



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:22 AM GMT

PDB ID : 3I6N  
Title : Mode of Binding of the Tuberculosis Prodrug Isoniazid to Peroxidases: Crystal Structure of Bovine Lactoperoxidase with Isoniazid at 2.7 Resolution  
Authors : Singh, A.K.; Kumar, R.P.; Pandey, N.; Singh, N.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2009-07-07  
Resolution : 2.70 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

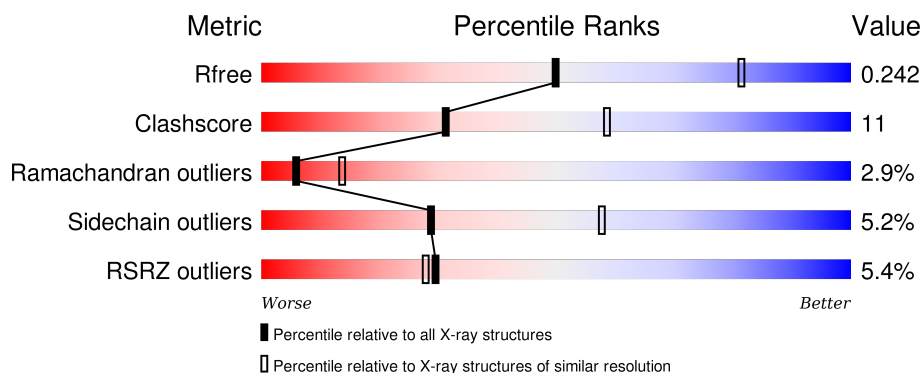
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>5%</div> <div>74%</div> <div>22%</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
5	ISZ	A	607	-	-	X	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5259 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

- 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		

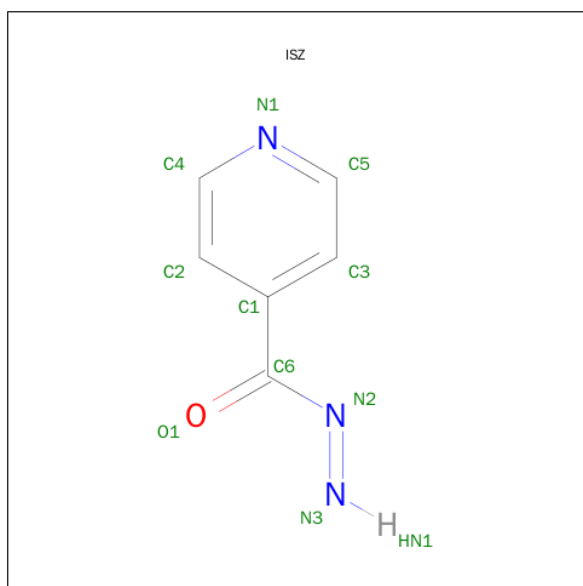
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is 4-(DIAZENYL CARBONYL)PYRIDINE (three-letter code: ISZ) (formula:  $C_6H_5N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	3	1		

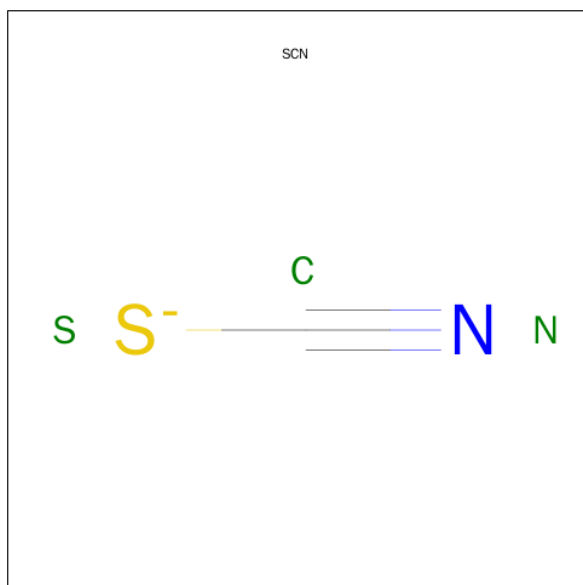
- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	I	0	0
			7	7		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

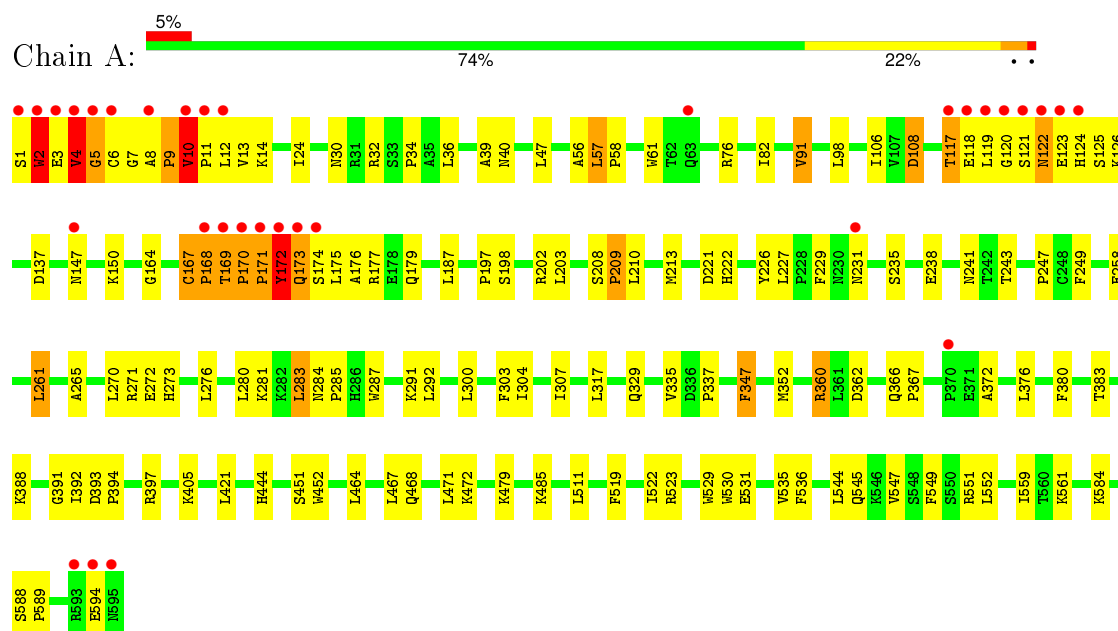
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	287	Total	O	0	0
			287	287		

### 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: Lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.49Å 80.55Å 77.78Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	75.81 – 2.70 16.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (75.81-2.70) 94.1 (16.74-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.232 0.201 , 0.242	Depositor DCC
$R_{free}$ test set	865 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 17002 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ISZ, SCN, NAG, SEP, CA, HEM, IOD, 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	0.52	1/4891 (0.0%)	0.83	7/6634 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	MET	CG-SD	-6.10	1.65	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	CA-CB-CG	9.59	134.50	113.40
1	A	10	VAL	CB-CA-C	7.66	125.96	111.40
1	A	173	GLN	N-CA-CB	6.30	121.95	110.60
1	A	147	ASN	CA-CB-CG	6.03	126.67	113.40
1	A	4	VAL	CA-CB-CG2	-5.31	102.94	110.90
1	A	2	TRP	CB-CA-C	-5.10	100.20	110.40
1	A	32	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	172	TYR	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	4688	102	0
2	A	43	0	30	1	0
3	A	78	0	68	2	0
4	A	56	0	50	2	0
5	A	10	0	5	5	0
6	A	7	0	0	0	0
7	A	1	0	0	0	0
8	A	3	0	0	0	0
9	A	287	0	0	0	0
All	All	5259	0	4841	106	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 11.

All (106) 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:167:CYS:HB3	1:A:168:PRO:HD3	1.55	0.86
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.57	0.85
1:A:169:THR:N	1:A:170:PRO:HD2	1.95	0.82
1:A:258:GLU:HB2	5:A:607:ISZ:H3	1.63	0.79
1:A:258:GLU:HG3	5:A:607:ISZ:H3	1.66	0.76
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.23	0.73
1:A:258:GLU:CB	5:A:607:ISZ:H3	2.21	0.69
1:A:197:PRO:HD2	1:A:198:SEP:O3P	1.92	0.69
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.07	0.69
1:A:175:LEU:HG	1:A:176:ALA:H	1.58	0.69
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.74	0.69
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.28	0.68
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.30	0.66
1:A:2:TRP:HA	1:A:2:TRP:HE3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:CG	5:A:607:ISZ:H3	2.25	0.65
1:A:167:CYS:CB	1:A:168:PRO:CD	2.75	0.65
1:A:2:TRP:HA	1:A:2:TRP:CE3	2.30	0.65
1:A:588:SER:OG	1:A:589:PRO:HD3	1.97	0.64
1:A:91:VAL:HG13	1:A:405:LYS:HG3	1.80	0.64
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.32	0.64
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.27	0.64
1:A:208:SER:HB3	4:A:599:NAG:H62	1.81	0.63
1:A:169:THR:HB	1:A:170:PRO:HD3	1.80	0.62
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.27	0.62
1:A:169:THR:N	1:A:170:PRO:CD	2.63	0.61
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.82	0.61
1:A:258:GLU:O	1:A:258:GLU:HG2	2.01	0.60
1:A:121:SER:O	1:A:122:ASN:CB	2.49	0.60
1:A:123:GLU:HB3	1:A:126:LYS:HE2	1.83	0.59
1:A:208:SER:HB2	1:A:210:LEU:HD12	1.85	0.57
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.33	0.57
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.39	0.57
1:A:202:ARG:NH2	1:A:231:ASN:HB2	2.20	0.56
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.87	0.56
1:A:535:VAL:HG12	1:A:536:PHE:CD1	2.40	0.56
1:A:123:GLU:HB3	1:A:126:LYS:HG3	1.87	0.56
1:A:281:LYS:O	1:A:281:LYS:HD2	2.06	0.56
1:A:360:ARG:HH11	1:A:372:ALA:HA	1.71	0.56
1:A:13:VAL:HG12	1:A:14:LYS:H	1.72	0.54
1:A:272:GLU:O	1:A:276:LEU:HB2	2.08	0.54
1:A:544:LEU:O	1:A:547:VAL:HG22	2.07	0.53
1:A:3:GLU:HG3	1:A:175:LEU:HD22	1.90	0.53
1:A:300:LEU:O	1:A:304:ILE:HG12	2.08	0.53
1:A:56:ALA:HB1	1:A:177:ARG:HD3	1.91	0.53
1:A:169:THR:HB	1:A:170:PRO:CD	2.39	0.52
1:A:519:PHE:HA	1:A:522:ILE:HG12	1.92	0.52
3:A:596:NAG:H61	3:A:597:NAG:C1	2.39	0.52
4:A:604:NAG:H61	4:A:606:NAG:O7	2.10	0.51
1:A:118:GLU:HG3	1:A:120:GLY:H	1.74	0.51
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.93	0.51
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.94	0.50
1:A:3:GLU:C	1:A:5:GLY:H	2.15	0.50
1:A:303:PHE:O	1:A:307:ILE:HG12	2.13	0.49
1:A:335:VAL:O	1:A:337:PRO:HD3	2.13	0.49
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:HB2	1:A:347:PHE:CE2	2.48	0.48
1:A:468:GLN:O	1:A:472:LYS:N	2.46	0.48
1:A:1:SER:O	1:A:2:TRP:HB2	2.13	0.48
1:A:76:ARG:NH2	1:A:150:LYS:HD2	2.29	0.48
1:A:10:VAL:HB	1:A:12:LEU:N	2.29	0.48
2:A:605:HEM:HBC2	2:A:605:HEM:HMC2	1.95	0.47
1:A:258:GLU:HG3	5:A:607:ISZ:C3	2.42	0.47
1:A:108:ASP:HB2	1:A:347:PHE:CD2	2.50	0.47
1:A:280:LEU:HA	1:A:283:LEU:CD1	2.44	0.47
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:123:GLU:HG3	1:A:125:SER:H	1.80	0.46
1:A:121:SER:O	1:A:122:ASN:HB2	2.14	0.46
1:A:170:PRO:HB3	1:A:171:PRO:CD	2.39	0.45
1:A:10:VAL:HB	1:A:11:PRO:CA	2.47	0.45
1:A:284:ASN:O	1:A:285:PRO:C	2.54	0.45
1:A:397:ARG:HG2	1:A:559:ILE:HD12	1.98	0.45
1:A:47:LEU:HD12	1:A:452:TRP:CH2	2.52	0.45
1:A:82:ILE:CD1	1:A:479:LYS:HB3	2.47	0.45
1:A:249:PHE:CE1	1:A:383:THR:HG22	2.52	0.45
1:A:235:SER:HB3	1:A:238:GLU:HG2	2.00	0.44
1:A:168:PRO:HB2	1:A:169:THR:H	1.35	0.44
1:A:271:ARG:NH1	1:A:392:ILE:HD11	2.33	0.43
1:A:169:THR:CB	1:A:170:PRO:CD	2.96	0.43
3:A:601:NAG:H62	3:A:602:NAG:N2	2.34	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.53	0.43
1:A:362:ASP:OD2	1:A:366:GLN:HB2	2.19	0.43
1:A:393:ASP:HB2	1:A:394:PRO:HD3	2.01	0.43
1:A:61:TRP:HH2	1:A:137:ASP:O	2.02	0.43
1:A:170:PRO:CB	1:A:171:PRO:CD	2.97	0.43
1:A:39:ALA:O	1:A:40:ASN:HB2	2.19	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.77	0.42
1:A:303:PHE:CE1	1:A:307:ILE:HD11	2.54	0.42
1:A:175:LEU:HG	1:A:176:ALA:N	2.31	0.42
1:A:283:LEU:C	1:A:285:PRO:HD3	2.40	0.42
1:A:171:PRO:HB2	1:A:172:TYR:H	1.67	0.41
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.19	0.41
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.85	0.41
1:A:549:PHE:CE1	1:A:552:LEU:HD22	2.55	0.41
1:A:209:PRO:HD2	1:A:210:LEU:HG	2.02	0.41
1:A:303:PHE:CD2	1:A:304:ILE:HD13	2.55	0.41
1:A:241:ASN:OD1	1:A:243:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ARG:HG3	1:A:529:TRP:CD2	2.56	0.41
1:A:168:PRO:O	1:A:169:THR:OG1	2.33	0.41
1:A:287:TRP:CG	1:A:291:LYS:HG2	2.56	0.41
1:A:119:LEU:HD21	1:A:170:PRO:HA	2.01	0.40
1:A:366:GLN:O	1:A:367:PRO:C	2.59	0.40
1:A:467:LEU:HG	1:A:471:LEU:HD22	2.03	0.40
1:A:380:PHE:CE2	1:A:421:LEU:HA	2.55	0.40
1:A:261:LEU:HA	1:A:261:LEU:HD12	1.85	0.40
1:A:30:ASN:O	1:A:34:PRO:HA	2.20	0.40
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

## 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%)	541 (91%)	34 (6%)	17 (3%)	<b>6</b> <b>14</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	10	VAL
1	A	122	ASN
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	170	PRO
1	A	171	PRO
1	A	485	LYS
1	A	174	SER
1	A	594	GLU

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Mol	Chain	Res	Type
1	A	2	TRP
1	A	6	CYS
1	A	5	GLY
1	A	7	GLY
1	A	209	PRO
1	A	9	PRO

### 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%)	490 (95%)	27 (5%)	29 58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	10	VAL
1	A	24	ILE
1	A	57	LEU
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	124	HIS
1	A	172	TYR
1	A	173	GLN
1	A	187	LEU
1	A	222	HIS
1	A	261	LEU
1	A	283	LEU
1	A	292	LEU
1	A	317	LEU
1	A	329	GLN
1	A	347	PHE
1	A	360	ARG

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	388	LYS
1	A	451	SER
1	A	464	LEU
1	A	511	LEU
1	A	545	GLN
1	A	561	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	8,9,10	1.52	1 (12%)	8,12,14	1.99	2 (25%)

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	-	0/6/8/10	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	P-O1P	2.95	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O-C-CA	-2.18	119.82	125.49
1	A	198	SEP	OG-CB-CA	4.56	112.16	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	0

## 5.5 Carbohydrates [i](#)

10 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	$\# Z  > 2$
3	NAG	A	596	1,3	14,14,15	0.86	0	15,19,21	1.38	2 (13%)
3	NAG	A	597	3	14,14,15	1.09	2 (14%)	15,19,21	1.17	2 (13%)
3	MAN	A	598	3	11,11,12	0.86	0	14,15,17	0.74	0
4	NAG	A	599	1,4	14,14,15	0.66	0	15,19,21	0.76	0
4	NAG	A	600	4	14,14,15	0.83	0	15,19,21	1.39	3 (20%)
3	NAG	A	601	1,3	14,14,15	0.50	0	15,19,21	0.95	1 (6%)
3	NAG	A	602	3	14,14,15	0.54	0	15,19,21	1.07	1 (6%)
3	MAN	A	603	3	11,11,12	0.66	0	14,15,17	0.43	0
4	NAG	A	604	1,4	14,14,15	0.94	1 (7%)	15,19,21	1.37	1 (6%)
4	NAG	A	606	4	14,14,15	1.00	2 (14%)	15,19,21	1.15	1 (6%)

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	NAG	A	596	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	597	3	-	0/6/23/26	0/1/1/1
3	MAN	A	598	3	-	0/2/19/22	0/1/1/1
4	NAG	A	599	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	600	4	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
3	MAN	A	603	3	-	0/2/19/22	1/1/1/1
4	NAG	A	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	606	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	NAG	C3-C2	2.00	1.57	1.52
3	A	597	NAG	C3-C2	2.13	1.57	1.52
4	A	604	NAG	C3-C2	2.17	1.57	1.52
3	A	597	NAG	C1-C2	2.19	1.55	1.52
4	A	606	NAG	C1-C2	2.81	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	597	NAG	C2-N2-C7	-3.01	119.17	123.04
3	A	596	NAG	C2-N2-C7	-2.82	119.42	123.04
3	A	602	NAG	C2-N2-C7	-2.72	119.55	123.04
3	A	601	NAG	C2-N2-C7	-2.34	120.03	123.04
4	A	600	NAG	C2-N2-C7	-2.05	120.40	123.04
4	A	600	NAG	C3-C4-C5	2.52	114.59	110.20
3	A	597	NAG	C4-C3-C2	2.92	115.76	111.23
3	A	596	NAG	C1-O5-C5	3.04	116.11	112.25
4	A	606	NAG	C4-C3-C2	3.53	116.72	111.23
4	A	600	NAG	C4-C3-C2	3.59	116.82	111.23
4	A	604	NAG	C4-C3-C2	4.45	118.15	111.23

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	603	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	596	NAG	1	0
3	A	597	NAG	1	0
4	A	599	NAG	1	0
3	A	601	NAG	1	0
3	A	602	NAG	1	0
4	A	604	NAG	1	0
4	A	606	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	605	1,9	30,50,50	2.72	12 (40%)	24,82,82	2.26	7 (29%)
5	ISZ	A	607	-	9,10,10	1.00	0	12,12,12	5.46	2 (16%)
8	SCN	A	616	-	2,2,2	2.13	1 (50%)	1,1,1	0.12	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	605	1,9	-	0/10/54/54	0/0/8/8
5	ISZ	A	607	-	-	0/4/6/6	0/1/1/1
8	SCN	A	616	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C4B	-9.36	1.43	1.51
2	A	605	HEM	C3D-C4D	-4.30	1.46	1.51
2	A	605	HEM	C2D-C1D	-4.05	1.38	1.51
2	A	605	HEM	C1A-CHA	-2.71	1.32	1.39
2	A	605	HEM	C2B-C1B	-2.27	1.44	1.51
2	A	605	HEM	CAD-CBD	2.00	1.62	1.52
2	A	605	HEM	CMC-C2C	2.28	1.58	1.53
2	A	605	HEM	CAA-C2A	2.39	1.56	1.52
8	A	616	SCN	C-S	2.84	1.81	1.63
2	A	605	HEM	FE-NC	3.23	2.08	1.95
2	A	605	HEM	CAD-C3D	3.36	1.60	1.54
2	A	605	HEM	C3B-CAB	3.51	1.57	1.51
2	A	605	HEM	C3C-CAC	4.10	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	CMD-C2D-C3D	2.02	123.29	114.35
2	A	605	HEM	CAD-C3D-C2D	2.52	120.46	113.22
2	A	605	HEM	C3C-CAC-CBC	2.67	128.55	124.46
2	A	605	HEM	C4B-CHC-C1C	2.78	130.47	125.82
5	A	607	ISZ	C1-C6-N2	3.31	120.58	114.16
2	A	605	HEM	CMC-C2C-C3C	3.65	125.65	116.53
2	A	605	HEM	CMB-C2B-C3B	4.10	126.76	116.53
2	A	605	HEM	CAD-C3D-C4D	6.88	136.72	112.47
5	A	607	ISZ	C6-N2-N3	18.38	157.72	117.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEM	1	0
5	A	607	ISZ	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 ⓘ

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%)	-0.10	32 (5%)	29 28	20, 39, 81, 98	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	8.0
1	A	2	TRP	7.9
1	A	1	SER	6.1
1	A	172	TYR	6.0
1	A	171	PRO	5.9
1	A	121	SER	5.6
1	A	595	ASN	5.2
1	A	169	THR	5.2
1	A	170	PRO	4.6
1	A	122	ASN	4.4
1	A	5	GLY	4.3
1	A	174	SER	4.2
1	A	119	LEU	3.9
1	A	173	GLN	3.8
1	A	8	ALA	3.7
1	A	12	LEU	3.7
1	A	10	VAL	3.5
1	A	124	HIS	3.4
1	A	3	GLU	3.2
1	A	6	CYS	3.2
1	A	120	GLY	3.0
1	A	11	PRO	2.8
1	A	123	GLU	2.7
1	A	593	ARG	2.6
1	A	147	ASN	2.5
1	A	594	GLU	2.3
1	A	231	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLN	2.1
1	A	118	GLU	2.1
1	A	168	PRO	2.1
1	A	117	THR	2.1
1	A	370	PRO	2.1

## 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
1	SEP	A	198	10/11	0.94	0.15	-	38,39,41,43	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
3	NAG	A	596	14/15	0.84	0.19	0.52	66,70,74,80	0
3	NAG	A	601	14/15	0.94	0.13	-0.74	55,58,61,66	0
4	NAG	A	599	14/15	0.91	0.16	-0.93	57,59,62,65	0
3	MAN	A	598	11/12	0.56	0.50	-	97,99,99,99	0
3	NAG	A	602	14/15	0.79	0.34	-	71,74,76,79	0
4	NAG	A	604	14/15	0.79	0.37	-	72,78,80,84	0
4	NAG	A	606	14/15	0.63	0.53	-	88,91,92,92	0
3	NAG	A	597	14/15	0.84	0.49	-	86,90,91,94	0
3	MAN	A	603	11/12	0.67	0.41	-	82,83,84,85	0
4	NAG	A	600	14/15	0.82	0.27	-	68,70,71,72	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
5	ISZ	A	607	10/10	0.85	0.29	5.91	27,30,34,35	0
2	HEM	A	605	43/43	0.95	0.15	0.33	28,34,38,39	0
6	IOD	A	612	1/1	0.96	0.12	0.07	54,54,54,54	1
6	IOD	A	613	1/1	0.96	0.16	-0.60	45,45,45,45	1
7	CA	A	615	1/1	0.97	0.09	-1.39	24,24,24,24	0
6	IOD	A	611	1/1	0.99	0.10	-1.66	44,44,44,44	1
6	IOD	A	608	1/1	1.00	0.07	-1.87	34,34,34,34	0
6	IOD	A	609	1/1	0.99	0.04	-1.88	51,51,51,51	1
8	SCN	A	616	3/3	0.95	0.11	-2.22	20,20,21,21	0
6	IOD	A	614	1/1	0.99	0.03	-	32,32,32,32	1
6	IOD	A	610	1/1	0.96	0.06	-	57,57,57,57	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.