

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 02:03 PM BST

PDB ID	:	4OBZ
Title	:	Structure of Cathepsin D with inhibitor 2-(3,4-dimethoxyphenyl)-N-[N-(4-me
		thylbenzyl) carbamimidoyl] acetamide
Authors	:	Graedler, U.; Czodrowski, P.; Tsaklakidis, C.; Klein, M.; Maskos, K.; Leuth-
		ner, B.
Deposited on	:	2014-01-08
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

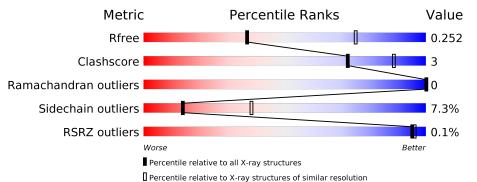
MolProbity		4.02b-467 1.8.5 (274361), CSD as541be (2020)
9		
Xtriage (Phenix)		1.13
EDS	:	2.13.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	А	103	85%	9% 6%
1	С	103	88%	11% •
2	В	243	85%	12% ••
2	D	243	84%	13% ••
3	Е	2	100%	



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5307 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 Cathepsin D light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	97	Total 753	C 481	11	0 147	${ m S}{ m 5}$	0	0	0
1	С	103	Total 792	C 505		O 156	${f S}5$	0	0	0

• Molecule 2 is a protein called Cathepsin D heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
0	В	240	Total	С	Ν	Ο	S	0	0	0
	D	240	1840	1182	301	346	11	0		
0	л	237	Total	С	Ν	0	S	0	0	0
	D	237	1817	1168	296	342	11	0	0	0

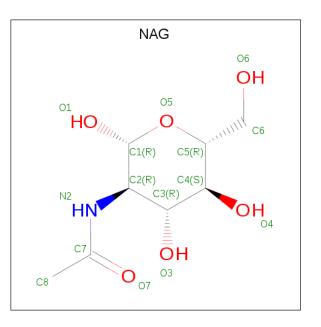
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

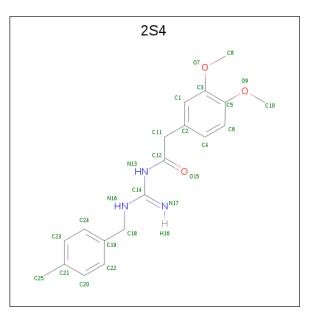
• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 5 is 2-(3,4-dimethoxyphenyl)-N-[N-(4-methylbenzyl)carbamimidoyl]acetamide (three-letter code: 2S4) (formula: $C_{19}H_{23}N_3O_3$).



\mathbf{N}	ſol	Chain	Residues	Atoms			ZeroOcc	AltConf
	5	В	1	Total 25		N 3	0	0

• Molecule 6 is water.

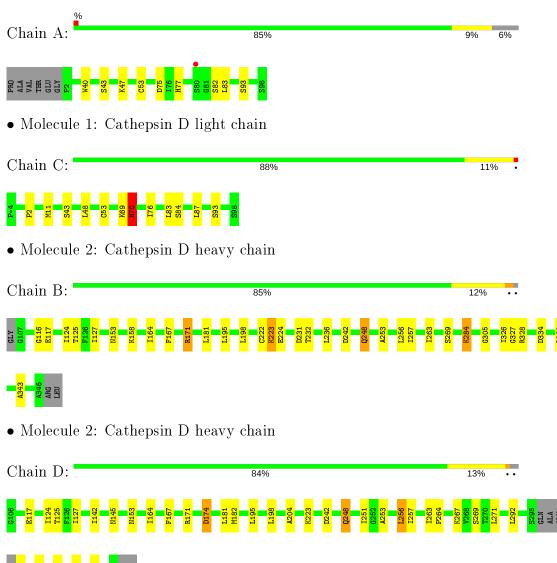


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	8	Total O 8 8	0	0
6	В	6	Total O 6 6	0	0
6	С	5	Total O 5 5	0	0
6	D	19	Total O 19 19	0	0



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: Cathepsin D light chain

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain E:

100%

NAG 1 NAG 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	230.34Å 42.45Å 73.22Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.26 - 2.90	Depositor
Resolution (A)	41.75 - 2.90	EDS
% Data completeness	98.9 (45.26-2.90)	Depositor
(in resolution range)	98.9(41.75-2.90)	EDS
R _{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.62 (at 2.90 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
D D.	0.177 , 0.233	Depositor
R, R_{free}	0.191 , 0.252	DCC
R_{free} test set	678 reflections $(4.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	54.0	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 64.8	EDS
L-test for twinning ²	$ \langle L \rangle = 0.44, \langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5307	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 2S4, 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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/776	0.68	0/1058	
1	С	0.54	0/816	0.77	$1/1114 \ (0.1\%)$	
2	В	0.48	0/1879	0.72	0/2546	
2	D	0.51	0/1855	0.75	0/2513	
All	All	0.50	0/5326	0.73	1/7231~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	70	ASN	CB-CG-ND2	6.52	132.36	116.70

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	А	753	0	708	4	0
1	С	792	0	747	3	0
2	В	1840	0	1847	17	0
2	D	1817	0	1820	17	0
3	Е	28	0	25	1	0
4	А	14	0	13	0	0

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	ů	Non-H		H(added)	Clashes	Symm-Clashes
5	В	25	0	22	2	0
6	А	8	0	0	0	0
6	В	6	0	0	0	0
6	С	5	0	0	0	0
6	D	19	0	0	0	0
All	All	5307	0	5182	35	0

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

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:77:HIS:CE1	2:D:174:ASP:HB2	2.29	0.67
1:C:43:SER:HB2	2:D:117:GLU:HB3	1.79	0.63
2:D:195:LEU:HD13	2:D:343:ALA:HB2	1.81	0.61
2:D:248:GLN:HG2	2:D:253:ALA:HB3	1.83	0.59
2:B:284:LYS:H	2:B:284:LYS:HD3	1.68	0.58
2:B:248:GLN:HG2	2:B:253:ALA:HB3	1.85	0.57
1:A:77:HIS:HE1	2:D:174:ASP:HB2	1.73	0.54
2:B:195:LEU:HD13	2:B:343:ALA:HB2	1.90	0.53
2:D:171:ARG:HD3	2:D:327:GLY:HA3	1.89	0.53
2:D:256:LEU:HD12	2:D:257:ILE:H	1.74	0.53
2:D:124:ILE:HA	2:D:127:ILE:HD12	1.91	0.51
2:B:124:ILE:HA	2:B:127:ILE:HD12	1.93	0.51
2:B:171:ARG:HD2	2:B:327:GLY:HA3	1.93	0.50
2:B:231:ASP:OD2	5:B:401:2S4:N17	2.44	0.50
1:A:43:SER:HB2	2:B:117:GLU:HB3	1.94	0.49
1:C:70:ASN:OD1	1:C:87:LEU:HB2	2.12	0.48
2:B:164:ILE:HG22	2:B:334:ASP:HA	1.96	0.47
2:D:256:LEU:CD1	2:D:257:ILE:H	2.28	0.46
2:B:236:LEU:HD22	2:B:305:GLY:HA2	1.99	0.45
2:B:253:ALA:HB2	2:B:263:ILE:HG12	1.99	0.45
2:B:167:PHE:CZ	2:B:181:LEU:HD13	2.52	0.44
2:D:164:ILE:HG22	2:D:334:ASP:HA	2.00	0.44
2:D:253:ALA:HB2	2:D:263:ILE:HG12	1.99	0.44
2:D:264:PRO:HG2	2:D:267:LYS:HE2	1.99	0.44
2:B:248:GLN:HE21	2:B:248:GLN:HB2	1.66	0.43
1:C:2:PRO:HB2	2:D:182:MET:SD	2.59	0.43
2:B:222:CYS:O	2:B:222:CYS:SG	2.76	0.43
2:D:142:ILE:HG23	2:D:204:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:LYS:H	2:B:223:LYS:HG2	1.60	0.42
2:B:231:ASP:OD2	5:B:401:2S4:H18	2.20	0.42
2:D:145:ASN:O	3:E:2:NAG:H83	2.19	0.42
2:D:167:PHE:CZ	2:D:181:LEU:HD13	2.55	0.42
2:D:251:ILE:HB	2:D:271:LEU:HD22	2.02	0.42
2:B:232:THR:HG22	2:B:326:ILE:HD13	2.03	0.41
1:A:40:TRP:HA	2:B:116:GLY:O	2.21	0.40

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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	Perce	ntiles
1	А	95/103~(92%)	93~(98%)	2(2%)	0	100	100
1	С	101/103~(98%)	100 (99%)	1 (1%)	0	100	100
2	В	238/243~(98%)	228~(96%)	10 (4%)	0	100	100
2	D	233/243~(96%)	223~(96%)	10 (4%)	0	100	100
All	All	667/692~(96%)	644 (97%)	23~(3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	87/91~(96%)	81~(93%)	6 (7%)	15	41
1	С	91/91~(100%)	82~(90%)	9 (10%)	8	24
2	В	199/201~(99%)	184 (92%)	15 (8%)	13	37
2	D	197/201~(98%)	185 (94%)	12~(6%)	18	48
All	All	574/584~(98%)	532~(93%)	42 (7%)	14	38

All (42) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	47	LYS
1	А	53	CYS
1	А	75	ASP
1	А	82	SER
1	А	83	LEU
1	А	93	SER
2	В	125	THR
2	В	153	ASN
2	В	158	LYS
2	В	171	ARG
2	В	198	LEU
2	В	223	LYS
2	В	224	GLU
2	В	242	ASP
2	В	248	GLN
2	В	256	LEU
2	В	257	ILE
2	В	269	SER
2	В	284	LYS
2	В	328	ARG
2	В	339	ARG
1	С	11	MET
1	С	48	LEU
1	С	53	CYS
1	С	69	LYS
1	C C C C	70	ASN
1	С	76	ILE
1	С	83	LEU
1	С	84	SER
1	С	93	SER
2	D	125	THR
2	D	153	ASN
2	D	174	ASP

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Conti	nuea fron	Continuea from previous page									
Mol	Chain	\mathbf{Res}	Type								
2	D	198	LEU								
2	D	223	LYS								
2	D	242	ASP								
2	D	248	GLN								
2	D	256	LEU								
2	D	269	SER								
2	D	292	LEU								
2	D	300	THR								
2	D	339	ARG								

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

Mol	Chain	Res	Type
2	В	162	GLN
2	D	162	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)

2 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).

Mal	Mol Type Chain		Type	Chain	n Res	Dog	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2			
3	NAG	Е	1	1,3	14,14,15	0.49	0	$17,\!19,\!21$	1.45	1(5%)			
3	NAG	Е	2	3	14,14,15	0.36	0	$17,\!19,\!21$	0.86	0			



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Е	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Е	1	NAG	C1-O5-C5	-4.97	105.45	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Е	2	NAG	C8-C7-N2-C2
3	Ε	2	NAG	O7-C7-N2-C2

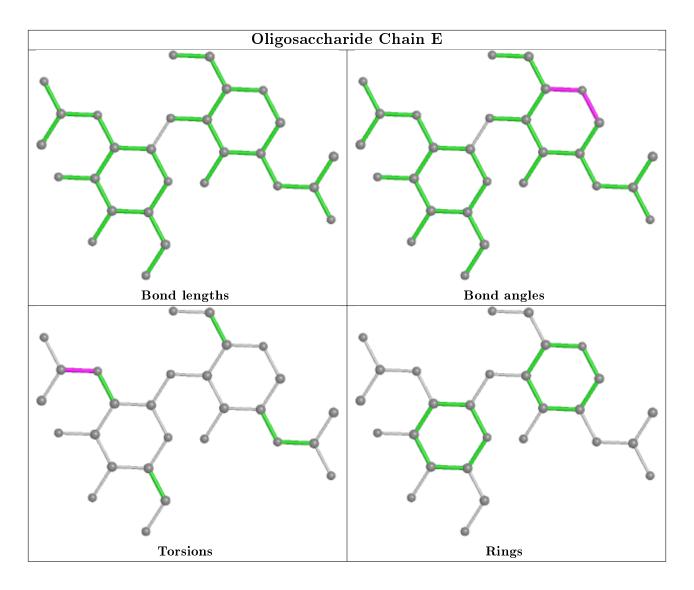
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Е	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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	Туре	Chain	Res	Link	Bo	Bond lengths			Bond angles		
INIOI			nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	NAG	А	400	1	14, 14, 15	0.34	0	$17,\!19,\!21$	0.83	1 (5%)	
5	2S4	В	401	-	24,26,26	0.65	0	34,34,34	2.28	12 (35%)	



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	\mathbf{Link}	Chirals	Torsions	Rings
4	NAG	А	400	1	-	0/6/23/26	0/1/1/1
5	2S4	В	401	-	-	2/17/17/17	0/2/2/2

There are no bond length outliers.

$\Delta 11$ ((13)) bond angle	outling	aro li	stad	bolow
AII ((10)) Donu angie	counters	are n	Isteu	Derow.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	401	2S4	C10-O9-C5	5.68	126.10	117.53
5	В	401	2S4	O9-C5-C3	5.23	122.70	115.41
5	В	401	2S4	O7-C3-C5	3.70	120.56	115.41
5	В	401	2S4	O7-C3-C1	-3.50	118.10	124.12
5	В	401	2S4	O9-C5-C6	-3.29	118.73	124.37
5	В	401	2S4	N13-C14-N16	3.22	126.35	118.08
5	В	401	2S4	C8-O7-C3	3.04	122.11	117.53
5	В	401	2S4	C19-C18-N16	2.79	119.04	113.05
5	В	401	2S4	N13-C14-N17	-2.73	112.18	121.58
4	А	400	NAG	C1-O5-C5	2.65	115.79	112.19
5	В	401	2S4	C11-C2-C4	-2.51	117.30	120.89
5	В	401	2S4	C18-C19-C22	-2.19	116.37	120.91
5	В	401	2S4	C11-C12-N13	2.05	116.98	114.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	401	2S4	C1-C3-O7-C8
5	В	401	2S4	C5-C3-O7-C8

There are no ring outliers.

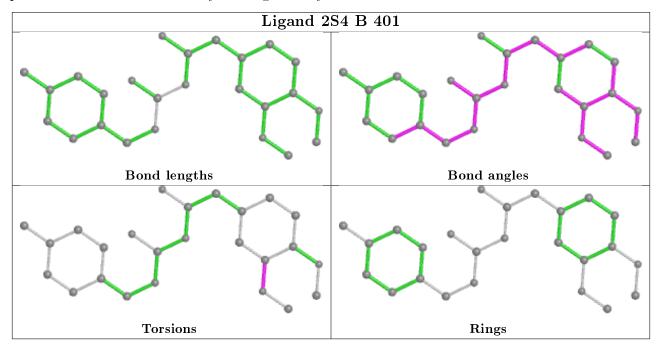
1 monomer is involved in 2 short contacts:

Mol	l Chain Res T		Type	Clashes	Symm-Clashes	
5	В	401	2S4	2	0	

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	97/103~(94%)	-0.14	1 (1%) 82	2 82	31,51,79,93	0
1	С	103/103~(100%)	-0.24	0 100	100	30,51,71,78	0
2	В	240/243~(98%)	-0.13	0 100	100	30,61,85,105	0
2	D	237/243~(97%)	-0.40	0 100	100	23, 49, 72, 96	0
All	All	677/692~(97%)	-0.24	1 (0%) 95	5 96	23, 54, 79, 105	0

All (1) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ	
1	А	80	SER	2.9	

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

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

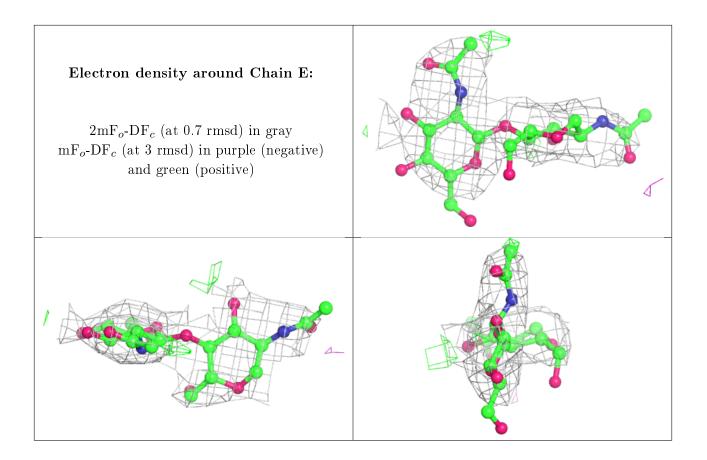
6.3 Carbohydrates (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	NAG	Е	1	14/15	0.80	0.23	$82,\!90,\!91,\!92$	0
3	NAG	Е	2	14/15	0.87	0.21	$85,\!95,\!98,\!101$	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





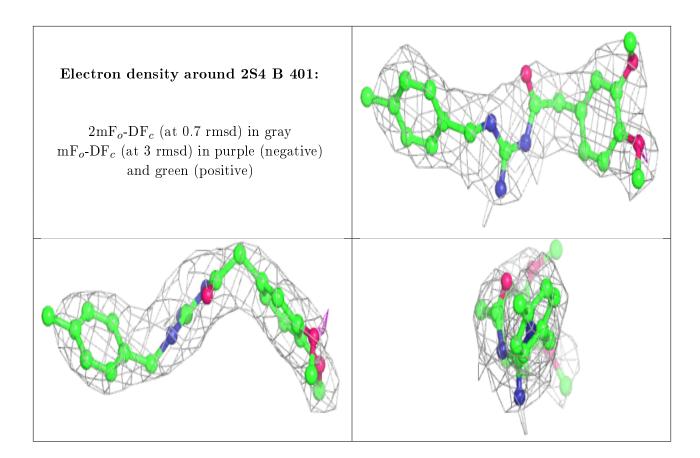
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	NAG	А	400	14/15	0.82	0.20	73,82,84,84	0
5	2S4	В	401	25/25	0.94	0.23	$39,\!45,\!68,\!71$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

