Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:50 AM GMT

PDB ID	:	2EHA
Title	:	Crystal structure of goat lactoperoxidase complexed with formate anion at 3.3 A resolution
Authors	:	Singh, A.K.; Ethayathulla, A.S.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-03-06
Resolution	:	3.30 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 ⓘ symbol.

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

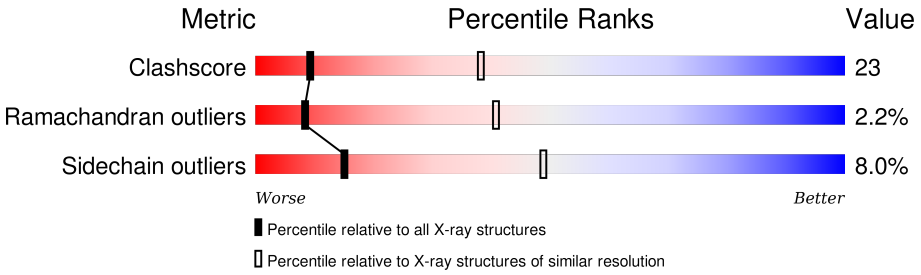
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.30 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	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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	61% 34% 5%
1	B	595	60% 35% 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
10	FMT	A	2002	-	-	X	-
10	FMT	B	2003	-	-	X	-
7	SCN	A	3002	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	OSM	B	3021	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10124 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			
1	B	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			

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

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

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

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

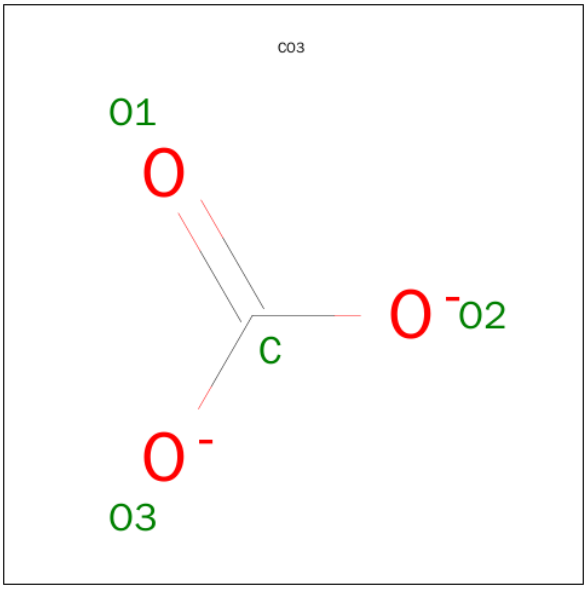
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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

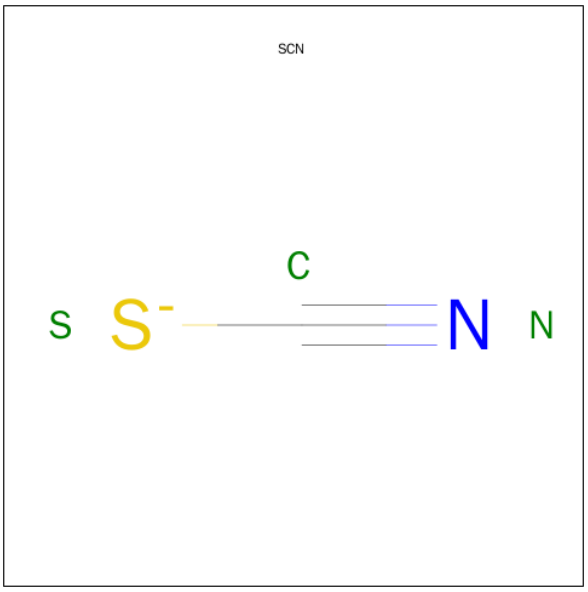
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0

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



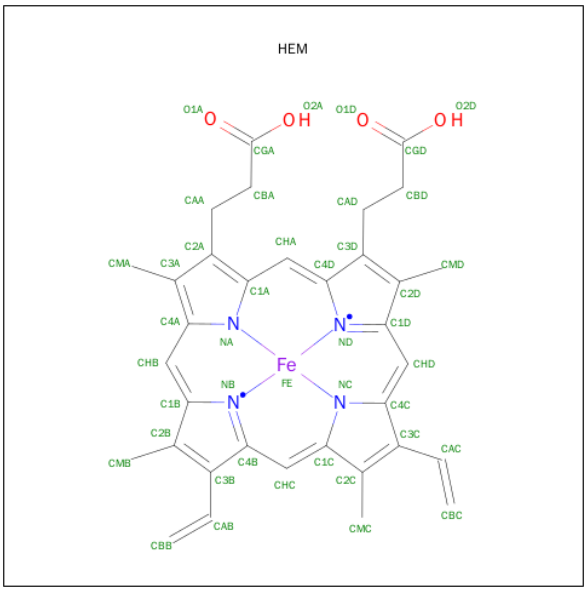
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



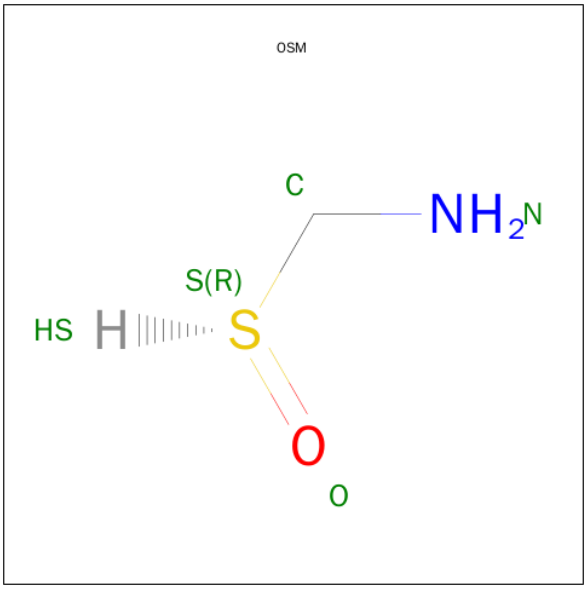
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

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



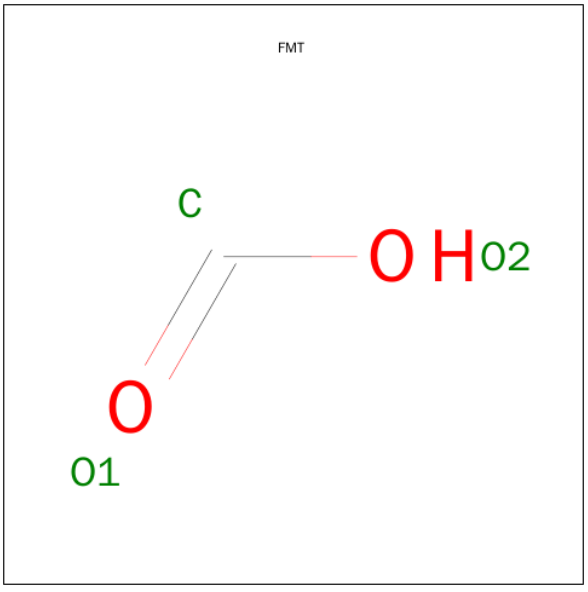
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
8	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 9 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



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

- Molecule 10 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	3	1	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 3 1 2	0	0
10	B	1	Total C O 3 1 2	0	0
10	B	1	Total C O 3 1 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	116	Total O 116 116	0	0
11	B	97	Total O 97 97	0	0

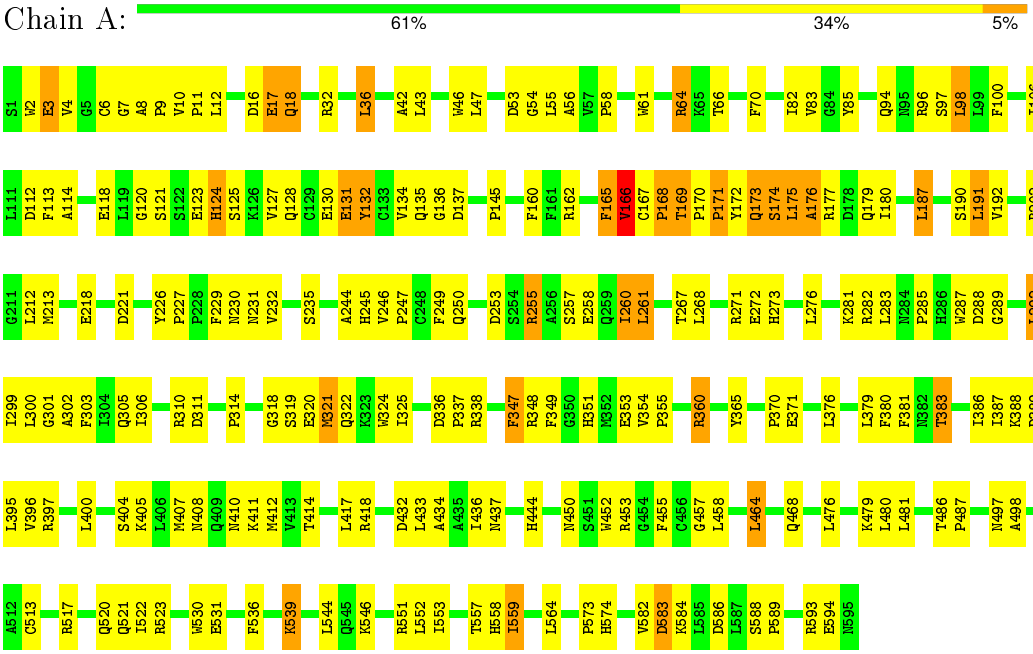
3 Residue-property plots (i)

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.

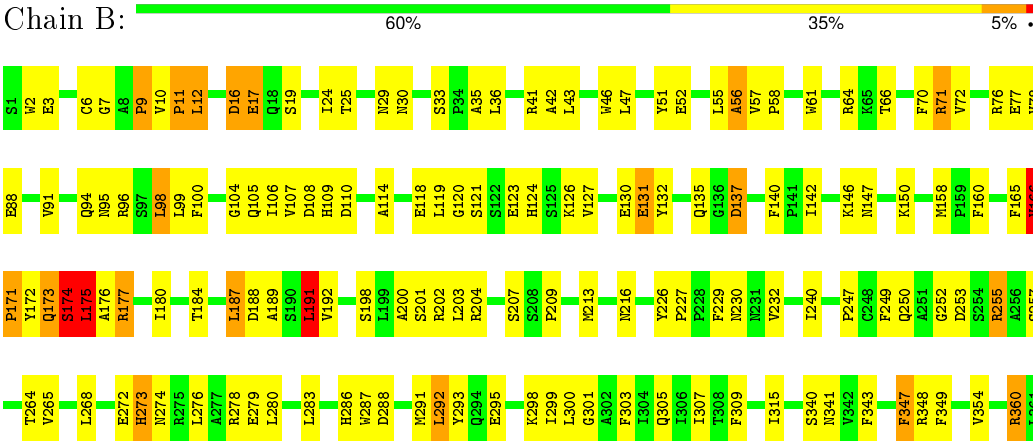
- Molecule 1: Lactoperoxidase

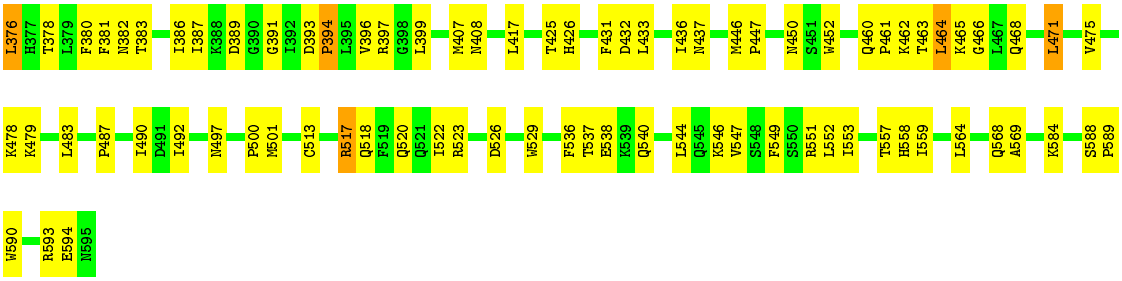
Chain A:



- Molecule 1: Lactoperoxidase

Chain B:




L376
H377
T378
L379
F380
F381
N382
T383
I386
I387
K388
D389
G390
G391
I392
D393
P394
L395
V396
R397
G398
L399
M407
N408
L417
T425
H426
F431
D432
L433
I436
N437
M446
P447
N450
S451
W452
Q460
P461
K462
T463
L464
K465
G466
L467
Q468
L471
V475
K478
K479
L483
P487
I490
D491
I492
N497
P500
M501
C513
R517
Q518
F519
Q520
Q521
I522
R523
D526
W529
F536
T537
E538
K539
Q540
L544
Q545
K546
V547
S548
F549
S550
R551
L552
I553
T557
H558
I559
L564
Q568
A569
K584
S588
P589
W590
R593
E594
N595

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	Depositor
Cell constants a, b, c, α, β, γ	57.99Å 72.27Å 83.65Å 85.45° 84.04° 75.89°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10124	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, SCN, NAG, FMT, BMA, OSM, HEM, CA, 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	0.44	0/4882	0.80	4/6632 (0.1%)
1	B	0.44	0/4882	0.82	7/6632 (0.1%)
All	All	0.44	0/9764	0.81	11/13264 (0.1%)

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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	VAL	N-CA-C	8.08	132.83	111.00
1	B	174	SER	N-CA-C	6.67	129.02	111.00
1	A	166	VAL	N-CA-C	6.65	128.96	111.00
1	A	559	ILE	N-CA-C	-6.14	94.42	111.00
1	B	12	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	173	GLN	N-CA-C	5.58	126.06	111.00
1	B	191	LEU	CA-CB-CG	5.31	127.50	115.30
1	B	12	LEU	N-CA-C	5.26	125.22	111.00
1	A	10	VAL	N-CA-C	-5.26	96.80	111.00
1	B	43	LEU	CA-CB-CG	5.16	127.18	115.30
1	B	175	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4753	0	4646	228	0
1	B	4753	0	4646	226	0
2	A	78	0	68	0	0
2	B	39	0	34	7	0
3	A	39	0	34	0	0
3	B	78	0	68	2	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	3	0	0	3	0
8	A	43	0	30	11	0
8	B	43	0	30	7	0
9	B	4	0	5	2	0
10	A	6	0	4	3	0
10	B	6	0	4	3	0
11	A	116	0	0	20	0
11	B	97	0	0	8	0
All	All	10124	0	9619	446	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 23.

All (446) 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:B:167:CYS:HB2	1:B:168:PRO:HD3	1.26	1.14
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.28	1.13
1:A:132:TYR:OH	1:B:120:GLY:HA2	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:HIS:HB2	1:B:137:ASP:CG	1.80	1.01
1:B:315:ILE:HG22	2:B:597:NAG:H82	1.40	1.01
1:B:432:ASP:O	1:B:436:ILE:HD13	1.67	0.95
1:B:172:TYR:O	1:B:173:GLN:HG3	1.69	0.93
1:A:202:ARG:HD2	1:A:250:GLN:HE22	1.34	0.92
1:B:172:TYR:CE2	1:B:174:SER:HB2	2.05	0.92
1:B:315:ILE:HG22	2:B:597:NAG:C8	2.00	0.91
7:A:3002:SCN:S	11:A:3077:HOH:O	2.27	0.91
1:B:175:LEU:HD22	1:B:176:ALA:H	1.36	0.90
1:B:487:PRO:HA	1:B:490:ILE:HD13	1.55	0.89
1:B:109:HIS:NE2	9:B:3021:OSM:S	2.46	0.88
1:A:258:GLU:OE2	8:A:3003:HEM:HMB3	1.72	0.88
1:A:64:ARG:HG2	11:A:3029:HOH:O	1.73	0.87
1:A:168:PRO:CB	1:A:170:PRO:HD2	2.05	0.87
1:B:258:GLU:OE2	8:B:1003:HEM:HMB3	1.75	0.87
1:B:168:PRO:CB	1:B:170:PRO:HD2	2.04	0.86
1:A:588:SER:OG	1:A:589:PRO:HD3	1.75	0.86
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.59	0.85
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.10	0.85
1:B:557:THR:OG1	1:B:559:ILE:HD12	1.78	0.84
1:A:169:THR:N	1:A:170:PRO:HD2	1.94	0.83
1:B:105:GLN:NE2	9:B:3021:OSM:O	2.11	0.81
1:B:9:PRO:O	1:B:11:PRO:HD3	1.81	0.81
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.61	0.81
1:A:169:THR:H	1:A:170:PRO:HD2	1.45	0.79
1:B:168:PRO:HB2	1:B:170:PRO:HD2	1.66	0.77
1:A:2:TRP:CG	1:A:175:LEU:HB3	2.19	0.77
1:B:169:THR:CG2	1:B:170:PRO:HD3	2.16	0.76
1:A:17:GLU:O	1:A:18:GLN:HG2	1.85	0.76
1:B:272:GLU:OE1	1:B:272:GLU:HA	1.84	0.76
1:B:167:CYS:CB	1:B:168:PRO:HD3	2.13	0.76
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.67	0.75
1:A:172:TYR:O	1:A:173:GLN:HG3	1.87	0.75
1:B:108:ASP:OD2	8:B:1003:HEM:HMD3	1.86	0.75
1:B:175:LEU:CD2	1:B:176:ALA:H	1.99	0.74
1:A:3:GLU:HG3	11:A:3078:HOH:O	1.87	0.74
1:B:106:ILE:HG23	1:B:191:LEU:HD11	1.71	0.73
1:A:145:PRO:HG2	11:A:3052:HOH:O	1.87	0.72
1:B:315:ILE:CG2	2:B:597:NAG:C8	2.66	0.72
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.54	0.72
1:A:169:THR:N	1:A:170:PRO:CD	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:O	1:A:11:PRO:HD3	1.90	0.72
1:A:517:ARG:O	1:A:521:GLN:HG3	1.90	0.72
1:A:108:ASP:OD1	8:A:3003:HEM:HMD3	1.90	0.72
1:B:78:VAL:HG13	1:B:82:ILE:HD13	1.72	0.72
1:A:124:HIS:CG	1:B:137:ASP:HB2	2.25	0.71
1:B:513:CYS:O	1:B:517:ARG:HG2	1.90	0.71
1:A:168:PRO:HD2	11:A:3083:HOH:O	1.88	0.71
1:B:168:PRO:HB3	1:B:170:PRO:HD2	1.73	0.71
1:B:537:THR:OG1	1:B:540:GLN:HG3	1.89	0.71
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.26	0.71
1:B:166:VAL:O	1:B:167:CYS:C	2.29	0.71
1:A:212:LEU:HB2	11:A:3080:HOH:O	1.90	0.70
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.89	0.70
1:B:202:ARG:HD2	1:B:250:GLN:HE22	1.54	0.70
1:B:175:LEU:HD22	1:B:176:ALA:N	2.05	0.70
1:B:169:THR:H	1:B:170:PRO:CD	2.05	0.70
1:A:557:THR:CB	1:A:559:ILE:HD12	2.22	0.69
1:B:167:CYS:HB2	1:B:168:PRO:CD	2.15	0.69
1:A:124:HIS:HB2	1:B:137:ASP:OD2	1.91	0.69
1:B:354:VAL:HG21	1:B:417:LEU:HD11	1.73	0.69
1:B:169:THR:N	1:B:170:PRO:CD	2.54	0.69
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.76	0.68
1:B:347:PHE:HB3	8:B:1003:HEM:HMD2	1.75	0.68
1:B:82:ILE:HD11	1:B:483:LEU:CD1	2.24	0.68
1:B:551:ARG:HD3	1:B:584:LYS:HA	1.74	0.68
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.39	0.68
1:A:255:ARG:HG2	7:A:3002:SCN:S	2.34	0.67
1:B:452:TRP:CD1	1:B:492:ILE:HD13	2.28	0.67
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.75	0.67
1:A:168:PRO:HB2	1:A:170:PRO:CD	2.17	0.67
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.30	0.67
1:A:202:ARG:HD2	1:A:250:GLN:NE2	2.07	0.66
8:A:3003:HEM:HBB2	8:A:3003:HEM:HMB1	1.77	0.66
1:A:414:THR:HG22	11:A:3098:HOH:O	1.96	0.66
1:A:36:LEU:HG	1:A:337:PRO:HD2	1.78	0.66
1:A:347:PHE:CD1	1:A:349:PHE:HE2	2.13	0.66
1:A:244:ALA:O	1:A:245:HIS:HB2	1.96	0.66
1:B:315:ILE:CG2	2:B:597:NAG:H81	2.26	0.66
1:A:407:MET:HB3	1:A:501:MET:CE	2.26	0.66
1:B:169:THR:HG23	1:B:170:PRO:HD3	1.75	0.66
1:A:272:GLU:HA	1:A:272:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:H	1:A:175:LEU:HD12	1.61	0.65
1:B:108:ASP:OD2	8:B:1003:HEM:CMD	2.44	0.65
1:A:370:PRO:HG2	1:A:371:GLU:HG3	1.78	0.65
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.32	0.65
1:A:258:GLU:OE2	8:A:3003:HEM:CMB	2.45	0.65
1:A:7:GLY:C	1:A:9:PRO:HD3	2.17	0.65
1:B:397:ARG:HE	10:B:2003:FMT:H	1.61	0.65
1:A:123:GLU:HG3	1:A:125:SER:H	1.61	0.65
1:A:255:ARG:HG2	7:A:3002:SCN:C	2.27	0.64
1:A:118:GLU:HG2	11:A:3117:HOH:O	1.98	0.64
1:A:108:ASP:CG	8:A:3003:HEM:HMD3	2.18	0.63
1:A:300:LEU:O	1:A:303:PHE:HB3	1.98	0.63
1:A:94:GLN:OE1	1:A:94:GLN:HA	1.98	0.63
1:A:124:HIS:ND1	1:B:137:ASP:HB3	2.13	0.63
1:A:557:THR:OG1	1:A:559:ILE:HD12	1.98	0.63
1:B:82:ILE:HD11	1:B:483:LEU:HD12	1.79	0.62
1:B:175:LEU:CD2	1:B:176:ALA:N	2.61	0.62
1:B:2:TRP:CD1	1:B:175:LEU:HA	2.35	0.62
1:A:53:ASP:C	1:A:55:LEU:H	2.03	0.62
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.29	0.61
1:A:168:PRO:HG2	1:A:172:TYR:CD1	2.35	0.61
1:A:124:HIS:CG	1:B:137:ASP:CB	2.83	0.61
1:B:168:PRO:HG2	1:B:172:TYR:CD1	2.36	0.61
1:B:588:SER:N	1:B:589:PRO:CD	2.63	0.61
1:A:397:ARG:HE	10:A:2001:FMT:H	1.66	0.61
1:A:132:TYR:HH	1:B:120:GLY:HA2	1.65	0.60
1:A:127:VAL:HG13	1:A:131:GLU:HG3	1.83	0.60
11:A:3067:HOH:O	1:B:170:PRO:HG3	2.00	0.60
1:A:457:GLY:O	1:A:458:LEU:HD23	2.01	0.60
1:B:106:ILE:HG13	1:B:265:VAL:HG11	1.83	0.60
1:A:124:HIS:ND1	1:B:137:ASP:CB	2.65	0.60
1:B:259:GLN:OE1	1:B:261:LEU:HB2	2.00	0.60
1:B:396:VAL:HG11	1:B:559:ILE:HD13	1.82	0.60
1:A:302:ALA:O	1:A:306:ILE:HG13	2.02	0.59
1:A:108:ASP:OD2	8:A:3003:HEM:HMD3	2.02	0.59
1:B:299:ILE:HD11	1:B:590:TRP:NE1	2.16	0.59
1:A:191:LEU:HD23	1:A:192:VAL:N	2.18	0.59
1:A:306:ILE:HD13	1:A:544:LEU:O	2.02	0.59
1:A:288:ASP:O	1:A:292:LEU:HD22	2.03	0.59
1:A:66:THR:HB	1:A:70:PHE:O	2.02	0.59
1:A:2:TRP:HB2	1:A:175:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:NH2	1:B:150:LYS:HD2	2.19	0.58
1:B:593:ARG:HB2	11:B:3103:HOH:O	2.03	0.58
1:B:487:PRO:HA	1:B:490:ILE:CD1	2.31	0.58
1:B:123:GLU:HB3	1:B:126:LYS:HE2	1.85	0.58
1:A:112:ASP:O	1:A:255:ARG:NH2	2.32	0.58
1:B:118:GLU:O	1:B:119:LEU:C	2.43	0.57
1:B:315:ILE:HG23	2:B:597:NAG:H81	1.86	0.57
1:B:7:GLY:O	1:B:9:PRO:HD3	2.05	0.57
1:A:289:GLY:HA2	1:A:292:LEU:CD2	2.34	0.57
1:A:347:PHE:CD1	1:A:349:PHE:CE2	2.93	0.57
1:A:347:PHE:HD1	1:A:349:PHE:CE2	2.23	0.57
1:B:258:GLU:OE2	8:B:1003:HEM:CMB	2.50	0.57
1:B:114:ALA:HA	1:B:180:ILE:O	2.05	0.57
1:B:407:MET:HB3	1:B:501:MET:CE	2.35	0.57
1:A:418:ARG:HG2	1:A:418:ARG:O	2.05	0.57
1:A:108:ASP:OD2	8:A:3003:HEM:CMD	2.52	0.56
1:B:123:GLU:HB3	1:B:126:LYS:HB2	1.87	0.56
1:B:343:PHE:CD1	1:B:518:GLN:HG2	2.40	0.56
1:B:94:GLN:HA	1:B:94:GLN:OE1	2.05	0.56
1:B:72:VAL:HA	11:B:3116:HOH:O	2.05	0.56
1:B:17:GLU:HG3	1:B:17:GLU:O	2.05	0.56
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.87	0.56
1:A:336:ASP:OD1	1:A:338:ARG:HB2	2.06	0.56
1:A:281:LYS:HE3	11:A:3066:HOH:O	2.05	0.56
1:B:568:GLN:OE1	2:B:596:NAG:H5	2.06	0.55
1:B:518:GLN:HE21	1:B:522:ILE:HG23	1.70	0.55
1:A:432:ASP:OD1	1:A:434:ALA:N	2.39	0.55
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.41	0.55
1:A:205:ASN:HB3	11:A:3080:HOH:O	2.06	0.55
1:B:288:ASP:O	1:B:292:LEU:HD22	2.04	0.55
1:B:393:ASP:HB2	1:B:394:PRO:HD3	1.89	0.55
1:B:118:GLU:HG3	1:B:119:LEU:H	1.72	0.55
1:A:320:GLU:O	1:A:324:TRP:HD1	1.88	0.55
1:A:322:GLN:HB3	11:A:3101:HOH:O	2.06	0.55
1:B:299:ILE:HD11	1:B:590:TRP:HE1	1.72	0.55
1:B:42:ALA:HB2	1:B:166:VAL:HG11	1.88	0.55
1:A:82:ILE:HD11	1:A:479:LYS:CB	2.36	0.55
1:A:386:ILE:HD12	1:A:386:ILE:H	1.73	0.54
1:B:142:ILE:HB	1:B:158:MET:HB2	1.89	0.54
1:A:583:ASP:OD1	1:A:583:ASP:N	2.40	0.54
1:B:417:LEU:HD22	1:B:433:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:THR:HG22	1:B:170:PRO:HD3	1.90	0.54
1:A:287:TRP:CZ3	1:A:295:GLU:HG3	2.43	0.54
1:A:348:ARG:NH1	1:A:437:ASN:HD22	2.06	0.54
1:B:274:ASN:HB3	1:B:278:ARG:NH1	2.22	0.54
1:A:557:THR:HB	1:A:559:ILE:HD12	1.90	0.53
1:B:25:THR:O	1:B:184:THR:HG22	2.08	0.53
1:B:341:ASN:HB3	1:B:446:MET:HE1	1.90	0.53
1:B:387:ILE:HA	11:B:3084:HOH:O	2.08	0.53
1:B:315:ILE:CG2	2:B:597:NAG:H82	2.24	0.53
1:B:95:ASN:HA	1:B:569:ALA:CB	2.38	0.53
1:B:140:PHE:O	1:B:160:PHE:HB3	2.08	0.53
1:B:167:CYS:SG	1:B:172:TYR:OH	2.53	0.53
1:A:289:GLY:HA2	1:A:292:LEU:HD23	1.91	0.52
1:B:120:GLY:HA3	1:B:123:GLU:OE1	2.09	0.52
1:A:347:PHE:HD1	1:A:349:PHE:HE2	1.55	0.52
1:A:387:ILE:HG22	1:A:388:LYS:HG3	1.90	0.52
1:A:17:GLU:O	1:A:17:GLU:HG3	2.09	0.52
1:A:17:GLU:O	1:A:18:GLN:CG	2.56	0.52
1:A:283:LEU:O	1:A:285:PRO:HD3	2.09	0.52
1:B:465:LYS:O	1:B:468:GLN:HB2	2.09	0.52
1:B:118:GLU:CG	1:B:119:LEU:H	2.23	0.52
1:A:165:PHE:N	1:A:165:PHE:CD1	2.77	0.52
1:A:83:VAL:O	1:A:412:MET:HB2	2.10	0.52
1:B:146:LYS:HG2	1:B:147:ASN:OD1	2.10	0.52
1:B:348:ARG:HH11	1:B:437:ASN:ND2	2.06	0.52
1:A:191:LEU:HD23	1:A:192:VAL:H	1.75	0.52
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.92	0.52
1:B:108:ASP:CG	8:B:1003:HEM:HMD3	2.30	0.51
1:A:229:PHE:HZ	1:A:387:ILE:HD13	1.75	0.51
1:B:16:ASP:HB3	1:B:19:SER:HB2	1.92	0.51
1:A:132:TYR:OH	1:B:119:LEU:O	2.26	0.51
1:A:118:GLU:O	11:A:3006:HOH:O	2.19	0.51
1:B:300:LEU:O	1:B:303:PHE:HB3	2.10	0.51
1:B:127:VAL:HG13	1:B:131:GLU:CG	2.40	0.51
1:B:165:PHE:O	1:B:180:ILE:HD11	2.11	0.51
1:A:82:ILE:HD11	1:A:479:LYS:HB3	1.93	0.50
1:B:47:LEU:HD12	1:B:452:TRP:CZ3	2.46	0.50
1:B:362:ASP:OD1	1:B:364:ASN:N	2.34	0.50
1:B:82:ILE:N	1:B:82:ILE:HD12	2.26	0.50
1:A:351:HIS:CG	1:A:433:LEU:HD21	2.47	0.50
1:B:257:SER:O	1:B:381:PHE:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PHE:CD1	1:B:529:TRP:HH2	2.30	0.50
1:A:191:LEU:HA	1:A:253:ASP:HB2	1.94	0.49
1:B:360:ARG:NH2	1:B:389:ASP:OD2	2.45	0.49
1:B:168:PRO:HB2	1:B:170:PRO:CD	2.40	0.49
1:A:166:VAL:O	1:A:167:CYS:C	2.49	0.49
1:A:260:ILE:HG12	1:A:386:ILE:HD11	1.94	0.49
1:B:170:PRO:O	1:B:171:PRO:C	2.51	0.49
1:B:191:LEU:HD23	1:B:192:VAL:HG23	1.94	0.49
1:A:347:PHE:CE1	1:A:349:PHE:HE2	2.31	0.49
1:B:35:ALA:HB2	1:B:41:ARG:NH2	2.28	0.49
1:B:426:HIS:CD2	1:B:431:PHE:CZ	3.00	0.49
1:B:127:VAL:HG13	1:B:131:GLU:HG3	1.95	0.49
1:A:7:GLY:O	1:A:9:PRO:HD3	2.12	0.49
1:B:463:THR:O	1:B:466:GLY:N	2.46	0.49
1:B:203:LEU:HD11	1:B:252:GLY:HA2	1.94	0.49
1:A:392:ILE:O	1:A:396:VAL:HG23	2.12	0.49
1:B:588:SER:N	1:B:589:PRO:HD3	2.28	0.48
1:B:475:VAL:O	1:B:479:LYS:HG3	2.13	0.48
1:B:10:VAL:HG12	1:B:10:VAL:O	2.13	0.48
1:A:118:GLU:C	1:A:120:GLY:N	2.65	0.48
3:B:599:NAG:H61	3:B:600:NAG:H82	1.94	0.48
1:A:168:PRO:CG	1:A:172:TYR:CD1	2.96	0.48
1:A:260:ILE:HD12	1:A:395:LEU:HD13	1.95	0.48
1:B:450:ASN:HD21	1:B:487:PRO:HB2	1.79	0.48
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.12	0.48
1:B:299:ILE:HD12	1:B:590:TRP:CZ2	2.49	0.48
1:A:353:GLU:HA	1:A:405:LYS:O	2.13	0.48
1:A:354:VAL:HG11	8:A:3003:HEM:CBB	2.44	0.48
1:B:461:PRO:O	1:B:487:PRO:HB2	2.14	0.48
1:B:104:GLY:HA3	8:B:1003:HEM:CBC	2.43	0.48
1:A:588:SER:N	1:A:589:PRO:CD	2.76	0.48
1:B:376:LEU:HD13	1:B:380:PHE:CZ	2.49	0.48
1:B:463:THR:O	1:B:464:LEU:C	2.52	0.48
1:B:471:LEU:HA	1:B:500:PRO:HD3	1.95	0.48
1:A:383:THR:HA	1:A:386:ILE:HD13	1.94	0.47
1:A:53:ASP:C	1:A:55:LEU:N	2.67	0.47
1:A:283:LEU:C	1:A:285:PRO:HD3	2.34	0.47
1:B:2:TRP:CE3	1:B:175:LEU:HG	2.49	0.47
1:A:260:ILE:CD1	1:A:395:LEU:HD13	2.44	0.47
1:B:287:TRP:CZ3	1:B:295:GLU:HG3	2.49	0.47
1:A:314:PRO:HG3	1:A:321:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:O	1:A:325:ILE:HG22	2.14	0.47
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.72	0.47
1:A:106:ILE:HG23	1:A:191:LEU:CD1	2.39	0.47
1:A:120:GLY:CA	1:A:123:GLU:OE1	2.63	0.47
1:A:574:HIS:C	1:A:574:HIS:ND1	2.68	0.47
1:B:230:ASN:OD1	1:B:232:VAL:HG23	2.14	0.47
1:B:131:GLU:HB2	1:B:132:TYR:CE1	2.49	0.47
1:B:30:ASN:HB3	1:B:33:SER:O	2.15	0.47
1:A:481:LEU:HD21	1:A:487:PRO:HG3	1.97	0.47
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.94	0.47
1:B:118:GLU:C	1:B:120:GLY:N	2.65	0.47
1:A:46:TRP:H	10:A:2002:FMT:C	2.28	0.47
1:B:198:SER:O	1:B:201:SER:HB3	2.14	0.47
1:A:170:PRO:O	1:A:171:PRO:C	2.53	0.47
1:B:120:GLY:CA	1:B:123:GLU:OE1	2.63	0.47
1:B:109:HIS:HA	1:B:255:ARG:HH12	1.80	0.47
1:B:347:PHE:C	1:B:349:PHE:H	2.18	0.47
1:B:174:SER:HB3	1:B:175:LEU:H	1.50	0.46
1:A:8:ALA:N	1:A:9:PRO:HD3	2.30	0.46
1:A:412:MET:HG3	11:A:3057:HOH:O	2.15	0.46
1:A:574:HIS:O	1:A:574:HIS:ND1	2.48	0.46
1:B:538:GLU:HG3	11:B:3083:HOH:O	2.16	0.46
1:A:450:ASN:HB2	11:A:3116:HOH:O	2.13	0.46
1:A:464:LEU:O	1:A:468:GLN:HG3	2.14	0.46
1:A:258:GLU:CD	8:A:3003:HEM:HMB3	2.36	0.46
1:B:363:GLU:HG3	11:B:3049:HOH:O	2.15	0.46
1:B:490:ILE:HD12	1:B:490:ILE:N	2.30	0.46
1:A:260:ILE:HD13	1:A:260:ILE:O	2.16	0.46
1:B:95:ASN:HA	1:B:569:ALA:HB3	1.98	0.46
1:B:286:HIS:NE2	1:B:594:GLU:OE2	2.48	0.46
1:B:169:THR:H	1:B:170:PRO:HD2	1.80	0.46
1:A:169:THR:CG2	1:A:170:PRO:CD	2.93	0.46
1:B:100:PHE:CE1	1:B:315:ILE:HG13	2.50	0.46
1:B:260:ILE:HG13	1:B:386:ILE:HD11	1.97	0.46
1:B:478:LYS:HB2	1:B:478:LYS:HE3	1.57	0.46
1:A:169:THR:H	1:A:170:PRO:CD	2.10	0.46
1:B:432:ASP:OD1	1:B:432:ASP:C	2.54	0.46
1:A:53:ASP:O	1:A:55:LEU:N	2.49	0.46
1:A:82:ILE:HD11	1:A:479:LYS:HB2	1.97	0.46
1:A:301:GLY:O	1:A:305:GLN:HG3	2.16	0.46
1:A:354:VAL:HA	1:A:355:PRO:HD3	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLY:O	1:B:305:GLN:HG3	2.15	0.46
1:B:396:VAL:CG1	1:B:559:ILE:HD13	2.46	0.46
1:B:160:PHE:CD1	1:B:160:PHE:C	2.89	0.46
1:B:393:ASP:OD1	1:B:557:THR:HB	2.16	0.45
1:A:320:GLU:HG3	1:A:502:VAL:HG11	1.98	0.45
1:A:551:ARG:O	1:A:552:LEU:C	2.55	0.45
1:A:551:ARG:HD2	1:A:582:VAL:HG12	1.97	0.45
1:A:393:ASP:N	1:A:394:PRO:CD	2.79	0.45
1:B:227:PRO:HD2	1:B:249:PHE:CE1	2.51	0.45
1:B:200:ALA:O	1:B:204:ARG:HG3	2.17	0.45
1:B:52:GLU:OE1	1:B:57:VAL:HG11	2.16	0.45
1:A:257:SER:O	1:A:381:PHE:HA	2.17	0.45
1:A:452:TRP:HH2	10:A:2002:FMT:H	1.81	0.45
1:A:58:PRO:HG3	1:A:162:ARG:NH2	2.31	0.45
1:B:299:ILE:N	1:B:299:ILE:HD13	2.31	0.45
1:A:314:PRO:HG3	1:A:321:MET:HE2	1.98	0.45
1:B:298:LYS:HG2	1:B:536:PHE:CE2	2.51	0.45
1:A:132:TYR:OH	1:B:120:GLY:CA	2.48	0.45
1:A:96:ARG:HD2	1:A:100:PHE:CG	2.52	0.45
1:B:51:TYR:CE2	1:B:177:ARG:HB3	2.51	0.45
1:A:417:LEU:HD21	8:A:3003:HEM:HMB1	1.99	0.45
1:B:559:ILE:HA	10:B:2003:FMT:C	2.47	0.45
3:B:603:NAG:O4	3:B:604:BMA:H61	2.17	0.45
1:A:260:ILE:HG23	1:A:261:LEU:HD13	1.99	0.45
1:B:363:GLU:CG	11:B:3049:HOH:O	2.65	0.45
1:A:169:THR:N	11:A:3083:HOH:O	2.49	0.45
1:B:292:LEU:O	1:B:293:TYR:C	2.55	0.45
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.52	0.45
1:A:175:LEU:HD13	11:A:3053:HOH:O	2.15	0.44
1:B:464:LEU:O	1:B:468:GLN:HG3	2.17	0.44
1:A:128:GLN:HG2	1:A:134:VAL:HB	1.98	0.44
1:B:96:ARG:NH2	1:B:315:ILE:HB	2.32	0.44
1:B:187:LEU:HA	1:B:187:LEU:HD23	1.78	0.44
1:B:88:GLU:O	1:B:91:VAL:HG22	2.18	0.44
1:B:349:PHE:HB2	1:B:497:ASN:HD21	1.82	0.44
1:A:175:LEU:N	1:A:175:LEU:CD1	2.80	0.44
1:B:272:GLU:OE1	1:B:272:GLU:CA	2.57	0.44
1:A:407:MET:SD	1:A:408:ASN:N	2.90	0.44
1:A:120:GLY:HA3	1:A:123:GLU:OE1	2.18	0.44
1:B:407:MET:SD	1:B:408:ASN:N	2.91	0.44
1:B:298:LYS:HG2	1:B:536:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD22	1:A:174:SER:O	2.17	0.44
1:A:318:GLY:O	1:A:320:GLU:N	2.50	0.44
1:B:55:LEU:HD22	1:B:175:LEU:O	2.17	0.44
1:A:166:VAL:HA	1:A:180:ILE:HD11	1.99	0.44
1:A:175:LEU:H	1:A:175:LEU:CD1	2.30	0.44
1:B:341:ASN:HB3	1:B:446:MET:CE	2.46	0.44
1:A:124:HIS:HB2	1:B:137:ASP:CB	2.46	0.44
1:B:188:ASP:O	1:B:189:ALA:HB3	2.16	0.44
1:A:160:PHE:HD2	1:A:436:ILE:HD13	1.83	0.44
1:A:191:LEU:CD2	1:A:191:LEU:N	2.81	0.44
1:A:43:LEU:HD12	1:A:179:GLN:HB2	2.00	0.44
1:B:452:TRP:HH2	10:B:2004:FMT:O2	2.01	0.43
1:A:169:THR:HG22	1:A:170:PRO:CD	2.43	0.43
1:A:513:CYS:O	1:A:517:ARG:HG2	2.18	0.43
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.83	0.43
1:B:71:ARG:HG2	1:B:71:ARG:NH1	2.33	0.43
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.85	0.43
1:B:551:ARG:O	1:B:552:LEU:C	2.55	0.43
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.77	0.43
1:B:55:LEU:HA	1:B:55:LEU:HD23	1.83	0.43
1:B:29:ASN:ND2	1:B:526:ASP:OD1	2.51	0.43
1:A:42:ALA:HB2	1:A:166:VAL:CG1	2.46	0.43
1:A:47:LEU:HD11	1:A:455:PHE:HB2	2.00	0.43
1:B:460:GLN:HA	1:B:461:PRO:HD2	1.84	0.43
1:B:393:ASP:OD2	1:B:558:HIS:HB2	2.18	0.43
1:A:407:MET:HB3	1:A:501:MET:HE3	1.99	0.43
1:B:307:ILE:HD12	1:B:307:ILE:N	2.33	0.43
1:A:287:TRP:CH2	1:A:295:GLU:HG3	2.54	0.43
1:B:240:ILE:HD11	1:B:382:ASN:HA	2.00	0.43
1:A:386:ILE:HD12	1:A:386:ILE:N	2.33	0.43
1:B:283:LEU:HD23	1:B:283:LEU:HA	1.87	0.43
1:B:490:ILE:CD1	1:B:490:ILE:H	2.32	0.42
1:B:57:VAL:HA	1:B:58:PRO:HD3	1.92	0.42
1:A:227:PRO:HD2	1:A:249:PHE:CE1	2.54	0.42
1:A:376:LEU:HD13	1:A:380:PHE:CZ	2.54	0.42
1:A:586:ASP:OD1	1:A:586:ASP:C	2.56	0.42
1:A:2:TRP:CB	1:A:175:LEU:HB3	2.48	0.42
1:A:2:TRP:CE3	1:A:2:TRP:N	2.87	0.42
1:A:365:TYR:CE1	1:A:397:ARG:HB3	2.54	0.42
1:A:310:ARG:NH2	1:A:311:ASP:OD2	2.52	0.42
1:A:97:SER:O	1:A:404:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LYS:NZ	11:A:3094:HOH:O	2.51	0.42
1:B:557:THR:CB	1:B:559:ILE:HD12	2.49	0.42
1:B:9:PRO:C	1:B:11:PRO:HD3	2.40	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.62	0.42
1:B:98:LEU:HB3	1:B:399:LEU:HD23	2.01	0.42
1:B:99:LEU:HD21	1:B:549:PHE:CD2	2.54	0.42
1:B:362:ASP:OD1	1:B:362:ASP:C	2.58	0.42
1:A:452:TRP:O	1:A:453:ARG:C	2.58	0.42
1:B:66:THR:HB	1:B:70:PHE:C	2.39	0.42
1:B:77:GLU:OE2	1:B:81:LYS:HE3	2.20	0.42
1:B:229:PHE:CD1	1:B:247:PRO:HG2	2.55	0.42
1:B:538:GLU:O	1:B:538:GLU:HG2	2.19	0.42
1:A:124:HIS:ND1	1:B:137:ASP:HB2	2.33	0.42
1:A:113:PHE:HA	8:A:3003:HEM:O2D	2.20	0.42
1:B:9:PRO:O	1:B:11:PRO:CD	2.61	0.42
1:B:226:TYR:CE1	1:B:387:ILE:HG12	2.54	0.42
1:B:95:ASN:HA	1:B:569:ALA:HB2	2.00	0.42
1:A:246:VAL:HA	1:A:247:PRO:HD3	1.80	0.42
1:A:229:PHE:CZ	1:A:387:ILE:HD13	2.54	0.42
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.33	0.42
1:A:85:TYR:HB3	1:A:411:LYS:HA	2.02	0.42
1:B:46:TRP:CE2	1:B:340:SER:HB3	2.55	0.42
1:A:107:VAL:O	1:A:110:ASP:HB3	2.20	0.42
1:A:486:THR:O	1:A:486:THR:HG23	2.20	0.42
1:A:114:ALA:HA	1:A:180:ILE:O	2.20	0.42
1:B:118:GLU:CG	1:B:119:LEU:N	2.83	0.42
1:B:544:LEU:O	1:B:547:VAL:HG22	2.19	0.42
1:A:61:TRP:CD2	1:A:135:GLN:NE2	2.87	0.41
1:B:107:VAL:O	1:B:110:ASP:HB3	2.19	0.41
1:A:108:ASP:OD2	1:A:347:PHE:CD2	2.74	0.41
1:A:191:LEU:CD2	1:A:192:VAL:HG23	2.50	0.41
1:A:175:LEU:N	1:A:175:LEU:HD12	2.31	0.41
1:B:77:GLU:O	1:B:81:LYS:HG3	2.20	0.41
1:B:169:THR:HA	11:B:3054:HOH:O	2.20	0.41
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.54	0.41
1:B:226:TYR:OH	1:B:391:GLY:HA2	2.21	0.41
1:B:168:PRO:CG	1:B:172:TYR:CD1	3.03	0.41
1:A:244:ALA:O	1:A:245:HIS:CB	2.66	0.41
1:A:32:ARG:HD2	11:A:3034:HOH:O	2.19	0.41
1:B:462:LYS:HD2	11:B:3089:HOH:O	2.21	0.41
1:A:593:ARG:HA	1:A:593:ARG:HD3	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:H	1:A:191:LEU:CD2	2.34	0.41
1:B:191:LEU:HA	1:B:253:ASP:HB2	2.03	0.41
1:B:261:LEU:HG	1:B:399:LEU:HD21	2.03	0.41
1:A:289:GLY:HA2	1:A:292:LEU:HD22	2.01	0.41
1:A:230:ASN:OD1	1:A:232:VAL:HB	2.21	0.41
1:B:191:LEU:CD2	1:B:192:VAL:HG23	2.51	0.41
1:A:457:GLY:C	1:A:458:LEU:HD23	2.41	0.41
1:A:376:LEU:HA	1:A:379:LEU:HD12	2.01	0.41
1:B:24:ILE:HA	1:B:24:ILE:HD13	1.91	0.41
1:A:522:ILE:HD12	1:A:523:ARG:N	2.35	0.41
1:B:61:TRP:CD2	1:B:135:GLN:NE2	2.89	0.41
1:A:175:LEU:O	1:A:176:ALA:C	2.59	0.41
1:A:17:GLU:C	1:A:18:GLN:HG2	2.40	0.41
1:A:210:LEU:HB2	1:A:212:LEU:HG	2.01	0.41
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.56	0.41
1:A:376:LEU:HD22	1:A:376:LEU:O	2.21	0.41
1:B:66:THR:HB	1:B:70:PHE:O	2.21	0.41
1:B:36:LEU:HD12	1:B:36:LEU:HA	1.71	0.41
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.78	0.41
1:A:120:GLY:HA2	1:A:123:GLU:OE1	2.21	0.41
1:A:295:GLU:O	1:A:299:ILE:HG12	2.21	0.41
1:B:446:MET:HA	1:B:447:PRO:HD3	1.84	0.41
1:B:35:ALA:HB2	1:B:41:ARG:HH21	1.86	0.41
1:A:393:ASP:HB2	1:A:394:PRO:HD3	2.03	0.41
1:A:267:THR:O	1:A:271:ARG:HG3	2.21	0.41
1:B:7:GLY:C	1:B:9:PRO:HD3	2.41	0.40
1:B:51:TYR:CD2	1:B:56:ALA:HA	2.56	0.40
1:A:282:ARG:HB3	11:A:3026:HOH:O	2.21	0.40
1:B:487:PRO:CA	1:B:490:ILE:HD13	2.38	0.40
1:A:190:SER:C	1:A:192:VAL:N	2.73	0.40
1:B:131:GLU:HG2	1:B:131:GLU:H	1.78	0.40
1:B:549:PHE:CE2	1:B:553:ILE:HD11	2.55	0.40
1:B:216:ASN:HB2	1:B:227:PRO: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	593/595 (100%)	526 (89%)	54 (9%)	13 (2%)	8	41
1	B	593/595 (100%)	529 (89%)	51 (9%)	13 (2%)	8	41
All	All	1186/1190 (100%)	1055 (89%)	105 (9%)	26 (2%)	8	41

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	VAL
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	594	GLU
1	B	17	GLU
1	B	168	PRO
1	B	169	THR
1	B	171	PRO
1	B	174	SER
1	A	17	GLU
1	A	18	GLN
1	A	136	GLY
1	A	176	ALA
1	B	166	VAL
1	A	56	ALA
1	A	231	ASN
1	A	319	SER
1	B	273	HIS
1	B	173	GLN
1	B	56	ALA
1	B	209	PRO
1	B	264	THR
1	A	54	GLY
1	B	11	PRO

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Mol	Chain	Res	Type
1	B	9	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	476 (92%)	41 (8%)	15	49
1	B	517/517 (100%)	475 (92%)	42 (8%)	15	48
All	All	1034/1034 (100%)	951 (92%)	83 (8%)	15	49

All (83) 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	12	LEU
1	A	16	ASP
1	A	36	LEU
1	A	64	ARG
1	A	98	LEU
1	A	121	SER
1	A	124	HIS
1	A	130	GLU
1	A	131	GLU
1	A	137	ASP
1	A	165	PHE
1	A	166	VAL
1	A	174	SER
1	A	175	LEU
1	A	177	ARG
1	A	187	LEU
1	A	191	LEU
1	A	218	GLU
1	A	235	SER

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Mol	Chain	Res	Type
1	A	255	ARG
1	A	260	ILE
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	292	LEU
1	A	321	MET
1	A	347	PHE
1	A	360	ARG
1	A	383	THR
1	A	410	ASN
1	A	464	LEU
1	A	480	LEU
1	A	520	GLN
1	A	539	LYS
1	A	546	LYS
1	A	564	LEU
1	A	573	PRO
1	A	583	ASP
1	B	3	GLU
1	B	6	CYS
1	B	12	LEU
1	B	16	ASP
1	B	64	ARG
1	B	71	ARG
1	B	98	LEU
1	B	121	SER
1	B	124	HIS
1	B	130	GLU
1	B	131	GLU
1	B	137	ASP
1	B	166	VAL
1	B	174	SER
1	B	175	LEU
1	B	177	ARG
1	B	187	LEU
1	B	191	LEU
1	B	207	SER
1	B	255	ARG
1	B	261	LEU
1	B	268	LEU
1	B	276	LEU

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Mol	Chain	Res	Type
1	B	279	GLU
1	B	280	LEU
1	B	291	MET
1	B	292	LEU
1	B	347	PHE
1	B	360	ARG
1	B	363	GLU
1	B	376	LEU
1	B	378	THR
1	B	383	THR
1	B	394	PRO
1	B	425	THR
1	B	464	LEU
1	B	471	LEU
1	B	517	ARG
1	B	520	GLN
1	B	523	ARG
1	B	546	LYS
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	135	GLN
1	A	222	HIS
1	A	245	HIS
1	A	250	GLN
1	A	329	GLN
1	A	364	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	545	GLN
1	A	565	HIS
1	A	595	ASN
1	B	135	GLN
1	B	250	GLN
1	B	437	ASN
1	B	468	GLN
1	B	497	ASN
1	B	518	GLN

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Mol	Chain	Res	Type
1	B	520	GLN
1	B	521	GLN
1	B	545	GLN

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

22 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	0.65	0	15,19,21	0.63	0
2	NAG	A	597	2	14,14,15	0.80	0	15,19,21	0.99	1 (6%)
2	MAN	A	598	2	11,11,12	0.72	0	14,15,17	0.78	1 (7%)
2	NAG	A	599	1,2	14,14,15	0.56	0	15,19,21	0.87	1 (6%)
2	NAG	A	600	2	14,14,15	0.65	0	15,19,21	1.26	1 (6%)
2	MAN	A	601	2	11,11,12	0.57	0	14,15,17	0.42	0
3	NAG	A	602	1,3	14,14,15	0.55	0	15,19,21	0.81	0
3	NAG	A	603	3	14,14,15	0.81	0	15,19,21	1.35	2 (13%)
3	BMA	A	604	3	11,11,12	0.67	0	14,15,17	1.27	2 (14%)
4	NAG	A	605	1,4	14,14,15	0.63	0	15,19,21	1.37	3 (20%)
4	NAG	A	606	4	14,14,15	0.60	0	15,19,21	1.40	3 (20%)
2	NAG	B	596	1,2	14,14,15	0.63	0	15,19,21	0.61	0
2	NAG	B	597	2	14,14,15	0.54	0	15,19,21	1.47	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	B	598	2	11,11,12	0.66	0	14,15,17	1.00	1 (7%)
3	NAG	B	599	1,3	14,14,15	0.50	0	15,19,21	1.00	2 (13%)
3	NAG	B	600	3	14,14,15	0.93	0	15,19,21	0.95	1 (6%)
3	BMA	B	601	3	11,11,12	0.84	0	14,15,17	1.94	4 (28%)
3	NAG	B	602	1,3	14,14,15	0.48	0	15,19,21	0.78	0
3	NAG	B	603	3	14,14,15	0.68	0	15,19,21	1.87	2 (13%)
3	BMA	B	604	3	11,11,12	0.66	0	14,15,17	1.03	2 (14%)
4	NAG	B	605	1,4	14,14,15	0.49	0	15,19,21	1.45	3 (20%)
4	NAG	B	606	4	14,14,15	0.49	0	15,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	1/1/1/1
2	NAG	A	599	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	2	-	0/6/23/26	0/1/1/1
2	MAN	A	601	2	-	0/2/19/22	1/1/1/1
3	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	BMA	A	604	3	-	0/2/19/22	1/1/1/1
4	NAG	A	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	606	4	-	0/6/23/26	0/1/1/1
2	NAG	B	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	597	2	-	0/6/23/26	0/1/1/1
2	MAN	B	598	2	-	0/2/19/22	1/1/1/1
3	NAG	B	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	600	3	-	0/6/23/26	0/1/1/1
3	BMA	B	601	3	-	0/2/19/22	0/1/1/1
3	NAG	B	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	603	3	-	0/6/23/26	0/1/1/1
3	BMA	B	604	3	-	0/2/19/22	1/1/1/1
4	NAG	B	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	606	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	NAG	C4-C3-C2	-5.36	102.90	111.23
3	B	603	NAG	C2-N2-C7	-3.53	118.51	123.04
3	A	603	NAG	C4-C3-C2	-2.92	106.68	111.23
2	A	599	NAG	C2-N2-C7	-2.66	119.62	123.04
3	B	601	BMA	C2-C3-C4	-2.64	106.56	111.04
2	B	597	NAG	C2-N2-C7	-2.44	119.91	123.04
4	B	605	NAG	C2-N2-C7	-2.40	119.96	123.04
4	A	606	NAG	C2-N2-C7	-2.39	119.96	123.04
2	B	598	MAN	C3-C4-C5	-2.27	106.25	110.20
3	B	599	NAG	C4-C3-C2	-2.23	107.77	111.23
3	A	603	NAG	C2-N2-C7	-2.19	120.22	123.04
4	A	605	NAG	C1-O5-C5	-2.11	109.58	112.25
3	B	599	NAG	C2-N2-C7	-2.07	120.38	123.04
4	A	606	NAG	C3-C4-C5	2.05	113.78	110.20
3	B	604	BMA	O6-C6-C5	2.06	118.15	111.33
2	A	598	MAN	C1-O5-C5	2.19	115.02	112.25
2	B	597	NAG	C4-C3-C2	2.20	114.64	111.23
4	B	605	NAG	C3-C4-C5	2.20	114.04	110.20
4	A	605	NAG	C3-C4-C5	2.28	114.16	110.20
3	A	604	BMA	O6-C6-C5	2.29	118.91	111.33
3	B	604	BMA	C1-O5-C5	2.35	115.22	112.25
3	B	601	BMA	O5-C1-C2	2.42	114.79	110.86
2	A	597	NAG	C3-C4-C5	2.63	114.79	110.20
3	B	600	NAG	C4-C3-C2	2.76	115.52	111.23
2	A	600	NAG	C4-C3-C2	2.87	115.69	111.23
4	A	605	NAG	C4-C3-C2	3.22	116.23	111.23
3	A	604	BMA	C1-O5-C5	3.48	116.67	112.25
2	B	597	NAG	C3-C4-C5	3.57	116.42	110.20
3	B	601	BMA	O6-C6-C5	3.57	123.14	111.33
4	B	605	NAG	C4-C3-C2	3.65	116.90	111.23
4	A	606	NAG	C4-C3-C2	3.77	117.09	111.23
3	B	601	BMA	C1-O5-C5	4.94	118.51	112.25

There are no chirality outliers.

There are no torsion outliers.

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MAN	C1-C2-C3-C4-C5-O5
2	A	598	MAN	C1-C2-C3-C4-C5-O5
3	B	604	BMA	C1-C2-C3-C4-C5-O5
2	B	598	MAN	C1-C2-C3-C4-C5-O5
3	A	604	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	596	NAG	1	0
2	B	597	NAG	6	0
3	B	599	NAG	1	0
3	B	600	NAG	1	0
3	B	603	NAG	1	0
3	B	604	BMA	1	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	CO3	A	1001	-	0,3,3	0.00	-	0,3,3	0.00	-
10	FMT	A	2001	-	0,2,2	0.00	-	0,1,1	0.00	-
10	FMT	A	2002	-	0,2,2	0.00	-	0,1,1	0.00	-
7	SCN	A	3002	-	2,2,2	1.79	1 (50%)	1,1,1	1.43	0
8	HEM	A	3003	1	30,50,50	2.60	10 (33%)	24,82,82	2.34	8 (33%)
6	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
8	HEM	B	1003	1	30,50,50	3.12	11 (36%)	24,82,82	2.46	9 (37%)
10	FMT	B	2003	-	0,2,2	0.00	-	0,1,1	0.00	-
10	FMT	B	2004	-	0,2,2	0.00	-	0,1,1	0.00	-
9	OSM	B	3021	-	1,3,3	0.60	0	0,2,2	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
6	CO3	A	1001	-	-	0/0/0/0	0/0/0/0
10	FMT	A	2001	-	-	0/0/0/0	0/0/0/0
10	FMT	A	2002	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SCN	A	3002	-	-	0/0/0/0	0/0/0/0
8	HEM	A	3003	1	-	0/10/54/54	0/0/8/8
6	CO3	B	1002	-	-	0/0/0/0	0/0/0/0
8	HEM	B	1003	1	-	0/10/54/54	0/0/8/8
10	FMT	B	2003	-	-	0/0/0/0	0/0/0/0
10	FMT	B	2004	-	-	0/0/0/0	0/0/0/0
9	OSM	B	3021	-	-	0/0/1/1	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1003	HEM	C3B-C4B	-8.21	1.44	1.51
8	A	3003	HEM	C3B-C4B	-7.44	1.45	1.51
8	A	3003	HEM	C3D-C4D	-5.81	1.44	1.51
8	B	1003	HEM	C3D-C4D	-4.19	1.46	1.51
8	B	1003	HEM	C1A-CHA	-4.08	1.28	1.39
8	B	1003	HEM	C2C-C1C	-3.90	1.45	1.52
8	A	3003	HEM	C2C-C1C	-3.30	1.46	1.52
7	A	3002	SCN	C-S	2.10	1.77	1.63
8	A	3003	HEM	C4C-NC	2.40	1.39	1.36
8	A	3003	HEM	FE-NB	2.47	2.10	1.97
8	B	1003	HEM	CMA-C3A	2.60	1.57	1.51
8	A	3003	HEM	FE-ND	2.74	2.12	1.97
8	B	1003	HEM	CHD-C4C	2.92	1.43	1.36
8	B	1003	HEM	C3B-CAB	3.00	1.57	1.51
8	A	3003	HEM	C3C-CAC	3.05	1.57	1.51
8	B	1003	HEM	FE-NB	3.15	2.14	1.97
8	A	3003	HEM	C3B-CAB	3.26	1.57	1.51
8	A	3003	HEM	CAA-C2A	3.60	1.58	1.52
8	B	1003	HEM	CHC-C1C	3.62	1.44	1.36
8	B	1003	HEM	CAA-C2A	5.05	1.60	1.52
8	A	3003	HEM	FE-NC	5.23	2.16	1.95
8	B	1003	HEM	FE-NC	8.76	2.30	1.95

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1003	HEM	CBD-CAD-C3D	-2.89	105.14	113.55
8	A	3003	HEM	CBD-CAD-C3D	-2.60	105.99	113.55
8	B	1003	HEM	C3B-C4B-NB	-2.24	107.34	111.63
8	A	3003	HEM	CMA-C3A-C4A	-2.22	124.70	128.36
8	A	3003	HEM	C2D-C3D-C4D	2.22	105.27	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	3003	HEM	CMD-C2D-C3D	2.48	125.30	114.35
8	B	1003	HEM	C2D-C3D-C4D	2.76	106.18	101.50
8	B	1003	HEM	CMD-C2D-C3D	2.80	126.75	114.35
8	B	1003	HEM	C3B-C4B-CHC	3.53	128.14	123.16
8	A	3003	HEM	CMB-C2B-C3B	3.92	126.32	116.53
8	A	3003	HEM	CAD-C3D-C4D	4.11	126.97	112.47
8	B	1003	HEM	CAD-C3D-C4D	4.15	127.12	112.47
8	B	1003	HEM	CMB-C2B-C3B	4.51	127.79	116.53
8	B	1003	HEM	CAD-C3D-C2D	4.69	126.70	113.22
8	A	3003	HEM	CAD-C3D-C2D	5.06	127.76	113.22
8	B	1003	HEM	CMC-C2C-C3C	5.51	130.28	116.53
8	A	3003	HEM	CMC-C2C-C3C	5.52	130.31	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2001	FMT	1	0
10	A	2002	FMT	2	0
7	A	3002	SCN	3	0
8	A	3003	HEM	11	0
8	B	1003	HEM	7	0
10	B	2003	FMT	2	0
10	B	2004	FMT	1	0
9	B	3021	OSM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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