



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N8F
Title : Crystal structure of the complex of goat lactoperoxidase with thiocyanate at 3.2 Å resolution
Authors : Vikram, G.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2010-05-28
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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

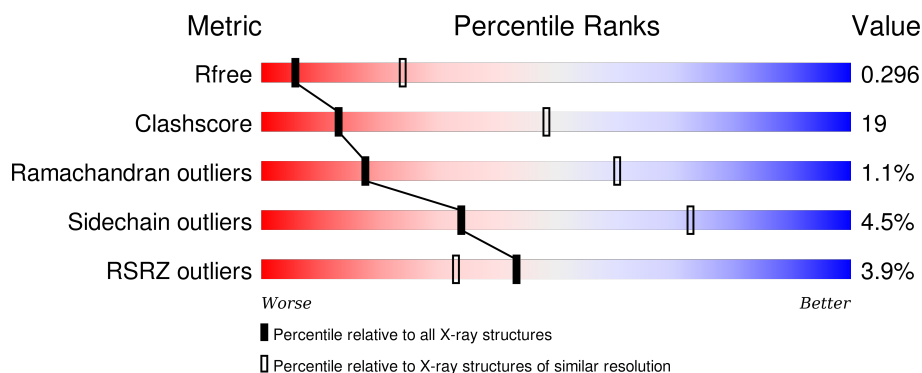
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (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.

Mol	Chain	Length	Quality of chain
1	A	595	<div> <div>4%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
1	B	595	<div> <div>4%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>

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
4	NO3	A	607	-	X	-	-
4	NO3	A	608	-	X	-	-
4	NO3	B	607	-	X	-	X
4	NO3	B	608	-	X	-	-
6	SCN	A	901	-	X	-	-
6	SCN	B	902	-	-	X	-
7	HEM	A	801	-	-	X	X
7	HEM	B	821	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10057 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	P	S	0	0	0
			4757	3021	844	865	1	26			
1	B	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			

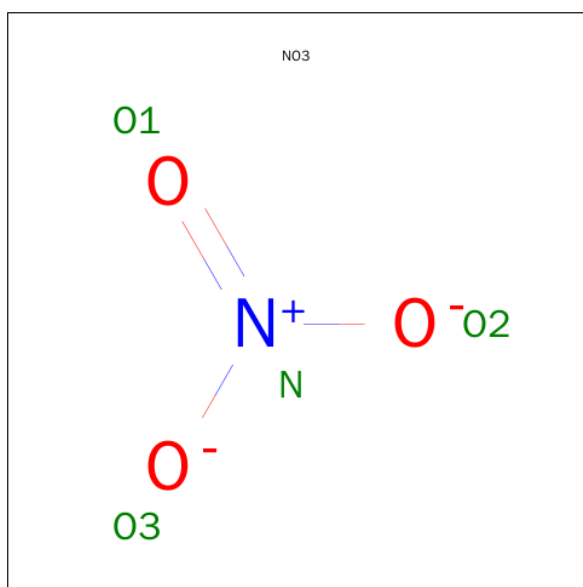
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

- 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		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).

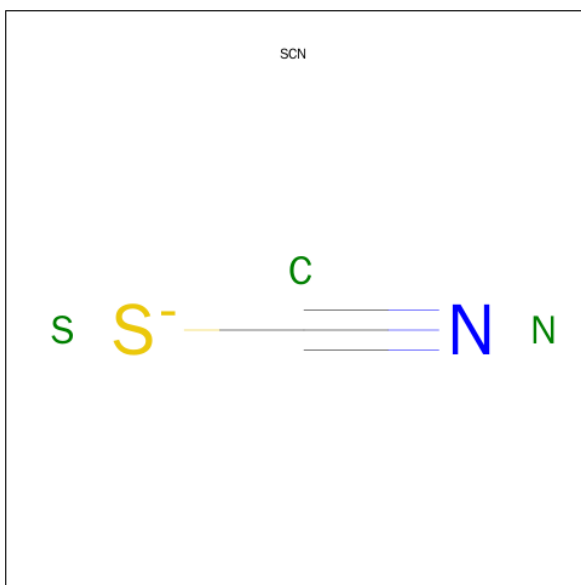


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		

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

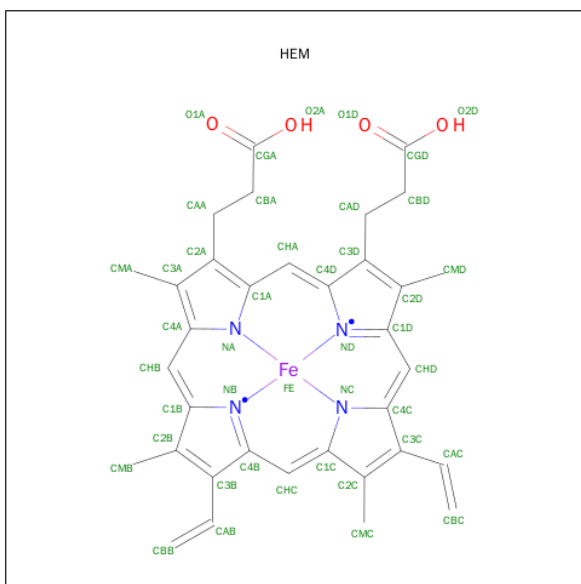
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

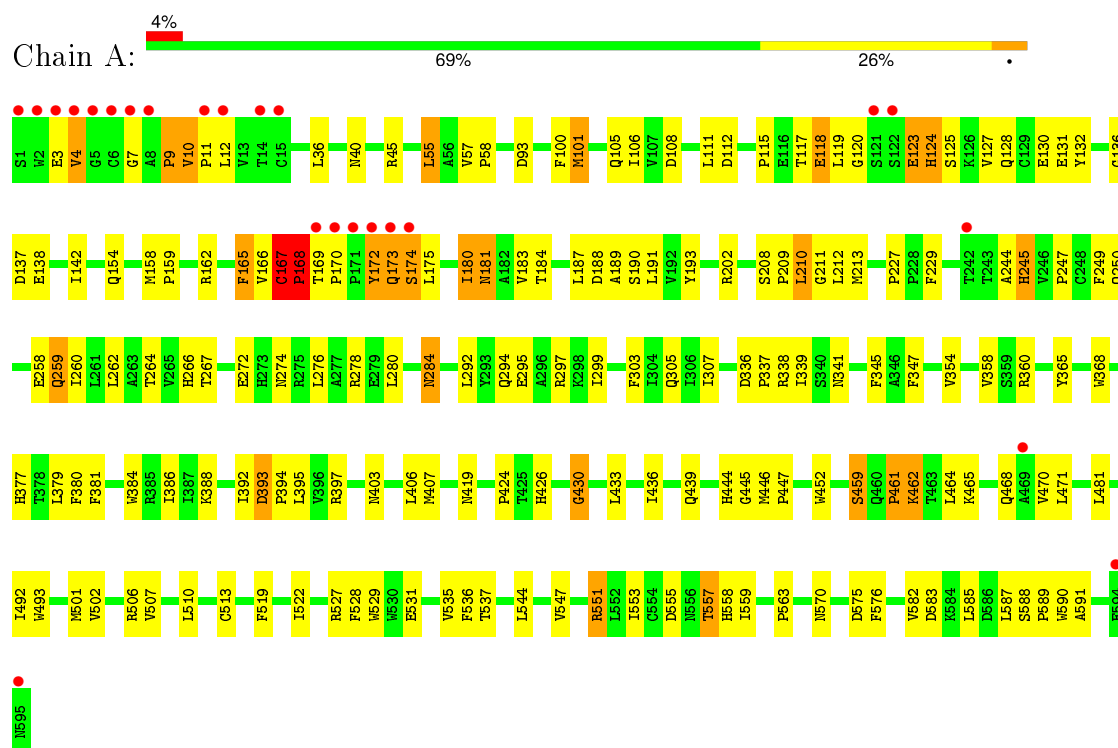
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	87	Total	O	0	0
			87	87		
8	B	100	Total	O	0	0
			100	100		

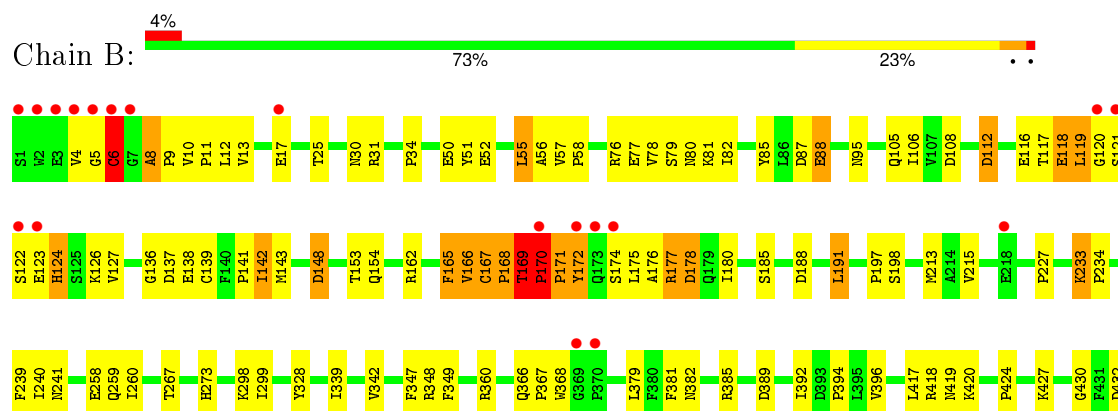
3 Residue-property plots [i](#)

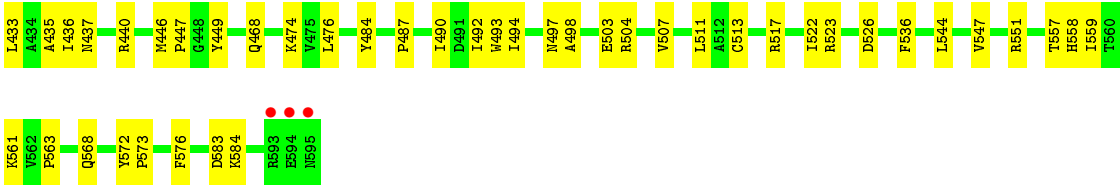
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoperoxidase



• Molecule 1: Lactoperoxidase





4 Data and refinement statistics

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)	24.98 – 3.25 24.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.6 (24.98-3.25) 92.9 (24.98-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.23Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.248 0.210 , 0.296	Depositor DCC
R_{free} test set	1011 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 71.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19767 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10057	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, BMA, HEM, NO3

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	0.58	0/4875	0.67	7/6621 (0.1%)
1	B	0.55	1/4875 (0.0%)	0.67	5/6621 (0.1%)
All	All	0.57	1/9750 (0.0%)	0.67	12/13242 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	PHE	CD1-CE1	-5.40	1.28	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	PRO	CA-N-CD	-13.40	92.74	111.50
1	B	169	THR	C-N-CD	-11.10	96.18	120.60
1	B	166	VAL	N-CA-C	6.07	127.39	111.00
1	A	10	VAL	N-CA-C	-5.80	95.35	111.00
1	A	7	GLY	N-CA-C	5.77	127.52	113.10
1	A	108	ASP	CB-CA-C	-5.69	99.02	110.40
1	B	166	VAL	C-N-CA	-5.62	107.65	121.70
1	A	167	CYS	C-N-CD	-5.58	108.31	120.60
1	B	170	PRO	C-N-CD	-5.48	108.55	120.60
1	B	6	CYS	N-CA-C	-5.33	96.62	111.00
1	A	471	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	244	ALA	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4757	0	4644	177	0
1	B	4757	0	4644	185	0
2	A	84	0	75	0	0
2	B	84	0	75	2	0
3	A	39	0	34	0	0
3	B	39	0	34	1	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	1	0
6	B	3	0	0	3	0
7	A	43	0	30	21	0
7	B	43	0	30	19	0
8	A	87	0	0	1	0
8	B	100	0	0	3	0
All	All	10057	0	9566	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (369) 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:258:GLU:OE2	7:B:821:HEM:CMB	1.63	1.46
1:B:108:ASP:OD2	7:B:821:HEM:CMD	1.65	1.45
1:A:258:GLU:OE2	7:A:801:HEM:CMB	1.67	1.39
1:B:170:PRO:CB	1:B:171:PRO:HD3	1.50	1.36
1:B:170:PRO:HB2	1:B:171:PRO:CD	1.46	1.36
1:A:258:GLU:OE2	7:A:801:HEM:HMB1	1.01	1.17
1:B:9:PRO:O	1:B:11:PRO:HD3	1.40	1.17
1:B:557:THR:HG22	1:B:558:HIS:H	1.11	1.12
1:B:108:ASP:OD2	7:B:821:HEM:HMD1	0.94	1.09
1:B:258:GLU:OE2	7:B:821:HEM:HMB3	0.89	1.07
1:B:120:GLY:HA3	1:B:123:GLU:CG	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:THR:HG22	1:B:170:PRO:HD3	1.41	1.02
1:A:168:PRO:HD2	1:A:168:PRO:O	1.60	1.01
1:A:284:ASN:ND2	1:A:591:ALA:HA	1.76	1.00
1:B:557:THR:HG22	1:B:558:HIS:N	1.75	0.98
1:A:360:ARG:HG2	1:A:394:PRO:HB2	1.43	0.98
1:B:167:CYS:CB	1:B:168:PRO:HD3	1.91	0.97
1:A:553:ILE:HB	1:A:559:ILE:HD11	1.47	0.96
1:B:4:VAL:HG22	1:B:5:GLY:N	1.80	0.95
1:B:4:VAL:CG2	1:B:5:GLY:N	2.30	0.95
1:B:120:GLY:HA3	1:B:123:GLU:HG3	1.49	0.94
1:B:166:VAL:HG12	1:B:180:ILE:CG2	1.97	0.94
1:A:210:LEU:N	1:A:210:LEU:CD1	2.30	0.93
1:B:258:GLU:CD	7:B:821:HEM:HMB3	1.89	0.93
1:B:169:THR:CG2	1:B:170:PRO:HD3	1.99	0.92
1:B:260:ILE:HD11	1:B:379:LEU:HD22	1.49	0.91
1:A:258:GLU:OE2	7:A:801:HEM:C2B	2.25	0.90
1:B:557:THR:CG2	1:B:558:HIS:H	1.86	0.89
1:A:209:PRO:C	1:A:210:LEU:CD1	2.41	0.88
1:A:210:LEU:N	1:A:210:LEU:HD13	1.88	0.88
1:A:4:VAL:HG13	1:A:4:VAL:O	1.72	0.88
1:B:168:PRO:HG2	1:B:172:TYR:CG	2.09	0.88
1:A:209:PRO:C	1:A:210:LEU:HD12	1.94	0.86
1:A:284:ASN:HD21	1:A:591:ALA:HA	1.40	0.86
1:A:258:GLU:OE1	7:A:801:HEM:C1B	2.28	0.86
1:B:432:ASP:O	1:B:436:ILE:HG12	1.76	0.85
1:B:137:ASP:OD1	1:B:138:GLU:HG2	1.77	0.85
1:B:167:CYS:HB3	1:B:168:PRO:HD3	1.58	0.85
7:B:821:HEM:C4A	6:B:902:SCN:S	2.70	0.85
1:B:9:PRO:O	1:B:11:PRO:CD	2.24	0.84
1:B:166:VAL:HG13	1:B:178:ASP:O	1.79	0.83
1:A:452:TRP:CD1	1:A:492:ILE:HD11	2.15	0.82
1:A:10:VAL:HG13	1:A:10:VAL:O	1.78	0.82
1:A:209:PRO:O	1:A:210:LEU:HD12	1.78	0.82
1:A:4:VAL:CG1	1:A:4:VAL:O	2.29	0.81
1:A:10:VAL:O	1:A:10:VAL:CG1	2.30	0.80
1:B:166:VAL:HG12	1:B:180:ILE:HG22	1.63	0.80
1:A:3:GLU:N	1:A:4:VAL:HA	1.96	0.80
1:B:123:GLU:HB2	1:B:126:LYS:HD2	1.64	0.78
1:B:197:PRO:HD2	1:B:198:SEP:O3P	1.84	0.78
7:A:801:HEM:HMC2	7:A:801:HEM:HBC2	1.66	0.77
1:B:88:GLU:HB2	8:B:626:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:HB2	1:B:490:ILE:HG13	1.64	0.77
1:B:118:GLU:HG2	1:B:118:GLU:O	1.67	0.77
1:B:166:VAL:HG12	1:B:180:ILE:HG23	1.66	0.76
1:B:8:ALA:N	1:B:9:PRO:CD	2.49	0.76
1:B:167:CYS:HB3	1:B:168:PRO:CD	2.16	0.76
1:B:260:ILE:CD1	1:B:379:LEU:HD22	2.15	0.76
1:A:259:GLN:HE21	7:A:801:HEM:CBB	1.99	0.75
1:B:120:GLY:HA3	1:B:123:GLU:HG2	1.68	0.75
1:B:260:ILE:HG13	1:B:379:LEU:HB3	1.66	0.75
1:A:115:PRO:HD2	1:A:180:ILE:CG2	2.16	0.75
1:B:174:SER:O	1:B:175:LEU:C	2.26	0.74
1:B:166:VAL:CG1	1:B:180:ILE:HG22	2.16	0.74
1:B:112:ASP:HB2	7:B:821:HEM:O1D	1.87	0.74
1:A:123:GLU:HG3	1:A:124:HIS:N	2.01	0.73
1:B:108:ASP:OD2	7:B:821:HEM:C2D	2.41	0.73
1:A:209:PRO:C	1:A:210:LEU:HD13	2.08	0.73
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.24	0.73
1:A:166:VAL:O	1:A:168:PRO:HD3	1.89	0.72
1:B:80:ASN:ND2	1:B:148:ASP:OD1	2.22	0.72
1:A:259:GLN:NE2	7:A:801:HEM:CAB	2.53	0.71
1:A:249:PHE:HE2	1:A:386:ILE:HD11	1.55	0.71
1:A:259:GLN:HE21	7:A:801:HEM:CAB	2.04	0.70
1:B:167:CYS:CB	1:B:168:PRO:CD	2.68	0.70
1:A:169:THR:N	1:A:170:PRO:HD2	2.06	0.70
1:B:8:ALA:N	1:B:9:PRO:HD3	2.06	0.70
1:B:381:PHE:CZ	1:B:424:PRO:HG3	2.27	0.70
7:A:801:HEM:HBB2	7:A:801:HEM:HMB2	1.74	0.69
1:B:419:ASN:O	1:B:420:LYS:HG3	1.92	0.69
1:B:446:MET:HE3	1:B:492:ILE:HD11	1.73	0.69
1:A:117:THR:HG22	1:A:162:ARG:O	1.93	0.69
1:A:124:HIS:CD2	1:A:124:HIS:H	2.09	0.69
1:B:169:THR:HG22	1:B:170:PRO:CD	2.22	0.69
1:A:166:VAL:O	1:A:168:PRO:CD	2.40	0.69
1:B:449:TYR:CB	1:B:490:ILE:HG13	2.23	0.69
1:A:123:GLU:HG3	1:A:125:SER:H	1.58	0.68
6:B:902:SCN:S	8:B:928:HOH:O	2.52	0.68
1:A:433:LEU:HA	1:A:436:ILE:HG22	1.76	0.67
1:A:142:ILE:HG12	1:A:439:GLN:HG3	1.77	0.67
1:A:527:ARG:HH21	1:A:528:PHE:HZ	1.40	0.67
1:A:452:TRP:NE1	1:A:492:ILE:HD11	2.09	0.67
1:A:117:THR:O	1:A:117:THR:HG23	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG12	1:A:180:ILE:HD12	1.76	0.67
1:A:168:PRO:O	1:A:168:PRO:CD	2.40	0.67
1:B:137:ASP:CG	1:B:138:GLU:H	1.96	0.66
1:B:417:LEU:HD13	1:B:433:LEU:HD23	1.77	0.66
1:A:173:GLN:O	1:A:174:SER:HB2	1.95	0.66
1:A:260:ILE:HG13	1:A:379:LEU:HD22	1.78	0.66
1:B:56:ALA:HB1	1:B:177:ARG:NH2	2.10	0.66
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.30	0.65
1:A:393:ASP:CG	1:A:557:THR:HG22	2.16	0.65
1:B:120:GLY:CA	1:B:123:GLU:HG2	2.27	0.65
1:B:168:PRO:HG2	1:B:172:TYR:CD1	2.31	0.65
1:B:4:VAL:HG22	1:B:5:GLY:H	1.58	0.65
1:A:461:PRO:O	1:A:462:LYS:HG2	1.97	0.64
1:A:360:ARG:CG	1:A:394:PRO:HB2	2.23	0.64
1:A:55:LEU:HD22	1:A:175:LEU:O	1.98	0.64
1:B:56:ALA:HB1	1:B:177:ARG:CZ	2.28	0.64
1:B:258:GLU:OE2	7:B:821:HEM:C2B	2.48	0.64
1:B:168:PRO:CG	1:B:172:TYR:CD2	2.82	0.63
1:B:168:PRO:HG2	1:B:172:TYR:CD2	2.34	0.63
1:A:193:TYR:CE2	1:A:213:MET:HE1	2.34	0.63
1:A:136:GLY:O	1:A:137:ASP:HB2	1.98	0.63
1:A:570:ASN:HB2	1:A:575:ASP:CB	2.28	0.63
1:B:108:ASP:OD2	7:B:821:HEM:HMD2	1.90	0.63
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.81	0.62
1:B:258:GLU:OE2	7:B:821:HEM:HMB2	1.87	0.62
1:B:551:ARG:HD3	1:B:583:ASP:O	1.98	0.62
7:B:821:HEM:C3A	6:B:902:SCN:S	2.92	0.62
1:B:120:GLY:C	1:B:123:GLU:HG2	2.19	0.62
1:A:393:ASP:OD2	1:A:557:THR:HG22	1.99	0.62
1:A:274:ASN:O	1:A:278:ARG:HG3	1.98	0.62
1:A:9:PRO:O	1:A:11:PRO:HD3	2.00	0.62
1:B:120:GLY:CA	1:B:123:GLU:CG	2.72	0.61
1:B:166:VAL:O	1:B:167:CYS:C	2.31	0.61
1:B:484:TYR:CD2	1:B:490:ILE:HG22	2.34	0.61
1:A:169:THR:N	1:A:170:PRO:CD	2.64	0.61
1:B:342:VAL:HA	1:B:446:MET:HE2	1.82	0.61
1:A:544:LEU:O	1:A:547:VAL:HG22	2.00	0.61
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.35	0.61
1:B:123:GLU:CB	1:B:126:LYS:HD2	2.31	0.61
1:A:407:MET:HB3	1:A:501:MET:CE	2.30	0.61
1:A:105:GLN:NE2	7:A:801:HEM:C4B	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:CYS:HB3	1:B:168:PRO:HG3	1.82	0.61
1:A:181:ASN:ND2	1:A:183:VAL:O	2.33	0.61
1:B:95:ASN:OD1	1:B:568:GLN:HB2	2.01	0.61
1:B:328:TYR:HA	1:B:523:ARG:HH12	1.65	0.61
1:A:258:GLU:CD	7:A:801:HEM:C2B	2.74	0.60
1:B:167:CYS:HB3	1:B:168:PRO:CG	2.31	0.60
1:A:258:GLU:CD	7:A:801:HEM:C1B	2.74	0.59
1:A:557:THR:HB	1:A:559:ILE:HG12	1.84	0.59
1:B:51:TYR:CD2	1:B:55:LEU:O	2.55	0.59
1:A:3:GLU:H	1:A:4:VAL:HA	1.67	0.59
1:B:446:MET:HE3	1:B:492:ILE:CD1	2.32	0.59
1:B:215:VAL:HG22	3:B:599:NAG:O7	2.02	0.58
1:B:137:ASP:CG	1:B:138:GLU:N	2.56	0.58
1:A:341:ASN:HD21	1:A:444:HIS:HB3	1.68	0.58
1:A:258:GLU:OE1	7:A:801:HEM:C2B	2.56	0.58
1:A:128:GLN:HE22	1:B:170:PRO:HB3	1.69	0.57
1:A:393:ASP:OD2	1:A:557:THR:CG2	2.52	0.57
1:B:112:ASP:OD2	1:B:112:ASP:N	2.37	0.57
1:B:493:TRP:O	1:B:497:ASN:HB2	2.04	0.57
1:B:368:TRP:CH2	1:B:389:ASP:O	2.58	0.57
1:B:239:PHE:CZ	1:B:427:LYS:HE2	2.39	0.57
1:A:105:GLN:NE2	7:A:801:HEM:CHC	2.68	0.56
1:A:262:LEU:O	1:A:266:HIS:HB2	2.06	0.56
1:B:507:VAL:HB	1:B:511:LEU:HB3	1.87	0.56
1:A:45:ARG:HH12	1:A:445:GLY:HA2	1.71	0.56
7:A:801:HEM:CMC	7:A:801:HEM:HBC2	2.35	0.56
1:A:386:ILE:HG22	1:A:395:LEU:HD11	1.88	0.56
1:B:168:PRO:HG3	1:B:172:TYR:CE2	2.40	0.56
1:A:118:GLU:C	1:A:120:GLY:H	2.08	0.56
1:B:8:ALA:H	1:B:9:PRO:HD3	1.68	0.55
1:B:522:ILE:O	1:B:526:ASP:HB2	2.06	0.55
1:A:419:ASN:O	1:A:430:GLY:HA2	2.06	0.55
1:A:258:GLU:CD	7:A:801:HEM:CHB	2.75	0.55
1:B:241:ASN:HD22	2:B:602:NAG:C7	2.20	0.55
1:A:249:PHE:CE2	1:A:386:ILE:HD11	2.40	0.55
1:B:17:GLU:O	1:B:31:ARG:NH2	2.37	0.55
1:B:76:ARG:O	1:B:76:ARG:CG	2.55	0.55
1:B:142:ILE:CD1	1:B:435:ALA:HB1	2.37	0.55
1:A:284:ASN:HD22	1:A:591:ALA:HA	1.66	0.54
1:B:449:TYR:CD2	1:B:490:ILE:HD11	2.42	0.54
1:B:468:GLN:HG2	1:B:474:LYS:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:HG3	1:A:125:SER:N	2.23	0.54
1:A:393:ASP:OD1	1:A:557:THR:HG22	2.08	0.54
1:A:259:GLN:NE2	7:A:801:HEM:HAB	2.23	0.54
1:B:197:PRO:CD	1:B:198:SEP:O3P	2.54	0.54
1:A:551:ARG:NH1	1:A:555:ASP:OD1	2.39	0.54
1:B:169:THR:H	1:B:170:PRO:HD2	1.72	0.53
7:A:801:HEM:HBB2	7:A:801:HEM:CMB	2.38	0.53
1:A:112:ASP:OD1	1:A:112:ASP:N	2.41	0.53
1:A:165:PHE:CD1	1:A:165:PHE:N	2.76	0.53
1:A:193:TYR:HE2	1:A:213:MET:HE1	1.73	0.53
1:B:116:GLU:HG3	1:B:440:ARG:HH22	1.73	0.53
7:B:821:HEM:HBC2	7:B:821:HEM:HMC1	1.90	0.53
1:B:136:GLY:O	1:B:137:ASP:HB3	2.09	0.53
1:B:503:GLU:O	1:B:504:ARG:HB2	2.08	0.53
1:A:40:ASN:N	1:A:181:ASN:O	2.41	0.53
1:A:245:HIS:ND1	1:A:245:HIS:N	2.56	0.52
1:B:56:ALA:CB	1:B:177:ARG:NH2	2.73	0.52
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.91	0.52
1:B:258:GLU:CD	7:B:821:HEM:CMB	2.63	0.51
1:A:3:GLU:HG3	1:A:175:LEU:HD13	1.92	0.51
1:B:487:PRO:O	1:B:490:ILE:HG12	2.10	0.51
1:B:112:ASP:HB3	1:B:339:ILE:HD11	1.91	0.51
1:B:167:CYS:N	1:B:168:PRO:CD	2.68	0.51
1:A:181:ASN:ND2	1:A:183:VAL:H	2.09	0.51
1:B:78:VAL:HG11	1:B:494:ILE:HD13	1.92	0.51
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.11	0.51
1:B:170:PRO:CB	1:B:171:PRO:CD	2.33	0.51
1:B:360:ARG:HB3	1:B:394:PRO:HB2	1.91	0.51
1:A:9:PRO:HG2	1:A:10:VAL:N	2.26	0.50
1:B:117:THR:HG23	1:B:118:GLU:N	2.20	0.50
1:A:115:PRO:HD2	1:A:180:ILE:HG23	1.89	0.50
1:B:513:CYS:O	1:B:517:ARG:HB2	2.12	0.50
1:B:167:CYS:N	1:B:168:PRO:HD3	2.24	0.50
1:A:45:ARG:HH12	1:A:445:GLY:CA	2.24	0.50
1:B:167:CYS:HB2	1:B:168:PRO:HD3	1.89	0.50
1:A:117:THR:CG2	1:A:162:ARG:O	2.60	0.50
1:B:105:GLN:NE2	7:B:821:HEM:C4B	2.80	0.49
1:A:452:TRP:CD1	1:A:492:ILE:CD1	2.91	0.49
1:B:241:ASN:ND2	2:B:602:NAG:C7	2.75	0.49
1:A:111:LEU:O	1:A:339:ILE:HG13	2.13	0.49
1:A:128:GLN:NE2	1:B:170:PRO:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TYR:CE2	1:A:213:MET:CE	2.96	0.49
1:A:181:ASN:HD22	1:A:183:VAL:H	1.59	0.49
1:B:88:GLU:HG2	1:B:88:GLU:O	2.12	0.49
1:B:298:LYS:HG2	1:B:536:PHE:CZ	2.48	0.49
1:B:169:THR:N	1:B:170:PRO:HD2	2.28	0.49
1:B:169:THR:O	1:B:169:THR:HG23	2.13	0.49
1:A:502:VAL:HG22	1:A:507:VAL:O	2.13	0.49
1:B:88:GLU:CG	1:B:88:GLU:O	2.61	0.48
1:B:171:PRO:HD2	1:B:171:PRO:O	2.13	0.48
1:B:117:THR:HB	1:B:162:ARG:O	2.13	0.48
1:B:185:SER:HB3	1:B:339:ILE:HG23	1.96	0.48
1:A:528:PHE:HA	1:A:535:VAL:HG11	1.95	0.48
1:A:551:ARG:HG3	1:A:583:ASP:O	2.13	0.48
1:B:446:MET:CE	1:B:492:ILE:HD11	2.42	0.48
1:B:170:PRO:HB2	1:B:171:PRO:HD3	0.62	0.48
1:B:166:VAL:CG1	1:B:178:ASP:O	2.56	0.48
1:A:202:ARG:HD2	1:A:250:GLN:NE2	2.28	0.48
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.96	0.48
1:A:276:LEU:HD13	1:A:299:ILE:HG23	1.96	0.48
1:A:124:HIS:CD2	1:A:124:HIS:N	2.81	0.48
1:A:358:VAL:HB	1:A:379:LEU:HD11	1.95	0.48
1:B:52:GLU:HB3	1:B:57:VAL:HG12	1.96	0.47
6:A:901:SCN:S	8:A:927:HOH:O	2.61	0.47
1:B:392:ILE:O	1:B:396:VAL:HG23	2.14	0.47
1:B:5:GLY:O	1:B:6:CYS:C	2.51	0.47
7:B:821:HEM:HBC2	7:B:821:HEM:CMC	2.44	0.47
1:B:10:VAL:HA	1:B:11:PRO:HD2	1.73	0.47
1:B:385:ARG:O	1:B:389:ASP:HB3	2.14	0.47
1:A:536:PHE:HE1	1:A:590:TRP:HH2	1.63	0.47
1:B:137:ASP:OD1	1:B:138:GLU:N	2.47	0.47
1:A:365:TYR:CE1	1:A:397:ARG:HG2	2.50	0.47
1:A:101:MET:HE2	1:A:354:VAL:HG22	1.96	0.47
1:A:123:GLU:CG	1:A:125:SER:H	2.27	0.46
1:B:106:ILE:HG23	1:B:191:LEU:HD21	1.97	0.46
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.50	0.46
1:A:168:PRO:C	1:A:170:PRO:HD2	2.35	0.46
1:B:124:HIS:O	1:B:127:VAL:HB	2.16	0.46
1:B:349:PHE:HB2	1:B:497:ASN:HD21	1.81	0.46
1:B:563:PRO:HD3	1:B:576:PHE:CE2	2.50	0.46
1:A:9:PRO:HB2	1:A:10:VAL:H	1.43	0.46
1:B:484:TYR:CE1	1:B:490:ILE:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:O	1:A:117:THR:CG2	2.61	0.46
1:A:570:ASN:HB2	1:A:575:ASP:HB2	1.98	0.46
1:B:258:GLU:OE1	7:B:821:HEM:C2B	2.69	0.46
1:B:76:ARG:HG2	1:B:76:ARG:O	2.16	0.46
1:A:202:ARG:HD2	1:A:250:GLN:HE22	1.81	0.46
1:A:464:LEU:O	1:A:468:GLN:HG3	2.15	0.46
1:A:360:ARG:HD2	1:A:368:TRP:CE3	2.50	0.45
1:A:464:LEU:HA	1:A:481:LEU:HD21	1.97	0.45
1:A:93:ASP:HA	1:A:406:LEU:HD12	1.98	0.45
1:B:77:GLU:O	1:B:81:LYS:HG3	2.16	0.45
1:A:57:VAL:HA	1:A:58:PRO:HD3	1.84	0.45
1:A:529:TRP:CD1	1:A:531:GLU:HB2	2.51	0.45
1:B:165:PHE:HB3	1:B:177:ARG:HD3	1.99	0.45
1:A:280:LEU:HD21	1:A:587:LEU:HD22	1.99	0.45
1:B:544:LEU:O	1:B:547:VAL:HG22	2.16	0.45
1:B:368:TRP:HH2	1:B:389:ASP:O	1.97	0.45
1:A:588:SER:OG	1:A:589:PRO:HD3	2.17	0.45
1:B:299:ILE:HG23	1:B:544:LEU:HD21	1.98	0.45
1:A:229:PHE:HB3	1:A:247:PRO:HG2	1.99	0.45
1:B:360:ARG:HH11	1:B:360:ARG:HG3	1.81	0.45
1:B:169:THR:CG2	1:B:170:PRO:CD	2.82	0.44
1:A:11:PRO:HB2	1:A:12:LEU:HD12	1.97	0.44
1:B:118:GLU:CG	1:B:118:GLU:O	2.46	0.44
1:A:258:GLU:OE1	7:A:801:HEM:CHB	2.66	0.44
1:A:384:TRP:O	1:A:388:LYS:HB2	2.17	0.44
1:B:511:LEU:HD12	1:B:511:LEU:HA	1.89	0.44
1:A:127:VAL:HG13	1:A:131:GLU:HG3	1.98	0.44
1:B:227:PRO:HD3	1:B:267:THR:HG23	2.00	0.44
1:A:184:THR:OG1	1:A:190:SER:OG	2.35	0.44
1:A:55:LEU:CD2	1:A:175:LEU:O	2.64	0.44
1:B:258:GLU:CD	7:B:821:HEM:C2B	2.90	0.44
1:A:557:THR:HG22	1:A:558:HIS:H	1.82	0.44
1:B:446:MET:CE	1:B:492:ILE:CD1	2.96	0.44
1:A:100:PHE:CE2	1:A:506:ARG:HG3	2.53	0.44
1:A:536:PHE:CE1	1:A:590:TRP:HH2	2.36	0.43
1:B:50:GLU:OE1	1:B:447:PRO:HA	2.18	0.43
1:A:299:ILE:HD11	1:A:585:LEU:HD21	2.00	0.43
1:A:189:ALA:O	1:A:193:TYR:HD1	2.01	0.43
1:A:295:GLU:O	1:A:299:ILE:HG22	2.18	0.43
1:B:30:ASN:O	1:B:34:PRO:HA	2.19	0.43
1:B:142:ILE:HD11	1:B:435:ALA:HB1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLN:HE22	1:B:430:GLY:HA3	1.84	0.43
1:B:561:LYS:HD2	1:B:576:PHE:HB3	2.01	0.43
1:B:171:PRO:CD	1:B:171:PRO:O	2.65	0.43
1:B:551:ARG:CZ	1:B:584:LYS:HG2	2.48	0.43
1:A:345:PHE:CE1	1:A:446:MET:HE3	2.53	0.43
1:A:294:GLN:HE22	1:A:297:ARG:HH11	1.66	0.43
1:A:154:GLN:HE22	1:A:430:GLY:HA3	1.84	0.43
1:A:36:LEU:HG	1:A:337:PRO:HD2	2.01	0.43
1:A:433:LEU:O	1:A:436:ILE:HG22	2.19	0.43
1:B:119:LEU:HA	1:B:119:LEU:HD13	1.40	0.43
1:A:303:PHE:CZ	1:A:307:ILE:HD12	2.54	0.43
7:A:801:HEM:HBA2	7:A:801:HEM:HHA	2.01	0.42
1:A:227:PRO:HD3	1:A:267:THR:HG23	2.01	0.42
1:B:52:GLU:OE1	1:B:57:VAL:HG11	2.19	0.42
1:A:210:LEU:O	1:A:211:GLY:C	2.54	0.42
1:B:11:PRO:O	1:B:12:LEU:HB2	2.20	0.42
1:B:166:VAL:O	1:B:166:VAL:HG23	2.18	0.42
1:B:168:PRO:CG	1:B:172:TYR:CE2	3.02	0.42
1:A:461:PRO:O	1:A:462:LYS:CG	2.67	0.42
1:A:210:LEU:HA	1:A:292:LEU:HD13	2.00	0.42
1:A:462:LYS:HD3	1:A:462:LYS:HA	1.91	0.42
1:B:259:GLN:HB2	7:B:821:HEM:HBB2	2.02	0.42
1:B:175:LEU:HD12	1:B:176:ALA:H	1.85	0.42
1:B:142:ILE:HD12	1:B:435:ALA:HB1	2.02	0.42
1:B:188:ASP:N	1:B:188:ASP:OD1	2.53	0.42
1:B:51:TYR:HB3	1:B:57:VAL:O	2.19	0.42
1:B:348:ARG:HH11	1:B:437:ASN:ND2	2.17	0.42
1:B:348:ARG:NH2	8:B:664:HOH:O	2.51	0.41
1:A:210:LEU:CB	1:A:212:LEU:HD13	2.50	0.41
1:A:131:GLU:HB2	1:A:132:TYR:CD1	2.55	0.41
1:B:233:LYS:HA	1:B:234:PRO:HA	1.88	0.41
1:A:137:ASP:HB3	1:A:138:GLU:H	1.62	0.41
1:A:459:SER:O	1:A:461:PRO:HD3	2.20	0.41
1:A:510:LEU:O	1:A:513:CYS:HB3	2.20	0.41
1:A:393:ASP:CG	1:A:557:THR:CG2	2.88	0.41
1:B:418:ARG:HA	1:B:433:LEU:H	1.85	0.41
1:B:240:ILE:HD11	1:B:382:ASN:HA	2.02	0.41
1:A:447:PRO:O	1:A:452:TRP:CD1	2.74	0.41
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.53	0.41
1:A:393:ASP:N	1:A:394:PRO:HD2	2.35	0.41
1:A:117:THR:HG21	1:A:138:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:MET:O	1:A:159:PRO:C	2.59	0.41
1:A:465:LYS:HA	1:A:468:GLN:HB2	2.03	0.41
1:A:187:LEU:HD13	1:A:305:GLN:HA	2.01	0.41
1:A:115:PRO:CD	1:A:180:ILE:HG23	2.49	0.41
1:A:124:HIS:HD1	1:B:137:ASP:CG	2.24	0.41
1:B:484:TYR:CG	1:B:490:ILE:HG22	2.56	0.41
1:B:139:CYS:SG	1:B:141:PRO:HG3	2.61	0.41
1:A:264:THR:HG23	1:A:392:ILE:HB	2.02	0.41
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.03	0.41
1:A:397:ARG:HE	1:A:559:ILE:HG22	1.86	0.40
1:B:260:ILE:HD12	1:B:379:LEU:HD13	2.03	0.40
1:B:25:THR:HG22	1:B:197:PRO:HG3	2.03	0.40
1:B:551:ARG:HD3	1:B:584:LYS:HA	2.03	0.40
1:B:57:VAL:HA	1:B:58:PRO:HD3	1.87	0.40
1:A:188:ASP:N	1:A:188:ASP:OD1	2.54	0.40
1:A:258:GLU:CD	7:A:801:HEM:HHB	2.41	0.40
1:B:476:LEU:HD21	1:B:498:ALA:HB1	2.03	0.40
1:B:85:TYR:CD2	1:B:87:ASP:O	2.74	0.40
1:A:124:HIS:CE1	1:B:137:ASP:HA	2.56	0.40
1:B:117:THR:CG2	1:B:117:THR:O	2.60	0.40
1:A:208:SER:OG	1:A:208:SER:O	2.30	0.40
1:B:366:GLN:O	1:B:367:PRO:C	2.60	0.40
1:A:168:PRO:HG2	1:A:172:TYR:HD2	1.86	0.40
1:A:445:GLY:H	1:A:446:MET:HB2	1.87	0.40
1:B:572:TYR:CG	1:B:573:PRO:HA	2.56	0.40
1:B:557:THR:HG21	1:B:559:ILE:HG13	2.02	0.40
1:A:492:ILE:O	1:A:493:TRP:C	2.60	0.40
1:A:551:ARG:HG2	1:A:582:VAL:HG12	2.03	0.40
1:A:93:ASP:O	1:A:403:ASN:CG	2.60	0.40
1:A:336:ASP:OD1	1:A:338:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	592/595 (100%)	555 (94%)	30 (5%)	7 (1%)	16	58
1	B	592/595 (100%)	556 (94%)	30 (5%)	6 (1%)	19	62
All	All	1184/1190 (100%)	1111 (94%)	60 (5%)	13 (1%)	17	60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	167	CYS
1	A	168	PRO
1	B	168	PRO
1	B	170	PRO
1	B	171	PRO
1	A	174	SER
1	A	462	LYS
1	B	233	LYS
1	B	8	ALA
1	A	461	PRO
1	B	169	THR
1	A	430	GLY

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	516/516 (100%)	493 (96%)	23 (4%)	34	73
1	B	516/516 (100%)	493 (96%)	23 (4%)	34	73
All	All	1032/1032 (100%)	986 (96%)	46 (4%)	34	73

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

Mol	Chain	Res	Type
1	A	4	VAL
1	A	55	LEU
1	A	101	MET
1	A	118	GLU
1	A	119	LEU
1	A	123	GLU
1	A	124	HIS
1	A	165	PHE
1	A	172	TYR
1	A	173	GLN
1	A	180	ILE
1	A	181	ASN
1	A	210	LEU
1	A	245	HIS
1	A	259	GLN
1	A	284	ASN
1	A	347	PHE
1	A	393	ASP
1	A	459	SER
1	A	470	VAL
1	A	537	THR
1	A	551	ARG
1	A	557	THR
1	B	6	CYS
1	B	13	VAL
1	B	55	LEU
1	B	79	SER
1	B	82	ILE
1	B	88	GLU
1	B	112	ASP
1	B	118	GLU
1	B	119	LEU
1	B	121	SER
1	B	122	SER
1	B	124	HIS
1	B	142	ILE
1	B	143	MET
1	B	148	ASP
1	B	153	THR
1	B	167	CYS
1	B	169	THR
1	B	172	TYR
1	B	177	ARG

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Mol	Chain	Res	Type
1	B	178	ASP
1	B	191	LEU
1	B	347	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	147	ASN
1	A	154	GLN
1	A	181	ASN
1	A	250	GLN
1	A	284	ASN
1	A	294	GLN
1	A	329	GLN
1	A	341	ASN
1	A	377	HIS
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	B	105	GLN
1	B	128	GLN
1	B	250	GLN
1	B	437	ASN
1	B	468	GLN
1	B	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	A	198	1	8,9,10	1.64	2 (25%)	8,12,14	1.65	1 (12%)
1	SEP	B	198	1	8,9,10	1.62	2 (25%)	8,12,14	1.35	1 (12%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	SEP	P-O2P	2.06	1.62	1.54
1	A	198	SEP	P-O2P	2.11	1.62	1.54
1	B	198	SEP	P-O1P	3.46	1.62	1.51
1	A	198	SEP	P-O1P	3.47	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	SEP	OG-CB-CA	2.33	110.26	108.27
1	A	198	SEP	OG-CB-CA	3.52	111.28	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates ⓘ

18 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	1.07	1 (7%)	15,19,21	1.01	1 (6%)
2	NAG	A	597	2	14,14,15	1.37	4 (28%)	15,19,21	1.51	2 (13%)
3	NAG	A	599	1,3	14,14,15	0.72	0	15,19,21	0.83	1 (6%)
3	NAG	A	600	3	14,14,15	0.78	0	15,19,21	1.61	2 (13%)
3	BMA	A	601	3	11,11,12	1.12	1 (9%)	14,15,17	1.77	4 (28%)
2	NAG	A	602	1,2	14,14,15	0.53	0	15,19,21	1.31	2 (13%)
2	NAG	A	603	2	14,14,15	0.55	0	15,19,21	1.94	3 (20%)
2	NAG	A	605	1,2	14,14,15	0.55	0	15,19,21	1.16	1 (6%)
2	NAG	A	606	2	14,14,15	0.62	0	15,19,21	1.49	2 (13%)
2	NAG	B	596	1,2	14,14,15	1.07	1 (7%)	15,19,21	1.01	1 (6%)
2	NAG	B	597	2	14,14,15	1.36	3 (21%)	15,19,21	1.50	2 (13%)
3	NAG	B	599	1,3	14,14,15	0.71	0	15,19,21	0.84	1 (6%)
3	NAG	B	600	3	14,14,15	0.78	0	15,19,21	1.61	2 (13%)
3	BMA	B	601	3	11,11,12	1.11	1 (9%)	14,15,17	1.77	4 (28%)
2	NAG	B	602	1,2	14,14,15	0.43	0	15,19,21	1.46	2 (13%)
2	NAG	B	603	2	14,14,15	0.57	0	15,19,21	1.25	2 (13%)
2	NAG	B	605	1,2	14,14,15	0.58	0	15,19,21	1.47	2 (13%)
2	NAG	B	606	2	14,14,15	0.51	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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	596	NAG	O4-C4	2.03	1.47	1.43
2	B	596	NAG	O4-C4	2.03	1.47	1.43
2	A	597	NAG	C1-C2	2.06	1.55	1.52
2	A	597	NAG	O4-C4	2.14	1.48	1.43
2	B	597	NAG	O4-C4	2.16	1.48	1.43
2	A	597	NAG	C4-C3	2.27	1.58	1.52
2	B	597	NAG	C4-C3	2.31	1.58	1.52
2	A	597	NAG	C3-C2	2.68	1.58	1.52
2	B	597	NAG	C3-C2	2.70	1.58	1.52
3	A	601	BMA	C2-C3	3.00	1.56	1.52
3	B	601	BMA	C2-C3	3.00	1.56	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	NAG	C2-N2-C7	-3.14	119.00	123.04
3	B	600	NAG	C2-N2-C7	-3.13	119.02	123.04
3	A	601	BMA	C1-O5-C5	-2.62	108.92	112.25
3	B	601	BMA	C1-O5-C5	-2.60	108.95	112.25
3	A	599	NAG	C2-N2-C7	-2.26	120.13	123.04
3	B	599	NAG	C2-N2-C7	-2.26	120.13	123.04
2	A	603	NAG	C4-C3-C2	-2.04	108.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAG	C4-C3-C2	2.21	114.66	111.23
2	A	602	NAG	C4-C3-C2	2.21	114.67	111.23
2	A	597	NAG	C3-C4-C5	2.23	114.08	110.20
2	B	597	NAG	C3-C4-C5	2.23	114.08	110.20
2	A	606	NAG	C3-C4-C5	2.30	114.21	110.20
2	B	603	NAG	C1-O5-C5	2.40	115.29	112.25
2	B	596	NAG	C4-C3-C2	2.76	115.53	111.23
2	A	596	NAG	C4-C3-C2	2.82	115.61	111.23
2	B	603	NAG	C4-C3-C2	2.88	115.70	111.23
2	B	605	NAG	C3-C4-C5	2.88	115.22	110.20
3	A	601	BMA	C3-C4-C5	2.94	115.32	110.20
3	B	601	BMA	C3-C4-C5	2.95	115.34	110.20
2	B	606	NAG	C1-O5-C5	3.01	116.07	112.25
2	A	605	NAG	C4-C3-C2	3.19	116.19	111.23
3	B	601	BMA	C2-C3-C4	3.36	116.75	111.04
3	A	601	BMA	C2-C3-C4	3.37	116.76	111.04
3	A	601	BMA	C1-C2-C3	3.45	113.62	109.54
3	B	601	BMA	C1-C2-C3	3.48	113.66	109.54
2	A	603	NAG	O4-C4-C3	3.60	118.44	110.34
2	A	602	NAG	C1-O5-C5	3.85	117.13	112.25
2	B	602	NAG	C1-O5-C5	4.12	117.48	112.25
2	A	606	NAG	C4-C3-C2	4.26	117.85	111.23
2	B	605	NAG	C4-C3-C2	4.39	118.05	111.23
2	B	597	NAG	C4-C3-C2	4.41	118.09	111.23
2	A	597	NAG	C4-C3-C2	4.44	118.14	111.23
3	A	600	NAG	C4-C3-C2	4.45	118.14	111.23
3	B	600	NAG	C4-C3-C2	4.48	118.19	111.23
2	A	603	NAG	C1-O5-C5	5.58	119.33	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	599	NAG	1	0
2	B	602	NAG	2	0

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NO3	A	607	-	3,3,3	3.43	3 (100%)	3,3,3	0.11	0
4	NO3	A	608	-	3,3,3	3.27	3 (100%)	3,3,3	0.11	0
7	HEM	A	801	1,8	30,50,50	2.28	10 (33%)	24,82,82	2.22	7 (29%)
6	SCN	A	901	-	2,2,2	2.47	1 (50%)	1,1,1	2.62	1 (100%)
4	NO3	B	607	-	3,3,3	3.41	3 (100%)	3,3,3	0.11	0
4	NO3	B	608	-	3,3,3	3.21	3 (100%)	3,3,3	0.28	0
7	HEM	B	821	1,8	30,50,50	2.32	10 (33%)	24,82,82	2.28	8 (33%)
6	SCN	B	902	-	2,2,2	2.43	1 (50%)	1,1,1	1.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NO3	A	607	-	-	0/0/0/0	0/0/0/0
4	NO3	A	608	-	-	0/0/0/0	0/0/0/0
7	HEM	A	801	1,8	-	0/10/54/54	0/0/8/8
6	SCN	A	901	-	-	0/0/0/0	0/0/0/0
4	NO3	B	607	-	-	0/0/0/0	0/0/0/0
4	NO3	B	608	-	-	0/0/0/0	0/0/0/0
7	HEM	B	821	1,8	-	0/10/54/54	0/0/8/8
6	SCN	B	902	-	-	0/0/0/0	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	821	HEM	C3B-C4B	-7.55	1.45	1.51
7	A	801	HEM	C3B-C4B	-7.10	1.45	1.51
7	B	821	HEM	C3D-C4D	-5.36	1.44	1.51
7	A	801	HEM	C3D-C4D	-5.06	1.45	1.51
7	B	821	HEM	C2C-C1C	-3.62	1.45	1.52
7	A	801	HEM	C2C-C1C	-3.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	821	HEM	CMA-C3A	2.05	1.55	1.51
7	B	821	HEM	FE-ND	2.08	2.08	1.97
7	B	821	HEM	C3B-CAB	2.21	1.55	1.51
7	A	801	HEM	C3B-CAB	2.25	1.55	1.51
7	B	821	HEM	C1C-NC	2.31	1.38	1.36
7	A	801	HEM	C4C-NC	2.32	1.38	1.36
7	B	821	HEM	C3C-CAC	2.37	1.55	1.51
7	B	821	HEM	C4C-NC	2.38	1.38	1.36
7	A	801	HEM	CAA-C2A	2.45	1.56	1.52
7	A	801	HEM	C3C-CAC	2.50	1.56	1.51
7	A	801	HEM	C1C-NC	2.53	1.39	1.36
4	B	608	NO3	O2-N	2.82	1.39	1.25
4	A	608	NO3	O2-N	2.86	1.40	1.25
4	A	608	NO3	O3-N	2.90	1.40	1.25
4	B	607	NO3	O2-N	2.97	1.40	1.25
6	A	901	SCN	C-S	2.99	1.82	1.63
4	B	608	NO3	O3-N	3.01	1.40	1.25
4	A	607	NO3	O2-N	3.01	1.40	1.25
7	A	801	HEM	FE-NB	3.01	2.13	1.97
6	B	902	SCN	C-S	3.05	1.83	1.63
4	B	607	NO3	O3-N	3.08	1.41	1.25
4	A	607	NO3	O3-N	3.12	1.41	1.25
7	A	801	HEM	FE-NC	3.22	2.08	1.95
7	B	821	HEM	FE-NC	3.46	2.09	1.95
4	B	608	NO3	O1-N	3.73	1.39	1.24
4	A	608	NO3	O1-N	3.93	1.40	1.24
4	A	607	NO3	O1-N	4.06	1.41	1.24
4	B	607	NO3	O1-N	4.07	1.41	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	901	SCN	S-C-N	-2.62	158.28	175.94
7	A	801	HEM	CBD-CAD-C3D	-2.61	105.96	113.55
7	B	821	HEM	CAA-C2A-C1A	-2.22	124.60	127.01
7	B	821	HEM	CBD-CAD-C3D	-2.09	107.48	113.55
7	A	801	HEM	CMD-C2D-C3D	2.29	124.47	114.35
7	A	801	HEM	C2D-C3D-C4D	2.31	105.41	101.50
7	B	821	HEM	CMD-C2D-C3D	2.43	125.12	114.35
7	B	821	HEM	C2D-C3D-C4D	2.64	105.97	101.50
7	B	821	HEM	CMB-C2B-C3B	3.86	126.17	116.53
7	A	801	HEM	CMC-C2C-C3C	4.14	126.88	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	821	HEM	CAD-C3D-C4D	4.23	127.40	112.47
7	B	821	HEM	CMC-C2C-C3C	4.47	127.69	116.53
7	A	801	HEM	CAD-C3D-C4D	4.50	128.36	112.47
7	A	801	HEM	CMB-C2B-C3B	4.52	127.82	116.53
7	A	801	HEM	CAD-C3D-C2D	4.52	126.22	113.22
7	B	821	HEM	CAD-C3D-C2D	4.66	126.63	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	801	HEM	21	0
6	A	901	SCN	1	0
7	B	821	HEM	19	0
6	B	902	SCN	3	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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	594/595 (99%)	-0.23	24 (4%)	42 32	6, 21, 48, 75	0
1	B	594/595 (99%)	-0.18	22 (3%)	45 35	4, 22, 46, 71	0
All	All	1188/1190 (99%)	-0.20	46 (3%)	43 33	4, 22, 47, 75	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	CYS	5.9
1	A	595	ASN	5.7
1	B	5	GLY	5.4
1	A	172	TYR	5.2
1	B	121	SER	5.2
1	A	121	SER	5.0
1	B	122	SER	5.0
1	A	4	VAL	4.8
1	A	7	GLY	4.6
1	B	1	SER	4.4
1	A	122	SER	4.4
1	A	2	TRP	4.1
1	B	2	TRP	4.0
1	B	595	ASN	3.8
1	B	594	GLU	3.7
1	A	171	PRO	3.6
1	A	8	ALA	3.6
1	A	3	GLU	3.6
1	B	174	SER	3.4
1	A	12	LEU	3.4
1	B	7	GLY	3.3
1	A	469	ALA	3.3
1	A	173	GLN	3.2
1	B	4	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	3.2
1	B	3	GLU	3.0
1	B	172	TYR	2.9
1	A	169	THR	2.8
1	A	11	PRO	2.7
1	B	593	ARG	2.7
1	A	6	CYS	2.7
1	A	170	PRO	2.6
1	B	170	PRO	2.6
1	A	174	SER	2.6
1	B	370	PRO	2.5
1	A	242	THR	2.4
1	B	120	GLY	2.3
1	A	14	THR	2.3
1	A	1	SER	2.3
1	B	123	GLU	2.3
1	B	17	GLU	2.2
1	A	15	CYS	2.1
1	B	218	GLU	2.1
1	B	369	GLY	2.1
1	B	173	GLN	2.1
1	A	594	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	B	198	10/11	0.89	0.34	-	29,30,35,35	0
1	SEP	A	198	10/11	0.84	0.52	-	31,32,38,39	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	600	14/15	0.83	0.32	0.77	30,37,39,39	0
3	NAG	A	599	14/15	0.91	0.21	0.46	30,35,39,39	0
3	NAG	B	599	14/15	0.92	0.19	-0.33	30,35,39,39	0
2	NAG	B	602	14/15	0.93	0.15	-0.67	38,40,42,46	0
2	NAG	A	602	14/15	0.93	0.16	-0.83	38,40,42,46	0
2	NAG	B	597	14/15	0.59	0.61	-	35,39,39,39	0
2	NAG	B	605	14/15	0.85	0.36	-	37,40,43,46	0
3	BMA	A	601	11/12	0.63	0.72	-	36,38,39,39	0
2	NAG	A	606	14/15	0.66	0.56	-	52,52,53,53	0
3	NAG	B	600	14/15	0.68	0.59	-	30,37,39,39	0
2	NAG	A	603	14/15	0.64	0.44	-	49,52,53,54	0
2	NAG	B	606	14/15	0.79	0.70	-	49,51,51,51	0
2	NAG	A	596	14/15	0.82	0.42	-	30,31,38,39	0
2	NAG	B	603	14/15	0.76	0.38	-	50,53,54,56	0
2	NAG	A	605	14/15	0.71	0.42	-	44,47,48,50	0
3	BMA	B	601	11/12	0.68	0.78	-	36,38,39,39	0
2	NAG	B	596	14/15	0.79	0.45	-	30,31,38,39	0
2	NAG	A	597	14/15	0.68	0.55	-	35,39,39,39	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
7	HEM	B	821	43/43	0.84	0.28	4.39	15,18,18,19	0
4	NO3	B	607	4/4	0.92	0.31	4.05	44,44,44,44	0
7	HEM	A	801	43/43	0.85	0.28	3.01	22,24,26,27	0
4	NO3	A	607	4/4	0.92	0.24	1.74	69,69,69,69	0
4	NO3	B	608	4/4	0.97	0.17	0.34	11,11,11,11	0
4	NO3	A	608	4/4	0.98	0.16	0.03	25,25,26,26	0
5	CA	B	724	1/1	0.99	0.10	-2.19	21,21,21,21	0
5	CA	A	704	1/1	0.95	0.09	-2.57	28,28,28,28	0
6	SCN	B	902	3/3	0.73	0.42	-	23,23,23,24	0
6	SCN	A	901	3/3	0.83	0.25	-	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.