



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:27 pm GMT

PDB ID : 4MSL  
Title : Crystal structure of the Vps10p domain of human sortilin/NTS3 in complex with AF40431  
Authors : Andersen, J.L.; Strandbygaard, D.; Thirup, S.  
Deposited on : 2013-09-18  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

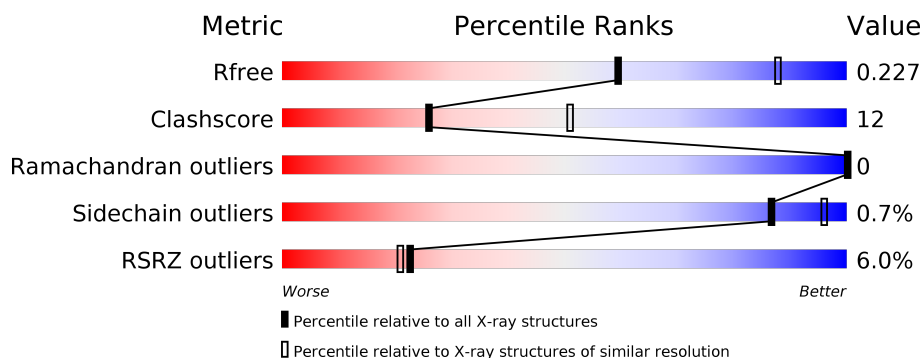
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	696	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5335 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 Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5143	3241	867	1006	29			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	MET	VAL	VARIANT	UNP Q99523
A	724	GLY	-	EXPRESSION TAG	UNP Q99523
A	725	SER	-	EXPRESSION TAG	UNP Q99523
A	726	ALA	-	EXPRESSION TAG	UNP Q99523
A	727	MET	-	EXPRESSION TAG	UNP Q99523
A	728	ILE	-	EXPRESSION TAG	UNP Q99523
A	729	GLU	-	EXPRESSION TAG	UNP Q99523
A	730	GLY	-	EXPRESSION TAG	UNP Q99523
A	731	ARG	-	EXPRESSION TAG	UNP Q99523
A	732	GLY	-	EXPRESSION TAG	UNP Q99523
A	733	VAL	-	EXPRESSION TAG	UNP Q99523
A	734	GLY	-	EXPRESSION TAG	UNP Q99523
A	735	HIS	-	EXPRESSION TAG	UNP Q99523
A	736	HIS	-	EXPRESSION TAG	UNP Q99523
A	737	HIS	-	EXPRESSION TAG	UNP Q99523
A	738	HIS	-	EXPRESSION TAG	UNP Q99523
A	739	HIS	-	EXPRESSION TAG	UNP Q99523
A	740	HIS	-	EXPRESSION TAG	UNP Q99523

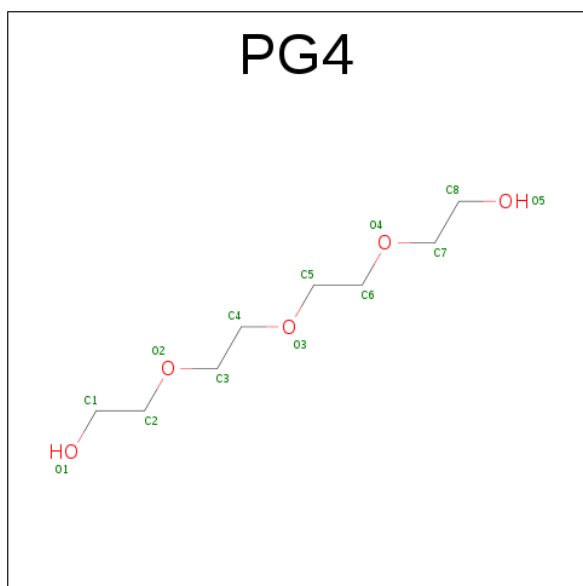
- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

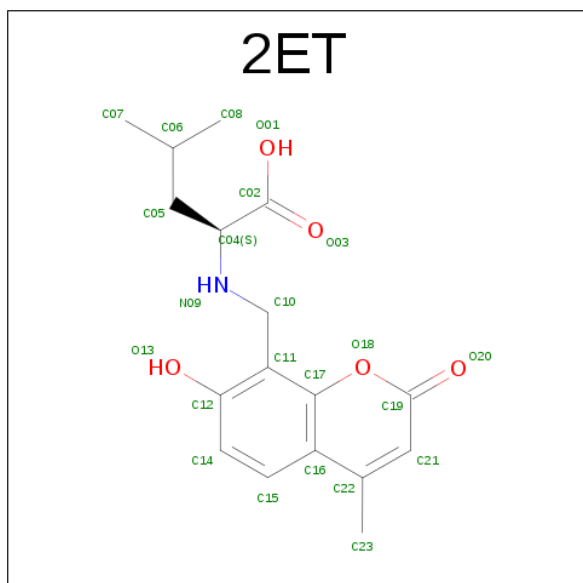
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is N-[(7-HYDROXY-4-METHYL-2-OXO-2H-CHROMEN-8-YL)METHYL]-L-L EUCINE (three-letter code: 2ET) (formula:  $C_{17}H_{21}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	17	1	5		

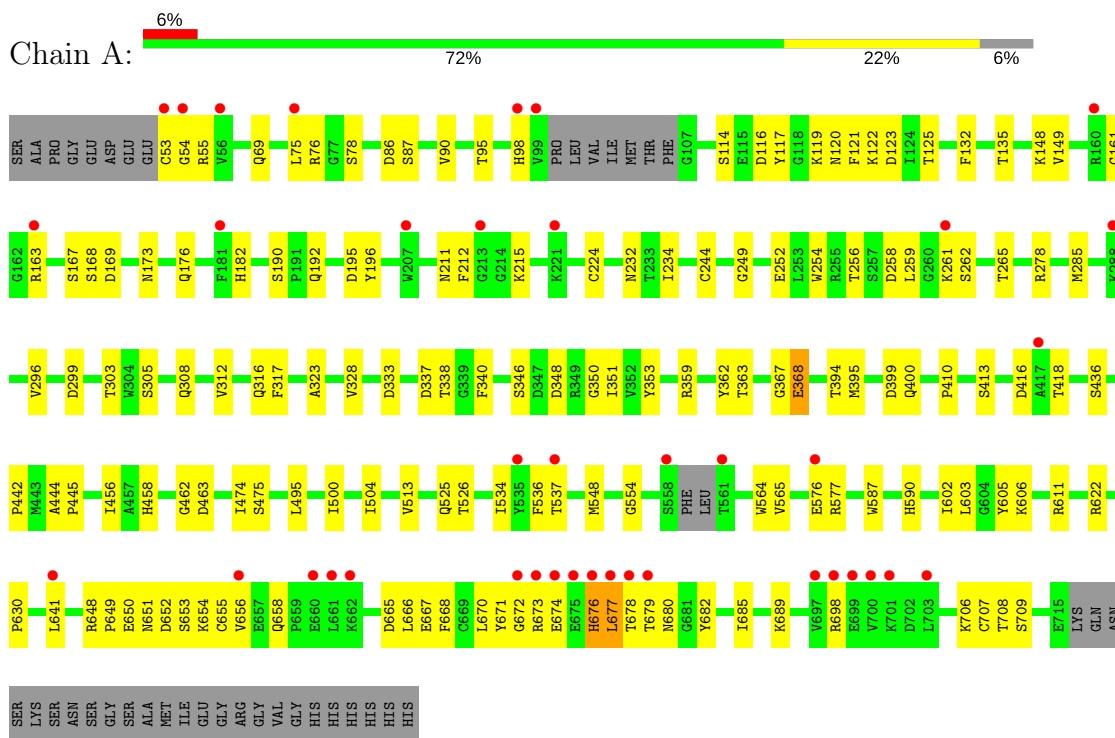
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		

### 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: Sortilin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.88Å 79.17Å 111.70Å 90.00° 127.27° 90.00°	Depositor
Resolution (Å)	46.95 – 2.70 46.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.95-2.70) 95.0 (46.95-2.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.205 , 0.227 0.205 , 0.227	Depositor DCC
$R_{free}$ test set	1542 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: PG4, BMA, NAG, 2ET, 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	0.47	0/5262	0.65	1/7125 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	677	LEU	CB-CG-CD2	-5.46	101.71	111.00

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	5143	0	4919	119	0
2	A	50	0	43	1	0
3	A	39	0	34	2	0
4	A	13	0	18	0	0
5	A	23	0	19	0	0
6	A	67	0	0	3	0
All	All	5335	0	5033	120	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 12.



All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HB3	1:A:564:TRP:CD1	1.99	0.96
1:A:75:LEU:HB3	1:A:564:TRP:HD1	1.32	0.95
1:A:75:LEU:HD22	1:A:564:TRP:NE1	1.85	0.91
1:A:416:ASP:OD1	1:A:418:THR:HG22	1.71	0.88
1:A:168:SER:HB3	1:A:212:PHE:CE2	2.12	0.84
1:A:258:ASP:OD2	1:A:261:LYS:HB2	1.81	0.81
1:A:258:ASP:OD2	1:A:261:LYS:CB	2.33	0.77
1:A:368:GLU:OE2	1:A:436:SER:HB2	1.86	0.75
1:A:658:GLN:O	1:A:706:LYS:NZ	2.21	0.74
1:A:258:ASP:CG	1:A:261:LYS:HB2	2.07	0.73
1:A:258:ASP:OD2	1:A:262:SER:N	2.23	0.71
1:A:116:ASP:OD2	1:A:119:LYS:HB2	1.91	0.70
1:A:537:THR:O	1:A:537:THR:HG22	1.90	0.70
1:A:75:LEU:HD22	1:A:564:TRP:CD1	2.26	0.70
1:A:75:LEU:HG	1:A:95:THR:HG21	1.73	0.68
1:A:75:LEU:HD13	1:A:564:TRP:CD1	2.31	0.66
1:A:148:LYS:NZ	1:A:195:ASP:OD1	2.29	0.65
1:A:75:LEU:CB	1:A:564:TRP:HD1	2.08	0.64
1:A:224:CYS:SG	1:A:244:CYS:CB	2.86	0.63
1:A:116:ASP:OD2	1:A:120:ASN:N	2.32	0.63
1:A:650:GLU:CG	1:A:652:ASP:H	2.12	0.63
1:A:368:GLU:OE2	1:A:436:SER:CB	2.48	0.62
1:A:75:LEU:CB	1:A:564:TRP:CD1	2.79	0.62
1:A:548:MET:HG2	3:A:805:NAG:H82	1.82	0.60
1:A:211:ASN:HD21	1:A:215:LYS:HD3	1.66	0.60
1:A:234:ILE:HB	1:A:256:THR:HG22	1.84	0.60
1:A:351:ILE:HD13	1:A:676:HIS:CE1	2.38	0.59
1:A:674:GLU:O	1:A:678:THR:HG22	2.03	0.59
1:A:116:ASP:CG	1:A:119:LYS:HB2	2.24	0.58
1:A:337:ASP:HA	6:A:953:HOH:O	2.04	0.58
1:A:53:CYS:SG	1:A:54:GLY:N	2.76	0.58
1:A:650:GLU:HG2	1:A:652:ASP:H	1.69	0.58
1:A:312:VAL:HB	1:A:316:GLN:HB3	1.87	0.57
1:A:495:LEU:HB2	1:A:500:ILE:HB	1.87	0.57
1:A:410:PRO:HB2	1:A:413:SER:OG	2.05	0.55
1:A:537:THR:O	1:A:537:THR:CG2	2.53	0.55
1:A:652:ASP:OD1	1:A:653:SER:N	2.39	0.55
1:A:418:THR:HG23	1:A:463:ASP:H	1.72	0.55
1:A:305:SER:OG	1:A:673:ARG:HD3	2.08	0.54
1:A:78:SER:OG	1:A:135:THR:HG21	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD12	1:A:554:GLY:HA3	1.89	0.53
1:A:363:THR:O	1:A:367:GLY:HA2	2.09	0.53
1:A:399:ASP:O	1:A:400:GLN:HB3	2.09	0.53
1:A:278:ARG:NH2	1:A:348:ASP:O	2.41	0.53
1:A:338:THR:HB	1:A:340:PHE:CE2	2.44	0.52
1:A:299:ASP:OD2	1:A:303:THR:N	2.43	0.52
1:A:90:VAL:HA	1:A:114:SER:O	2.10	0.52
1:A:312:VAL:HB	1:A:316:GLN:CB	2.40	0.52
1:A:650:GLU:CG	1:A:651:ASN:N	2.73	0.52
1:A:655:CYS:HB2	1:A:682:TYR:CZ	2.45	0.51
1:A:169:ASP:OD2	1:A:173:ASN:N	2.43	0.51
1:A:234:ILE:HB	1:A:256:THR:CG2	2.41	0.51
1:A:668:PHE:O	1:A:672:GLY:N	2.41	0.51
1:A:399:ASP:O	1:A:400:GLN:CB	2.58	0.51
1:A:299:ASP:CG	1:A:303:THR:H	2.15	0.50
1:A:55:ARG:HB3	1:A:525:GLN:NE2	2.26	0.50
1:A:706:LYS:O	1:A:709:SER:HB3	2.11	0.50
1:A:149:VAL:HB	1:A:167:SER:OG	2.12	0.50
1:A:652:ASP:OD2	1:A:654:LYS:CB	2.60	0.50
1:A:456:ILE:HG12	1:A:474:ILE:HG13	1.93	0.50
1:A:513:VAL:HG11	1:A:526:THR:HG23	1.94	0.49
1:A:605:TYR:CD1	1:A:689:LYS:HB2	2.47	0.49
1:A:652:ASP:OD2	1:A:654:LYS:HB2	2.12	0.49
1:A:416:ASP:CG	1:A:418:THR:HG22	2.32	0.49
1:A:648:ARG:HD3	1:A:653:SER:HA	1.95	0.49
1:A:641:LEU:HD23	1:A:685:ILE:HA	1.94	0.49
1:A:116:ASP:O	1:A:117:TYR:HB2	2.12	0.49
1:A:649:PRO:O	1:A:650:GLU:HG2	2.12	0.49
1:A:394:THR:O	1:A:395:MET:HE2	2.13	0.48
1:A:114:SER:OG	1:A:116:ASP:OD1	2.32	0.48
1:A:513:VAL:CG1	1:A:526:THR:HG23	2.43	0.48
1:A:652:ASP:CG	1:A:654:LYS:H	2.17	0.48
1:A:666:LEU:O	1:A:670:LEU:HG	2.14	0.48
1:A:98:HIS:NE2	1:A:132:PHE:HZ	2.12	0.47
1:A:504:ILE:HG21	1:A:536:PHE:CD2	2.50	0.47
1:A:86:ASP:O	1:A:87:SER:HB2	2.13	0.47
1:A:116:ASP:OD1	1:A:119:LYS:N	2.48	0.47
1:A:69:GLN:HE21	1:A:565:VAL:HG21	1.80	0.46
1:A:296:VAL:HG21	1:A:350:GLY:O	2.16	0.46
1:A:442:PRO:HD2	1:A:458:HIS:CE1	2.49	0.46
1:A:75:LEU:HD13	1:A:564:TRP:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLU:O	1:A:671:TYR:HD2	1.99	0.46
1:A:323:ALA:CB	1:A:328:VAL:HG12	2.46	0.46
1:A:650:GLU:HG3	1:A:652:ASP:H	1.81	0.46
1:A:346:SER:HB3	1:A:353:TYR:CE2	2.52	0.45
1:A:76:ARG:HH11	1:A:76:ARG:HG2	1.82	0.45
1:A:606:LYS:O	1:A:630:PRO:HA	2.16	0.45
1:A:161:GLY:C	1:A:182:HIS:CE1	2.90	0.44
1:A:308:GLN:NE2	1:A:665:ASP:OD1	2.50	0.44
1:A:323:ALA:O	6:A:908:HOH:O	2.21	0.44
1:A:252:GLU:HB3	1:A:254:TRP:HE1	1.81	0.44
1:A:680:ASN:OD1	1:A:698:ARG:HG3	2.17	0.44
1:A:123:ASP:OD1	1:A:125:THR:OG1	2.28	0.44
1:A:442:PRO:HD2	1:A:458:HIS:NE2	2.33	0.44
1:A:416:ASP:OD1	1:A:462:GLY:HA3	2.17	0.44
1:A:340:PHE:CD1	1:A:359:ARG:HA	2.53	0.44
1:A:622:ARG:NH1	3:A:805:NAG:O7	2.49	0.43
1:A:254:TRP:CE2	1:A:265:THR:HG22	2.53	0.43
1:A:192:GLN:HB3	1:A:232:ASN:OD1	2.19	0.43
1:A:444:ALA:HB1	1:A:445:PRO:HD2	2.00	0.43
1:A:474:ILE:HG12	1:A:475:SER:N	2.34	0.43
1:A:590:HIS:CG	1:A:602:ILE:HG13	2.54	0.43
1:A:670:LEU:HB2	1:A:671:TYR:CD2	2.54	0.42
1:A:163:ARG:HD3	1:A:176:GLN:HG3	2.02	0.42
1:A:299:ASP:OD2	1:A:303:THR:OG1	2.27	0.42
1:A:649:PRO:HG3	1:A:656:VAL:HG21	2.01	0.42
1:A:116:ASP:CG	1:A:120:ASN:H	2.22	0.42
1:A:190:SER:HB3	1:A:196:TYR:HB2	2.00	0.42
1:A:677:LEU:HD12	1:A:678:THR:N	2.35	0.42
1:A:121:PHE:O	1:A:122:LYS:HD2	2.18	0.42
1:A:148:LYS:HD2	1:A:212:PHE:CE1	2.55	0.42
2:A:803:BMA:H62	2:A:804:MAN:H2	1.65	0.42
1:A:576:GLU:HG3	1:A:577:ARG:N	2.34	0.41
1:A:708:THR:O	6:A:919:HOH:O	2.22	0.41
1:A:399:ASP:O	1:A:603:LEU:HD11	2.20	0.41
1:A:249:GLY:HA3	1:A:285:MET:HE3	2.01	0.41
1:A:317:PHE:H	1:A:333:ASP:HB3	1.86	0.40
1:A:258:ASP:O	1:A:259:LEU:HB2	2.21	0.40
1:A:587:TRP:CE3	1:A:611:ARG:HD2	2.55	0.40
1:A:679:THR:OG1	1:A:680:ASN:N	2.55	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	A	648/696 (93%)	634 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/605 (94%)	566 (99%)	4 (1%)	87	96

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

Mol	Chain	Res	Type
1	A	362	TYR
1	A	368	GLU
1	A	676	HIS
1	A	707	CYS

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

Mol	Chain	Res	Type
1	A	69	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 ⓘ

7 carbohydrates 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$
2	NAG	A	801	1,2	14,14,15	0.32	0	15,19,21	0.67	0
2	NAG	A	802	2	14,14,15	1.08	1 (7%)	15,19,21	0.77	0
2	BMA	A	803	2	11,11,12	0.81	1 (9%)	13,15,17	1.05	0
2	MAN	A	804	2	11,11,12	1.26	2 (18%)	13,15,17	1.28	1 (7%)
3	NAG	A	805	1,3	14,14,15	0.54	0	15,19,21	0.80	0
3	NAG	A	806	3	14,14,15	0.64	1 (7%)	15,19,21	0.57	0
3	BMA	A	807	3	11,11,12	1.38	2 (18%)	13,15,17	1.58	3 (23%)

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	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	BMA	A	803	2	-	0/2/19/22	0/1/1/1
2	MAN	A	804	2	-	0/2/19/22	0/1/1/1
3	NAG	A	805	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	806	3	-	0/6/23/26	0/1/1/1
3	BMA	A	807	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	O5-C1	-3.95	1.37	1.43
3	A	806	NAG	O5-C1	-2.05	1.40	1.43
2	A	803	BMA	C4-C5	2.04	1.57	1.53
2	A	804	MAN	C4-C5	2.07	1.57	1.53
3	A	807	BMA	C4-C3	2.08	1.57	1.52
2	A	804	MAN	C4-C3	2.10	1.57	1.52
3	A	807	BMA	C2-C3	3.13	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	807	BMA	O2-C2-C3	-2.39	105.47	110.17
3	A	807	BMA	C2-C3-C4	2.54	115.31	110.88
2	A	804	MAN	C1-O5-C5	2.58	115.72	112.17
3	A	807	BMA	C1-O5-C5	3.06	116.38	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	BMA	1	0
2	A	804	MAN	1	0
3	A	805	NAG	2	0

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PG4	A	808	-	12,12,12	0.51	0	11,11,11	1.51	0
5	2ET	A	809	-	19,24,24	2.31	4 (21%)	22,34,34	1.30	4 (18%)

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	PG4	A	808	-	-	0/10/10/10	0/0/0/0
5	2ET	A	809	-	-	0/9/13/13	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	809	2ET	C12-C11	2.94	1.40	1.37
5	A	809	2ET	C22-C16	3.16	1.49	1.42
5	A	809	2ET	C21-C19	4.81	1.47	1.37
5	A	809	2ET	O18-C17	6.49	1.47	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	809	2ET	C14-C12-C11	-3.07	119.75	121.41
5	A	809	2ET	C11-C10-N09	2.04	117.39	111.78
5	A	809	2ET	C21-C22-C16	2.06	119.81	117.73
5	A	809	2ET	O18-C17-C11	2.65	119.18	116.03

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	654/696 (93%)	0.47	39 (5%) 23 21	48, 94, 157, 223	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	LEU	7.0
1	A	675	GLU	6.0
1	A	699	GLU	4.5
1	A	697	VAL	4.4
1	A	703	LEU	4.3
1	A	98	HIS	4.2
1	A	661	LEU	3.9
1	A	700	VAL	3.8
1	A	677	LEU	3.5
1	A	99	VAL	3.5
1	A	656	VAL	3.4
1	A	660	GLU	3.4
1	A	53	CYS	3.3
1	A	561	THR	3.3
1	A	160	ARG	3.2
1	A	181	PHE	3.0
1	A	676	HIS	2.9
1	A	672	GLY	2.9
1	A	641	LEU	2.8
1	A	698	ARG	2.8
1	A	674	GLU	2.7
1	A	662	LYS	2.7
1	A	673	ARG	2.5
1	A	679	THR	2.5
1	A	537	THR	2.5
1	A	678	THR	2.4
1	A	56	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	207	TRP	2.4
1	A	54	GLY	2.4
1	A	701	LYS	2.3
1	A	535	TYR	2.3
1	A	576	GLU	2.3
1	A	213	GLY	2.3
1	A	288	LYS	2.1
1	A	221	LYS	2.1
1	A	163	ARG	2.0
1	A	558	SER	2.0
1	A	261	LYS	2.0
1	A	417	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	801	14/15	0.97	0.22	-0.16	51,51,51,51	0
3	NAG	A	805	14/15	0.94	0.12	-1.75	83,83,83,83	0
2	NAG	A	802	14/15	0.93	0.21	-	84,84,84,84	0
3	BMA	A	807	11/12	0.71	0.23	-	170,170,170,170	0
2	MAN	A	804	11/12	0.85	0.17	-	142,142,142,142	0
3	NAG	A	806	14/15	0.94	0.10	-	103,103,103,103	0
2	BMA	A	803	11/12	0.80	0.18	-	139,139,139,139	0

## 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, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PG4	A	808	13/13	0.80	0.26	0.53	104,104,104,104	0
5	2ET	A	809	23/23	0.94	0.21	0.41	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.