Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:52 AM GMT

PDB ID	:	2OJV
Title	:	Crystal structure of a ternary complex of goat lactoperoxidase with cyanide and iodide ions at 2.4 A resolution
Authors	:	Singh, A.K.; Singh, N.; Singh, S.B.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-01-15
Resolution	:	2.40 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

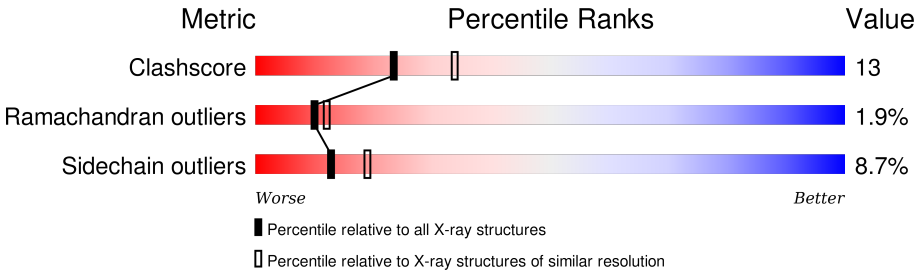
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	595	75% 19% 5%

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	CYN	A	2844	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5362 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	S	0	0	0
			4753	3021	844	862	26			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

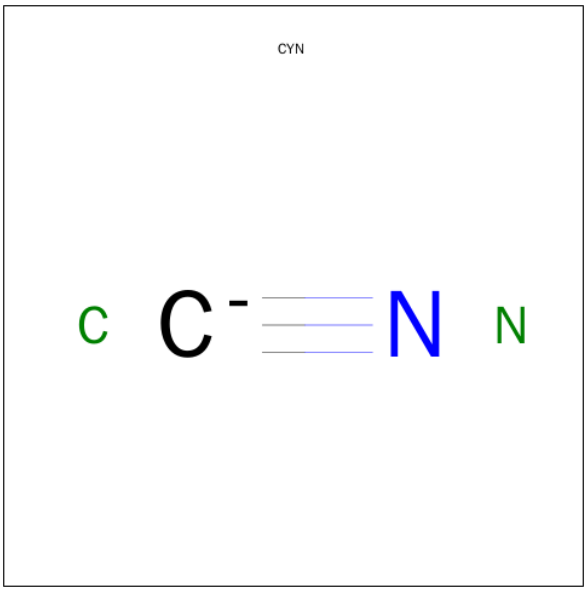
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

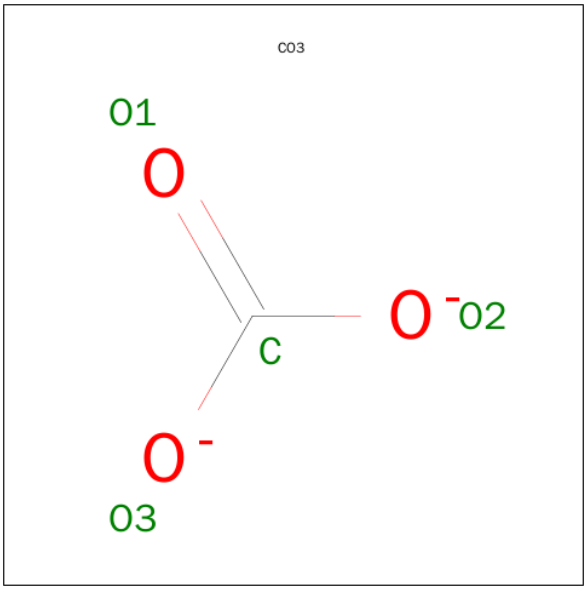
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 2 1 1	0	0

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

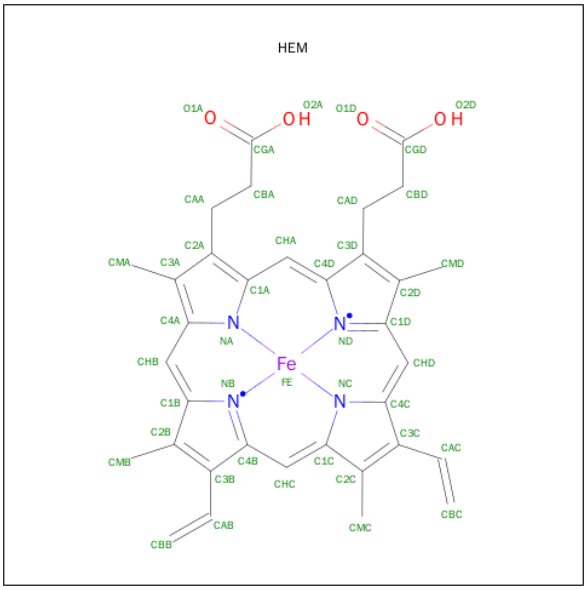


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	8	Total I 8 8	0	0

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	406	Total O 406 406	0	0

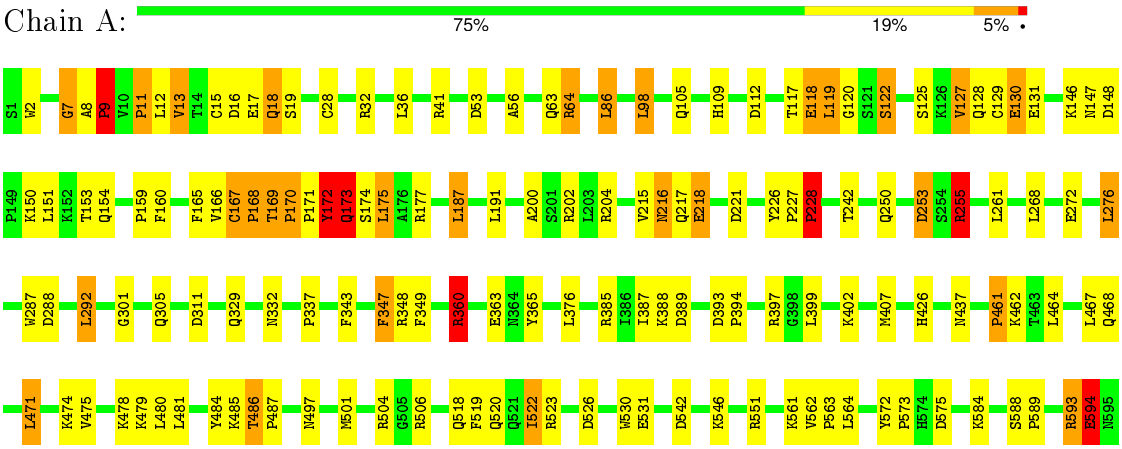
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: Lactoperoxidase

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.20Å 80.81Å 77.05Å 90.00° 102.96° 90.00°	Depositor
Resolution (Å)	74.54 – 2.40	Depositor
% Data completeness (in resolution range)	97.8 (74.54-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.178 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5362	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, NAG, CA, 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	0.71	1/4882 (0.0%)	1.00	23/6632 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PRO	N-CA	6.27	1.57	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	TYR	CA-CB-CG	-9.83	94.73	113.40
1	A	11	PRO	C-N-CA	-8.82	99.66	121.70
1	A	11	PRO	N-CA-C	7.41	131.36	112.10
1	A	11	PRO	CA-C-N	6.55	131.60	117.20
1	A	255	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	228	PRO	CA-N-CD	-6.18	102.85	111.50
1	A	13	VAL	N-CA-C	6.11	127.49	111.00
1	A	18	GLN	CB-CA-C	5.98	122.37	110.40
1	A	112	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	461	PRO	CA-N-CD	-5.85	103.31	111.50
1	A	171	PRO	CA-N-CD	-5.80	103.38	111.50
1	A	360	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	311	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	172	TYR	N-CA-C	5.28	125.26	111.00
1	A	575	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	53	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	506	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	542	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	7	GLY	N-CA-C	5.23	126.17	113.10
1	A	253	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	LEU	N-CA-C	5.18	124.99	111.00
1	A	11	PRO	O-C-N	-5.13	114.48	122.70
1	A	11	PRO	CA-N-CD	-5.11	104.35	111.50

There are no chirality outliers.

There are no planarity outliers.

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	4753	0	4647	122	0
2	A	117	0	102	4	0
3	A	28	0	25	0	0
4	A	1	0	0	0	0
5	A	2	0	0	2	0
6	A	4	0	0	0	0
7	A	8	0	0	2	0
8	A	43	0	30	3	0
9	A	406	0	0	17	0
All	All	5362	0	4804	129	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 13.

All (129) 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:168:PRO:HG2	1:A:172:TYR:CE1	1.85	1.11
1:A:63:GLN:HG2	9:A:3178:HOH:O	1.50	1.10
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.34	1.09
1:A:426:HIS:HB3	9:A:3202:HOH:O	1.55	1.05
1:A:2:TRP:HB2	1:A:175:LEU:HD12	1.35	1.03
1:A:169:THR:CG2	1:A:170:PRO:HD3	1.89	1.02
1:A:64:ARG:HG3	9:A:3237:HOH:O	1.64	0.96
1:A:119:LEU:HD11	1:A:169:THR:HG21	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.97	0.95
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.49	0.93
1:A:169:THR:HG22	1:A:170:PRO:CD	2.00	0.91
1:A:118:GLU:HB3	9:A:3243:HOH:O	1.72	0.90
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.55	0.87
1:A:216:ASN:ND2	1:A:218:GLU:H	1.72	0.87
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.07	0.84
1:A:481:LEU:HD21	1:A:487:PRO:HD3	1.56	0.84
5:A:2844:CYN:N	7:A:2852:IOD:I	2.82	0.82
1:A:202:ARG:NH2	7:A:2848:IOD:I	2.83	0.81
1:A:119:LEU:HD11	1:A:169:THR:CG2	2.11	0.81
1:A:169:THR:HG23	1:A:170:PRO:HD3	1.61	0.81
1:A:19:SER:HB3	9:A:3189:HOH:O	1.79	0.81
1:A:130:GLU:HG2	1:A:159:PRO:HG3	1.62	0.80
1:A:172:TYR:O	1:A:173:GLN:HB3	1.81	0.80
1:A:146:LYS:HE2	9:A:3257:HOH:O	1.84	0.77
1:A:216:ASN:HD22	1:A:218:GLU:H	1.31	0.76
1:A:169:THR:CG2	1:A:170:PRO:CD	2.59	0.76
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.87	0.75
1:A:172:TYR:HD2	1:A:173:GLN:H	1.34	0.74
1:A:481:LEU:CD2	1:A:487:PRO:HD3	2.18	0.73
1:A:167:CYS:CB	1:A:168:PRO:CD	2.63	0.72
1:A:561:LYS:HE2	9:A:2905:HOH:O	1.89	0.72
1:A:365:TYR:CZ	1:A:397:ARG:HG2	2.25	0.72
1:A:146:LYS:O	1:A:147:ASN:HB2	1.88	0.71
1:A:130:GLU:HG3	9:A:3201:HOH:O	1.93	0.69
1:A:174:SER:OG	1:A:175:LEU:N	2.25	0.69
1:A:216:ASN:HD22	1:A:217:GLN:N	1.93	0.67
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.77	0.66
1:A:169:THR:HG22	1:A:170:PRO:HD2	1.77	0.66
1:A:288:ASP:O	1:A:292:LEU:HD22	1.96	0.66
1:A:169:THR:H	1:A:170:PRO:HD2	1.61	0.64
1:A:8:ALA:HB3	9:A:3247:HOH:O	1.97	0.64
1:A:129:CYS:HB2	9:A:3188:HOH:O	1.98	0.63
1:A:119:LEU:CD1	1:A:169:THR:HG21	2.25	0.63
1:A:168:PRO:CG	1:A:172:TYR:CE1	2.75	0.63
8:A:2853:HEM:HBC2	8:A:2853:HEM:HMC2	1.81	0.62
1:A:2:TRP:HB2	1:A:175:LEU:CD1	2.22	0.61
2:A:596:NAG:H61	2:A:597:NAG:C1	2.31	0.61
1:A:168:PRO:HG2	1:A:172:TYR:HE1	1.58	0.61
1:A:475:VAL:HG12	1:A:479:LYS:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:OE2	1:A:594:GLU:HA	2.02	0.59
1:A:8:ALA:N	1:A:9:PRO:CD	2.65	0.59
1:A:64:ARG:HD3	9:A:3249:HOH:O	2.02	0.59
1:A:7:GLY:HA2	1:A:167:CYS:HA	1.84	0.59
1:A:8:ALA:N	1:A:9:PRO:HD2	2.18	0.58
1:A:15:CYS:HG	1:A:28:CYS:HG	0.60	0.58
1:A:216:ASN:HD22	1:A:216:ASN:C	2.07	0.57
1:A:125:SER:HA	1:A:128:GLN:HB3	1.87	0.57
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.03	0.57
1:A:169:THR:H	1:A:170:PRO:CD	2.18	0.57
1:A:202:ARG:HD2	1:A:250:GLN:HE22	1.69	0.57
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.40	0.56
1:A:119:LEU:CD1	1:A:169:THR:CG2	2.80	0.56
1:A:125:SER:C	1:A:127:VAL:N	2.60	0.55
1:A:172:TYR:HD2	1:A:173:GLN:N	2.04	0.54
1:A:462:LYS:HD2	9:A:3136:HOH:O	2.09	0.53
1:A:588:SER:N	1:A:589:PRO:CD	2.71	0.53
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.44	0.53
1:A:16:ASP:O	1:A:17:GLU:HB2	2.09	0.52
2:A:602:NAG:H62	2:A:603:NAG:C1	2.40	0.52
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.23	0.52
1:A:172:TYR:CD2	1:A:173:GLN:N	2.77	0.51
2:A:597:NAG:H3	2:A:598:MAN:O5	2.11	0.51
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.92	0.51
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.92	0.51
1:A:216:ASN:HB2	1:A:227:PRO:O	2.11	0.50
1:A:16:ASP:HB3	9:A:3189:HOH:O	2.11	0.50
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.45	0.50
1:A:365:TYR:CE1	1:A:397:ARG:HG2	2.48	0.49
1:A:287:TRP:HE3	1:A:292:LEU:HD13	1.78	0.49
1:A:301:GLY:O	1:A:305:GLN:HG3	2.14	0.47
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.80	0.47
1:A:593:ARG:HA	1:A:593:ARG:HD3	1.79	0.47
1:A:216:ASN:ND2	1:A:217:GLN:N	2.63	0.47
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.96	0.47
1:A:36:LEU:HG	1:A:337:PRO:HD2	1.96	0.47
1:A:485:LYS:O	1:A:486:THR:HB	2.15	0.47
1:A:105:GLN:HE21	5:A:2844:CYN:C	2.28	0.46
1:A:109:HIS:ND1	9:A:2881:HOH:O	2.28	0.46
1:A:148:ASP:O	1:A:151:LEU:HB2	2.15	0.46
1:A:125:SER:C	1:A:127:VAL:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:O	1:A:173:GLN:CB	2.59	0.46
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.63	0.45
2:A:603:NAG:H4	2:A:604:MAN:H2	1.65	0.45
1:A:407:MET:HB3	1:A:501:MET:CE	2.47	0.45
1:A:169:THR:N	1:A:170:PRO:HD2	2.31	0.45
1:A:215:VAL:HA	1:A:228:PRO:HD3	1.97	0.45
1:A:15:CYS:CB	1:A:28:CYS:HG	2.24	0.44
1:A:131:GLU:HA	1:A:131:GLU:OE2	2.17	0.44
1:A:150:LYS:O	1:A:154:GLN:N	2.46	0.44
1:A:478:LYS:HB2	1:A:478:LYS:HE3	1.50	0.44
1:A:120:GLY:C	1:A:122:SER:H	2.19	0.43
1:A:332:ASN:ND2	9:A:3196:HOH:O	2.41	0.43
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.51	0.43
1:A:202:ARG:HD2	1:A:250:GLN:NE2	2.34	0.43
1:A:15:CYS:CB	1:A:28:CYS:SG	3.06	0.43
1:A:572:TYR:HA	1:A:573:PRO:HA	1.62	0.43
1:A:119:LEU:HD21	1:A:169:THR:HG23	2.00	0.43
1:A:272:GLU:HG3	1:A:276:LEU:HD22	2.01	0.43
1:A:562:VAL:HB	1:A:563:PRO:HD2	2.01	0.43
1:A:484:TYR:O	1:A:485:LYS:HB2	2.19	0.42
1:A:9:PRO:CG	1:A:41:ARG:CZ	2.96	0.42
1:A:481:LEU:HA	1:A:481:LEU:HD23	1.74	0.42
1:A:385:ARG:O	1:A:389:ASP:HB3	2.19	0.42
1:A:160:PHE:HA	9:A:3144:HOH:O	2.19	0.42
8:A:2853:HEM:CMC	8:A:2853:HEM:HBC2	2.48	0.42
1:A:594:GLU:OE2	1:A:594:GLU:CA	2.66	0.42
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.55	0.42
1:A:7:GLY:C	1:A:9:PRO:HD2	2.40	0.42
1:A:387:ILE:HG22	1:A:388:LYS:HG3	2.02	0.42
1:A:588:SER:N	1:A:589:PRO:HD2	2.35	0.41
1:A:98:LEU:HD13	1:A:399:LEU:HD23	2.01	0.41
1:A:347:PHE:HB3	8:A:2853:HEM:HMD3	2.02	0.41
1:A:200:ALA:O	1:A:204:ARG:HG3	2.21	0.41
1:A:86:LEU:HD13	9:A:3037:HOH:O	2.21	0.41
1:A:522:ILE:O	1:A:526:ASP:HB2	2.20	0.41
1:A:9:PRO:O	1:A:11:PRO:HD3	2.20	0.40
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.95	0.40
1:A:165:PHE:N	1:A:165:PHE:CD1	2.90	0.40
1:A:216:ASN:ND2	1:A:216:ASN:C	2.74	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	593/595 (100%)	557 (94%)	25 (4%)	11 (2%)	10 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	173	GLN
1	A	594	GLU
1	A	242	THR
1	A	486	THR
1	A	56	ALA
1	A	172	TYR
1	A	9	PRO
1	A	166	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	472 (91%)	45 (9%)	13 19

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	13	VAL
1	A	18	GLN
1	A	32	ARG
1	A	64	ARG
1	A	86	LEU
1	A	98	LEU
1	A	117	THR
1	A	118	GLU
1	A	119	LEU
1	A	122	SER
1	A	127	VAL
1	A	130	GLU
1	A	153	THR
1	A	172	TYR
1	A	173	GLN
1	A	175	LEU
1	A	177	ARG
1	A	187	LEU
1	A	191	LEU
1	A	216	ASN
1	A	218	GLU
1	A	228	PRO
1	A	255	ARG
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	292	LEU
1	A	329	GLN
1	A	347	PHE
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	461	PRO
1	A	464	LEU
1	A	471	LEU
1	A	480	LEU
1	A	504	ARG
1	A	520	GLN
1	A	522	ILE
1	A	523	ARG
1	A	546	LYS
1	A	564	LEU

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Mol	Chain	Res	Type
1	A	593	ARG
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	147	ASN
1	A	216	ASN
1	A	222	HIS
1	A	245	HIS
1	A	250	GLN
1	A	329	GLN
1	A	423	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	570	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	$\#\|Z\|>2$
2	NAG	A	596	1,2	14,14,15	0.56	0	15,19,21	1.39	2 (13%)
2	NAG	A	597	2	14,14,15	0.53	0	15,19,21	1.49	3 (20%)
2	MAN	A	598	2	11,11,12	0.66	0	14,15,17	1.57	2 (14%)
2	NAG	A	599	1,2	14,14,15	0.58	0	15,19,21	0.62	0
2	NAG	A	600	2	14,14,15	0.71	0	15,19,21	1.52	3 (20%)
2	MAN	A	601	2	11,11,12	0.55	0	14,15,17	1.04	1 (7%)
2	NAG	A	602	1,2	14,14,15	0.77	1 (7%)	15,19,21	1.19	1 (6%)
2	NAG	A	603	2	14,14,15	0.55	0	15,19,21	1.85	3 (20%)
2	MAN	A	604	2	11,11,12	0.51	0	14,15,17	1.77	2 (14%)
3	NAG	A	605	1,3	14,14,15	0.62	0	15,19,21	1.99	4 (26%)
3	NAG	A	606	3	14,14,15	0.50	0	15,19,21	0.85	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	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	0/1/1/1
2	NAG	A	599	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	2	-	0/6/23/26	0/1/1/1
2	MAN	A	601	2	-	0/2/19/22	0/1/1/1
2	NAG	A	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	603	2	-	0/6/23/26	0/1/1/1
2	MAN	A	604	2	-	0/2/19/22	1/1/1/1
3	NAG	A	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	606	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	NAG	O5-C1	-2.09	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	605	NAG	C1-O5-C5	-3.98	107.20	112.25
2	A	596	NAG	C2-N2-C7	-3.73	118.25	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	605	NAG	C2-N2-C7	-2.95	119.25	123.04
2	A	602	NAG	C6-C5-C4	-2.88	105.91	113.02
2	A	603	NAG	C2-N2-C7	-2.78	119.47	123.04
2	A	600	NAG	C3-C2-N2	-2.33	104.98	110.56
2	A	600	NAG	C2-N2-C7	-2.32	120.06	123.04
2	A	603	NAG	C4-C3-C2	-2.30	107.66	111.23
2	A	597	NAG	O4-C4-C3	2.06	114.97	110.34
2	A	596	NAG	O4-C4-C5	2.08	114.76	109.24
2	A	601	MAN	C1-O5-C5	2.46	115.37	112.25
2	A	597	NAG	O5-C5-C6	2.54	112.85	107.35
2	A	604	MAN	C1-C2-C3	2.61	112.62	109.54
3	A	605	NAG	O5-C5-C6	3.55	115.04	107.35
2	A	598	MAN	C1-C2-C3	3.56	113.76	109.54
2	A	598	MAN	C1-O5-C5	3.72	116.97	112.25
2	A	597	NAG	C4-C3-C2	3.75	117.06	111.23
3	A	605	NAG	C4-C3-C2	4.03	117.49	111.23
2	A	600	NAG	C1-O5-C5	4.06	117.41	112.25
2	A	604	MAN	C1-O5-C5	5.40	119.10	112.25
2	A	603	NAG	C1-O5-C5	5.59	119.34	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	604	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	596	NAG	1	0
2	A	597	NAG	2	0
2	A	598	MAN	1	0
2	A	602	NAG	1	0
2	A	603	NAG	2	0
2	A	604	MAN	1	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 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	$\#\|Z\| > 2$
5	CYN	A	2844	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	A	2853	1,5	30,50,50	2.02	8 (26%)	24,82,82	2.17	5 (20%)
6	CO3	A	688	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYN	A	2844	8	-	0/0/0/0	0/0/0/0
8	HEM	A	2853	1,5	-	0/10/54/54	0/0/8/8
6	CO3	A	688	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2853	HEM	C3B-C4B	-6.62	1.46	1.51
8	A	2853	HEM	C3D-C4D	-3.83	1.46	1.51
8	A	2853	HEM	C2C-C1C	-3.27	1.46	1.52
8	A	2853	HEM	C2D-C1D	-2.22	1.44	1.51
8	A	2853	HEM	C3B-CAB	2.10	1.55	1.51
8	A	2853	HEM	C3C-CAC	2.48	1.56	1.51
8	A	2853	HEM	CAA-C2A	2.57	1.56	1.52
8	A	2853	HEM	FE-NC	3.07	2.07	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2853	HEM	CMD-C2D-C3D	3.03	127.77	114.35
8	A	2853	HEM	CMB-C2B-C3B	4.03	126.58	116.53
8	A	2853	HEM	CMC-C2C-C3C	4.33	127.33	116.53
8	A	2853	HEM	CAD-C3D-C4D	4.62	128.75	112.47
8	A	2853	HEM	CAD-C3D-C2D	4.85	127.15	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2844	CYN	2	0
8	A	2853	HEM	3	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.