



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:51 AM GMT

PDB ID : 3GC1
Title : Crystal structure of bovine lactoperoxidase
Authors : Singh, A.K.; Singh, N.; Sinha, M.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on : 2009-02-21
Resolution : 2.50 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

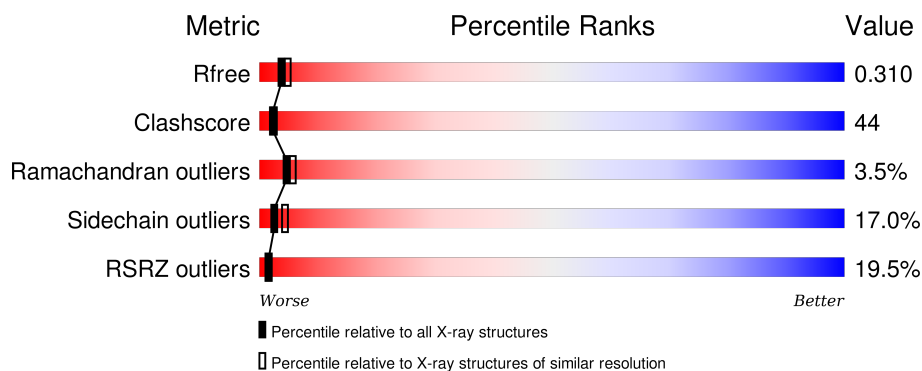
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	A	605	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	IOD	A	610	-	-	X	-
7	IOD	A	613	-	-	X	-

2 Entry composition [i](#)

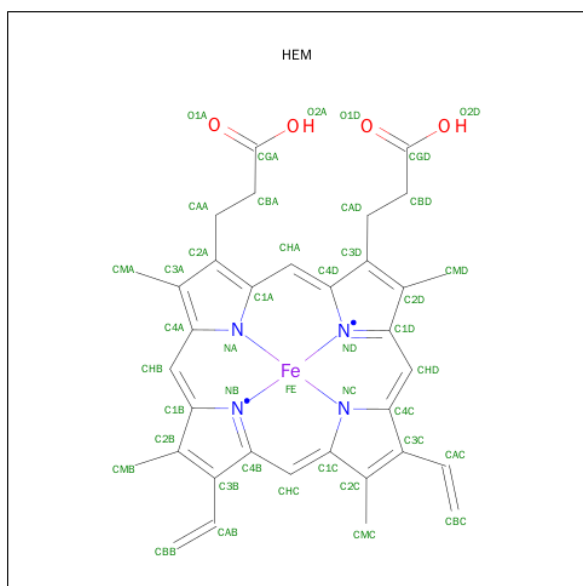
There are 8 unique types of molecules in this entry. The entry contains 5258 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4774	3037	847	863	1	26			

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

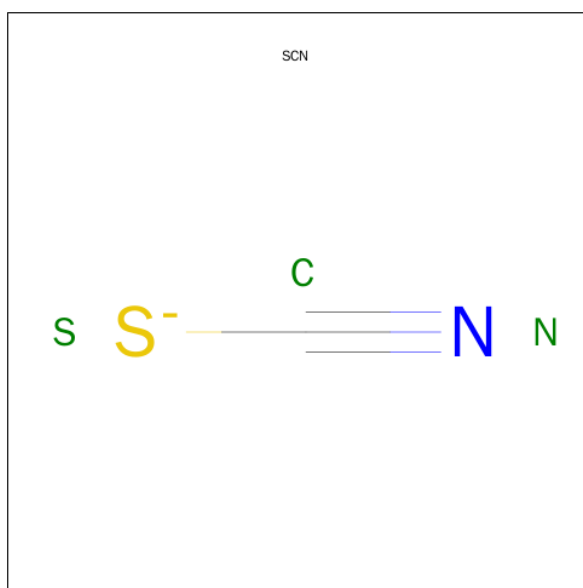


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

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

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

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

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

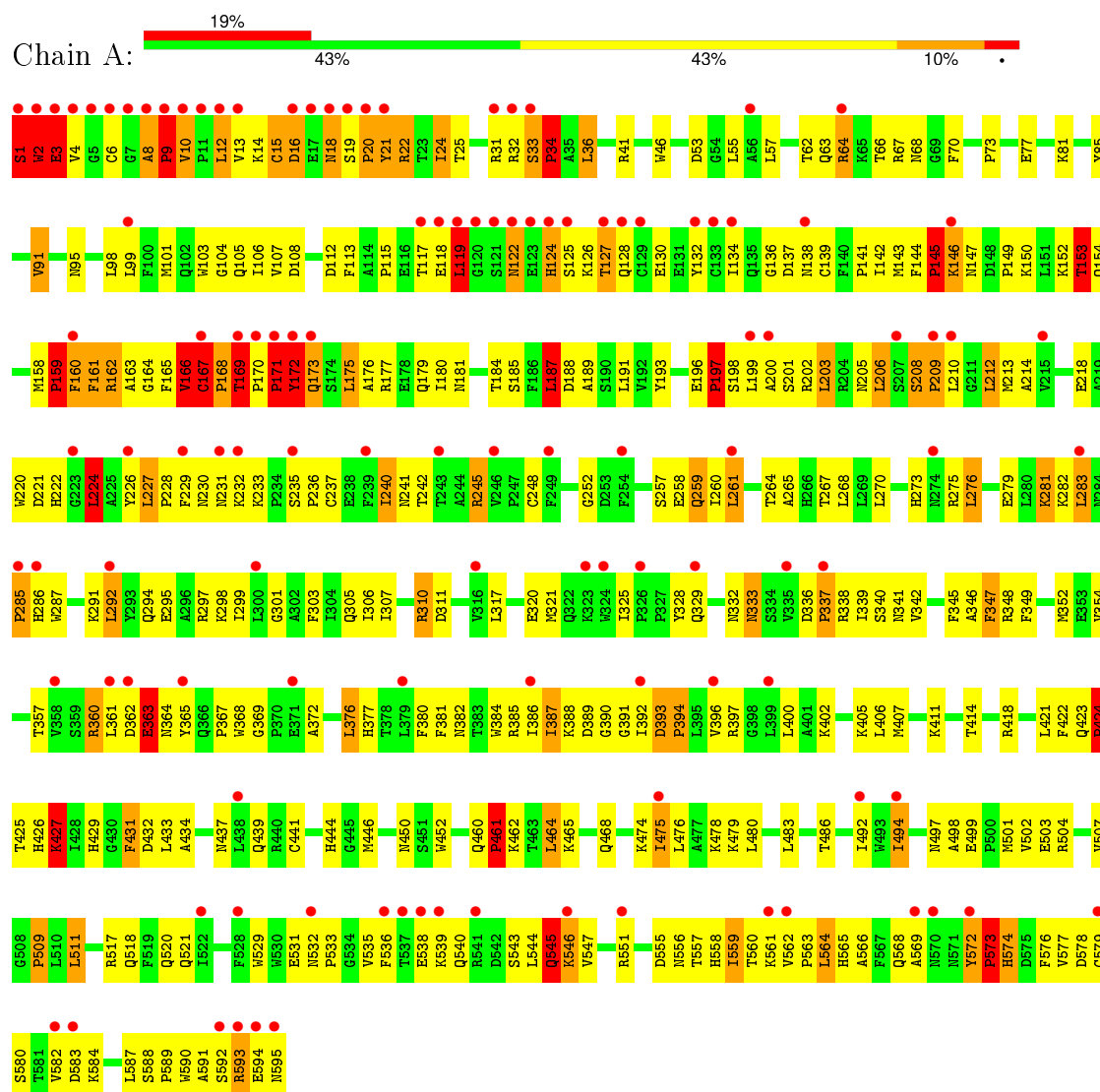
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	296	Total 296	O 296	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.65Å 80.71Å 75.68Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	24.97 – 2.50 24.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.97-2.50) 95.4 (24.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.247 , 0.268 0.262 , 0.310	Depositor DCC
R_{free} test set	1073 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20970 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	7/4891 (0.1%)	1.25	44/6634 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	TRP	CB-CG	-6.67	1.38	1.50
1	A	145	PRO	CA-C	-6.62	1.39	1.52
1	A	461	PRO	CA-C	-6.30	1.40	1.52
1	A	171	PRO	N-CA	6.11	1.57	1.47
1	A	33	SER	C-N	5.38	1.44	1.34
1	A	34	PRO	N-CA	5.15	1.56	1.47
1	A	208	SER	C-N	5.08	1.44	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	PRO	CA-N-CD	-18.07	86.20	111.50
1	A	572	TYR	C-N-CD	-14.29	89.15	120.60
1	A	2	TRP	N-CA-C	13.15	146.51	111.00
1	A	573	PRO	N-CA-CB	13.11	119.03	103.30
1	A	572	TYR	C-N-CA	12.57	174.80	122.00
1	A	573	PRO	N-CD-CG	12.27	121.61	103.20
1	A	461	PRO	CA-N-CD	-10.50	96.80	111.50
1	A	172	TYR	CB-CG-CD1	-9.05	115.57	121.00
1	A	172	TYR	CB-CG-CD2	8.58	126.15	121.00
1	A	159	PRO	CA-N-CD	-7.97	100.34	111.50
1	A	9	PRO	CA-N-CD	-7.96	100.36	111.50
1	A	336	ASP	C-N-CD	-7.70	103.66	120.60
1	A	15	CYS	N-CA-C	7.35	130.85	111.00
1	A	2	TRP	CB-CA-C	-7.33	95.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	CYS	N-CA-C	-6.59	93.21	111.00
1	A	167	CYS	CB-CA-C	6.45	123.30	110.40
1	A	171	PRO	N-CA-C	6.43	128.82	112.10
1	A	197	PRO	CA-N-CD	-6.18	102.85	111.50
1	A	169	THR	N-CA-C	-6.14	94.42	111.00
1	A	145	PRO	CA-N-CD	-6.13	102.92	111.50
1	A	233	LYS	N-CA-C	-6.07	94.61	111.00
1	A	427	LYS	N-CA-C	6.02	127.25	111.00
1	A	2	TRP	CA-C-N	-5.98	104.04	117.20
1	A	332	ASN	N-CA-C	-5.92	95.01	111.00
1	A	34	PRO	CA-N-CD	-5.91	103.23	111.50
1	A	166	VAL	N-CA-C	5.82	126.71	111.00
1	A	222	HIS	CA-CB-CG	-5.75	103.83	113.60
1	A	574	HIS	N-CA-C	5.72	126.43	111.00
1	A	12	LEU	C-N-CA	-5.69	107.47	121.70
1	A	224	LEU	CA-CB-CG	-5.68	102.23	115.30
1	A	222	HIS	CB-CA-C	5.55	121.51	110.40
1	A	390	GLY	N-CA-C	5.40	126.60	113.10
1	A	21	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	A	169	THR	N-CA-CB	5.38	120.52	110.30
1	A	232	LYS	N-CA-C	5.36	125.48	111.00
1	A	545	GLN	N-CA-CB	5.25	120.05	110.60
1	A	6	CYS	N-CA-C	-5.22	96.91	111.00
1	A	21	TYR	CB-CG-CD1	5.13	124.08	121.00
1	A	122	ASN	N-CA-C	-5.08	97.28	111.00
1	A	187	LEU	N-CA-C	-5.08	97.28	111.00
1	A	10	VAL	CB-CA-C	-5.07	101.77	111.40
1	A	1	SER	C-N-CA	5.03	134.28	121.70
1	A	153	THR	N-CA-C	5.01	124.53	111.00
1	A	337	PRO	CA-N-CD	-5.00	104.50	111.50

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	4774	0	4688	420	0
2	A	43	0	30	31	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	78	0	68	8	0
6	A	56	0	50	3	0
7	A	7	0	0	6	0
8	A	296	0	0	43	0
All	All	5258	0	4836	428	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 44.

All (428) 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:105:GLN:HB2	2:A:605:HEM:C2C	1.64	1.32
1:A:221:ASP:HB2	1:A:226:TYR:CZ	1.81	1.16
1:A:104:GLY:HA3	2:A:605:HEM:HBC1	1.26	1.09
1:A:22:ARG:CG	1:A:22:ARG:HH11	1.66	1.08
1:A:22:ARG:NH1	1:A:22:ARG:HG2	1.53	1.06
1:A:202:ARG:HH22	1:A:231:ASN:HB2	1.14	1.06
1:A:504:ARG:NH2	5:A:596:NDG:H4	1.73	1.03
1:A:504:ARG:HH22	5:A:596:NDG:H4	1.18	1.03
1:A:3:GLU:HG2	1:A:175:LEU:HD22	1.41	1.03
1:A:104:GLY:HA3	2:A:605:HEM:CBC	1.91	1.01
1:A:105:GLN:HB2	2:A:605:HEM:CMC	1.91	1.01
1:A:104:GLY:CA	2:A:605:HEM:HBC1	1.96	0.96
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.01	0.95
1:A:9:PRO:HG2	1:A:167:CYS:O	1.66	0.95
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.46	0.95
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.48	0.94
1:A:21:TYR:CG	1:A:294:GLN:HB3	2.06	0.90
1:A:539:LYS:HE2	1:A:589:PRO:HB3	1.53	0.89
1:A:424:PRO:O	7:A:610:IOD:I	2.61	0.89
1:A:202:ARG:NH2	1:A:231:ASN:HB2	1.88	0.88
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.36	0.87
1:A:465:LYS:HA	1:A:468:GLN:NE2	1.89	0.87
1:A:19:SER:N	1:A:20:PRO:HD3	1.88	0.87
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.75	0.87
1:A:392:ILE:O	1:A:396:VAL:HG23	1.75	0.87
1:A:161:PHE:N	1:A:161:PHE:HD1	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:C	2:A:605:HEM:CBC	2.43	0.86
1:A:105:GLN:N	2:A:605:HEM:CAC	2.40	0.85
1:A:104:GLY:CA	2:A:605:HEM:CBC	2.54	0.85
1:A:494:ILE:O	1:A:494:ILE:HD13	1.77	0.85
1:A:227:LEU:HD21	1:A:267:THR:HA	1.57	0.84
1:A:18:ASN:HB3	1:A:20:PRO:HD3	1.58	0.84
1:A:105:GLN:CB	2:A:605:HEM:C2C	2.57	0.83
1:A:260:ILE:HD13	1:A:382:ASN:O	1.79	0.83
1:A:3:GLU:CG	1:A:175:LEU:HD22	2.08	0.82
1:A:568:GLN:HE21	5:A:596:NDG:C6	1.93	0.82
1:A:141:PRO:HB2	1:A:143:MET:CE	2.11	0.81
1:A:224:LEU:HD13	8:A:778:HOH:O	1.79	0.81
1:A:161:PHE:CD1	1:A:161:PHE:N	2.45	0.81
1:A:175:LEU:HG	1:A:176:ALA:H	1.45	0.80
1:A:544:LEU:O	1:A:547:VAL:HG13	1.82	0.78
1:A:504:ARG:HH22	5:A:596:NDG:C4	1.97	0.78
1:A:199:LEU:HD12	1:A:199:LEU:O	1.83	0.78
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.67	0.76
1:A:105:GLN:N	2:A:605:HEM:CBC	2.48	0.76
1:A:19:SER:N	1:A:20:PRO:CD	2.49	0.76
1:A:199:LEU:CD1	1:A:203:LEU:HD22	2.16	0.76
1:A:104:GLY:C	2:A:605:HEM:CAC	2.54	0.75
1:A:295:GLU:O	1:A:299:ILE:HG13	1.86	0.75
6:A:607:NAG:H4	8:A:904:HOH:O	1.87	0.74
1:A:231:ASN:HB3	8:A:847:HOH:O	1.87	0.74
1:A:166:VAL:CG1	1:A:180:ILE:HG12	2.18	0.74
1:A:521:GLN:NE2	8:A:753:HOH:O	2.20	0.74
1:A:161:PHE:H	1:A:161:PHE:HD1	1.36	0.73
1:A:22:ARG:HG2	1:A:22:ARG:HH11	0.72	0.72
1:A:18:ASN:CB	1:A:20:PRO:HD3	2.19	0.72
1:A:146:LYS:O	1:A:147:ASN:HB2	1.89	0.71
1:A:504:ARG:HD3	8:A:791:HOH:O	1.89	0.71
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.73	0.71
1:A:545:GLN:N	1:A:545:GLN:HE21	1.88	0.71
1:A:200:ALA:O	1:A:203:LEU:HB2	1.90	0.71
1:A:565:HIS:CB	1:A:568:GLN:HG2	2.21	0.71
1:A:105:GLN:HA	2:A:605:HEM:C3C	2.27	0.70
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.04	0.69
1:A:16:ASP:N	1:A:16:ASP:OD1	2.25	0.69
1:A:63:GLN:HB3	8:A:844:HOH:O	1.91	0.69
1:A:465:LYS:HD2	1:A:468:GLN:NE2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:O	1:A:245:ARG:HG2	1.91	0.69
1:A:283:LEU:C	1:A:285:PRO:HD3	2.13	0.69
1:A:14:LYS:HE3	1:A:34:PRO:CG	2.23	0.68
1:A:465:LYS:HA	1:A:468:GLN:HE21	1.59	0.68
1:A:346:ALA:HA	8:A:802:HOH:O	1.93	0.68
1:A:365:TYR:CE1	1:A:576:PHE:CE2	2.81	0.68
1:A:565:HIS:HB2	1:A:568:GLN:HG2	1.76	0.68
1:A:579:CYS:O	1:A:582:VAL:HB	1.93	0.68
1:A:294:GLN:NE2	8:A:829:HOH:O	2.25	0.68
1:A:245:ARG:NH2	8:A:909:HOH:O	2.26	0.68
1:A:341:ASN:OD1	1:A:444:HIS:ND1	2.23	0.68
1:A:221:ASP:HB2	1:A:226:TYR:OH	1.94	0.67
1:A:105:GLN:HB2	2:A:605:HEM:C3C	2.25	0.66
1:A:159:PRO:HB3	1:A:161:PHE:HE1	1.60	0.66
1:A:531:GLU:O	1:A:533:PRO:HD3	1.95	0.66
1:A:568:GLN:HB3	5:A:596:NDG:O6	1.95	0.66
1:A:173:GLN:HG2	1:A:173:GLN:O	1.96	0.66
1:A:199:LEU:HD11	1:A:203:LEU:CD2	2.26	0.66
1:A:517:ARG:HD3	8:A:753:HOH:O	1.96	0.66
1:A:2:TRP:CE3	1:A:2:TRP:N	2.64	0.66
1:A:433:LEU:HD13	2:A:605:HEM:HMA3	1.78	0.66
1:A:18:ASN:ND2	1:A:20:PRO:HG3	2.12	0.65
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.76	0.65
1:A:237:CYS:HA	1:A:381:PHE:O	1.96	0.65
1:A:113:PHE:O	1:A:115:PRO:HD2	1.97	0.65
1:A:310:ARG:NE	1:A:311:ASP:OD1	2.24	0.65
1:A:158:MET:SD	8:A:692:HOH:O	2.54	0.65
1:A:342:VAL:HG12	7:A:608:IOD:I	2.66	0.65
1:A:127:THR:HB	8:A:711:HOH:O	1.97	0.65
1:A:588:SER:N	1:A:589:PRO:HD2	2.12	0.65
1:A:214:ALA:O	1:A:228:PRO:HG3	1.97	0.65
1:A:224:LEU:HD11	1:A:558:HIS:CE1	2.32	0.65
1:A:461:PRO:O	1:A:462:LYS:HD3	1.97	0.65
1:A:105:GLN:CA	2:A:605:HEM:CAC	2.74	0.64
1:A:1:SER:N	1:A:2:TRP:CE3	2.64	0.64
1:A:360:ARG:HH11	1:A:372:ALA:HA	1.62	0.64
1:A:551:ARG:HD3	1:A:583:ASP:O	1.98	0.64
6:A:599:NAG:H61	6:A:600:NAG:C7	2.27	0.64
1:A:105:GLN:CA	2:A:605:HEM:C3C	2.81	0.64
1:A:139:CYS:SG	1:A:141:PRO:HG3	2.37	0.64
1:A:545:GLN:NE2	1:A:545:GLN:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:SER:O	1:A:381:PHE:HA	1.97	0.64
1:A:119:LEU:HD21	1:A:138:ASN:ND2	2.13	0.64
1:A:593:ARG:C	1:A:595:ASN:H	2.02	0.63
1:A:105:GLN:HA	2:A:605:HEM:CAC	2.29	0.63
1:A:321:MET:SD	1:A:325:ILE:HD12	2.39	0.63
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.29	0.63
1:A:425:THR:O	1:A:425:THR:HG22	1.98	0.63
1:A:130:GLU:HG3	1:A:159:PRO:CG	2.29	0.63
1:A:199:LEU:HD11	1:A:203:LEU:HD22	1.79	0.62
2:A:605:HEM:HMB1	2:A:605:HEM:HBB2	1.81	0.62
1:A:425:THR:O	1:A:425:THR:CG2	2.48	0.62
1:A:209:PRO:HB3	8:A:635:HOH:O	1.99	0.62
1:A:400:LEU:HD13	1:A:563:PRO:HD3	1.81	0.62
1:A:166:VAL:CG1	1:A:180:ILE:CG1	2.78	0.61
1:A:2:TRP:HE3	1:A:2:TRP:N	1.99	0.61
1:A:275:ARG:CD	1:A:555:ASP:HB3	2.30	0.61
1:A:227:LEU:HD23	1:A:267:THR:HG23	1.82	0.61
1:A:545:GLN:H	1:A:545:GLN:HE21	1.48	0.61
1:A:139:CYS:O	1:A:141:PRO:HD3	2.00	0.60
1:A:303:PHE:CE1	1:A:307:ILE:HD11	2.35	0.60
1:A:276:LEU:CD1	1:A:587:LEU:HD21	2.30	0.60
1:A:117:THR:HB	1:A:119:LEU:CD2	2.30	0.60
1:A:205:ASN:HD22	1:A:212:LEU:HD12	1.65	0.60
1:A:14:LYS:HG3	1:A:15:CYS:H	1.66	0.60
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.01	0.59
1:A:283:LEU:HD23	1:A:591:ALA:HB2	1.82	0.59
1:A:407:MET:HB3	1:A:501:MET:HE2	1.84	0.59
1:A:153:THR:HG22	1:A:154:GLN:HG3	1.83	0.59
1:A:105:GLN:CB	2:A:605:HEM:CMC	2.77	0.59
1:A:21:TYR:HB3	8:A:796:HOH:O	2.01	0.59
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.35	0.58
1:A:328:TYR:CE2	1:A:531:GLU:HB2	2.37	0.58
1:A:1:SER:C	1:A:2:TRP:HE3	2.07	0.58
1:A:265:ALA:HA	1:A:268:LEU:HD23	1.83	0.58
1:A:578:ASP:OD1	1:A:579:CYS:N	2.37	0.58
1:A:130:GLU:HG3	1:A:159:PRO:CD	2.33	0.58
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.32	0.58
1:A:14:LYS:CG	1:A:15:CYS:H	2.16	0.58
1:A:160:PHE:CE1	1:A:439:GLN:HB3	2.39	0.58
1:A:8:ALA:CB	1:A:9:PRO:CD	2.80	0.58
1:A:138:ASN:O	1:A:161:PHE:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD12	1:A:587:LEU:HD21	1.86	0.58
1:A:475:ILE:HG13	1:A:479:LYS:HE3	1.86	0.57
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.27	0.57
1:A:188:ASP:O	1:A:189:ALA:HB3	2.04	0.57
1:A:203:LEU:HB3	1:A:213:MET:CE	2.33	0.57
1:A:393:ASP:N	1:A:394:PRO:HD2	2.19	0.57
1:A:175:LEU:HD23	8:A:863:HOH:O	2.04	0.57
1:A:339:ILE:HA	1:A:518:GLN:NE2	2.20	0.57
1:A:556:ASN:O	1:A:557:THR:CG2	2.53	0.57
1:A:465:LYS:CD	1:A:468:GLN:NE2	2.67	0.57
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.86	0.57
1:A:433:LEU:CD1	2:A:605:HEM:HMA3	2.34	0.57
1:A:464:LEU:HD22	1:A:468:GLN:HG3	1.86	0.57
1:A:544:LEU:O	1:A:546:LYS:N	2.38	0.57
1:A:227:LEU:CD2	1:A:267:THR:HA	2.31	0.57
1:A:21:TYR:OH	1:A:291:LYS:HD2	2.05	0.56
1:A:544:LEU:C	1:A:546:LYS:H	2.09	0.56
1:A:210:LEU:O	1:A:292:LEU:HD23	2.06	0.56
1:A:294:GLN:O	1:A:298:LYS:HB2	2.05	0.56
1:A:431:PHE:N	1:A:431:PHE:CD1	2.73	0.56
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.05	0.56
1:A:431:PHE:N	1:A:431:PHE:HD1	2.04	0.56
1:A:21:TYR:CD1	1:A:294:GLN:HB3	2.40	0.56
1:A:565:HIS:HB3	1:A:568:GLN:HG2	1.87	0.56
1:A:150:LYS:HD2	1:A:158:MET:HE3	1.87	0.55
1:A:180:ILE:HG22	1:A:181:ASN:N	2.21	0.55
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.86	0.55
1:A:494:ILE:HD13	1:A:494:ILE:C	2.26	0.55
1:A:338:ARG:CD	8:A:859:HOH:O	2.54	0.55
1:A:146:LYS:O	1:A:147:ASN:CB	2.54	0.55
1:A:465:LYS:HD3	1:A:468:GLN:HE22	1.70	0.55
1:A:365:TYR:CD2	1:A:572:TYR:CD1	2.95	0.55
1:A:287:TRP:HB2	1:A:292:LEU:HD11	1.88	0.55
1:A:301:GLY:O	1:A:305:GLN:HG3	2.06	0.55
1:A:529:TRP:O	1:A:535:VAL:HG11	2.07	0.55
1:A:203:LEU:HB3	1:A:213:MET:HE3	1.88	0.55
1:A:465:LYS:CD	1:A:468:GLN:HE22	2.20	0.55
1:A:138:ASN:HA	1:A:162:ARG:HG3	1.89	0.55
1:A:14:LYS:HE3	1:A:34:PRO:HG3	1.87	0.55
1:A:147:ASN:O	1:A:149:PRO:HD3	2.07	0.54
1:A:113:PHE:CG	1:A:115:PRO:HD3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG13	1:A:180:ILE:CG1	2.38	0.54
1:A:568:GLN:NE2	5:A:596:NDG:O6	2.34	0.54
1:A:393:ASP:CB	1:A:394:PRO:CD	2.85	0.54
1:A:393:ASP:HB2	1:A:394:PRO:CD	2.37	0.54
1:A:25:THR:CG2	1:A:197:PRO:HD3	2.38	0.54
1:A:532:ASN:O	1:A:535:VAL:HB	2.07	0.54
1:A:63:GLN:CB	8:A:844:HOH:O	2.52	0.54
1:A:185:SER:HB3	1:A:337:PRO:O	2.08	0.54
1:A:175:LEU:HG	1:A:176:ALA:N	2.19	0.53
1:A:169:THR:N	1:A:170:PRO:CD	2.68	0.53
1:A:264:THR:HG23	1:A:392:ILE:HB	1.89	0.53
1:A:283:LEU:O	1:A:285:PRO:HD3	2.09	0.53
1:A:214:ALA:O	1:A:228:PRO:CG	2.56	0.53
1:A:376:LEU:HG	8:A:824:HOH:O	2.09	0.53
1:A:259:GLN:HG2	2:A:605:HEM:CBB	2.38	0.53
1:A:101:MET:SD	2:A:605:HEM:CMC	2.97	0.53
1:A:166:VAL:HG12	1:A:180:ILE:CG1	2.38	0.53
1:A:465:LYS:HD2	1:A:468:GLN:HE21	1.71	0.53
5:A:603:MAN:H3	8:A:659:HOH:O	2.07	0.53
1:A:105:GLN:CB	2:A:605:HEM:C3C	2.89	0.53
1:A:1:SER:CA	1:A:2:TRP:HE3	2.22	0.53
1:A:275:ARG:NE	1:A:555:ASP:HB3	2.23	0.53
1:A:539:LYS:HB3	1:A:589:PRO:HB3	1.91	0.52
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.40	0.52
1:A:22:ARG:NH1	1:A:22:ARG:CG	2.38	0.52
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.92	0.52
1:A:240:ILE:HG12	1:A:241:ASN:N	2.24	0.52
1:A:169:THR:H	1:A:170:PRO:CD	2.17	0.52
1:A:407:MET:HB3	1:A:501:MET:CE	2.39	0.52
1:A:560:THR:O	1:A:561:LYS:HD3	2.09	0.52
1:A:188:ASP:HA	8:A:679:HOH:O	2.10	0.52
1:A:199:LEU:HD12	1:A:203:LEU:HD22	1.88	0.52
1:A:117:THR:HB	1:A:119:LEU:HD21	1.91	0.52
1:A:365:TYR:CE1	1:A:576:PHE:HE2	2.28	0.52
1:A:66:THR:HB	1:A:70:PHE:N	2.25	0.52
1:A:345:PHE:CE2	1:A:441:CYS:HA	2.45	0.52
1:A:187:LEU:CD1	1:A:305:GLN:HA	2.40	0.52
1:A:31:ARG:HD2	8:A:768:HOH:O	2.09	0.52
1:A:108:ASP:OD1	2:A:605:HEM:C2D	2.59	0.51
1:A:64:ARG:HG2	1:A:64:ARG:O	2.10	0.51
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLN:HB2	2:A:605:HEM:HMC2	1.90	0.51
1:A:113:PHE:CD1	1:A:115:PRO:HD3	2.46	0.51
1:A:77:GLU:HB2	1:A:145:PRO:HG3	1.91	0.51
1:A:193:TYR:O	1:A:200:ALA:HA	2.10	0.51
1:A:173:GLN:CG	1:A:173:GLN:O	2.59	0.51
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.41	0.51
1:A:229:PHE:HD2	7:A:613:IOD:I	2.64	0.51
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.29	0.51
1:A:275:ARG:HH11	1:A:275:ARG:HG2	1.76	0.51
1:A:561:LYS:NZ	1:A:578:ASP:HB2	2.25	0.51
1:A:36:LEU:HD12	8:A:709:HOH:O	2.09	0.51
1:A:22:ARG:HD3	8:A:783:HOH:O	2.11	0.50
1:A:21:TYR:CD2	1:A:294:GLN:HB3	2.46	0.50
1:A:574:HIS:C	1:A:574:HIS:CD2	2.84	0.50
1:A:1:SER:CA	1:A:2:TRP:CE3	2.95	0.50
1:A:202:ARG:NH2	1:A:231:ASN:CB	2.66	0.50
1:A:551:ARG:CZ	1:A:584:LYS:HG2	2.41	0.50
1:A:540:GLN:HG2	1:A:590:TRP:CD2	2.46	0.50
1:A:260:ILE:HG23	1:A:261:LEU:HD13	1.93	0.50
1:A:433:LEU:HD11	2:A:605:HEM:C3A	2.47	0.50
1:A:543:SER:OG	1:A:589:PRO:HG3	2.11	0.50
1:A:393:ASP:CB	1:A:394:PRO:HD3	2.42	0.49
1:A:53:ASP:HB2	8:A:678:HOH:O	2.12	0.49
1:A:361:LEU:O	1:A:397:ARG:HD2	2.12	0.49
1:A:286:HIS:N	1:A:286:HIS:ND1	2.55	0.49
1:A:556:ASN:O	1:A:557:THR:HG23	2.11	0.49
1:A:106:ILE:HG22	1:A:107:VAL:N	2.28	0.49
1:A:14:LYS:HE3	1:A:34:PRO:HG2	1.94	0.49
1:A:41:ARG:O	1:A:180:ILE:HG23	2.13	0.49
1:A:62:THR:O	1:A:63:GLN:C	2.49	0.49
1:A:113:PHE:CE2	1:A:115:PRO:HG3	2.48	0.49
1:A:150:LYS:HD2	1:A:158:MET:CE	2.42	0.49
1:A:342:VAL:HG11	1:A:452:TRP:CH2	2.47	0.49
1:A:22:ARG:CD	8:A:783:HOH:O	2.60	0.49
1:A:580:SER:C	1:A:582:VAL:H	2.16	0.49
1:A:166:VAL:HG13	1:A:180:ILE:HG13	1.95	0.49
1:A:328:TYR:CD2	1:A:531:GLU:HB2	2.48	0.49
1:A:127:THR:HG22	1:A:128:GLN:N	2.28	0.49
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.12	0.49
1:A:572:TYR:CD2	1:A:573:PRO:N	2.81	0.49
1:A:345:PHE:HZ	1:A:444:HIS:CG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG23	1:A:132:TYR:HE1	1.78	0.49
1:A:24:ILE:HG13	1:A:200:ALA:HB2	1.94	0.49
1:A:572:TYR:HD2	1:A:573:PRO:HD3	1.78	0.48
1:A:169:THR:N	1:A:170:PRO:HD2	2.28	0.48
1:A:384:TRP:CZ3	1:A:385:ARG:HD3	2.48	0.48
7:A:610:IOD:I	8:A:717:HOH:O	2.90	0.48
1:A:365:TYR:CZ	1:A:576:PHE:CE2	3.02	0.48
1:A:171:PRO:HD3	8:A:716:HOH:O	2.13	0.48
1:A:101:MET:SD	2:A:605:HEM:HMC1	2.53	0.48
1:A:21:TYR:CD1	1:A:294:GLN:CB	2.96	0.48
1:A:298:LYS:HE3	1:A:536:PHE:CE2	2.48	0.48
1:A:16:ASP:HB3	8:A:900:HOH:O	2.13	0.48
6:A:607:NAG:H5	6:A:607:NAG:N2	2.28	0.48
1:A:348:ARG:NH1	2:A:605:HEM:HBA1	2.29	0.48
1:A:127:THR:HG23	1:A:132:TYR:CE1	2.48	0.48
1:A:360:ARG:C	1:A:361:LEU:HD23	2.34	0.47
1:A:423:GLN:O	1:A:425:THR:N	2.46	0.47
1:A:177:ARG:HA	8:A:774:HOH:O	2.14	0.47
1:A:338:ARG:HD2	8:A:859:HOH:O	2.15	0.47
1:A:377:HIS:O	1:A:429:HIS:CD2	2.67	0.47
1:A:142:ILE:HG23	8:A:651:HOH:O	2.15	0.47
1:A:545:GLN:NE2	1:A:545:GLN:N	2.56	0.47
1:A:237:CYS:SG	1:A:381:PHE:HB3	2.54	0.47
1:A:281:LYS:HD3	1:A:285:PRO:HA	1.96	0.47
1:A:229:PHE:CD2	7:A:613:IOD:I	3.38	0.47
1:A:446:MET:HA	1:A:446:MET:CE	2.44	0.47
1:A:230:ASN:OD1	1:A:231:ASN:N	2.47	0.47
1:A:556:ASN:C	1:A:557:THR:HG23	2.34	0.47
2:A:605:HEM:ND	8:A:616:HOH:O	2.35	0.47
1:A:164:GLY:O	1:A:179:GLN:HA	2.14	0.47
1:A:354:VAL:HG11	1:A:376:LEU:HD11	1.97	0.47
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.56	0.47
1:A:12:LEU:HB2	8:A:723:HOH:O	2.13	0.47
1:A:532:ASN:O	1:A:533:PRO:C	2.51	0.47
1:A:593:ARG:C	1:A:595:ASN:N	2.67	0.47
1:A:101:MET:HG2	2:A:605:HEM:HMC3	1.96	0.47
1:A:421:LEU:HD21	1:A:423:GLN:NE2	2.30	0.47
1:A:85:TYR:CD2	1:A:411:LYS:HA	2.50	0.47
1:A:369:GLY:HA3	8:A:752:HOH:O	2.14	0.47
1:A:141:PRO:HB2	1:A:143:MET:HE3	1.91	0.46
1:A:347:PHE:O	1:A:347:PHE:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:HB3	1:A:161:PHE:CE1	2.46	0.46
1:A:381:PHE:CZ	1:A:424:PRO:HD3	2.50	0.46
1:A:64:ARG:CG	1:A:64:ARG:NH1	2.73	0.46
1:A:468:GLN:OE1	1:A:474:LYS:HG3	2.16	0.46
1:A:432:ASP:OD1	1:A:434:ALA:N	2.47	0.46
1:A:202:ARG:HH21	1:A:231:ASN:ND2	2.13	0.46
1:A:593:ARG:O	1:A:595:ASN:N	2.48	0.46
1:A:180:ILE:CG2	1:A:181:ASN:N	2.79	0.46
1:A:95:ASN:HA	1:A:569:ALA:HB2	1.98	0.46
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.97	0.46
1:A:229:PHE:HB2	7:A:613:IOD:I	2.86	0.45
1:A:19:SER:O	1:A:21:TYR:N	2.50	0.45
1:A:287:TRP:CB	1:A:292:LEU:HD11	2.45	0.45
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.97	0.45
1:A:275:ARG:HG2	1:A:275:ARG:NH1	2.32	0.45
1:A:240:ILE:HD12	1:A:381:PHE:O	2.17	0.45
1:A:517:ARG:CD	8:A:753:HOH:O	2.60	0.45
1:A:551:ARG:HD2	1:A:582:VAL:HG12	1.98	0.45
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.98	0.45
1:A:113:PHE:C	1:A:115:PRO:CD	2.85	0.45
1:A:433:LEU:HD13	2:A:605:HEM:CMA	2.47	0.45
1:A:544:LEU:O	1:A:547:VAL:HG22	2.16	0.45
1:A:14:LYS:HG3	1:A:15:CYS:N	2.32	0.45
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.80	0.45
1:A:14:LYS:HD2	1:A:14:LYS:HA	1.82	0.45
1:A:365:TYR:CZ	1:A:576:PHE:HE2	2.34	0.45
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.57	0.45
1:A:53:ASP:C	1:A:55:LEU:H	2.18	0.45
1:A:203:LEU:HD21	1:A:252:GLY:HA2	1.98	0.44
1:A:36:LEU:CD1	8:A:709:HOH:O	2.65	0.44
1:A:418:ARG:O	1:A:432:ASP:HB2	2.18	0.44
1:A:136:GLY:O	1:A:137:ASP:C	2.56	0.44
1:A:167:CYS:CB	1:A:168:PRO:CD	2.93	0.44
1:A:103:TRP:O	1:A:106:ILE:HB	2.18	0.44
1:A:562:VAL:O	1:A:577:VAL:HG22	2.17	0.44
1:A:362:ASP:HB3	1:A:368:TRP:HD1	1.83	0.44
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.99	0.44
1:A:166:VAL:HB	1:A:167:CYS:H	1.23	0.44
1:A:113:PHE:C	1:A:115:PRO:HD3	2.39	0.44
1:A:543:SER:O	1:A:546:LYS:HB2	2.18	0.43
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:VAL:HG13	1:A:507:VAL:O	2.19	0.43
1:A:387:ILE:HG12	1:A:388:LYS:HG3	2.00	0.43
1:A:345:PHE:CZ	1:A:444:HIS:HB2	2.53	0.43
1:A:220:TRP:HB2	8:A:712:HOH:O	2.18	0.43
1:A:242:THR:O	1:A:245:ARG:CG	2.63	0.43
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.54	0.43
1:A:67:ARG:O	1:A:68:ASN:HB2	2.18	0.43
1:A:260:ILE:HD11	1:A:386:ILE:CG1	2.31	0.43
1:A:134:ILE:O	1:A:139:CYS:SG	2.76	0.43
1:A:588:SER:N	1:A:589:PRO:CD	2.81	0.43
1:A:475:ILE:O	1:A:479:LYS:HG3	2.19	0.43
1:A:557:THR:OG1	1:A:559:ILE:HG13	2.18	0.43
1:A:260:ILE:CD1	1:A:382:ASN:O	2.60	0.43
1:A:14:LYS:CG	1:A:15:CYS:N	2.80	0.43
1:A:468:GLN:HB2	1:A:468:GLN:HE21	1.66	0.42
1:A:153:THR:HG23	1:A:153:THR:O	2.18	0.42
1:A:10:VAL:HG21	8:A:908:HOH:O	2.18	0.42
1:A:578:ASP:OD1	1:A:580:SER:N	2.52	0.42
1:A:414:THR:O	1:A:414:THR:HG23	2.19	0.42
1:A:134:ILE:HG22	1:A:134:ILE:O	2.20	0.42
1:A:345:PHE:CZ	1:A:444:HIS:CG	3.07	0.42
1:A:12:LEU:O	1:A:13:VAL:C	2.58	0.42
1:A:544:LEU:C	1:A:546:LYS:N	2.73	0.42
1:A:8:ALA:O	1:A:10:VAL:N	2.46	0.42
5:A:602:NAG:H4	5:A:603:MAN:H2	1.61	0.42
1:A:545:GLN:CA	1:A:545:GLN:HE21	2.31	0.42
1:A:450:ASN:OD1	1:A:460:GLN:HB3	2.18	0.42
1:A:162:ARG:HB3	1:A:162:ARG:HE	1.63	0.42
1:A:572:TYR:HD2	1:A:573:PRO:CD	2.32	0.42
1:A:169:THR:CB	1:A:170:PRO:CD	2.98	0.42
1:A:22:ARG:NE	8:A:783:HOH:O	2.53	0.41
1:A:193:TYR:OH	1:A:297:ARG:HA	2.20	0.41
1:A:561:LYS:HZ2	1:A:578:ASP:HB2	1.83	0.41
1:A:189:ALA:C	1:A:191:LEU:N	2.73	0.41
1:A:63:GLN:N	8:A:844:HOH:O	2.53	0.41
1:A:276:LEU:HD11	1:A:587:LEU:HD21	2.00	0.41
1:A:258:GLU:O	1:A:380:PHE:HA	2.20	0.41
1:A:283:LEU:O	1:A:285:PRO:CD	2.68	0.41
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.37	0.41
1:A:333:ASN:ND2	1:A:333:ASN:O	2.54	0.41
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD13	1:A:305:GLN:HG2	2.02	0.41
1:A:199:LEU:O	1:A:200:ALA:C	2.59	0.41
1:A:213:MET:HG2	1:A:273:HIS:NE2	2.34	0.41
1:A:494:ILE:CD1	1:A:494:ILE:C	2.89	0.41
1:A:393:ASP:N	1:A:394:PRO:CD	2.75	0.41
1:A:363:GLU:H	1:A:363:GLU:HG2	1.40	0.41
1:A:236:PRO:HD2	1:A:248:CYS:SG	2.61	0.41
1:A:18:ASN:HB3	1:A:19:SER:H	1.27	0.41
1:A:144:PHE:CE2	1:A:150:LYS:HB2	2.56	0.41
1:A:212:LEU:HG	1:A:212:LEU:H	1.44	0.41
1:A:73:PRO:HG3	1:A:483:LEU:O	2.20	0.41
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.20	0.41
1:A:421:LEU:HG	1:A:422:PHE:N	2.35	0.41
1:A:270:LEU:HD13	8:A:620:HOH:O	2.21	0.41
1:A:152:LYS:HG2	1:A:152:LYS:H	1.63	0.41
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.49	0.41
1:A:364:ASN:HB3	8:A:864:HOH:O	2.20	0.41
1:A:203:LEU:HA	1:A:203:LEU:HD12	1.93	0.40
1:A:18:ASN:C	1:A:20:PRO:HD3	2.38	0.40
1:A:117:THR:HG23	1:A:164:GLY:CA	2.50	0.40
1:A:165:PHE:HA	1:A:179:GLN:HA	2.03	0.40
1:A:172:TYR:HA	1:A:172:TYR:HD1	1.27	0.40
1:A:124:HIS:HA	8:A:711:HOH:O	2.20	0.40
1:A:206:LEU:HG	1:A:206:LEU:H	1.69	0.40
1:A:405:LYS:HG2	1:A:406:LEU:N	2.37	0.40
1:A:117:THR:HG23	1:A:163:ALA:C	2.42	0.40
1:A:306:ILE:O	1:A:310:ARG:CB	2.69	0.40
1:A:127:THR:CG2	1:A:128:GLN:N	2.82	0.40
1:A:53:ASP:C	1:A:55:LEU:N	2.75	0.40
1:A:221:ASP:HB2	1:A:226:TYR:CE1	2.46	0.40
1:A:426:HIS:CD2	1:A:426:HIS:N	2.89	0.40
1:A:91:VAL:HG23	1:A:411:LYS:HD3	2.04	0.40
1:A:511:LEU:HA	1:A:511:LEU:HD12	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/595 (100%)	505 (85%)	66 (11%)	21 (4%)	4 6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	424	PRO
1	A	427	LYS
1	A	573	PRO
1	A	3	GLU
1	A	119	LEU
1	A	363	GLU
1	A	594	GLU
1	A	20	PRO
1	A	122	ASN
1	A	171	PRO
1	A	545	GLN
1	A	9	PRO
1	A	32	ARG
1	A	166	VAL
1	A	8	ALA
1	A	367	PRO
1	A	509	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	429 (83%)	88 (17%)	2 4

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	TRP
1	A	3	GLU
1	A	4	VAL
1	A	16	ASP
1	A	18	ASN
1	A	22	ARG
1	A	24	ILE
1	A	33	SER
1	A	34	PRO
1	A	57	LEU
1	A	64	ARG
1	A	91	VAL
1	A	98	LEU
1	A	112	ASP
1	A	118	GLU
1	A	119	LEU
1	A	124	HIS
1	A	125	SER
1	A	126	LYS
1	A	127	THR
1	A	145	PRO
1	A	146	LYS
1	A	153	THR
1	A	159	PRO
1	A	160	PHE
1	A	161	PHE
1	A	162	ARG
1	A	169	THR
1	A	172	TYR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	197	PRO
1	A	201	SER

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	206	LEU
1	A	208	SER
1	A	209	PRO
1	A	212	LEU
1	A	218	GLU
1	A	224	LEU
1	A	227	LEU
1	A	235	SER
1	A	240	ILE
1	A	245	ARG
1	A	259	GLN
1	A	261	LEU
1	A	276	LEU
1	A	279	GLU
1	A	281	LYS
1	A	282	LYS
1	A	283	LEU
1	A	285	PRO
1	A	292	LEU
1	A	310	ARG
1	A	317	LEU
1	A	329	GLN
1	A	333	ASN
1	A	347	PHE
1	A	352	MET
1	A	357	THR
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	387	ILE
1	A	393	ASP
1	A	394	PRO
1	A	402	LYS
1	A	424	PRO
1	A	427	LYS
1	A	431	PHE
1	A	461	PRO
1	A	464	LEU
1	A	475	ILE
1	A	480	LEU
1	A	486	THR

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Mol	Chain	Res	Type
1	A	494	ILE
1	A	503	GLU
1	A	511	LEU
1	A	520	GLN
1	A	538	GLU
1	A	545	GLN
1	A	546	LYS
1	A	559	ILE
1	A	564	LEU
1	A	592	SER
1	A	593	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	147	ASN
1	A	273	HIS
1	A	288	ASN
1	A	333	ASN
1	A	423	GLN
1	A	429	HIS
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	A	558	HIS
1	A	568	GLN
1	A	574	HIS
1	A	595	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	SEP	A	198	1	8,9,10	1.48	1 (12%)	8,12,14	3.21	3 (37%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	2.44	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	-4.51	93.57	106.56
1	A	198	SEP	O3P-P-O1P	-3.42	99.57	110.58
1	A	198	SEP	O3P-P-OG	6.52	125.35	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates

10 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NDG	A	596	1,5	14,14,15	1.40	3 (21%)	15,19,21	1.57	2 (13%)
5	NAG	A	597	5	14,14,15	1.77	3 (21%)	15,19,21	2.44	5 (33%)
5	MAN	A	598	5	11,11,12	0.95	1 (9%)	14,15,17	2.48	2 (14%)
6	NAG	A	599	1,6	14,14,15	1.25	2 (14%)	15,19,21	2.05	5 (33%)
6	NAG	A	600	6	14,14,15	0.89	1 (7%)	15,19,21	1.02	0
5	NDG	A	601	1,5	14,14,15	1.12	1 (7%)	15,19,21	1.78	5 (33%)
5	NAG	A	602	5	14,14,15	0.68	0	15,19,21	1.36	2 (13%)
5	MAN	A	603	5	11,11,12	0.79	0	14,15,17	0.83	0
6	NAG	A	604	1,6	14,14,15	1.27	2 (14%)	15,19,21	1.66	2 (13%)
6	NAG	A	607	6	14,14,15	1.21	1 (7%)	15,19,21	0.86	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
5	NDG	A	596	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	597	5	-	0/6/23/26	0/1/1/1
5	MAN	A	598	5	-	0/2/19/22	0/1/1/1
6	NAG	A	599	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	600	6	-	0/6/23/26	0/1/1/1
5	NDG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	0/1/1/1
5	MAN	A	603	5	-	0/2/19/22	1/1/1/1
6	NAG	A	604	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	607	6	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	604	NAG	C8-C7	2.02	1.54	1.50
6	A	599	NAG	O5-C5	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	597	NAG	C4-C5	2.14	1.57	1.53
5	A	596	NDG	O4-C4	2.18	1.48	1.43
6	A	604	NAG	C4-C5	2.23	1.57	1.53
5	A	596	NDG	C4-C3	2.26	1.58	1.52
5	A	596	NDG	O-C1	2.32	1.47	1.43
5	A	598	MAN	C2-C3	2.42	1.55	1.52
6	A	599	NAG	O5-C1	2.48	1.47	1.43
6	A	600	NAG	C1-C2	2.48	1.55	1.52
5	A	601	NDG	C1-C2	3.13	1.56	1.52
5	A	597	NAG	C8-C7	3.19	1.57	1.50
6	A	607	NAG	C1-C2	3.68	1.57	1.52
5	A	597	NAG	C1-C2	3.80	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	599	NAG	C4-C3-C2	-6.02	101.86	111.23
5	A	597	NAG	C2-N2-C7	-5.24	116.31	123.04
6	A	604	NAG	C2-N2-C7	-4.60	117.13	123.04
5	A	597	NAG	C3-C2-N2	-4.43	99.95	110.56
5	A	601	NDG	C2-N2-C7	-4.19	117.66	123.04
5	A	596	NDG	C3-C4-C5	-4.04	103.15	110.20
5	A	597	NAG	C6-C5-C4	-3.88	103.43	113.02
5	A	601	NDG	C3-C4-C5	-2.88	105.18	110.20
5	A	602	NAG	C4-C3-C2	-2.75	106.95	111.23
5	A	602	NAG	C2-N2-C7	-2.71	119.55	123.04
6	A	599	NAG	C2-N2-C7	-2.35	120.02	123.04
6	A	599	NAG	C3-C4-C5	-2.28	106.22	110.20
5	A	597	NAG	O7-C7-C8	-2.28	117.87	122.06
6	A	599	NAG	O7-C7-C8	-2.16	118.09	122.06
5	A	601	NDG	C1-O-C5	-2.11	109.57	112.25
5	A	601	NDG	C6-C5-C4	2.13	118.27	113.02
6	A	599	NAG	C8-C7-N2	2.15	120.22	116.11
5	A	601	NDG	C8-C7-N2	2.20	120.31	116.11
5	A	597	NAG	C8-C7-N2	2.24	120.40	116.11
6	A	604	NAG	C4-C3-C2	2.73	115.47	111.23
5	A	596	NDG	C1-O-C5	2.84	115.85	112.25
5	A	598	MAN	C2-C3-C4	2.93	116.02	111.04
5	A	598	MAN	C1-C2-C3	8.39	119.47	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	603	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	596	NDG	6	0
6	A	599	NAG	1	0
6	A	600	NAG	1	0
5	A	602	NAG	1	0
5	A	603	MAN	2	0
6	A	607	NAG	2	0

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
2	HEM	A	605	1	30,50,50	3.86	17 (56%)	24,82,82	2.93	13 (54%)
4	SCN	A	615	-	2,2,2	2.59	1 (50%)	1,1,1	0.21	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	HEM	A	605	1	-	0/10/54/54	0/0/8/8
4	SCN	A	615	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C4B	-8.47	1.44	1.51
2	A	605	HEM	C2C-C1C	-3.99	1.45	1.52
2	A	605	HEM	C3D-C4D	-3.88	1.46	1.51
2	A	605	HEM	C1C-NC	-3.39	1.31	1.36
2	A	605	HEM	C2D-C1D	-2.70	1.43	1.51
2	A	605	HEM	C1A-CHA	-2.43	1.33	1.39
2	A	605	HEM	CHC-C4B	-2.16	1.32	1.38
2	A	605	HEM	CHD-C4C	2.07	1.41	1.36
2	A	605	HEM	CMC-C2C	2.26	1.58	1.53
2	A	605	HEM	FE-ND	2.32	2.09	1.97
2	A	605	HEM	CHD-C1D	2.52	1.45	1.38
2	A	605	HEM	CMB-C2B	2.69	1.59	1.53
2	A	605	HEM	CAD-C3D	2.78	1.59	1.54
2	A	605	HEM	C3C-CAC	3.11	1.57	1.51
4	A	615	SCN	C-S	3.60	1.86	1.63
2	A	605	HEM	CMA-C3A	4.73	1.61	1.51
2	A	605	HEM	C3B-CAB	5.70	1.62	1.51
2	A	605	HEM	FE-NC	13.94	2.50	1.95

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	CBD-CAD-C3D	-4.95	99.13	113.55
2	A	605	HEM	C3B-C4B-CHC	-3.39	118.39	123.16
2	A	605	HEM	C2C-C1C-CHC	-3.15	118.88	123.68
2	A	605	HEM	CAA-CBA-CGA	-3.10	107.07	112.75
2	A	605	HEM	C1D-CHD-C4C	-2.97	120.86	125.82
2	A	605	HEM	CAA-C2A-C3A	-2.31	122.41	129.00
2	A	605	HEM	C2D-C3D-C4D	2.05	104.98	101.50
2	A	605	HEM	CMB-C2B-C3B	2.31	122.30	116.53
2	A	605	HEM	CMD-C2D-C3D	3.03	127.76	114.35
2	A	605	HEM	CAA-C2A-C1A	4.20	131.56	127.01
2	A	605	HEM	CAD-C3D-C2D	4.20	125.30	113.22
2	A	605	HEM	CAD-C3D-C4D	4.89	129.72	112.47
2	A	605	HEM	CMC-C2C-C3C	6.32	132.31	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEM	31	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%)	1.21	116 (19%) 1 1	28, 47, 86, 100	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	HIS	9.4
1	A	592	SER	9.4
1	A	582	VAL	8.8
1	A	172	TYR	8.6
1	A	2	TRP	8.5
1	A	12	LEU	7.8
1	A	170	PRO	7.2
1	A	125	SER	7.0
1	A	173	GLN	6.8
1	A	4	VAL	6.4
1	A	120	GLY	6.3
1	A	119	LEU	6.2
1	A	9	PRO	6.1
1	A	10	VAL	5.4
1	A	123	GLU	5.3
1	A	5	GLY	5.2
1	A	7	GLY	4.9
1	A	18	ASN	4.9
1	A	121	SER	4.6
1	A	593	ARG	4.6
1	A	169	THR	4.4
1	A	539	LYS	4.4
1	A	128	GLN	4.3
1	A	33	SER	4.3
1	A	1	SER	4.2
1	A	595	ASN	4.0
1	A	246	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	3.9
1	A	17	GLU	3.9
1	A	127	THR	3.8
1	A	6	CYS	3.7
1	A	361	LEU	3.7
1	A	13	VAL	3.6
1	A	20	PRO	3.6
1	A	209	PRO	3.6
1	A	122	ASN	3.5
1	A	16	ASP	3.4
1	A	64	ARG	3.4
1	A	19	SER	3.4
1	A	215	VAL	3.3
1	A	129	CYS	3.3
1	A	583	ASP	3.3
1	A	118	GLU	3.3
1	A	532	ASN	3.3
1	A	167	CYS	3.2
1	A	292	LEU	3.2
1	A	594	GLU	3.1
1	A	210	LEU	3.1
1	A	261	LEU	3.1
1	A	11	PRO	3.1
1	A	438	LEU	3.1
1	A	569	ALA	3.1
1	A	358	VAL	3.1
1	A	337	PRO	3.1
1	A	229	PHE	3.0
1	A	541	ARG	3.0
1	A	399	LEU	3.0
1	A	492	ILE	3.0
1	A	283	LEU	2.9
1	A	3	GLU	2.9
1	A	522	ILE	2.9
1	A	8	ALA	2.9
1	A	21	TYR	2.8
1	A	286	HIS	2.8
1	A	160	PHE	2.8
1	A	572	TYR	2.8
1	A	254	PHE	2.7
1	A	386	ILE	2.7
1	A	133	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	371	GLU	2.7
1	A	31	ARG	2.7
1	A	249	PHE	2.7
1	A	232	LYS	2.6
1	A	392	ILE	2.6
1	A	329	GLN	2.6
1	A	537	THR	2.6
1	A	134	ILE	2.5
1	A	300	LEU	2.5
1	A	231	ASN	2.5
1	A	494	ILE	2.5
1	A	579	CYS	2.5
1	A	379	LEU	2.5
1	A	316	VAL	2.4
1	A	56	ALA	2.4
1	A	132	TYR	2.4
1	A	323	LYS	2.4
1	A	365	TYR	2.4
1	A	32	ARG	2.4
1	A	199	LEU	2.4
1	A	562	VAL	2.4
1	A	538	GLU	2.3
1	A	324	TRP	2.3
1	A	326	PRO	2.3
1	A	475	ILE	2.3
1	A	528	PHE	2.3
1	A	362	ASP	2.3
1	A	146	LYS	2.3
1	A	138	ASN	2.2
1	A	335	VAL	2.2
1	A	561	LYS	2.2
1	A	235	SER	2.2
1	A	570	ASN	2.2
1	A	396	VAL	2.1
1	A	99	LEU	2.1
1	A	536	PHE	2.1
1	A	207	SER	2.1
1	A	239	PHE	2.1
1	A	200	ALA	2.1
1	A	546	LYS	2.1
1	A	226	TYR	2.1
1	A	285	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	THR	2.1
1	A	223	GLY	2.0
1	A	117	THR	2.0
1	A	551	ARG	2.0
1	A	274	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.94	0.24	-	31,48,50,50	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
5	NDG	A	596	14/15	0.78	0.37	1.69	68,70,74,78	0
5	NDG	A	601	14/15	0.87	0.24	0.21	56,57,58,62	0
6	NAG	A	599	14/15	0.80	0.20	-0.80	72,73,75,77	0
5	MAN	A	603	11/12	0.64	0.48	-	78,80,81,82	0
6	NAG	A	607	14/15	0.32	0.58	-	86,89,91,91	0
5	NAG	A	597	14/15	0.68	0.47	-	83,87,89,91	0
5	MAN	A	598	11/12	0.42	0.40	-	94,95,96,96	0
6	NAG	A	604	14/15	0.76	0.32	-	71,74,77,82	0
6	NAG	A	600	14/15	0.59	0.45	-	80,82,83,84	0
5	NAG	A	602	14/15	0.80	0.31	-	64,66,70,74	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	HEM	A	605	43/43	0.80	0.27	2.02	22,27,34,38	0
7	IOD	A	608	1/1	0.99	0.13	-1.47	43,43,43,43	0
4	SCN	A	615	3/3	0.96	0.21	-1.74	17,17,21,25	0
7	IOD	A	612	1/1	0.96	0.06	-2.02	75,75,75,75	0
7	IOD	A	609	1/1	0.98	0.05	-2.22	60,60,60,60	0
3	CA	A	606	1/1	0.86	0.10	-2.49	44,44,44,44	0
7	IOD	A	610	1/1	0.99	0.03	-4.44	56,56,56,56	0
7	IOD	A	611	1/1	0.97	0.07	-4.96	57,57,57,57	0
7	IOD	A	614	1/1	0.96	0.19	-	54,54,54,54	0
7	IOD	A	613	1/1	0.95	0.05	-	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.