wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 07:37 PM EDT

PDB ID	:	1L6M
Title	:	Neutrophil Gelatinase-associated Lipocalin is a Novel Bacteriostatic Agent that Interferes with Siderophore-mediated Iron Acquisition
Authors	:	Goetz, D.H.; Borregaard, N.; Bluhm, M.E.; Raymond, K.N.; Strong, R.K.
Deposited on	:	2002-03-11
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

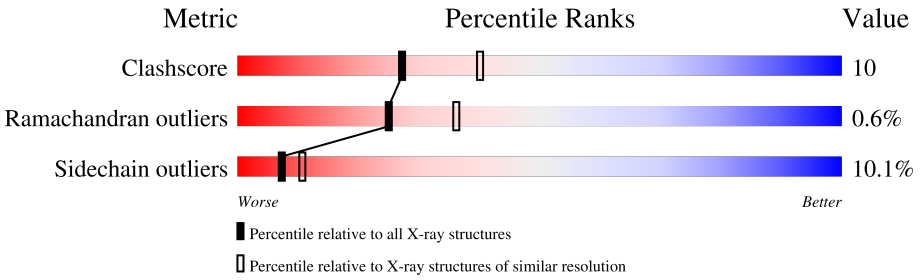
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 of 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	180	71% 22% • • •
1	B	180	57% 33% • • 6%
1	C	180	73% 21% • •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DBH	A	202	-	-	X	-
4	DBH	C	401	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4318 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	2	0
			1418	917	234	263	4			
1	B	169	Total	C	N	O	S	0	1	0
			1351	876	228	243	4			
1	C	172	Total	C	N	O	S	0	0	0
			1364	887	226	247	4			

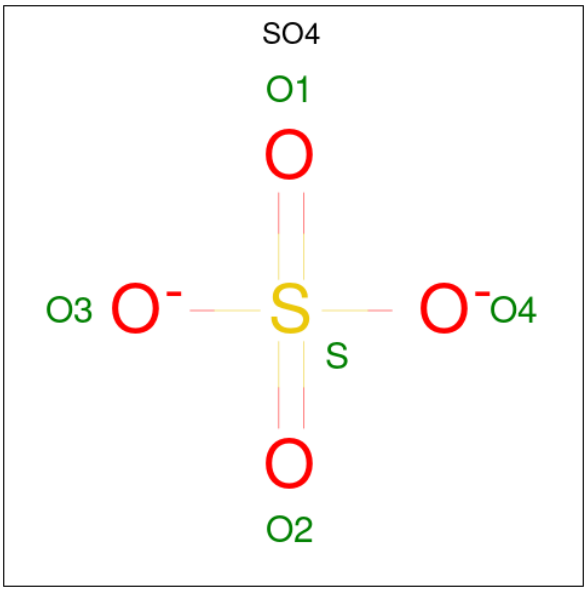
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP P80188
A	0	SER	-	cloning artifact	UNP P80188
A	87	SER	CYS	engineered mutation	UNP P80188
B	-1	GLY	-	cloning artifact	UNP P80188
B	0	SER	-	cloning artifact	UNP P80188
B	87	SER	CYS	engineered mutation	UNP P80188
C	-1	GLY	-	cloning artifact	UNP P80188
C	0	SER	-	cloning artifact	UNP P80188
C	87	SER	CYS	engineered mutation	UNP P80188

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

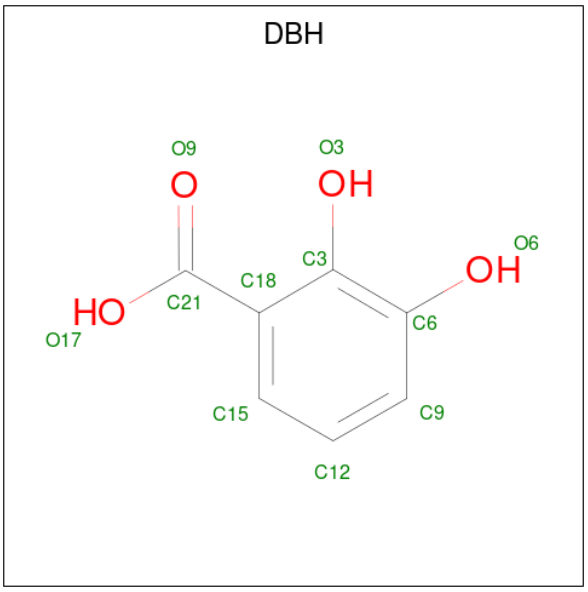
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



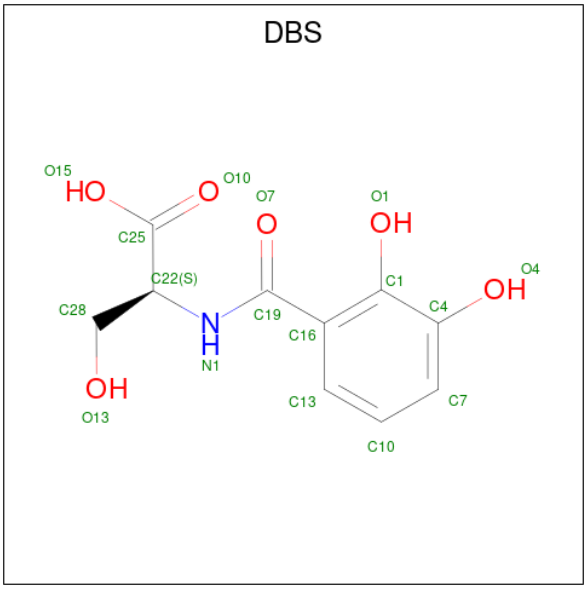
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is 2,3-DIHYDROXY-BENZOIC ACID (three-letter code: DBH) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 7 4	0	0
4	A	1	Total C O 11 7 4	0	0
4	B	1	Total C O 11 7 4	0	0
4	B	1	Total C O 11 7 4	0	0
4	C	1	Total C O 11 7 4	0	0

- Molecule 5 is 2-(2,3-DIHYDROXY-BENZOYLAMINO)-3-HYDROXY-PROPIONIC ACID (three-letter code: DBS) (formula: $C_{10}H_{11}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 17 10 1 6	0	0
5	B	1	Total C N O 17 10 1 6	0	0
5	C	1	Total C N O 17 10 1 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total O 26 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	8	Total O 8 8	0	0
6	C	27	Total O 27 27	0	0

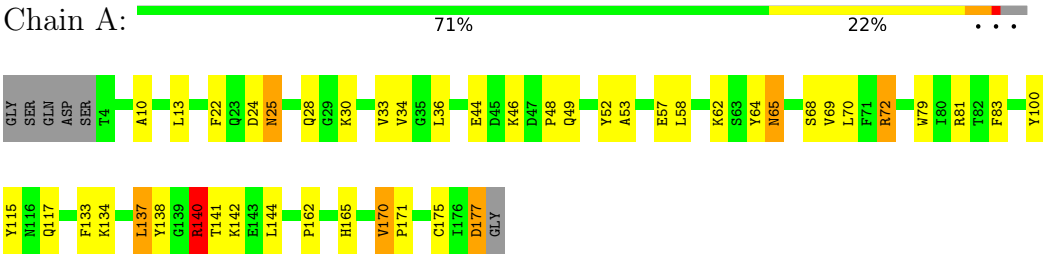
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

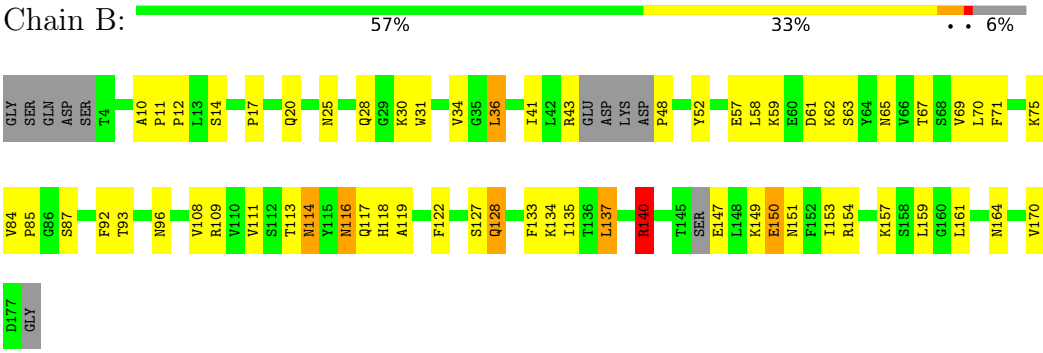
• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain A:



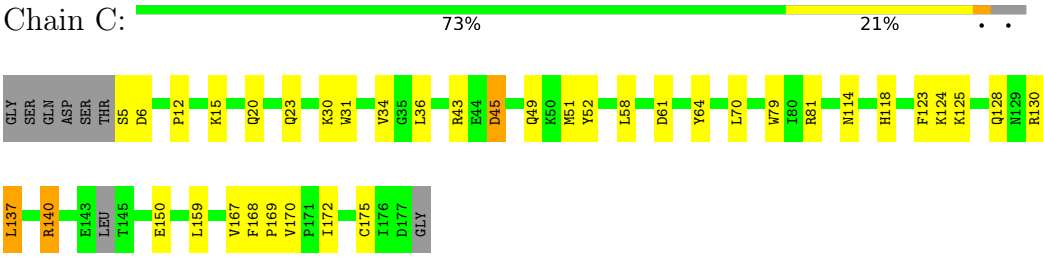
• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain B:



• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.08Å 115.08Å 115.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.40	Depositor
% Data completeness (in resolution range)	96.5 (19.76-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.232 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4318	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

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: SO4, FE, DBS, DBH

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	1.13	1/1455 (0.1%)	1.16	5/1974 (0.3%)
1	B	0.94	0/1384	1.01	1/1874 (0.1%)
1	C	1.12	1/1400 (0.1%)	1.11	5/1900 (0.3%)
All	All	1.07	2/4239 (0.0%)	1.10	11/5748 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	PHE	CE1-CZ	5.73	1.48	1.37
1	C	150	GLU	CG-CD	5.40	1.60	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	C	140	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	C	140	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	A	140	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	115	TYR	CB-CG-CD2	6.34	124.80	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
1	A	64	TYR	Sidechain
1	B	48	PRO	Mainchain
1	C	43	ARG	Sidechain

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	1418	0	1386	30	0
1	B	1351	0	1318	38	0
1	C	1364	0	1326	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
4	A	22	0	7	5	0
4	B	22	0	7	0	0
4	C	11	0	4	0	0
5	A	17	0	9	0	0
5	B	17	0	9	0	0
5	C	17	0	9	2	0
6	A	26	0	0	0	0
6	B	8	0	0	1	0
6	C	27	0	0	0	0
All	All	4318	0	4075	84	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 10.

The worst 5 of 84 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:B:122:PHE:HD2	1:B:135:ILE:HD11	1.17	1.06
1:B:34:VAL:HG23	1:B:137:LEU:HD13	1.44	0.95
1:A:141:THR:HB	1:C:20:GLN:HE21	1.34	0.92
1:C:5:SER:HA	1:C:130:ARG:HH22	1.39	0.88
1:B:122:PHE:CD2	1:B:135:ILE:HD11	2.09	0.83

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	174/180 (97%)	165 (95%)	8 (5%)	1 (1%)	25	36
1	B	164/180 (91%)	153 (93%)	10 (6%)	1 (1%)	25	36
1	C	168/180 (93%)	158 (94%)	9 (5%)	1 (1%)	25	36
All	All	506/540 (94%)	476 (94%)	27 (5%)	3 (1%)	25	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	CYS
1	B	175	CYS
1	C	175	CYS

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	157/164 (96%)	141 (90%)	16 (10%)	7 10
1	B	145/164 (88%)	124 (86%)	21 (14%)	3 3
1	C	147/164 (90%)	138 (94%)	9 (6%)	18 30
All	All	449/492 (91%)	403 (90%)	46 (10%)	7 10

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	109	ARG
1	B	164	ASN
1	B	114	ASN
1	B	137	LEU
1	C	6	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	ASN
1	C	20	GLN
1	C	128	GLN
1	C	118	HIS
1	B	114	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	DBS	B	303	2	17,17,17	1.96	3 (17%)	22,23,23	1.23	2 (9%)
3	SO4	C	330	-	4,4,4	0.29	0	6,6,6	0.13	0
5	DBS	C	403	2	17,17,17	2.18	5 (29%)	22,23,23	1.80	8 (36%)
4	DBH	A	202	2	11,11,11	2.52	5 (45%)	15,15,15	1.39	1 (6%)
3	SO4	C	430	-	4,4,4	0.31	0	6,6,6	0.31	0
3	SO4	A	230	-	4,4,4	0.34	0	6,6,6	0.18	0
4	DBH	A	201	2	11,11,11	2.83	3 (27%)	15,15,15	1.72	3 (20%)
4	DBH	B	302	4,2	11,11,11	2.56	5 (45%)	15,15,15	1.62	4 (26%)
4	DBH	B	301	4,2	11,11,11	2.50	3 (27%)	15,15,15	1.51	3 (20%)
5	DBS	A	203	2	17,17,17	1.96	2 (11%)	22,23,23	1.45	4 (18%)
4	DBH	C	401	2	11,11,11	2.73	7 (63%)	15,15,15	1.70	5 (33%)

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	DBS	B	303	2	-	2/14/14/14	0/1/1/1
5	DBS	C	403	2	-	4/14/14/14	0/1/1/1
4	DBH	A	202	2	-	0/4/4/4	0/1/1/1
4	DBH	B	302	4,2	-	0/4/4/4	0/1/1/1
4	DBH	A	201	2	-	0/4/4/4	0/1/1/1
4	DBH	B	301	4,2	-	0/4/4/4	0/1/1/1
5	DBS	A	203	2	-	2/14/14/14	0/1/1/1
4	DBH	C	401	2	-	4/4/4/4	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	DBH	C6-C3	6.55	1.47	1.40
5	A	203	DBS	C4-C1	6.47	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	303	DBS	C4-C1	6.21	1.47	1.40
5	C	403	DBS	C4-C1	6.06	1.47	1.40
4	A	202	DBH	C15-C18	5.92	1.49	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	201	DBH	C3-C18-C21	3.84	124.06	119.83
5	C	403	DBS	C16-C1-C4	-3.50	117.77	119.99
4	C	401	DBH	C3-C18-C21	3.42	123.60	119.83
5	C	403	DBS	O4-C4-C7	3.37	128.49	119.33
4	B	302	DBH	C18-C3-C6	3.23	122.03	119.99

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	303	DBS	N1-C22-C28-O13
5	C	403	DBS	C25-C22-C28-O13
5	C	403	DBS	C28-C22-C25-O10
4	C	401	DBH	C3-C18-C21-O9
4	C	401	DBH	C3-C18-C21-O17

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	DBS	2	0
4	A	202	DBH	4	0
4	A	201	DBH	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.