Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:53 AM GMT

PDB ID	:	2YP1
Title	:	Crystallization of a 45 kDa peroxygenase- peroxidase from the mushroom Agrocybe aegerita and structure determination by SAD utilizing only the haem iron
Authors	:	Piontek, K.; Strittmatter, E.; Ullrich, R.; Plattner, D.A.; Hofrichter, M.
Deposited on	:	2012-10-29
Resolution	:	2.31 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 (1)) were used in the production of this report:

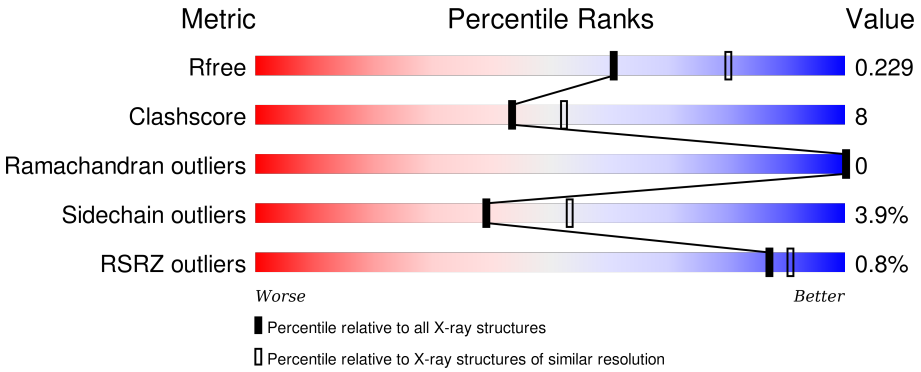
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	325	84% 14%
1	B	325	83% 15%
1	C	325	% 88% 11%
1	D	325	2% 78% 20%

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
11	NAG	D	391	-	-	-	X
5	NAG	A	372	-	-	-	X
5	NAG	B	361	-	-	-	X
6	NAG	C	372	-	-	-	X
6	NAG	C	391	-	-	-	X
7	NAG	A	391	-	-	-	X
8	ACT	A	1327	-	-	-	X
8	ACT	B	1328	-	-	-	X
8	ACT	C	1329	-	-	-	X
8	ACT	D	1327	-	-	-	X
9	SO4	A	1331	-	-	X	X
9	SO4	B	1331	-	-	X	X

2 Entry composition

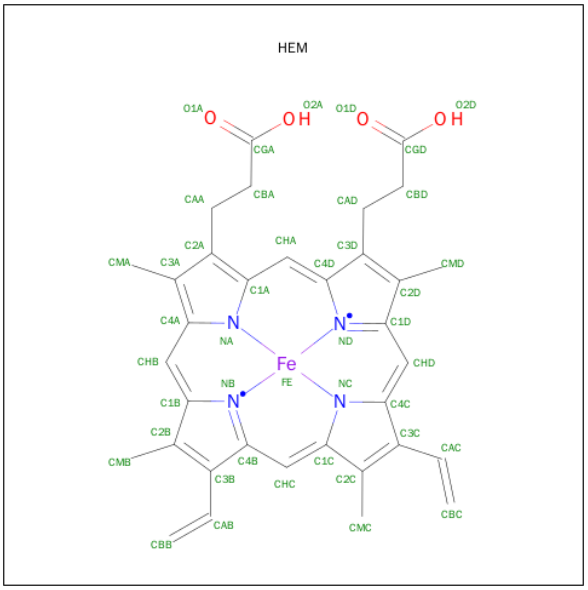
There are 12 unique types of molecules in this entry. The entry contains 12290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AROMATIC PEROXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2506	1589	434	475	8			
1	B	324	Total	C	N	O	S	0	4	0
			2537	1608	442	479	8			
1	C	325	Total	C	N	O	S	0	1	0
			2526	1599	440	479	8			
1	D	323	Total	C	N	O	S	0	1	0
			2507	1590	435	474	8			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total C N O 72 40 2 30	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total C N O 61 34 2 25	0	0
5	B	5	Total C N O 61 34 2 25	0	0

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

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

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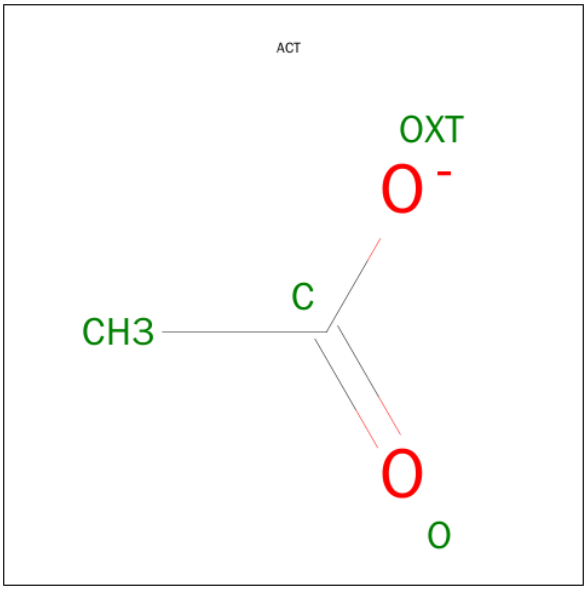
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total C N O 28 16 2 10	0	0
6	C	2	Total C N O 28 16 2 10	0	0
6	C	2	Total C N O 28 16 2 10	0	0
6	C	2	Total C N O 28 16 2 10	0	0
6	D	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	8	Total C N O 94 52 2 40	0	0
7	B	8	Total C N O 94 52 2 40	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

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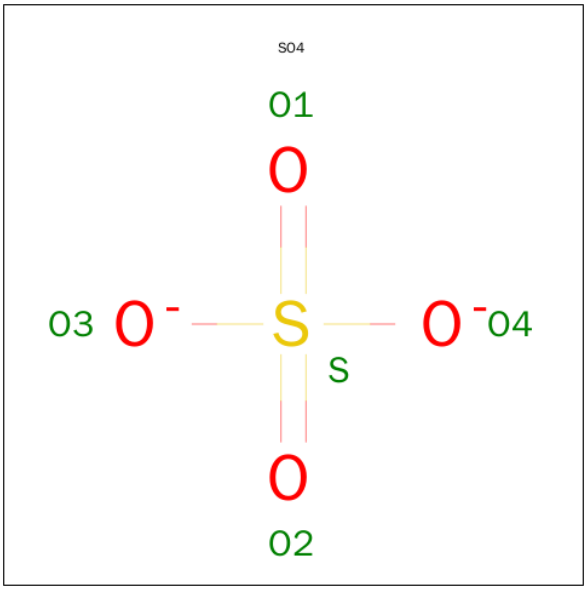
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0

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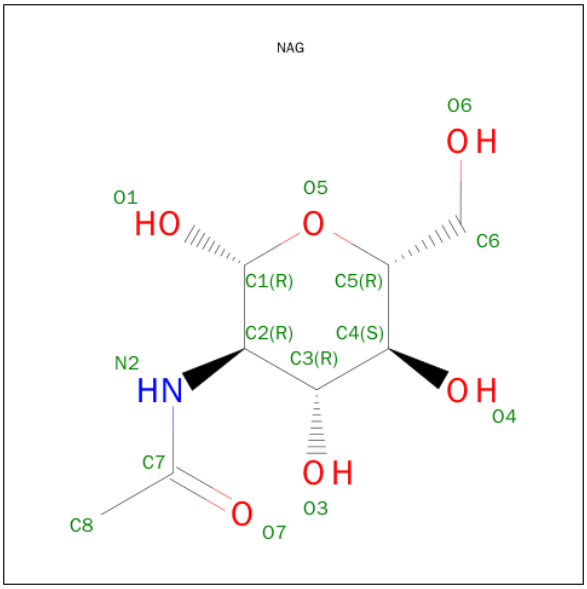
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is water.

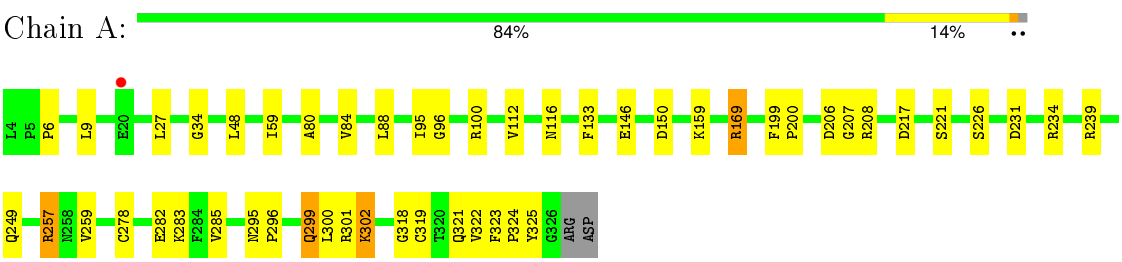
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	327	Total O 327 327	0	0
12	B	369	Total O 369 369	0	0
12	C	291	Total O 291 291	0	0
12	D	198	Total O 198 198	0	0

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.

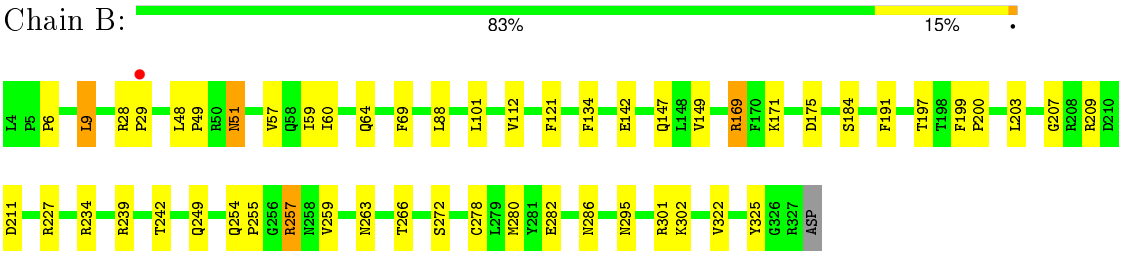
- Molecule 1: AROMATIC PEROXYGENASE

Chain A:



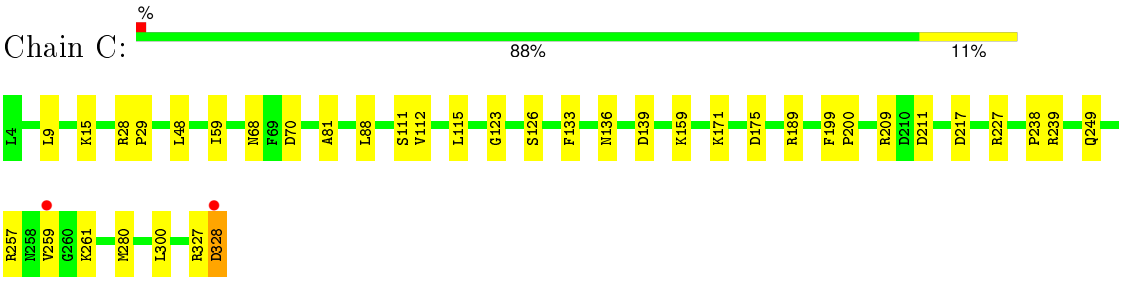
- Molecule 1: AROMATIC PEROXYGENASE

Chain B:



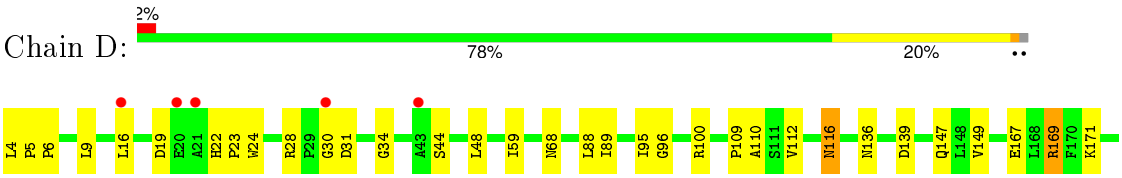
- Molecule 1: AROMATIC PEROXYGENASE

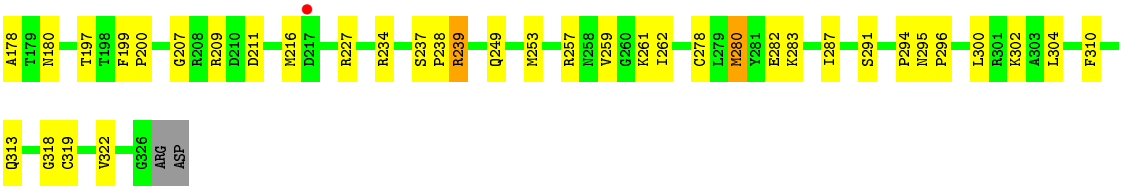
Chain C:



- Molecule 1: AROMATIC PEROXYGENASE

Chain D:




A178
T179
N180
T197
T198
F199
P200
G207
R208
R209
D210
D211
M216
D217
R227
R234
S237
P238
R239
Q249
M253
R257
N258
V259
G260
K261
I262
C278
L279
M280
Y281
E282
K283
I287
S291
P294
N295
P296
L300
R301
K302
A303
L304
F310
Q313
G318
C319
V322
G326
ARG
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.75Å 144.88Å 134.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.31 48.93 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-2.31) 99.4 (48.93-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.01 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.230 0.177 , 0.229	Depositor DCC
R_{free} test set	4841 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 97006 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12290	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, SO4, ACT, HEM, 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	0.48	0/2579	0.56	0/3512
1	B	0.52	0/2619	0.57	0/3564
1	C	0.52	0/2599	0.53	0/3538
1	D	0.44	0/2580	0.51	0/3513
All	All	0.49	0/10377	0.54	0/14127

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	30	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2386	40	0
1	B	2537	0	2426	41	0
1	C	2526	0	2405	20	0
1	D	2507	0	2390	52	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	72	0	61	2	0
5	A	61	0	52	2	0
5	B	61	0	52	2	0
6	A	56	0	50	6	0
6	B	84	0	75	2	0
6	C	84	0	75	0	0
6	D	28	0	25	0	0
7	A	94	0	79	4	0
7	B	94	0	79	2	0
8	A	4	0	3	0	0
8	B	4	0	3	0	0
8	C	8	0	6	0	0
8	D	4	0	3	0	0
9	A	20	0	0	2	0
9	B	15	0	0	2	0
9	C	20	0	0	0	0
9	D	10	0	0	2	0
10	C	39	0	34	0	0
10	D	39	0	34	0	0
11	C	14	0	13	1	0
11	D	42	0	39	0	0
12	A	327	0	0	9	0
12	B	369	0	0	13	0
12	C	291	0	0	5	0
12	D	198	0	0	6	0
All	All	12290	0	10410	174	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 8.

All (174) 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)
2:D:350:HEM:HMC2	2:D:350:HEM:HBC2	1.29	1.11
1:A:259:VAL:O	1:A:259:VAL:HG23	1.68	0.94
1:A:299:GLN:HG2	12:A:2271:HOH:O	1.73	0.88
1:A:299:GLN:NE2	12:A:2273:HOH:O	2.07	0.88
1:D:89:ILE:HD11	1:D:300:LEU:HD13	1.56	0.88
2:D:350:HEM:HBC2	2:D:350:HEM:CMC	2.02	0.85
1:D:100:ARG:N	9:D:1328:SO4:O1	2.13	0.81
1:D:259:VAL:CG1	1:D:259:VAL:O	2.29	0.81
1:B:278:CYS:HB2	9:B:1331:SO4:O2	1.81	0.80
7:A:394:MAN:C6	7:A:395:MAN:H3	2.11	0.80
1:D:296:PRO:HB2	1:D:300:LEU:HB3	1.65	0.79
7:A:394:MAN:H62	7:A:395:MAN:H3	1.66	0.76
2:A:350:HEM:HHD	2:A:350:HEM:HBC2	1.68	0.74
1:B:134:PHE:CD1	5:B:362:NAG:H62	2.21	0.74
1:B:282:GLU:HG3	1:B:322:VAL:HG11	1.69	0.74
1:D:282:GLU:HG2	1:D:322:VAL:HG11	1.71	0.71
1:B:302:LYS:HE3	12:B:2319:HOH:O	1.91	0.70
6:B:372:NAG:O6	12:B:2351:HOH:O	2.08	0.70
1:A:217[A]:ASP:OD2	12:A:2203:HOH:O	2.08	0.69
1:B:254:GLN:NE2	12:B:2267:HOH:O	2.25	0.69
7:B:396:MAN:H62	7:B:398:MAN:H3	1.74	0.69
1:B:259:VAL:HG12	1:B:259:VAL:O	1.90	0.69
1:A:133:PHE:CE1	6:A:381:NAG:H82	2.27	0.68
1:D:5:PRO:O	12:D:2003:HOH:O	2.11	0.68
1:D:31:ASP:N	12:D:2024:HOH:O	2.27	0.67
1:D:259:VAL:HG13	1:D:259:VAL:O	1.94	0.67
1:A:112:VAL:HG12	1:A:112:VAL:O	1.97	0.65
1:D:167:GLU:OE2	12:D:2103:HOH:O	2.14	0.64
1:A:48:LEU:HD21	1:A:59:ILE:HA	1.80	0.64
1:B:263:ASN:ND2	12:B:2277:HOH:O	2.16	0.63
1:D:147:GLN:OE1	1:D:171:LYS:HE3	1.98	0.63
1:D:88:LEU:HD23	1:D:304:LEU:HG	1.80	0.63
1:D:291:SER:HB2	12:D:2158:HOH:O	1.99	0.62
1:A:249:GLN:NE2	1:C:249:GLN:OE1	2.33	0.61
1:C:227:ARG:CD	12:C:2199:HOH:O	2.49	0.61
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.66	0.60
1:A:206:ASP:OD2	12:A:2183:HOH:O	2.16	0.60
1:D:96:GLY:HA2	1:D:116:ASN:ND2	2.17	0.59
1:C:259:VAL:HG12	1:C:259:VAL:O	2.02	0.58
1:B:249:GLN:OE1	12:B:2261:HOH:O	2.17	0.58
1:D:310:PHE:O	1:D:313[A]:GLN:HB2	2.03	0.58
1:B:278:CYS:HB2	9:B:1331:SO4:S	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLN:NE2	1:B:171:LYS:HE2	2.19	0.57
1:C:327:ARG:O	1:C:328:ASP:HB2	2.05	0.57
1:C:123:GLY:HA3	1:C:189:ARG:HD3	1.87	0.57
1:C:209:ARG:HD2	1:C:211:ASP:OD2	2.05	0.56
2:C:350:HEM:HBC2	2:C:350:HEM:CMC	2.36	0.56
1:C:171:LYS:HE2	1:C:175:ASP:OD1	2.05	0.56
1:A:208:ARG:NH2	1:A:231:ASP:O	2.39	0.56
1:B:184:SER:HA	1:B:257[A]:ARG:HB3	1.88	0.56
1:D:4:LEU:N	12:D:2002:HOH:O	2.38	0.56
1:A:259:VAL:O	1:A:259:VAL:CG2	2.42	0.55
2:A:350:HEM:HHD	2:A:350:HEM:CBC	2.37	0.55
1:D:5:PRO:HD3	1:D:310:PHE:CE1	2.41	0.55
1:D:209:ARG:HD2	1:D:211:ASP:OD2	2.07	0.54
7:B:396:MAN:H62	7:B:398:MAN:C3	2.36	0.54
1:B:254:GLN:HB3	1:B:255:PRO:HD2	1.89	0.54
6:A:411:NAG:C6	6:A:412:NAG:C1	2.83	0.54
1:C:48:LEU:HD21	1:C:59:ILE:HA	1.90	0.54
12:B:2100:HOH:O	1:D:313[B]:GLN:HG3	2.08	0.53
1:B:6:PRO:HD3	1:B:57:VAL:HG22	1.89	0.53
1:B:191:PHE:HB2	12:B:2090:HOH:O	2.07	0.53
1:D:180:ASN:C	1:D:180:ASN:OD1	2.45	0.53
1:A:296:PRO:HG2	1:A:301:ARG:HB2	1.89	0.53
1:D:16:LEU:HG	1:D:19:ASP:HB3	1.90	0.53
1:A:282:GLU:HG3	1:A:322:VAL:HG21	1.91	0.53
1:D:278:CYS:HB2	9:D:1329:SO4:O3	2.09	0.53
6:A:381:NAG:H61	6:A:382:NAG:C7	2.39	0.52
6:A:411:NAG:H62	6:A:412:NAG:C1	2.39	0.52
1:A:100:ARG:HD2	12:A:2099:HOH:O	2.10	0.52
1:B:207:GLY:HA3	1:B:234:ARG:O	2.10	0.52
2:D:350:HEM:HMC2	2:D:350:HEM:CBC	2.20	0.51
1:A:207:GLY:HA3	1:A:234:ARG:O	2.10	0.51
7:A:394:MAN:C6	7:A:395:MAN:C3	2.67	0.51
2:B:350:HEM:HHC	2:B:350:HEM:HBB2	1.91	0.51
1:D:68:ASN:O	1:D:238:PRO:HA	2.10	0.51
1:A:278:CYS:HB2	9:A:1331:SO4:O1	2.10	0.51
1:A:285:VAL:CG1	1:A:324:PRO:HD3	2.41	0.51
2:A:350:HEM:HBC2	2:A:350:HEM:CHD	2.37	0.51
1:D:282:GLU:HG2	1:D:322:VAL:CG1	2.39	0.51
1:D:259:VAL:HG12	1:D:259:VAL:O	2.06	0.50
1:D:112:VAL:O	1:D:112:VAL:HG12	2.11	0.50
1:D:48:LEU:HD21	1:D:59:ILE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:NZ	12:A:2252:HOH:O	2.00	0.49
1:D:24:TRP:CG	1:D:227:ARG:HG3	2.47	0.49
1:B:9:LEU:HD13	1:B:64:GLN:HB3	1.94	0.49
1:B:48:LEU:HD21	1:B:59:ILE:HA	1.94	0.49
2:C:350:HEM:HBC2	2:C:350:HEM:HMC1	1.95	0.49
6:A:411:NAG:H62	6:A:412:NAG:O5	2.13	0.49
1:D:237:SER:O	1:D:239:ARG:NE	2.43	0.49
1:A:27:LEU:N	12:A:2028:HOH:O	2.30	0.49
1:B:48:LEU:O	1:B:49:PRO:C	2.51	0.49
1:B:112:VAL:HG12	1:B:112:VAL:O	2.11	0.48
1:C:126:SER:OG	2:C:350:HEM:O2A	2.31	0.48
1:C:227:ARG:HD2	12:C:2199:HOH:O	2.12	0.48
1:B:51:ASN:HD22	1:B:51:ASN:H	1.60	0.48
1:D:318:GLY:O	1:D:319:CYS:HB2	2.12	0.48
1:D:136:ASN:ND2	1:D:139:ASP:OD2	2.35	0.48
1:B:28:ARG:HB3	1:B:29:PRO:CD	2.44	0.47
1:D:199:PHE:N	1:D:200:PRO:CD	2.77	0.47
1:D:22:HIS:N	1:D:23:PRO:CD	2.77	0.47
1:D:28:ARG:O	12:D:2024:HOH:O	2.20	0.47
1:B:259:VAL:O	1:B:259:VAL:CG1	2.61	0.47
1:B:266:THR:HA	12:B:2278:HOH:O	2.14	0.47
1:D:207:GLY:HA3	1:D:234:ARG:O	2.14	0.47
1:B:60:ILE:O	1:B:64:GLN:HG3	2.15	0.47
1:C:28:ARG:HB3	1:C:29:PRO:HD2	1.96	0.47
1:A:301:ARG:NH2	1:A:325:TYR:O	2.43	0.47
1:B:249:GLN:NE2	1:D:249:GLN:OE1	2.44	0.47
4:A:363:BMA:C6	4:A:366:MAN:O2	2.62	0.47
1:A:133:PHE:CD1	6:A:381:NAG:H82	2.49	0.46
1:B:203:LEU:HD13	2:B:350:HEM:CBC	2.45	0.46
1:B:171:LYS:HE3	1:B:175:ASP:OD1	2.15	0.46
1:A:257:ARG:HD3	1:A:257:ARG:N	2.30	0.46
1:C:111:SER:HB2	12:C:2111:HOH:O	2.16	0.46
1:B:301:ARG:NH1	1:B:325:TYR:O	2.50	0.45
1:A:199:PHE:HB3	2:A:350:HEM:HBC2	1.99	0.45
1:B:191:PHE:HD1	12:B:2090:HOH:O	2.00	0.45
1:A:318:GLY:O	1:A:319:CYS:HB2	2.17	0.45
5:B:364:MAN:O5	5:B:365:MAN:H2	2.17	0.45
1:B:227:ARG:NH2	12:B:2241:HOH:O	2.17	0.45
1:A:80:ALA:O	1:A:84:VAL:HG22	2.17	0.44
1:A:257:ARG:CD	1:A:257:ARG:N	2.81	0.44
5:A:373:BMA:H61	5:A:374:MAN:C5	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:HA	1:A:302:LYS:HD2	1.48	0.44
1:C:189:ARG:HA	12:C:2128:HOH:O	2.17	0.44
1:B:203:LEU:HD13	2:B:350:HEM:HBC2	1.99	0.44
1:B:28:ARG:HE	1:B:28:ARG:HB2	1.57	0.43
1:D:280:MET:C	1:D:280:MET:HE3	2.39	0.43
1:D:253:MET:CE	1:D:253:MET:HA	2.48	0.43
7:A:394:MAN:H61	7:A:395:MAN:H2	1.37	0.43
1:C:81:ALA:HB1	1:C:115:LEU:HD21	2.00	0.43
1:D:149:VAL:HG22	1:D:216:MET:SD	2.58	0.43
1:A:146:GLU:HG2	1:B:149:VAL:HG11	2.00	0.43
1:C:136:ASN:ND2	1:C:139:ASP:OD2	2.45	0.43
1:D:109:PRO:O	1:D:110:ALA:C	2.56	0.43
1:C:68:ASN:O	1:C:238:PRO:HA	2.19	0.43
1:A:34:GLY:HA3	1:A:95:ILE:O	2.19	0.43
1:D:24:TRP:HA	1:D:44:SER:O	2.18	0.43
1:D:280:MET:HE3	1:D:280:MET:O	2.19	0.42
1:B:209:ARG:HD2	1:B:211:ASP:OD2	2.18	0.42
1:D:283:LYS:O	1:D:287:ILE:HB	2.19	0.42
1:A:217[A]:ASP:OD1	12:A:2201:HOH:O	2.21	0.42
1:D:5:PRO:HA	1:D:6:PRO:HD3	1.90	0.42
1:D:280:MET:C	1:D:280:MET:CE	2.88	0.42
1:D:178:ALA:O	1:D:262:ILE:HB	2.19	0.42
1:A:278:CYS:HB2	9:A:1331:SO4:S	2.59	0.42
1:A:323:PHE:HA	1:A:324:PRO:HD2	1.92	0.42
1:C:199:PHE:N	1:C:200:PRO:CD	2.83	0.42
1:A:150:ASP:OD1	1:B:142:GLU:OE2	2.37	0.42
1:C:133:PHE:CE2	11:C:381:NAG:H82	2.55	0.42
4:A:361:NAG:H61	4:A:362:NAG:C1	2.49	0.42
1:B:199:PHE:N	1:B:200:PRO:CD	2.82	0.42
1:B:302:LYS:CE	12:B:2319:HOH:O	2.58	0.41
1:A:169:ARG:HD3	1:A:169:ARG:HH11	1.75	0.41
1:D:24:TRP:CD1	1:D:227:ARG:HG3	2.55	0.41
1:D:169:ARG:HB2	1:D:197:THR:HG21	2.01	0.41
1:D:294:PRO:O	1:D:295:ASN:HB3	2.20	0.41
1:D:34:GLY:HA3	1:D:95:ILE:O	2.20	0.41
1:A:96:GLY:HA2	1:A:116:ASN:ND2	2.35	0.41
1:D:209:ARG:HG2	1:D:211:ASP:OD2	2.21	0.41
1:D:89:ILE:CD1	1:D:300:LEU:HD13	2.40	0.41
1:A:199:PHE:HB3	2:A:350:HEM:CBC	2.50	0.41
6:B:371:NAG:H83	1:D:278:CYS:SG	2.61	0.41
1:A:321:GLN:HG2	1:A:323:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:HG22	12:B:2259:HOH:O	2.21	0.41
1:B:301:ARG:NH2	12:B:2316:HOH:O	2.53	0.41
1:B:169:ARG:HB2	1:B:197:THR:HG21	2.03	0.41
1:A:6:PRO:HG3	12:A:2057:HOH:O	2.21	0.40
5:A:373:BMA:H61	5:A:374:MAN:H5	2.03	0.40
1:B:272:SER:OG	1:B:280:MET:HB2	2.21	0.40
1:A:199:PHE:N	1:A:200:PRO:CD	2.84	0.40
1:C:112:VAL:O	1:C:112:VAL:HG12	2.21	0.40
1:C:15:LYS:HE3	12:C:2019:HOH:O	2.20	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	322/325 (99%)	301 (94%)	21 (6%)	0	100	100
1	B	326/325 (100%)	307 (94%)	19 (6%)	0	100	100
1	C	324/325 (100%)	304 (94%)	20 (6%)	0	100	100
1	D	322/325 (99%)	298 (92%)	24 (8%)	0	100	100
All	All	1294/1300 (100%)	1210 (94%)	84 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	270/271 (100%)	258 (96%)	12 (4%)	35 47
1	B	274/271 (101%)	262 (96%)	12 (4%)	35 47
1	C	272/271 (100%)	261 (96%)	11 (4%)	38 52
1	D	270/271 (100%)	262 (97%)	8 (3%)	48 65
All	All	1086/1084 (100%)	1043 (96%)	43 (4%)	39 52

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	88	LEU
1	A	159	LYS
1	A	169	ARG
1	A	221	SER
1	A	226	SER
1	A	239	ARG
1	A	257	ARG
1	A	295	ASN
1	A	299	GLN
1	A	300	LEU
1	A	302	LYS
1	B	9	LEU
1	B	51	ASN
1	B	69	PHE
1	B	88	LEU
1	B	101	LEU
1	B	121	PHE
1	B	169	ARG
1	B	239	ARG
1	B	257[A]	ARG
1	B	257[B]	ARG
1	B	286	ASN
1	B	295	ASN
1	C	9	LEU
1	C	70	ASP
1	C	88	LEU
1	C	159	LYS
1	C	217	ASP
1	C	239	ARG
1	C	257	ARG
1	C	261	LYS
1	C	280	MET

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Mol	Chain	Res	Type
1	C	300	LEU
1	C	328	ASP
1	D	9	LEU
1	D	116	ASN
1	D	169	ARG
1	D	239	ARG
1	D	257	ARG
1	D	261	LYS
1	D	280	MET
1	D	302	LYS

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	82	HIS
1	A	116	ASN
1	A	138	HIS
1	A	249	GLN
1	A	299	GLN
1	B	51	ASN
1	B	147	GLN
1	C	61	ASN
1	C	249	GLN
1	D	116	ASN
1	D	263	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

56 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	361	1,4	14,14,15	0.43	0	15,19,21	1.20	2 (13%)
4	NAG	A	362	4	14,14,15	0.44	0	15,19,21	0.92	0
4	BMA	A	363	4	11,11,12	0.53	0	14,15,17	1.01	1 (7%)
4	MAN	A	364	4	11,11,12	0.50	0	14,15,17	1.06	1 (7%)
4	MAN	A	365	4	11,11,12	0.57	0	14,15,17	0.86	1 (7%)
4	MAN	A	366	4	11,11,12	0.52	0	14,15,17	1.29	1 (7%)
5	NAG	A	371	1,5	14,14,15	0.66	0	15,19,21	1.06	0
5	NAG	A	372	5	14,14,15	0.77	0	15,19,21	1.15	1 (6%)
5	BMA	A	373	5	11,11,12	0.55	0	14,15,17	1.11	1 (7%)
5	MAN	A	374	5	11,11,12	0.57	0	14,15,17	1.07	1 (7%)
5	MAN	A	375	5	11,11,12	0.53	0	14,15,17	1.04	2 (14%)
6	NAG	A	381	1,6	14,14,15	0.50	0	15,19,21	1.28	2 (13%)
6	NAG	A	382	6	14,14,15	0.51	0	15,19,21	1.28	1 (6%)
7	NAG	A	391	1,7	14,14,15	0.62	0	15,19,21	1.81	2 (13%)
7	NAG	A	392	7	14,14,15	0.66	0	15,19,21	1.17	1 (6%)
7	BMA	A	393	7	11,11,12	0.66	0	14,15,17	1.29	2 (14%)
7	MAN	A	394	7	11,11,12	0.57	0	14,15,17	0.90	0
7	MAN	A	395	7	11,11,12	0.56	0	14,15,17	1.31	1 (7%)
7	MAN	A	396	7	11,11,12	0.51	0	14,15,17	1.00	0
7	MAN	A	397	7	11,11,12	0.57	0	14,15,17	1.27	3 (21%)
7	MAN	A	398	7	11,11,12	0.42	0	14,15,17	1.17	2 (14%)
6	NAG	A	411	1,6	14,14,15	0.48	0	15,19,21	2.02	5 (33%)
6	NAG	A	412	6	14,14,15	0.47	0	15,19,21	0.93	1 (6%)
5	NAG	B	361	1,5	14,14,15	0.58	0	15,19,21	1.13	1 (6%)
5	NAG	B	362	5	14,14,15	0.40	0	15,19,21	2.00	3 (20%)
5	BMA	B	363	5	11,11,12	0.55	0	14,15,17	1.38	2 (14%)
5	MAN	B	364	5	11,11,12	0.59	0	14,15,17	1.33	3 (21%)
5	MAN	B	365	5	11,11,12	0.60	0	14,15,17	1.69	2 (14%)
6	NAG	B	371	1,6	14,14,15	0.53	0	15,19,21	1.65	2 (13%)
6	NAG	B	372	6	14,14,15	0.57	0	15,19,21	1.07	1 (6%)
6	NAG	B	381	1,6	14,14,15	0.73	0	15,19,21	1.24	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	382	6	14,14,15	0.54	0	15,19,21	0.81	0
7	NAG	B	391	1,7	14,14,15	0.61	0	15,19,21	1.89	4 (26%)
7	NAG	B	392	7	14,14,15	0.71	0	15,19,21	1.22	2 (13%)
7	BMA	B	393	7	11,11,12	0.77	0	14,15,17	1.35	1 (7%)
7	MAN	B	394	7	11,11,12	0.64	0	14,15,17	1.23	1 (7%)
7	MAN	B	395	7	11,11,12	0.42	0	14,15,17	1.61	2 (14%)
7	MAN	B	396	7	11,11,12	0.52	0	14,15,17	2.11	4 (28%)
7	MAN	B	397	7	11,11,12	0.47	0	14,15,17	0.86	0
7	MAN	B	398	7	11,11,12	0.71	0	14,15,17	1.63	2 (14%)
6	NAG	B	411	1,6	14,14,15	0.54	0	15,19,21	0.88	1 (6%)
6	NAG	B	412	6	14,14,15	0.49	0	15,19,21	0.59	0
10	NAG	C	361	1,10	14,14,15	0.57	0	15,19,21	0.75	0
10	NAG	C	362	10	14,14,15	0.47	0	15,19,21	0.79	1 (6%)
10	BMA	C	363	10	11,11,12	0.50	0	14,15,17	2.07	4 (28%)
6	NAG	C	371	1,6	14,14,15	0.69	0	15,19,21	1.52	2 (13%)
6	NAG	C	372	6	14,14,15	0.50	0	15,19,21	1.18	1 (6%)
6	NAG	C	391	1,6	14,14,15	0.54	0	15,19,21	1.80	3 (20%)
6	NAG	C	392	6	14,14,15	0.47	0	15,19,21	0.73	0
6	NAG	C	411	1,6	14,14,15	0.57	0	15,19,21	0.80	1 (6%)
6	NAG	C	412	6	14,14,15	0.54	0	15,19,21	0.69	0
6	NAG	D	361	1,6	14,14,15	0.65	0	15,19,21	1.13	2 (13%)
6	NAG	D	362	6	14,14,15	0.47	0	15,19,21	0.59	0
10	NAG	D	371	1,10	14,14,15	0.62	0	15,19,21	1.05	1 (6%)
10	NAG	D	372	10	14,14,15	0.55	0	15,19,21	0.51	0
10	BMA	D	373	10	11,11,12	0.49	0	14,15,17	1.46	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	361	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	362	4	-	0/6/23/26	0/1/1/1
4	BMA	A	363	4	-	0/2/19/22	0/1/1/1
4	MAN	A	364	4	-	0/2/19/22	0/1/1/1
4	MAN	A	365	4	-	0/2/19/22	0/1/1/1
4	MAN	A	366	4	-	0/2/19/22	1/1/1/1
5	NAG	A	371	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	372	5	-	0/6/23/26	0/1/1/1
5	BMA	A	373	5	-	0/2/19/22	0/1/1/1
5	MAN	A	374	5	-	0/2/19/22	0/1/1/1
5	MAN	A	375	5	-	0/2/19/22	0/1/1/1
6	NAG	A	381	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	382	6	-	0/6/23/26	0/1/1/1
7	NAG	A	391	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	392	7	-	0/6/23/26	0/1/1/1
7	BMA	A	393	7	-	0/2/19/22	0/1/1/1
7	MAN	A	394	7	-	0/2/19/22	0/1/1/1
7	MAN	A	395	7	-	0/2/19/22	0/1/1/1
7	MAN	A	396	7	-	0/2/19/22	0/1/1/1
7	MAN	A	397	7	-	0/2/19/22	0/1/1/1
7	MAN	A	398	7	-	0/2/19/22	0/1/1/1
6	NAG	A	411	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	412	6	-	0/6/23/26	0/1/1/1
5	NAG	B	361	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	362	5	-	0/6/23/26	0/1/1/1
5	BMA	B	363	5	-	0/2/19/22	0/1/1/1
5	MAN	B	364	5	-	0/2/19/22	0/1/1/1
5	MAN	B	365	5	-	0/2/19/22	0/1/1/1
6	NAG	B	371	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	372	6	-	0/6/23/26	0/1/1/1
6	NAG	B	381	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	382	6	-	0/6/23/26	0/1/1/1
7	NAG	B	391	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	392	7	-	0/6/23/26	0/1/1/1
7	BMA	B	393	7	-	0/2/19/22	0/1/1/1
7	MAN	B	394	7	-	0/2/19/22	0/1/1/1
7	MAN	B	395	7	-	0/2/19/22	0/1/1/1
7	MAN	B	396	7	-	0/2/19/22	0/1/1/1
7	MAN	B	397	7	-	0/2/19/22	0/1/1/1
7	MAN	B	398	7	-	0/2/19/22	0/1/1/1
6	NAG	B	411	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	412	6	-	0/6/23/26	0/1/1/1
10	NAG	C	361	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	362	10	-	0/6/23/26	0/1/1/1
10	BMA	C	363	10	-	0/2/19/22	0/1/1/1
6	NAG	C	371	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	372	6	-	0/6/23/26	0/1/1/1
6	NAG	C	391	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	392	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	411	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	412	6	-	0/6/23/26	0/1/1/1
6	NAG	D	361	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	362	6	-	0/6/23/26	0/1/1/1
10	NAG	D	371	1,10	-	0/6/23/26	0/1/1/1
10	NAG	D	372	10	-	0/6/23/26	0/1/1/1
10	BMA	D	373	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	362	NAG	C2-N2-C7	-5.57	115.89	123.04
6	B	371	NAG	C2-N2-C7	-4.07	117.82	123.04
7	A	395	MAN	C1-C2-C3	-3.92	104.91	109.54
7	A	391	NAG	C2-N2-C7	-3.87	118.07	123.04
7	A	392	NAG	C1-O5-C5	-3.57	107.72	112.25
7	B	396	MAN	C6-C5-C4	-3.50	104.38	113.02
5	B	362	NAG	C4-C3-C2	-3.38	105.97	111.23
5	B	361	NAG	C2-N2-C7	-3.28	118.83	123.04
6	B	372	NAG	C1-O5-C5	-3.23	108.15	112.25
6	B	381	NAG	C2-N2-C7	-3.22	118.90	123.04
6	A	411	NAG	C4-C3-C2	-3.20	106.25	111.23
6	C	372	NAG	C2-N2-C7	-3.17	118.97	123.04
5	A	372	NAG	C2-N2-C7	-2.96	119.24	123.04
7	B	394	MAN	C2-C3-C4	-2.92	106.09	111.04
6	C	371	NAG	C2-N2-C7	-2.87	119.36	123.04
7	B	398	MAN	O2-C2-C3	-2.86	104.36	110.12
6	C	391	NAG	C3-C4-C5	-2.84	105.25	110.20
4	A	366	MAN	C2-C3-C4	-2.79	106.31	111.04
6	C	371	NAG	O4-C4-C3	-2.73	104.18	110.34
7	B	391	NAG	C6-C5-C4	-2.73	106.28	113.02
6	A	381	NAG	C3-C4-C5	-2.70	105.49	110.20
6	C	391	NAG	C2-N2-C7	-2.61	119.68	123.04
4	A	361	NAG	C2-N2-C7	-2.60	119.70	123.04
7	B	392	NAG	C3-C4-C5	-2.56	105.74	110.20
5	A	375	MAN	O5-C1-C2	-2.52	106.77	110.86
10	D	373	BMA	O5-C1-C2	-2.45	106.88	110.86
7	B	392	NAG	C1-O5-C5	-2.45	109.14	112.25
7	A	397	MAN	C1-C2-C3	-2.31	106.81	109.54
7	A	397	MAN	C2-C3-C4	-2.30	107.13	111.04
10	C	363	BMA	C2-C3-C4	-2.21	107.28	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	396	MAN	O3-C3-C4	-2.16	105.47	110.34
6	C	411	NAG	C2-N2-C7	-2.15	120.28	123.04
4	A	364	MAN	C2-C3-C4	-2.15	107.40	111.04
4	A	361	NAG	O7-C7-C8	-2.12	118.18	122.06
7	A	397	MAN	O5-C1-C2	-2.06	107.51	110.86
7	A	398	MAN	C2-C3-C4	-2.06	107.55	111.04
10	D	371	NAG	O4-C4-C3	-2.03	105.77	110.34
7	B	391	NAG	O7-C7-C8	-2.01	118.36	122.06
7	A	393	BMA	C1-O5-C5	2.00	114.79	112.25
5	A	375	MAN	C3-C4-C5	2.01	113.70	110.20
10	D	373	BMA	O5-C5-C6	2.02	111.71	107.35
6	A	381	NAG	O3-C3-C4	2.02	114.89	110.34
10	C	363	BMA	O5-C1-C2	2.03	114.14	110.86
5	B	364	MAN	C2-C3-C4	2.03	114.48	111.04
6	A	411	NAG	C3-C2-N2	2.03	115.43	110.56
6	B	411	NAG	O5-C5-C6	2.04	111.77	107.35
6	A	411	NAG	C3-C4-C5	2.07	113.80	110.20
6	A	411	NAG	O3-C3-C2	2.14	113.35	109.11
7	B	395	MAN	O5-C1-C2	2.15	114.34	110.86
4	A	365	MAN	C1-C2-C3	2.15	112.08	109.54
10	C	362	NAG	O5-C5-C6	2.18	112.06	107.35
5	B	364	MAN	O2-C2-C1	2.21	113.64	109.21
6	D	361	NAG	C3-C4-C5	2.22	114.06	110.20
6	A	412	NAG	C1-O5-C5	2.25	115.11	112.25
7	B	391	NAG	C3-C4-C5	2.27	114.16	110.20
6	D	361	NAG	C1-O5-C5	2.30	115.17	112.25
10	D	373	BMA	C1-O5-C5	2.37	115.26	112.25
5	A	373	BMA	C1-C2-C3	2.42	112.40	109.54
6	A	382	NAG	C3-C4-C5	2.56	114.65	110.20
4	A	363	BMA	C1-O5-C5	2.63	115.59	112.25
5	B	363	BMA	C1-O5-C5	2.72	115.70	112.25
5	B	362	NAG	C1-O5-C5	2.74	115.72	112.25
7	A	398	MAN	C1-O5-C5	2.87	115.89	112.25
7	A	393	BMA	C1-C2-C3	2.88	112.95	109.54
6	B	371	NAG	C1-O5-C5	3.07	116.14	112.25
5	B	363	BMA	C1-C2-C3	3.08	113.19	109.54
5	B	364	MAN	C1-C2-C3	3.15	113.26	109.54
5	A	374	MAN	C1-C2-C3	3.15	113.27	109.54
5	B	365	MAN	C1-O5-C5	3.24	116.36	112.25
7	B	393	BMA	C1-O5-C5	3.64	116.87	112.25
7	B	396	MAN	C1-O5-C5	4.29	117.69	112.25
7	B	396	MAN	C3-C4-C5	4.36	117.79	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	398	MAN	C1-C2-C3	4.40	114.75	109.54
7	B	395	MAN	C1-O5-C5	4.41	117.85	112.25
10	C	363	BMA	C1-C2-C3	4.59	114.97	109.54
10	C	363	BMA	C1-O5-C5	4.68	118.19	112.25
7	A	391	NAG	C1-O5-C5	4.69	118.20	112.25
6	C	391	NAG	C1-O5-C5	4.78	118.31	112.25
5	B	365	MAN	C3-C4-C5	4.80	118.57	110.20
7	B	391	NAG	C1-O5-C5	5.17	118.81	112.25
6	A	411	NAG	C1-O5-C5	5.47	119.19	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	366	MAN	C1-C2-C3-C4-C5-O5

19 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	361	NAG	1	0
4	A	362	NAG	1	0
4	A	363	BMA	1	0
4	A	366	MAN	1	0
5	A	373	BMA	2	0
5	A	374	MAN	2	0
6	A	381	NAG	3	0
6	A	382	NAG	1	0
7	A	394	MAN	4	0
7	A	395	MAN	4	0
6	A	411	NAG	3	0
6	A	412	NAG	3	0
5	B	362	NAG	1	0
5	B	364	MAN	1	0
5	B	365	MAN	1	0
6	B	371	NAG	1	0
6	B	372	NAG	1	0
7	B	396	MAN	2	0
7	B	398	MAN	2	0

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ACT	A	1327	-	1,3,3	0.86	0	0,3,3	0.00	-
9	SO4	A	1328	-	4,4,4	0.13	0	6,6,6	0.12	0
9	SO4	A	1329	-	4,4,4	0.20	0	6,6,6	0.22	0
9	SO4	A	1330	-	4,4,4	0.15	0	6,6,6	0.20	0
9	SO4	A	1331	-	4,4,4	0.08	0	6,6,6	0.29	0
2	HEM	A	350	1,3	30,50,50	2.19	7 (23%)	24,82,82	2.16	9 (37%)
8	ACT	B	1328	2	1,3,3	0.99	0	0,3,3	0.00	-
9	SO4	B	1329	-	4,4,4	0.05	0	6,6,6	0.33	0
9	SO4	B	1330	-	4,4,4	0.14	0	6,6,6	0.19	0
9	SO4	B	1331	-	4,4,4	0.17	0	6,6,6	0.19	0
2	HEM	B	350	1,8,3	30,50,50	2.34	7 (23%)	24,82,82	2.35	9 (37%)
8	ACT	C	1329	-	1,3,3	1.79	0	0,3,3	0.00	-
9	SO4	C	1330	-	4,4,4	0.26	0	6,6,6	0.18	0
9	SO4	C	1331	-	4,4,4	0.15	0	6,6,6	0.14	0
9	SO4	C	1332	-	4,4,4	0.12	0	6,6,6	0.21	0
9	SO4	C	1333	-	4,4,4	0.18	0	6,6,6	0.14	0
8	ACT	C	1334	-	1,3,3	1.28	0	0,3,3	0.00	-
2	HEM	C	350	1,3	30,50,50	2.29	9 (30%)	24,82,82	2.39	11 (45%)
11	NAG	C	381	1	14,14,15	0.62	0	15,19,21	1.34	2 (13%)
8	ACT	D	1327	-	1,3,3	1.00	0	0,3,3	0.00	-
9	SO4	D	1328	-	4,4,4	0.20	0	6,6,6	0.31	0
9	SO4	D	1329	-	4,4,4	0.17	0	6,6,6	0.14	0
2	HEM	D	350	1,3	30,50,50	2.12	6 (20%)	24,82,82	2.51	11 (45%)
11	NAG	D	381	1	14,14,15	0.62	0	15,19,21	0.67	0
11	NAG	D	391	1	14,14,15	0.52	0	15,19,21	1.38	3 (20%)
11	NAG	D	411	1	14,14,15	0.53	0	15,19,21	0.70	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
8	ACT	A	1327	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1328	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1329	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1330	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1331	-	-	0/0/0/0	0/0/0/0
2	HEM	A	350	1,3	-	0/10/54/54	0/0/8/8
8	ACT	B	1328	2	-	0/0/0/0	0/0/0/0
9	SO4	B	1329	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1330	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1331	-	-	0/0/0/0	0/0/0/0
2	HEM	B	350	1,8,3	-	0/10/54/54	0/0/8/8
8	ACT	C	1329	-	-	0/0/0/0	0/0/0/0
9	SO4	C	1330	-	-	0/0/0/0	0/0/0/0
9	SO4	C	1331	-	-	0/0/0/0	0/0/0/0
9	SO4	C	1332	-	-	0/0/0/0	0/0/0/0
9	SO4	C	1333	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1334	-	-	0/0/0/0	0/0/0/0
2	HEM	C	350	1,3	-	0/10/54/54	0/0/8/8
11	NAG	C	381	1	-	0/6/23/26	0/1/1/1
8	ACT	D	1327	-	-	0/0/0/0	0/0/0/0
9	SO4	D	1328	-	-	0/0/0/0	0/0/0/0
9	SO4	D	1329	-	-	0/0/0/0	0/0/0/0
2	HEM	D	350	1,3	-	0/10/54/54	0/0/8/8
11	NAG	D	381	1	-	0/6/23/26	0/1/1/1
11	NAG	D	391	1	-	0/6/23/26	0/1/1/1
11	NAG	D	411	1	-	0/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	HEM	C3B-C4B	-8.44	1.44	1.51
2	C	350	HEM	C3B-C4B	-7.21	1.45	1.51
2	A	350	HEM	C3B-C4B	-7.13	1.45	1.51
2	D	350	HEM	C3B-C4B	-6.52	1.46	1.51
2	B	350	HEM	C3D-C4D	-5.74	1.44	1.51
2	D	350	HEM	C3D-C4D	-5.66	1.44	1.51
2	C	350	HEM	C3D-C4D	-5.29	1.44	1.51
2	A	350	HEM	C3D-C4D	-4.95	1.45	1.51
2	D	350	HEM	C2C-C1C	-3.88	1.45	1.52
2	C	350	HEM	C2C-C1C	-3.81	1.45	1.52
2	A	350	HEM	C2C-C1C	-3.57	1.45	1.52
2	B	350	HEM	C2C-C1C	-3.45	1.46	1.52
2	D	350	HEM	C2D-C1D	-2.25	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	HEM	C2D-C1D	-2.18	1.44	1.51
2	C	350	HEM	C2B-C1B	-2.11	1.44	1.51
2	D	350	HEM	C2B-C1B	-2.10	1.45	1.51
2	B	350	HEM	C3C-CAC	2.03	1.55	1.51
2	B	350	HEM	FE-NB	2.07	2.08	1.97
2	B	350	HEM	FE-ND	2.09	2.08	1.97
2	A	350	HEM	CMA-C3A	2.23	1.56	1.51
2	B	350	HEM	C1C-NC	2.31	1.38	1.36
2	A	350	HEM	FE-ND	2.40	2.10	1.97
2	C	350	HEM	CAA-C2A	2.70	1.56	1.52
2	A	350	HEM	C1C-NC	2.74	1.39	1.36
2	A	350	HEM	C4C-NC	2.80	1.39	1.36
2	D	350	HEM	C1C-NC	2.83	1.39	1.36
2	C	350	HEM	FE-ND	2.89	2.12	1.97
2	C	350	HEM	C4C-NC	2.97	1.39	1.36
2	C	350	HEM	C1C-NC	3.49	1.40	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	350	HEM	C3C-CAC-CBC	-5.11	116.62	124.46
2	B	350	HEM	C3C-CAC-CBC	-4.26	117.92	124.46
2	C	350	HEM	C3C-CAC-CBC	-3.78	118.65	124.46
2	A	350	HEM	C3C-CAC-CBC	-3.21	119.54	124.46
2	A	350	HEM	C3B-CAB-CBB	-3.02	119.82	124.46
11	D	391	NAG	C4-C3-C2	-2.67	107.08	111.23
2	C	350	HEM	C3B-CAB-CBB	-2.65	120.39	124.46
2	C	350	HEM	CBD-CAD-C3D	-2.39	106.59	113.55
2	B	350	HEM	C3B-C4B-NB	-2.38	107.08	111.63
2	D	350	HEM	C4B-CHC-C1C	-2.20	122.15	125.82
2	D	350	HEM	C3B-CAB-CBB	-2.17	121.12	124.46
2	C	350	HEM	C4B-CHC-C1C	-2.17	122.20	125.82
2	B	350	HEM	CAA-C2A-C1A	-2.16	124.67	127.01
11	D	391	NAG	C3-C4-C5	-2.14	106.47	110.20
2	A	350	HEM	C2D-C3D-C4D	2.01	104.91	101.50
2	B	350	HEM	C3B-C4B-CHC	2.18	126.24	123.16
2	D	350	HEM	C2D-C3D-C4D	2.22	105.26	101.50
2	C	350	HEM	C2D-C3D-C4D	2.29	105.38	101.50
11	C	381	NAG	C3-C4-C5	2.34	114.27	110.20
2	D	350	HEM	C2C-C1C-CHC	2.43	127.38	123.68
2	A	350	HEM	CMD-C2D-C3D	2.45	125.19	114.35
2	A	350	HEM	C3B-C4B-CHC	2.47	126.64	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	350	HEM	CMD-C2D-C3D	2.54	125.60	114.35
2	C	350	HEM	C3B-C4B-CHC	2.76	127.05	123.16
2	D	350	HEM	CMD-C2D-C3D	2.82	126.81	114.35
2	D	350	HEM	C3B-C4B-CHC	2.98	127.36	123.16
2	B	350	HEM	CMD-C2D-C3D	3.02	127.70	114.35
2	A	350	HEM	CMC-C2C-C3C	3.19	124.49	116.53
11	D	391	NAG	C1-O5-C5	3.30	116.44	112.25
11	C	381	NAG	C4-C3-C2	3.32	116.39	111.23
2	A	350	HEM	CMB-C2B-C3B	3.49	125.25	116.53
2	C	350	HEM	CMB-C2B-C3B	3.63	125.59	116.53
2	D	350	HEM	CMB-C2B-C3B	3.67	125.69	116.53
2	B	350	HEM	CMC-C2C-C3C	3.68	125.72	116.53
2	D	350	HEM	CMC-C2C-C3C	3.70	125.78	116.53
2	B	350	HEM	CMB-C2B-C3B	3.89	126.24	116.53
2	B	350	HEM	CAD-C3D-C4D	4.05	126.75	112.47
2	C	350	HEM	CAD-C3D-C4D	4.21	127.33	112.47
2	A	350	HEM	CAD-C3D-C2D	4.27	125.50	113.22
2	C	350	HEM	CMC-C2C-C3C	4.39	127.49	116.53
2	D	350	HEM	CAD-C3D-C2D	4.50	126.16	113.22
2	D	350	HEM	CAD-C3D-C4D	4.56	128.54	112.47
2	A	350	HEM	CAD-C3D-C4D	4.85	129.56	112.47
2	C	350	HEM	CAD-C3D-C2D	4.88	127.25	113.22
2	B	350	HEM	CAD-C3D-C2D	5.30	128.46	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1331	SO4	2	0
2	A	350	HEM	5	0
9	B	1331	SO4	2	0
2	B	350	HEM	3	0
2	C	350	HEM	3	0
11	C	381	NAG	1	0
9	D	1328	SO4	1	0
9	D	1329	SO4	1	0
2	D	350	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

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^{th} 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	323/325 (99%)	-0.25	1 (0%)	94	96	12, 26, 42, 56	0
1	B	324/325 (99%)	-0.40	1 (0%)	94	96	11, 21, 34, 53	0
1	C	325/325 (100%)	-0.27	2 (0%)	90	93	14, 24, 37, 68	0
1	D	323/325 (99%)	-0.01	6 (1%)	70	77	16, 32, 47, 59	0
All	All	1295/1300 (99%)	-0.23	10 (0%)	87	91	11, 26, 43, 68	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	328	ASP	4.0
1	D	20	GLU	3.8
1	A	20	GLU	3.0
1	C	259	VAL	2.7
1	D	16	LEU	2.6
1	D	217	ASP	2.6
1	D	21	ALA	2.4
1	D	43	ALA	2.4
1	D	30	GLY	2.1
1	B	29	PRO	2.0

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

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

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^{th} 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
6	NAG	C	391	14/15	0.88	0.22	6.09	31,42,48,51	0
5	NAG	B	361	14/15	0.95	0.15	4.52	30,34,41,45	0
6	NAG	C	372	14/15	0.81	0.23	3.92	47,53,55,58	0
5	NAG	A	372	14/15	0.88	0.14	2.36	37,42,46,52	0
7	NAG	A	391	14/15	0.93	0.20	2.31	34,39,42,43	0
4	NAG	A	361	14/15	0.95	0.16	1.90	33,36,41,41	0
6	NAG	B	372	14/15	0.86	0.20	1.82	43,49,52,53	0
7	MAN	A	394	11/12	0.84	0.20	1.72	46,49,55,59	0
10	NAG	D	372	14/15	0.91	0.18	1.21	48,52,58,58	0
7	NAG	B	391	14/15	0.97	0.14	1.15	26,30,32,37	0
6	NAG	C	371	14/15	0.96	0.11	0.31	25,30,36,42	0
10	NAG	D	371	14/15	0.94	0.11	0.24	26,34,39,43	0
7	MAN	B	397	11/12	0.97	0.15	-0.09	27,31,32,34	0
6	NAG	B	371	14/15	0.96	0.10	-0.36	16,23,29,36	0
7	MAN	B	396	11/12	0.96	0.10	-0.76	26,30,36,45	0
5	NAG	A	371	14/15	0.97	0.10	-1.08	18,21,26,30	0
6	NAG	D	362	14/15	0.81	0.35	-	60,62,65,66	0
5	MAN	A	374	11/12	0.71	0.38	-	79,81,84,88	0
7	MAN	A	395	11/12	0.81	0.25	-	60,61,63,64	0
6	NAG	A	411	14/15	0.91	0.30	-	56,64,68,70	0
7	MAN	B	394	11/12	0.93	0.16	-	40,43,45,50	0
6	NAG	C	392	14/15	0.86	0.47	-	56,60,63,65	0
6	NAG	C	412	14/15	0.82	0.48	-	73,76,77,78	0
6	NAG	A	381	14/15	0.95	0.17	-	39,43,47,54	0
5	MAN	A	375	11/12	0.76	0.52	-	88,90,90,91	0
7	MAN	A	396	11/12	0.93	0.22	-	52,53,54,55	0
4	MAN	A	366	11/12	0.71	0.24	-	64,65,66,67	0
4	MAN	A	365	11/12	0.78	0.35	-	66,68,70,71	0
5	BMA	B	363	11/12	0.65	0.32	-	59,62,64,66	0
10	NAG	C	361	14/15	0.93	0.22	-	41,46,49,54	0
5	NAG	B	362	14/15	0.76	0.26	-	45,50,52,56	0
6	NAG	A	382	14/15	0.81	0.26	-	57,61,65,66	0
10	BMA	C	363	11/12	0.71	0.48	-	75,78,79,79	0
4	BMA	A	363	11/12	0.89	0.23	-	49,54,59,62	0
4	MAN	A	364	11/12	0.89	0.23	-	51,54,58,63	0
6	NAG	B	382	14/15	0.82	0.30	-	57,59,63,64	0
7	MAN	A	397	11/12	0.87	0.27	-	55,59,60,62	0
6	NAG	D	361	14/15	0.93	0.22	-	50,54,56,59	0
5	MAN	B	365	11/12	0.42	0.46	-	78,80,81,81	0
10	BMA	D	373	11/12	0.71	0.25	-	58,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BMA	A	373	11/12	0.72	0.33	-	56,58,68,74	0
10	NAG	C	362	14/15	0.91	0.32	-	58,61,65,70	0
7	NAG	B	392	14/15	0.97	0.13	-	23,31,34,40	0
7	MAN	B	395	11/12	0.88	0.36	-	52,55,57,58	0
6	NAG	B	411	14/15	0.93	0.26	-	51,57,62,69	0
6	NAG	B	412	14/15	0.80	0.61	-	74,77,79,81	0
5	MAN	B	364	11/12	0.75	0.30	-	67,69,72,75	0
7	MAN	A	398	11/12	0.69	0.41	-	58,64,65,65	0
7	BMA	A	393	11/12	0.94	0.12	-	40,44,47,48	0
6	NAG	C	411	14/15	0.89	0.28	-	55,60,64,69	0
6	NAG	B	381	14/15	0.95	0.13	-	39,42,46,53	0
7	MAN	B	398	11/12	0.90	0.21	-	47,50,52,52	0
7	BMA	B	393	11/12	0.96	0.13	-	30,33,36,37	0
7	NAG	A	392	14/15	0.96	0.18	-	42,45,47,47	0
6	NAG	A	412	14/15	0.77	0.51	-	75,78,81,81	0
4	NAG	A	362	14/15	0.90	0.23	-	40,46,53,56	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, 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
9	SO4	A	1331	5/5	0.95	0.21	8.51	60,60,61,63	0
8	ACT	C	1329	4/4	0.94	0.19	7.47	31,34,37,38	0
9	SO4	B	1331	5/5	0.93	0.19	7.26	68,69,69,71	0
8	ACT	D	1327	4/4	0.95	0.20	4.87	48,49,49,50	0
8	ACT	A	1327	4/4	0.93	0.18	4.09	30,32,32,32	0
11	NAG	D	391	14/15	0.89	0.25	3.78	46,48,51,53	0
8	ACT	B	1328	4/4	0.95	0.15	2.59	25,25,30,32	0
9	SO4	D	1329	5/5	0.96	0.14	1.84	55,56,58,58	0
8	ACT	C	1334	4/4	0.98	0.11	0.93	24,27,29,30	0
2	HEM	C	350	43/43	0.98	0.13	0.83	13,17,22,26	0
9	SO4	C	1332	5/5	0.95	0.14	0.83	62,62,63,63	0
2	HEM	A	350	43/43	0.97	0.12	0.49	12,19,21,27	0
2	HEM	B	350	43/43	0.98	0.11	0.08	6,13,16,22	0
9	SO4	C	1330	5/5	0.97	0.11	0.05	61,62,63,63	0
2	HEM	D	350	43/43	0.98	0.12	-0.01	18,23,28,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	D	353	1/1	0.92	0.06	-3.21	26,26,26,26	0
3	MG	A	353	1/1	0.95	0.06	-4.16	18,18,18,18	0
3	MG	C	353	1/1	0.96	0.03	-4.17	19,19,19,19	0
3	MG	B	353	1/1	0.99	0.03	-11.05	12,12,12,12	0
9	SO4	A	1330	5/5	0.95	0.15	-	59,62,63,63	0
11	NAG	D	381	14/15	0.80	0.25	-	54,57,61,62	0
11	NAG	C	381	14/15	0.87	0.33	-	50,54,57,58	0
11	NAG	D	411	14/15	0.92	0.17	-	53,56,58,59	0
9	SO4	C	1331	5/5	0.89	0.20	-	87,88,88,89	0
9	SO4	B	1330	5/5	0.92	0.18	-	65,65,65,66	0
9	SO4	D	1328	5/5	0.95	0.13	-	60,60,61,62	0
9	SO4	B	1329	5/5	0.90	0.23	-	57,58,61,62	0
9	SO4	A	1329	5/5	0.95	0.18	-	70,71,71,72	0
9	SO4	A	1328	5/5	0.97	0.14	-	56,56,58,59	0
9	SO4	C	1333	5/5	0.94	0.32	-	74,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.