Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 04:47 AM GMT

PDB ID	:	2O86
Title	:	Crystal structure of a ternary complex of buffalo lactoperoxidase with nitrate and iodide at 2.8 A resolution
Authors	:	Sheikh, I.A.; Singh, N.; Singh, A.K.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2006-12-12
Resolution	:	2.80 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:

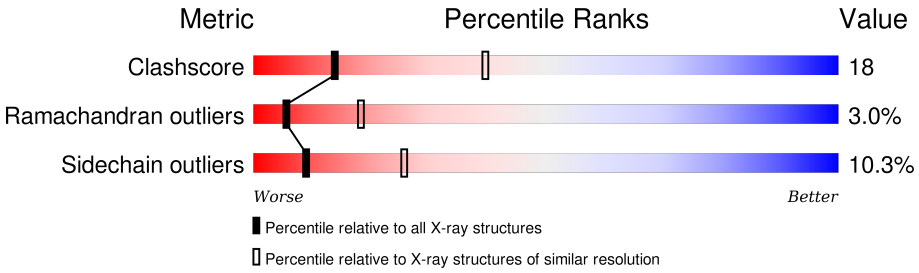
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	65% 28% 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
6	IOD	A	2003	-	-	X	-
7	NO3	A	3001	-	X	-	-
7	NO3	A	3002	-	X	-	-
7	NO3	A	3003	-	X	-	-
7	NO3	A	3004	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NO3	A	3007	-	X	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5219 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
			4766	3032	845	862	27			

- 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		

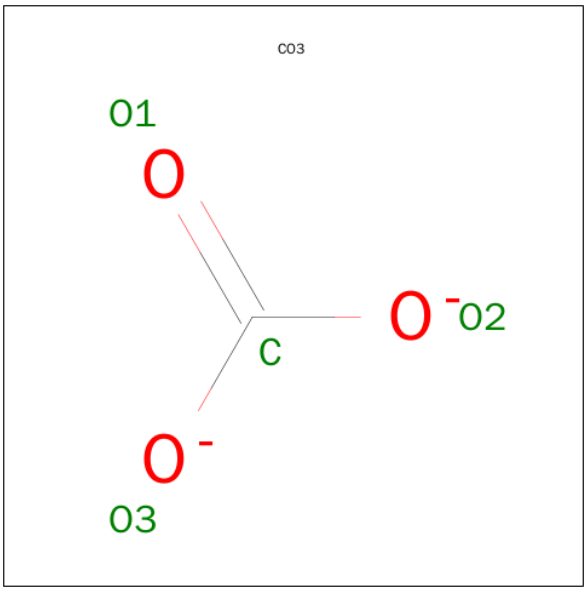
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
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 CARBONATE ION (three-letter code: CO3) (formula: CO_3).

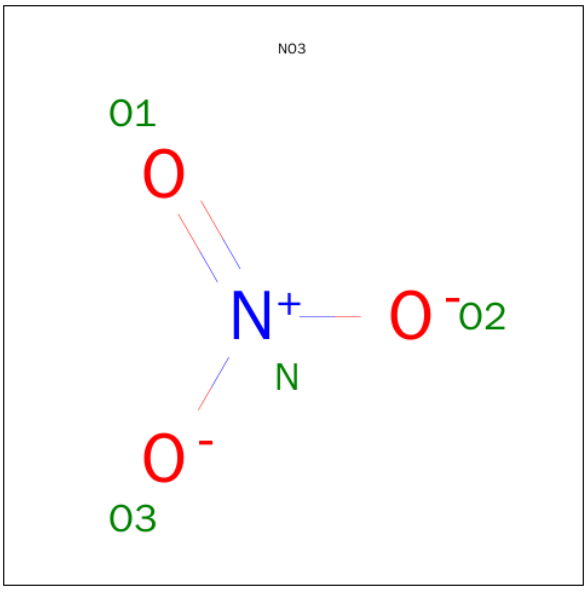


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 1 3	0	0

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

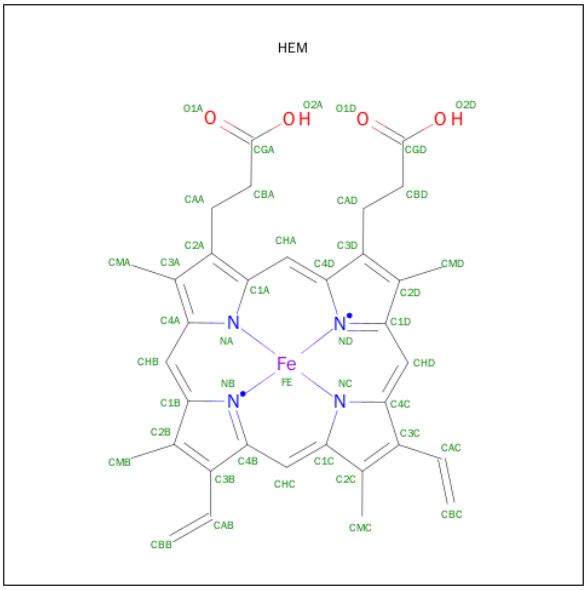
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total I 7 7	0	0

- Molecule 7 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	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	236	Total O 236 236	0	0

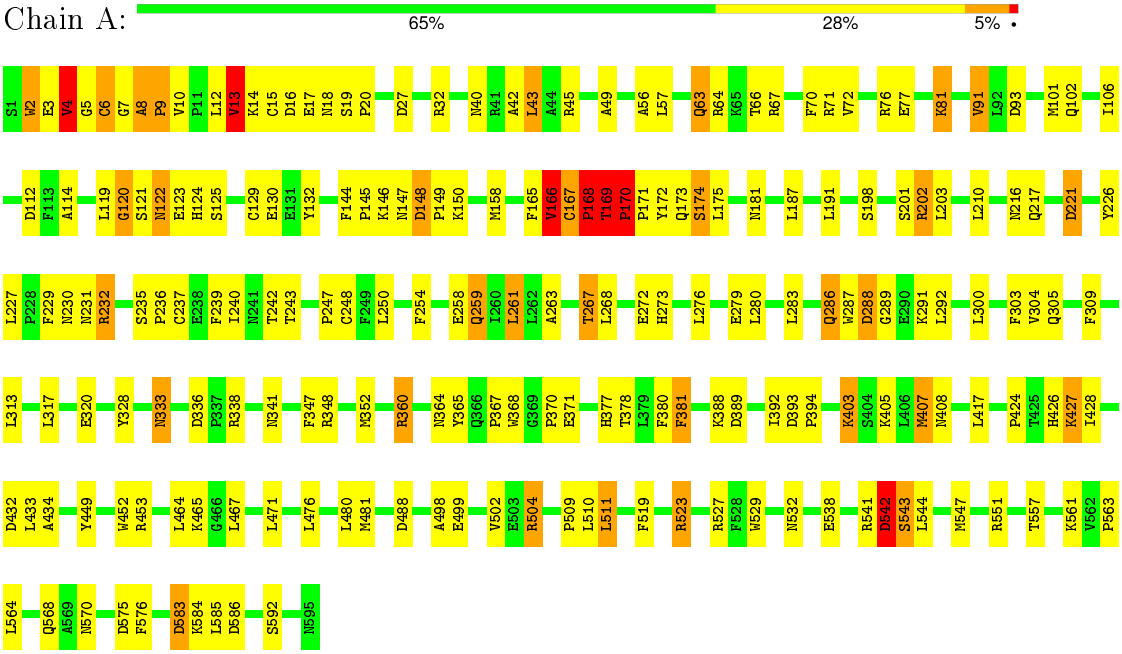
3 Residue-property plots (i)

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	54.53Å 80.83Å 77.66Å 90.00° 102.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	96.5 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.209 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5219	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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, NO3, 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	0.81	0/4893	1.01	12/6638 (0.2%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	THR	N-CA-C	-9.20	86.16	111.00
1	A	221	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	27	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	288	ASP	CB-CA-C	-6.54	97.32	110.40
1	A	542	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	583	ASP	CB-CG-OD2	5.59	123.34	118.30
1	A	148	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	488	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	112	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	287	TRP	C-N-CA	5.35	135.08	121.70
1	A	575	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	93	ASP	CB-CG-OD2	5.17	122.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	THR	Mainchain

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	4766	0	4676	173	0
2	A	78	0	68	2	0
3	A	56	0	50	2	0
4	A	1	0	0	0	0
5	A	4	0	0	0	0
6	A	7	0	0	5	0
7	A	28	0	0	4	0
8	A	43	0	30	6	0
9	A	236	0	0	37	0
All	All	5219	0	4824	179	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 18.

All (179) 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:7:GLY:HA3	9:A:3187:HOH:O	1.51	1.09
1:A:289:GLY:HA3	9:A:3196:HOH:O	1.57	1.04
1:A:8:ALA:HB1	1:A:9:PRO:CD	1.88	1.03
1:A:258:GLU:OE2	8:A:3008:HEM:HMB1	0.85	1.02
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.43	0.98
3:A:605:NAG:H5	9:A:3206:HOH:O	1.62	0.98
1:A:292:LEU:HG	9:A:3225:HOH:O	1.64	0.97
1:A:8:ALA:O	1:A:10:VAL:HG22	1.65	0.96
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.45	0.95
8:A:3008:HEM:HMC2	8:A:3008:HEM:HBC2	1.51	0.91
1:A:42:ALA:HB2	1:A:166:VAL:HG21	1.57	0.86
1:A:263:ALA:O	1:A:267:THR:HG22	1.76	0.86
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.04	0.85
1:A:288:ASP:HB2	1:A:291:LYS:HB3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:CB	1:A:9:PRO:CD	2.55	0.84
1:A:173:GLN:HG3	1:A:174:SER:H	1.43	0.83
1:A:232:ARG:O	1:A:232:ARG:HG3	1.78	0.82
1:A:32:ARG:HG3	9:A:3209:HOH:O	1.78	0.82
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.09	0.82
1:A:333:ASN:HD22	1:A:333:ASN:C	1.84	0.81
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.63	0.80
1:A:132:TYR:HE1	9:A:3228:HOH:O	1.66	0.78
1:A:254:PHE:HD2	9:A:3160:HOH:O	1.68	0.75
1:A:63:GLN:HG2	9:A:3135:HOH:O	1.87	0.75
1:A:288:ASP:HB2	1:A:291:LYS:CB	2.20	0.72
1:A:360:ARG:HD2	9:A:3200:HOH:O	1.90	0.71
1:A:367:PRO:HG3	6:A:2007:IOD:I	2.60	0.71
1:A:146:LYS:O	1:A:147:ASN:HB2	1.90	0.71
1:A:77:GLU:HG3	7:A:3004:NO3:O2	1.91	0.70
8:A:3008:HEM:HBC2	8:A:3008:HEM:CMC	2.21	0.70
1:A:129:CYS:HB2	9:A:3033:HOH:O	1.92	0.70
1:A:258:GLU:OE2	8:A:3008:HEM:C2B	2.47	0.68
1:A:403:LYS:NZ	9:A:3118:HOH:O	2.26	0.68
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.77	0.67
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.30	0.67
1:A:171:PRO:HD3	9:A:3084:HOH:O	1.92	0.67
1:A:360:ARG:HA	1:A:394:PRO:O	1.95	0.67
1:A:527:ARG:O	1:A:532:ASN:ND2	2.28	0.66
1:A:169:THR:HB	1:A:170:PRO:HD3	1.78	0.66
1:A:2:TRP:CB	1:A:4:VAL:HG22	2.27	0.65
1:A:2:TRP:HB3	1:A:4:VAL:HG22	1.79	0.64
1:A:544:LEU:CD2	1:A:547:MET:HE1	2.29	0.63
1:A:8:ALA:HB1	1:A:9:PRO:HD3	1.76	0.62
1:A:120:GLY:C	1:A:122:ASN:H	2.02	0.62
1:A:145:PRO:HG2	1:A:148:ASP:HB2	1.80	0.62
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.63	0.62
1:A:169:THR:HB	1:A:170:PRO:CD	2.29	0.61
1:A:173:GLN:HB3	9:A:3221:HOH:O	2.00	0.61
1:A:243:THR:HG22	9:A:3215:HOH:O	2.00	0.60
1:A:9:PRO:O	1:A:10:VAL:HG13	2.00	0.60
1:A:407:MET:HG3	9:A:3177:HOH:O	2.01	0.60
1:A:64:ARG:HA	9:A:3219:HOH:O	2.02	0.59
1:A:333:ASN:ND2	1:A:333:ASN:C	2.56	0.59
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.85	0.59
1:A:542:ASP:HB3	9:A:3223:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:CD	8:A:3008:HEM:CMB	2.66	0.59
1:A:101:MET:HE3	1:A:102:GLN:HA	1.85	0.59
1:A:114:ALA:HB3	9:A:3027:HOH:O	2.03	0.58
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.27	0.58
1:A:393:ASP:OD1	1:A:557:THR:HB	2.05	0.57
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.40	0.56
1:A:232:ARG:HG2	9:A:3188:HOH:O	2.05	0.55
1:A:187:LEU:HD22	1:A:304:VAL:HG12	1.87	0.55
1:A:259:GLN:HE22	1:A:261:LEU:HB2	1.71	0.54
1:A:288:ASP:HB3	1:A:291:LYS:H	1.72	0.54
1:A:43:LEU:HD13	1:A:181:ASN:HB2	1.88	0.54
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.90	0.54
1:A:232:ARG:HH21	1:A:248:CYS:CB	2.21	0.53
1:A:544:LEU:HD23	1:A:547:MET:CE	2.38	0.53
1:A:336:ASP:OD2	1:A:338:ARG:NH2	2.33	0.53
1:A:467:LEU:HD22	1:A:481:MET:HE1	1.91	0.53
2:A:597:NAG:H3	2:A:598:MAN:H61	1.91	0.53
1:A:352:MET:HB2	1:A:407:MET:HG2	1.91	0.52
1:A:167:CYS:CB	1:A:168:PRO:CD	2.81	0.52
2:A:598:MAN:H3	9:A:3151:HOH:O	2.09	0.52
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.40	0.52
1:A:273:HIS:C	1:A:273:HIS:CD2	2.83	0.51
1:A:173:GLN:HG3	1:A:174:SER:N	2.20	0.51
1:A:76:ARG:NE	1:A:148:ASP:OD2	2.43	0.51
1:A:504:ARG:HD2	9:A:3210:HOH:O	2.09	0.51
1:A:10:VAL:HG12	1:A:40:ASN:O	2.11	0.51
1:A:101:MET:O	1:A:101:MET:HG2	2.09	0.51
1:A:66:THR:HB	1:A:70:PHE:N	2.26	0.51
1:A:216:ASN:HA	6:A:2001:IOD:I	2.80	0.51
1:A:9:PRO:C	1:A:10:VAL:HG13	2.32	0.51
1:A:64:ARG:HB3	9:A:3024:HOH:O	2.11	0.50
1:A:2:TRP:HB2	1:A:4:VAL:HG22	1.93	0.50
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.36	0.50
1:A:239:PHE:CZ	1:A:427:LYS:HG2	2.46	0.50
8:A:3008:HEM:HMC2	8:A:3008:HEM:CBC	2.35	0.49
1:A:173:GLN:CG	1:A:174:SER:H	2.09	0.49
1:A:144:PHE:CE2	1:A:158:MET:HG3	2.48	0.49
1:A:538:GLU:HG3	1:A:541:ARG:NH2	2.28	0.49
1:A:42:ALA:HB2	1:A:166:VAL:CG2	2.38	0.49
1:A:43:LEU:HB2	9:A:3045:HOH:O	2.11	0.48
1:A:198:SER:HB2	7:A:3003:NO3:O2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:MET:HE2	1:A:585:LEU:HD22	1.95	0.48
1:A:511:LEU:HB2	9:A:3101:HOH:O	2.14	0.48
1:A:43:LEU:HG	1:A:341:ASN:HA	1.96	0.48
1:A:165:PHE:HE2	1:A:172:TYR:HB3	1.78	0.48
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.95	0.47
1:A:393:ASP:HB2	1:A:394:PRO:CD	2.44	0.47
1:A:424:PRO:O	6:A:2003:IOD:I	3.01	0.47
1:A:216:ASN:HB2	1:A:227:LEU:O	2.14	0.47
1:A:9:PRO:O	1:A:10:VAL:CG1	2.63	0.47
1:A:286:GLN:CD	1:A:286:GLN:H	2.19	0.47
1:A:481:MET:HA	1:A:481:MET:HE2	1.97	0.46
1:A:166:VAL:C	1:A:167:CYS:O	2.53	0.46
1:A:453:ARG:NH1	1:A:499:GLU:OE2	2.46	0.46
1:A:217:GLN:HE21	3:A:599:NAG:C7	2.28	0.46
1:A:551:ARG:CZ	1:A:584:LYS:HG2	2.45	0.46
1:A:19:SER:HA	1:A:20:PRO:HD3	1.81	0.46
1:A:237:CYS:HA	1:A:381:PHE:O	2.15	0.46
1:A:123:GLU:HG3	1:A:124:HIS:N	2.31	0.46
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.15	0.46
1:A:132:TYR:CE1	9:A:3228:HOH:O	2.53	0.46
1:A:3:GLU:O	1:A:5:GLY:N	2.49	0.46
1:A:259:GLN:HB2	1:A:259:GLN:HE21	1.46	0.46
1:A:91:VAL:HG13	1:A:405:LYS:HG3	1.98	0.45
1:A:130:GLU:OE2	1:A:426:HIS:HB3	2.17	0.45
1:A:388:LYS:HA	9:A:3216:HOH:O	2.16	0.45
1:A:119:LEU:HD22	9:A:3084:HOH:O	2.16	0.45
1:A:544:LEU:HD22	1:A:547:MET:HE1	1.98	0.45
1:A:67:ARG:NH1	9:A:3034:HOH:O	2.47	0.45
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.52	0.45
1:A:568:GLN:HE21	1:A:570:ASN:HD21	1.64	0.45
1:A:254:PHE:CD2	9:A:3160:HOH:O	2.55	0.45
1:A:364:ASN:O	1:A:365:TYR:HB2	2.17	0.44
1:A:368:TRP:CH2	1:A:389:ASP:O	2.70	0.44
1:A:544:LEU:HD23	1:A:547:MET:HE1	1.98	0.44
1:A:202:ARG:HD3	1:A:250:LEU:HD21	1.98	0.44
1:A:481:MET:HE3	1:A:481:MET:HB2	1.47	0.44
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.99	0.44
1:A:360:ARG:NH2	1:A:371:GLU:O	2.51	0.44
1:A:300:LEU:O	1:A:303:PHE:HB3	2.18	0.43
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.53	0.43
1:A:543:SER:OG	1:A:586:ASP:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:CB	1:A:291:LYS:H	2.31	0.43
1:A:171:PRO:HG3	9:A:3242:HOH:O	2.17	0.43
1:A:71:ARG:CZ	9:A:3219:HOH:O	2.66	0.43
1:A:101:MET:CE	1:A:102:GLN:HA	2.46	0.43
1:A:313:LEU:HD11	1:A:519:PHE:CG	2.54	0.43
1:A:544:LEU:HD23	1:A:547:MET:HE3	2.01	0.43
1:A:258:GLU:HG3	6:A:2002:IOD:I	2.89	0.43
1:A:561:LYS:HE2	9:A:3197:HOH:O	2.18	0.43
1:A:544:LEU:CD2	1:A:547:MET:CE	2.96	0.43
1:A:279:GLU:OE1	1:A:279:GLU:HA	2.18	0.43
1:A:13:VAL:HB	1:A:14:LYS:H	1.71	0.42
1:A:232:ARG:CG	9:A:3188:HOH:O	2.67	0.42
1:A:452:TRP:HB3	1:A:510:LEU:HD11	2.01	0.42
1:A:348:ARG:NH2	9:A:3179:HOH:O	2.51	0.42
1:A:258:GLU:O	1:A:380:PHE:HA	2.20	0.42
1:A:167:CYS:O	1:A:168:PRO:O	2.37	0.42
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.20	0.42
1:A:378:THR:HG22	7:A:3007:NO3:O1	2.19	0.42
1:A:432:ASP:OD1	1:A:434:ALA:N	2.53	0.42
1:A:377:HIS:NE2	7:A:3007:NO3:O1	2.52	0.42
1:A:561:LYS:CE	9:A:3197:HOH:O	2.67	0.42
1:A:235:SER:HA	1:A:236:PRO:HD3	1.89	0.42
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.55	0.42
1:A:125:SER:HB3	9:A:3226:HOH:O	2.20	0.41
1:A:309:PHE:CD1	1:A:529:TRP:HH2	2.39	0.41
1:A:146:LYS:O	1:A:147:ASN:CB	2.57	0.41
1:A:169:THR:CB	1:A:170:PRO:CD	2.98	0.41
1:A:370:PRO:HD2	1:A:371:GLU:H	1.86	0.41
1:A:236:PRO:HG3	6:A:2003:IOD:I	2.90	0.41
1:A:320:GLU:HG3	1:A:502:VAL:HG11	2.03	0.41
1:A:417:LEU:HD13	1:A:433:LEU:HD23	2.03	0.41
1:A:481:MET:CA	1:A:481:MET:HE2	2.51	0.41
1:A:15:CYS:O	1:A:16:ASP:C	2.59	0.41
1:A:148:ASP:O	1:A:149:PRO:C	2.59	0.40
1:A:407:MET:HE3	1:A:408:ASN:N	2.37	0.40
1:A:338:ARG:HB2	1:A:338:ARG:HE	1.67	0.40
1:A:432:ASP:OD1	1:A:432:ASP:C	2.60	0.40
1:A:232:ARG:HH21	1:A:248:CYS:HB2	1.87	0.40
1:A:2:TRP:C	1:A:4:VAL:H	2.24	0.40
1:A:449:TYR:CZ	1:A:453:ARG:HD3	2.56	0.40
1:A:230:ASN:HB3	9:A:3188:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASP:CB	1:A:394:PRO:CD	3.00	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	593/595 (100%)	527 (89%)	48 (8%)	18 (3%)	5 18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	8	ALA
1	A	122	ASN
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	170	PRO
1	A	174	SER
1	A	6	CYS
1	A	9	PRO
1	A	17	GLU
1	A	56	ALA
1	A	150	LYS
1	A	63	GLN
1	A	166	VAL
1	A	381	PHE
1	A	13	VAL
1	A	120	GLY

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%)	464 (90%)	53 (10%)	9 26

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	6	CYS
1	A	12	LEU
1	A	13	VAL
1	A	18	ASN
1	A	43	LEU
1	A	57	LEU
1	A	72	VAL
1	A	81	LYS
1	A	91	VAL
1	A	121	SER
1	A	166	VAL
1	A	168	PRO
1	A	170	PRO
1	A	175	LEU
1	A	201	SER
1	A	202	ARG
1	A	203	LEU
1	A	210	LEU
1	A	231	ASN
1	A	232	ARG
1	A	240	ILE
1	A	242	THR
1	A	259	GLN
1	A	261	LEU
1	A	267	THR
1	A	268	LEU
1	A	276	LEU
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	286	GLN
1	A	317	LEU
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	392	ILE
1	A	403	LYS
1	A	407	MET
1	A	427	LYS
1	A	428	ILE
1	A	464	LEU
1	A	465	LYS
1	A	471	LEU
1	A	480	LEU
1	A	504	ARG
1	A	511	LEU
1	A	523	ARG
1	A	542	ASP
1	A	543	SER
1	A	564	LEU
1	A	583	ASP
1	A	592	SER

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	259	GLN
1	A	286	GLN
1	A	333	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	558	HIS
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 (i)

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

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	$\#\|Z\| > 2$
2	NAG	A	596	1,2	14,14,15	0.71	0	15,19,21	1.76	4 (26%)
2	NAG	A	597	2	14,14,15	0.76	1 (7%)	15,19,21	1.45	1 (6%)
2	MAN	A	598	2	11,11,12	0.56	0	14,15,17	1.06	1 (7%)
3	NAG	A	599	1,3	14,14,15	0.65	1 (7%)	15,19,21	1.38	2 (13%)
3	NAG	A	600	3	14,14,15	0.89	0	15,19,21	2.18	2 (13%)
2	NAG	A	601	1,2	14,14,15	0.67	0	15,19,21	2.00	5 (33%)
2	NAG	A	602	2	14,14,15	0.47	0	15,19,21	2.33	3 (20%)
2	MAN	A	603	2	11,11,12	0.86	0	14,15,17	2.05	2 (14%)
3	NAG	A	604	1,3	14,14,15	0.78	0	15,19,21	1.59	2 (13%)
3	NAG	A	605	3	14,14,15	0.69	0	15,19,21	1.31	3 (20%)

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	1/1/1/1
3	NAG	A	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	600	3	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	603	2	-	0/2/19/22	1/1/1/1
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	597	NAG	O5-C1	-2.19	1.40	1.43
3	A	599	NAG	O5-C1	-2.04	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	596	NAG	C2-N2-C7	-3.74	118.24	123.04
3	A	605	NAG	C1-O5-C5	-3.30	108.06	112.25
3	A	604	NAG	C2-N2-C7	-2.79	119.46	123.04
2	A	601	NAG	C6-C5-C4	-2.65	106.48	113.02
2	A	602	NAG	C4-C3-C2	-2.45	107.42	111.23
3	A	599	NAG	O7-C7-C8	-2.40	117.65	122.06
2	A	601	NAG	O7-C7-C8	-2.36	117.73	122.06
2	A	596	NAG	O6-C6-C5	2.11	118.30	111.33
3	A	605	NAG	O3-C3-C2	2.18	113.42	109.11
2	A	602	NAG	C2-N2-C7	2.26	125.94	123.04
3	A	605	NAG	O5-C5-C6	2.34	112.41	107.35
2	A	596	NAG	C4-C3-C2	2.51	115.14	111.23
2	A	601	NAG	O7-C7-N2	2.58	127.12	121.86
2	A	598	MAN	O5-C5-C6	2.58	112.94	107.35
3	A	600	NAG	O3-C3-C2	2.66	114.39	109.11
2	A	601	NAG	C3-C4-C5	2.79	115.06	110.20
2	A	596	NAG	C1-O5-C5	3.20	116.30	112.25
2	A	603	MAN	C1-C2-C3	3.45	113.62	109.54
3	A	599	NAG	C1-O5-C5	3.50	116.69	112.25
2	A	597	NAG	C4-C3-C2	3.61	116.85	111.23
3	A	604	NAG	C4-C3-C2	3.85	117.21	111.23
2	A	601	NAG	C1-O5-C5	4.22	117.61	112.25
2	A	603	MAN	C1-O5-C5	5.86	119.68	112.25
3	A	600	NAG	C1-O5-C5	7.09	121.25	112.25
2	A	602	NAG	C1-O5-C5	7.53	121.80	112.25

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	MAN	C1-C2-C3-C4-C5-O5
2	A	598	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	597	NAG	1	0
2	A	598	MAN	2	0
3	A	599	NAG	1	0
3	A	605	NAG	1	0

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
7	NO3	A	3001	-	3,3,3	3.07	3 (100%)	3,3,3	0.50	0
7	NO3	A	3002	-	3,3,3	3.39	3 (100%)	3,3,3	0.36	0
7	NO3	A	3003	-	3,3,3	3.95	3 (100%)	3,3,3	1.00	0
7	NO3	A	3004	-	3,3,3	3.05	3 (100%)	3,3,3	0.46	0
7	NO3	A	3005	-	3,3,3	1.95	1 (33%)	3,3,3	0.88	0
7	NO3	A	3006	-	3,3,3	2.39	2 (66%)	3,3,3	0.52	0
7	NO3	A	3007	-	3,3,3	3.11	3 (100%)	3,3,3	1.38	0
8	HEM	A	3008	1	30,50,50	2.14	8 (26%)	24,82,82	2.07	8 (33%)
5	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
7	NO3	A	3001	-	-	0/0/0/0	0/0/0/0
7	NO3	A	3002	-	-	0/0/0/0	0/0/0/0
7	NO3	A	3003	-	-	0/0/0/0	0/0/0/0
7	NO3	A	3004	-	-	0/0/0/0	0/0/0/0
7	NO3	A	3005	-	-	0/0/0/0	0/0/0/0
7	NO3	A	3006	-	-	0/0/0/0	0/0/0/0
7	NO3	A	3007	-	-	0/0/0/0	0/0/0/0
8	HEM	A	3008	1	-	0/10/54/54	0/0/8/8
5	CO3	A	688	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3008	HEM	C3B-C4B	-6.96	1.45	1.51
8	A	3008	HEM	C2C-C1C	-4.34	1.44	1.52
8	A	3008	HEM	C3D-C4D	-2.61	1.48	1.51
8	A	3008	HEM	C2D-C1D	-2.45	1.43	1.51
8	A	3008	HEM	C3C-CAC	2.35	1.55	1.51
7	A	3006	NO3	O2-N	2.36	1.37	1.25
7	A	3004	NO3	O2-N	2.41	1.37	1.25
7	A	3004	NO3	O3-N	2.50	1.38	1.25
8	A	3008	HEM	C3B-CAB	2.52	1.56	1.51
7	A	3005	NO3	O1-N	2.63	1.35	1.24
8	A	3008	HEM	CAA-C2A	2.80	1.56	1.52
7	A	3001	NO3	O2-N	2.90	1.40	1.25
7	A	3007	NO3	O3-N	2.93	1.40	1.25
7	A	3002	NO3	O2-N	2.98	1.40	1.25
7	A	3007	NO3	O2-N	3.00	1.40	1.25
7	A	3001	NO3	O3-N	3.10	1.41	1.25
7	A	3003	NO3	O3-N	3.13	1.41	1.25
7	A	3003	NO3	O2-N	3.13	1.41	1.25
7	A	3006	NO3	O1-N	3.14	1.37	1.24
7	A	3002	NO3	O3-N	3.15	1.41	1.25
7	A	3001	NO3	O1-N	3.20	1.37	1.24
7	A	3007	NO3	O1-N	3.38	1.38	1.24
7	A	3002	NO3	O1-N	3.96	1.40	1.24
7	A	3004	NO3	O1-N	3.97	1.40	1.24
8	A	3008	HEM	FE-NC	4.51	2.13	1.95
7	A	3003	NO3	O1-N	5.21	1.45	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	3008	HEM	CAA-CBA-CGA	-2.06	108.97	112.75
8	A	3008	HEM	C2D-C3D-C4D	2.26	105.33	101.50
8	A	3008	HEM	CMB-C2B-C3B	2.48	122.72	116.53
8	A	3008	HEM	C4B-CHC-C1C	2.52	130.04	125.82
8	A	3008	HEM	CMD-C2D-C3D	3.16	128.34	114.35
8	A	3008	HEM	CMC-C2C-C3C	3.81	126.04	116.53
8	A	3008	HEM	CAD-C3D-C2D	4.42	125.92	113.22
8	A	3008	HEM	CAD-C3D-C4D	4.61	128.75	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3003	NO3	1	0
7	A	3004	NO3	1	0
7	A	3007	NO3	2	0
8	A	3008	HEM	6	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

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.