



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2017 – 02:27 PM EDT

PDB ID : 5YD9  
Title : Crystal structure of bovine lactoperoxidase with iodide ion at the substrate binding site on the distal heme side at 1.91 Å resolution  
Authors : Singh, P.K.; Sirohi, H.V.; kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : unknown  
Resolution : 1.92 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

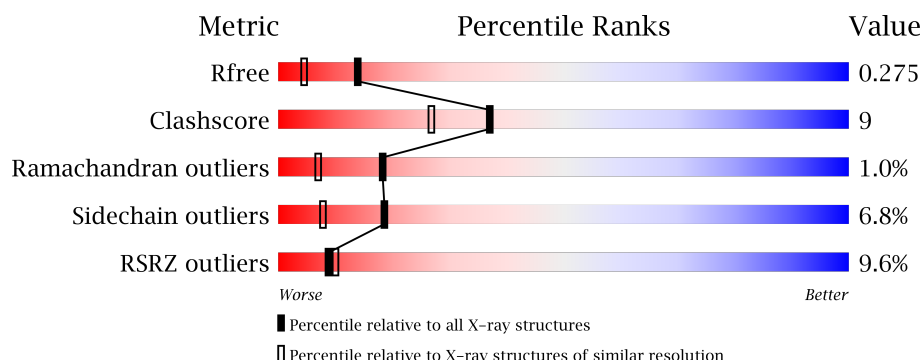
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	595	<div> <div>10%</div> <div>83%</div> <div>14%</div> <div>..</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
6	SCN	A	614	-	-	-	X
6	SCN	A	617	-	-	-	X





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

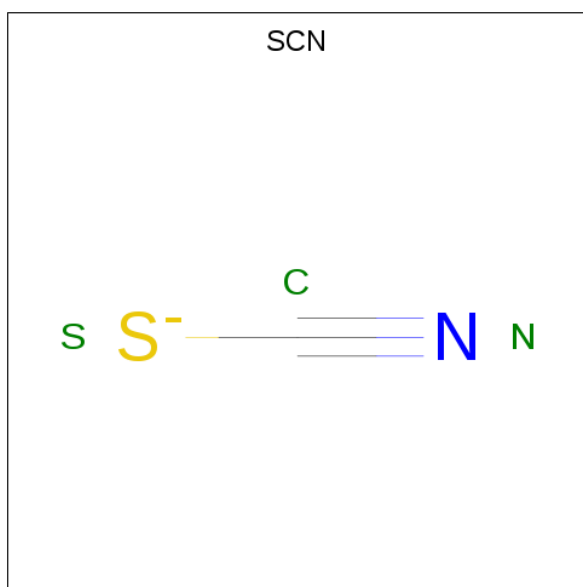
- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	I	0	0
			4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	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	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	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		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	208	Total	O	0	0
			208	208		

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.74Å 79.80Å 65.18Å 90.00° 91.43° 90.00°	Depositor
Resolution (Å)	65.16 – 1.92 50.47 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.2 (65.16-1.92) 95.3 (50.47-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.227 , 0.277 0.230 , 0.275	Depositor DCC
$R_{free}$ test set	1886 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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, 0.333 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: SCN, NAG, SEP, CA, HEC, IOD

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	0.70	0/4891	0.86	5/6634 (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	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	348	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	167	CYS	C-N-CD	-6.14	107.09	120.60
1	A	16	ASP	N-CA-C	-6.05	94.67	111.00
1	A	432	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	108	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	VAL	Peptide
1	A	9	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	4774	0	4687	81	1
2	A	43	0	32	12	0
3	A	70	0	64	0	0
4	A	4	0	0	2	0
5	A	1	0	0	0	0
6	A	21	0	0	2	0
7	A	208	0	0	5	0
All	All	5121	0	4783	86	1

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 9.

All (86) 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:108:ASP:OD2	2:A:601:HEC:CMD	1.83	1.25
1:A:258:GLU:OE2	2:A:601:HEC:CMB	1.88	1.21
1:A:108:ASP:OD2	2:A:601:HEC:HMD3	0.90	1.08
1:A:258:GLU:OE2	2:A:601:HEC:HMB3	0.91	1.07
1:A:170:PRO:HG2	1:A:171:PRO:HD3	1.40	1.03
1:A:168:PRO:CG	1:A:173:GLN:HG2	1.92	0.99
1:A:168:PRO:CD	1:A:173:GLN:HG2	1.96	0.94
1:A:108:ASP:CG	2:A:601:HEC:HMD3	1.88	0.94
1:A:258:GLU:CD	2:A:601:HEC:HMB3	1.96	0.86
1:A:170:PRO:CG	1:A:171:PRO:HD3	2.06	0.85
1:A:593:ARG:C	1:A:595:ASN:HD22	1.79	0.84
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.22	0.84
1:A:593:ARG:C	1:A:595:ASN:ND2	2.32	0.82
1:A:204:ARG:NH1	1:A:290:GLU:OE2	2.15	0.80
1:A:168:PRO:HG3	1:A:173:GLN:HG2	1.64	0.79
1:A:424:PRO:O	4:A:610:IOD:I	2.71	0.79
1:A:146:LYS:O	1:A:147:ASN:HB2	1.86	0.73
1:A:29:ASN:OD1	7:A:701:HOH:O	2.05	0.73
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.71	0.72
1:A:167:CYS:CB	1:A:168:PRO:CD	2.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.72	0.71
1:A:168:PRO:CD	1:A:173:GLN:CG	2.69	0.71
1:A:593:ARG:HD2	1:A:593:ARG:N	2.06	0.71
6:A:614:SCN:N	7:A:702:HOH:O	2.26	0.69
1:A:170:PRO:HG2	1:A:171:PRO:CD	2.21	0.67
1:A:306:ILE:HA	6:A:616:SCN:S	2.35	0.66
1:A:295:GLU:O	1:A:299:ILE:HD12	1.95	0.66
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.25	0.66
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.27	0.64
1:A:170:PRO:CG	1:A:171:PRO:CD	2.77	0.63
1:A:169:THR:HG23	1:A:170:PRO:HD3	1.83	0.58
1:A:82:ILE:HD13	1:A:480:LEU:CD1	2.34	0.57
2:A:601:HEC:CBB	2:A:601:HEC:HMB1	2.32	0.57
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.88	0.56
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.88	0.56
1:A:350:GLY:HA3	2:A:601:HEC:HBC2	1.87	0.56
1:A:593:ARG:HA	1:A:595:ASN:HD21	1.71	0.54
1:A:204:ARG:CZ	1:A:290:GLU:OE2	2.56	0.54
1:A:170:PRO:HD2	1:A:171:PRO:HD2	1.90	0.54
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.44	0.53
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.43	0.53
2:A:601:HEC:HBB3	2:A:601:HEC:HMB1	1.91	0.52
1:A:204:ARG:NH2	1:A:290:GLU:OE2	2.43	0.52
1:A:593:ARG:CA	1:A:595:ASN:ND2	2.72	0.52
1:A:385:ARG:NE	7:A:707:HOH:O	2.41	0.51
1:A:593:ARG:CA	1:A:595:ASN:HD21	2.23	0.51
1:A:168:PRO:HD2	1:A:173:GLN:HG2	1.87	0.51
1:A:168:PRO:HD3	1:A:173:GLN:CG	2.42	0.50
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.42	0.50
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.42	0.50
1:A:146:LYS:O	1:A:147:ASN:CB	2.53	0.49
1:A:165:PHE:CE2	1:A:172:TYR:HD1	2.30	0.49
1:A:32:ARG:NH1	7:A:711:HOH:O	2.45	0.49
1:A:170:PRO:CD	1:A:171:PRO:HD2	2.42	0.49
1:A:224:LEU:HD12	1:A:558:HIS:CE1	2.48	0.48
2:A:601:HEC:HMC1	2:A:601:HEC:CBC	2.44	0.48
1:A:335:VAL:O	1:A:337:PRO:HD3	2.14	0.48
1:A:8:ALA:N	1:A:9:PRO:CD	2.77	0.48
1:A:106:ILE:HD11	1:A:265:ALA:HB3	1.96	0.47
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.95	0.47
1:A:165:PHE:HE2	1:A:172:TYR:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLN:HG2	1:A:218:GLU:H	1.80	0.47
1:A:203:LEU:HB3	1:A:213:MET:CE	2.46	0.45
1:A:255:ARG:HD2	4:A:607:IOD:I	2.87	0.45
1:A:503:GLU:HG2	7:A:883:HOH:O	2.16	0.45
1:A:288:ASN:N	1:A:288:ASN:OD1	2.46	0.44
1:A:170:PRO:CD	1:A:171:PRO:CD	2.95	0.44
1:A:595:ASN:N	1:A:595:ASN:ND2	2.65	0.44
1:A:102:GLN:HE21	1:A:106:ILE:HD12	1.83	0.43
1:A:216:ASN:OD1	1:A:218:GLU:N	2.51	0.43
1:A:260:ILE:HG23	1:A:261:LEU:HD13	2.01	0.43
1:A:549:PHE:HE1	1:A:553:ILE:HD11	1.83	0.43
1:A:464:LEU:O	1:A:468:GLN:HG3	2.19	0.42
1:A:467:LEU:HG	1:A:471:LEU:HD22	2.01	0.42
2:A:601:HEC:HMC1	2:A:601:HEC:HBC3	2.01	0.42
1:A:407:MET:HB3	1:A:501:MET:CE	2.50	0.42
1:A:242:THR:O	1:A:245:ARG:NH2	2.53	0.41
1:A:7:GLY:C	1:A:9:PRO:HD2	2.41	0.41
1:A:350:GLY:CA	2:A:601:HEC:HBC2	2.50	0.41
1:A:8:ALA:O	1:A:10:VAL:N	2.54	0.41
1:A:168:PRO:HD2	1:A:173:GLN:CG	2.48	0.41
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.56	0.41
1:A:217:GLN:HG2	1:A:218:GLU:N	2.36	0.40
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.56	0.40
1:A:172:TYR:OH	1:A:175:LEU:O	2.22	0.40
1:A:148:ASP:O	1:A:151:LEU:HB2	2.21	0.40

All (1) 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)
1:A:368:TRP:CZ3	1:A:594:GLU:O[2_555]	2.02	0.18

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	592/595 (100%)	558 (94%)	28 (5%)	6 (1%)	18	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	168	PRO
1	A	9	PRO
1	A	11	PRO
1	A	171	PRO
1	A	10	VAL

### 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	517/517 (100%)	482 (93%)	35 (7%)	18	8

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	12	LEU
1	A	13	VAL
1	A	91	VAL
1	A	98	LEU
1	A	106	ILE
1	A	119	LEU
1	A	124	HIS
1	A	128	GLN
1	A	153	THR
1	A	175	LEU
1	A	187	LEU
1	A	202	ARG

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	217	GLN
1	A	220	TRP
1	A	235	SER
1	A	238	GLU
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	282	LYS
1	A	290	GLU
1	A	292	LEU
1	A	317	LEU
1	A	347	PHE
1	A	376	LEU
1	A	464	LEU
1	A	471	LEU
1	A	480	LEU
1	A	511	LEU
1	A	542	ASP
1	A	564	LEU
1	A	593	ARG
1	A	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	SEP	A	198	1	9,9,10	1.48	1 (11%)	9,12,14	3.19	3 (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
1	SEP	A	198	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-C	3.06	1.54	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-O1P	2.28	119.43	110.50
1	A	198	SEP	P-OG-CB	5.71	134.03	118.30
1	A	198	SEP	OG-CB-CA	7.21	115.28	108.17

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	HEC	A	601	1,7	28,50,50	2.13	7 (25%)	16,82,82	1.56	4 (25%)
3	NAG	A	602	1	14,14,15	0.59	0	15,19,21	1.29	1 (6%)
3	NAG	A	603	1,3	14,14,15	0.30	0	15,19,21	1.67	3 (20%)
3	NAG	A	604	3	14,14,15	0.37	0	15,19,21	1.03	1 (6%)
3	NAG	A	605	1	14,14,15	0.52	0	15,19,21	1.00	1 (6%)
3	NAG	A	606	1	14,14,15	0.85	1 (7%)	15,19,21	1.29	2 (13%)
6	SCN	A	612	-	1,2,2	0.39	0	0,1,1	0.00	-
6	SCN	A	613	-	1,2,2	0.41	0	0,1,1	0.00	-
6	SCN	A	614	-	1,2,2	0.42	0	0,1,1	0.00	-
6	SCN	A	615	-	1,2,2	0.40	0	0,1,1	0.00	-
6	SCN	A	616	-	1,2,2	0.43	0	0,1,1	0.00	-
6	SCN	A	617	-	1,2,2	3.37	1 (100%)	0,1,1	0.00	-
6	SCN	A	618	4	1,2,2	0.72	0	0,1,1	0.00	-

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	HEC	A	601	1,7	-	0/6/54/54	0/0/8/8
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	604	3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
3	NAG	A	606	1	-	0/6/23/26	0/1/1/1
6	SCN	A	612	-	-	0/0/0/0	0/0/0/0
6	SCN	A	613	-	-	0/0/0/0	0/0/0/0
6	SCN	A	614	-	-	0/0/0/0	0/0/0/0
6	SCN	A	615	-	-	0/0/0/0	0/0/0/0
6	SCN	A	616	-	-	0/0/0/0	0/0/0/0
6	SCN	A	617	-	-	0/0/0/0	0/0/0/0
6	SCN	A	618	4	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEC	C3B-C2B	-6.25	1.34	1.40
2	A	601	HEC	CBC-CAC	-4.14	1.33	1.49
2	A	601	HEC	C4B-NB	-4.07	1.32	1.36
2	A	601	HEC	CBB-CAB	-3.96	1.33	1.49
2	A	601	HEC	C4C-NC	-3.11	1.33	1.36
2	A	601	HEC	C3C-C2C	-2.75	1.37	1.40
3	A	606	NAG	C1-C2	2.24	1.55	1.52
2	A	601	HEC	C3B-C4B	2.85	1.48	1.43
6	A	617	SCN	C-N	3.37	1.27	1.15

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAG	C1-C2-N2	-3.57	104.39	110.49
3	A	603	NAG	O4-C4-C3	-3.06	103.69	110.36
2	A	601	HEC	CMC-C2C-C1C	-2.77	124.21	128.46
3	A	603	NAG	O5-C1-C2	-2.43	108.10	111.47
3	A	605	NAG	O5-C1-C2	-2.38	108.16	111.47
2	A	601	HEC	C3B-C4B-NB	-2.32	106.56	110.94
2	A	601	HEC	CBD-CAD-C3D	-2.18	108.32	112.48
2	A	601	HEC	CBA-CAA-C2A	-2.10	108.47	112.47
3	A	606	NAG	O3-C3-C2	2.03	113.73	109.39
3	A	604	NAG	C1-O5-C5	2.16	115.14	112.17
3	A	606	NAG	O4-C4-C5	2.26	114.97	109.28
3	A	603	NAG	C3-C4-C5	3.99	117.25	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	12	0
6	A	614	SCN	1	0
6	A	616	SCN	1	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 ⓘ

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	594/595 (99%)	0.70	57 (9%) 9 10	29, 52, 113, 192	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	SER	27.6
1	A	7	GLY	19.7
1	A	2	TRP	18.7
1	A	1	SER	13.7
1	A	119	LEU	12.6
1	A	120	GLY	11.5
1	A	174	SER	11.0
1	A	11	PRO	10.9
1	A	122	ASN	9.2
1	A	170	PRO	9.1
1	A	117	THR	8.4
1	A	118	GLU	7.9
1	A	172	TYR	7.5
1	A	171	PRO	7.4
1	A	169	THR	6.1
1	A	10	VAL	6.0
1	A	8	ALA	4.6
1	A	13	VAL	4.4
1	A	583	ASP	3.7
1	A	292	LEU	3.7
1	A	254	PHE	3.7
1	A	587	LEU	3.6
1	A	593	ARG	3.6
1	A	591	ALA	3.6
1	A	126	LYS	3.6
1	A	20	PRO	3.4
1	A	21	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	124	HIS	3.3
1	A	16	ASP	3.3
1	A	12	LEU	3.3
1	A	283	LEU	3.3
1	A	231	ASN	2.9
1	A	220	TRP	2.9
1	A	4	VAL	2.9
1	A	222	HIS	2.8
1	A	279	GLU	2.8
1	A	173	GLN	2.8
1	A	128	GLN	2.8
1	A	287	TRP	2.7
1	A	209	PRO	2.7
1	A	132	TYR	2.6
1	A	226	TYR	2.6
1	A	15	CYS	2.6
1	A	595	ASN	2.5
1	A	9	PRO	2.4
1	A	286	HIS	2.4
1	A	581	THR	2.4
1	A	63	GLN	2.3
1	A	3	GLU	2.3
1	A	585	LEU	2.3
1	A	285	PRO	2.1
1	A	584	LYS	2.1
1	A	425	THR	2.1
1	A	547	VAL	2.1
1	A	229	PHE	2.1
1	A	200	ALA	2.0
1	A	280	LEU	2.0

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

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
1	SEP	A	198	10/11	0.93	0.18	-	52,64,73,77	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
6	SCN	A	614	3/3	0.96	0.13	3.80	54,54,55,59	0
6	SCN	A	617	3/3	0.98	0.16	3.40	24,24,31,33	0
6	SCN	A	615	3/3	0.77	0.21	1.61	42,42,42,69	3
3	NAG	A	603	14/15	0.84	0.16	0.89	64,73,80,85	0
6	SCN	A	612	3/3	0.95	0.14	0.19	62,62,63,70	0
4	IOD	A	608	1/1	0.98	0.10	-0.43	53,53,53,53	1
3	NAG	A	605	14/15	0.90	0.12	-0.47	54,62,70,77	0
2	HEC	A	601	43/43	0.98	0.10	-0.69	24,30,40,42	0
4	IOD	A	610	1/1	0.98	0.08	-1.58	63,63,63,63	1
6	SCN	A	618	3/3	0.99	0.09	-1.63	44,44,46,48	3
6	SCN	A	616	3/3	0.99	0.08	-3.15	22,22,24,31	3
4	IOD	A	609	1/1	0.99	0.08	-3.31	55,55,55,55	1
5	CA	A	611	1/1	0.97	0.06	-3.58	43,43,43,43	0
3	NAG	A	606	14/15	0.68	0.22	-	65,79,96,100	0
6	SCN	A	613	3/3	0.96	0.18	-	52,52,55,59	0
3	NAG	A	602	14/15	0.76	0.21	-	76,84,97,110	0
4	IOD	A	607	1/1	0.96	0.04	-	67,67,67,67	1
3	NAG	A	604	14/15	0.72	0.23	-	81,92,97,109	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.