



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DNU  
Title : STRUCTURAL ANALYSES OF HUMAN MYELOPEROXIDASE-THIOCYANATE COMPLEX  
Authors : Blair-Johnson, M.; Fiedler, T.J.; Fenna, R.E.  
Deposited on : 1999-12-16  
Resolution : 1.85 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  
<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

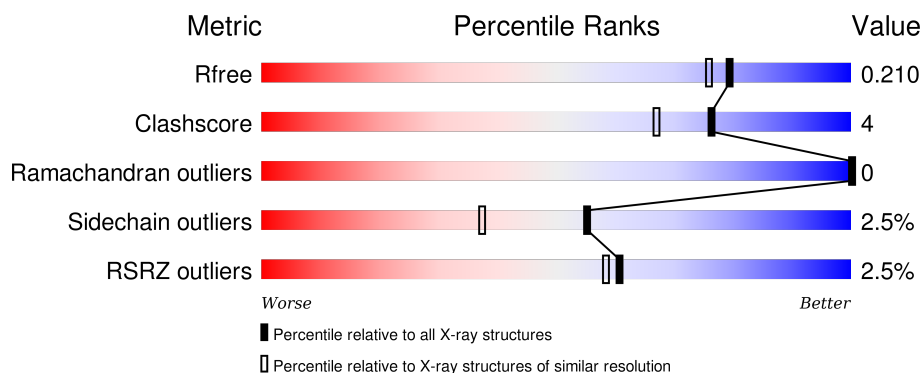
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	104	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
1	B	104	<div> <div>93%</div> <div>7%</div> </div>
2	C	466	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
2	D	466	<div> <div>3%</div> <div>89%</div> <div>10%</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
3	NAG	D	630	-	-	-	X
9	ACY	C	15	-	-	X	X
9	ACY	D	14	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10318 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 MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			
2	D	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	MODIFIED RESIDUE	UNP P05164
D	150	CSO	CYS	MODIFIED RESIDUE	UNP P05164

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

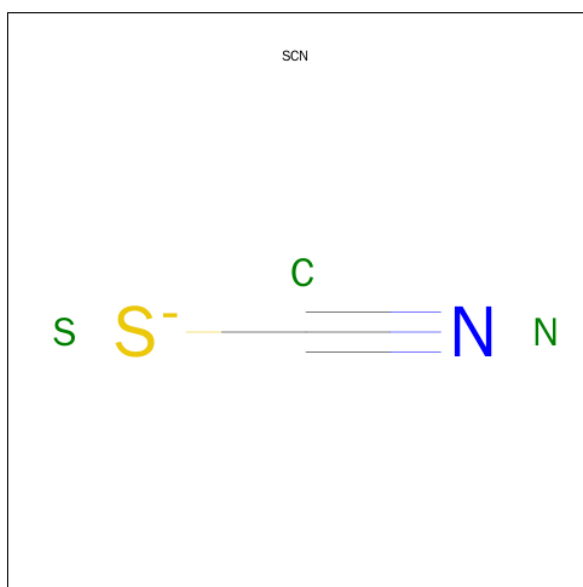
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	6	Total	C	N	O	0	0
			71	40	2	29		
4	D	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

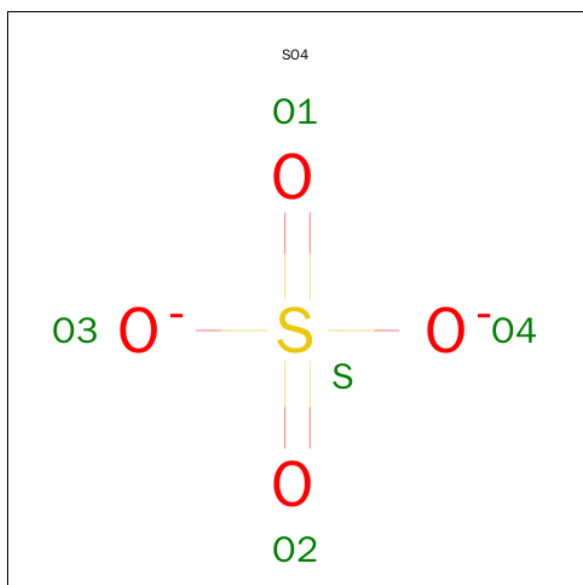
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



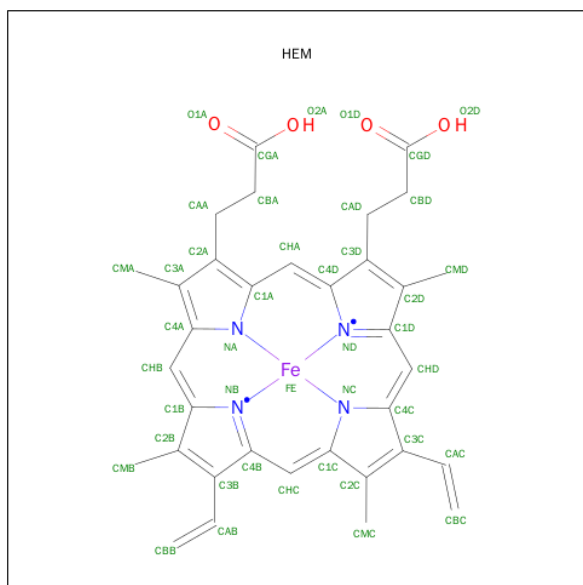
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			3	1	1	1		
6	A	1	Total	C	N	S	0	0
			3	1	1	1		
6	B	1	Total	C	N	S	0	0
			3	1	1	1		
6	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 9 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is water.

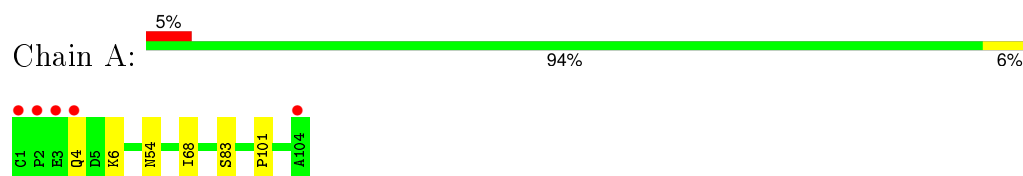
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	92	Total	O	0	0
			92	92		
10	B	103	Total	O	0	0
			103	103		
10	C	334	Total	O	0	0
			334	334		
10	D	310	Total	O	0	0
			310	310		



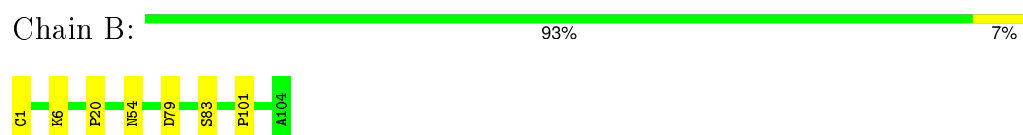
### 3 Residue-property plots

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.

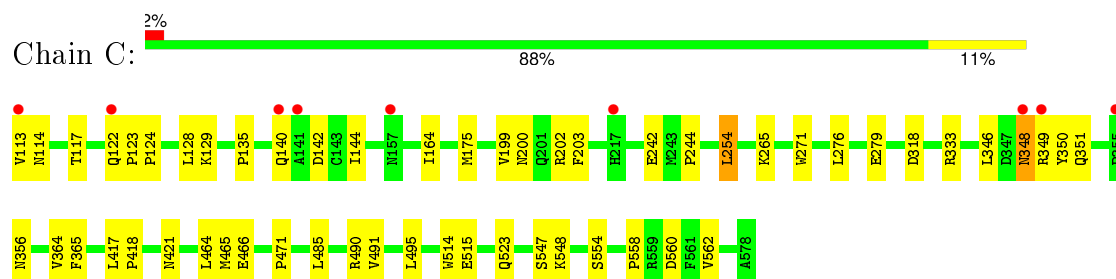
- Molecule 1: MYELOPEROXIDASE



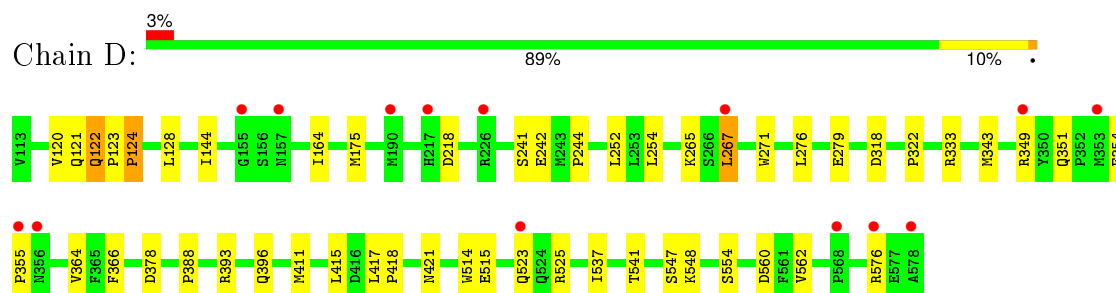
- Molecule 1: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.24Å 63.87Å 92.62Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85 48.79 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.7 (10.00-1.85) 98.1 (48.79-1.86)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.51 (at 1.86Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.178 , 0.210 0.177 , 0.210	Depositor DCC
$R_{free}$ test set	5356 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 106892 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: CSO, SCN, NAG, CA, BMA, SO4, HEM, ACY, MAN, FUC

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	0.64	0/863	0.70	0/1174
1	B	0.60	0/863	0.73	0/1174
2	C	0.60	0/3811	0.63	0/5168
2	D	0.57	0/3811	0.61	0/5168
All	All	0.59	0/9348	0.64	0/12684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	838	0	798	4	0
1	B	838	0	798	5	0
2	C	3733	0	3725	37	0
2	D	3733	0	3725	31	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	C	71	0	61	0	0
4	D	71	0	61	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
7	A	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	B	43	0	30	2	0
8	C	43	0	30	2	0
9	C	12	0	9	2	0
9	D	12	0	9	1	0
10	A	92	0	0	1	0
10	B	103	0	0	0	0
10	C	334	0	0	2	0
10	D	310	0	0	0	0
All	All	10318	0	9298	72	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 4.

All (72) 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)
2:C:135:PRO:HG2	10:C:897:HOH:O	1.84	0.77
2:D:525:ARG:HH11	9:D:13:ACY:H2	1.48	0.75
2:C:348:ASN:H	2:C:348:ASN:HD22	1.37	0.71
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.77	0.66
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.33	0.63
2:D:265:LYS:HD3	2:D:276:LEU:HD11	1.80	0.62
10:A:188:HOH:O	2:C:129:LYS:HD3	2.00	0.60
2:C:333:ARG:HH21	2:C:421:ASN:HD22	1.50	0.60
2:C:200:ASN:HD22	2:C:203:PHE:H	1.49	0.59
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.85	0.58
2:C:200:ASN:ND2	2:C:202:ARG:H	2.01	0.58
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.85	0.58
2:C:200:ASN:HD22	2:C:202:ARG:H	1.51	0.57
2:D:411:MET:CE	2:D:415:LEU:HD21	2.34	0.57
2:C:142:ASP:HB3	10:C:928:HOH:O	2.05	0.57
8:B:107:HEM:HMC2	8:B:107:HEM:HBC2	1.87	0.56
2:C:465:MET:HE1	2:C:471:PRO:HD3	1.90	0.55
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.90	0.53
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.52
2:D:333:ARG:HH21	2:D:421:ASN:HD22	1.57	0.52
2:D:120:VAL:HG12	2:D:122:GLN:CG	2.41	0.51
2:D:244:PRO:HD3	2:D:364:VAL:O	2.09	0.51
2:C:348:ASN:ND2	2:C:348:ASN:H	2.06	0.50
1:A:101:PRO:HD2	2:C:164:ILE:O	2.12	0.50
2:C:548:LYS:HG2	2:C:562:VAL:HG13	1.93	0.50
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.94	0.49
2:C:333:ARG:HH21	2:C:421:ASN:ND2	2.11	0.48
8:B:107:HEM:HBB2	2:D:242:GLU:OE1	2.13	0.48
2:C:200:ASN:ND2	2:C:203:PHE:H	2.12	0.48
1:B:83:SER:HB3	2:D:554:SER:O	2.13	0.47
2:D:267:LEU:HD13	2:D:576:ARG:NE	2.29	0.47
1:B:1:CYS:SG	1:B:20:PRO:HB3	2.55	0.47
1:A:68:ILE:HD13	2:C:464:LEU:HD23	1.96	0.47
2:D:393:ARG:HB2	2:D:396:GLN:HB2	1.97	0.47
2:D:378:ASP:OD1	2:D:541:THR:HB	2.15	0.46
2:D:333:ARG:HH21	2:D:421:ASN:ND2	2.12	0.46
2:D:271:TRP:CZ3	2:D:279:GLU:HG3	2.50	0.46
2:C:554:SER:HB3	2:C:560:ASP:HB3	1.97	0.46
1:A:83:SER:HB3	2:C:554:SER:O	2.15	0.46
8:C:10:HEM:HMC2	8:C:10:HEM:HBC2	1.98	0.46
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.50	0.46
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.97	0.46
2:C:123:PRO:HB3	9:C:15:ACY:H3	1.98	0.46
2:D:120:VAL:HG12	2:D:122:GLN:HG2	1.96	0.46
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.98	0.45
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.98	0.44
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.99	0.44
2:D:244:PRO:HB2	2:D:343:MET:SD	2.58	0.44
2:D:349:ARG:HG3	2:D:351:GLN:CG	2.46	0.43
2:C:124:PRO:HA	9:C:15:ACY:CH3	2.49	0.43
2:D:554:SER:HB3	2:D:560:ASP:HB3	2.01	0.43
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.54	0.43
2:D:252:LEU:HD11	2:D:537:ILE:HA	2.02	0.42
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.34	0.42
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.00	0.42
2:C:244:PRO:HD3	2:C:364:VAL:O	2.19	0.42
2:D:121:GLN:C	2:D:122:GLN:HG2	2.39	0.42
1:B:79:ASP:O	2:D:388:PRO:HB3	2.19	0.42
2:C:346:LEU:HB3	2:C:350:TYR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.50	0.42
2:C:123:PRO:HA	2:C:124:PRO:HA	1.84	0.42
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.42
2:D:123:PRO:HA	2:D:124:PRO:HA	1.89	0.41
2:D:120:VAL:HG12	2:D:122:GLN:HG3	2.03	0.41
2:C:242:GLU:OE1	8:C:10:HEM:HBB2	2.21	0.41
2:D:241:SER:O	2:D:366:PHE:HA	2.20	0.41
2:C:113:VAL:HG12	2:C:114:ASN:N	2.35	0.41
2:C:114:ASN:HB3	2:C:117:THR:OG1	2.20	0.41
1:B:6:LYS:HB2	1:B:6:LYS:HE2	1.99	0.41
2:D:128:LEU:HB2	2:D:144:ILE:HB	2.03	0.41
2:C:242:GLU:O	2:C:365:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
1	B	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	450 (97%)	13 (3%)	0	100	100
2	D	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
All	All	1130/1140 (99%)	1101 (97%)	29 (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	Percentiles	
1	A	90/90 (100%)	87 (97%)	3 (3%)	45	25
1	B	90/90 (100%)	89 (99%)	1 (1%)	80	72
2	C	410/410 (100%)	399 (97%)	11 (3%)	52	34
2	D	410/410 (100%)	400 (98%)	10 (2%)	57	39
All	All	1000/1000 (100%)	975 (98%)	25 (2%)	55	37

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	LYS
1	A	54	ASN
2	C	122	GLN
2	C	140	GLN
2	C	175	MET
2	C	254	LEU
2	C	318	ASP
2	C	348	ASN
2	C	356	ASN
2	C	466	GLU
2	C	523	GLN
2	C	547	SER
2	C	558	PRO
1	B	54	ASN
2	D	122	GLN
2	D	124	PRO
2	D	175	MET
2	D	218	ASP
2	D	254	LEU
2	D	267	LEU
2	D	318	ASP
2	D	322	PRO
2	D	523	GLN
2	D	547	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	200	ASN
2	C	348	ASN
2	C	421	ASN
1	B	54	ASN
2	D	421	ASN
2	D	549	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CSO	C	150	2	3,6,7	0.66	0	1,6,8	2.27	1 (100%)
2	CSO	D	150	2	3,6,7	0.61	0	1,6,8	1.82	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	CSO	C	150	2	-	0/1/5/7	0/0/0/0
2	CSO	D	150	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	CSO	O-C-CA	-2.27	119.57	125.49



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

12 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	C	640	2,4	14,14,15	0.76	0	15,19,21	0.87	0
4	NAG	C	641	4	14,14,15	0.57	0	15,19,21	0.77	0
4	BMA	C	642	4	11,11,12	0.73	0	14,15,17	0.55	0
4	MAN	C	643	4	11,11,12	1.02	1 (9%)	14,15,17	0.57	0
4	MAN	C	644	4	11,11,12	0.59	0	14,15,17	0.72	1 (7%)
4	FUC	C	645	4	10,10,11	0.54	0	14,14,16	0.66	0
4	NAG	D	640	2,4	14,14,15	0.59	0	15,19,21	0.86	0
4	NAG	D	641	4	14,14,15	0.55	0	15,19,21	0.80	1 (6%)
4	BMA	D	642	4	11,11,12	0.58	0	14,15,17	0.61	0
4	MAN	D	643	4	11,11,12	0.87	0	14,15,17	0.74	1 (7%)
4	MAN	D	644	4	11,11,12	0.59	0	14,15,17	0.62	1 (7%)
4	FUC	D	645	4	10,10,11	0.50	0	14,14,16	0.59	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
4	NAG	C	640	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	641	4	-	0/6/23/26	0/1/1/1
4	BMA	C	642	4	-	0/2/19/22	0/1/1/1
4	MAN	C	643	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	644	4	-	0/2/19/22	0/1/1/1
4	FUC	C	645	4	-	0/0/17/20	0/1/1/1
4	NAG	D	640	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	641	4	-	0/6/23/26	0/1/1/1
4	BMA	D	642	4	-	0/2/19/22	0/1/1/1
4	MAN	D	643	4	-	0/2/19/22	0/1/1/1
4	MAN	D	644	4	-	0/2/19/22	0/1/1/1
4	FUC	D	645	4	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	643	MAN	C2-C3	2.13	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	641	NAG	C4-C3-C2	-2.22	107.78	111.23
4	C	644	MAN	C1-O5-C5	2.08	114.89	112.25
4	D	644	MAN	C1-O5-C5	2.15	114.98	112.25
4	D	643	MAN	C1-O5-C5	2.17	115.01	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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
6	SCN	A	105	-	2,2,2	1.08	0	1,1,1	0.51	0
7	SO4	A	106	-	4,4,4	0.08	0	6,6,6	0.07	0
6	SCN	A	107	-	2,2,2	1.17	0	1,1,1	0.53	0
6	SCN	B	105	-	2,2,2	1.20	0	1,1,1	0.55	0
6	SCN	B	106	-	2,2,2	1.11	0	1,1,1	0.53	0
8	HEM	B	107	1,10,2	30,50,50	2.62	9 (30%)	24,82,82	2.09	6 (25%)
8	HEM	C	10	1,2	30,50,50	2.49	9 (30%)	24,82,82	2.05	6 (25%)
9	ACY	C	15	-	1,3,3	0.89	0	0,3,3	0.00	-
9	ACY	C	16	-	1,3,3	2.85	1 (100%)	0,3,3	0.00	-
9	ACY	C	17	-	1,3,3	1.80	0	0,3,3	0.00	-
3	NAG	C	620	2	14,14,15	0.79	1 (7%)	15,19,21	1.08	1 (6%)
3	NAG	C	630	2	14,14,15	0.75	0	15,19,21	0.78	0
7	SO4	C	9	-	4,4,4	0.46	0	6,6,6	0.20	0
9	ACY	D	12	-	1,3,3	2.51	1 (100%)	0,3,3	0.00	-
9	ACY	D	13	-	1,3,3	2.60	1 (100%)	0,3,3	0.00	-
9	ACY	D	14	-	1,3,3	2.76	1 (100%)	0,3,3	0.00	-
3	NAG	D	620	2	14,14,15	0.65	0	15,19,21	0.73	0
3	NAG	D	630	2	14,14,15	0.58	0	15,19,21	0.64	0
7	SO4	D	7	-	4,4,4	0.36	0	6,6,6	0.13	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
6	SCN	A	105	-	-	0/0/0/0	0/0/0/0
7	SO4	A	106	-	-	0/0/0/0	0/0/0/0
6	SCN	A	107	-	-	0/0/0/0	0/0/0/0
6	SCN	B	105	-	-	0/0/0/0	0/0/0/0
6	SCN	B	106	-	-	0/0/0/0	0/0/0/0
8	HEM	B	107	1,10,2	-	0/10/54/54	0/0/8/8
8	HEM	C	10	1,2	-	0/10/54/54	0/0/8/8
9	ACY	C	15	-	-	0/0/0/0	0/0/0/0
9	ACY	C	16	-	-	0/0/0/0	0/0/0/0
9	ACY	C	17	-	-	0/0/0/0	0/0/0/0
3	NAG	C	620	2	-	0/6/23/26	0/1/1/1
3	NAG	C	630	2	-	0/6/23/26	0/1/1/1
7	SO4	C	9	-	-	0/0/0/0	0/0/0/0
9	ACY	D	12	-	-	0/0/0/0	0/0/0/0
9	ACY	D	13	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ACY	D	14	-	-	0/0/0/0	0/0/0/0
3	NAG	D	620	2	-	0/6/23/26	0/1/1/1
3	NAG	D	630	2	-	0/6/23/26	0/1/1/1
7	SO4	D	7	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	10	HEM	C2D-C3D	-6.59	1.34	1.54
8	B	107	HEM	C3B-C4B	-6.54	1.46	1.51
8	B	107	HEM	C2D-C3D	-6.32	1.35	1.54
8	C	10	HEM	C3C-CAC	-5.56	1.40	1.51
8	C	10	HEM	C3B-C4B	-5.19	1.47	1.51
8	B	107	HEM	C3C-CAC	-5.12	1.41	1.51
8	B	107	HEM	C3D-C4D	-4.96	1.45	1.51
8	C	10	HEM	C3B-CAB	-4.93	1.42	1.51
8	B	107	HEM	C3B-CAB	-4.54	1.42	1.51
8	B	107	HEM	C2C-C1C	-3.98	1.45	1.52
8	C	10	HEM	C3D-C4D	-3.85	1.46	1.51
8	C	10	HEM	C2C-C1C	-3.44	1.46	1.52
8	C	10	HEM	C4C-NC	2.09	1.38	1.36
3	C	620	NAG	C1-C2	2.10	1.55	1.52
8	B	107	HEM	C4C-NC	2.18	1.38	1.36
9	D	12	ACY	CH3-C	2.51	1.52	1.48
8	B	107	HEM	CBC-CAC	2.52	1.43	1.29
9	D	13	ACY	CH3-C	2.60	1.52	1.48
8	C	10	HEM	CBC-CAC	2.67	1.44	1.29
9	D	14	ACY	CH3-C	2.76	1.52	1.48
9	C	16	ACY	CH3-C	2.85	1.52	1.48
8	C	10	HEM	CBB-CAB	2.89	1.46	1.29
8	B	107	HEM	CBB-CAB	2.95	1.46	1.29

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	10	HEM	CMD-C2D-C3D	2.64	126.01	114.35
8	B	107	HEM	CMD-C2D-C3D	2.66	126.13	114.35
8	C	10	HEM	C2D-C3D-C4D	2.90	106.42	101.50
3	C	620	NAG	C1-O5-C5	2.97	116.02	112.25
8	B	107	HEM	C2D-C3D-C4D	2.98	106.55	101.50
8	B	107	HEM	CAD-C3D-C4D	3.82	125.95	112.47
8	C	10	HEM	CAD-C3D-C4D	4.08	126.86	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed( <sup>o</sup> )	Ideal( <sup>o</sup> )
8	B	107	HEM	CMB-C2B-C3B	4.38	127.47	116.53
8	C	10	HEM	CMB-C2B-C3B	4.40	127.51	116.53
8	C	10	HEM	CAD-C3D-C2D	4.51	126.18	113.22
8	C	10	HEM	CMC-C2C-C3C	4.76	128.40	116.53
8	B	107	HEM	CAD-C3D-C2D	4.76	126.92	113.22
8	B	107	HEM	CMC-C2C-C3C	4.93	128.85	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	107	HEM	2	0
8	C	10	HEM	2	0
9	C	15	ACY	2	0
9	D	13	ACY	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	104/104 (100%)	0.04	5 (4%) 34 32	6, 9, 23, 46	0
1	B	104/104 (100%)	-0.04	0 100 100	6, 10, 19, 24	0
2	C	465/466 (99%)	-0.07	9 (1%) 70 69	5, 10, 24, 39	0
2	D	465/466 (99%)	0.16	14 (3%) 54 51	6, 12, 27, 43	0
All	All	1138/1140 (99%)	0.04	28 (2%) 61 58	5, 11, 25, 46	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	14.1
2	D	217	HIS	6.1
2	C	355	PRO	6.0
2	D	355	PRO	5.8
2	D	578	ALA	5.8
1	A	1	CYS	4.8
1	A	3	GLU	4.7
1	A	4	GLN	4.5
2	D	267	LEU	3.9
2	C	217	HIS	3.7
2	C	140	GLN	3.6
2	D	576	ARG	3.5
2	D	568	PRO	3.5
2	D	190	MET	2.9
2	D	155	GLY	2.7
2	D	356	ASN	2.7
2	C	349	ARG	2.5
2	C	348	ASN	2.5
2	D	157	ASN	2.5
2	D	226	ARG	2.3
2	D	349	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	2.3
2	D	353	MET	2.3
2	D	523	GLN	2.3
1	A	104	ALA	2.1
2	C	141	ALA	2.1
2	C	122	GLN	2.0
2	C	157	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSO	D	150	7/8	0.94	0.10	-	6,8,10,14	0
2	CSO	C	150	7/8	0.94	0.09	-	8,10,11,15	0

## 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
4	BMA	C	642	11/12	0.94	0.12	0.47	11,13,16,21	0
4	NAG	C	641	14/15	0.96	0.11	0.21	8,10,11,11	0
4	NAG	D	641	14/15	0.97	0.11	-0.11	8,11,12,13	0
4	BMA	D	642	11/12	0.96	0.09	-0.55	10,12,15,19	0
4	FUC	D	645	10/11	0.96	0.09	-	14,15,17,18	0
4	MAN	D	644	11/12	0.93	0.12	-	13,14,16,17	0
4	MAN	D	643	11/12	0.89	0.12	-	22,24,28,30	0
4	MAN	C	643	11/12	0.90	0.11	-	24,26,27,27	0
4	FUC	C	645	10/11	0.95	0.09	-	15,16,18,19	0
4	NAG	C	640	14/15	0.94	0.10	-	8,12,16,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	C	644	11/12	0.95	0.14	-	13,15,17,18	0
4	NAG	D	640	14/15	0.96	0.11	-	10,12,17,20	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( $\text{\AA}^2$ )	Q<0.9
9	ACY	C	15	4/4	0.79	0.14	8.13	27,28,29,30	0
9	ACY	D	14	4/4	0.91	0.13	4.56	20,21,21,24	0
3	NAG	D	630	14/15	0.82	0.19	2.61	32,34,37,38	0
3	NAG	D	620	14/15	0.89	0.17	1.71	17,24,28,29	0
3	NAG	C	630	14/15	0.85	0.14	0.98	23,28,36,36	0
3	NAG	C	620	14/15	0.92	0.11	0.88	15,17,21,22	0
8	HEM	C	10	43/43	0.96	0.10	0.71	4,8,9,10	0
6	SCN	A	105	3/3	0.98	0.14	0.40	12,12,12,17	0
6	SCN	B	105	3/3	0.98	0.14	0.36	11,11,16,17	0
6	SCN	A	107	3/3	0.98	0.09	0.34	15,15,18,20	0
8	HEM	B	107	43/43	0.96	0.11	0.15	5,8,10,12	0
5	CA	D	2	1/1	1.00	0.11	-0.30	9,9,9,9	0
5	CA	C	1	1/1	1.00	0.09	-0.45	10,10,10,10	0
9	ACY	C	16	4/4	0.88	0.14	-	27,28,29,29	0
7	SO4	D	7	5/5	0.68	0.35	-	46,47,47,47	5
9	ACY	C	17	4/4	0.92	0.20	-	17,20,20,21	0
9	ACY	D	12	4/4	0.93	0.14	-	30,31,31,32	0
9	ACY	D	13	4/4	0.34	0.39	-	38,38,38,39	0
7	SO4	C	9	5/5	0.95	0.15	-	27,29,31,33	0
7	SO4	A	106	5/5	0.98	0.08	-	25,25,28,29	0
6	SCN	B	106	3/3	0.97	0.10	-	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.