



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:40 PM GMT

PDB ID : 4A5G  
Title : Raphanus sativus anionic peroxidase.  
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Deposited on : 2011-10-25  
Resolution : 2.05 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](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 (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

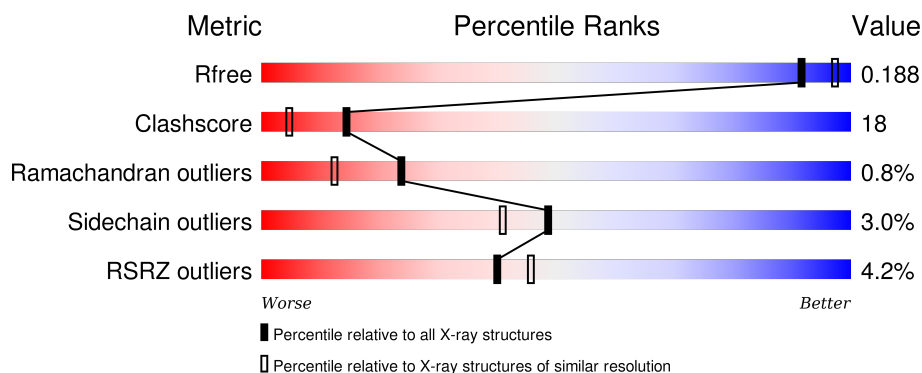
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	308	<div> <div>4%</div> <div>81% 16% .</div> </div>
1	B	308	<div> <div>5%</div> <div>83% 14% .</div> </div>

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
10	NAG	B	1326	X	-	-	X
10	NAG	B	1328	X	-	-	-
11	1PE	A	1338	-	-	-	X
11	1PE	B	1329	-	-	-	X
11	1PE	B	1330	-	-	X	-
12	NAG	B	1311	X	-	-	-
12	MAN	B	1314	X	-	-	X
15	NAG	B	1322	X	-	-	-
16	PG0	B	1331	-	-	-	X
5	NAG	A	1316	-	-	-	X
5	BMA	A	1318	X	-	-	-
8	NAG	A	1330	X	-	-	-

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 5969 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 ANIONIC PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	7	0
			2277	1395	400	467	15			
1	B	307	Total	C	N	O	S	0	5	0
			2258	1388	395	462	13			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total C N O 69 39 2 28	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total C N O 49 28 2 19	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total C N O 49 28 2 19	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total C N O 49 28 2 19	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	6	Total C N O 69 39 2 28	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

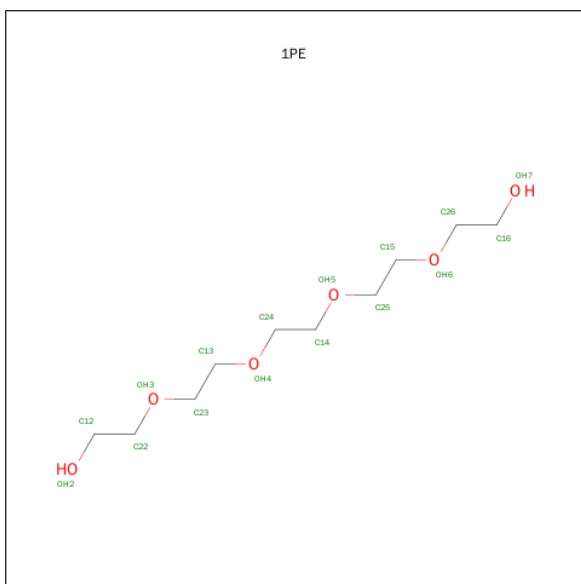
- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG)

(formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			5	3	2		
11	A	1	Total	C	O	0	0
			10	6	4		
11	B	1	Total	C	O	0	0
			15	10	5		
11	B	1	Total	C	O	0	0
			16	10	6		
11	B	1	Total	C	O	0	0
			5	3	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 12 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	6	Total	C	N	O	0	0
			69	39	2	28		

- Molecule 13 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	4	Total	C	N	O	0	0
			49	28	2	19		

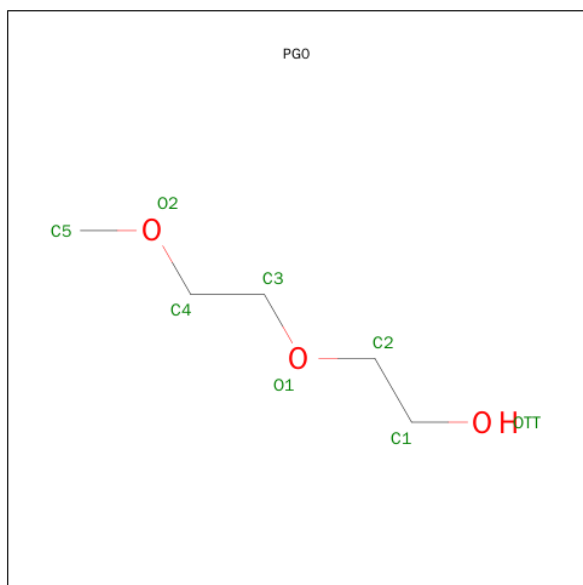
- Molecule 14 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 15 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 16 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 17 is water.

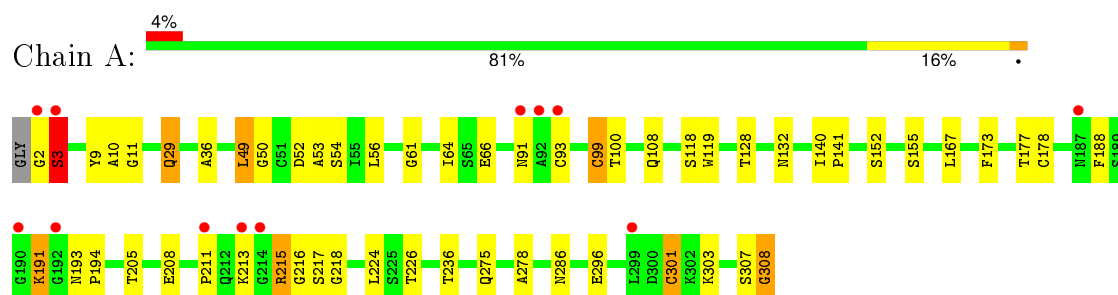
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	364	Total	O	0	0
			364	364		
17	B	336	Total	O	0	0
			336	336		



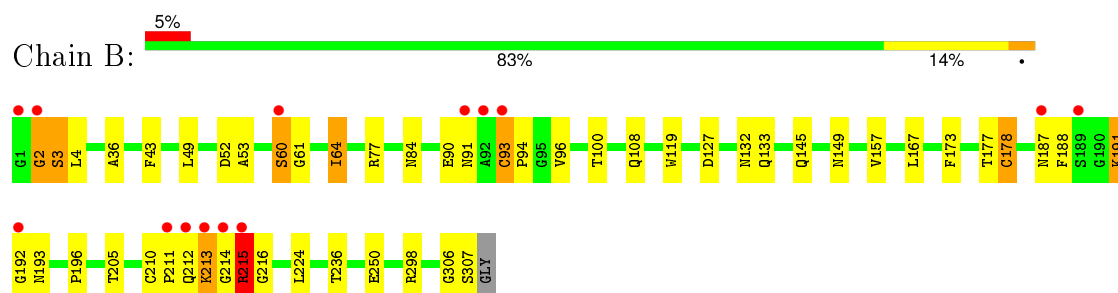
### 3 Residue-property plots [i](#)

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: ANIONIC PEROXIDASE



#### • Molecule 1: ANIONIC PEROXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.15Å 41.19Å 137.80Å 90.00° 96.91° 90.00°	Depositor
Resolution (Å)	35.29 – 2.05 35.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.29-2.05) 98.6 (35.29-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.163 , 0.185 0.165 , 0.188	Depositor DCC
$R_{free}$ test set	2118 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 51681 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.06% 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, 0.375 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: XYP, BMA, NAG, CA, 1PE, FUC, PG0, HEM, FUL, 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	1.57	7/2314 (0.3%)	0.79	2/3144 (0.1%)
1	B	1.57	3/2301 (0.1%)	0.83	3/3128 (0.1%)
All	All	1.57	10/4615 (0.2%)	0.81	5/6272 (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	A	0	4
1	B	0	3
5	A	1	0
8	A	1	0
12	B	2	0
15	B	1	0
All	All	5	7

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ASN	C-N	-11.08	1.08	1.34
1	B	90	GLU	C-N	-8.77	1.13	1.34
1	A	91	ASN	C-N	-8.60	1.14	1.34
1	B	250	GLU	CD-OE2	-5.56	1.19	1.25
1	A	66	GLU	CD-OE1	-5.41	1.19	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	GLY	N-CA-C	-6.29	97.39	113.10
1	A	91	ASN	O-C-N	-5.91	113.25	122.70
1	B	157[A]	VAL	CA-C-N	5.27	126.75	116.20
1	B	157[B]	VAL	CA-C-N	5.27	126.75	116.20
1	A	308	GLY	N-CA-C	5.20	126.11	113.10

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1318	BMA	C1
8	A	1330	NAG	C1
12	B	1311	NAG	C1
12	B	1314	MAN	C1
15	B	1322	NAG	C1

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3[B]	SER	Mainchain
1	A	301[B]	CYS	Mainchain
1	A	93[B]	CYS	Mainchain
1	A	99[B]	CYS	Mainchain
1	B	212	GLN	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	2277	0	2185	74	0
1	B	2258	0	2177	79	1
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	69	0	59	4	0
5	A	49	0	43	0	0
6	A	49	0	43	2	0
7	A	49	0	43	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	69	0	59	1	0
9	A	28	0	25	0	0
10	A	14	0	13	2	0
10	B	42	0	39	2	0
11	A	15	0	17	5	0
11	B	47	0	55	14	0
12	B	69	0	59	6	0
13	B	49	0	43	4	0
14	B	38	0	34	0	0
15	B	49	0	43	1	0
16	B	8	0	12	1	0
17	A	364	0	0	31	9
17	B	336	0	0	29	2
All	All	5969	0	5009	182	11

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 18.

The worst 5 of 182 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:177:THR:HG23	17:A:2200:HOH:O	1.22	1.31
1:A:99[B]:CYS:SG	1:A:301[B]:CYS:HB3	1.73	1.27
1:A:56:LEU:CD1	1:A:99[B]:CYS:SG	2.30	1.20
1:B:60:SER:HA	17:B:2089:HOH:O	1.02	1.20
1:A:308:GLY:O	17:A:2328:HOH:O	1.57	1.19

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1327:FUC:C6	17:B:2137:HOH:O[1_445]	1.72	0.48
17:A:2194:HOH:O	17:A:2212:HOH:O[2_556]	1.95	0.25
1:B:93[B]:CYS:O	17:A:2353:HOH:O[1_665]	2.00	0.20
17:A:2076:HOH:O	17:A:2122:HOH:O[2_556]	2.02	0.18
17:A:2159:HOH:O	17:A:2358:HOH:O[2_656]	2.03	0.17

## 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	312/308 (101%)	305 (98%)	5 (2%)	2 (1%)	30	18
1	B	310/308 (101%)	297 (96%)	7 (2%)	6 (2%)	10	2
All	All	622/616 (101%)	602 (97%)	12 (2%)	8 (1%)	24	5

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	ARG
1	A	3[A]	SER
1	A	3[B]	SER
1	B	94	PRO
1	B	178[A]	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	257/250 (103%)	251 (98%)	6 (2%)	58	51
1	B	255/250 (102%)	246 (96%)	9 (4%)	43	35
All	All	512/500 (102%)	497 (97%)	15 (3%)	48	42

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	SER

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Mol	Chain	Res	Type
1	B	43	PHE
1	B	213	LYS
1	A	224	LEU
1	B	191	LYS

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 ⓘ

43 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	$\# Z  > 2$
4	NAG	A	1310	1,4	14,14,15	1.81	4 (28%)	15,19,21	1.23	1 (6%)
4	NAG	A	1311	4	14,14,15	1.86	6 (42%)	15,19,21	1.40	2 (13%)
4	BMA	A	1312	4	11,11,12	2.11	2 (18%)	14,15,17	0.89	0
4	FUC	A	1313	4	10,10,11	2.08	2 (20%)	14,14,16	0.97	0
4	MAN	A	1314	4	11,11,12	1.98	2 (18%)	14,15,17	0.96	1 (7%)
4	XYP	A	1315	4	9,9,10	2.32	3 (33%)	12,12,14	1.18	2 (16%)
5	NAG	A	1316	1,5	14,14,15	1.75	4 (28%)	15,19,21	1.09	1 (6%)
5	NAG	A	1317	5	14,14,15	1.80	5 (35%)	15,19,21	1.03	0
5	BMA	A	1318	5	11,11,12	1.93	2 (18%)	14,15,17	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FUC	A	1319	5	10,10,11	2.02	2 (20%)	14,14,16	0.84	0
6	NAG	A	1320	1,6	14,14,15	1.86	4 (28%)	15,19,21	1.87	3 (20%)
6	NAG	A	1321	6	14,14,15	1.91	4 (28%)	15,19,21	1.15	2 (13%)
6	MAN	A	1322	6	11,11,12	2.18	2 (18%)	14,15,17	1.13	0
6	FUL	A	1323	6	10,10,11	2.18	2 (20%)	14,14,16	1.37	1 (7%)
7	NAG	A	1324	1,7	14,14,15	1.73	3 (21%)	15,19,21	0.98	0
7	NAG	A	1325	7	14,14,15	1.80	5 (35%)	15,19,21	1.53	2 (13%)
7	MAN	A	1326	7	11,11,12	1.94	2 (18%)	14,15,17	1.20	2 (14%)
7	FUC	A	1327	7	10,10,11	2.08	2 (20%)	14,14,16	1.33	3 (21%)
8	NAG	A	1328	1,8	14,14,15	1.82	4 (28%)	15,19,21	1.55	3 (20%)
8	FUL	A	1329	8	10,10,11	2.10	2 (20%)	14,14,16	1.22	1 (7%)
8	NAG	A	1330	8	14,14,15	1.84	5 (35%)	15,19,21	1.20	1 (6%)
8	BMA	A	1331	8	11,11,12	1.95	2 (18%)	14,15,17	0.82	1 (7%)
8	BMA	A	1332	8	11,11,12	1.86	2 (18%)	14,15,17	1.07	1 (7%)
8	XYP	A	1333	8	9,9,10	2.30	3 (33%)	12,12,14	1.10	1 (8%)
9	NAG	A	1334	1,9	14,14,15	1.86	5 (35%)	15,19,21	1.10	2 (13%)
9	NAG	A	1335	9	14,14,15	1.80	5 (35%)	15,19,21	1.21	1 (6%)
12	NAG	B	1309	1,12	14,14,15	1.81	4 (28%)	15,19,21	1.18	1 (6%)
12	FUC	B	1310	12	10,10,11	2.03	2 (20%)	14,14,16	1.21	1 (7%)
12	NAG	B	1311	12	14,14,15	1.79	5 (35%)	15,19,21	1.63	4 (26%)
12	BMA	B	1312	12	11,11,12	2.00	2 (18%)	14,15,17	0.77	0
12	XYP	B	1313	12	9,9,10	2.37	3 (33%)	12,12,14	1.43	3 (25%)
12	MAN	B	1314	12	11,11,12	1.91	2 (18%)	14,15,17	1.01	0
13	NAG	B	1315	1,13	14,14,15	1.83	4 (28%)	15,19,21	1.21	2 (13%)
13	NAG	B	1316	13	14,14,15	1.83	4 (28%)	15,19,21	1.41	2 (13%)
13	FUL	B	1317	13	10,10,11	2.18	2 (20%)	14,14,16	1.26	1 (7%)
13	BMA	B	1318	13	11,11,12	1.92	2 (18%)	14,15,17	1.08	1 (7%)
14	NAG	B	1319	1,14	14,14,15	1.82	4 (28%)	15,19,21	1.43	2 (13%)
14	FUC	B	1320	14	10,10,11	2.13	2 (20%)	14,14,16	0.93	1 (7%)
14	NAG	B	1321	14	14,14,15	1.83	5 (35%)	15,19,21	1.27	2 (13%)
15	NAG	B	1322	1,15	14,14,15	1.79	4 (28%)	15,19,21	1.69	4 (26%)
15	NAG	B	1323	15	14,14,15	1.83	6 (42%)	15,19,21	1.21	1 (6%)
15	FUC	B	1324	15	10,10,11	2.02	2 (20%)	14,14,16	1.07	0
15	MAN	B	1325	15	11,11,12	1.93	2 (18%)	14,15,17	1.41	3 (21%)



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	NAG	A	1310	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1311	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1312	4	-	0/2/19/22	0/1/1/1
4	FUC	A	1313	4	-	0/0/17/20	0/1/1/1
4	MAN	A	1314	4	-	0/2/19/22	0/1/1/1
4	XYP	A	1315	4	-	0/0/14/17	0/1/1/1
5	NAG	A	1316	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1317	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1318	5	1/1/4/5	0/2/19/22	0/1/1/1
5	FUC	A	1319	5	-	0/0/17/20	0/1/1/1
6	NAG	A	1320	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1321	6	-	0/6/23/26	0/1/1/1
6	MAN	A	1322	6	-	0/2/19/22	0/1/1/1
6	FUL	A	1323	6	-	0/0/17/20	0/1/1/1
7	NAG	A	1324	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1325	7	-	0/6/23/26	0/1/1/1
7	MAN	A	1326	7	-	0/2/19/22	0/1/1/1
7	FUC	A	1327	7	-	0/0/17/20	0/1/1/1
8	NAG	A	1328	1,8	-	0/6/23/26	0/1/1/1
8	FUL	A	1329	8	-	0/0/17/20	0/1/1/1
8	NAG	A	1330	8	1/1/5/7	0/6/23/26	0/1/1/1
8	BMA	A	1331	8	-	0/2/19/22	0/1/1/1
8	BMA	A	1332	8	-	0/2/19/22	1/1/1/1
8	XYP	A	1333	8	-	0/0/14/17	0/1/1/1
9	NAG	A	1334	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1335	9	-	0/6/23/26	0/1/1/1
12	NAG	B	1309	1,12	-	0/6/23/26	0/1/1/1
12	FUC	B	1310	12	-	0/0/17/20	0/1/1/1
12	NAG	B	1311	12	1/1/5/7	0/6/23/26	0/1/1/1
12	BMA	B	1312	12	-	0/2/19/22	0/1/1/1
12	XYP	B	1313	12	-	0/0/14/17	0/1/1/1
12	MAN	B	1314	12	1/1/4/5	0/2/19/22	1/1/1/1
13	NAG	B	1315	1,13	-	0/6/23/26	0/1/1/1
13	NAG	B	1316	13	-	0/6/23/26	0/1/1/1
13	FUL	B	1317	13	-	0/0/17/20	0/1/1/1
13	BMA	B	1318	13	-	0/2/19/22	0/1/1/1
14	NAG	B	1319	1,14	-	0/6/23/26	0/1/1/1
14	FUC	B	1320	14	-	0/0/17/20	0/1/1/1
14	NAG	B	1321	14	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	B	1322	1,15	1/1/5/7	0/6/23/26	0/1/1/1
15	NAG	B	1323	15	-	0/6/23/26	0/1/1/1
15	FUC	B	1324	15	-	0/0/17/20	0/1/1/1
15	MAN	B	1325	15	-	0/2/19/22	0/1/1/1

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1322	MAN	C2-C3	-6.14	1.44	1.52
4	A	1312	BMA	C2-C3	-6.03	1.44	1.52
6	A	1323	FUL	C2-C3	-5.91	1.44	1.52
13	B	1317	FUL	C2-C3	-5.85	1.44	1.52
8	A	1329	FUL	C2-C3	-5.71	1.44	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1320	NAG	C2-N2-C7	-4.34	117.46	123.04
6	A	1320	NAG	C1-O5-C5	-4.06	107.09	112.25
4	A	1311	NAG	C2-N2-C7	-4.06	117.83	123.04
13	B	1316	NAG	C2-N2-C7	-3.91	118.02	123.04
7	A	1325	NAG	C2-N2-C7	-3.88	118.05	123.04

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	1314	MAN	C1
5	A	1318	BMA	C1
8	A	1330	NAG	C1
15	B	1322	NAG	C1
12	B	1311	NAG	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1332	BMA	C1-C2-C3-C4-C5-O5
12	B	1314	MAN	C1-C2-C3-C4-C5-O5

17 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1314	MAN	1	0
4	A	1315	XYP	4	0
6	A	1320	NAG	1	0
6	A	1322	MAN	1	0
6	A	1323	FUL	1	0
7	A	1324	NAG	1	0
7	A	1325	NAG	1	0
7	A	1326	MAN	1	0
7	A	1327	FUC	0	1
8	A	1332	BMA	1	0
12	B	1311	NAG	1	0
12	B	1313	XYP	1	0
12	B	1314	MAN	4	0
13	B	1316	NAG	2	0
13	B	1318	BMA	2	0
15	B	1323	NAG	1	0
15	B	1324	FUC	1	0

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z  > 2$
2	HEM	A	1307	1	30,50,50	2.30	7 (23%)	24,82,82	2.53	13 (54%)
10	NAG	A	1336	-	14,14,15	1.98	5 (35%)	15,19,21	1.25	1 (6%)
11	1PE	A	1337	-	4,4,15	0.48	0	3,3,14	0.83	0
11	1PE	A	1338	-	9,9,15	0.64	0	8,8,14	1.43	0
2	HEM	B	1306	1	30,50,50	2.13	10 (33%)	24,82,82	2.51	12 (50%)
10	NAG	B	1326	1	14,14,15	1.80	5 (35%)	15,19,21	1.29	2 (13%)
10	NAG	B	1327	1	14,14,15	1.82	5 (35%)	15,19,21	1.35	2 (13%)
10	NAG	B	1328	1	14,14,15	1.81	5 (35%)	15,19,21	1.41	2 (13%)
11	1PE	B	1329	-	14,14,15	0.64	0	13,13,14	1.60	1 (7%)
11	1PE	B	1330	-	15,15,15	0.67	0	14,14,14	1.59	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	PG0	B	1331	-	7,7,7	0.35	0	6,6,6	0.61	0
11	1PE	B	1332	-	4,4,15	0.47	0	3,3,14	0.90	0
11	1PE	B	1333	-	5,5,15	0.56	0	4,4,14	1.14	0
11	1PE	B	1334	-	4,4,15	0.51	0	3,3,14	0.79	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
2	HEM	A	1307	1	-	0/10/54/54	0/0/8/8
10	NAG	A	1336	-	-	0/6/23/26	0/1/1/1
11	1PE	A	1337	-	-	0/2/2/13	0/0/0/0
11	1PE	A	1338	-	-	0/7/7/13	0/0/0/0
2	HEM	B	1306	1	-	0/10/54/54	0/0/8/8
10	NAG	B	1326	1	1/1/5/7	0/6/23/26	0/1/1/1
10	NAG	B	1327	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1328	1	1/1/5/7	0/6/23/26	0/1/1/1
11	1PE	B	1329	-	-	0/12/12/13	0/0/0/0
11	1PE	B	1330	-	-	0/13/13/13	0/0/0/0
16	PG0	B	1331	-	-	0/5/5/5	0/0/0/0
11	1PE	B	1332	-	-	0/2/2/13	0/0/0/0
11	1PE	B	1333	-	-	0/3/3/13	0/0/0/0
11	1PE	B	1334	-	-	0/2/2/13	0/0/0/0

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1307	HEM	C3B-C4B	-7.30	1.45	1.51
2	B	1306	HEM	C3B-C4B	-6.52	1.46	1.51
2	A	1307	HEM	C3D-C4D	-5.58	1.44	1.51
2	B	1306	HEM	C3D-C4D	-5.55	1.44	1.51
2	A	1307	HEM	C2C-C1C	-3.70	1.45	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1307	HEM	CBD-CAD-C3D	-4.27	101.11	113.55
2	B	1306	HEM	CBD-CAD-C3D	-4.20	101.32	113.55
10	B	1328	NAG	C2-N2-C7	-3.80	118.15	123.04
2	A	1307	HEM	C3B-CAB-CBB	-3.68	118.81	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
10	B	1326	NAG	C2-N2-C7	-2.61	119.69	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	1326	NAG	C1
10	B	1328	NAG	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1307	HEM	2	0
10	A	1336	NAG	2	0
11	A	1337	1PE	5	0
2	B	1306	HEM	3	0
10	B	1326	NAG	1	0
10	B	1327	NAG	1	0
11	B	1330	1PE	9	0
16	B	1331	PG0	1	0
11	B	1333	1PE	3	0
11	B	1334	1PE	3	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 [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<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	307/308 (99%)	-0.09	12 (3%) 43 48	18, 23, 35, 50	0
1	B	307/308 (99%)	-0.06	14 (4%) 36 41	17, 25, 41, 67	0
All	All	614/616 (99%)	-0.08	26 (4%) 40 46	17, 24, 39, 67	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	6.2
1	B	215	ARG	5.7
1	B	212	GLN	4.6
1	B	189	SER	4.2
1	A	214	GLY	4.0

### 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
5	NAG	A	1316	14/15	0.92	0.22	19.37	29,36,40,48	0
12	MAN	B	1314	11/12	0.78	0.24	7.36	43,50,61,63	0
7	NAG	A	1325	14/15	0.84	0.21	1.95	31,37,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	NAG	B	1309	14/15	0.81	0.16	1.46	23,32,49,51	0
4	XYP	A	1315	9/10	0.86	0.13	0.98	35,44,49,49	0
13	NAG	B	1315	14/15	0.94	0.09	0.09	23,30,35,37	0
4	MAN	A	1314	11/12	0.88	0.09	-0.34	32,36,39,44	0
12	FUC	B	1310	10/11	0.91	0.11	-0.50	30,37,42,43	0
6	NAG	A	1320	14/15	0.95	0.09	-0.65	21,28,33,38	0
4	NAG	A	1310	14/15	0.91	0.10	-0.68	25,27,32,37	0
7	NAG	A	1324	14/15	0.90	0.19	-	25,30,35,40	0
7	FUC	A	1327	10/11	0.89	0.31	-	28,37,41,49	0
6	MAN	A	1322	11/12	0.81	0.27	-	55,63,71,72	0
8	BMA	A	1332	11/12	0.77	0.46	-	55,60,65,70	0
15	NAG	B	1323	14/15	0.72	0.17	-	36,50,60,63	0
13	BMA	B	1318	11/12	0.55	0.27	-	52,63,67,68	0
5	BMA	A	1318	11/12	0.68	0.28	-	61,70,75,78	0
14	NAG	B	1319	14/15	0.86	0.42	-	46,56,64,66	0
15	FUC	B	1324	10/11	0.74	0.35	-	56,64,71,77	0
5	NAG	A	1317	14/15	0.73	0.33	-	36,51,63,75	0
9	NAG	A	1335	14/15	0.69	0.40	-	57,72,88,88	0
4	BMA	A	1312	11/12	0.93	0.18	-	42,44,49,56	0
12	XYP	B	1313	9/10	0.88	0.17	-	41,47,52,56	0
5	FUC	A	1319	10/11	0.89	0.24	-	39,48,50,52	0
8	NAG	A	1330	14/15	0.78	0.41	-	52,60,66,68	0
13	FUL	B	1317	10/11	0.80	0.16	-	30,41,53,55	0
14	FUC	B	1320	10/11	0.62	0.48	-	66,71,77,82	0
12	BMA	B	1312	11/12	0.53	0.55	-	52,60,67,70	0
4	FUC	A	1313	10/11	0.92	0.09	-	26,31,33,35	0
4	NAG	A	1311	14/15	0.89	0.14	-	31,38,41,44	0
9	NAG	A	1334	14/15	0.41	0.36	-	52,61,67,72	0
15	MAN	B	1325	11/12	0.57	0.38	-	73,77,80,86	0
6	NAG	A	1321	14/15	0.88	0.17	-	32,42,49,53	0
7	MAN	A	1326	11/12	0.71	0.29	-	47,56,60,61	0
13	NAG	B	1316	14/15	0.87	0.17	-	32,48,53,60	0
15	NAG	B	1322	14/15	0.78	0.25	-	37,50,58,60	0
8	BMA	A	1331	11/12	0.79	0.47	-	58,61,64,64	0
14	NAG	B	1321	14/15	0.75	0.50	-	60,71,82,86	0
8	NAG	A	1328	14/15	0.64	0.41	-	47,53,60,62	0
12	NAG	B	1311	14/15	0.53	0.30	-	29,52,59,61	0
8	FUL	A	1329	10/11	0.78	0.64	-	59,63,68,69	0
8	XYP	A	1333	9/10	0.67	0.34	-	56,64,70,70	0
6	FUL	A	1323	10/11	0.84	0.15	-	30,43,51,57	0

## 6.4 Ligands ⓘ

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
10	NAG	B	1326	14/15	0.54	0.53	6.77	57,65,72,75	0
11	1PE	B	1329	15/16	0.81	0.17	2.68	32,42,54,61	0
11	1PE	A	1338	10/16	0.81	0.15	2.53	32,37,46,47	0
16	PG0	B	1331	8/8	0.86	0.15	2.30	41,52,54,55	0
3	CA	A	1309	1/1	0.99	0.11	0.30	20,20,20,20	0
11	1PE	B	1330	16/16	0.82	0.16	0.24	41,49,57,57	0
11	1PE	B	1333	6/16	0.92	0.15	0.08	30,43,51,55	0
2	HEM	A	1307	43/43	0.94	0.12	-0.10	14,18,24,29	0
2	HEM	B	1306	43/43	0.95	0.11	-0.31	15,21,26,35	0
3	CA	B	1307	1/1	0.98	0.10	-0.47	25,25,25,25	0
3	CA	A	1308	1/1	0.99	0.10	-0.75	22,22,22,22	0
11	1PE	A	1337	5/16	0.93	0.14	-0.75	31,31,42,48	0
3	CA	B	1308	1/1	0.99	0.09	-0.95	22,22,22,22	0
10	NAG	B	1327	14/15	0.61	0.42	-	49,66,75,78	0
10	NAG	A	1336	14/15	0.78	0.35	-	48,61,67,86	0
11	1PE	B	1334	5/16	0.75	0.23	-	49,50,57,60	0
11	1PE	B	1332	5/16	0.91	0.29	-	40,48,50,59	0
10	NAG	B	1328	14/15	0.73	0.47	-	59,74,80,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.