



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2E9E
Title : Crystal structure of the complex of goat lactoperoxidase with Nitrate at 3.25 Å resolution
Authors : Singh, A.K.; Prem kumar, R.; Singh, N.; Sharma, S.; Singh, S.B.; Bhushan, A.; Kaur, P.; Singh, T.P.
Deposited on : 2007-01-25
Resolution : 3.25 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

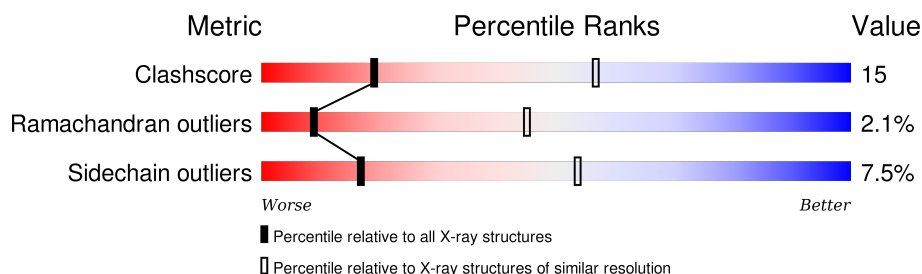
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)

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 $\leq 5\%$. 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	
1	B	595	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NO3	A	607	-	X	-	-
5	NO3	A	608	-	X	-	-
5	NO3	B	607	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NO3	B	608	-	X	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10299 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
			4754	3021	844	863	26			
1	B	595	Total	C	N	O	S	0	0	0
			4754	3021	844	863	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	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

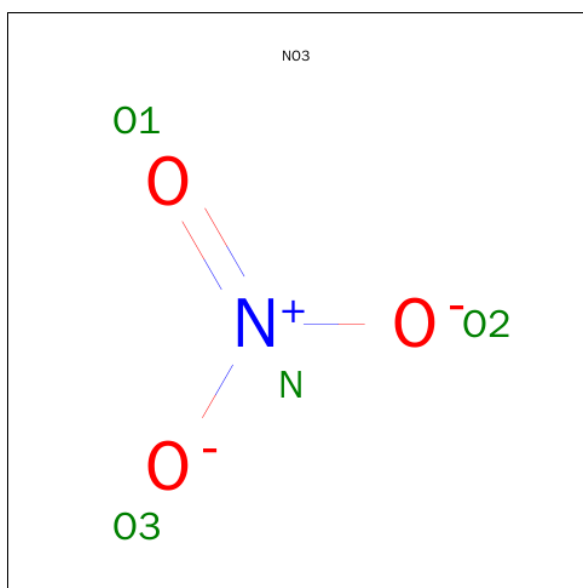
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

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

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

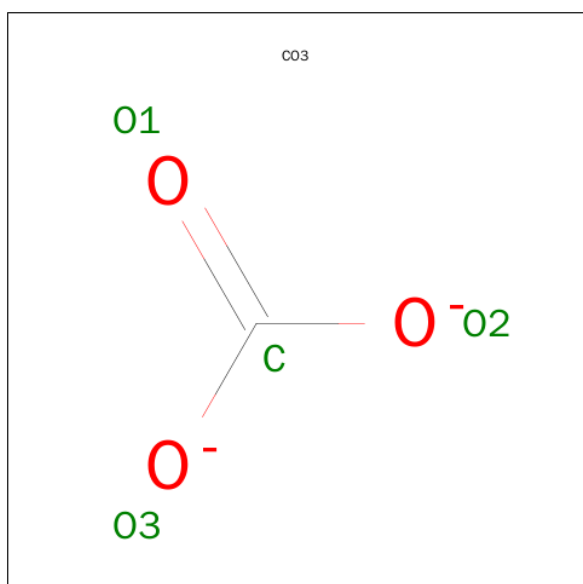
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



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

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

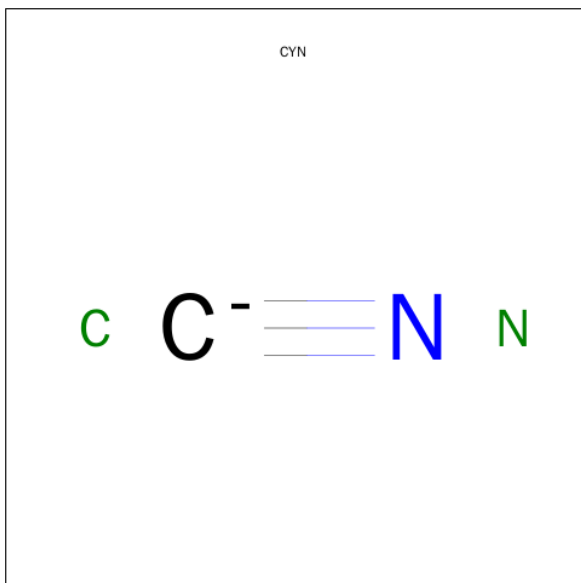


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

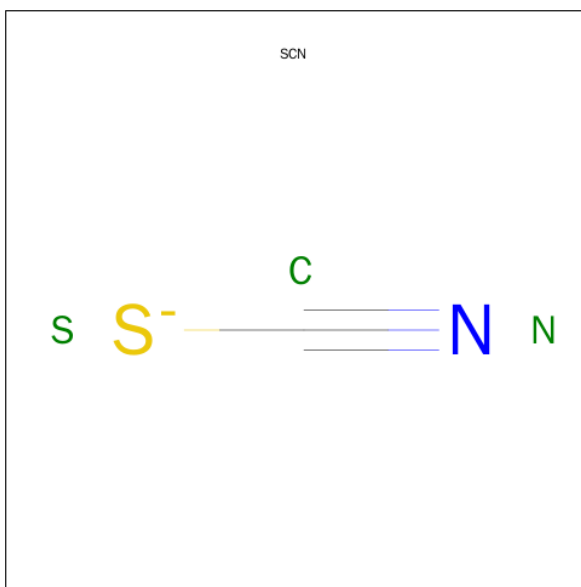
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CYANIDE ION (three-letter code: CYN) (formula: CN).



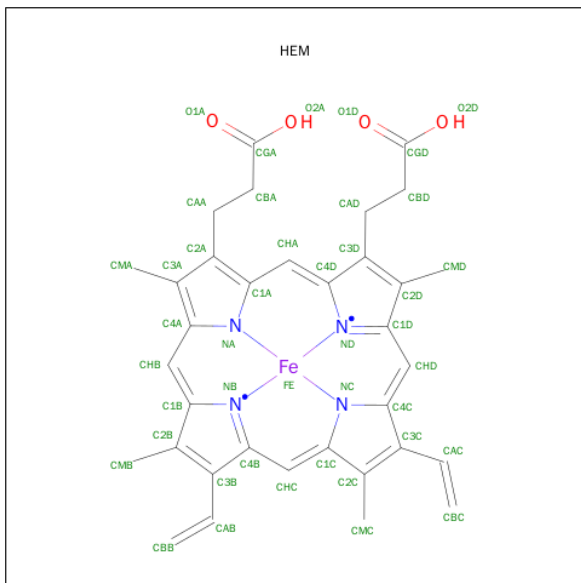
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	0	0
			2	1	1		

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



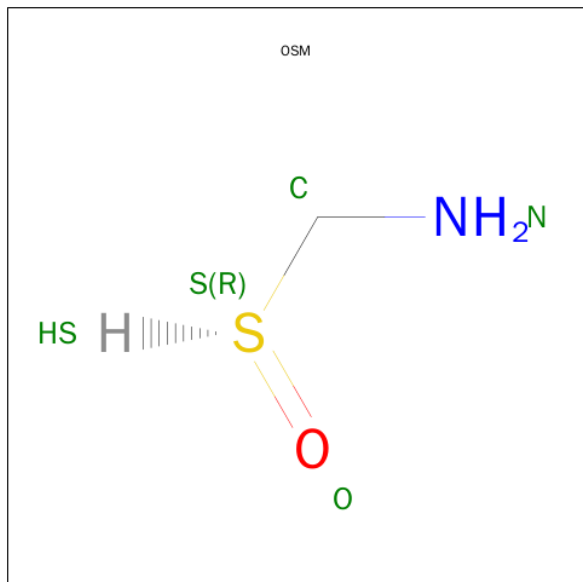
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH₅NOS).



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

- Molecule 12 is water.

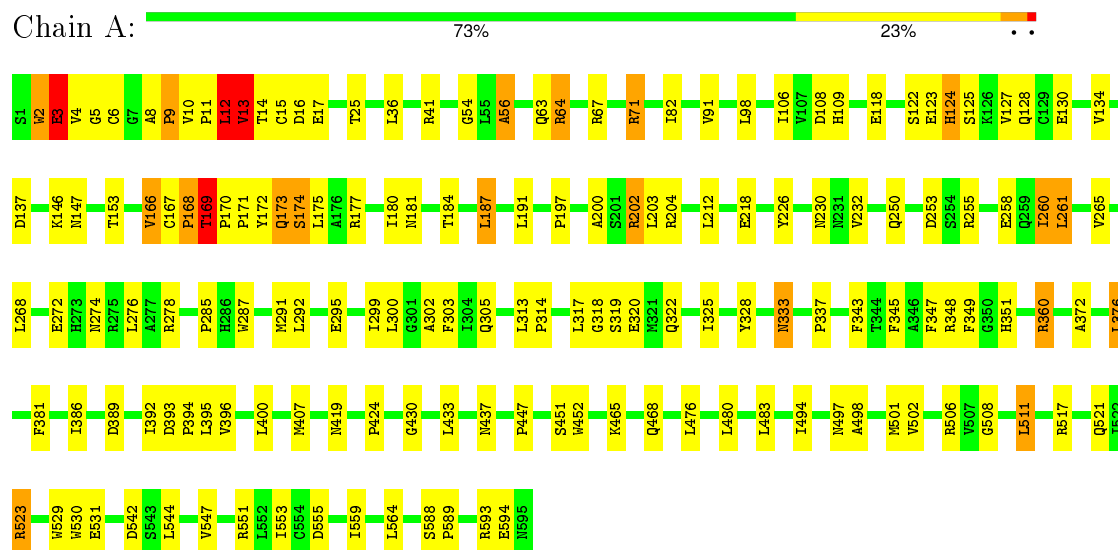
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	180	Total	O	0	0
			180	180		
12	B	200	Total	O	0	0
			200	200		

3 Residue-property plots

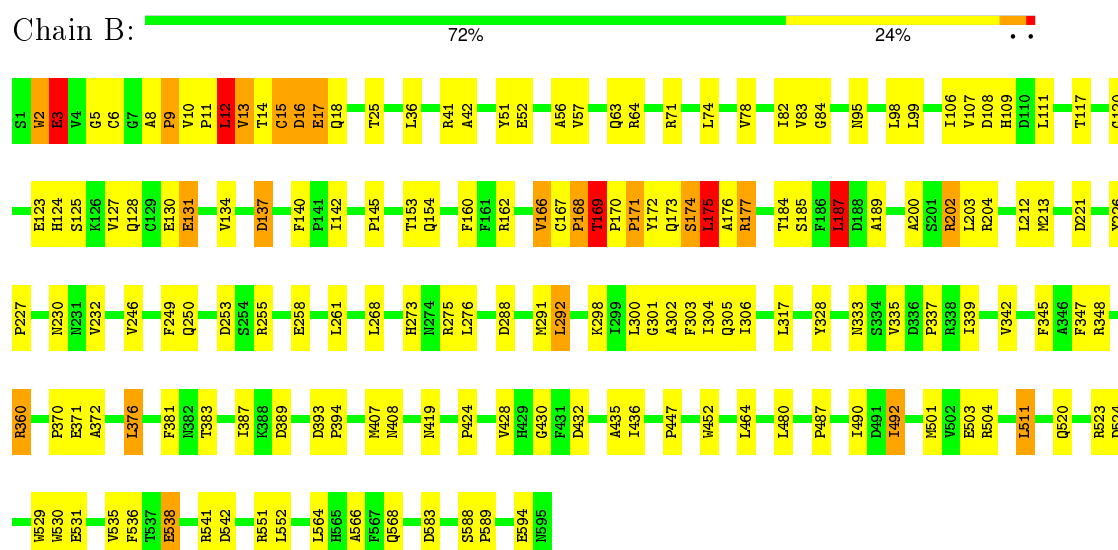
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Lactoperoxidase



• Molecule 1: Lactoperoxidase



4 Data and refinement statistics

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	58.52Å 72.54Å 83.98Å 85.30° 84.06° 75.68°	Depositor
Resolution (Å)	20.00 – 3.25	Depositor
% Data completeness (in resolution range)	94.8 (20.00-3.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10299	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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, CA, BMA, OSM, HEM, NO3, CYN, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.55	0/4883	0.73	5/6632 (0.1%)
1	B	0.54	0/4883	0.74	7/6632 (0.1%)
All	All	0.54	0/9766	0.73	12/13264 (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 (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	13	VAL	CA-CB-CG2	-6.31	101.43	110.90
1	A	15	CYS	CA-CB-SG	-6.10	103.03	114.00
1	B	13	VAL	CA-CB-CG1	6.03	119.94	110.90
1	B	13	VAL	CB-CA-C	-6.00	100.01	111.40
1	B	12	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	13	VAL	N-CA-C	5.78	126.59	111.00
1	B	13	VAL	CA-CB-CG2	-5.44	102.75	110.90
1	B	15	CYS	CA-CB-SG	-5.43	104.23	114.00
1	A	13	VAL	N-CA-C	5.42	125.63	111.00
1	A	12	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	13	VAL	CA-CB-CG1	5.01	118.42	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	LEU	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	4754	0	4647	127	0
1	B	4754	0	4645	152	0
2	A	78	0	68	3	0
2	B	39	0	34	4	0
3	A	39	0	34	0	0
3	B	78	0	68	6	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	8	0	0	0	0
5	B	8	0	0	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	2	0	0	1	0
9	A	3	0	0	0	0
10	A	43	0	30	7	0
10	B	43	0	30	8	0
11	B	4	0	5	1	0
12	A	180	0	0	14	0
12	B	200	0	0	15	0
All	All	10299	0	9611	292	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 15.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HB2	1:A:13:VAL:HG23	1.21	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.36	1.08
1:B:12:LEU:HB2	1:B:13:VAL:HG23	1.13	1.08
1:B:258:GLU:OE2	10:B:821:HEM:HMB3	1.54	1.06
1:A:13:VAL:HG12	1:A:14:THR:H	1.16	1.05
1:B:13:VAL:HG12	1:B:14:THR:H	1.16	1.05
1:B:175:LEU:HD12	1:B:176:ALA:H	1.17	1.05
1:A:258:GLU:OE2	10:A:801:HEM:HMB3	1.54	1.04
1:B:487:PRO:HA	1:B:490:ILE:HD13	1.37	1.02
1:B:8:ALA:HB1	1:B:9:PRO:HD2	1.41	0.99
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.43	0.97
1:B:12:LEU:HB2	1:B:13:VAL:CG2	1.97	0.95
1:A:108:ASP:OD2	10:A:801:HEM:HMD3	1.66	0.94
1:B:175:LEU:CD1	1:B:176:ALA:H	1.82	0.93
1:A:12:LEU:HB2	1:A:13:VAL:CG2	1.99	0.92
1:B:167:CYS:HB2	1:B:168:PRO:HD3	1.51	0.92
1:B:13:VAL:CG1	1:B:14:THR:H	1.79	0.91
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.01	0.90
1:B:108:ASP:OD2	10:B:821:HEM:HMD3	1.71	0.89
1:A:109:HIS:NE2	8:A:901:CYN:C	2.37	0.87
1:A:13:VAL:CG1	1:A:14:THR:H	1.81	0.87
1:A:230:ASN:HD21	1:A:232:VAL:HG12	1.42	0.84
1:A:230:ASN:ND2	1:A:232:VAL:HG12	1.93	0.83
1:A:134:VAL:HG12	12:A:951:HOH:O	1.78	0.83
1:B:8:ALA:CB	1:B:9:PRO:HD2	2.08	0.82
1:B:487:PRO:HA	1:B:490:ILE:CD1	2.11	0.81
1:B:52:GLU:HB3	1:B:57:VAL:HG12	1.61	0.80
1:A:13:VAL:HG12	1:A:14:THR:N	1.97	0.80
1:B:381:PHE:CZ	1:B:424:PRO:HG3	2.16	0.80
1:B:13:VAL:HG12	1:B:14:THR:N	1.95	0.80
1:A:169:THR:H	1:A:170:PRO:CD	1.96	0.77
1:A:123:GLU:HG3	1:A:125:SER:H	1.50	0.77
1:B:2:TRP:HB3	1:B:175:LEU:HD23	1.66	0.77
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.15	0.75
1:B:2:TRP:HZ3	1:B:174:SER:HB3	1.53	0.74
1:B:12:LEU:CB	1:B:13:VAL:HG23	2.06	0.74
2:A:601:MAN:H4	12:A:945:HOH:O	1.88	0.74
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.87	0.73
1:B:169:THR:H	1:B:170:PRO:CD	2.01	0.73
1:A:2:TRP:HZ3	1:A:174:SER:HB3	1.53	0.73
1:A:260:ILE:HD12	1:A:395:LEU:HD13	1.70	0.73
1:B:2:TRP:CB	1:B:175:LEU:HD23	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:CZ	1:B:250:GLN:HE22	2.01	0.73
1:B:109:HIS:NE2	11:B:921:OSM:S	2.62	0.72
1:A:260:ILE:HD11	1:A:386:ILE:HG12	1.69	0.72
1:A:2:TRP:CB	1:A:175:LEU:HD12	2.19	0.72
1:A:230:ASN:HD21	1:A:232:VAL:CG1	2.02	0.71
1:A:63:GLN:O	1:A:71:ARG:NH2	2.23	0.71
1:A:124:HIS:HB2	1:B:137:ASP:CG	2.12	0.70
3:B:601:BMA:H4	12:B:999:HOH:O	1.91	0.70
1:A:2:TRP:HB2	1:A:175:LEU:CD1	2.22	0.69
1:B:432:ASP:O	1:B:436:ILE:HG12	1.91	0.69
1:B:56:ALA:HB1	1:B:177:ARG:HD3	1.75	0.69
1:B:8:ALA:HB1	1:B:9:PRO:CD	2.20	0.68
1:B:169:THR:H	1:B:170:PRO:HD2	1.57	0.68
1:B:173:GLN:HG2	12:B:986:HOH:O	1.92	0.68
3:B:603:NAG:H62	3:B:604:BMA:O2	1.94	0.67
1:A:124:HIS:HD2	1:A:127:VAL:HG21	1.59	0.67
1:A:260:ILE:CD1	1:A:395:LEU:HD13	2.25	0.66
1:A:169:THR:H	1:A:170:PRO:HD2	1.60	0.66
1:B:95:ASN:ND2	1:B:95:ASN:O	2.28	0.66
1:B:487:PRO:CA	1:B:490:ILE:HD13	2.22	0.66
1:B:10:VAL:HG11	1:B:41:ARG:CZ	2.26	0.65
10:A:801:HEM:HBB2	10:A:801:HEM:HMB1	1.76	0.65
1:B:407:MET:HB3	1:B:501:MET:CE	2.26	0.65
1:B:123:GLU:HG3	1:B:125:SER:H	1.59	0.65
3:B:600:NAG:H61	3:B:601:BMA:O2	1.97	0.65
1:A:2:TRP:HB3	1:A:175:LEU:HD12	1.77	0.65
1:A:106:ILE:HD11	1:A:265:VAL:HG11	1.79	0.64
1:A:300:LEU:O	1:A:303:PHE:HB3	1.97	0.64
1:A:260:ILE:HD13	1:A:260:ILE:O	1.98	0.64
1:A:465:LYS:HD2	1:A:468:GLN:NE2	2.13	0.64
1:B:8:ALA:C	1:B:10:VAL:H	2.01	0.64
1:B:246:VAL:HG11	1:B:387:ILE:HD13	1.80	0.64
1:B:108:ASP:CG	10:B:821:HEM:HMD3	2.18	0.63
1:B:407:MET:HB3	1:B:501:MET:HE3	1.80	0.63
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.79	0.62
1:A:260:ILE:HG23	1:A:261:LEU:HD13	1.80	0.62
10:A:801:HEM:HMC2	10:A:801:HEM:HBC2	1.82	0.61
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.33	0.61
1:A:407:MET:HB3	1:A:501:MET:CE	2.30	0.61
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.36	0.61
1:B:253:ASP:OD2	1:B:255:ARG:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:PRO:HD2	1:A:452:TRP:HE1	1.64	0.61
1:B:108:ASP:OD2	10:B:821:HEM:HMD2	2.00	0.61
1:A:376:LEU:HD22	1:A:376:LEU:O	2.00	0.61
2:A:596:NAG:H3	12:A:1082:HOH:O	2.00	0.61
10:B:821:HEM:HBC2	10:B:821:HEM:HMC1	1.83	0.60
1:B:134:VAL:HA	12:B:995:HOH:O	2.01	0.60
10:B:821:HEM:HBB2	10:B:821:HEM:HMB1	1.83	0.60
1:B:12:LEU:C	1:B:13:VAL:CG2	2.69	0.60
1:B:13:VAL:CG1	1:B:14:THR:N	2.56	0.60
1:B:175:LEU:HD12	1:B:176:ALA:N	2.02	0.60
1:A:106:ILE:HD11	1:A:265:VAL:CG1	2.32	0.59
1:A:260:ILE:CD1	1:A:395:LEU:CD1	2.81	0.59
1:B:230:ASN:CG	1:B:232:VAL:HG12	2.23	0.59
1:A:202:ARG:NH1	1:A:250:GLN:HE22	2.01	0.59
1:B:51:TYR:OH	1:B:177:ARG:HB3	2.03	0.59
1:B:227:PRO:HD2	12:B:949:HOH:O	2.02	0.59
1:A:2:TRP:HB2	1:A:175:LEU:HD12	1.85	0.58
1:B:568:GLN:HB3	2:B:596:NAG:C5	2.33	0.58
1:B:503:GLU:HG2	1:B:504:ARG:HG3	1.85	0.58
1:B:212:LEU:HB2	12:B:958:HOH:O	2.03	0.57
1:A:108:ASP:CG	10:A:801:HEM:HMD3	2.24	0.57
1:A:128:GLN:NE2	1:B:170:PRO:HB3	2.20	0.56
1:A:106:ILE:CD1	1:A:265:VAL:HG11	2.35	0.56
1:A:274:ASN:O	1:A:278:ARG:HG2	2.06	0.56
1:B:551:ARG:HD3	1:B:583:ASP:O	2.04	0.56
1:A:8:ALA:C	1:A:10:VAL:H	2.08	0.56
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.28	0.56
1:B:168:PRO:HB2	1:B:170:PRO:HD2	1.87	0.56
1:B:202:ARG:CZ	1:B:250:GLN:NE2	2.68	0.56
1:A:8:ALA:CB	1:A:9:PRO:CD	2.80	0.56
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.86	0.56
1:A:169:THR:N	1:A:170:PRO:CD	2.66	0.56
1:A:2:TRP:HZ3	1:A:174:SER:CB	2.19	0.56
1:B:8:ALA:O	1:B:10:VAL:N	2.39	0.55
1:B:249:PHE:CE2	12:B:949:HOH:O	2.60	0.55
1:B:11:PRO:HB2	1:B:12:LEU:HD12	1.88	0.55
1:A:13:VAL:CG1	1:A:14:THR:N	2.59	0.55
1:B:2:TRP:CZ3	1:B:174:SER:HB3	2.38	0.55
1:B:2:TRP:HZ3	1:B:174:SER:CB	2.19	0.55
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.89	0.54
1:B:169:THR:N	1:B:170:PRO:CD	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLN:OE1	2:B:596:NAG:H5	2.08	0.54
1:A:285:PRO:HB3	12:A:1025:HOH:O	2.07	0.54
1:B:10:VAL:HG11	1:B:41:ARG:NH2	2.23	0.54
1:A:544:LEU:O	1:A:547:VAL:HG22	2.08	0.53
1:A:260:ILE:HD12	1:A:395:LEU:CD1	2.35	0.53
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.42	0.53
1:A:12:LEU:HD11	1:A:197:PRO:HG2	1.91	0.53
2:A:600:NAG:H61	2:A:601:MAN:H2	1.91	0.53
1:B:383:THR:O	1:B:387:ILE:HD12	2.09	0.53
1:A:529:TRP:CD1	1:A:531:GLU:HB2	2.44	0.53
1:B:302:ALA:O	1:B:306:ILE:HG13	2.08	0.53
1:B:15:CYS:C	1:B:17:GLU:H	2.13	0.52
1:B:13:VAL:HB	12:B:1084:HOH:O	2.10	0.52
1:B:230:ASN:ND2	1:B:232:VAL:HG12	2.25	0.52
1:B:16:ASP:O	1:B:18:GLN:N	2.40	0.52
1:B:300:LEU:O	1:B:303:PHE:HB3	2.10	0.52
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.45	0.52
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.40	0.51
1:B:301:GLY:O	1:B:305:GLN:HG3	2.10	0.51
1:B:78:VAL:HG13	1:B:82:ILE:HD12	1.92	0.51
1:A:118:GLU:HA	12:A:932:HOH:O	2.10	0.51
1:A:12:LEU:C	1:A:13:VAL:CG2	2.79	0.51
1:B:166:VAL:O	1:B:167:CYS:C	2.48	0.51
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.09	0.51
1:A:260:ILE:HD11	1:A:386:ILE:CG1	2.39	0.51
1:B:84:GLY:HA2	12:B:963:HOH:O	2.11	0.50
1:B:568:GLN:HB3	2:B:596:NAG:C6	2.42	0.50
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.11	0.50
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.93	0.50
3:B:601:BMA:H62	12:B:971:HOH:O	2.11	0.50
1:A:396:VAL:HB	1:A:559:ILE:HD11	1.92	0.50
1:B:169:THR:HB	12:B:926:HOH:O	2.10	0.49
1:B:249:PHE:CZ	12:B:949:HOH:O	2.54	0.49
1:B:588:SER:OG	1:B:589:PRO:HD3	2.13	0.49
1:B:436:ILE:HD13	1:B:436:ILE:N	2.27	0.49
3:B:604:BMA:H4	12:B:1101:HOH:O	2.12	0.49
1:A:333:ASN:HD22	1:A:333:ASN:C	2.15	0.49
1:A:56:ALA:HB1	1:A:177:ARG:HD3	1.94	0.49
1:B:2:TRP:HB2	1:B:175:LEU:HD23	1.92	0.49
1:B:56:ALA:CB	1:B:177:ARG:HD3	2.42	0.49
1:B:490:ILE:H	1:B:490:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:HIS:HD2	1:A:127:VAL:CG2	2.25	0.49
1:B:246:VAL:CG1	1:B:387:ILE:HD13	2.43	0.49
1:B:393:ASP:HB2	1:B:394:PRO:HD3	1.95	0.49
1:B:588:SER:N	1:B:589:PRO:CD	2.76	0.48
1:A:260:ILE:HD11	1:A:395:LEU:CD1	2.43	0.48
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.96	0.48
1:B:52:GLU:OE1	1:B:57:VAL:HG11	2.14	0.48
1:B:360:ARG:NH1	1:B:372:ALA:HA	2.28	0.48
1:B:594:GLU:CD	1:B:594:GLU:H	2.15	0.48
1:A:8:ALA:O	1:A:10:VAL:N	2.46	0.48
1:B:370:PRO:HG2	1:B:371:GLU:HG3	1.95	0.48
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.48	0.48
1:B:108:ASP:OD1	10:B:821:HEM:HMD3	2.13	0.48
1:A:8:ALA:O	1:A:10:VAL:HG23	2.13	0.48
1:B:360:ARG:NH2	1:B:389:ASP:OD2	2.47	0.48
1:A:2:TRP:HB2	1:A:175:LEU:HD11	1.96	0.47
1:B:298:LYS:HG2	1:B:536:PHE:CZ	2.50	0.47
1:B:328:TYR:CD1	1:B:523:ARG:HD3	2.49	0.47
1:A:258:GLU:CD	10:A:801:HEM:HMB3	2.29	0.47
1:A:392:ILE:O	1:A:396:VAL:HG23	2.14	0.47
1:B:12:LEU:C	1:B:13:VAL:HG22	2.35	0.47
1:B:523:ARG:HD2	1:B:524:ASP:OD1	2.15	0.47
1:A:25:THR:O	1:A:184:THR:HG22	2.13	0.47
1:B:335:VAL:O	1:B:337:PRO:HD3	2.15	0.47
1:B:8:ALA:O	1:B:10:VAL:HG23	2.15	0.47
1:A:588:SER:OG	1:A:589:PRO:HD3	2.15	0.47
1:B:328:TYR:HD1	1:B:523:ARG:HD3	1.80	0.47
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.79	0.47
1:B:142:ILE:HD12	1:B:160:PHE:HB2	1.97	0.47
1:A:180:ILE:HG22	1:A:181:ASN:N	2.30	0.47
1:B:2:TRP:HB2	1:B:175:LEU:CD2	2.45	0.47
1:B:120:GLY:HA2	1:B:123:GLU:HB2	1.96	0.47
1:A:212:LEU:HB2	12:A:937:HOH:O	2.15	0.47
1:A:299:ILE:O	1:A:302:ALA:HB3	2.15	0.46
1:B:3:GLU:C	1:B:5:GLY:H	2.18	0.46
1:B:8:ALA:CB	1:B:9:PRO:CD	2.86	0.46
10:A:801:HEM:CMC	10:A:801:HEM:HBC2	2.45	0.46
1:B:432:ASP:HB3	1:B:435:ALA:HB3	1.98	0.46
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.31	0.46
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.97	0.46
1:A:517:ARG:O	1:A:521:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ALA:HB2	1:B:166:VAL:HG11	1.98	0.46
1:A:3:GLU:C	1:A:5:GLY:H	2.20	0.46
1:A:2:TRP:CZ3	1:A:174:SER:HB3	2.40	0.46
1:B:511:LEU:HD12	1:B:511:LEU:HA	1.77	0.46
1:B:568:GLN:HB3	2:B:596:NAG:H5	1.98	0.45
1:A:407:MET:HB3	1:A:501:MET:HE3	1.97	0.45
1:A:594:GLU:HG2	12:A:931:HOH:O	2.15	0.45
1:A:551:ARG:NH2	1:A:555:ASP:OD1	2.45	0.45
1:A:10:VAL:CG1	1:A:41:ARG:CZ	2.94	0.45
1:B:529:TRP:CD1	1:B:531:GLU:HB2	2.52	0.45
1:B:111:LEU:O	1:B:339:ILE:HD13	2.16	0.45
1:A:167:CYS:N	12:A:1000:HOH:O	2.50	0.45
1:B:106:ILE:HG22	1:B:107:VAL:N	2.31	0.45
1:B:360:ARG:NH1	1:B:371:GLU:O	2.48	0.45
1:A:325:ILE:O	1:A:325:ILE:HG22	2.17	0.45
1:A:502:VAL:HG13	1:A:508:GLY:HA2	1.99	0.45
10:B:821:HEM:HBB2	10:B:821:HEM:CMB	2.47	0.44
1:A:200:ALA:O	1:A:204:ARG:HG3	2.16	0.44
1:A:593:ARG:NH2	12:A:1011:HOH:O	2.50	0.44
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.99	0.44
1:A:67:ARG:NH1	12:A:966:HOH:O	2.43	0.44
1:A:447:PRO:HD2	1:A:452:TRP:NE1	2.30	0.44
1:B:490:ILE:N	1:B:490:ILE:HD12	2.32	0.44
1:B:127:VAL:CG1	1:B:131:GLU:HG3	2.48	0.44
1:A:123:GLU:HG2	1:A:125:SER:HB3	2.00	0.44
1:A:511:LEU:HA	1:A:511:LEU:HD12	1.66	0.44
1:B:8:ALA:C	1:B:10:VAL:N	2.70	0.44
1:B:117:THR:HG23	1:B:162:ARG:O	2.18	0.44
1:A:64:ARG:H	1:A:64:ARG:HG3	1.68	0.43
1:B:288:ASP:O	1:B:292:LEU:HD22	2.18	0.43
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.54	0.43
1:B:530:TRP:CE2	1:B:531:GLU:HG3	2.53	0.43
1:B:538:GLU:HG2	1:B:541:ARG:NH2	2.33	0.43
1:B:170:PRO:HB3	1:B:171:PRO:HD2	2.00	0.43
1:B:99:LEU:HD23	1:B:566:ALA:O	2.18	0.43
3:B:600:NAG:H61	3:B:601:BMA:C2	2.49	0.43
1:A:12:LEU:CB	1:A:13:VAL:HG23	2.16	0.43
1:B:168:PRO:HB2	1:B:169:THR:H	1.53	0.43
1:A:260:ILE:HD11	1:A:395:LEU:HD11	2.01	0.43
1:B:551:ARG:O	1:B:552:LEU:C	2.56	0.43
1:B:230:ASN:ND2	1:B:232:VAL:CG1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:O	1:B:173:GLN:HG3	2.19	0.42
1:A:202:ARG:HG3	12:A:1013:HOH:O	2.19	0.42
1:B:189:ALA:HB2	1:B:304:ILE:HD12	2.01	0.42
1:B:345:PHE:HA	1:B:348:ARG:HG3	2.01	0.42
1:B:83:VAL:HG12	1:B:83:VAL:O	2.20	0.42
1:A:146:LYS:O	1:A:147:ASN:HB2	2.20	0.42
1:B:175:LEU:CD1	1:B:176:ALA:N	2.66	0.42
1:B:185:SER:HA	1:B:339:ILE:CD1	2.50	0.42
1:B:452:TRP:CD1	1:B:492:ILE:HG13	2.55	0.42
1:B:63:GLN:O	1:B:71:ARG:NH2	2.52	0.42
1:B:74:LEU:HD12	1:B:145:PRO:HB3	2.01	0.42
1:B:95:ASN:HB3	12:B:996:HOH:O	2.20	0.42
1:B:140:PHE:O	1:B:160:PHE:HB3	2.20	0.42
1:B:298:LYS:NZ	1:B:535:VAL:O	2.34	0.42
1:B:127:VAL:HG13	1:B:131:GLU:HG3	2.00	0.42
1:B:154:GLN:HB3	1:B:154:GLN:HE21	1.56	0.42
1:B:187:LEU:HD13	1:B:305:GLN:HA	2.02	0.41
1:A:506:ARG:HD2	12:A:1020:HOH:O	2.20	0.41
1:A:291:MET:HE1	12:A:984:HOH:O	2.21	0.41
1:B:490:ILE:CD1	1:B:490:ILE:H	2.33	0.41
1:B:342:VAL:HG12	5:B:608:NO3:O1	2.20	0.41
1:A:588:SER:N	1:A:589:PRO:CD	2.84	0.41
1:A:419:ASN:O	1:A:430:GLY:HA2	2.21	0.41
1:A:36:LEU:HG	1:A:337:PRO:HD2	2.02	0.41
1:B:447:PRO:HD2	1:B:452:TRP:HE1	1.85	0.41
1:A:343:PHE:O	1:A:345:PHE:N	2.53	0.41
1:A:287:TRP:CZ3	1:A:295:GLU:HG3	2.56	0.41
1:A:41:ARG:NH1	12:A:1005:HOH:O	2.49	0.41
1:B:2:TRP:HZ3	1:B:174:SER:HG	1.68	0.41
1:B:95:ASN:OD1	12:B:977:HOH:O	2.22	0.41
1:A:318:GLY:C	1:A:320:GLU:H	2.23	0.41
1:B:407:MET:SD	1:B:408:ASN:N	2.94	0.40
1:A:318:GLY:C	1:A:320:GLU:N	2.74	0.40
1:A:172:TYR:O	1:A:173:GLN:HG3	2.21	0.40
1:B:523:ARG:CD	1:B:524:ASP:OD1	2.69	0.40
1:B:36:LEU:HA	1:B:36:LEU:HD12	1.87	0.40
1:B:419:ASN:O	1:B:430:GLY:HA2	2.22	0.40
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.90	0.40
1:B:376:LEU:O	1:B:376:LEU:HD22	2.20	0.40
1:B:25:THR:O	1:B:184:THR:HG22	2.21	0.40
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HB2	1:A:169:THR:H	1.61	0.40
1:B:200:ALA:O	1:B:204:ARG:HG3	2.21	0.40
1:A:313:LEU:N	1:A:314:PRO:CD	2.84	0.40
1:B:275:ARG:NH1	12:B:1045:HOH:O	2.53	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%)	538 (91%)	40 (7%)	15 (2%)	7	40
1	B	593/595 (100%)	541 (91%)	42 (7%)	10 (2%)	11	50
All	All	1186/1190 (100%)	1079 (91%)	82 (7%)	25 (2%)	9	45

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	12	LEU
1	A	169	THR
1	A	171	PRO
1	B	9	PRO
1	B	12	LEU
1	B	17	GLU
1	B	168	PRO
1	B	169	THR
1	B	174	SER
1	A	168	PRO
1	B	171	PRO
1	A	3	GLU
1	A	174	SER

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Mol	Chain	Res	Type
1	B	3	GLU
1	A	17	GLU
1	A	54	GLY
1	A	56	ALA
1	B	187	LEU
1	A	166	VAL
1	A	173	GLN
1	A	319	SER
1	B	166	VAL
1	A	11	PRO
1	A	4	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	477 (92%)	40 (8%)	16	52
1	B	517/517 (100%)	479 (93%)	38 (7%)	17	54
All	All	1034/1034 (100%)	956 (92%)	78 (8%)	17	53

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	3	GLU
1	A	6	CYS
1	A	12	LEU
1	A	13	VAL
1	A	16	ASP
1	A	64	ARG
1	A	71	ARG
1	A	91	VAL
1	A	98	LEU
1	A	122	SER
1	A	124	HIS

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Mol	Chain	Res	Type
1	A	130	GLU
1	A	137	ASP
1	A	153	THR
1	A	166	VAL
1	A	169	THR
1	A	187	LEU
1	A	202	ARG
1	A	203	LEU
1	A	218	GLU
1	A	226	TYR
1	A	260	ILE
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	451	SER
1	A	480	LEU
1	A	494	ILE
1	A	511	LEU
1	A	523	ARG
1	A	542	ASP
1	A	564	LEU
1	B	2	TRP
1	B	3	GLU
1	B	6	CYS
1	B	12	LEU
1	B	16	ASP
1	B	64	ARG
1	B	98	LEU
1	B	124	HIS
1	B	128	GLN
1	B	130	GLU
1	B	131	GLU
1	B	137	ASP
1	B	153	THR
1	B	169	THR

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Mol	Chain	Res	Type
1	B	175	LEU
1	B	177	ARG
1	B	187	LEU
1	B	202	ARG
1	B	203	LEU
1	B	261	LEU
1	B	268	LEU
1	B	276	LEU
1	B	291	MET
1	B	292	LEU
1	B	317	LEU
1	B	333	ASN
1	B	347	PHE
1	B	360	ARG
1	B	376	LEU
1	B	428	VAL
1	B	464	LEU
1	B	480	LEU
1	B	492	ILE
1	B	511	LEU
1	B	520	GLN
1	B	538	GLU
1	B	542	ASP
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	128	GLN
1	A	147	ASN
1	A	217	GLN
1	A	222	HIS
1	A	230	ASN
1	A	250	GLN
1	A	333	ASN
1	A	341	ASN
1	A	364	ASN
1	A	408	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	545	GLN
1	A	558	HIS
1	A	571	ASN
1	B	250	GLN
1	B	333	ASN
1	B	341	ASN
1	B	366	GLN
1	B	408	ASN
1	B	437	ASN
1	B	468	GLN
1	B	497	ASN
1	B	521	GLN
1	B	571	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 ⓘ

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	0.60	0	15,19,21	0.68	0
2	NAG	A	597	2	14,14,15	0.67	0	15,19,21	1.37	3 (20%)
2	MAN	A	598	2	11,11,12	0.48	0	14,15,17	1.51	1 (7%)
2	NAG	A	599	1,2	14,14,15	0.71	1 (7%)	15,19,21	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	600	2	14,14,15	0.78	0	15,19,21	1.18	1 (6%)
2	MAN	A	601	2	11,11,12	0.60	0	14,15,17	0.78	0
3	NAG	A	602	1,3	14,14,15	0.68	0	15,19,21	1.20	1 (6%)
3	NAG	A	603	3	14,14,15	0.54	0	15,19,21	1.51	2 (13%)
3	BMA	A	604	3	11,11,12	0.72	0	14,15,17	1.63	2 (14%)
4	NAG	A	605	1,4	14,14,15	0.60	0	15,19,21	1.53	2 (13%)
4	NAG	A	606	4	14,14,15	0.66	0	15,19,21	1.57	1 (6%)
2	NAG	B	596	1,2	14,14,15	0.74	0	15,19,21	1.64	4 (26%)
2	NAG	B	597	2	14,14,15	0.62	0	15,19,21	2.58	1 (6%)
2	MAN	B	598	2	11,11,12	0.89	0	14,15,17	1.96	3 (21%)
3	NAG	B	599	1,3	14,14,15	0.50	0	15,19,21	1.04	1 (6%)
3	NAG	B	600	3	14,14,15	0.72	0	15,19,21	1.42	2 (13%)
3	BMA	B	601	3	11,11,12	0.71	0	14,15,17	2.43	4 (28%)
3	NAG	B	602	1,3	14,14,15	0.72	0	15,19,21	1.46	2 (13%)
3	NAG	B	603	3	14,14,15	0.71	0	15,19,21	1.38	1 (6%)
3	BMA	B	604	3	11,11,12	0.65	0	14,15,17	1.72	2 (14%)
4	NAG	B	605	1,4	14,14,15	0.62	0	15,19,21	1.70	3 (20%)
4	NAG	B	606	4	14,14,15	0.68	0	15,19,21	0.97	1 (6%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	599	NAG	C1-C2	2.24	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	NAG	O3-C3-C4	-2.21	105.37	110.34
3	A	603	NAG	C2-N2-C7	-2.18	120.24	123.04
3	B	599	NAG	C2-N2-C7	-2.09	120.35	123.04
2	B	596	NAG	O7-C7-C8	-2.06	118.27	122.06
2	B	596	NAG	O4-C4-C5	-2.03	103.86	109.24
4	B	606	NAG	C4-C3-C2	2.02	114.36	111.23
3	A	604	BMA	O2-C2-C1	2.02	113.25	109.21
2	B	598	MAN	O5-C5-C6	2.07	111.83	107.35
2	A	597	NAG	C1-O5-C5	2.09	114.90	112.25
3	B	600	NAG	C1-O5-C5	2.11	114.93	112.25
3	B	604	BMA	O5-C5-C6	2.20	112.10	107.35
4	A	605	NAG	C3-C4-C5	2.24	114.10	110.20
3	B	602	NAG	C4-C3-C2	2.48	115.08	111.23
3	B	601	BMA	O2-C2-C1	2.49	114.20	109.21
2	A	599	NAG	C1-O5-C5	2.65	115.61	112.25
2	A	597	NAG	C3-C4-C5	2.82	115.11	110.20
4	B	605	NAG	C3-C4-C5	2.84	115.15	110.20
2	B	596	NAG	C6-C5-C4	2.89	120.16	113.02
3	B	601	BMA	C1-C2-C3	2.97	113.05	109.54
3	B	601	BMA	O5-C1-C2	3.01	115.73	110.86
2	A	597	NAG	C4-C3-C2	3.02	115.92	111.23
3	A	602	NAG	C1-O5-C5	3.12	116.20	112.25
2	B	596	NAG	C4-C3-C2	3.20	116.20	111.23
2	A	600	NAG	C4-C3-C2	3.39	116.50	111.23
2	B	598	MAN	C1-C2-C3	3.49	113.67	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAG	C1-O5-C5	3.49	116.68	112.25
3	B	600	NAG	C4-C3-C2	4.06	117.54	111.23
3	B	603	NAG	C1-O5-C5	4.18	117.56	112.25
4	B	605	NAG	C4-C3-C2	4.23	117.81	111.23
4	A	606	NAG	C4-C3-C2	4.31	117.93	111.23
4	A	605	NAG	C4-C3-C2	4.44	118.13	111.23
3	A	604	BMA	C1-O5-C5	4.54	118.01	112.25
3	A	603	NAG	C1-O5-C5	4.69	118.19	112.25
2	A	598	MAN	C1-O5-C5	4.93	118.50	112.25
3	B	604	BMA	C1-O5-C5	5.42	119.13	112.25
2	B	598	MAN	C1-O5-C5	5.58	119.33	112.25
3	B	601	BMA	C1-O5-C5	7.46	121.72	112.25
2	B	597	NAG	C1-O5-C5	8.94	123.60	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	B	598	MAN	C1-C2-C3-C4-C5-O5
2	A	601	MAN	C1-C2-C3-C4-C5-O5
3	B	604	BMA	C1-C2-C3-C4-C5-O5
3	A	604	BMA	C1-C2-C3-C4-C5-O5
2	A	598	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	596	NAG	1	0
2	A	600	NAG	1	0
2	A	601	MAN	2	0
2	B	596	NAG	4	0
3	B	600	NAG	2	0
3	B	601	BMA	4	0
3	B	603	NAG	1	0
3	B	604	BMA	2	0

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NO3	A	607	-	3,3,3	3.51	3 (100%)	3,3,3	0.22	0
5	NO3	A	608	-	3,3,3	3.09	3 (100%)	3,3,3	0.10	0
6	CO3	A	609	-	0,3,3	0.00	-	0,3,3	0.00	-
10	HEM	A	801	1,8	30,50,50	2.46	9 (30%)	24,82,82	2.23	7 (29%)
8	CYN	A	901	10	0,1,1	0.00	-	0,0,0	0.00	-
9	SCN	A	902	-	2,2,2	1.96	1 (50%)	1,1,1	1.75	0
5	NO3	B	607	-	3,3,3	3.50	3 (100%)	3,3,3	0.24	0
5	NO3	B	608	-	3,3,3	2.96	3 (100%)	3,3,3	0.16	0
6	CO3	B	609	-	0,3,3	0.00	-	0,3,3	0.00	-
10	HEM	B	821	1,11	30,50,50	2.53	10 (33%)	24,82,82	2.25	9 (37%)
11	OSM	B	921	10	1,3,3	0.48	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
5	NO3	A	607	-	-	0/0/0/0	0/0/0/0
5	NO3	A	608	-	-	0/0/0/0	0/0/0/0
6	CO3	A	609	-	-	0/0/0/0	0/0/0/0
10	HEM	A	801	1,8	-	0/10/54/54	0/0/8/8
8	CYN	A	901	10	-	0/0/0/0	0/0/0/0
9	SCN	A	902	-	-	0/0/0/0	0/0/0/0
5	NO3	B	607	-	-	0/0/0/0	0/0/0/0
5	NO3	B	608	-	-	0/0/0/0	0/0/0/0
6	CO3	B	609	-	-	0/0/0/0	0/0/0/0
10	HEM	B	821	1,11	-	0/10/54/54	0/0/8/8
11	OSM	B	921	10	-	0/0/1/1	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	801	HEM	C3B-C4B	-7.98	1.44	1.51
10	B	821	HEM	C3B-C4B	-7.29	1.45	1.51
10	B	821	HEM	C3D-C4D	-5.05	1.45	1.51
10	A	801	HEM	C3D-C4D	-4.84	1.45	1.51
10	A	801	HEM	C2C-C1C	-3.60	1.45	1.52
10	B	821	HEM	C2C-C1C	-3.11	1.46	1.52
10	A	801	HEM	C4C-NC	2.04	1.38	1.36
10	B	821	HEM	CAA-C2A	2.31	1.56	1.52
10	A	801	HEM	C3C-CAC	2.37	1.55	1.51
10	B	821	HEM	FE-NB	2.47	2.10	1.97
5	B	608	NO3	O2-N	2.55	1.38	1.25
9	A	902	SCN	C-S	2.58	1.80	1.63
10	A	801	HEM	CAA-C2A	2.68	1.56	1.52
5	B	608	NO3	O3-N	2.69	1.39	1.25
5	A	608	NO3	O3-N	2.69	1.39	1.25
5	A	608	NO3	O2-N	2.76	1.39	1.25
10	B	821	HEM	C3C-CAC	2.76	1.56	1.51
10	B	821	HEM	C1C-NC	2.78	1.39	1.36
10	B	821	HEM	C4C-NC	2.82	1.39	1.36
10	A	801	HEM	C3B-CAB	2.89	1.56	1.51
5	B	607	NO3	O2-N	2.93	1.40	1.25
5	A	607	NO3	O2-N	2.98	1.40	1.25
10	B	821	HEM	C3B-CAB	3.07	1.57	1.51
5	A	607	NO3	O3-N	3.14	1.41	1.25
5	B	607	NO3	O3-N	3.15	1.41	1.25
5	B	608	NO3	O1-N	3.53	1.38	1.24
5	A	608	NO3	O1-N	3.72	1.39	1.24
10	A	801	HEM	FE-NC	4.25	2.12	1.95
5	A	607	NO3	O1-N	4.26	1.41	1.24
5	B	607	NO3	O1-N	4.26	1.41	1.24
10	A	801	HEM	FE-NB	4.40	2.20	1.97
10	B	821	HEM	FE-NC	6.42	2.21	1.95

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	801	HEM	CBD-CAD-C3D	-2.74	105.59	113.55
10	B	821	HEM	CBD-CAD-C3D	-2.60	105.97	113.55
10	B	821	HEM	CAA-C2A-C1A	-2.42	124.38	127.01
10	B	821	HEM	CBA-CAA-C2A	-2.41	108.21	112.53
10	B	821	HEM	CMD-C2D-C3D	2.03	123.31	114.35
10	A	801	HEM	CMD-C2D-C3D	2.17	123.95	114.35
10	B	821	HEM	C2D-C3D-C4D	2.50	105.75	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	801	HEM	C2D-C3D-C4D	2.74	106.14	101.50
10	B	821	HEM	CMB-C2B-C3B	3.49	125.25	116.53
10	B	821	HEM	CAD-C3D-C2D	4.03	124.81	113.22
10	A	801	HEM	CMB-C2B-C3B	4.13	126.84	116.53
10	A	801	HEM	CAD-C3D-C4D	4.38	127.91	112.47
10	A	801	HEM	CAD-C3D-C2D	4.43	125.94	113.22
10	A	801	HEM	CMC-C2C-C3C	4.75	128.39	116.53
10	B	821	HEM	CAD-C3D-C4D	4.81	129.43	112.47
10	B	821	HEM	CMC-C2C-C3C	4.83	128.59	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	801	HEM	7	0
8	A	901	CYN	1	0
5	B	608	NO3	1	0
10	B	821	HEM	8	0
11	B	921	OSM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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