



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:55 PM GMT

PDB ID : 4N7E
Title : Crystal structure of the Vps10p domain of human sortilin/NTS3 in complex with AF38469
Authors : Andersen, J.L.; Strandbygaard, D.; Thirup, S.
Deposited on : 2013-10-15
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
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

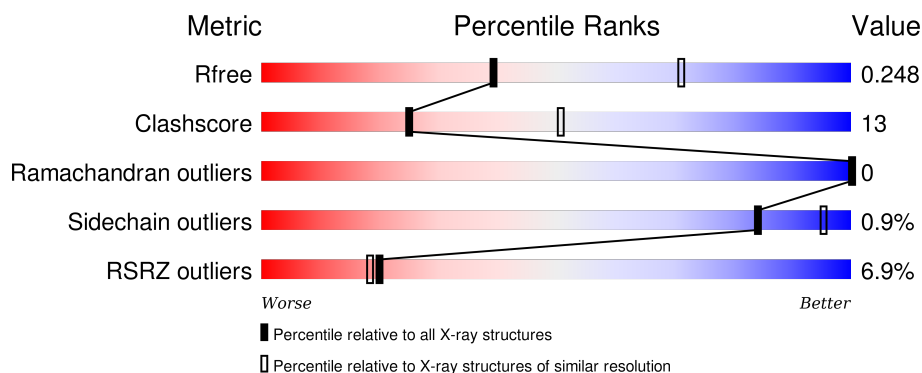
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 ≥ 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	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5291 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	653	Total	C	N	O	S	0	0	0
			5140	3241	866	1005	28			

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

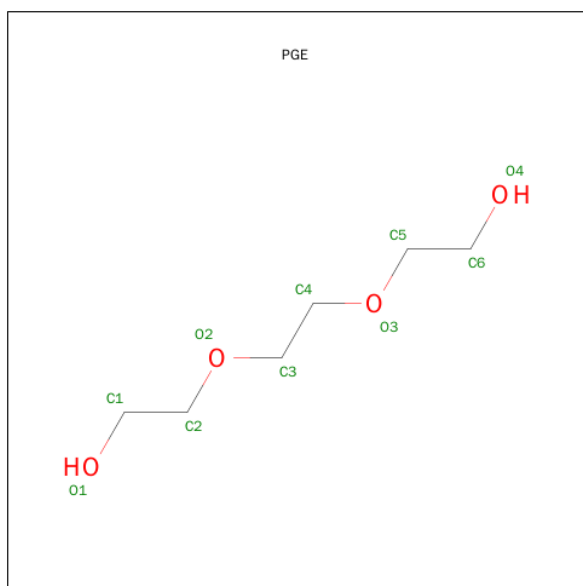
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

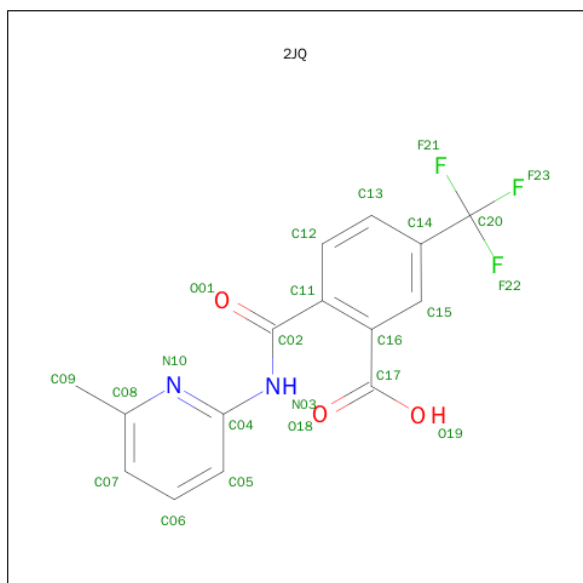
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 5 is 2-[(6-METHYLPYRIDIN-2-YL)CARBAMOYL]-5-(TRIFLUOROMETHYL) BENZOIC ACID (three-letter code: 2JQ) (formula: C₁₅H₁₁F₃N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			23	15	3	2	3		

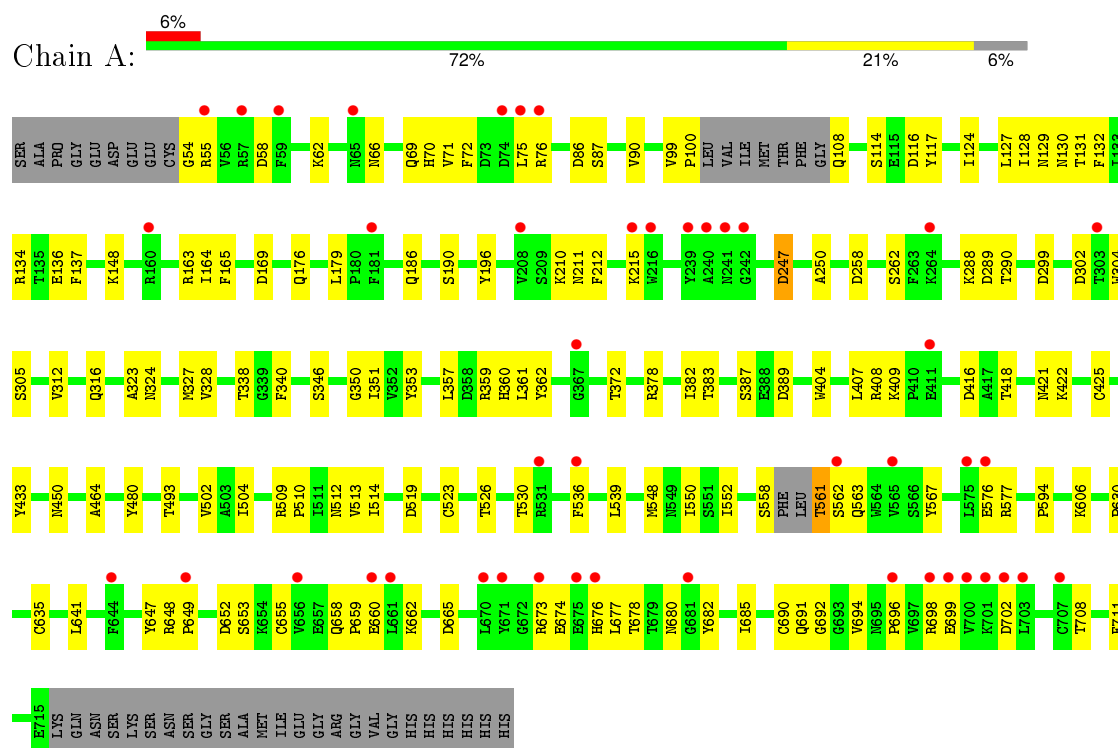
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)

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

• Molecule 1: Sortilin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.95Å 77.40Å 111.18Å 90.00° 127.06° 90.00°	Depositor
Resolution (Å)	44.40 – 2.70 44.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.40-2.70) 94.1 (44.36-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.201 , 0.242 0.212 , 0.248	Depositor DCC
R_{free} test set	2224 reflections (8.37%)	DCC
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30394 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5291	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: BMA, PGE, 2JQ, NAG

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	0.53	1/5260 (0.0%)	0.68	0/7124

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	594	PRO	N-CD	5.24	1.55	1.47

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	5140	0	4918	129	0
2	A	39	0	34	0	0
3	A	28	0	25	3	0
4	A	10	0	14	0	0
5	A	23	0	10	1	0
6	A	51	0	0	2	0
All	All	5291	0	5001	130	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 13.

All (130) 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:536:PHE:CE1	1:A:552:ILE:HG23	1.94	1.01
1:A:694:VAL:HG12	1:A:696:PRO:HD3	1.67	0.76
1:A:304:TRP:N	1:A:673:ARG:HH22	1.85	0.74
1:A:536:PHE:CE1	1:A:552:ILE:CG2	2.70	0.74
1:A:305:SER:OG	1:A:673:ARG:NH1	2.21	0.74
1:A:647:TYR:CE2	1:A:649:PRO:HB3	2.28	0.67
1:A:493:THR:HG23	1:A:539:LEU:HD13	1.78	0.66
1:A:338:THR:HB	1:A:340:PHE:CE2	2.31	0.66
1:A:86:ASP:O	1:A:87:SER:HB2	1.97	0.65
1:A:351:ILE:HD13	1:A:676:HIS:CE1	2.33	0.64
1:A:54:GLY:O	1:A:55:ARG:HB2	1.97	0.64
1:A:129:ASN:O	1:A:130:ASN:HB2	1.99	0.63
1:A:71:VAL:HG12	1:A:72:PHE:N	2.13	0.63
1:A:680:ASN:HB3	1:A:698:ARG:H	1.65	0.62
1:A:383:THR:HG22	1:A:404:TRP:CZ3	2.34	0.62
1:A:163:ARG:HD2	1:A:176:GLN:OE1	2.00	0.61
1:A:680:ASN:O	1:A:698:ARG:HB2	2.00	0.61
1:A:648:ARG:NE	1:A:653:SER:O	2.34	0.61
1:A:351:ILE:CD1	1:A:676:HIS:CE1	2.84	0.61
1:A:163:ARG:HD2	1:A:176:GLN:HG3	1.83	0.60
1:A:75:LEU:HB2	1:A:76:ARG:HG2	1.83	0.60
1:A:408:ARG:NH1	1:A:480:TYR:O	2.35	0.59
1:A:116:ASP:O	1:A:117:TYR:HB2	2.02	0.59
1:A:71:VAL:CG1	1:A:72:PHE:N	2.65	0.59
1:A:504:ILE:HG21	1:A:536:PHE:CD2	2.38	0.58
1:A:350:GLY:O	1:A:353:TYR:CE1	2.57	0.58
1:A:163:ARG:CD	1:A:176:GLN:CG	2.82	0.57
1:A:562:SER:OG	1:A:563:GLN:N	2.36	0.57
1:A:659:PRO:O	1:A:660:GLU:HG3	2.05	0.57
1:A:548:MET:H	3:A:804:NAG:H82	1.70	0.57
1:A:90:VAL:HA	1:A:114:SER:O	2.06	0.56
1:A:351:ILE:HD13	1:A:676:HIS:NE2	2.21	0.56
1:A:163:ARG:HD2	1:A:176:GLN:CG	2.36	0.56
1:A:338:THR:HB	1:A:340:PHE:CD2	2.41	0.55
1:A:548:MET:HG3	3:A:804:NAG:H82	1.88	0.55
1:A:536:PHE:HE1	1:A:552:ILE:HG23	1.65	0.55
1:A:674:GLU:N	1:A:674:GLU:OE1	2.38	0.55
1:A:128:ILE:O	1:A:129:ASN:HB2	2.08	0.54
1:A:99:VAL:HB	1:A:100:PRO:HD2	1.89	0.54
1:A:211:ASN:HD21	1:A:215:LYS:N	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:TRP:H	1:A:673:ARG:HH22	1.56	0.53
1:A:289:ASP:OD1	1:A:290:THR:N	2.37	0.53
1:A:124:ILE:HB	1:A:127:LEU:HD22	1.91	0.53
1:A:360:HIS:NE2	1:A:383:THR:OG1	2.41	0.53
1:A:418:THR:HG21	1:A:464:ALA:N	2.25	0.52
1:A:163:ARG:CD	1:A:176:GLN:HG3	2.39	0.52
1:A:536:PHE:CD1	1:A:552:ILE:CG2	2.93	0.52
1:A:514:ILE:HD12	1:A:552:ILE:HD11	1.91	0.51
1:A:360:HIS:CD2	1:A:383:THR:OG1	2.63	0.51
1:A:699:GLU:OE1	1:A:699:GLU:N	2.36	0.51
1:A:163:ARG:HD2	1:A:176:GLN:CD	2.31	0.51
1:A:134:ARG:NE	1:A:136:GLU:OE2	2.45	0.50
1:A:312:VAL:HB	1:A:316:GLN:HB2	1.92	0.50
1:A:416:ASP:OD1	1:A:418:THR:HB	2.12	0.50
1:A:196:TYR:CE1	1:A:210:LYS:HG3	2.47	0.50
1:A:137:PHE:O	1:A:186:GLN:NE2	2.44	0.50
1:A:247:ASP:O	1:A:250:ALA:HB3	2.13	0.49
1:A:75:LEU:HD12	1:A:75:LEU:C	2.33	0.49
1:A:108:GLN:HA	1:A:132:PHE:HD1	1.77	0.49
1:A:350:GLY:O	1:A:353:TYR:HE1	1.96	0.48
1:A:635:CYS:HB2	1:A:692:GLY:O	2.14	0.48
1:A:58:ASP:O	1:A:62:LYS:HE3	2.14	0.48
1:A:548:MET:N	3:A:804:NAG:H82	2.29	0.47
1:A:75:LEU:HD12	1:A:75:LEU:O	2.13	0.47
1:A:652:ASP:OD1	1:A:653:SER:N	2.48	0.47
1:A:288:LYS:HG3	1:A:289:ASP:HB2	1.96	0.47
1:A:519:ASP:OD2	1:A:523:CYS:HB2	2.15	0.47
1:A:539:LEU:HB3	1:A:550:ILE:HD11	1.96	0.47
1:A:114:SER:OG	1:A:116:ASP:OD1	2.33	0.47
1:A:606:LYS:O	1:A:630:PRO:HA	2.15	0.47
1:A:163:ARG:HH11	1:A:176:GLN:CD	2.19	0.46
1:A:72:PHE:O	1:A:563:GLN:HB3	2.16	0.46
5:A:807:2JQ:O01	5:A:807:2JQ:H4	2.14	0.46
1:A:655:CYS:HB2	1:A:682:TYR:CE1	2.51	0.46
1:A:387:SER:HB3	1:A:389:ASP:OD1	2.16	0.46
1:A:512:ASN:HB2	1:A:530:THR:O	2.16	0.46
1:A:409:LYS:HD3	1:A:425:CYS:SG	2.57	0.45
1:A:148:LYS:HD2	1:A:212:PHE:CE1	2.51	0.45
1:A:340:PHE:CD1	1:A:359:ARG:HA	2.52	0.45
1:A:71:VAL:CG1	1:A:72:PHE:H	2.29	0.45
1:A:131:THR:OG1	1:A:132:PHE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HG23	1:A:179:LEU:HD11	1.98	0.45
1:A:163:ARG:CD	1:A:176:GLN:CD	2.85	0.45
1:A:641:LEU:HD23	1:A:685:ILE:HA	1.99	0.45
1:A:351:ILE:HD13	1:A:676:HIS:CD2	2.52	0.45
1:A:678:THR:HG22	1:A:702:ASP:HA	1.99	0.44
1:A:407:LEU:H	1:A:407:LEU:HD12	1.81	0.44
1:A:165:PHE:CE2	1:A:176:GLN:HB2	2.52	0.44
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.82	0.44
1:A:86:ASP:O	1:A:87:SER:CB	2.66	0.44
1:A:190:SER:HB3	1:A:196:TYR:HB2	1.99	0.44
1:A:357:LEU:CD2	1:A:383:THR:HG21	2.48	0.44
1:A:361:LEU:HD21	1:A:433:TYR:CD1	2.53	0.44
1:A:323:ALA:HB2	1:A:328:VAL:HG12	1.99	0.43
1:A:258:ASP:OD2	1:A:262:SER:OG	2.24	0.43
1:A:108:GLN:HA	1:A:132:PHE:CD1	2.53	0.43
1:A:304:TRP:H	1:A:673:ARG:NH2	2.16	0.43
1:A:163:ARG:HD3	1:A:176:GLN:CG	2.49	0.43
1:A:212:PHE:CG	1:A:212:PHE:O	2.72	0.43
1:A:211:ASN:HD21	1:A:215:LYS:H	1.67	0.43
1:A:69:GLN:HB2	1:A:567:TYR:CE2	2.54	0.43
1:A:299:ASP:OD1	1:A:302:ASP:N	2.51	0.43
1:A:128:ILE:HG13	1:A:130:ASN:H	1.83	0.42
1:A:690:CYS:O	1:A:691:GLN:HG2	2.20	0.42
1:A:708:THR:HA	1:A:711:PHE:HD1	1.85	0.42
1:A:372:THR:HB	1:A:382:ILE:HG13	2.01	0.42
1:A:662:LYS:O	1:A:665:ASP:HB2	2.20	0.42
1:A:536:PHE:HE1	1:A:552:ILE:CG2	2.28	0.42
1:A:75:LEU:HA	1:A:76:ARG:HA	1.74	0.42
1:A:247:ASP:O	1:A:250:ALA:N	2.48	0.42
1:A:62:LYS:O	1:A:66:ASN:ND2	2.52	0.42
1:A:708:THR:O	6:A:1017:HOH:O	2.22	0.42
1:A:576:GLU:HG3	1:A:577:ARG:N	2.35	0.41
1:A:648:ARG:HA	1:A:649:PRO:HD2	1.94	0.41
1:A:698:ARG:NH1	1:A:699:GLU:OE1	2.53	0.41
1:A:378:ARG:HD2	6:A:1050:HOH:O	2.20	0.41
1:A:346:SER:HB3	1:A:353:TYR:CE2	2.56	0.41
1:A:407:LEU:N	1:A:407:LEU:HD12	2.35	0.41
1:A:324:ASN:OD1	1:A:327:MET:N	2.49	0.41
1:A:134:ARG:NH2	1:A:137:PHE:CE2	2.88	0.41
1:A:536:PHE:CD1	1:A:552:ILE:HG23	2.48	0.41
1:A:418:THR:HG21	1:A:464:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:VAL:CG1	1:A:526:THR:HG23	2.51	0.41
1:A:558:SER:HB3	1:A:561:THR:HG23	2.03	0.41
1:A:169:ASP:N	1:A:169:ASP:OD1	2.49	0.41
1:A:548:MET:HE2	1:A:548:MET:HB3	1.99	0.40
1:A:509:ARG:HB3	1:A:510:PRO:CD	2.51	0.40
1:A:69:GLN:HG2	1:A:70:HIS:N	2.36	0.40
1:A:421:ASN:OD1	1:A:422:LYS:N	2.53	0.40
1:A:502:VAL:CG1	1:A:514:ILE:HD11	2.51	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	647/696 (93%)	633 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/605 (94%)	565 (99%)	5 (1%)	84	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
1	A	362	TYR
1	A	450	ASN
1	A	561	THR
1	A	658	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	0.67	0	15,19,21	0.35	0
2	NAG	A	802	2	14,14,15	0.28	0	15,19,21	0.53	0
2	BMA	A	803	2	11,11,12	0.26	0	14,15,17	0.60	0
3	NAG	A	804	1,3	14,14,15	0.59	0	15,19,21	0.79	1 (6%)
3	NAG	A	805	3	14,14,15	0.47	0	15,19,21	0.84	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
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
3	NAG	A	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	NAG	C1-O5-C5	2.39	115.28	112.25
3	A	805	NAG	C1-O5-C5	2.82	115.83	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	NAG	3	0

5.6 Ligand geometry ⓘ

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	PGE	A	806	-	9,9,9	0.36	0	8,8,8	0.29	0
5	2JQ	A	807	-	21,24,24	0.85	1 (4%)	30,35,35	1.39	4 (13%)

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	PGE	A	806	-	-	0/7/7/7	0/0/0/0
5	2JQ	A	807	-	-	0/14/18/18	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807	2JQ	C02-N03	2.36	1.41	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	807	2JQ	F23-C20-C14	-3.60	105.25	112.95
5	A	807	2JQ	C07-C06-C05	-2.51	116.66	120.24
5	A	807	2JQ	C06-C05-C04	2.06	121.06	117.70
5	A	807	2JQ	C09-C08-N10	2.16	119.93	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	807	2JQ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	653/696 (93%)	0.58	45 (6%) 20 18	43, 87, 154, 222	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	GLU	7.9
1	A	76	ARG	6.1
1	A	660	GLU	4.9
1	A	676	HIS	4.5
1	A	75	LEU	4.2
1	A	701	LYS	4.1
1	A	160	ARG	3.9
1	A	699	GLU	3.7
1	A	703	LEU	3.5
1	A	702	ASP	3.5
1	A	57	ARG	3.4
1	A	700	VAL	3.3
1	A	565	VAL	3.3
1	A	240	ALA	3.3
1	A	575	LEU	3.1
1	A	216	TRP	3.1
1	A	531	ARG	3.1
1	A	74	ASP	3.1
1	A	59	PHE	2.9
1	A	649	PRO	2.9
1	A	671	TYR	2.9
1	A	656	VAL	2.8
1	A	411	GLU	2.8
1	A	215	LYS	2.8
1	A	65	ASN	2.7
1	A	55	ARG	2.6
1	A	698	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	670	LEU	2.6
1	A	576	GLU	2.6
1	A	673	ARG	2.4
1	A	661	LEU	2.4
1	A	696	PRO	2.4
1	A	264	LYS	2.4
1	A	562	SER	2.4
1	A	303	THR	2.3
1	A	536	PHE	2.3
1	A	239	TYR	2.3
1	A	181	PHE	2.3
1	A	644	PHE	2.3
1	A	242	GLY	2.3
1	A	707	CYS	2.3
1	A	241	ASN	2.1
1	A	367	GLY	2.1
1	A	681	GLY	2.0
1	A	208	VAL	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. 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	NAG	A	801	14/15	0.96	0.23	0.06	50,50,50,50	0
3	NAG	A	804	14/15	0.97	0.15	-1.47	78,78,78,78	0
3	NAG	A	805	14/15	0.92	0.13	-	96,96,96,96	0
2	NAG	A	802	14/15	0.87	0.25	-	92,92,92,92	0
2	BMA	A	803	11/12	0.75	0.30	-	166,166,166,166	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, 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(\AA^2)	Q<0.9
4	PGE	A	806	10/10	0.85	0.30	0.08	83,83,83,83	0
5	2JQ	A	807	23/23	0.95	0.19	-0.46	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.