



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:19 AM GMT

PDB ID : 3FAQ  
Title : Crystal structure of lactoperoxidase complex with cyanide  
Authors : Sheikh, I.A.; Singh, N.; Sharma, S.; Kaur, P.; Srinivasan, A.; Singh, T.P.  
Deposited on : 2008-11-18  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

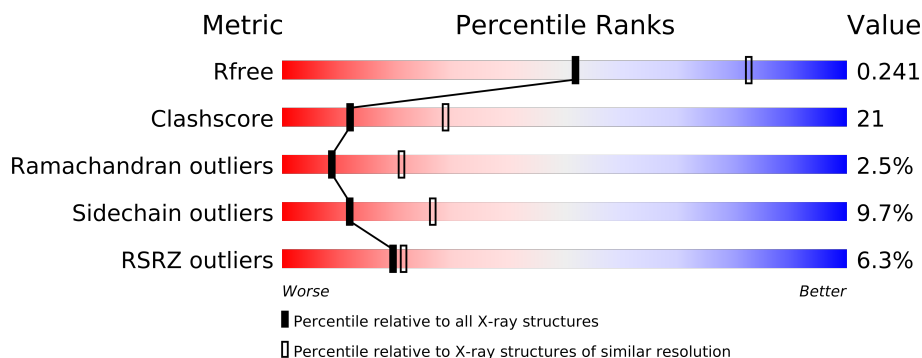
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 5256 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

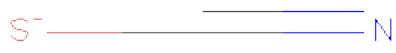
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4778	3040	847	864	1	26	0	0	0

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

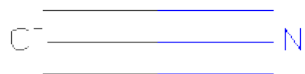


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			2	1	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 a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	4	Total	C	N	O	0	0
			50	28	2	20		

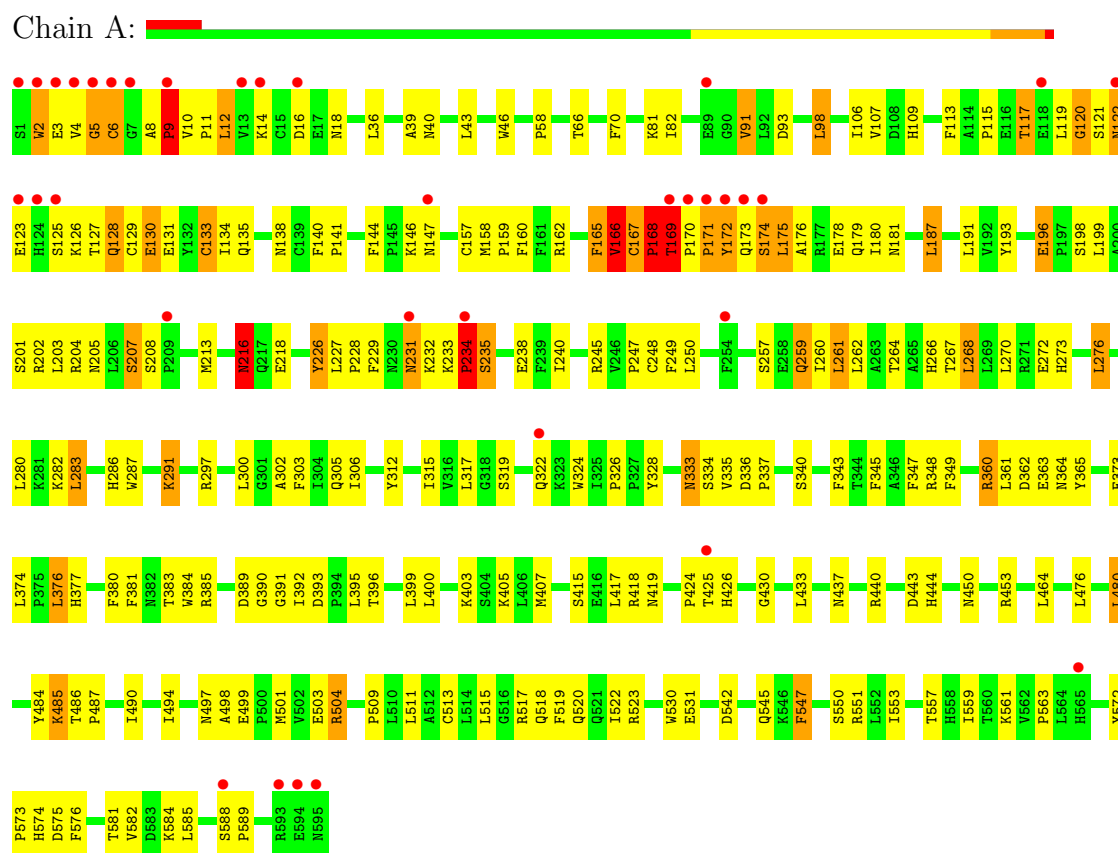
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	274	Total	O	0	0
			274	274		

### 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	54.45Å 80.67Å 77.80Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	11.94 – 2.70 11.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (11.94-2.70) 89.1 (11.93-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.208 , 0.235 0.206 , 0.241	Depositor DCC
$R_{free}$ test set	824 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15982 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, BMA, HEM, IOD, CYN, 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	0.51	3/4896 (0.1%)	0.96	22/6640 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	PRO	N-CD	6.71	1.57	1.47
1	A	234	PRO	CA-C	-6.24	1.40	1.52
1	A	234	PRO	C-N	-5.04	1.22	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	PRO	CA-N-CD	-23.12	79.14	111.50
1	A	234	PRO	N-CA-CB	17.15	123.88	103.30
1	A	234	PRO	N-CD-CG	15.44	126.36	103.20
1	A	233	LYS	C-N-CA	12.60	174.93	122.00
1	A	233	LYS	C-N-CD	-11.27	95.82	120.60
1	A	234	PRO	C-N-CA	-8.61	100.19	121.70
1	A	166	VAL	N-CA-C	8.54	134.06	111.00
1	A	9	PRO	CA-N-CD	-8.12	100.13	111.50
1	A	216	ASN	CA-CB-CG	6.55	127.80	113.40
1	A	233	LYS	CA-C-N	-5.93	100.51	117.10
1	A	547	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	A	121	SER	N-CA-C	-5.90	95.08	111.00
1	A	122	ASN	N-CA-CB	5.87	121.17	110.60
1	A	233	LYS	CB-CA-C	5.46	121.32	110.40
1	A	173	GLN	N-CA-C	5.33	125.38	111.00
1	A	233	LYS	O-C-N	5.30	131.17	121.10
1	A	196	GLU	C-N-CD	-5.18	109.20	120.60
1	A	122	ASN	N-CA-C	-5.16	97.08	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	CA-CB-CG	5.06	124.53	113.40
1	A	120	GLY	N-CA-C	5.04	125.71	113.10
1	A	390	GLY	N-CA-C	5.03	125.68	113.10
1	A	174	SER	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4778	0	4690	198	0
2	A	43	0	30	0	0
3	A	6	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	1	0
6	A	7	0	0	0	0
7	A	56	0	50	2	0
8	A	39	0	34	5	0
9	A	50	0	43	4	0
10	A	274	0	0	15	0
All	All	5256	0	4847	209	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (209) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:547:PHE:HE2	1:A:585:LEU:HD22	1.33	0.93
1:A:175:LEU:CD2	1:A:176:ALA:H	1.88	0.86
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.74	0.85
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.57	0.85
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.15	0.82
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:THR:HB	1:A:426:HIS:CD2	2.19	0.78
1:A:123:GLU:HG3	1:A:125:SER:H	1.50	0.77
1:A:91:VAL:HG13	1:A:405:LYS:HG3	1.68	0.75
1:A:581:THR:HG22	1:A:581:THR:O	1.86	0.75
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.22	0.75
1:A:127:THR:HG23	1:A:131:GLU:HG3	1.68	0.74
1:A:302:ALA:O	1:A:306:ILE:HG13	1.90	0.72
1:A:123:GLU:HB3	1:A:126:LYS:NZ	2.05	0.71
1:A:588:SER:OG	1:A:589:PRO:HD3	1.91	0.70
1:A:10:VAL:HB	10:A:668:HOH:O	1.91	0.70
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.72	0.70
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.72	0.69
1:A:175:LEU:HD22	1:A:176:ALA:H	1.56	0.69
7:A:610:NAG:H61	10:A:775:HOH:O	1.92	0.69
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.75	0.69
1:A:503:GLU:O	1:A:504:ARG:HB2	1.90	0.68
1:A:175:LEU:HD23	1:A:176:ALA:H	1.58	0.68
1:A:123:GLU:HB3	1:A:126:LYS:CE	2.25	0.67
1:A:123:GLU:HB3	1:A:126:LYS:HE3	1.77	0.67
1:A:260:ILE:HD11	1:A:385:ARG:CB	2.25	0.67
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.75	0.67
1:A:260:ILE:HD11	1:A:385:ARG:HB2	1.76	0.66
9:A:616:NAG:H2	10:A:843:HOH:O	1.94	0.66
1:A:204:ARG:HD3	10:A:849:HOH:O	1.96	0.66
1:A:146:LYS:O	1:A:147:ASN:HB2	1.94	0.66
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.77	0.66
1:A:130:GLU:HA	1:A:159:PRO:HG3	1.76	0.66
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.79	0.65
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.31	0.65
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.60	0.65
1:A:169:THR:N	1:A:170:PRO:CD	2.58	0.65
1:A:235:SER:HB3	1:A:238:GLU:HB2	1.80	0.64
1:A:547:PHE:CE2	1:A:585:LEU:HD22	2.24	0.63
1:A:126:LYS:NZ	1:A:126:LYS:HB2	2.13	0.63
1:A:165:PHE:CE2	1:A:172:TYR:HB2	2.34	0.63
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.33	0.63
1:A:81:LYS:HD2	10:A:763:HOH:O	1.98	0.62
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.00	0.62
1:A:487:PRO:HA	1:A:490:ILE:HG13	1.80	0.62
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.47	0.61
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.36	0.61
9:A:615:NAG:H61	9:A:616:NAG:C7	2.31	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:TRP:CE2	1:A:291:LYS:HE3	2.36	0.60
8:A:613:NAG:H2	8:A:613:NAG:H61	1.84	0.60
1:A:381:PHE:CZ	1:A:424:PRO:HB3	2.36	0.60
1:A:324:TRP:O	1:A:326:PRO:HD2	2.03	0.59
1:A:165:PHE:HE2	1:A:172:TYR:HB2	1.65	0.59
1:A:393:ASP:HB2	10:A:652:HOH:O	2.03	0.59
1:A:574:HIS:HD2	1:A:575:ASP:OD1	1.86	0.59
1:A:205:ASN:OD1	1:A:207:SER:HB2	2.02	0.59
1:A:348:ARG:HD3	1:A:437:ASN:ND2	2.17	0.59
1:A:58:PRO:HD3	1:A:162:ARG:CZ	2.33	0.59
1:A:123:GLU:HB3	1:A:126:LYS:HZ2	1.67	0.59
1:A:166:VAL:CG2	1:A:178:GLU:HB2	2.32	0.58
1:A:168:PRO:HG2	1:A:169:THR:N	2.18	0.58
1:A:109:HIS:NE2	5:A:596:CYN:N	2.50	0.58
1:A:106:ILE:HG23	1:A:191:LEU:CD1	2.33	0.58
1:A:425:THR:HB	1:A:426:HIS:HD2	1.67	0.58
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.86	0.58
1:A:557:THR:OG1	1:A:559:ILE:HG12	2.04	0.58
1:A:126:LYS:HZ2	1:A:126:LYS:HB2	1.70	0.57
1:A:123:GLU:CB	1:A:126:LYS:HE3	2.34	0.57
1:A:333:ASN:HD22	1:A:333:ASN:N	2.03	0.57
1:A:417:LEU:HD22	1:A:433:LEU:HD22	1.86	0.57
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.56
1:A:169:THR:N	1:A:170:PRO:HD3	2.20	0.56
1:A:561:LYS:HE2	10:A:707:HOH:O	2.05	0.56
1:A:335:VAL:O	1:A:337:PRO:HD3	2.06	0.56
1:A:376:LEU:HD22	1:A:376:LEU:O	2.06	0.56
9:A:615:NAG:H61	9:A:616:NAG:O7	2.06	0.56
1:A:257:SER:O	1:A:381:PHE:HA	2.06	0.56
1:A:550:SER:HB2	1:A:582:VAL:HG11	1.86	0.56
1:A:175:LEU:HD22	1:A:176:ALA:N	2.21	0.55
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.10	0.55
1:A:129:CYS:HB2	10:A:811:HOH:O	2.07	0.55
1:A:407:MET:HB3	1:A:501:MET:CE	2.37	0.55
9:A:616:NAG:O4	9:A:617:BMA:H61	2.06	0.55
1:A:165:PHE:O	1:A:180:ILE:HD11	2.06	0.54
1:A:3:GLU:HG2	1:A:5:GLY:H	1.72	0.54
1:A:513:CYS:O	1:A:517:ARG:HG3	2.07	0.54
1:A:2:TRP:CG	1:A:3:GLU:N	2.75	0.53
1:A:166:VAL:HG22	1:A:178:GLU:O	2.09	0.53
1:A:216:ASN:HB2	1:A:228:PRO:HA	1.89	0.53
1:A:123:GLU:HG3	1:A:125:SER:N	2.21	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.44	0.52
1:A:98:LEU:HD11	1:A:261:LEU:HD21	1.92	0.52
1:A:202:ARG:HD2	1:A:250:LEU:HD21	1.90	0.52
1:A:165:PHE:N	1:A:165:PHE:CD1	2.78	0.52
1:A:260:ILE:CD1	1:A:385:ARG:HB2	2.39	0.52
1:A:407:MET:HE2	10:A:874:HOH:O	2.09	0.51
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.45	0.51
1:A:175:LEU:CD2	1:A:176:ALA:N	2.66	0.51
1:A:426:HIS:CD2	1:A:426:HIS:N	2.78	0.51
1:A:117:THR:HG21	1:A:138:ASN:CG	2.31	0.51
1:A:324:TRP:HZ3	10:A:869:HOH:O	1.93	0.50
1:A:504:ARG:HG3	10:A:693:HOH:O	2.11	0.50
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.47	0.50
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.46	0.50
1:A:6:CYS:HB3	1:A:167:CYS:SG	2.53	0.49
1:A:8:ALA:N	1:A:9:PRO:CD	2.76	0.49
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.77	0.49
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.47	0.49
1:A:98:LEU:CD1	1:A:261:LEU:HD21	2.43	0.49
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.13	0.49
1:A:43:LEU:CD2	1:A:181:ASN:HB2	2.43	0.49
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.48	0.48
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.48	0.48
1:A:260:ILE:HD11	1:A:385:ARG:HB3	1.93	0.48
1:A:484:TYR:O	1:A:486:THR:N	2.44	0.48
1:A:126:LYS:HB3	10:A:867:HOH:O	2.14	0.48
1:A:581:THR:CG2	1:A:581:THR:O	2.56	0.47
1:A:187:LEU:CD1	1:A:305:GLN:HA	2.44	0.47
1:A:453:ARG:NH1	1:A:499:GLU:OE2	2.45	0.47
1:A:240:ILE:HD11	1:A:384:TRP:HD1	1.79	0.47
1:A:286:HIS:HB2	10:A:780:HOH:O	2.13	0.47
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.47	0.47
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.94	0.47
1:A:16:ASP:OD1	1:A:16:ASP:O	2.32	0.47
1:A:245:ARG:HH21	1:A:245:ARG:HG3	1.79	0.47
1:A:503:GLU:O	1:A:504:ARG:CB	2.57	0.47
1:A:272:GLU:O	1:A:276:LEU:HD22	2.15	0.46
1:A:168:PRO:CG	1:A:169:THR:N	2.75	0.46
1:A:166:VAL:HG21	1:A:178:GLU:HB2	1.96	0.46
1:A:187:LEU:HB3	1:A:305:GLN:HG2	1.96	0.46
1:A:144:PHE:HE2	1:A:158:MET:CE	2.29	0.46
1:A:162:ARG:HA	1:A:443:ASP:OD2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:TRP:NE1	1:A:291:LYS:HE3	2.32	0.45
1:A:362:ASP:C	1:A:362:ASP:OD1	2.55	0.45
1:A:262:LEU:O	1:A:266:HIS:HD2	2.00	0.45
8:A:613:NAG:C2	8:A:613:NAG:H61	2.46	0.45
1:A:166:VAL:CG2	1:A:178:GLU:O	2.64	0.45
1:A:484:TYR:C	1:A:486:THR:H	2.18	0.45
1:A:127:THR:HG23	1:A:131:GLU:CG	2.42	0.45
1:A:400:LEU:HD11	1:A:553:ILE:CD1	2.44	0.45
8:A:613:NAG:H2	8:A:613:NAG:C6	2.46	0.45
8:A:613:NAG:H4	8:A:614:MAN:H2	1.71	0.45
1:A:70:PHE:CD1	1:A:485:LYS:HB2	2.52	0.45
1:A:120:GLY:HA2	1:A:123:GLU:OE1	2.17	0.45
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.30	0.45
1:A:419:ASN:O	1:A:430:GLY:HA2	2.16	0.44
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.81	0.44
1:A:333:ASN:ND2	1:A:333:ASN:N	2.65	0.44
1:A:407:MET:HB3	1:A:501:MET:HE2	1.98	0.44
1:A:333:ASN:H	1:A:333:ASN:ND2	2.15	0.44
1:A:133:CYS:SG	1:A:157:CYS:CB	3.06	0.44
1:A:227:LEU:HD22	10:A:623:HOH:O	2.16	0.44
1:A:319:SER:OG	1:A:503:GLU:HB3	2.18	0.44
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.99	0.44
1:A:572:TYR:HA	1:A:573:PRO:HA	1.70	0.44
1:A:193:TYR:CE2	1:A:297:ARG:HG3	2.52	0.44
1:A:547:PHE:CE2	1:A:585:LEU:HD13	2.52	0.44
1:A:300:LEU:O	1:A:303:PHE:HB3	2.18	0.44
1:A:199:LEU:C	1:A:201:SER:H	2.21	0.44
1:A:58:PRO:HD3	1:A:162:ARG:NH1	2.32	0.44
1:A:268:LEU:HD11	1:A:392:ILE:CD1	2.48	0.44
1:A:345:PHE:HZ	1:A:440:ARG:HG3	1.83	0.43
1:A:312:TYR:O	1:A:315:ILE:HG12	2.19	0.43
1:A:135:GLN:HB2	1:A:141:PRO:HD2	2.00	0.43
1:A:249:PHE:CE2	1:A:383:THR:HG22	2.52	0.43
1:A:282:LYS:HB2	1:A:282:LYS:HE3	1.67	0.43
1:A:8:ALA:N	1:A:9:PRO:HD2	2.33	0.43
1:A:264:THR:O	1:A:267:THR:HB	2.19	0.43
8:A:613:NAG:C2	8:A:613:NAG:C6	2.96	0.43
1:A:268:LEU:HD11	1:A:392:ILE:HD11	2.01	0.43
1:A:4:VAL:HG23	1:A:4:VAL:O	2.18	0.43
1:A:264:THR:HG23	1:A:392:ILE:HB	2.01	0.42
1:A:364:ASN:O	1:A:365:TYR:HB2	2.19	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.71	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:ASP:O	1:A:403:LYS:HD3	2.19	0.42
7:A:604:NAG:C6	7:A:606:NAG:C1	2.97	0.42
1:A:202:ARG:HD3	10:A:669:HOH:O	2.19	0.42
1:A:333:ASN:HD22	1:A:334:SER:N	2.16	0.42
1:A:283:LEU:HD22	1:A:283:LEU:O	2.19	0.42
1:A:3:GLU:OE1	1:A:6:CYS:SG	2.76	0.41
1:A:240:ILE:C	1:A:240:ILE:HD12	2.40	0.41
1:A:199:LEU:C	1:A:201:SER:N	2.73	0.41
1:A:130:GLU:HG2	1:A:426:HIS:CE1	2.55	0.41
1:A:202:ARG:CD	1:A:250:LEU:HD21	2.49	0.41
1:A:360:ARG:O	1:A:361:LEU:HD23	2.20	0.41
1:A:248:CYS:HA	1:A:383:THR:HG21	2.02	0.41
1:A:376:LEU:HD13	1:A:380:PHE:CZ	2.55	0.41
1:A:396:THR:O	1:A:399:LEU:HB2	2.19	0.41
1:A:113:PHE:O	1:A:115:PRO:HD3	2.20	0.41
1:A:345:PHE:CZ	1:A:440:ARG:HG3	2.55	0.41
1:A:336:ASP:HA	1:A:337:PRO:HD2	1.96	0.41
1:A:276:LEU:O	1:A:280:LEU:HG	2.21	0.41
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.93	0.41
1:A:373:GLU:O	1:A:374:LEU:HD23	2.20	0.41
1:A:240:ILE:HD11	1:A:384:TRP:CD1	2.56	0.41
1:A:125:SER:HA	1:A:128:GLN:HB3	2.02	0.41
1:A:160:PHE:CD1	1:A:160:PHE:C	2.94	0.41
1:A:235:SER:CB	1:A:238:GLU:HB2	2.50	0.41
1:A:39:ALA:O	1:A:40:ASN:HB2	2.21	0.41
1:A:66:THR:HB	1:A:70:PHE:N	2.36	0.41
1:A:324:TRP:CZ2	1:A:513:CYS:HB2	2.56	0.40
1:A:106:ILE:O	1:A:107:VAL:C	2.59	0.40
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.56	0.40
1:A:345:PHE:HE2	1:A:440:ARG:HB3	1.86	0.40
1:A:515:LEU:HA	1:A:515:LEU:HD23	1.92	0.40
1:A:12:LEU:H	1:A:12:LEU:HG	1.57	0.40
1:A:259:GLN:O	1:A:260:ILE:C	2.60	0.40
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.85	0.40
1:A:140:PHE:O	1:A:160:PHE:HB3	2.22	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%)	537 (91%)	40 (7%)	15 (2%)	9 21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	12	LEU
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	174	SER
1	A	234	PRO
1	A	14	LYS
1	A	485	LYS
1	A	2	TRP
1	A	122	ASN
1	A	9	PRO
1	A	18	ASN
1	A	133	CYS
1	A	5	GLY

### 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%)	467 (90%)	50 (10%)	12 27

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	9	PRO
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	119	LEU
1	A	128	GLN
1	A	130	GLU
1	A	134	ILE
1	A	165	PHE
1	A	166	VAL
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	172	TYR
1	A	175	LEU
1	A	187	LEU
1	A	203	LEU
1	A	207	SER
1	A	208	SER
1	A	216	ASN
1	A	218	GLU
1	A	226	TYR
1	A	231	ASN
1	A	232	LYS
1	A	234	PRO
1	A	235	SER
1	A	259	GLN
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	283	LEU
1	A	291	LYS
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	415	SER
1	A	418	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	464	LEU
1	A	480	LEU
1	A	504	ARG
1	A	511	LEU
1	A	520	GLN
1	A	542	ASP
1	A	545	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	284	ASN
1	A	322	GLN
1	A	333	ASN
1	A	341	ASN
1	A	423	GLN
1	A	437	ASN
1	A	497	ASN
1	A	574	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	7.19	2 (22%)	10,12,14	2.83	5 (50%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	20.76	1.25	1.11
1	A	198	SEP	CA-C	5.33	1.58	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	4.83	115.52	108.69
1	A	198	SEP	C-CA-N	-4.32	109.51	113.83
1	A	198	SEP	O2P-P-OG	3.75	116.99	106.65
1	A	198	SEP	O3P-P-O1P	-3.08	100.36	110.44
1	A	198	SEP	O3P-P-O2P	2.64	117.90	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	$\# Z  > 2$
7	NAG	A	604	1,7	12,14,15	0.52	0	15,19,21	1.16	3 (20%)
7	NAG	A	606	7	12,14,15	0.71	0	15,19,21	1.34	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	610	1,7	12,14,15	0.61	0	15,19,21	0.81	0
7	NAG	A	611	7	12,14,15	0.60	0	15,19,21	1.63	4 (26%)
8	NAG	A	612	1,8	12,14,15	0.74	0	15,19,21	0.84	0
8	NAG	A	613	8	12,14,15	0.72	0	15,19,21	0.86	0
8	MAN	A	614	8	10,11,12	0.58	0	11,15,17	1.30	1 (9%)
9	NAG	A	615	1,9	12,14,15	0.95	1 (8%)	15,19,21	1.16	1 (6%)
9	NAG	A	616	9	12,14,15	1.15	0	15,19,21	1.45	2 (13%)
9	BMA	A	617	9	10,11,12	0.55	0	11,15,17	0.73	1 (9%)
9	MAN	A	618	9	10,11,12	0.41	0	11,15,17	0.34	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
7	NAG	A	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	606	7	-	0/6/23/26	0/1/1/1
7	NAG	A	610	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	611	7	-	0/6/23/26	0/1/1/1
8	NAG	A	612	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	613	8	-	0/6/23/26	1/1/1/1
8	MAN	A	614	8	-	0/2/19/22	0/1/1/1
9	NAG	A	615	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	616	9	-	0/6/23/26	0/1/1/1
9	BMA	A	617	9	-	0/2/19/22	0/1/1/1
9	MAN	A	618	9	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	615	NAG	C3-C2	2.07	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	614	MAN	C4-C3-C2	3.72	115.50	110.50
7	A	611	NAG	C6-C5-C4	3.14	120.57	113.00
7	A	611	NAG	O5-C5-C4	2.85	114.27	110.65
7	A	606	NAG	C3-C2-N2	-2.83	107.46	111.76
9	A	615	NAG	C4-C3-C2	2.69	117.91	111.32

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	611	NAG	C3-C4-C5	2.50	114.67	110.20
7	A	611	NAG	C2-N2-C7	-2.50	118.89	123.09
7	A	604	NAG	C4-C3-C2	-2.40	105.44	111.32
7	A	604	NAG	C2-N2-C7	-2.38	119.09	123.09
7	A	606	NAG	C4-C3-C2	2.32	116.99	111.32
7	A	604	NAG	C3-C4-C5	-2.31	106.07	110.20
9	A	616	NAG	C3-C2-N2	-2.10	108.57	111.76
9	A	616	NAG	O5-C5-C6	2.08	109.16	106.98
9	A	617	BMA	O5-C5-C6	2.08	109.16	106.98
7	A	606	NAG	C2-N2-C7	-2.06	119.64	123.09

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	613	NAG	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
5	CYN	A	596	-	1,1,1	0.29	0	0,0,0	0.00	-
2	HEM	A	605	1	49,50,50	3.28	14 (28%)	46,82,82	2.26	10 (21%)
3	SCN	A	607	-	2,2,2	1.54	1 (50%)	1,1,1	0.22	0
3	SCN	A	608	-	2,2,2	1.52	1 (50%)	1,1,1	0.18	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
5	CYN	A	596	-	-	0/0/0/0	0/0/0/0
2	HEM	A	605	1	-	0/14/114/114	0/0/8/8
3	SCN	A	607	-	-	0/0/0/0	0/0/0/0
3	SCN	A	608	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3D-C4D	12.70	1.47	1.44
2	A	605	HEM	C2D-C1D	-10.55	1.41	1.44
2	A	605	HEM	C4A-C3A	5.97	1.47	1.40
2	A	605	HEM	C3B-C2B	-5.93	1.33	1.43
2	A	605	HEM	C2B-C1B	5.73	1.46	1.44
2	A	605	HEM	C3C-C2C	-4.34	1.36	1.43
2	A	605	HEM	C3B-CAB	4.19	1.53	1.40
2	A	605	HEM	C3D-C2D	4.13	1.51	1.43
2	A	605	HEM	C3C-CAC	4.08	1.53	1.40
2	A	605	HEM	CHA-C4D	3.25	1.40	1.35
2	A	605	HEM	FE-NC	2.82	2.08	1.97
2	A	605	HEM	CMC-C2C	2.53	1.55	1.47
2	A	605	HEM	CAA-C2A	2.37	1.56	1.52
2	A	605	HEM	C1A-C2A	2.30	1.47	1.43
3	A	607	SCN	C-S	2.17	1.77	1.63
3	A	608	SCN	C-S	2.14	1.77	1.63

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	C3B-C4B-NB	-8.85	107.67	114.00
2	A	605	HEM	CHC-C4B-NB	5.08	128.80	124.58
2	A	605	HEM	C4D-ND-C1D	4.33	109.60	105.16
2	A	605	HEM	C4A-C3A-C2A	3.95	109.75	107.00
2	A	605	HEM	CMA-C3A-C4A	-3.62	123.05	128.62
2	A	605	HEM	CAD-C3D-C4D	3.38	130.61	124.53
2	A	605	HEM	C4A-CHB-C1B	-3.21	123.25	127.47
2	A	605	HEM	CHD-C1D-ND	2.64	126.78	124.58
2	A	605	HEM	C1A-CHA-C4D	2.18	130.34	127.47
2	A	605	HEM	CHD-C4C-NC	-2.04	122.96	124.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	595/595 (100%)	0.00	35 (5%)	22 23	10, 28, 72, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	8.1
1	A	122	ASN	8.1
1	A	13	VAL	6.1
1	A	1	SER	5.9
1	A	595	ASN	5.6
1	A	124	HIS	5.2
1	A	123	GLU	5.2
1	A	5	GLY	5.2
1	A	173	GLN	5.1
1	A	593	ARG	4.7
1	A	118	GLU	4.6
1	A	7	GLY	4.3
1	A	171	PRO	4.2
1	A	170	PRO	4.1
1	A	6	CYS	4.1
1	A	425	THR	3.4
1	A	231	ASN	3.3
1	A	172	TYR	3.2
1	A	594	GLU	3.1
1	A	2	TRP	3.0
1	A	125	SER	2.9
1	A	147	ASN	2.7
1	A	3	GLU	2.6
1	A	588	SER	2.6
1	A	4	VAL	2.6
1	A	89	GLU	2.5
1	A	322	GLN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	2.5
1	A	254	PHE	2.2
1	A	565	HIS	2.2
1	A	169	THR	2.2
1	A	16	ASP	2.1
1	A	14	LYS	2.0
1	A	9	PRO	2.0
1	A	209	PRO	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.15	-0.31	31,40,42,43	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	A	611	14/15	0.43	20.03	59,62,63,63	0
9	NAG	A	615	14/15	0.39	15.35	58,64,67,69	0
8	NAG	A	613	14/15	0.35	8.00	68,72,75,76	0
9	NAG	A	616	14/15	0.69	4.58	74,77,79,80	0
7	NAG	A	610	14/15	0.21	2.84	48,50,55,57	0
7	NAG	A	606	14/15	0.37	1.99	73,75,77,77	0
7	NAG	A	604	14/15	0.29	1.86	57,63,66,70	0
8	NAG	A	612	14/15	0.18	0.58	51,53,55,61	0
9	BMA	A	617	11/12	0.54	-	79,80,80,80	0
9	MAN	A	618	11/12	0.61	-	77,79,79,79	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MAN	A	614	11/12	0.49	-	79,81,81,81	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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SCN	A	607	3/3	0.16	0.11	16,16,16,19	0
2	HEM	A	605	43/43	0.15	-0.01	18,26,30,35	0
3	SCN	A	608	3/3	0.13	-0.36	32,32,36,37	0
6	IOD	A	597	1/1	0.14	-0.82	52,52,52,52	1
6	IOD	A	598	1/1	0.10	-1.00	56,56,56,56	1
6	IOD	A	603	1/1	0.04	-2.32	61,61,61,61	0
6	IOD	A	600	1/1	0.06	-2.60	90,90,90,90	0
4	CA	A	609	1/1	0.04	-3.44	17,17,17,17	0
6	IOD	A	601	1/1	0.04	-3.69	66,66,66,66	0
6	IOD	A	602	1/1	0.02	-4.87	21,21,21,21	0
6	IOD	A	599	1/1	0.04	-5.44	79,79,79,79	0
5	CYN	A	596	2/2	0.12	-9.95	35,35,35,38	0

## 6.5 Other polymers

There are no such residues in this entry.