



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:04 AM GMT

PDB ID : 3KRQ  
Title : Crystal structure of the complex of lactoperoxidase with a potent inhibitor amino-triazole at 2.2a resolution  
Authors : Singh, A.K.; Singh, N.; Sinha, M.; Kushwaha, G.S.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.  
Deposited on : 2009-11-19  
Resolution : 2.25 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

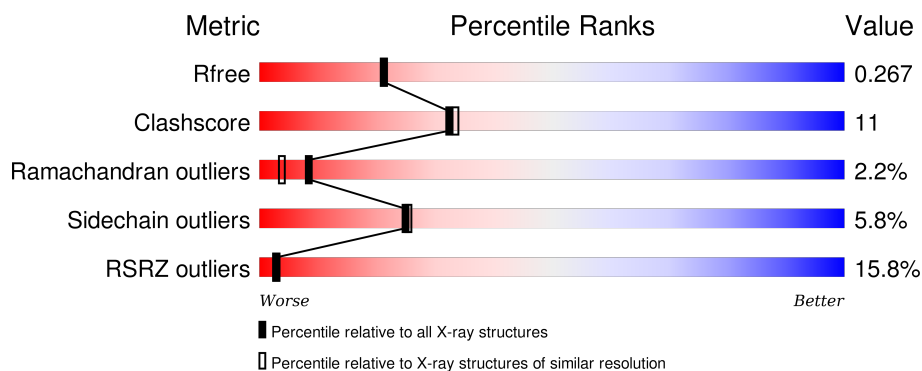
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	

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
7	IOD	A	615	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	3TR	A	607	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5418 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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

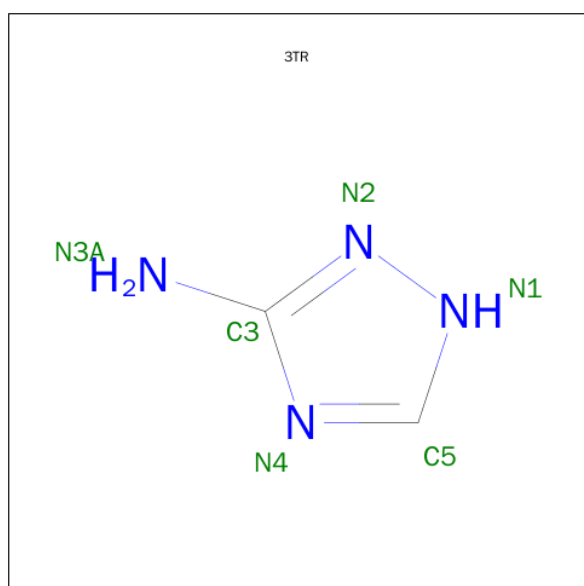
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

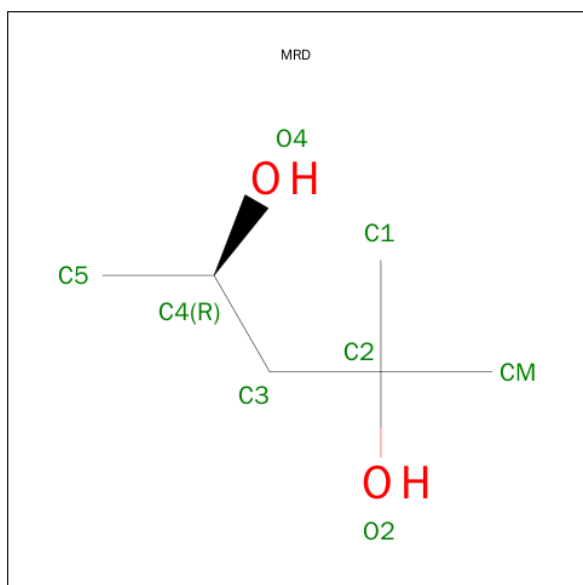
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total I 7 7	0	0

- Molecule 8 is 3-AMINO-1,2,4-TRIAZOLE (three-letter code: 3TR) (formula: C<sub>2</sub>H<sub>4</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	0	0
			6	2	4		
8	A	1	Total	C	N	0	0
			6	2	4		

- Molecule 9 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

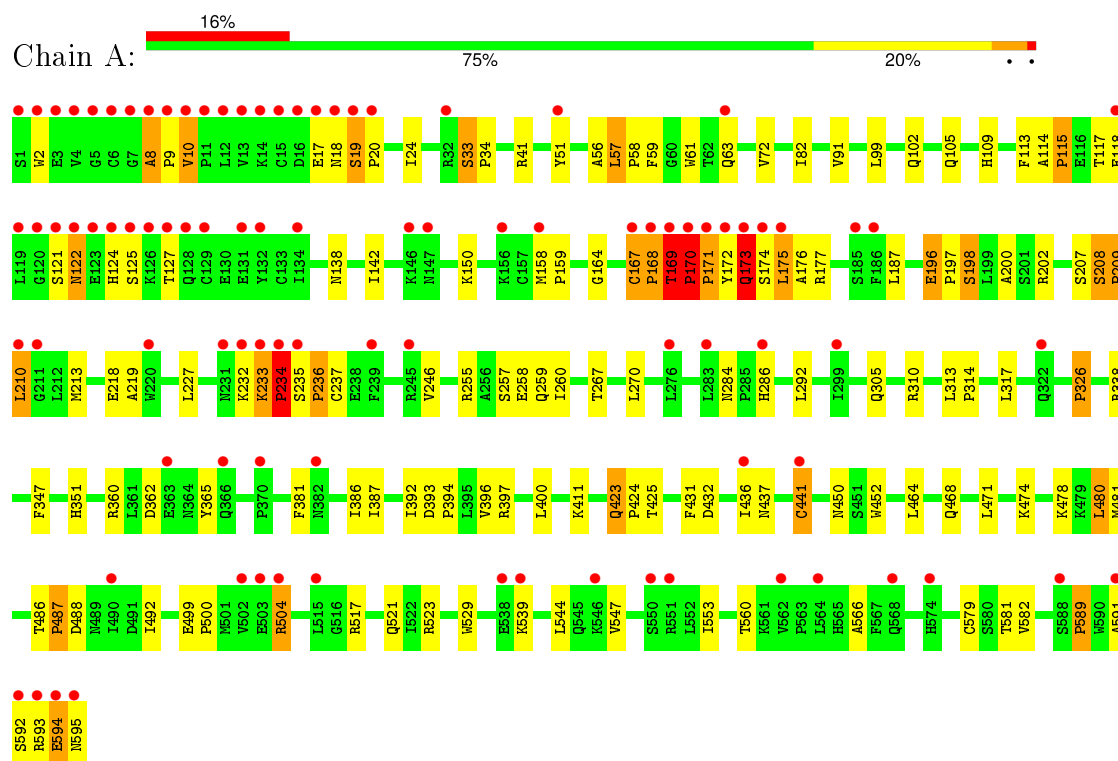
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	421	Total	O	0	0
			421	421		

### 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: 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 81.11Å 73.93Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.91 – 2.25 19.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.91-2.25) 99.9 (19.91-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.26Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.226 , 0.249 0.238 , 0.267	Depositor DCC
$R_{free}$ test set	1527 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.5	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 30048 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: BMA, PEG, NAG, SEP, CA, NDG, 3TR, MRD, 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	0.78	9/4891 (0.2%)	1.09	27/6634 (0.4%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	PRO	N-CA	7.87	1.60	1.47
1	A	504	ARG	NE-CZ	7.14	1.42	1.33
1	A	122	ASN	N-CA	6.32	1.58	1.46
1	A	504	ARG	CG-CD	6.31	1.67	1.51
1	A	170	PRO	C-N	6.06	1.45	1.34
1	A	504	ARG	CB-CG	6.01	1.68	1.52
1	A	504	ARG	CD-NE	5.95	1.56	1.46
1	A	170	PRO	N-CA	5.87	1.57	1.47
1	A	169	THR	N-CA	-5.11	1.36	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	PRO	CA-N-CD	-15.05	90.42	111.50
1	A	168	PRO	CA-N-CD	-12.63	93.82	111.50
1	A	167	CYS	C-N-CD	-11.05	96.29	120.60
1	A	169	THR	C-N-CD	-10.26	98.04	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	C-N-CD	-9.15	100.46	120.60
1	A	233	LYS	N-CA-C	-8.84	87.12	111.00
1	A	234	PRO	N-CD-CG	8.74	116.30	103.20
1	A	171	PRO	CA-N-CD	-8.59	99.47	111.50
1	A	504	ARG	CB-CA-C	8.24	126.89	110.40
1	A	168	PRO	N-CD-CG	7.98	115.17	103.20
1	A	594	GLU	N-CA-C	7.65	131.65	111.00
1	A	168	PRO	N-CA-CB	7.40	112.18	103.30
1	A	592	SER	C-N-CA	7.22	139.75	121.70
1	A	589	PRO	CA-N-CD	-7.09	101.58	111.50
1	A	121	SER	C-N-CA	7.02	139.26	121.70
1	A	591	ALA	N-CA-C	6.74	129.21	111.00
1	A	234	PRO	N-CA-CB	6.71	111.35	103.30
1	A	57	LEU	C-N-CD	-6.07	107.25	120.60
1	A	167	CYS	C-N-CA	6.05	147.42	122.00
1	A	592	SER	CA-C-N	-5.90	104.21	117.20
1	A	504	ARG	CG-CD-NE	5.59	123.54	111.80
1	A	504	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	504	ARG	CB-CG-CD	5.44	125.73	111.60
1	A	169	THR	CB-CA-C	5.27	125.83	111.60
1	A	19	SER	CA-C-N	-5.24	102.43	117.10
1	A	159	PRO	CA-N-CD	-5.19	104.23	111.50
1	A	326	PRO	CA-N-CD	-5.05	104.43	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	SEP	Peptide
1	A	423	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	4774	0	4687	100	0
2	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	78	0	68	0	0
5	A	39	0	34	0	0
6	A	28	0	25	0	0
7	A	7	0	0	2	0
8	A	12	0	8	5	0
9	A	8	0	14	0	0
10	A	7	0	10	0	0
11	A	421	0	0	3	0
All	All	5418	0	4876	104	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 (104) 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)
8:A:607:3TR:H5	8:A:608:3TR:H5	1.44	0.99
1:A:18:ASN:O	1:A:20:PRO:HD3	1.66	0.94
1:A:424:PRO:O	7:A:615:IOD:I	2.65	0.85
1:A:432:ASP:O	1:A:436:ILE:HD13	1.77	0.84
1:A:208:SER:HB2	1:A:210:LEU:HD12	1.60	0.82
1:A:175:LEU:HD22	1:A:176:ALA:H	1.48	0.78
1:A:284:ASN:HD22	1:A:286:HIS:CE1	2.02	0.77
1:A:72:VAL:HG13	1:A:72:VAL:O	1.83	0.75
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.70	0.73
1:A:158:MET:SD	1:A:431:PHE:HA	2.30	0.72
1:A:392:ILE:O	1:A:396:VAL:HG23	1.89	0.71
1:A:208:SER:CB	1:A:210:LEU:HD12	2.22	0.70
8:A:607:3TR:C5	8:A:608:3TR:H5	2.21	0.68
1:A:234:PRO:O	1:A:236:PRO:HD3	1.94	0.67
1:A:234:PRO:HB3	7:A:615:IOD:I	2.65	0.67
1:A:18:ASN:O	1:A:20:PRO:CD	2.40	0.67
1:A:197:PRO:O	1:A:198:SEP:C	2.43	0.66
1:A:172:TYR:C	1:A:173:GLN:HG3	2.14	0.66
1:A:202:ARG:HG2	1:A:202:ARG:O	1.96	0.66
1:A:105:GLN:HE22	1:A:259:GLN:HE21	1.44	0.65
1:A:51:TYR:HB3	1:A:57:LEU:O	1.95	0.65
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.27	0.65
1:A:113:PHE:CE2	1:A:115:PRO:HG3	2.33	0.64
1:A:58:PRO:HB2	1:A:61:TRP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HB3	1:A:233:LYS:O	2.01	0.60
1:A:72:VAL:O	1:A:72:VAL:CG1	2.49	0.60
1:A:481:MET:SD	1:A:487:PRO:HD3	2.41	0.59
1:A:284:ASN:HD22	1:A:286:HIS:HE1	1.50	0.58
1:A:10:VAL:HG13	1:A:10:VAL:O	2.04	0.57
1:A:257:SER:O	1:A:381:PHE:HA	2.05	0.56
1:A:10:VAL:O	1:A:10:VAL:HG22	2.06	0.56
1:A:227:LEU:CD1	1:A:267:THR:HA	2.36	0.56
1:A:58:PRO:O	1:A:59:PHE:C	2.44	0.55
1:A:210:LEU:HA	1:A:292:LEU:CD1	2.37	0.54
1:A:517:ARG:O	1:A:521:GLN:HG3	2.07	0.54
1:A:310:ARG:O	1:A:314:PRO:HG2	2.08	0.54
1:A:258:GLU:HG3	8:A:607:3TR:C5	2.39	0.52
1:A:210:LEU:HA	1:A:292:LEU:HD12	1.90	0.52
1:A:313:LEU:N	1:A:314:PRO:CD	2.72	0.52
1:A:175:LEU:HD22	1:A:176:ALA:N	2.20	0.52
1:A:544:LEU:O	1:A:547:VAL:HG22	2.09	0.52
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.92	0.51
1:A:170:PRO:CB	1:A:171:PRO:CD	2.89	0.50
1:A:227:LEU:HD13	1:A:267:THR:HA	1.93	0.50
1:A:33:SER:N	1:A:34:PRO:CD	2.75	0.49
1:A:208:SER:C	1:A:210:LEU:H	2.16	0.49
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.43	0.49
1:A:471:LEU:HD21	1:A:480:LEU:HD23	1.95	0.49
1:A:210:LEU:HB3	11:A:962:HOH:O	2.13	0.48
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.48
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.95	0.48
1:A:486:THR:C	1:A:488:ASP:N	2.65	0.48
1:A:286:HIS:CD2	1:A:594:GLU:OE1	2.67	0.48
1:A:33:SER:N	1:A:34:PRO:HD3	2.28	0.48
1:A:117:THR:HG21	1:A:138:ASN:CG	2.34	0.48
1:A:113:PHE:CG	1:A:115:PRO:HD3	2.49	0.47
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.95	0.47
1:A:196:GLU:HG3	1:A:197:PRO:N	2.29	0.47
1:A:56:ALA:O	1:A:58:PRO:HD3	2.15	0.47
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.54	0.47
1:A:213:MET:HB3	1:A:270:LEU:HD11	1.97	0.46
1:A:393:ASP:N	1:A:394:PRO:CD	2.77	0.46
1:A:164:GLY:HA2	11:A:708:HOH:O	2.15	0.46
1:A:560:THR:HA	1:A:579:CYS:SG	2.55	0.46
1:A:539:LYS:HB3	1:A:589:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.98	0.46
1:A:464:LEU:HD21	1:A:478:LYS:HE2	1.98	0.46
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.82	0.45
1:A:57:LEU:HA	1:A:58:PRO:HD2	1.72	0.45
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.79	0.45
1:A:169:THR:H	1:A:170:PRO:HD2	1.82	0.45
1:A:362:ASP:O	1:A:365:TYR:N	2.46	0.45
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.99	0.45
1:A:24:ILE:HD12	1:A:200:ALA:HB2	1.98	0.44
1:A:19:SER:HA	1:A:20:PRO:HD2	1.22	0.44
1:A:452:TRP:CD1	1:A:492:ILE:HD13	2.53	0.44
1:A:393:ASP:O	1:A:397:ARG:HG3	2.17	0.44
1:A:486:THR:O	1:A:488:ASP:N	2.51	0.43
1:A:218:GLU:O	1:A:219:ALA:HB2	2.17	0.43
1:A:187:LEU:HD23	1:A:305:GLN:HA	2.00	0.43
1:A:255:ARG:HA	8:A:608:3TR:N4	2.34	0.43
1:A:499:GLU:HA	1:A:500:PRO:HD3	1.89	0.43
1:A:213:MET:CB	1:A:270:LEU:HD11	2.48	0.42
1:A:423:GLN:HA	1:A:424:PRO:HD3	1.67	0.42
1:A:208:SER:HA	1:A:209:PRO:HD2	1.64	0.42
1:A:468:GLN:HG2	1:A:474:LYS:HA	2.01	0.42
1:A:362:ASP:OD1	1:A:362:ASP:C	2.57	0.42
1:A:246:VAL:CG1	1:A:387:ILE:HD12	2.49	0.42
1:A:109:HIS:NE2	8:A:607:3TR:N3A	2.68	0.42
1:A:234:PRO:O	1:A:236:PRO:CD	2.63	0.42
2:A:655:HEM:HBC2	2:A:655:HEM:HMC1	2.02	0.42
1:A:486:THR:C	1:A:488:ASP:H	2.23	0.41
1:A:8:ALA:CB	1:A:9:PRO:CD	2.98	0.41
1:A:82:ILE:HD12	1:A:480:LEU:HD13	2.03	0.41
1:A:124:HIS:O	1:A:127:THR:N	2.54	0.41
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.56	0.41
1:A:351:HIS:CE1	1:A:437:ASN:HD21	2.37	0.41
1:A:114:ALA:HB3	11:A:624:HOH:O	2.21	0.41
1:A:91:VAL:HG12	1:A:411:LYS:HD3	2.02	0.41
1:A:150:LYS:HD3	1:A:158:MET:HE2	2.03	0.41
2:A:655:HEM:HBB2	2:A:655:HEM:CMB	2.50	0.41
1:A:208:SER:CB	1:A:210:LEU:CD1	2.98	0.40
1:A:142:ILE:HB	1:A:158:MET:HB2	2.03	0.40
1:A:102:GLN:HE22	1:A:105:GLN:HE21	1.68	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	592/595 (100%)	541 (91%)	38 (6%)	13 (2%)	8 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	VAL
1	A	168	PRO
1	A	170	PRO
1	A	234	PRO
1	A	338	ARG
1	A	209	PRO
1	A	115	PRO
1	A	118	GLU
1	A	173	GLN
1	A	174	SER
1	A	169	THR
1	A	167	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	517/517 (100%)	487 (94%)	30 (6%)	25 25

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	17	GLU
1	A	33	SER
1	A	41	ARG
1	A	63	GLN
1	A	122	ASN
1	A	125	SER
1	A	169	THR
1	A	173	GLN
1	A	175	LEU
1	A	177	ARG
1	A	196	GLU
1	A	207	SER
1	A	208	SER
1	A	210	LEU
1	A	235	SER
1	A	236	PRO
1	A	317	LEU
1	A	326	PRO
1	A	347	PHE
1	A	360	ARG
1	A	425	THR
1	A	441	CYS
1	A	480	LEU
1	A	487	PRO
1	A	504	ARG
1	A	581	THR
1	A	582	VAL
1	A	593	ARG
1	A	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	284	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	8,9,10	1.03	0	8,12,14	3.85	5 (62%)

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

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	198	SEP	O3P-P-O1P	-3.12	100.53	110.58
1	A	198	SEP	O2P-P-O1P	-2.70	101.88	110.58
1	A	198	SEP	OG-P-O1P	2.15	112.61	107.14
1	A	198	SEP	O3P-P-OG	5.54	122.52	106.56
1	A	198	SEP	OG-CB-CA	7.84	114.96	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 ⓘ

11 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	596	1,4	14,14,15	1.08	1 (7%)	15,19,21	1.01	1 (6%)
4	NAG	A	597	4	14,14,15	1.36	4 (28%)	15,19,21	1.50	2 (13%)
4	MAN	A	598	4	11,11,12	1.17	1 (9%)	14,15,17	0.83	0
5	NAG	A	599	1,5	14,14,15	0.72	0	15,19,21	0.84	1 (6%)
5	NAG	A	600	5	14,14,15	0.77	0	15,19,21	1.61	2 (13%)
5	BMA	A	601	5	11,11,12	1.13	1 (9%)	14,15,17	1.77	4 (28%)
4	NAG	A	602	1,4	14,14,15	0.52	0	15,19,21	0.80	1 (6%)
4	NAG	A	603	4	14,14,15	0.69	0	15,19,21	1.05	1 (6%)
4	MAN	A	604	4	11,11,12	0.62	0	14,15,17	0.96	1 (7%)
6	NAG	A	605	1,6	14,14,15	0.49	0	15,19,21	0.79	1 (6%)
6	NDG	A	606	6	14,14,15	0.62	0	15,19,21	1.15	2 (13%)

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	596	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	597	4	-	0/6/23/26	0/1/1/1
4	MAN	A	598	4	-	0/2/19/22	0/1/1/1
5	NAG	A	599	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	600	5	-	0/6/23/26	0/1/1/1
5	BMA	A	601	5	-	0/2/19/22	0/1/1/1
4	NAG	A	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	603	4	-	0/6/23/26	0/1/1/1
4	MAN	A	604	4	-	0/2/19/22	0/1/1/1
6	NAG	A	605	1,6	-	0/6/23/26	0/1/1/1
6	NDG	A	606	6	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	597	NAG	C1-C2	2.01	1.55	1.52
4	A	596	NAG	O4-C4	2.04	1.47	1.43
4	A	597	NAG	O4-C4	2.15	1.48	1.43
4	A	597	NAG	C4-C3	2.27	1.58	1.52
4	A	597	NAG	C3-C2	2.69	1.58	1.52
4	A	598	MAN	C2-C3	2.95	1.56	1.52
5	A	601	BMA	C2-C3	3.03	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	NAG	C2-N2-C7	-3.10	119.06	123.04
6	A	606	NDG	C2-N2-C7	-2.69	119.58	123.04
5	A	601	BMA	C1-O5-C5	-2.62	108.92	112.25
4	A	602	NAG	C2-N2-C7	-2.38	119.97	123.04
5	A	599	NAG	C2-N2-C7	-2.31	120.07	123.04
6	A	605	NAG	C2-N2-C7	-2.12	120.31	123.04
4	A	604	MAN	C1-C2-C3	2.02	111.93	109.54
4	A	597	NAG	C3-C4-C5	2.21	114.05	110.20
4	A	603	NAG	C4-C3-C2	2.64	115.33	111.23
4	A	596	NAG	C4-C3-C2	2.78	115.55	111.23
6	A	606	NDG	C1-O-C5	2.81	115.82	112.25
5	A	601	BMA	C3-C4-C5	2.94	115.33	110.20
5	A	601	BMA	C2-C3-C4	3.37	116.76	111.04
5	A	601	BMA	C1-C2-C3	3.44	113.62	109.54
4	A	597	NAG	C4-C3-C2	4.44	118.14	111.23
5	A	600	NAG	C4-C3-C2	4.47	118.17	111.23

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 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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
8	3TR	A	607	-	4,6,6	3.27	1 (25%)	1,7,7	1.67	0
10	PEG	A	6071	-	6,6,6	1.55	1 (16%)	5,5,5	0.73	0
8	3TR	A	608	-	4,6,6	3.29	1 (25%)	1,7,7	1.64	0
9	MRD	A	609	-	6,7,7	0.35	0	7,10,10	0.64	0
2	HEM	A	655	1	30,50,50	2.40	12 (40%)	24,82,82	2.47	11 (45%)

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
8	3TR	A	607	-	-	0/0/0/0	0/1/1/1
10	PEG	A	6071	-	-	0/4/4/4	0/0/0/0
8	3TR	A	608	-	-	0/0/0/0	0/1/1/1
9	MRD	A	609	-	-	0/5/5/5	0/0/0/0
2	HEM	A	655	1	-	0/10/54/54	0/0/8/8

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	608	3TR	N1-N2	-6.44	1.23	1.37
8	A	607	3TR	N1-N2	-6.39	1.23	1.37
2	A	655	HEM	C3D-C4D	-5.82	1.44	1.51
2	A	655	HEM	C2C-C1C	-5.38	1.42	1.52
2	A	655	HEM	C3B-C4B	-4.12	1.48	1.51
2	A	655	HEM	C2D-C1D	-2.67	1.43	1.51
2	A	655	HEM	C2D-C3D	-2.30	1.47	1.54
2	A	655	HEM	CMC-C2C	2.08	1.58	1.53
2	A	655	HEM	CMA-C3A	2.22	1.56	1.51
2	A	655	HEM	C1C-NC	2.25	1.38	1.36
10	A	6071	PEG	O2-C3	2.27	1.51	1.42
2	A	655	HEM	FE-ND	2.67	2.11	1.97
2	A	655	HEM	CAA-C2A	3.01	1.57	1.52
2	A	655	HEM	C3B-CAB	3.22	1.57	1.51
2	A	655	HEM	C3C-CAC	4.08	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	655	HEM	CBD-CAD-C3D	-4.04	101.78	113.55
2	A	655	HEM	CBA-CAA-C2A	-3.13	106.92	112.53
2	A	655	HEM	CAD-CBD-CGD	-2.49	102.85	113.02
2	A	655	HEM	C3C-CAC-CBC	2.18	127.80	124.46
2	A	655	HEM	C3B-C4B-CHC	2.24	126.32	123.16
2	A	655	HEM	C1D-CHD-C4C	2.60	130.17	125.82
2	A	655	HEM	CMB-C2B-C3B	2.94	123.88	116.53
2	A	655	HEM	CMD-C2D-C3D	3.28	128.87	114.35
2	A	655	HEM	CAD-C3D-C4D	4.67	128.95	112.47
2	A	655	HEM	CAD-C3D-C2D	4.73	126.82	113.22
2	A	655	HEM	CMC-C2C-C3C	4.91	128.78	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	607	3TR	4	0
8	A	608	3TR	3	0
2	A	655	HEM	2	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	594/595 (99%)	1.05	94 (15%) ⓘ ⓘ	30, 51, 94, 100	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	14.4
1	A	1	SER	13.2
1	A	8	ALA	10.5
1	A	121	SER	9.2
1	A	595	ASN	8.9
1	A	7	GLY	7.9
1	A	173	GLN	7.8
1	A	4	VAL	7.7
1	A	172	TYR	7.4
1	A	13	VAL	7.4
1	A	122	ASN	7.0
1	A	591	ALA	6.3
1	A	3	GLU	6.2
1	A	124	HIS	6.2
1	A	169	THR	6.1
1	A	593	ARG	6.1
1	A	118	GLU	6.0
1	A	128	GLN	5.8
1	A	125	SER	5.7
1	A	16	ASP	5.6
1	A	126	LYS	5.6
1	A	12	LEU	5.6
1	A	175	LEU	5.5
1	A	594	GLU	5.3
1	A	119	LEU	5.3
1	A	6	CYS	5.0
1	A	170	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	4.6
1	A	167	CYS	4.6
1	A	233	LYS	4.3
1	A	286	HIS	4.2
1	A	129	CYS	4.1
1	A	11	PRO	4.1
1	A	120	GLY	4.1
1	A	234	PRO	4.1
1	A	5	GLY	3.9
1	A	32	ARG	3.9
1	A	322	GLN	3.9
1	A	174	SER	3.8
1	A	132	TYR	3.8
1	A	134	ILE	3.4
1	A	538	GLU	3.4
1	A	564	LEU	3.3
1	A	539	LYS	3.2
1	A	17	GLU	3.1
1	A	245	ARG	3.1
1	A	235	SER	3.1
1	A	123	GLU	3.0
1	A	231	ASN	3.0
1	A	20	PRO	3.0
1	A	574	HIS	2.9
1	A	18	ASN	2.9
1	A	592	SER	2.9
1	A	168	PRO	2.8
1	A	562	VAL	2.8
1	A	436	ILE	2.8
1	A	283	LEU	2.7
1	A	370	PRO	2.7
1	A	568	GLN	2.7
1	A	232	LYS	2.7
1	A	19	SER	2.6
1	A	502	VAL	2.6
1	A	63	GLN	2.6
1	A	156	LYS	2.6
1	A	550	SER	2.6
1	A	15	CYS	2.6
1	A	366	GLN	2.5
1	A	211	GLY	2.5
1	A	131	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	158	MET	2.5
1	A	127	THR	2.5
1	A	276	LEU	2.5
1	A	9	PRO	2.5
1	A	186	PHE	2.4
1	A	546	LYS	2.4
1	A	10	VAL	2.4
1	A	147	ASN	2.4
1	A	14	LYS	2.3
1	A	490	ILE	2.3
1	A	503	GLU	2.3
1	A	551	ARG	2.3
1	A	515	LEU	2.3
1	A	441	CYS	2.3
1	A	382	ASN	2.2
1	A	185	SER	2.2
1	A	51	TYR	2.2
1	A	146	LYS	2.2
1	A	504	ARG	2.1
1	A	299	ILE	2.1
1	A	210	LEU	2.1
1	A	239	PHE	2.0
1	A	588	SER	2.0
1	A	363	GLU	2.0
1	A	220	TRP	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	0.83	0.24	-	49,55,64,64	0

## 6.3 Carbohydrates ⓘ

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	NAG	A	596	14/15	0.75	0.31	1.15	75,81,83,89	0
4	NAG	A	602	14/15	0.81	0.21	0.20	62,67,71,77	0
5	NAG	A	599	14/15	0.90	0.17	-0.65	74,77,80,83	0
4	NAG	A	597	14/15	0.61	0.39	-	95,99,99,99	0
4	NAG	A	603	14/15	0.73	0.31	-	83,88,89,93	0
6	NDG	A	606	14/15	0.44	0.52	-	96,99,99,99	0
5	NAG	A	600	14/15	0.80	0.31	-	86,87,90,93	0
6	NAG	A	605	14/15	0.67	0.37	-	82,88,92,93	0
4	MAN	A	604	11/12	0.54	0.36	-	96,98,98,99	0
5	BMA	A	601	11/12	0.71	0.51	-	96,98,99,99	0
4	MAN	A	598	11/12	0.42	0.74	-	100,100,100,100	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
9	MRD	A	609	8/8	0.83	0.27	1.26	38,44,46,46	0
3	CA	A	656	1/1	0.98	0.20	0.24	6,6,6,6	0
2	HEM	A	655	43/43	0.96	0.12	-1.03	24,31,38,46	0
7	IOD	A	610	1/1	1.00	0.10	-2.32	39,39,39,39	0
7	IOD	A	615	1/1	0.90	0.05	-2.44	70,70,70,70	0
7	IOD	A	614	1/1	0.96	0.04	-2.49	82,82,82,82	0
7	IOD	A	612	1/1	0.97	0.06	-3.05	84,84,84,84	0
7	IOD	A	613	1/1	0.96	0.09	-3.39	62,62,62,62	0
7	IOD	A	616	1/1	0.89	0.09	-	87,87,87,87	1
10	PEG	A	6071	7/7	0.77	0.42	-	43,46,49,49	0
8	3TR	A	607	6/6	0.83	0.32	-	22,30,33,36	0
8	3TR	A	608	6/6	0.89	0.25	-	45,47,49,50	0
7	IOD	A	611	1/1	0.94	0.07	-	93,93,93,93	0

## 6.5 Other polymers

There are no such residues in this entry.