



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 12:00 PM EDT

PDB ID : 3D78  
Title : Dimeric crystal structure of a pheromone binding protein mutant D35N, from *Apis mellifera*, at pH 7.0  
Authors : Pesenti, M.E.; Spinelli, S.; Bezirard, V.; Briand, L.; Pernollet, J.C.; Tegoni, M.; Cambillau, C.  
Deposited on : 2008-05-20  
Resolution : 1.60 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

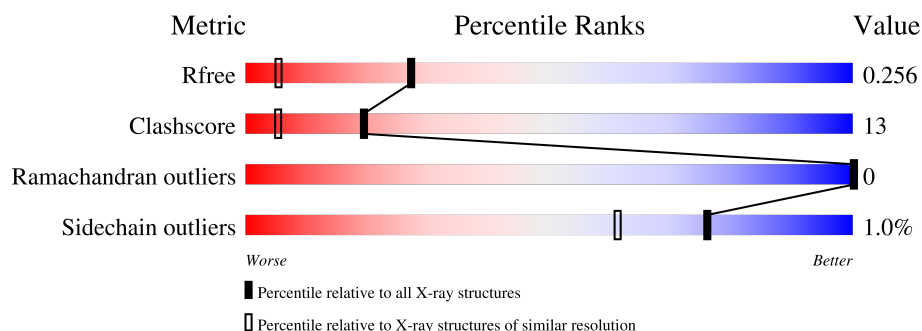
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	119	
1	B	119	

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
2	NBB	A	120	-	X	-	-
3	EDO	A	122	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2213 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.

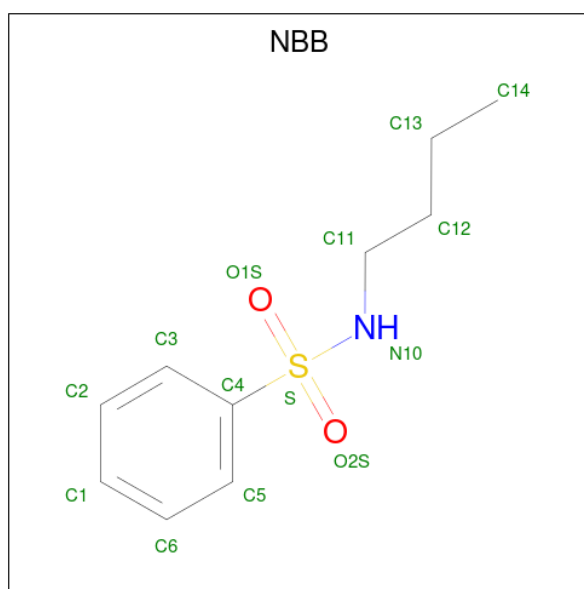
- Molecule 1 is a protein called Pheromone-binding protein ASP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	7	0
			957	604	149	192	12			
1	B	119	Total	C	N	O	S	0	7	0
			948	597	147	193	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ASN	ASP	engineered mutation	UNP Q9U9J6
B	35	ASN	ASP	engineered mutation	UNP Q9U9J6

- Molecule 2 is N-BUTYL-BENZENESULFONAMIDE (three-letter code: NBB) (formula:  $C_{10}H_{15}NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			14	10	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			14	10	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			14	10	1	2	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	127	Total 127	O 127	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.

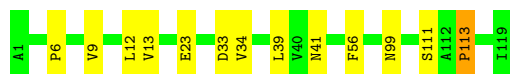
- Molecule 1: Pheromone-binding protein ASP1

Chain A:  84% 15%



- Molecule 1: Pheromone-binding protein ASP1

Chain B:  89% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.05Å 60.95Å 57.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 34.65 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-1.60) 99.5 (34.65-1.55)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.159 , 0.206 0.214 , 0.256	Depositor DCC
$R_{free}$ test set	1309 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8250e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NBB, EDO

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	0.60	0/997	0.68	0/1356
1	B	0.63	0/986	0.77	2/1342 (0.1%)
All	All	0.62	0/1983	0.73	2/2698 (0.1%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	111[A]	SER	CB-CA-C	5.61	120.76	110.10
1	B	111[B]	SER	CB-CA-C	5.61	120.76	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	113	PRO	Peptide

### 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	A	957	0	930	27	0
1	B	948	0	925	18	0
2	A	14	0	15	5	0
2	B	28	0	30	4	0
3	A	20	0	30	9	0
3	B	4	0	6	2	0
4	A	115	0	0	8	0
4	B	127	0	0	3	0
All	All	2213	0	1936	50	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 (50) 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:41:ASN:HD22	3:B:122:EDO:H22	1.38	0.85
1:A:8:GLU:CG	4:A:203:HOH:O	2.25	0.85
1:A:34:VAL:HG11	1:A:118:VAL:HG23	1.62	0.82
1:A:34:VAL:HG11	1:A:118:VAL:CG2	2.14	0.77
1:A:34:VAL:HG13	1:A:116[A]:TRP:CH2	2.22	0.74
1:A:8:GLU:HG3	4:A:203:HOH:O	1.87	0.74
1:B:23:GLU:HG2	4:B:229:HOH:O	1.89	0.73
1:B:13[B]:VAL:HG12	1:B:56:PHE:CZ	2.23	0.73
1:A:34:VAL:HG13	1:A:116[A]:TRP:CZ3	2.23	0.71
1:A:8:GLU:OE1	1:A:12[A]:LEU:HD11	1.92	0.70
1:A:34:VAL:HG22	1:A:39:LEU:HD13	1.74	0.69
1:A:34:VAL:CG1	1:A:116[A]:TRP:CZ3	2.75	0.69
1:A:21:MET:O	3:A:124:EDO:H11	1.96	0.65
1:A:116[A]:TRP:HA	2:A:120:NBB:H143	1.79	0.64
1:B:41:ASN:HD21	1:B:99:ASN:HD21	1.49	0.60
2:A:120:NBB:H142	3:A:122:EDO:O1	2.01	0.60
1:A:41:ASN:HD21	1:A:99:ASN:ND2	2.02	0.58
1:A:8:GLU:HG2	4:A:203:HOH:O	1.98	0.58
1:B:34:VAL:HG22	1:B:39:LEU:HD13	1.87	0.56
1:B:41:ASN:HD21	1:B:99:ASN:ND2	2.03	0.55
1:B:23:GLU:CG	4:B:229:HOH:O	2.51	0.55
1:B:12[B]:LEU:CD1	2:B:121:NBB:H141	2.37	0.54
1:A:73:LEU:HD23	3:A:123:EDO:H22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116[B]:TRP:HA	2:A:120:NBB:H143	1.91	0.53
3:A:124:EDO:H21	4:A:232:HOH:O	2.08	0.53
1:B:13[B]:VAL:HG12	1:B:56:PHE:HZ	1.70	0.51
1:A:86[B]:MET:HG2	3:A:122:EDO:O2	2.10	0.51
1:B:13[B]:VAL:HG12	1:B:56:PHE:CE2	2.46	0.50
1:B:12[B]:LEU:HD11	2:B:121:NBB:H141	1.92	0.50
1:A:41:ASN:HD21	1:A:99:ASN:HD21	1.58	0.50
1:A:34:VAL:HG11	1:A:118:VAL:HG21	1.92	0.49
1:A:77:GLN:HG2	1:A:78:LEU:HD22	1.94	0.49
2:A:120:NBB:C14	3:A:122:EDO:O1	2.60	0.49
1:A:70[B]:MET:SD	3:A:122:EDO:H12	2.53	0.49
1:B:6:PRO:O	1:B:9[B]:VAL:HG12	2.13	0.48
3:A:125:EDO:C2	4:A:175:HOH:O	2.62	0.48
1:B:9[A]:VAL:HG11	2:B:121:NBB:O1S	2.15	0.47
1:B:6:PRO:HB2	1:B:9[A]:VAL:HG13	1.96	0.47
1:A:119:ILE:HD12	4:A:174:HOH:O	2.15	0.46
1:A:36:LYS:HE3	1:A:36:LYS:HB3	1.67	0.45
3:A:124:EDO:H22	4:A:200:HOH:O	2.16	0.45
1:A:88:LYS:NZ	4:A:230:HOH:O	2.50	0.44
1:A:34:VAL:CG1	1:A:118:VAL:HG23	2.42	0.43
1:A:52:LEU:HD21	1:A:119:ILE:HG23	2.01	0.43
1:B:113:PRO:HD2	4:B:162:HOH:O	2.18	0.43
1:A:116[B]:TRP:CD2	2:A:120:NBB:H121	2.54	0.43
1:A:75:PRO:HG2	1:A:78:LEU:HD23	2.01	0.41
1:B:9[A]:VAL:HG12	2:B:121:NBB:C13	2.51	0.41
1:B:41:ASN:HD22	3:B:122:EDO:C2	2.20	0.41

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	124/119 (104%)	123 (99%)	1 (1%)	0	100	100
1	B	124/119 (104%)	122 (98%)	2 (2%)	0	100	100
All	All	248/238 (104%)	245 (99%)	3 (1%)	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	112/105 (107%)	111 (99%)	1 (1%)	78	65
1	B	112/105 (107%)	110 (98%)	2 (2%)	59	36
All	All	224/210 (107%)	221 (99%)	3 (1%)	76	50

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	B	33[A]	ASP
1	B	33[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	B	38	ASN
1	B	41	ASN
1	B	77	GLN
1	B	79	GLN
1	B	83	GLN
1	B	99	ASN
1	B	103	ASN

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

9 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$
3	EDO	A	122	-	3,3,3	0.37	0	2,2,2	0.29	0
2	NBB	B	120	-	14,14,14	2.74	4 (28%)	18,18,18	1.92	6 (33%)
3	EDO	A	125	-	3,3,3	0.50	0	2,2,2	0.24	0
3	EDO	A	123	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	B	122	-	3,3,3	0.54	0	2,2,2	0.34	0
3	EDO	A	124	-	3,3,3	0.48	0	2,2,2	0.10	0
2	NBB	B	121	-	14,14,14	2.76	4 (28%)	18,18,18	1.76	6 (33%)
2	NBB	A	120	-	14,14,14	3.19	5 (35%)	18,18,18	4.06	9 (50%)
3	EDO	A	121	-	3,3,3	0.49	0	2,2,2	0.28	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	EDO	A	122	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBB	B	120	-	-	0/12/12/12	0/1/1/1
3	EDO	A	125	-	-	1/1/1/1	-
3	EDO	A	123	-	-	0/1/1/1	-
3	EDO	B	122	-	-	1/1/1/1	-
3	EDO	A	124	-	-	1/1/1/1	-
2	NBB	B	121	-	-	2/12/12/12	0/1/1/1
2	NBB	A	120	-	-	5/12/12/12	0/1/1/1
3	EDO	A	121	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	120	NBB	C4-S	-9.01	1.62	1.76
2	B	120	NBB	C4-S	-8.12	1.63	1.76
2	B	121	NBB	C4-S	-7.43	1.65	1.76
2	A	120	NBB	O2S-S	6.44	1.50	1.43
2	B	121	NBB	S-N10	-4.59	1.54	1.61
2	B	121	NBB	O1S-S	4.08	1.48	1.43
2	B	120	NBB	O2S-S	3.84	1.47	1.43
2	B	120	NBB	S-N10	-3.71	1.55	1.61
2	B	121	NBB	O2S-S	3.49	1.47	1.43
2	B	120	NBB	O1S-S	2.68	1.46	1.43
2	A	120	NBB	O1S-S	2.51	1.46	1.43
2	A	120	NBB	C11-N10	2.34	1.53	1.47
2	A	120	NBB	S-N10	-2.24	1.58	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	120	NBB	O2S-S-O1S	-13.39	103.09	119.55
2	A	120	NBB	O2S-S-N10	5.75	116.02	107.04
2	A	120	NBB	C6-C5-C4	4.75	123.88	118.95
2	B	120	NBB	O2S-S-O1S	-4.61	113.89	119.55
2	B	121	NBB	C6-C5-C4	4.24	123.35	118.95
2	A	120	NBB	O1S-S-N10	4.18	113.56	107.04
2	A	120	NBB	C12-C11-N10	3.65	119.03	111.03
2	B	120	NBB	C6-C5-C4	3.49	122.58	118.95
2	B	121	NBB	C3-C4-C5	-3.13	116.08	120.44
2	A	120	NBB	O2S-S-C4	3.08	111.75	107.97
2	B	120	NBB	O2S-S-C4	3.03	111.70	107.97
2	B	121	NBB	C5-C4-S	2.69	122.69	119.77
2	B	120	NBB	O1S-S-N10	2.46	110.88	107.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	NBB	C2-C3-C4	2.28	121.32	118.95
2	B	121	NBB	C2-C3-C4	2.27	121.31	118.95
2	B	120	NBB	C3-C4-C5	-2.17	117.42	120.44
2	B	121	NBB	C12-C11-N10	-2.15	106.32	111.03
2	A	120	NBB	C11-N10-S	2.07	127.11	120.41
2	A	120	NBB	C4-S-N10	-2.07	104.69	107.55
2	B	121	NBB	O2S-S-N10	-2.05	103.84	107.04
2	A	120	NBB	C3-C4-C5	-2.03	117.61	120.44

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	120	NBB	C11-N10-S-C4
2	B	121	NBB	N10-C11-C12-C13
2	A	120	NBB	C11-N10-S-O2S
3	A	122	EDO	O1-C1-C2-O2
3	A	125	EDO	O1-C1-C2-O2
2	A	120	NBB	C11-N10-S-O1S
2	B	121	NBB	C11-C12-C13-C14
2	A	120	NBB	C11-C12-C13-C14
3	A	121	EDO	O1-C1-C2-O2
3	B	122	EDO	O1-C1-C2-O2
3	A	124	EDO	O1-C1-C2-O2
2	A	120	NBB	C3-C4-S-O1S

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	122	EDO	4	0
3	A	125	EDO	1	0
3	A	123	EDO	1	0
3	B	122	EDO	2	0
3	A	124	EDO	3	0
2	B	121	NBB	4	0
2	A	120	NBB	5	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.