WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

PDB ID	:	2QQT
Title	:	Crystal structure of the complex of bovine lactoperoxidase with acetyl salicylic acid at 2.5 A resolution
Authors	:	Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-07-27
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		19
Ramachandran outliers		1.9%
Sidechain outliers		8.9%
RSRZ outliers		9.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
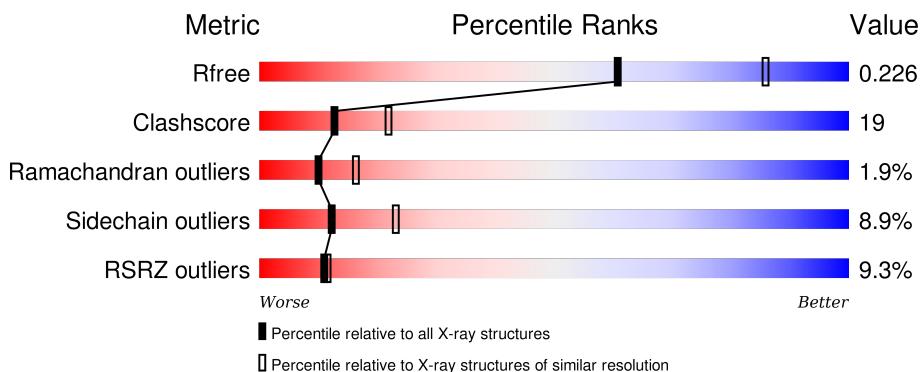
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	595	9% 66% 27% 6% ·

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
2	NAG	A	1001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AIN	A	596	-	-	X	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5295 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 4774	C 3037	N 847	O 863	P 1	S 26	0	0	0

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

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

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

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

- Molecule 4 is 2-(ACETYLOXY)BENZOIC ACID (three-letter code: AIN) (formula: $C_9H_8O_4$).
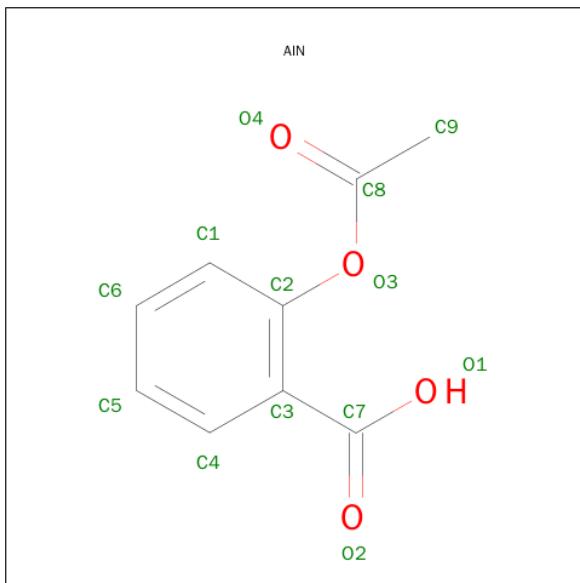
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 9	O 4	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).
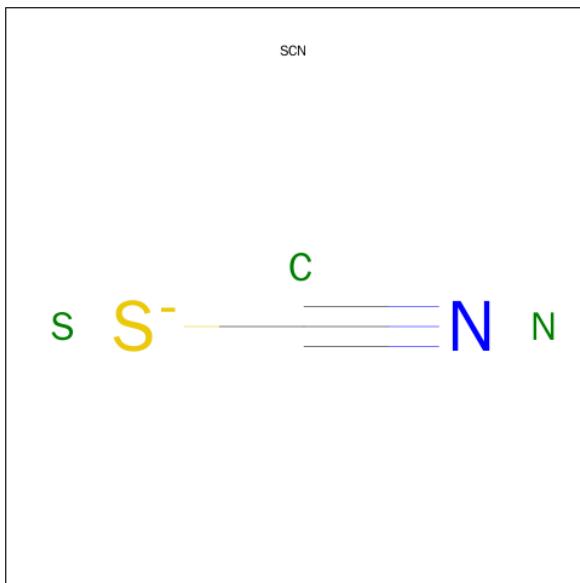
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
6	A	1	3	1	1	1	0	0

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

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

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
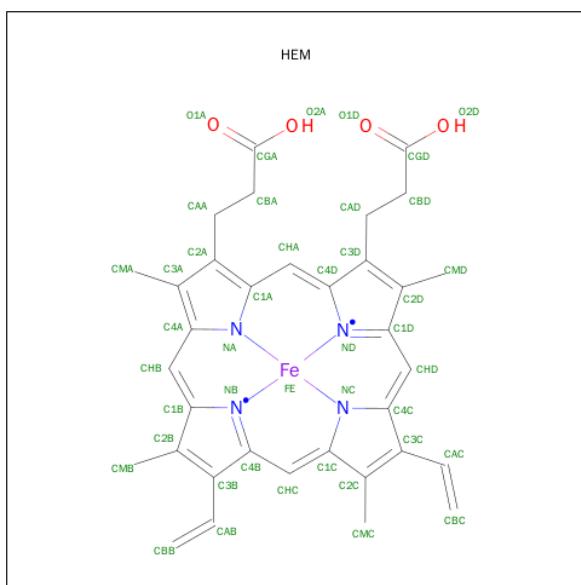
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	43	34	1	4	4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	320	320	320	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoperoxidase
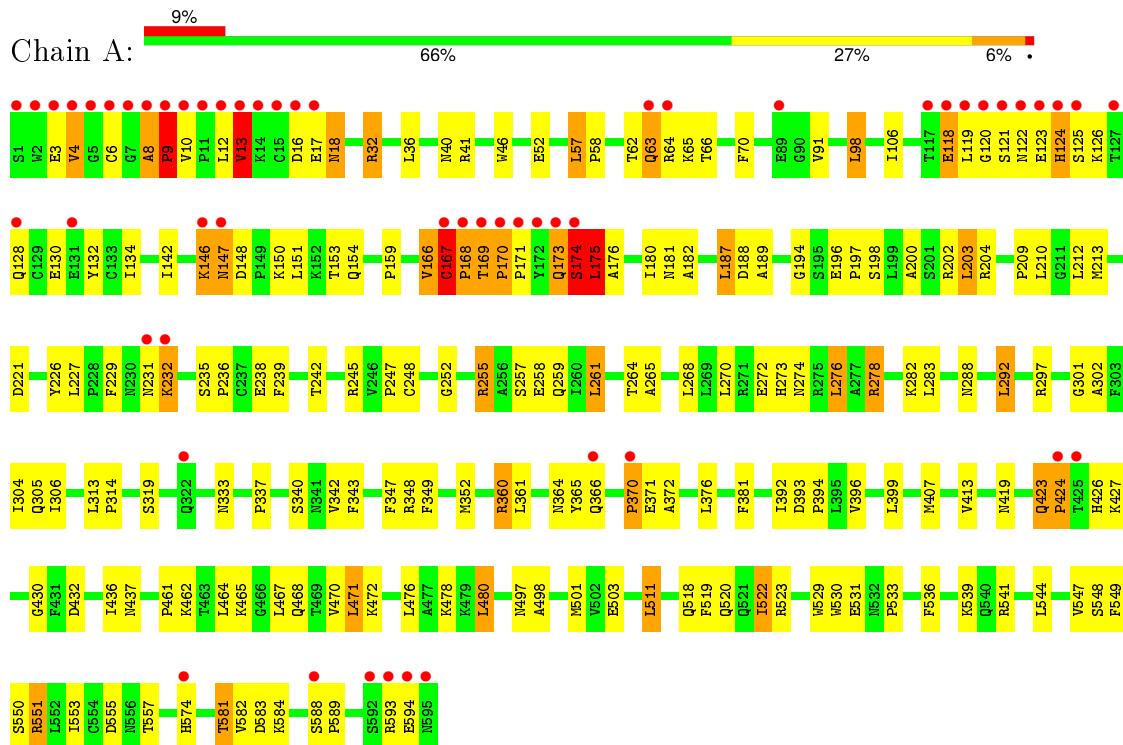
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.66Å　　80.52Å　　77.97Å 90.00°　　102.65°　　90.00°	Depositor
Resolution (Å)	19.44　–　2.50 19.44　–　2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.44-2.50) 98.8 (19.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.85 (at 2.49Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.194　,　0.211 0.192　,　0.226	Depositor DCC
R_{free} test set	1161 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 67.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 22614 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, AIN, 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	0.51	2/4891 (0.0%)	0.82	11/6634 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ARG	CD-NE	-11.42	1.27	1.46
1	A	9	PRO	CA-C	-5.43	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	PRO	CA-C-N	-8.82	97.80	117.20
1	A	167	CYS	N-CA-C	-7.28	91.34	111.00
1	A	423	GLN	CB-CA-C	6.42	123.24	110.40
1	A	167	CYS	CB-CA-C	6.39	123.18	110.40
1	A	9	PRO	CA-N-CD	-6.32	102.65	111.50
1	A	17	GLU	N-CA-C	5.89	126.89	111.00
1	A	232	LYS	N-CA-C	5.52	125.91	111.00
1	A	424	PRO	O-C-N	5.48	131.47	122.70
1	A	166	VAL	CA-C-N	-5.40	105.32	117.20
1	A	175	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	174	SER	N-CA-C	5.11	124.80	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4686	176	0
2	A	78	0	68	5	0
3	A	56	0	50	0	0
4	A	13	0	7	19	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	7	0	0	1	0
8	A	43	0	30	9	0
9	A	320	0	0	24	0
All	All	5295	0	4841	189	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 19.

All (189) 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:196:GLU:HB3	1:A:198:SEP:O2P	1.54	1.07
1:A:175:LEU:HD22	1:A:176:ALA:H	1.18	1.03
1:A:424:PRO:HG3	4:A:596:AIN:H4	1.42	1.01
1:A:235:SER:HB3	1:A:238:GLU:HG2	1.44	0.99
1:A:424:PRO:HD3	4:A:596:AIN:H5	1.45	0.97
1:A:4:VAL:O	1:A:4:VAL:HG13	1.65	0.94
1:A:173:GLN:HG2	1:A:174:SER:H	1.33	0.92
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.50	0.92
1:A:146:LYS:HE2	9:A:1256:HOH:O	1.71	0.91
1:A:8:ALA:C	1:A:10:VAL:H	1.74	0.91
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.55	0.89
1:A:175:LEU:CD2	1:A:176:ALA:H	1.86	0.87
1:A:424:PRO:CD	4:A:596:AIN:H5	2.04	0.87
1:A:32:ARG:HH11	1:A:32:ARG:HB3	1.38	0.86
1:A:424:PRO:CG	4:A:596:AIN:H4	2.06	0.84
1:A:282:LYS:HD3	9:A:1234:HOH:O	1.78	0.83
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.59	0.82
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.11	0.79
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.65	0.78
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.18	0.73
1:A:239:PHE:CZ	1:A:427:LYS:HG2	2.24	0.73
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.71	0.71
1:A:258:GLU:OE1	1:A:259:GLN:HG2	1.90	0.71
1:A:4:VAL:O	1:A:4:VAL:CG1	2.36	0.71
8:A:605:HEM:HMB1	8:A:605:HEM:HBB2	1.71	0.71
1:A:319:SER:HB3	9:A:1301:HOH:O	1.91	0.71
1:A:52:GLU:HG2	1:A:65:LYS:HE3	1.72	0.70
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.28	0.69
4:A:596:AIN:H1	8:A:605:HEM:CMA	2.22	0.69
4:A:596:AIN:H1	8:A:605:HEM:HMA2	1.74	0.69
1:A:119:LEU:HD21	1:A:170:PRO:HG3	1.75	0.69
1:A:173:GLN:CG	1:A:174:SER:H	2.04	0.68
1:A:123:GLU:HG3	1:A:125:SER:H	1.58	0.68
1:A:10:VAL:HG12	1:A:40:ASN:O	1.93	0.67
1:A:130:GLU:HG3	1:A:159:PRO:HG3	1.75	0.67
1:A:173:GLN:HG2	1:A:174:SER:N	2.09	0.67
1:A:302:ALA:O	1:A:306:ILE:HG13	1.95	0.66
1:A:255:ARG:CD	4:A:596:AIN:H92	2.26	0.65
1:A:170:PRO:CB	1:A:171:PRO:CD	2.75	0.64
1:A:381:PHE:HZ	4:A:596:AIN:C4	2.11	0.64
1:A:381:PHE:HZ	4:A:596:AIN:H4	1.61	0.63
1:A:274:ASN:O	1:A:278:ARG:HG2	2.00	0.62
1:A:392:ILE:O	1:A:396:VAL:HG23	2.00	0.62
1:A:8:ALA:C	1:A:10:VAL:N	2.43	0.62
1:A:173:GLN:CG	1:A:174:SER:N	2.63	0.62
1:A:197:PRO:HB2	1:A:198:SEP:O3P	2.00	0.62
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.98	0.62
1:A:12:LEU:HB2	9:A:1305:HOH:O	2.00	0.61
1:A:122:ASN:N	9:A:1196:HOH:O	2.33	0.61
1:A:533:PRO:HB3	9:A:1186:HOH:O	2.00	0.61
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.61
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.80	0.61
1:A:301:GLY:O	1:A:305:GLN:HG3	1.99	0.60
1:A:424:PRO:CG	4:A:596:AIN:C4	2.78	0.60
1:A:121:SER:O	1:A:122:ASN:HB3	2.02	0.60
1:A:12:LEU:O	1:A:13:VAL:HG13	2.02	0.60
1:A:32:ARG:NH1	1:A:32:ARG:HB3	2.13	0.60
1:A:255:ARG:HD2	4:A:596:AIN:H92	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:O	1:A:547:VAL:HG13	2.03	0.59
1:A:282:LYS:HG2	9:A:1171:HOH:O	2.03	0.59
1:A:10:VAL:HG23	9:A:1305:HOH:O	2.02	0.58
1:A:407:MET:HB3	1:A:501:MET:CE	2.34	0.58
1:A:255:ARG:HG2	4:A:596:AIN:O2	2.03	0.58
1:A:8:ALA:O	1:A:10:VAL:N	2.36	0.58
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.38	0.58
1:A:426:HIS:HB3	9:A:1167:HOH:O	2.03	0.57
1:A:393:ASP:OD1	1:A:557:THR:HB	2.04	0.57
2:A:1005:NAG:H62	2:A:1006:NAG:C1	2.34	0.57
1:A:424:PRO:CD	4:A:596:AIN:C5	2.80	0.57
1:A:550:SER:O	1:A:553:ILE:HB	2.06	0.56
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.84	0.56
2:A:1009:MAN:H61	9:A:1324:HOH:O	2.06	0.56
1:A:175:LEU:HD22	1:A:176:ALA:N	2.03	0.55
1:A:146:LYS:HE3	9:A:1052:HOH:O	2.05	0.55
1:A:582:VAL:HA	9:A:1308:HOH:O	2.07	0.55
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.22	0.55
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.89	0.55
1:A:258:GLU:OE1	1:A:259:GLN:CG	2.54	0.54
1:A:66:THR:HB	1:A:70:PHE:O	2.07	0.54
1:A:170:PRO:HB3	1:A:171:PRO:CD	2.38	0.54
1:A:200:ALA:O	1:A:204:ARG:HG3	2.08	0.54
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.54
1:A:10:VAL:HG21	1:A:41:ARG:NH2	2.23	0.53
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.90	0.53
1:A:462:LYS:HD2	9:A:1085:HOH:O	2.09	0.53
1:A:549:PHE:O	1:A:553:ILE:HG12	2.09	0.53
1:A:364:ASN:O	1:A:365:TYR:HB2	2.09	0.52
1:A:188:ASP:O	1:A:189:ALA:HB3	2.10	0.52
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.45	0.52
1:A:8:ALA:HB1	9:A:1226:HOH:O	2.09	0.51
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.91	0.51
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.92	0.51
1:A:381:PHE:CZ	4:A:596:AIN:C4	2.92	0.51
1:A:239:PHE:CE1	1:A:427:LYS:HG2	2.46	0.51
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.40	0.51
1:A:120:GLY:HA2	1:A:123:GLU:HB2	1.93	0.50
1:A:370:PRO:HG2	1:A:371:GLU:HG3	1.93	0.50
1:A:62:THR:HG21	1:A:64:ARG:NH1	2.27	0.50
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:HD2	1:A:248:CYS:SG	2.52	0.50
1:A:519:PHE:HD1	1:A:522:ILE:HD11	1.73	0.50
1:A:62:THR:HG21	1:A:64:ARG:HH11	1.77	0.49
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.76	0.49
1:A:146:LYS:HG3	1:A:147:ASN:ND2	2.28	0.49
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.94	0.49
1:A:551:ARG:NH2	1:A:555:ASP:OD1	2.36	0.48
1:A:370:PRO:HG2	1:A:371:GLU:H	1.78	0.48
1:A:142:ILE:CD1	1:A:436:ILE:HD13	2.44	0.48
1:A:360:ARG:C	1:A:361:LEU:HD23	2.34	0.48
1:A:132:TYR:HB3	9:A:1243:HOH:O	2.13	0.48
1:A:257:SER:O	1:A:381:PHE:HA	2.14	0.47
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.14	0.47
4:A:596:AIN:C1	8:A:605:HEM:HMA2	2.43	0.47
1:A:203:LEU:HD21	1:A:252:GLY:HA2	1.96	0.47
1:A:588:SER:N	1:A:589:PRO:CD	2.76	0.47
8:A:605:HEM:HMC2	8:A:605:HEM:HBC2	1.96	0.47
1:A:272:GLU:O	1:A:276:LEU:HB2	2.14	0.47
1:A:134:ILE:HD11	9:A:1243:HOH:O	2.14	0.47
1:A:36:LEU:HG	1:A:337:PRO:HD2	1.97	0.47
1:A:549:PHE:CE2	1:A:553:ILE:HD11	2.50	0.47
1:A:313:LEU:N	1:A:314:PRO:CD	2.78	0.47
1:A:168:PRO:HB3	1:A:170:PRO:HD2	1.97	0.46
1:A:478:LYS:HB2	1:A:478:LYS:HE3	1.82	0.46
1:A:8:ALA:CB	1:A:9:PRO:CD	2.78	0.46
1:A:187:LEU:HD21	1:A:304:ILE:HG22	1.98	0.46
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.50	0.46
1:A:242:THR:O	1:A:245:ARG:NH2	2.48	0.46
1:A:231:ASN:HB3	9:A:1099:HOH:O	2.15	0.46
1:A:166:VAL:HB	1:A:167:CYS:H	1.48	0.46
1:A:381:PHE:CZ	4:A:596:AIN:H4	2.46	0.46
1:A:106:ILE:CD1	1:A:265:ALA:HB1	2.35	0.45
1:A:182:ALA:HB1	9:A:1064:HOH:O	2.16	0.45
1:A:32:ARG:HH11	1:A:32:ARG:CB	2.20	0.45
1:A:541:ARG:NH2	9:A:1102:HOH:O	2.49	0.45
1:A:9:PRO:HG2	1:A:167:CYS:O	2.17	0.45
1:A:352:MET:HG2	1:A:413:VAL:HG23	1.99	0.45
1:A:342:VAL:HG12	7:A:608:IOD:I	2.87	0.45
1:A:126:LYS:NZ	9:A:1196:HOH:O	2.46	0.45
1:A:574:HIS:HB2	9:A:1228:HOH:O	2.17	0.45
1:A:461:PRO:HG3	1:A:470:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:HB3	1:A:119:LEU:H	1.56	0.44
1:A:581:THR:O	1:A:581:THR:HG23	2.18	0.44
1:A:98:LEU:HD13	1:A:399:LEU:HD23	1.99	0.43
1:A:10:VAL:HG21	1:A:41:ARG:CZ	2.48	0.43
1:A:424:PRO:HD3	4:A:596:AIN:C5	2.32	0.43
4:A:596:AIN:C1	8:A:605:HEM:CMA	2.94	0.43
1:A:581:THR:O	1:A:581:THR:CG2	2.65	0.43
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.46	0.43
2:A:1005:NAG:C6	2:A:1006:NAG:C1	2.97	0.43
1:A:194:GLY:HA2	1:A:252:GLY:O	2.18	0.43
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.78	0.43
1:A:361:LEU:HB3	1:A:365:TYR:HA	2.00	0.43
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.22	0.42
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.42
1:A:432:ASP:O	1:A:436:ILE:HG12	2.19	0.42
1:A:588:SER:OG	1:A:589:PRO:HD3	2.18	0.42
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.55	0.42
1:A:407:MET:HB3	1:A:501:MET:HE2	2.01	0.42
1:A:148:ASP:O	1:A:151:LEU:HB2	2.19	0.42
1:A:150:LYS:O	1:A:154:GLN:N	2.48	0.42
1:A:32:ARG:CB	1:A:32:ARG:NH1	2.82	0.42
1:A:150:LYS:HZ2	1:A:154:GLN:HE22	1.68	0.42
1:A:202:ARG:HG2	1:A:202:ARG:O	2.19	0.42
1:A:503:GLU:HG3	9:A:1268:HOH:O	2.19	0.42
1:A:288:ASN:O	1:A:292:LEU:CD2	2.68	0.42
1:A:175:LEU:CD2	1:A:176:ALA:N	2.68	0.42
4:A:596:AIN:H1	8:A:605:HEM:C3A	2.54	0.41
1:A:364:ASN:O	1:A:366:GLN:NE2	2.47	0.41
1:A:468:GLN:O	1:A:472:LYS:N	2.53	0.41
1:A:423:GLN:HA	1:A:424:PRO:HD2	1.68	0.41
2:A:1001:NAG:H61	2:A:1002:NAG:C1	2.49	0.41
2:A:1006:NAG:H4	2:A:1009:MAN:H2	1.55	0.41
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.55	0.41
1:A:419:ASN:O	1:A:430:GLY:HA2	2.20	0.41
1:A:124:HIS:O	1:A:128:GLN:N	2.42	0.41
1:A:297:ARG:HG2	9:A:1192:HOH:O	2.21	0.41
1:A:511:LEU:HA	1:A:511:LEU:HD12	1.79	0.41
1:A:146:LYS:HG3	1:A:147:ASN:N	2.35	0.41
1:A:63:GLN:NE2	1:A:63:GLN:N	2.68	0.41
1:A:264:THR:HG23	1:A:392:ILE:HB	2.02	0.41
8:A:605:HEM:HBB2	8:A:605:HEM:CMB	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HB2	1:A:212:LEU:HG	2.04	0.40
1:A:348:ARG:NH1	8:A:605:HEM:HBA2	2.35	0.40
1:A:146:LYS:CG	1:A:147:ASN:ND2	2.85	0.40
1:A:480:LEU:HA	1:A:480:LEU:HD12	1.93	0.40
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.56	0.40
1:A:180:ILE:HG22	1:A:181:ASN:N	2.36	0.40
1:A:536:PHE:HB2	9:A:1208:HOH:O	2.21	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%)	542 (92%)	39 (7%)	11 (2%)	10	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	174	SER
1	A	593	ARG
1	A	170	PRO
1	A	18	ASN
1	A	9	PRO
1	A	13	VAL
1	A	370	PRO

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%)	471 (91%)	46 (9%)	12	23

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	VAL
1	A	6	CYS
1	A	9	PRO
1	A	13	VAL
1	A	16	ASP
1	A	18	ASN
1	A	32	ARG
1	A	57	LEU
1	A	63	GLN
1	A	91	VAL
1	A	98	LEU
1	A	118	GLU
1	A	124	HIS
1	A	146	LYS
1	A	147	ASN
1	A	153	THR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	203	LEU
1	A	209	PRO
1	A	232	LYS
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	278	ARG
1	A	283	LEU
1	A	292	LEU
1	A	333	ASN

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Mol	Chain	Res	Type
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	464	LEU
1	A	465	LYS
1	A	471	LEU
1	A	480	LEU
1	A	511	LEU
1	A	520	GLN
1	A	522	ILE
1	A	539	LYS
1	A	548	SER
1	A	551	ARG
1	A	581	THR
1	A	583	ASP
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	147	ASN
1	A	154	GLN
1	A	217	GLN
1	A	333	ASN
1	A	364	ASN
1	A	423	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	SEP	A	198	1	8,9,10	1.63	2 (25%)	8,12,14	3.65	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	OG-CB	2.18	1.53	1.44
1	A	198	SEP	P-OG	3.13	1.70	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	3.10	115.03	107.14
1	A	198	SEP	OG-CB-CA	9.55	116.42	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

5.5 Carbohydrates (i)

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	NAG	A	1001	1,2	14,14,15	0.68	0	15,19,21	1.11	1 (6%)
2	NAG	A	1002	2	14,14,15	0.87	1 (7%)	15,19,21	0.82	1 (6%)
3	NAG	A	1003	1,3	14,14,15	0.53	0	15,19,21	0.79	1 (6%)
3	NAG	A	1004	3	14,14,15	0.57	0	15,19,21	1.15	1 (6%)
2	NAG	A	1005	1,2	14,14,15	0.50	0	15,19,21	0.92	1 (6%)
2	NAG	A	1006	2	14,14,15	0.78	0	15,19,21	1.49	3 (20%)
3	NAG	A	1007	1,3	14,14,15	1.47	2 (14%)	15,19,21	0.74	0
3	NAG	A	1008	3	14,14,15	1.44	1 (7%)	15,19,21	1.39	2 (13%)
2	MAN	A	1009	2	11,11,12	0.72	0	14,15,17	1.42	1 (7%)
2	MAN	A	1010	2	11,11,12	0.76	0	14,15,17	0.94	1 (7%)

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	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1003	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	3	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	3	-	0/6/23/26	0/1/1/1
2	MAN	A	1009	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1010	2	-	0/2/19/22	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	NAG	C1-C2	2.02	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	NAG	C3-C2	2.57	1.58	1.52
3	A	1007	NAG	C1-C2	3.82	1.57	1.52
3	A	1008	NAG	C1-C2	4.85	1.59	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1006	NAG	C4-C3-C2	-3.58	105.66	111.23
2	A	1001	NAG	C2-N2-C7	-2.65	119.64	123.04
3	A	1008	NAG	C3-C2-N2	-2.60	104.33	110.56
2	A	1006	NAG	C2-N2-C7	-2.58	119.72	123.04
3	A	1004	NAG	C2-N2-C7	-2.46	119.88	123.04
3	A	1003	NAG	C2-N2-C7	-2.18	120.24	123.04
2	A	1005	NAG	C2-N2-C7	-2.17	120.25	123.04
2	A	1002	NAG	C2-N2-C7	-2.16	120.26	123.04
2	A	1010	MAN	C1-C2-C3	2.23	112.18	109.54
2	A	1006	NAG	C1-O5-C5	2.89	115.91	112.25
3	A	1008	NAG	C1-O5-C5	3.55	116.75	112.25
2	A	1009	MAN	C1-C2-C3	4.64	115.03	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1010	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
2	A	1002	NAG	1	0
2	A	1005	NAG	2	0
2	A	1006	NAG	3	0
2	A	1009	MAN	2	0

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	AIN	A	596	-	10,13,13	4.16	5 (50%)	13,17,17	4.28	9 (69%)
8	HEM	A	605	1,9	30,50,50	2.19	9 (30%)	24,82,82	2.20	7 (29%)
6	SCN	A	607	-	2,2,2	2.49	1 (50%)	1,1,1	0.13	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
4	AIN	A	596	-	-	0/4/8/8	0/1/1/1
8	HEM	A	605	1,9	-	0/10/54/54	0/0/8/8
6	SCN	A	607	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	605	HEM	C3B-C4B	-5.58	1.46	1.51
8	A	605	HEM	C2C-C1C	-4.78	1.43	1.52
8	A	605	HEM	C1A-CHA	-2.12	1.34	1.39
8	A	605	HEM	CAD-C3D	2.07	1.58	1.54
8	A	605	HEM	CMC-C2C	2.90	1.59	1.53
8	A	605	HEM	FE-NC	2.97	2.07	1.95
6	A	607	SCN	C-S	3.43	1.85	1.63
8	A	605	HEM	C3C-CAC	3.44	1.57	1.51
8	A	605	HEM	C3B-CAB	3.60	1.58	1.51
8	A	605	HEM	C4C-NC	4.12	1.41	1.36
4	A	596	AIN	O3-C8	4.68	1.51	1.36
4	A	596	AIN	C6-C1	5.04	1.49	1.38
4	A	596	AIN	C1-C2	6.03	1.52	1.39
4	A	596	AIN	C3-C2	6.14	1.51	1.40
4	A	596	AIN	C4-C3	6.55	1.51	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	596	AIN	O3-C8-C9	-5.75	98.33	110.90
4	A	596	AIN	C5-C6-C1	-3.10	115.65	120.19
4	A	596	AIN	C4-C3-C7	-3.03	115.57	120.23
4	A	596	AIN	C1-C2-C3	-2.67	116.26	121.19
8	A	605	HEM	CBD-CAD-C3D	-2.66	105.81	113.55
4	A	596	AIN	O3-C2-C1	2.04	124.04	118.77
8	A	605	HEM	CBA-CAA-C2A	2.32	116.69	112.53
4	A	596	AIN	C6-C5-C4	2.37	123.65	120.19
4	A	596	AIN	C6-C1-C2	2.45	124.32	119.79
8	A	605	HEM	CMD-C2D-C3D	2.84	126.89	114.35
8	A	605	HEM	CMB-C2B-C3B	3.50	125.27	116.53
8	A	605	HEM	CAD-C3D-C2D	4.42	125.93	113.22
8	A	605	HEM	CAD-C3D-C4D	4.88	129.69	112.47
8	A	605	HEM	CMC-C2C-C3C	5.21	129.55	116.53
4	A	596	AIN	O3-C8-O4	8.26	141.63	122.37
4	A	596	AIN	C2-O3-C8	9.45	139.46	117.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	596	AIN	19	0
8	A	605	HEM	9	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	594/595 (99%)	0.40	55 (9%)	11	11	12, 30, 75, 100	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	10.7
1	A	5	GLY	10.5
1	A	7	GLY	10.0
1	A	595	ASN	9.3
1	A	8	ALA	9.2
1	A	121	SER	8.4
1	A	119	LEU	8.4
1	A	4	VAL	7.4
1	A	170	PRO	7.4
1	A	122	ASN	7.2
1	A	594	GLU	7.1
1	A	6	CYS	6.9
1	A	593	ARG	6.2
1	A	10	VAL	5.9
1	A	120	GLY	5.7
1	A	3	GLU	5.5
1	A	173	GLN	5.3
1	A	169	THR	4.8
1	A	171	PRO	4.8
1	A	172	TYR	4.6
1	A	63	GLN	4.6
1	A	231	ASN	4.5
1	A	174	SER	4.4
1	A	118	GLU	4.4
1	A	1	SER	4.2
1	A	574	HIS	4.0
1	A	15	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	GLU	3.8
1	A	124	HIS	3.7
1	A	131	GLU	3.6
1	A	592	SER	3.5
1	A	13	VAL	3.4
1	A	16	ASP	3.3
1	A	12	LEU	3.0
1	A	167	CYS	2.8
1	A	146	LYS	2.7
1	A	125	SER	2.6
1	A	14	LYS	2.6
1	A	232	LYS	2.6
1	A	9	PRO	2.5
1	A	168	PRO	2.5
1	A	147	ASN	2.5
1	A	322	GLN	2.5
1	A	588	SER	2.5
1	A	370	PRO	2.3
1	A	117	THR	2.2
1	A	424	PRO	2.2
1	A	64	ARG	2.2
1	A	17	GLU	2.2
1	A	11	PRO	2.1
1	A	366	GLN	2.0
1	A	89	GLU	2.0
1	A	127	THR	2.0
1	A	128	GLN	2.0
1	A	425	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
1	SEP	A	198	10/11	0.92	0.22	-	28,32,44,48	0

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
2	NAG	A	1001	14/15	0.84	0.29	3.29	55,58,64,71	0
3	NAG	A	1003	14/15	0.91	0.20	0.42	42,49,52,56	0
2	NAG	A	1005	14/15	0.91	0.16	-0.42	52,55,57,62	0
2	NAG	A	1002	14/15	0.67	0.45	-	78,83,85,88	0
2	MAN	A	1010	11/12	0.55	0.54	-	90,91,93,93	0
3	NAG	A	1007	14/15	0.65	0.44	-	58,64,67,74	0
3	NAG	A	1008	14/15	0.48	0.56	-	79,83,86,86	0
2	MAN	A	1009	11/12	0.57	0.55	-	80,80,81,82	0
3	NAG	A	1004	14/15	0.73	0.46	-	61,65,67,67	0
2	NAG	A	1006	14/15	0.77	0.43	-	67,69,73,77	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
4	AIN	A	596	13/13	0.81	0.38	3.47	63,67,73,74	0
8	HEM	A	605	43/43	0.95	0.14	-0.32	8,16,21,23	0
5	CA	A	606	1/1	0.96	0.14	-0.35	16,16,16,16	0
6	SCN	A	607	3/3	0.84	0.14	-1.38	32,32,35,41	0
7	IOD	A	609	1/1	0.98	0.07	-1.40	90,90,90,90	0
7	IOD	A	611	1/1	0.98	0.09	-1.92	79,79,79,79	0
7	IOD	A	612	1/1	0.95	0.09	-2.57	95,95,95,95	0
7	IOD	A	608	1/1	1.00	0.07	-2.58	26,26,26,26	0
7	IOD	A	613	1/1	0.99	0.05	-4.33	70,70,70,70	0
7	IOD	A	610	1/1	0.95	0.12	-	100,100,100,100	0
7	IOD	A	614	1/1	0.98	0.07	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.