	5:C:1419:NAG:O3	2.67	0.43
1:C:93:PHE:HE2	1:C:228:CYS:HB2	1.84	0.43
3:L:190:LYS:HG3	3:L:191:VAL:HG23	2.00	0.43
1:C:458:GLY:O	1:C:459:CYS:HB2	2.18	0.42
3:L:79:LYS:O	3:L:82:ASP:HB2	2.19	0.42
1:C:254:VAL:HG21	1:C:262:ASN:HB2	2.00	0.42
2:H:163:VAL:HG22	2:H:182:VAL:HG22	2.02	0.42
1:C:334:ILE:HG21	1:C:390:LEU:HD21	2.01	0.41
4:A:1:NAG:HO3	4:A:2:NAG:C1	2.29	0.41
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.02	0.40
2:H:11:VAL:HG23	2:H:147:PRO:HG3	2.02	0.40
1:C:123:THR:HG22	1:C:198:THR:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	329/347 (95%)	314 (95%)	15 (5%)	0	100	100
2	H	212/233 (91%)	202 (95%)	10 (5%)	0	100	100
3	L	200/216 (93%)	179 (90%)	20 (10%)	1 (0%)	29	68
All	All	741/796 (93%)	695 (94%)	45 (6%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	ALA

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	C	283/308 (92%)	282 (100%)	1 (0%)	91	97
2	H	180/199 (90%)	179 (99%)	1 (1%)	86	94
3	L	145/192 (76%)	143 (99%)	2 (1%)	67	85
All	All	608/699 (87%)	604 (99%)	4 (1%)	84	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	397	ASN
2	H	71	ARG
3	L	29	GLN
3	L	47	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	29	GLN
3	L	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

5 monosaccharides 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	1	1,4	14,14,15	1.95	3 (21%)	17,19,21	1.38	3 (17%)
4	NAG	A	2	4	14,14,15	1.92	3 (21%)	17,19,21	1.06	1 (5%)
4	BMA	A	3	4	11,11,12	1.78	2 (18%)	15,15,17	1.50	3 (20%)
4	MAN	A	4	4	11,11,12	1.88	3 (27%)	15,15,17	1.07	1 (6%)
4	MAN	A	5	4	11,11,12	1.78	3 (27%)	15,15,17	0.97	1 (6%)

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	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	4	4	-	2/2/19/22	1/1/1/1
4	MAN	A	5	4	-	0/2/19/22	1/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4	MAN	O5-C1	5.04	1.51	1.43
4	A	5	MAN	O5-C1	4.67	1.51	1.43
4	A	3	BMA	O5-C1	4.59	1.51	1.43
4	A	1	NAG	O5-C1	4.45	1.50	1.43
4	A	2	NAG	O5-C1	4.29	1.50	1.43
4	A	2	NAG	C7-N2	3.89	1.47	1.34
4	A	1	NAG	C7-N2	3.87	1.47	1.34
4	A	3	BMA	C2-C3	-2.90	1.48	1.52
4	A	1	NAG	C2-N2	2.53	1.50	1.46
4	A	2	NAG	C2-N2	2.44	1.50	1.46
4	A	4	MAN	C2-C3	-2.40	1.49	1.52
4	A	5	MAN	C2-C3	-2.30	1.49	1.52
4	A	5	MAN	O5-C5	2.16	1.47	1.43
4	A	4	MAN	O5-C5	2.05	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	BMA	C3-C4-C5	3.56	116.59	110.24
4	A	1	NAG	O5-C1-C2	2.86	115.80	111.29
4	A	4	MAN	C1-C2-C3	2.74	113.03	109.67
4	A	3	BMA	O3-C3-C4	-2.62	104.29	110.35
4	A	3	BMA	C6-C5-C4	-2.56	107.01	113.00
4	A	1	NAG	C8-C7-N2	2.54	120.40	116.10
4	A	5	MAN	C1-C2-C3	2.53	112.77	109.67
4	A	2	NAG	C8-C7-N2	2.31	120.01	116.10
4	A	1	NAG	C2-N2-C7	-2.05	119.99	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4	MAN	O5-C5-C6-O6
4	A	4	MAN	C4-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	3	BMA	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4	MAN	C1-C2-C3-C4-C5-O5
4	A	5	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	2	0
4	A	2	NAG	3	0
4	A	3	BMA	1	0

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 5 are monoatomic and 4 are modelled with single atom - leaving 13 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	$\# Z > 2$
5	NAG	C	1420	1	14,14,15	1.91	3 (21%)	17,19,21	1.04	1 (5%)
5	NAG	C	1424	1	14,14,15	1.83	3 (21%)	17,19,21	1.23	3 (17%)
5	NAG	C	1418	1	14,14,15	1.91	3 (21%)	17,19,21	1.05	2 (11%)
5	NAG	C	1423	1	14,14,15	1.93	3 (21%)	17,19,21	1.09	2 (11%)
5	NAG	C	1401	1	14,14,15	2.07	4 (28%)	17,19,21	1.51	5 (29%)
5	NAG	C	1419	1	14,14,15	2.13	4 (28%)	17,19,21	1.97	3 (17%)
7	EDO	C	1406	-	3,3,3	0.47	0	2,2,2	0.31	0
5	NAG	C	1421	1	14,14,15	1.93	3 (21%)	17,19,21	1.09	2 (11%)
5	NAG	C	1417	1	14,14,15	1.96	3 (21%)	17,19,21	1.70	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PEG	H	301	-	6,6,6	0.48	0	5,5,5	0.27	0
5	NAG	C	1422	1	14,14,15	1.99	3 (21%)	17,19,21	1.23	2 (11%)
7	EDO	C	1405	-	3,3,3	0.47	0	2,2,2	0.29	0
8	PEG	C	1407	-	6,6,6	0.48	0	5,5,5	0.30	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
5	NAG	C	1420	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1424	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1418	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1423	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1419	1	-	4/6/23/26	0/1/1/1
7	EDO	C	1406	-	-	0/1/1/1	-
5	NAG	C	1421	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1417	1	-	6/6/23/26	0/1/1/1
8	PEG	H	301	-	-	1/4/4/4	-
5	NAG	C	1422	1	-	1/6/23/26	0/1/1/1
7	EDO	C	1405	-	-	0/1/1/1	-
8	PEG	C	1407	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1419	NAG	O5-C1	5.18	1.52	1.43
5	C	1401	NAG	O5-C1	4.88	1.51	1.43
5	C	1422	NAG	O5-C1	4.57	1.51	1.43
5	C	1417	NAG	O5-C1	4.50	1.50	1.43
5	C	1418	NAG	O5-C1	4.32	1.50	1.43
5	C	1423	NAG	O5-C1	4.31	1.50	1.43
5	C	1421	NAG	O5-C1	4.28	1.50	1.43
5	C	1420	NAG	O5-C1	4.21	1.50	1.43
5	C	1417	NAG	C7-N2	4.01	1.48	1.34
5	C	1424	NAG	O5-C1	3.98	1.50	1.43
5	C	1424	NAG	C7-N2	3.98	1.48	1.34
5	C	1419	NAG	C7-N2	3.90	1.47	1.34
5	C	1420	NAG	C7-N2	3.89	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1418	NAG	C7-N2	3.89	1.47	1.34
5	C	1423	NAG	C7-N2	3.87	1.47	1.34
5	C	1421	NAG	C7-N2	3.83	1.47	1.34
5	C	1422	NAG	C7-N2	3.83	1.47	1.34
5	C	1401	NAG	C7-N2	3.75	1.47	1.34
5	C	1401	NAG	C2-N2	2.72	1.50	1.46
5	C	1419	NAG	C2-N2	2.63	1.50	1.46
5	C	1422	NAG	C2-N2	2.61	1.50	1.46
5	C	1417	NAG	C2-N2	2.58	1.50	1.46
5	C	1421	NAG	C2-N2	2.48	1.50	1.46
5	C	1420	NAG	C2-N2	2.46	1.50	1.46
5	C	1423	NAG	C2-N2	2.36	1.50	1.46
5	C	1418	NAG	C2-N2	2.24	1.50	1.46
5	C	1419	NAG	O5-C5	2.22	1.47	1.43
5	C	1401	NAG	O5-C5	2.10	1.47	1.43
5	C	1424	NAG	C2-N2	2.06	1.49	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1419	NAG	C1-O5-C5	5.67	119.88	112.19
5	C	1417	NAG	C8-C7-N2	4.88	124.36	116.10
5	C	1401	NAG	C1-O5-C5	3.05	116.32	112.19
5	C	1419	NAG	O5-C5-C6	2.64	111.33	107.20
5	C	1401	NAG	O5-C5-C6	2.61	111.29	107.20
5	C	1419	NAG	C8-C7-N2	2.59	120.48	116.10
5	C	1424	NAG	C8-C7-N2	2.43	120.21	116.10
5	C	1417	NAG	O7-C7-N2	-2.41	117.52	121.95
5	C	1422	NAG	C8-C7-N2	2.33	120.04	116.10
5	C	1422	NAG	C1-O5-C5	2.33	115.34	112.19
5	C	1420	NAG	C8-C7-N2	2.32	120.03	116.10
5	C	1424	NAG	C2-N2-C7	-2.28	119.66	122.90
5	C	1421	NAG	C8-C7-N2	2.27	119.94	116.10
5	C	1418	NAG	C8-C7-N2	2.25	119.92	116.10
5	C	1424	NAG	C3-C4-C5	2.25	114.25	110.24
5	C	1418	NAG	C2-N2-C7	-2.24	119.71	122.90
5	C	1423	NAG	C8-C7-N2	2.22	119.86	116.10
5	C	1401	NAG	C8-C7-N2	2.15	119.74	116.10
5	C	1417	NAG	C2-N2-C7	2.14	125.95	122.90
5	C	1417	NAG	O7-C7-C8	-2.12	118.12	122.06
5	C	1401	NAG	C6-C5-C4	-2.11	108.07	113.00
5	C	1423	NAG	C2-N2-C7	-2.10	119.92	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1401	NAG	C1-C2-N2	-2.09	106.91	110.49
5	C	1421	NAG	C2-N2-C7	-2.05	119.98	122.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1419	NAG	O5-C5-C6-O6
5	C	1419	NAG	C4-C5-C6-O6
5	C	1419	NAG	C1-C2-N2-C7
5	C	1417	NAG	C8-C7-N2-C2
5	C	1417	NAG	O7-C7-N2-C2
5	C	1418	NAG	O5-C5-C6-O6
5	C	1423	NAG	C4-C5-C6-O6
5	C	1423	NAG	O5-C5-C6-O6
5	C	1420	NAG	O5-C5-C6-O6
5	C	1417	NAG	C4-C5-C6-O6
5	C	1421	NAG	C4-C5-C6-O6
8	C	1407	PEG	C4-C3-O2-C2
5	C	1418	NAG	C4-C5-C6-O6
8	H	301	PEG	O1-C1-C2-O2
5	C	1417	NAG	O5-C5-C6-O6
5	C	1419	NAG	C3-C2-N2-C7
5	C	1421	NAG	O5-C5-C6-O6
5	C	1422	NAG	O5-C5-C6-O6
5	C	1417	NAG	C1-C2-N2-C7
8	C	1407	PEG	O1-C1-C2-O2
5	C	1417	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1419	NAG	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	C	333/347 (95%)	-0.05	1 (0%) 94 88	42, 79, 124, 160	0
2	H	216/233 (92%)	0.46	15 (6%) 16 10	51, 89, 164, 183	0
3	L	204/216 (94%)	0.30	4 (1%) 65 49	67, 114, 142, 181	0
All	All	753/796 (94%)	0.19	20 (2%) 54 38	42, 91, 149, 183	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	GLY	3.8
2	H	206	LYS	3.6
2	H	187	SER	3.5
3	L	192	TYR	3.3
2	H	1	GLN	3.3
2	H	186	SER	3.2
2	H	183	THR	3.0
2	H	194	TYR	2.9
2	H	184	VAL	2.6
3	L	208	SER	2.5
2	H	134	GLY	2.5
2	H	126	PRO	2.4
2	H	211	VAL	2.3
2	H	157	GLY	2.3
3	L	210	ASN	2.3
2	H	189	LEU	2.2
2	H	125	ALA	2.1
3	L	201	LEU	2.1
2	H	154	TRP	2.0
1	C	91	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. 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	B-factors(Å ²)	Q<0.9
4	MAN	A	5	11/12	0.71	0.32	134,168,197,202	0
4	MAN	A	4	11/12	0.76	0.32	131,170,203,238	0
4	BMA	A	3	11/12	0.81	0.27	153,178,211,214	0
4	NAG	A	2	14/15	0.89	0.20	102,129,152,167	0
4	NAG	A	1	14/15	0.94	0.21	39,98,126,139	0

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. 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	B-factors(Å ²)	Q<0.9
7	EDO	C	1405	4/4	0.65	0.73	57,75,91,91	0
5	NAG	C	1417	14/15	0.70	0.45	120,151,182,189	0
6	NH4	C	1404	1/1	0.71	0.34	20,24,24,24	0
6	NH4	C	1403	1/1	0.71	2.01	55,66,66,66	0
5	NAG	C	1422	14/15	0.74	0.40	122,154,186,210	0
8	PEG	C	1407	7/7	0.75	0.30	37,74,91,91	0
5	NAG	C	1419	14/15	0.76	0.32	112,137,165,168	0
9	NA	H	302	1/1	0.76	0.66	45,45,45,45	0
5	NAG	C	1421	14/15	0.79	0.37	132,169,205,217	0
5	NAG	C	1424	14/15	0.79	0.34	107,143,177,178	0
5	NAG	C	1401	14/15	0.80	0.56	116,162,194,208	0
9	NA	C	1410	1/1	0.84	0.96	38,38,38,38	1
6	NH4	L	301	1/1	0.84	0.21	44,53,53,53	0
8	PEG	H	301	7/7	0.84	0.36	84,110,164,164	17
6	NH4	C	1402	1/1	0.84	0.93	70,84,84,84	0
5	NAG	C	1418	14/15	0.86	0.40	69,129,155,191	0
7	EDO	C	1406	4/4	0.87	0.46	37,55,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	C	1423	14/15	0.87	0.32	70,87,104,111	0
9	NA	C	1408	1/1	0.92	0.44	13,13,13,13	0
5	NAG	C	1420	14/15	0.92	0.30	86,114,134,138	0
10	CL	C	1411	1/1	0.93	0.42	119,119,119,119	0
9	NA	C	1409	1/1	0.96	1.06	27,27,27,27	1

6.5 Other polymers [i](#)

There are no such residues in this entry.