



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:25 PM EDT

PDB ID : 3DDR / pdb_00003ddr
Title : Structure of the *Serratia marcescens* hemophore receptor HasR-Ile671Gly mutant in complex with its hemophore HasA and heme
Authors : Krieg, S.; Diederichs, K.
Deposited on : 2008-06-06
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

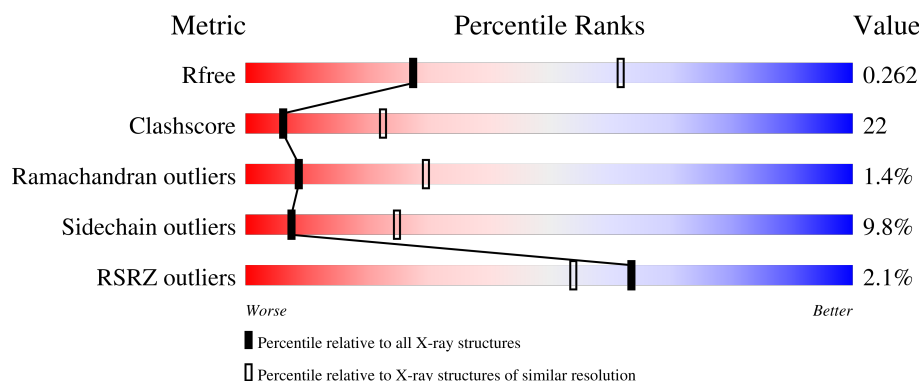
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	865	2% 52% 31% • 13%
1	B	865	% 51% 32% • 13%
2	C	206	2% 56% 20% • 21%
2	D	206	2% 56% 20% • 21%

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
3	NA	A	866	-	-	-	X
3	NA	B	866	-	-	-	X
4	GOL	B	871	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14259 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 HasR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	0	0
			5885	3670	1043	1159	13			
1	B	753	Total	C	N	O	S	0	0	0
			5885	3670	1043	1159	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q79AD2
A	2	GLN	-	expression tag	UNP Q79AD2
A	3	ALA	-	expression tag	UNP Q79AD2
A	4	GLU	-	expression tag	UNP Q79AD2
A	5	ALA	-	expression tag	UNP Q79AD2
A	6	SER	-	expression tag	UNP Q79AD2
A	7	SER	-	expression tag	UNP Q79AD2
A	8	ALA	-	expression tag	UNP Q79AD2
A	9	GLN	-	expression tag	UNP Q79AD2
A	10	ALA	-	expression tag	UNP Q79AD2
A	11	ALA	-	expression tag	UNP Q79AD2
A	12	GLN	-	expression tag	UNP Q79AD2
A	13	GLN	-	expression tag	UNP Q79AD2
A	645	ALA	GLY	SEE REMARK 999	UNP Q79AD2
A	671	GLY	ILE	engineered mutation	UNP Q79AD2
B	1	ALA	-	expression tag	UNP Q79AD2
B	2	GLN	-	expression tag	UNP Q79AD2
B	3	ALA	-	expression tag	UNP Q79AD2
B	4	GLU	-	expression tag	UNP Q79AD2
B	5	ALA	-	expression tag	UNP Q79AD2
B	6	SER	-	expression tag	UNP Q79AD2
B	7	SER	-	expression tag	UNP Q79AD2
B	8	ALA	-	expression tag	UNP Q79AD2
B	9	GLN	-	expression tag	UNP Q79AD2
B	10	ALA	-	expression tag	UNP Q79AD2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	-	expression tag	UNP Q79AD2
B	12	GLN	-	expression tag	UNP Q79AD2
B	13	GLN	-	expression tag	UNP Q79AD2
B	645	ALA	GLY	SEE REMARK 999	UNP Q79AD2
B	671	GLY	ILE	engineered mutation	UNP Q79AD2

- Molecule 2 is a protein called Hemophore HasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	162	Total	C	N	O	S	0	0	0
			1176	739	188	248	1			
2	D	162	Total	C	N	O	S	0	0	0
			1176	739	188	248	1			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	expression tag	UNP Q54450
C	-16	ARG	-	expression tag	UNP Q54450
C	-15	GLY	-	expression tag	UNP Q54450
C	-14	SER	-	expression tag	UNP Q54450
C	-13	HIS	-	expression tag	UNP Q54450
C	-12	HIS	-	expression tag	UNP Q54450
C	-11	HIS	-	expression tag	UNP Q54450
C	-10	HIS	-	expression tag	UNP Q54450
C	-9	HIS	-	expression tag	UNP Q54450
C	-8	HIS	-	expression tag	UNP Q54450
C	-7	GLY	-	expression tag	UNP Q54450
C	-6	ILE	-	expression tag	UNP Q54450
C	-5	ARG	-	expression tag	UNP Q54450
C	-4	MET	-	expression tag	UNP Q54450
C	-3	ARG	-	expression tag	UNP Q54450
C	-2	ALA	-	expression tag	UNP Q54450
C	-1	ARG	-	expression tag	UNP Q54450
C	0	TYR	-	expression tag	UNP Q54450
C	1	PRO	-	expression tag	UNP Q54450
D	-17	MET	-	expression tag	UNP Q54450
D	-16	ARG	-	expression tag	UNP Q54450
D	-15	GLY	-	expression tag	UNP Q54450
D	-14	SER	-	expression tag	UNP Q54450
D	-13	HIS	-	expression tag	UNP Q54450
D	-12	HIS	-	expression tag	UNP Q54450

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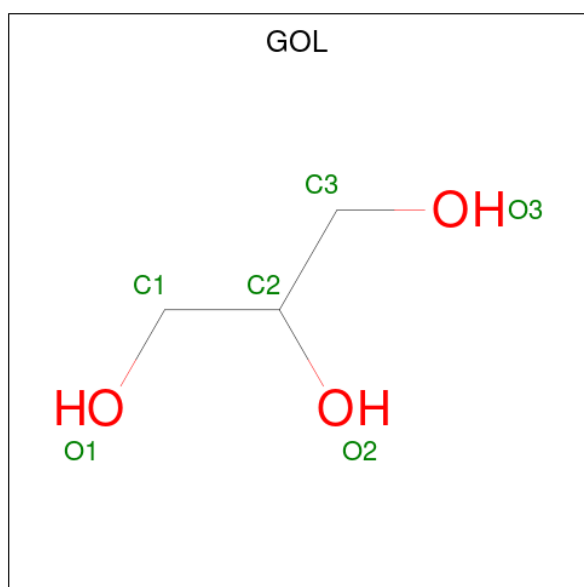
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP Q54450
D	-10	HIS	-	expression tag	UNP Q54450
D	-9	HIS	-	expression tag	UNP Q54450
D	-8	HIS	-	expression tag	UNP Q54450
D	-7	GLY	-	expression tag	UNP Q54450
D	-6	ILE	-	expression tag	UNP Q54450
D	-5	ARG	-	expression tag	UNP Q54450
D	-4	MET	-	expression tag	UNP Q54450
D	-3	ARG	-	expression tag	UNP Q54450
D	-2	ALA	-	expression tag	UNP Q54450
D	-1	ARG	-	expression tag	UNP Q54450
D	0	TYR	-	expression tag	UNP Q54450
D	1	PRO	-	expression tag	UNP Q54450

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

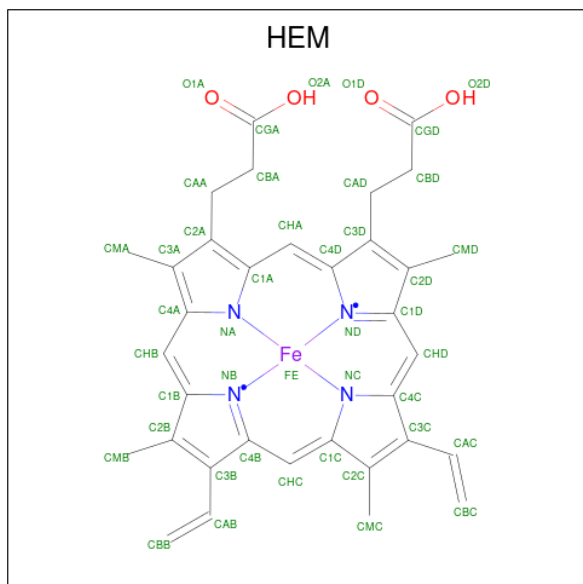
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



[illegible]

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0

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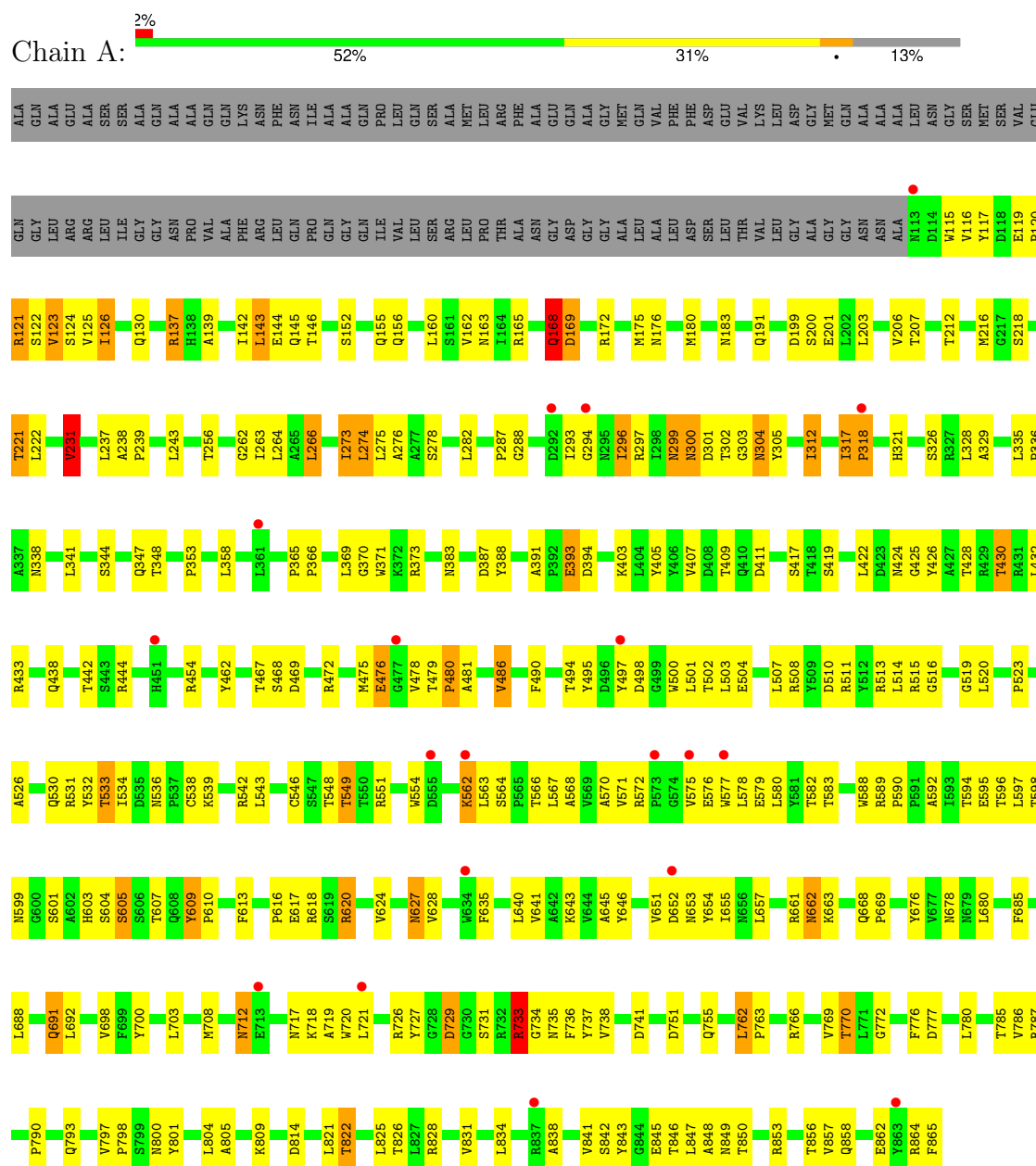
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	6	Total 6	O 6	0	0
6	D	1	Total 1	O 1	0	0

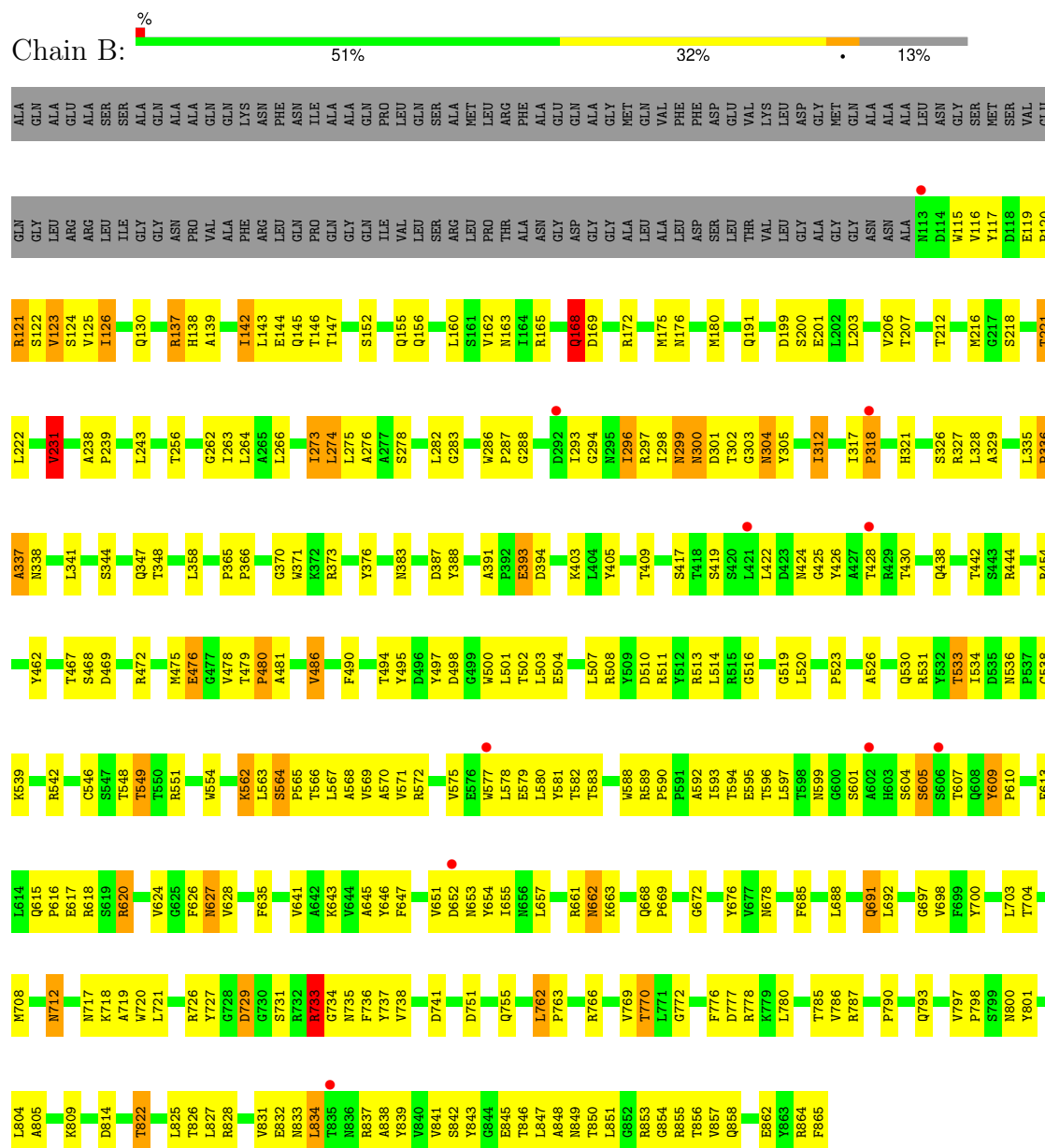
3 Residue-property plots

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

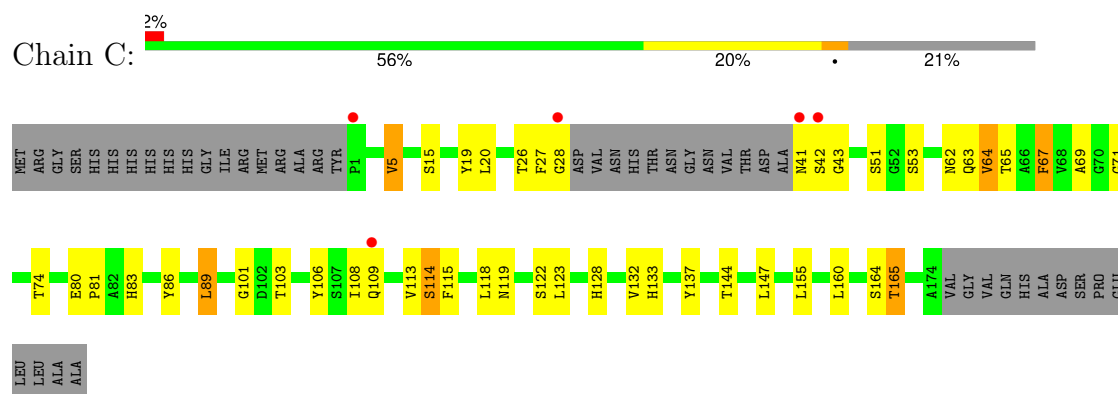
• Molecule 1: HasR protein



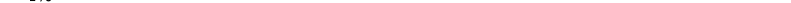
• Molecule 1: HasR protein

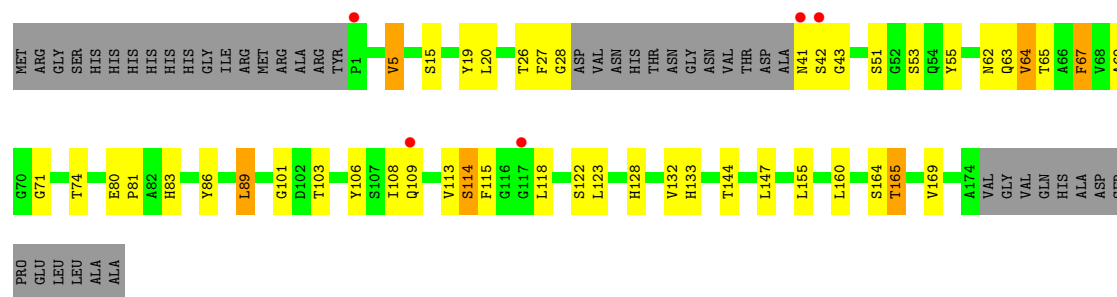


- Molecule 2: Hemophore HasA



- Molecule 2: Hemophore HasA

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.41Å 162.72Å 597.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.25 – 2.80 39.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.25-2.80) 98.4 (39.25-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.226 , 0.262 0.225 , 0.262	Depositor DCC
R_{free} test set	4636 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14259	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, HEM, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/6023	0.88	8/8182 (0.1%)
1	B	0.43	0/6023	0.88	9/8182 (0.1%)
2	C	0.34	0/1203	0.76	0/1638
2	D	0.35	0/1203	0.78	0/1638
All	All	0.42	0/14452	0.86	17/19640 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ILE	CA-C-N	6.28	127.69	119.84
1	B	317	ILE	C-N-CA	6.28	127.69	119.84
1	A	137	ARG	N-CA-C	-6.19	106.70	114.56
1	B	168	GLN	N-CA-C	6.16	123.91	110.80
1	A	317	ILE	CA-C-N	6.04	127.39	119.84
1	A	317	ILE	C-N-CA	6.04	127.39	119.84
1	A	168	GLN	N-CA-C	6.00	123.57	110.80
1	B	137	ARG	N-CA-C	-5.79	107.21	114.56
1	B	751	ASP	CB-CA-C	-5.62	110.12	116.63
1	A	609	TYR	CA-C-N	5.36	125.27	119.85
1	A	609	TYR	C-N-CA	5.36	125.27	119.85
1	A	751	ASP	CB-CA-C	-5.36	110.42	116.63
1	B	609	TYR	CA-C-N	5.23	125.44	120.31
1	B	609	TYR	C-N-CA	5.23	125.44	120.31
1	A	169	ASP	N-CA-C	5.18	117.76	110.14
1	B	536	ASN	CA-C-N	5.09	125.30	120.31
1	B	536	ASN	C-N-CA	5.09	125.30	120.31

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	5885	0	5589	261	0
1	B	5885	0	5589	280	0
2	C	1176	0	1073	36	0
2	D	1176	0	1073	32	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	1	0
4	B	30	0	40	13	0
5	C	43	0	30	14	0
5	D	43	0	30	13	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
6	D	1	0	0	0	0
All	All	14259	0	13432	619	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 22.

All (619) 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:137:ARG:HD3	1:A:853:ARG:HD2	1.35	1.08
1:B:137:ARG:HD3	1:B:853:ARG:HD2	1.37	1.06
1:A:162:VAL:HG23	1:A:175:MET:HE3	1.38	1.02
1:B:300:ASN:HB3	1:B:302:THR:HG23	1.41	1.01
1:B:162:VAL:HG23	1:B:175:MET:HE3	1.39	1.00
1:A:300:ASN:HB3	1:A:302:THR:HG23	1.41	0.99
1:A:733:ARG:CG	1:A:734:GLY:H	1.72	0.99
1:B:575:VAL:HG22	1:B:577:TRP:H	1.26	0.99
5:C:200:HEM:HHD	5:C:200:HEM:HBC2	1.44	0.98
1:B:733:ARG:CG	1:B:734:GLY:H	1.75	0.97
5:D:200:HEM:HBC2	5:D:200:HEM:HHD	1.45	0.96
1:A:575:VAL:HG22	1:A:577:TRP:H	1.27	0.96
5:C:200:HEM:HBA2	5:C:200:HEM:HHA	1.48	0.93
1:B:318:PRO:HG2	1:B:371:TRP:HB2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:A:221:THR:HB	1.68	0.92
1:A:733:ARG:HG2	1:A:734:GLY:H	1.33	0.92
1:B:218:SER:O	1:B:221:THR:HB	1.70	0.92
5:C:200:HEM:HBD2	5:C:200:HEM:HMD1	1.53	0.91
1:A:318:PRO:HG2	1:A:371:TRP:HB2	1.52	0.89
1:A:592:ALA:HB3	1:A:595:GLU:HG2	1.54	0.89
1:B:539:LYS:HA	1:B:734:GLY:HA2	1.53	0.89
1:A:539:LYS:HA	1:A:734:GLY:HA2	1.54	0.88
1:B:733:ARG:HG2	1:B:734:GLY:H	1.35	0.88
1:B:589:ARG:NH2	1:B:595:GLU:OE2	2.08	0.85
2:D:51:SER:HB2	2:D:74:THR:HG22	1.58	0.84
2:C:51:SER:HB2	2:C:74:THR:HG22	1.60	0.83
1:A:191:GLN:HG2	1:A:845:GLU:HG3	1.60	0.83
1:A:538:CYS:O	1:A:539:LYS:HB2	1.77	0.83
5:C:200:HEM:HHC	5:C:200:HEM:HBB2	1.61	0.83
1:B:520:LEU:HD11	1:B:609:TYR:CD1	2.14	0.82
2:C:137:TYR:HB2	5:C:200:HEM:HBC1	1.60	0.82
1:B:191:GLN:HG2	1:B:845:GLU:HG3	1.62	0.81
1:B:592:ALA:HB3	1:B:595:GLU:HG2	1.61	0.81
2:C:41:ASN:HB2	2:C:42:SER:HA	1.63	0.81
1:A:301:ASP:HA	1:A:304:ASN:HA	1.63	0.80
1:A:480:PRO:HD3	1:A:594:THR:HA	1.63	0.79
1:A:720:TRP:CE3	1:A:721:LEU:HG	2.17	0.79
1:B:301:ASP:HA	1:B:304:ASN:HA	1.64	0.79
1:A:520:LEU:HD11	1:A:609:TYR:CD1	2.18	0.78
1:A:341:LEU:HD23	1:A:388:TYR:HD1	1.48	0.78
1:B:341:LEU:HD23	1:B:388:TYR:HD1	1.46	0.78
1:B:538:CYS:O	1:B:539:LYS:HB2	1.82	0.78
1:A:720:TRP:CZ3	1:A:721:LEU:HG	2.19	0.77
1:B:480:PRO:HD3	1:B:594:THR:HA	1.64	0.77
1:B:643:LYS:HB3	1:B:691:GLN:HG3	1.65	0.77
1:B:610:PRO:O	1:B:720:TRP:HZ3	1.67	0.77
2:D:41:ASN:HB2	2:D:42:SER:HA	1.65	0.77
1:A:568:ALA:HB2	1:A:583:THR:HG22	1.67	0.77
1:B:720:TRP:CE3	1:B:721:LEU:HG	2.20	0.77
1:A:643:LYS:HB3	1:A:691:GLN:HG3	1.67	0.76
1:A:216:MET:SD	1:A:438:GLN:HB2	2.25	0.76
1:B:720:TRP:CZ3	1:B:721:LEU:HG	2.21	0.76
1:A:562:LYS:HE2	1:A:618:ARG:CD	2.15	0.76
1:A:610:PRO:O	1:A:720:TRP:HZ3	1.68	0.75
1:B:297:ARG:HH22	1:B:847:LEU:HA	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:LYS:HE2	1:B:618:ARG:CD	2.16	0.75
1:B:376:TYR:CE1	4:B:871:GOL:H2	2.21	0.75
2:D:20:LEU:HB3	2:D:144:THR:HG21	1.69	0.75
1:A:216:MET:HE2	1:A:490:PHE:HE2	1.52	0.74
1:B:520:LEU:CD1	1:B:609:TYR:HD1	2.00	0.74
1:A:462:TYR:CE1	1:A:486:VAL:HG13	2.23	0.73
1:B:376:TYR:HE1	4:B:871:GOL:H2	1.53	0.73
5:D:200:HEM:HBD2	5:D:200:HEM:HHA	1.70	0.73
1:A:297:ARG:HH22	1:A:847:LEU:HA	1.52	0.73
1:A:733:ARG:HG2	1:A:734:GLY:N	2.04	0.73
1:B:520:LEU:HD11	1:B:609:TYR:HD1	1.53	0.73
2:C:20:LEU:HB3	2:C:144:THR:HG21	1.71	0.73
5:D:200:HEM:HHC	5:D:200:HEM:HBB2	1.69	0.73
1:B:393:GLU:O	1:B:394:ASP:HB2	1.89	0.72
1:B:462:TYR:CE1	1:B:486:VAL:HG13	2.25	0.72
1:A:562:LYS:HE2	1:A:618:ARG:HD2	1.71	0.72
1:A:165:ARG:HA	1:A:708:MET:HE1	1.71	0.72
1:A:300:ASN:HB3	1:A:302:THR:CG2	2.19	0.72
1:A:520:LEU:CD1	1:A:609:TYR:HD1	2.02	0.72
1:B:216:MET:SD	1:B:438:GLN:HB2	2.30	0.71
1:B:562:LYS:HE2	1:B:618:ARG:HD2	1.72	0.71
1:B:300:ASN:HB3	1:B:302:THR:CG2	2.19	0.70
1:B:831:VAL:HG22	1:B:857:VAL:HG22	1.71	0.70
1:B:426:TYR:CE2	1:B:472:ARG:HD2	2.25	0.70
1:A:831:VAL:HG22	1:A:857:VAL:HG22	1.74	0.70
1:B:274:LEU:HD12	1:B:275:LEU:N	2.07	0.70
1:B:216:MET:HE2	1:B:490:PHE:HE2	1.55	0.69
1:B:165:ARG:HA	1:B:708:MET:HE1	1.73	0.69
1:A:274:LEU:HD12	1:A:275:LEU:N	2.06	0.69
1:B:278:SER:OG	1:B:326:SER:HB2	1.93	0.69
1:A:733:ARG:HG3	1:A:734:GLY:H	1.58	0.69
5:C:200:HEM:HBA2	5:C:200:HEM:CHA	2.22	0.69
1:A:520:LEU:O	1:A:551:ARG:HD3	1.92	0.69
1:A:180:MET:HE3	1:A:405:TYR:HB2	1.75	0.68
1:A:604:SER:O	1:A:605:SER:HB3	1.92	0.68
1:B:770:THR:HG22	1:B:785:THR:HG23	1.76	0.68
1:A:657:LEU:O	1:A:755:GLN:O	2.11	0.67
1:A:568:ALA:CB	1:A:583:THR:HG22	2.24	0.67
1:A:163:ASN:ND2	1:A:168:GLN:HB3	2.10	0.67
1:A:393:GLU:O	1:A:394:ASP:HB2	1.92	0.67
1:A:770:THR:HG22	1:A:785:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HG2	1:A:597:LEU:HB2	1.77	0.67
1:B:321:HIS:CE1	4:B:871:GOL:HO1	2.13	0.67
1:A:661:ARG:HH11	1:A:718:LYS:HA	1.59	0.67
1:A:798:PRO:HB2	1:A:800:ASN:OD1	1.95	0.67
1:B:520:LEU:O	1:B:551:ARG:HD3	1.94	0.66
1:B:733:ARG:HG2	1:B:734:GLY:N	2.07	0.66
1:A:278:SER:OG	1:A:326:SER:HB2	1.95	0.66
1:B:604:SER:O	1:B:605:SER:HB3	1.94	0.66
1:B:798:PRO:HB2	1:B:800:ASN:OD1	1.96	0.66
2:C:122:SER:HB2	2:C:132:VAL:HG22	1.76	0.66
1:B:480:PRO:HG2	1:B:597:LEU:HB2	1.76	0.66
1:A:426:TYR:CE2	1:A:472:ARG:HD2	2.30	0.66
1:B:657:LEU:O	1:B:755:GLN:O	2.13	0.66
1:A:604:SER:O	1:A:605:SER:CB	2.43	0.66
1:B:163:ASN:ND2	1:B:168:GLN:HB3	2.11	0.66
1:A:798:PRO:HD2	1:A:801:TYR:CE2	2.29	0.66
2:C:41:ASN:CB	2:C:42:SER:HA	2.23	0.66
2:D:122:SER:HB2	2:D:132:VAL:HG22	1.77	0.66
1:B:539:LYS:HD2	1:B:734:GLY:HA3	1.78	0.65
1:B:568:ALA:HB2	1:B:583:THR:HG22	1.78	0.65
1:A:237:LEU:O	4:A:867:GOL:H11	1.96	0.65
1:A:475:MET:HA	1:A:478:VAL:HG23	1.78	0.65
1:B:604:SER:O	1:B:605:SER:CB	2.44	0.65
1:B:733:ARG:HG3	1:B:734:GLY:H	1.61	0.65
1:A:216:MET:HE2	1:A:490:PHE:CE2	2.31	0.65
1:A:603:HIS:HE1	5:C:200:HEM:HMA3	1.62	0.65
1:B:661:ARG:HH11	1:B:718:LYS:HA	1.62	0.64
1:B:231:VAL:HG12	1:B:274:LEU:HD21	1.79	0.64
1:B:180:MET:HE3	1:B:405:TYR:HB2	1.79	0.64
1:A:610:PRO:O	1:A:720:TRP:CZ3	2.51	0.64
1:B:373:ARG:HH12	4:B:871:GOL:H12	1.63	0.64
1:A:539:LYS:HD2	1:A:734:GLY:HA3	1.79	0.64
1:B:798:PRO:HD2	1:B:801:TYR:CE2	2.32	0.64
1:B:610:PRO:O	1:B:720:TRP:CZ3	2.50	0.64
1:A:231:VAL:HG12	1:A:274:LEU:HD21	1.79	0.64
1:A:566:THR:O	1:A:567:LEU:HD12	1.97	0.64
1:A:341:LEU:CD2	1:A:388:TYR:HD1	2.11	0.63
1:A:303:GLY:O	1:A:304:ASN:HB2	1.97	0.63
1:B:475:MET:HA	1:B:478:VAL:HG23	1.78	0.63
1:B:417:SER:HB2	1:B:424:ASN:OD1	1.99	0.63
1:B:697:GLY:HA3	1:B:778:ARG:HH21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:MET:HE2	1:B:490:PHE:CE2	2.34	0.63
1:B:301:ASP:HB3	1:B:304:ASN:OD1	1.98	0.63
1:B:822:THR:HG23	1:B:825:LEU:HB2	1.81	0.63
1:B:373:ARG:CZ	4:B:871:GOL:H11	2.28	0.63
1:B:508:ARG:O	1:B:563:LEU:HD12	1.98	0.63
1:B:504:GLU:HB3	1:B:568:ALA:HB3	1.81	0.63
1:A:822:THR:HG23	1:A:825:LEU:HB2	1.81	0.62
1:B:341:LEU:CD2	1:B:388:TYR:HD1	2.11	0.62
1:A:301:ASP:HB3	1:A:304:ASN:OD1	1.99	0.62
1:A:853:ARG:HH11	1:A:856:THR:HG21	1.64	0.62
1:B:373:ARG:HH12	4:B:871:GOL:C1	2.12	0.62
1:B:568:ALA:CB	1:B:583:THR:HG22	2.30	0.61
1:A:417:SER:HB2	1:A:424:ASN:OD1	2.00	0.61
1:B:566:THR:O	1:B:567:LEU:HD12	2.00	0.61
1:B:328:LEU:HD12	1:B:329:ALA:N	2.15	0.61
1:B:373:ARG:NH1	4:B:871:GOL:H11	2.15	0.61
2:C:15:SER:HA	2:C:165:THR:HA	1.82	0.61
1:A:508:ARG:O	1:A:563:LEU:HD12	2.01	0.61
1:B:508:ARG:HD2	1:B:510:ASP:OD1	2.00	0.61
1:A:299:ASN:HA	1:A:305:TYR:HD2	1.65	0.61
1:A:341:LEU:CD2	1:A:388:TYR:CD1	2.84	0.61
1:B:341:LEU:CD2	1:B:388:TYR:CD1	2.83	0.61
1:B:341:LEU:HD23	1:B:388:TYR:CD1	2.34	0.61
2:C:137:TYR:HB2	5:C:200:HEM:CBC	2.31	0.61
1:B:609:TYR:CZ	1:B:663:LYS:HE2	2.36	0.60
1:B:299:ASN:HA	1:B:305:TYR:HD2	1.66	0.60
1:A:137:ARG:HD3	1:A:853:ARG:CD	2.23	0.60
1:B:605:SER:OG	5:D:200:HEM:C1D	2.55	0.60
1:B:137:ARG:HD3	1:B:853:ARG:CD	2.25	0.60
1:B:548:THR:HG22	1:B:549:THR:N	2.16	0.60
1:B:562:LYS:HG3	1:B:563:LEU:N	2.16	0.60
1:B:303:GLY:O	1:B:304:ASN:HB2	2.02	0.59
1:B:328:LEU:HD12	1:B:329:ALA:H	1.67	0.59
1:B:534:ILE:HD12	1:B:737:TYR:CZ	2.37	0.59
1:A:609:TYR:CZ	1:A:663:LYS:HE2	2.37	0.59
1:A:419:SER:OG	1:A:422:LEU:HB2	2.02	0.59
2:D:15:SER:HA	2:D:165:THR:HA	1.85	0.59
1:B:165:ARG:HA	1:B:708:MET:CE	2.33	0.59
1:B:520:LEU:CD1	1:B:609:TYR:CD1	2.82	0.59
1:A:579:GLU:HB3	1:A:627:ASN:ND2	2.18	0.59
1:B:579:GLU:HB3	1:B:627:ASN:ND2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:THR:HG22	1:A:549:THR:N	2.17	0.59
1:A:526:ALA:HB2	1:A:531:ARG:HA	1.85	0.58
1:A:562:LYS:HG3	1:A:563:LEU:N	2.17	0.58
1:B:620:ARG:HG2	1:B:620:ARG:O	2.02	0.58
1:A:700:TYR:CE2	1:A:772:GLY:HA3	2.39	0.58
1:B:299:ASN:HD22	1:B:300:ASN:N	2.00	0.58
1:B:419:SER:OG	1:B:422:LEU:HB2	2.03	0.58
1:B:526:ALA:HB2	1:B:531:ARG:HA	1.85	0.58
1:A:200:SER:HA	1:A:203:LEU:HD12	1.85	0.58
1:A:263:ILE:HG23	1:A:274:LEU:HD11	1.86	0.58
1:B:172:ARG:NH1	1:B:655:ILE:HG13	2.19	0.58
1:A:727:TYR:CD2	2:C:109:GLN:HG3	2.38	0.58
1:B:358:LEU:HD12	1:B:370:GLY:O	2.03	0.58
1:A:520:LEU:CD1	1:A:609:TYR:CD1	2.83	0.58
1:A:126:ILE:HG13	1:A:206:VAL:HB	1.86	0.58
1:A:328:LEU:HD12	1:A:329:ALA:N	2.19	0.58
1:B:497:TYR:HB3	1:B:501:LEU:HB3	1.84	0.58
1:B:500:TRP:O	1:B:571:VAL:HA	2.03	0.58
1:A:165:ARG:HA	1:A:708:MET:CE	2.34	0.57
1:A:655:ILE:HD12	1:A:655:ILE:O	2.03	0.57
1:B:126:ILE:HG13	1:B:206:VAL:HB	1.85	0.57
1:B:263:ILE:HG23	1:B:274:LEU:HD11	1.87	0.57
1:A:534:ILE:HD12	1:A:737:TYR:CZ	2.38	0.57
1:B:655:ILE:O	1:B:655:ILE:HD12	2.04	0.57
2:C:115:PHE:HB3	2:C:118:LEU:HD11	1.86	0.57
1:A:605:SER:OG	5:C:200:HEM:C4A	2.58	0.57
1:A:720:TRP:O	1:A:721:LEU:HB2	2.03	0.57
1:A:191:GLN:HG2	1:A:845:GLU:CG	2.33	0.57
1:A:163:ASN:HD22	1:A:168:GLN:HB3	1.70	0.57
2:C:101:GLY:HA3	2:C:106:TYR:CE2	2.40	0.57
1:B:373:ARG:NH2	4:B:871:GOL:H11	2.18	0.56
1:B:539:LYS:HD2	1:B:734:GLY:CA	2.34	0.56
1:A:115:TRP:H	1:A:115:TRP:CD1	2.23	0.56
1:A:475:MET:SD	1:A:478:VAL:HG21	2.45	0.56
1:A:520:LEU:HD11	1:A:609:TYR:HD1	1.58	0.56
1:A:508:ARG:HD2	1:A:510:ASP:OD1	2.04	0.56
1:B:274:LEU:HD12	1:B:274:LEU:C	2.30	0.56
1:B:426:TYR:CD2	1:B:472:ARG:HD2	2.39	0.56
1:B:526:ALA:HB1	1:B:530:GLN:O	2.05	0.56
1:A:120:PRO:O	1:A:121:ARG:HB3	2.05	0.56
1:A:539:LYS:HD2	1:A:734:GLY:CA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ARG:HH22	1:B:513:ARG:HD2	1.71	0.56
2:D:115:PHE:HB3	2:D:118:LEU:HD11	1.88	0.56
1:B:191:GLN:HG2	1:B:845:GLU:CG	2.34	0.56
1:B:700:TYR:CE2	1:B:772:GLY:HA3	2.41	0.56
1:B:727:TYR:CD2	2:D:109:GLN:HG3	2.40	0.56
1:B:588:TRP:CH2	1:B:590:PRO:HG3	2.41	0.55
1:B:655:ILE:HD12	1:B:655:ILE:C	2.32	0.55
2:C:67:PHE:CD1	2:C:67:PHE:C	2.84	0.55
1:A:733:ARG:CG	1:A:734:GLY:N	2.46	0.55
1:A:328:LEU:HD12	1:A:329:ALA:H	1.72	0.55
2:D:67:PHE:CD1	2:D:67:PHE:C	2.85	0.55
1:A:299:ASN:HD22	1:A:300:ASN:N	2.04	0.55
1:A:426:TYR:CD2	1:A:472:ARG:HD2	2.41	0.55
1:A:511:ARG:HH22	1:A:513:ARG:HD2	1.71	0.55
1:B:299:ASN:HD22	1:B:300:ASN:CG	2.15	0.55
1:A:655:ILE:HD12	1:A:655:ILE:C	2.32	0.55
1:A:712:ASN:HD22	1:A:712:ASN:N	2.05	0.55
1:B:645:ALA:O	1:B:688:LEU:HD23	2.07	0.55
1:B:733:ARG:CG	1:B:734:GLY:N	2.49	0.55
1:A:462:TYR:CE1	1:A:486:VAL:CG1	2.90	0.54
1:A:299:ASN:ND2	1:A:300:ASN:CG	2.64	0.54
2:C:113:VAL:HG12	2:C:114:SER:N	2.22	0.54
1:A:526:ALA:CB	1:A:531:ARG:HA	2.38	0.54
1:B:299:ASN:ND2	1:B:300:ASN:CG	2.64	0.54
1:A:358:LEU:HD12	1:A:370:GLY:O	2.08	0.54
1:B:853:ARG:HH11	1:B:856:THR:HG21	1.71	0.54
1:A:661:ARG:NH1	1:A:718:LYS:HA	2.23	0.54
1:B:373:ARG:NH1	4:B:871:GOL:C1	2.70	0.54
1:A:172:ARG:NH1	1:A:655:ILE:HG13	2.23	0.54
1:B:712:ASN:N	1:B:712:ASN:HD22	2.05	0.54
1:B:300:ASN:C	1:B:302:THR:H	2.16	0.54
1:A:620:ARG:O	1:A:620:ARG:HG2	2.08	0.54
1:A:692:LEU:C	1:A:692:LEU:HD23	2.32	0.54
1:A:299:ASN:HD22	1:A:300:ASN:CG	2.16	0.53
1:A:500:TRP:O	1:A:571:VAL:HA	2.07	0.53
1:A:601:SER:HB3	1:A:607:THR:HA	1.90	0.53
1:B:864:ARG:O	1:B:865:PHE:HB3	2.07	0.53
1:B:697:GLY:CA	1:B:778:ARG:HH21	2.22	0.53
1:A:273:ILE:HD11	1:A:275:LEU:HG	1.90	0.53
1:A:646:TYR:HB2	1:A:688:LEU:HD21	1.90	0.53
1:A:864:ARG:O	1:A:865:PHE:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ASN:HB2	2:C:42:SER:CA	2.37	0.53
5:D:200:HEM:HHD	5:D:200:HEM:CBC	2.30	0.53
1:A:588:TRP:CH2	1:A:590:PRO:HG3	2.44	0.53
1:A:726:ARG:HB2	1:A:741:ASP:HB2	1.89	0.53
1:A:729:ASP:OD1	1:A:729:ASP:N	2.40	0.53
1:B:137:ARG:HH11	1:B:155:GLN:HB3	1.73	0.53
1:B:163:ASN:HD22	1:B:168:GLN:HB3	1.73	0.53
1:B:200:SER:HA	1:B:203:LEU:HD12	1.91	0.53
1:B:692:LEU:HD23	1:B:692:LEU:C	2.33	0.53
1:B:729:ASP:OD1	1:B:729:ASP:N	2.41	0.53
1:A:300:ASN:C	1:A:302:THR:H	2.15	0.53
1:B:769:VAL:HG12	1:B:786:VAL:HB	1.91	0.53
1:A:504:GLU:HB3	1:A:568:ALA:HB3	1.91	0.53
1:A:274:LEU:HD12	1:A:274:LEU:C	2.34	0.53
1:A:645:ALA:O	1:A:688:LEU:HD23	2.08	0.53
1:B:278:SER:HG	1:B:326:SER:HB2	1.74	0.53
1:B:526:ALA:CB	1:B:531:ARG:HA	2.39	0.53
2:C:86:TYR:HA	2:C:132:VAL:HG21	1.91	0.53
2:D:113:VAL:HG12	2:D:114:SER:N	2.23	0.53
1:B:601:SER:HB3	1:B:607:THR:HA	1.92	0.52
1:B:199:ASP:O	1:B:200:SER:HB3	2.10	0.52
1:A:144:GLU:HG2	1:A:766:ARG:NH1	2.25	0.52
1:B:790:PRO:O	1:B:809:LYS:HB3	2.09	0.52
1:B:519:GLY:HA3	1:B:551:ARG:NH1	2.25	0.52
5:C:200:HEM:HHD	5:C:200:HEM:CBC	2.28	0.52
1:A:790:PRO:O	1:A:809:LYS:HB3	2.10	0.52
1:B:273:ILE:HD12	1:B:274:LEU:N	2.25	0.52
1:A:577:TRP:HD1	1:A:578:LEU:HB2	1.74	0.52
2:D:101:GLY:HA3	2:D:106:TYR:CE2	2.44	0.52
1:A:669:PRO:C	2:C:43:GLY:O	2.52	0.52
1:B:720:TRP:O	1:B:721:LEU:HB2	2.08	0.52
2:D:86:TYR:HA	2:D:132:VAL:HG21	1.92	0.51
1:A:338:ASN:HB3	1:A:391:ALA:O	2.10	0.51
1:B:462:TYR:CE1	1:B:486:VAL:CG1	2.92	0.51
1:A:273:ILE:HD12	1:A:274:LEU:N	2.25	0.51
2:C:128:HIS:HA	2:C:133:HIS:CD2	2.45	0.51
2:D:128:HIS:HA	2:D:133:HIS:CD2	2.44	0.51
1:A:497:TYR:HB3	1:A:501:LEU:HB3	1.91	0.51
1:B:296:ILE:HG22	1:B:804:LEU:HD13	1.93	0.51
1:B:646:TYR:HB2	1:B:688:LEU:HD21	1.93	0.51
1:A:117:TYR:CG	1:A:641:VAL:HG22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASP:HA	1:A:304:ASN:CA	2.36	0.51
1:A:462:TYR:CZ	1:A:486:VAL:CG1	2.94	0.51
1:A:479:THR:O	1:A:594:THR:HG23	2.11	0.51
1:B:669:PRO:C	2:D:43:GLY:O	2.54	0.51
1:B:120:PRO:O	1:B:121:ARG:HB3	2.09	0.51
1:B:199:ASP:C	1:B:201:GLU:H	2.19	0.51
1:B:338:ASN:HB3	1:B:391:ALA:O	2.12	0.50
1:A:282:LEU:O	1:A:321:HIS:HB2	2.11	0.50
1:B:828:ARG:NH1	1:B:862:GLU:OE1	2.42	0.50
1:A:137:ARG:HH11	1:A:155:GLN:HB3	1.75	0.50
1:A:828:ARG:NH1	1:A:862:GLU:OE1	2.42	0.50
2:D:55:TYR:CE1	5:D:200:HEM:CBB	2.94	0.50
1:A:169:ASP:O	1:A:172:ARG:HG3	2.10	0.50
1:B:273:ILE:HD11	1:B:275:LEU:HG	1.94	0.50
1:B:373:ARG:HH22	4:B:871:GOL:C1	2.24	0.50
1:B:596:THR:HG22	1:B:597:LEU:HD23	1.93	0.50
1:A:628:VAL:O	1:A:641:VAL:HA	2.12	0.50
1:B:144:GLU:HG2	1:B:766:ARG:NH1	2.26	0.50
1:B:156:GLN:HG3	1:B:850:THR:HG21	1.94	0.50
1:B:180:MET:HE1	1:B:383:ASN:HB3	1.93	0.50
1:B:588:TRP:CZ3	1:B:590:PRO:HG3	2.46	0.50
1:A:199:ASP:O	1:A:200:SER:HB3	2.12	0.50
1:A:199:ASP:C	1:A:201:GLU:H	2.20	0.50
1:A:296:ILE:HG22	1:A:804:LEU:HD13	1.93	0.50
1:A:526:ALA:HB1	1:A:530:GLN:O	2.12	0.50
1:A:635:PHE:CD1	1:A:635:PHE:N	2.76	0.50
1:A:853:ARG:NH1	1:A:856:THR:HG21	2.27	0.50
1:B:661:ARG:NH1	1:B:718:LYS:HA	2.25	0.50
2:C:19:TYR:C	2:C:19:TYR:CD2	2.90	0.50
5:D:200:HEM:HH1	5:D:200:HEM:CBB	2.41	0.50
1:A:199:ASP:O	1:A:199:ASP:OD1	2.29	0.50
1:A:116:VAL:HG23	1:A:123:VAL:HG13	1.94	0.49
1:B:301:ASP:HA	1:B:304:ASN:CA	2.37	0.49
1:B:577:TRP:HD1	1:B:578:LEU:HB2	1.77	0.49
1:A:562:LYS:HE2	1:A:618:ARG:NE	2.27	0.49
1:A:596:THR:HG22	1:A:597:LEU:HD23	1.95	0.49
1:B:570:ALA:HA	1:B:580:LEU:O	2.13	0.49
1:A:301:ASP:CA	1:A:304:ASN:HA	2.38	0.49
1:A:595:GLU:HA	1:A:676:TYR:CD1	2.47	0.49
1:B:662:ASN:OD1	1:B:718:LYS:HE3	2.13	0.49
1:B:115:TRP:H	1:B:115:TRP:CD1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:TYR:CZ	1:B:486:VAL:CG1	2.95	0.49
5:D:200:HEM:HHA	5:D:200:HEM:CBD	2.41	0.49
1:B:734:GLY:O	1:B:736:PHE:N	2.45	0.49
1:A:130:GLN:OE1	1:A:145:GLN:HB2	2.12	0.49
1:A:519:GLY:HA3	1:A:551:ARG:NH1	2.27	0.49
1:A:570:ALA:HA	1:A:580:LEU:O	2.13	0.49
2:C:26:THR:C	2:C:28:GLY:H	2.21	0.49
2:D:26:THR:C	2:D:28:GLY:H	2.20	0.49
1:A:139:ALA:HB1	1:A:160:LEU:HD22	1.95	0.49
1:A:507:LEU:HD12	1:A:507:LEU:O	2.13	0.49
1:B:726:ARG:HB2	1:B:741:ASP:HB2	1.94	0.49
1:A:797:VAL:HB	1:A:801:TYR:CD2	2.48	0.49
1:B:475:MET:SD	1:B:478:VAL:HG21	2.53	0.49
2:D:27:PHE:HB2	2:D:65:THR:HG21	1.95	0.49
1:B:628:VAL:O	1:B:641:VAL:HA	2.13	0.48
1:B:231:VAL:CG1	1:B:274:LEU:HD21	2.42	0.48
1:A:300:ASN:C	1:A:302:THR:N	2.71	0.48
1:A:734:GLY:O	1:A:736:PHE:N	2.45	0.48
1:B:117:TYR:CG	1:B:641:VAL:HG22	2.48	0.48
1:B:282:LEU:O	1:B:321:HIS:HB2	2.13	0.48
2:C:133:HIS:CE1	5:C:200:HEM:CBC	2.96	0.48
1:B:672:GLY:HA2	5:D:200:HEM:HBC1	1.96	0.48
2:C:62:ASN:O	2:C:64:VAL:HG12	2.13	0.48
1:A:769:VAL:HG12	1:A:786:VAL:HB	1.94	0.48
1:B:327:ARG:HB3	4:B:867:GOL:H31	1.95	0.48
1:B:169:ASP:O	1:B:172:ARG:HG3	2.13	0.48
1:B:539:LYS:CA	1:B:734:GLY:HA2	2.35	0.48
1:B:661:ARG:HD3	1:B:718:LYS:HA	1.96	0.48
1:A:231:VAL:CG1	1:A:274:LEU:HD21	2.42	0.48
1:B:797:VAL:HB	1:B:801:TYR:CD2	2.48	0.48
2:C:53:SER:HA	2:C:71:GLY:O	2.14	0.48
2:D:19:TYR:C	2:D:19:TYR:CD2	2.91	0.48
1:A:539:LYS:CA	1:A:734:GLY:HA2	2.35	0.48
1:A:577:TRP:CD1	1:A:578:LEU:HB2	2.48	0.48
2:D:62:ASN:O	2:D:64:VAL:HG12	2.14	0.48
1:B:243:LEU:C	1:B:243:LEU:HD23	2.38	0.48
1:B:130:GLN:OE1	1:B:145:GLN:HB2	2.13	0.48
1:B:299:ASN:C	1:B:301:ASP:H	2.22	0.47
1:B:635:PHE:CD1	1:B:635:PHE:N	2.79	0.47
2:C:113:VAL:CG1	2:C:114:SER:N	2.76	0.47
1:A:661:ARG:HD3	1:A:718:LYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:SER:OG	1:B:733:ARG:NH2	2.47	0.47
1:A:523:PRO:HG3	1:A:668:GLN:OE1	2.14	0.47
1:A:685:PHE:N	1:A:685:PHE:CD2	2.82	0.47
1:B:301:ASP:CA	1:B:304:ASN:HA	2.38	0.47
1:B:793:GLN:HA	1:B:805:ALA:O	2.14	0.47
1:B:655:ILE:HG22	1:B:678:ASN:ND2	2.30	0.47
1:B:116:VAL:HG23	1:B:123:VAL:HG13	1.97	0.47
1:A:655:ILE:HG22	1:A:678:ASN:ND2	2.29	0.47
1:A:793:GLN:HA	1:A:805:ALA:O	2.14	0.47
1:B:238:ALA:HB1	1:B:239:PRO:HD2	1.97	0.47
1:B:262:GLY:O	1:B:276:ALA:HA	2.15	0.47
1:B:554:TRP:CZ3	1:B:613:PHE:HZ	2.33	0.47
1:B:798:PRO:C	1:B:800:ASN:H	2.23	0.47
1:A:717:ASN:C	1:A:719:ALA:H	2.21	0.47
1:B:199:ASP:O	1:B:199:ASP:OD1	2.33	0.47
1:B:776:PHE:O	1:B:777:ASP:HB2	2.14	0.47
1:A:116:VAL:CG2	1:A:123:VAL:HG13	2.45	0.47
1:A:798:PRO:C	1:A:800:ASN:H	2.22	0.47
2:C:62:ASN:O	2:C:63:GLN:HB2	2.15	0.47
2:D:113:VAL:CG1	2:D:114:SER:N	2.78	0.47
1:A:513:ARG:HH12	1:A:515:ARG:NH1	2.13	0.47
1:B:119:GLU:HA	1:B:120:PRO:HD3	1.68	0.46
1:A:669:PRO:O	2:C:43:GLY:O	2.33	0.46
1:A:238:ALA:HB1	1:A:239:PRO:HD2	1.97	0.46
1:A:662:ASN:OD1	1:A:718:LYS:HE3	2.15	0.46
1:B:562:LYS:HE2	1:B:618:ARG:NE	2.30	0.46
1:B:685:PHE:N	1:B:685:PHE:CD2	2.84	0.46
1:A:296:ILE:HD13	1:A:296:ILE:N	2.31	0.46
1:A:579:GLU:HB3	1:A:627:ASN:HD21	1.80	0.46
1:B:387:ASP:OD1	1:B:403:LYS:HD3	2.15	0.46
5:D:200:HEM:HBB2	5:D:200:HEM:CHC	2.40	0.46
1:B:577:TRP:CD1	1:B:578:LEU:HB2	2.50	0.46
1:A:262:GLY:O	1:A:276:ALA:HA	2.15	0.46
1:B:160:LEU:O	1:B:175:MET:HE1	2.15	0.46
1:B:712:ASN:N	1:B:712:ASN:ND2	2.63	0.46
2:D:55:TYR:CE1	5:D:200:HEM:HBB1	2.51	0.46
1:B:321:HIS:CE1	4:B:871:GOL:O1	2.67	0.46
1:B:719:ALA:C	1:B:720:TRP:O	2.54	0.46
5:D:200:HEM:HBC2	5:D:200:HEM:CHD	2.24	0.46
1:B:501:LEU:HD12	1:B:502:THR:H	1.80	0.46
1:B:575:VAL:CG1	1:B:577:TRP:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HD11	1:A:358:LEU:HD11	1.98	0.46
1:A:494:THR:HG22	1:A:495:TYR:N	2.31	0.46
1:B:468:SER:HB3	1:B:476:GLU:O	2.16	0.46
1:B:854:GLY:O	1:B:855:ARG:C	2.59	0.46
1:B:523:PRO:HG3	1:B:668:GLN:OE1	2.16	0.45
1:A:121:ARG:O	1:A:643:LYS:HE3	2.15	0.45
1:A:299:ASN:C	1:A:301:ASP:H	2.23	0.45
1:B:139:ALA:HB1	1:B:160:LEU:HD22	1.97	0.45
1:B:669:PRO:O	2:D:43:GLY:O	2.35	0.45
1:A:712:ASN:N	1:A:712:ASN:ND2	2.64	0.45
1:B:162:VAL:CG2	1:B:175:MET:HE3	2.28	0.45
1:A:847:LEU:HA	1:A:847:LEU:HD12	1.73	0.45
1:B:216:MET:SD	1:B:438:GLN:CB	3.03	0.45
1:B:365:PRO:HA	1:B:366:PRO:C	2.42	0.45
1:B:373:ARG:NH2	4:B:871:GOL:C1	2.79	0.45
1:B:498:ASP:HB2	1:B:500:TRP:CD1	2.51	0.45
1:B:609:TYR:OH	1:B:663:LYS:HE2	2.17	0.45
1:A:776:PHE:O	1:A:777:ASP:HB2	2.16	0.45
1:B:299:ASN:O	1:B:301:ASP:N	2.49	0.45
2:D:27:PHE:O	2:D:27:PHE:CD1	2.70	0.45
1:A:498:ASP:HB2	1:A:500:TRP:CD1	2.52	0.45
1:A:588:TRP:CZ3	1:A:590:PRO:HG3	2.52	0.45
1:B:300:ASN:C	1:B:302:THR:N	2.71	0.45
1:B:533:THR:OG1	1:B:534:ILE:N	2.50	0.45
1:B:579:GLU:HB3	1:B:627:ASN:HD21	1.81	0.45
2:C:27:PHE:CD1	2:C:27:PHE:O	2.70	0.45
1:A:501:LEU:HD12	1:A:502:THR:H	1.79	0.45
2:C:27:PHE:HB2	2:C:65:THR:HG21	1.98	0.45
2:C:74:THR:OG1	2:C:86:TYR:CE2	2.70	0.45
1:A:719:ALA:C	1:A:720:TRP:O	2.55	0.45
1:B:312:ILE:HD11	1:B:358:LEU:HD11	1.97	0.45
1:B:299:ASN:ND2	1:B:300:ASN:N	2.65	0.45
1:A:299:ASN:O	1:A:301:ASP:N	2.50	0.44
2:D:53:SER:HA	2:D:71:GLY:O	2.17	0.44
1:A:156:GLN:HG3	1:A:850:THR:HG21	1.98	0.44
1:A:180:MET:HE1	1:A:383:ASN:HB3	1.99	0.44
1:A:595:GLU:OE2	1:A:655:ILE:HG12	2.16	0.44
1:B:256:THR:HG21	1:B:858:GLN:OE1	2.17	0.44
1:B:286:TRP:HA	1:B:287:PRO:HD3	1.78	0.44
1:B:595:GLU:HA	1:B:676:TYR:CD1	2.53	0.44
1:B:847:LEU:HA	1:B:847:LEU:HD12	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:HIS:O	2:D:128:HIS:HE1	2.00	0.44
1:B:717:ASN:C	1:B:719:ALA:H	2.24	0.44
2:D:74:THR:OG1	2:D:86:TYR:CE2	2.70	0.44
1:A:119:GLU:HA	1:A:120:PRO:HD3	1.70	0.44
1:A:162:VAL:CG2	1:A:175:MET:HE3	2.27	0.44
1:A:243:LEU:HD23	1:A:243:LEU:C	2.43	0.44
1:A:301:ASP:C	1:A:303:GLY:N	2.76	0.44
2:C:69:ALA:HB1	2:C:89:LEU:HD21	1.99	0.44
1:A:121:ARG:O	1:A:643:LYS:CE	2.65	0.44
1:B:479:THR:O	1:B:594:THR:HG23	2.18	0.44
1:B:853:ARG:NH1	1:B:856:THR:HG21	2.32	0.44
1:B:717:ASN:O	1:B:719:ALA:N	2.43	0.44
1:B:298:ILE:O	1:B:299:ASN:HB3	2.18	0.44
1:A:201:GLU:OE1	1:A:201:GLU:HA	2.17	0.44
1:A:288:GLY:HA3	1:A:838:ALA:HA	2.00	0.44
1:A:589:ARG:NH2	1:A:595:GLU:OE2	2.29	0.44
2:C:155:LEU:HB3	2:C:160:LEU:HB2	1.99	0.44
1:A:373:ARG:O	1:A:373:ARG:HG2	2.18	0.43
1:A:387:ASP:OD1	1:A:403:LYS:HD3	2.18	0.43
1:A:717:ASN:C	1:A:719:ALA:N	2.75	0.43
1:B:490:PHE:CD1	1:B:490:PHE:C	2.96	0.43
1:B:444:ARG:HG3	1:B:454:ARG:HG3	1.99	0.43
2:C:27:PHE:O	2:C:27:PHE:CG	2.71	0.43
2:D:62:ASN:O	2:D:63:GLN:HB2	2.18	0.43
1:B:123:VAL:HG22	1:B:124:SER:N	2.33	0.43
1:B:293:ILE:HG13	1:B:294:GLY:N	2.33	0.43
1:B:373:ARG:O	1:B:373:ARG:HG2	2.18	0.43
1:B:548:THR:HG22	1:B:549:THR:H	1.81	0.43
2:C:83:HIS:O	2:C:128:HIS:HE1	2.01	0.43
1:A:444:ARG:HG3	1:A:454:ARG:HG3	2.00	0.43
1:B:657:LEU:HB2	1:B:676:TYR:CE2	2.54	0.43
1:B:841:VAL:O	1:B:842:SER:C	2.61	0.43
2:D:155:LEU:HB3	2:D:160:LEU:HB2	1.99	0.43
1:A:533:THR:OG1	1:A:534:ILE:N	2.51	0.43
1:A:609:TYR:OH	1:A:663:LYS:HE2	2.18	0.43
1:B:296:ILE:N	1:B:296:ILE:HD13	2.32	0.43
1:B:697:GLY:HA3	1:B:778:ARG:NH2	2.30	0.43
1:B:717:ASN:C	1:B:719:ALA:N	2.76	0.43
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.80	0.43
1:B:762:LEU:HD12	1:B:762:LEU:HA	1.82	0.43
1:A:160:LEU:O	1:A:175:MET:HE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:THR:HG22	1:A:549:THR:H	1.81	0.43
1:A:731:SER:OG	1:A:733:ARG:NH2	2.51	0.43
1:B:494:THR:HG22	1:B:495:TYR:N	2.32	0.43
1:A:500:TRP:HA	1:A:572:ARG:HG3	2.01	0.43
1:A:554:TRP:CZ3	1:A:613:PHE:HZ	2.36	0.43
1:B:123:VAL:CG2	1:B:124:SER:N	2.81	0.43
1:B:165:ARG:HD3	1:B:647:PHE:CE2	2.54	0.43
1:B:787:ARG:NH1	1:B:814:ASP:OD2	2.50	0.43
2:C:83:HIS:CE1	5:C:200:HEM:C2A	3.06	0.43
1:A:652:ASP:O	1:A:653:ASN:HB2	2.19	0.42
1:B:116:VAL:CG2	1:B:123:VAL:HG13	2.49	0.42
1:B:139:ALA:O	1:B:142:ILE:HG23	2.19	0.42
1:B:201:GLU:OE1	1:B:201:GLU:HA	2.18	0.42
1:B:301:ASP:C	1:B:303:GLY:N	2.77	0.42
1:B:833:ASN:O	1:B:855:ARG:HA	2.20	0.42
1:B:590:PRO:HA	1:B:616:PRO:HB3	2.00	0.42
1:A:480:PRO:HB2	1:A:481:ALA:H	1.48	0.42
1:A:490:PHE:CD1	1:A:490:PHE:C	2.98	0.42
1:A:657:LEU:HB2	1:A:676:TYR:CE2	2.54	0.42
1:A:821:LEU:HA	1:A:821:LEU:HD12	1.76	0.42
1:B:121:ARG:O	1:B:643:LYS:CE	2.68	0.42
1:A:365:PRO:HA	1:A:366:PRO:C	2.43	0.42
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.92	0.42
1:A:680:LEU:HD11	1:A:717:ASN:OD1	2.19	0.42
1:A:763:PRO:HA	1:A:843:TYR:CD2	2.55	0.42
1:B:172:ARG:HH12	1:B:655:ILE:HG13	1.82	0.42
1:B:417:SER:HB3	1:B:425:GLY:N	2.34	0.42
5:C:200:HEM:HBC2	5:C:200:HEM:CHD	2.25	0.42
2:D:27:PHE:O	2:D:27:PHE:CG	2.72	0.42
1:A:299:ASN:ND2	1:A:300:ASN:N	2.67	0.42
1:A:575:VAL:CG1	1:A:577:TRP:HB3	2.50	0.42
1:A:599:ASN:CG	1:A:599:ASN:O	2.61	0.42
1:B:599:ASN:CG	1:B:599:ASN:O	2.62	0.42
1:B:763:PRO:HA	1:B:843:TYR:CD2	2.54	0.42
1:A:293:ILE:HG13	1:A:294:GLY:N	2.34	0.42
1:A:543:LEU:HD23	1:A:543:LEU:HA	1.89	0.42
1:A:572:ARG:HA	1:A:578:LEU:O	2.19	0.42
1:B:301:ASP:C	1:B:303:GLY:H	2.28	0.42
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.91	0.42
1:A:168:GLN:HG3	1:A:169:ASP:OD1	2.19	0.42
1:A:256:THR:HG21	1:A:858:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:THR:HG23	1:B:704:THR:HB	2.02	0.42
1:B:479:THR:O	1:B:594:THR:OG1	2.33	0.42
1:B:507:LEU:O	1:B:507:LEU:HD12	2.19	0.42
1:A:468:SER:HB3	1:A:476:GLU:O	2.19	0.42
1:A:480:PRO:HG3	1:A:598:THR:HA	2.01	0.42
1:A:603:HIS:CE1	5:C:200:HEM:HMA3	2.49	0.42
1:A:841:VAL:O	1:A:842:SER:C	2.63	0.42
1:A:300:ASN:O	1:A:302:THR:N	2.52	0.42
1:B:299:ASN:HD22	1:B:300:ASN:CB	2.33	0.42
1:B:572:ARG:HA	1:B:578:LEU:O	2.20	0.42
2:D:80:GLU:HG2	2:D:81:PRO:HA	2.01	0.42
1:A:301:ASP:C	1:A:303:GLY:H	2.26	0.41
1:A:516:GLY:HA3	1:A:597:LEU:HD11	2.02	0.41
1:B:832:GLU:OE1	1:B:853:ARG:NH2	2.53	0.41
2:C:118:LEU:O	2:C:119:ASN:C	2.63	0.41
1:A:338:ASN:HB3	1:A:391:ALA:C	2.45	0.41
1:A:575:VAL:HG22	1:A:576:GLU:N	2.35	0.41
1:A:609:TYR:HA	1:A:610:PRO:HD3	1.85	0.41
1:B:336:PRO:C	1:B:337:ALA:O	2.64	0.41
1:B:834:LEU:HD23	1:B:834:LEU:HA	1.86	0.41
1:A:762:LEU:HD12	1:A:762:LEU:HA	1.81	0.41
1:B:137:ARG:HB2	1:B:282:LEU:HD13	2.02	0.41
1:B:516:GLY:HA3	1:B:597:LEU:HD11	2.03	0.41
1:B:564:SER:HA	1:B:565:PRO:HD3	1.73	0.41
1:A:216:MET:SD	1:A:438:GLN:CB	3.03	0.41
1:B:569:VAL:O	1:B:581:TYR:HA	2.20	0.41
1:A:137:ARG:HB2	1:A:282:LEU:HD13	2.03	0.41
1:A:562:LYS:HB3	1:A:588:TRP:CD2	2.55	0.41
1:A:640:LEU:HG	1:A:641:VAL:N	2.35	0.41
1:B:297:ARG:NH2	1:B:846:THR:O	2.53	0.41
1:B:652:ASP:O	1:B:653:ASN:HB2	2.21	0.41
1:B:848:ALA:O	1:B:849:ASN:C	2.62	0.41
2:C:122:SER:HB2	2:C:132:VAL:CG2	2.48	0.41
1:B:712:ASN:HD22	1:B:712:ASN:H	1.67	0.41
5:D:200:HEM:CBD	5:D:200:HEM:CHA	2.99	0.41
1:A:417:SER:HB3	1:A:425:GLY:N	2.35	0.41
1:A:543:LEU:HD21	1:A:736:PHE:CD1	2.55	0.41
1:A:566:THR:O	1:A:567:LEU:CD1	2.66	0.41
1:B:121:ARG:O	1:B:643:LYS:HE3	2.20	0.41
1:B:520:LEU:HA	1:B:520:LEU:HD12	1.78	0.41
1:B:593:ILE:HD12	1:B:593:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:NH2	1:A:846:THR:O	2.54	0.41
2:D:122:SER:HB2	2:D:132:VAL:CG2	2.47	0.41
2:D:165:THR:O	2:D:169:VAL:HG23	2.21	0.41
1:A:532:TYR:HA	1:A:536:ASN:O	2.20	0.41
1:A:595:GLU:OE1	1:A:655:ILE:HD13	2.21	0.41
1:B:288:GLY:HA3	1:B:838:ALA:HA	2.03	0.41
1:B:338:ASN:HB3	1:B:391:ALA:C	2.46	0.41
1:B:480:PRO:HB2	1:B:481:ALA:H	1.38	0.41
1:B:495:TYR:CD1	1:B:495:TYR:C	2.96	0.41
1:B:609:TYR:HA	1:B:610:PRO:HD3	1.88	0.41
1:B:615:GLN:HA	1:B:616:PRO:HD3	1.95	0.41
2:C:80:GLU:HG2	2:C:81:PRO:HA	2.03	0.41
2:D:69:ALA:HB1	2:D:89:LEU:HD21	2.03	0.41
1:A:507:LEU:HD12	1:A:507:LEU:C	2.46	0.41
1:A:590:PRO:HA	1:A:616:PRO:HB3	2.02	0.41
1:A:787:ARG:NH1	1:A:814:ASP:OD2	2.51	0.41
1:A:848:ALA:O	1:A:849:ASN:C	2.64	0.40
1:A:183:ASN:C	1:A:432:LEU:HD23	2.47	0.40
1:A:617:GLU:OE2	1:A:654:TYR:HA	2.21	0.40
1:B:839:TYR:O	1:B:851:LEU:HA	2.22	0.40
1:A:407:VAL:O	1:A:433:ARG:HA	2.21	0.40
1:B:283:GLY:HA2	1:B:321:HIS:CB	2.51	0.40
1:B:288:GLY:HA3	1:B:837:ARG:C	2.47	0.40
1:B:617:GLU:OE2	1:B:654:TYR:HA	2.22	0.40
1:A:287:PRO:HG3	1:A:317:ILE:HD11	2.03	0.40
1:A:321:HIS:CE1	1:A:353:PRO:HG2	2.56	0.40
1:A:411:ASP:HB3	1:A:430:THR:HG23	2.03	0.40
1:B:626:PHE:CD2	1:B:626:PHE:C	2.99	0.40
1:B:827:LEU:HD23	1:B:827:LEU:HA	1.83	0.40
1:A:123:VAL:CG2	1:A:124:SER:N	2.84	0.40
1:B:138:HIS:O	1:B:139:ALA:C	2.64	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	751/865 (87%)	664 (88%)	76 (10%)	11 (2%)	8	28
1	B	751/865 (87%)	666 (89%)	73 (10%)	12 (2%)	7	27
2	C	158/206 (77%)	141 (89%)	16 (10%)	1 (1%)	21	51
2	D	158/206 (77%)	142 (90%)	15 (10%)	1 (1%)	21	51
All	All	1818/2142 (85%)	1613 (89%)	180 (10%)	25 (1%)	9	30

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	PRO
1	B	480	PRO
2	C	5	VAL
2	D	5	VAL
1	A	299	ASN
1	A	300	ASN
1	A	304	ASN
1	A	605	SER
1	A	733	ARG
1	B	299	ASN
1	B	300	ASN
1	B	304	ASN
1	B	605	SER
1	B	733	ARG
1	A	121	ARG
1	B	318	PRO
1	B	735	ASN
1	A	318	PRO
1	A	735	ASN
1	B	121	ARG
1	B	337	ALA
1	A	336	PRO
1	B	336	PRO
1	A	231	VAL
1	B	231	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	615/694 (89%)	554 (90%)	61 (10%)	7	24
1	B	615/694 (89%)	554 (90%)	61 (10%)	7	24
2	C	123/158 (78%)	112 (91%)	11 (9%)	9	29
2	D	123/158 (78%)	112 (91%)	11 (9%)	9	29
All	All	1476/1704 (87%)	1332 (90%)	144 (10%)	7	25

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	123	VAL
1	A	125	VAL
1	A	126	ILE
1	A	142	ILE
1	A	143	LEU
1	A	146	THR
1	A	152	SER
1	A	168	GLN
1	A	176	ASN
1	A	207	THR
1	A	212	THR
1	A	221	THR
1	A	222	LEU
1	A	231	VAL
1	A	264	LEU
1	A	266	LEU
1	A	273	ILE
1	A	274	LEU
1	A	296	ILE
1	A	312	ILE
1	A	335	LEU
1	A	344	SER
1	A	347	GLN

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Mol	Chain	Res	Type
1	A	348	THR
1	A	393	GLU
1	A	409	THR
1	A	428	THR
1	A	430	THR
1	A	442	THR
1	A	467	THR
1	A	469	ASP
1	A	476	GLU
1	A	486	VAL
1	A	503	LEU
1	A	514	LEU
1	A	533	THR
1	A	542	ARG
1	A	546	CYS
1	A	549	THR
1	A	562	LYS
1	A	564	SER
1	A	582	THR
1	A	620	ARG
1	A	624	VAL
1	A	627	ASN
1	A	651	VAL
1	A	662	ASN
1	A	691	GLN
1	A	698	VAL
1	A	703	LEU
1	A	712	ASN
1	A	729	ASP
1	A	733	ARG
1	A	738	VAL
1	A	762	LEU
1	A	770	THR
1	A	780	LEU
1	A	822	THR
1	A	826	THR
1	A	834	LEU
1	B	122	SER
1	B	123	VAL
1	B	125	VAL
1	B	126	ILE
1	B	142	ILE

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Mol	Chain	Res	Type
1	B	143	LEU
1	B	146	THR
1	B	152	SER
1	B	168	GLN
1	B	176	ASN
1	B	207	THR
1	B	212	THR
1	B	221	THR
1	B	222	LEU
1	B	231	VAL
1	B	264	LEU
1	B	266	LEU
1	B	273	ILE
1	B	274	LEU
1	B	296	ILE
1	B	312	ILE
1	B	335	LEU
1	B	344	SER
1	B	347	GLN
1	B	348	THR
1	B	393	GLU
1	B	409	THR
1	B	428	THR
1	B	430	THR
1	B	442	THR
1	B	467	THR
1	B	469	ASP
1	B	476	GLU
1	B	486	VAL
1	B	503	LEU
1	B	514	LEU
1	B	533	THR
1	B	542	ARG
1	B	546	CYS
1	B	549	THR
1	B	562	LYS
1	B	564	SER
1	B	582	THR
1	B	620	ARG
1	B	624	VAL
1	B	627	ASN
1	B	651	VAL

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Mol	Chain	Res	Type
1	B	662	ASN
1	B	691	GLN
1	B	698	VAL
1	B	703	LEU
1	B	712	ASN
1	B	729	ASP
1	B	733	ARG
1	B	738	VAL
1	B	762	LEU
1	B	770	THR
1	B	780	LEU
1	B	822	THR
1	B	826	THR
1	B	834	LEU
2	C	5	VAL
2	C	64	VAL
2	C	67	PHE
2	C	89	LEU
2	C	103	THR
2	C	108	ILE
2	C	114	SER
2	C	123	LEU
2	C	147	LEU
2	C	164	SER
2	C	165	THR
2	D	5	VAL
2	D	64	VAL
2	D	67	PHE
2	D	89	LEU
2	D	103	THR
2	D	108	ILE
2	D	114	SER
2	D	123	LEU
2	D	147	LEU
2	D	164	SER
2	D	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	441	ASN

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	603	HIS
1	B	182	GLN
1	B	299	ASN
1	B	441	ASN
1	B	456	ASN
2	C	63	GLN
2	D	63	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	HEM	C	200	2	50,50,50	1.93	9 (18%)	67,82,82	1.33	4 (5%)
5	HEM	D	200	2	50,50,50	1.92	10 (20%)	67,82,82	1.45	7 (10%)
4	GOL	B	867	-	5,5,5	0.45	0	5,5,5	0.25	0
4	GOL	B	868	-	5,5,5	0.41	0	5,5,5	0.31	0
4	GOL	B	871	-	5,5,5	0.33	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	869	-	5,5,5	0.39	0	5,5,5	0.28	0
4	GOL	B	870	-	5,5,5	0.48	0	5,5,5	0.43	0
4	GOL	A	867	-	5,5,5	0.41	0	5,5,5	0.22	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	HEM	C	200	2	-	6/14/54/54	-
5	HEM	D	200	2	-	6/14/54/54	-
4	GOL	B	867	-	-	4/4/4/4	-
4	GOL	B	868	-	-	2/4/4/4	-
4	GOL	B	871	-	-	2/4/4/4	-
4	GOL	B	869	-	-	2/4/4/4	-
4	GOL	B	870	-	-	0/4/4/4	-
4	GOL	A	867	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	200	HEM	C3D-C2D	7.96	1.53	1.36
5	D	200	HEM	C3D-C2D	7.84	1.53	1.36
5	D	200	HEM	FE-NB	5.46	2.11	1.94
5	C	200	HEM	FE-NB	4.66	2.09	1.94
5	C	200	HEM	FE-ND	4.59	2.09	1.94
5	C	200	HEM	FE-NA	4.32	2.09	1.95
5	D	200	HEM	FE-NC	3.83	2.07	1.95
5	D	200	HEM	FE-NA	3.68	2.07	1.95
5	C	200	HEM	CAB-C3B	2.91	1.55	1.47
5	C	200	HEM	CAC-C3C	2.69	1.54	1.47
5	D	200	HEM	CAB-C3B	2.66	1.54	1.47
5	D	200	HEM	CAC-C3C	2.53	1.54	1.47
5	D	200	HEM	CMD-C2D	2.36	1.55	1.50
5	D	200	HEM	C2A-C3A	-2.21	1.33	1.38
5	D	200	HEM	CMB-C2B	2.06	1.55	1.50
5	C	200	HEM	CMC-C2C	2.05	1.55	1.50
5	C	200	HEM	CMB-C2B	2.05	1.55	1.50
5	D	200	HEM	CMC-C2C	2.04	1.54	1.50
5	C	200	HEM	CMA-C3A	2.01	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	200	HEM	C4D-ND-C1D	5.75	112.02	105.21
5	C	200	HEM	C4D-ND-C1D	5.05	111.18	105.21
5	D	200	HEM	CBD-CAD-C3D	-2.69	105.10	112.53
5	C	200	HEM	C3B-C2B-C1B	2.48	108.28	106.41
5	D	200	HEM	C3B-C4B-NB	-2.26	107.84	109.47
5	D	200	HEM	CHD-C1D-ND	2.18	126.77	124.42
5	C	200	HEM	C1B-NB-C4B	2.08	107.67	105.21
5	D	200	HEM	CAA-CBA-CGA	-2.07	108.16	113.67
5	D	200	HEM	C2A-C1A-NA	-2.01	107.92	110.15
5	C	200	HEM	CHD-C4C-NC	2.01	126.64	124.45
5	D	200	HEM	C4C-C3C-C2C	2.00	108.55	106.81

There are no chirality outliers.

All (24) torsion outliers are listed below:

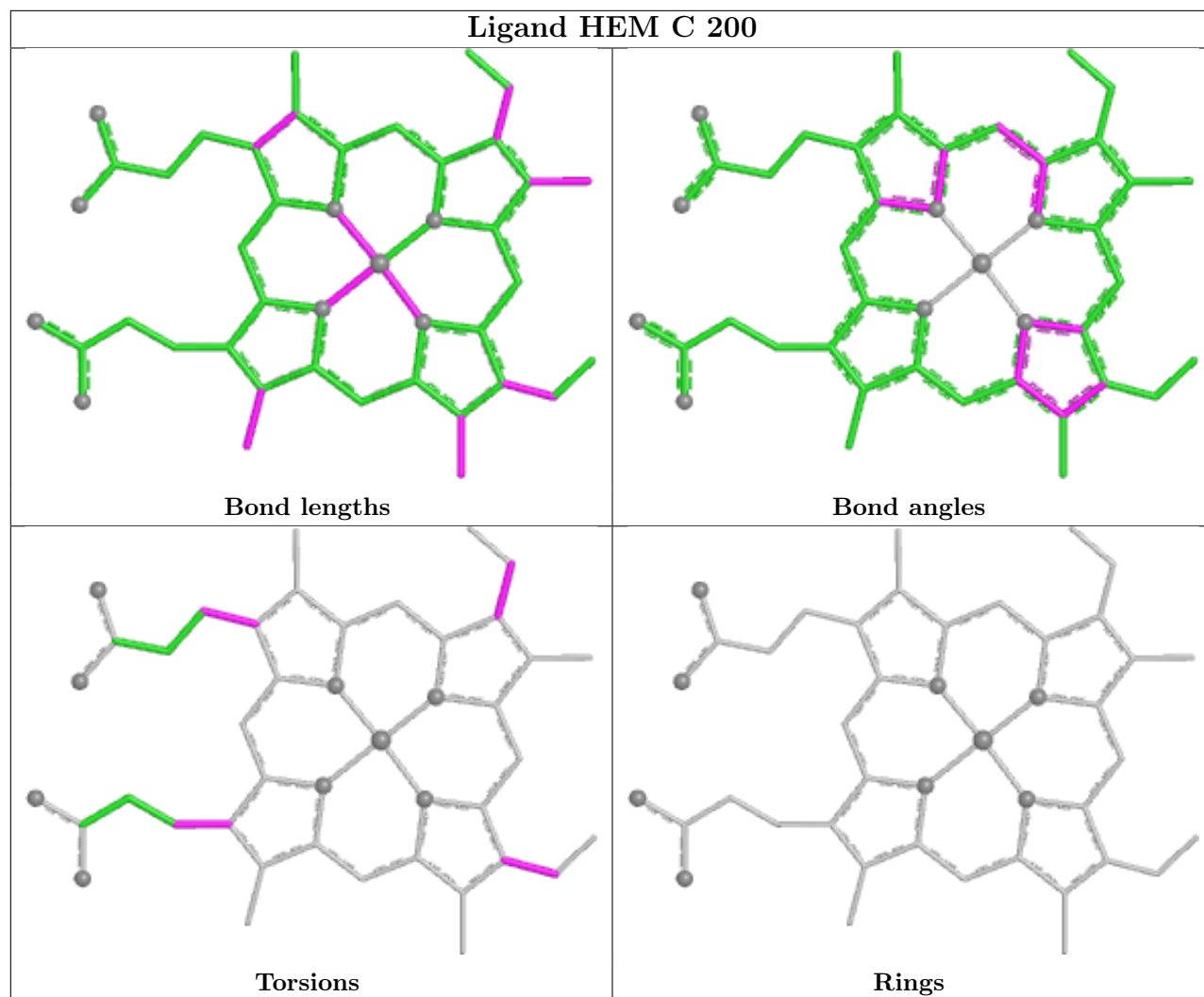
Mol	Chain	Res	Type	Atoms
4	B	867	GOL	O1-C1-C2-C3
4	B	867	GOL	C1-C2-C3-O3
4	B	868	GOL	O1-C1-C2-C3
4	B	869	GOL	O1-C1-C2-C3
4	B	871	GOL	O1-C1-C2-C3
5	C	200	HEM	C1A-C2A-CAA-CBA
5	C	200	HEM	C2D-C3D-CAD-CBD
5	C	200	HEM	C4D-C3D-CAD-CBD
5	C	200	HEM	C3A-C2A-CAA-CBA
4	B	867	GOL	O1-C1-C2-O2
4	A	867	GOL	O1-C1-C2-C3
5	D	200	HEM	C4D-C3D-CAD-CBD
4	B	867	GOL	O2-C2-C3-O3
4	B	868	GOL	O1-C1-C2-O2
4	B	871	GOL	O1-C1-C2-O2
5	D	200	HEM	C2D-C3D-CAD-CBD
4	A	867	GOL	O1-C1-C2-O2
4	B	869	GOL	O1-C1-C2-O2
5	C	200	HEM	C4B-C3B-CAB-CBB
5	C	200	HEM	C4C-C3C-CAC-CBC
5	D	200	HEM	C4C-C3C-CAC-CBC
5	D	200	HEM	C1A-C2A-CAA-CBA
5	D	200	HEM	CAD-CBD-CGD-O2D
5	D	200	HEM	CAD-CBD-CGD-O1D

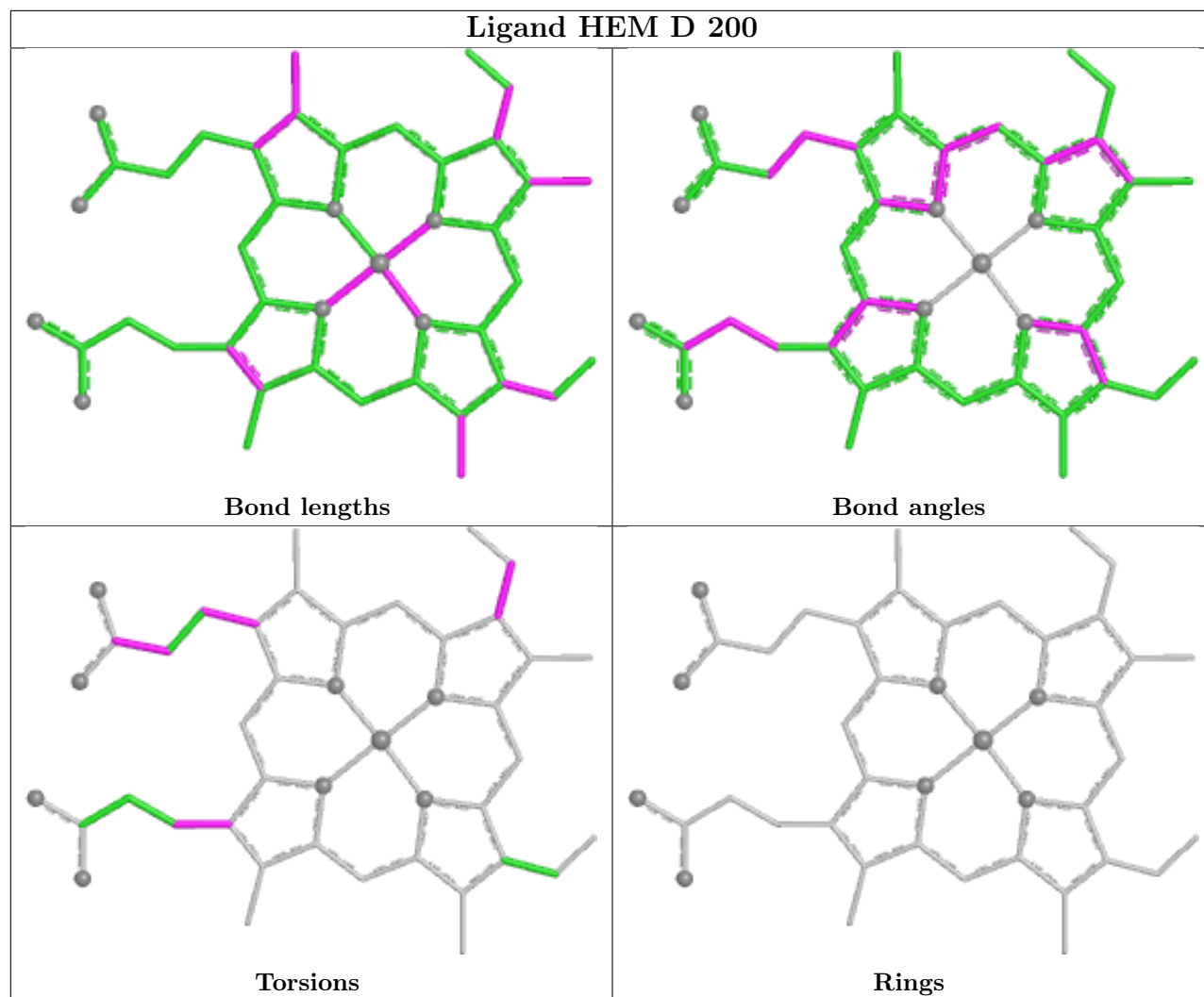
There are no ring outliers.

5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	200	HEM	14	0
5	D	200	HEM	13	0
4	B	867	GOL	1	0
4	B	871	GOL	12	0
4	A	867	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	753/865 (87%)	0.08	19 (2%) 58 48	65, 96, 140, 198	0
1	B	753/865 (87%)	0.05	10 (1%) 75 66	66, 99, 142, 195	0
2	C	162/206 (78%)	-0.02	5 (3%) 51 41	67, 118, 145, 161	5 (3%)
2	D	162/206 (78%)	-0.12	5 (3%) 51 41	73, 118, 144, 163	5 (3%)
All	All	1830/2142 (85%)	0.04	39 (2%) 63 54	65, 101, 142, 198	10 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	PRO	4.6
2	C	41	ASN	4.6
1	B	292	ASP	4.5
2	D	109	GLN	3.7
2	D	1	PRO	3.7
1	A	577	TRP	3.3
2	D	41	ASN	3.0
1	A	318	PRO	2.9
1	B	318	PRO	2.7
1	A	575	VAL	2.7
1	A	634	TRP	2.7
1	B	577	TRP	2.7
2	C	28	GLY	2.6
2	C	109	GLN	2.6
1	A	837	ARG	2.5
2	C	42	SER	2.4
1	A	113	ASN	2.4
1	A	451	HIS	2.4
1	A	361	LEU	2.4
1	B	652	ASP	2.4
1	A	721	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	421	LEU	2.3
1	A	863	TYR	2.3
2	D	42	SER	2.2
2	D	117	GLY	2.2
1	B	606	SER	2.2
1	A	562	LYS	2.2
1	A	713	GLU	2.2
1	A	652	ASP	2.2
1	A	477	GLY	2.2
1	A	555	ASP	2.2
1	A	294	GLY	2.1
1	A	573	PRO	2.1
1	A	292	ASP	2.1
1	B	428	THR	2.1
1	B	113	ASN	2.0
1	A	497	TYR	2.0
1	B	602	ALA	2.0
1	B	835	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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. 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.

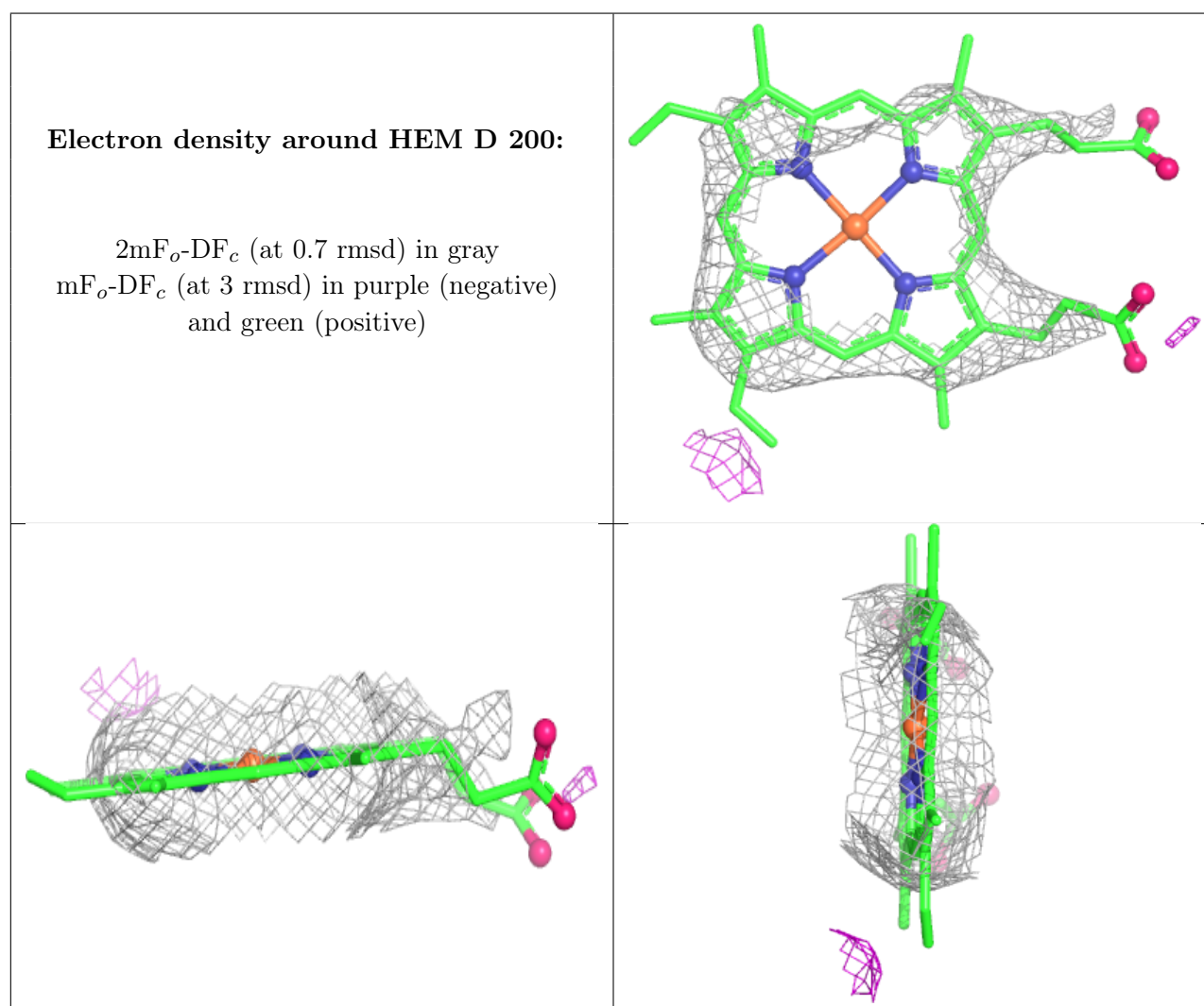
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	871	6/6	0.48	0.28	101,168,171,176	0
3	NA	B	866	1/1	0.58	0.97	131,131,131,131	0
3	NA	A	866	1/1	0.67	0.75	103,103,103,103	0
4	GOL	B	868	6/6	0.75	0.16	82,102,134,135	0
4	GOL	B	869	6/6	0.79	0.19	105,129,146,149	0

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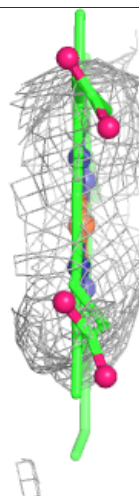
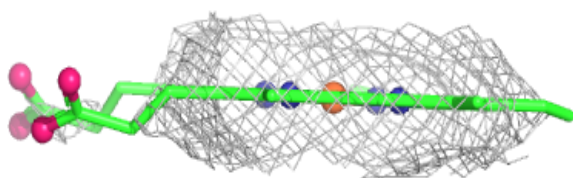
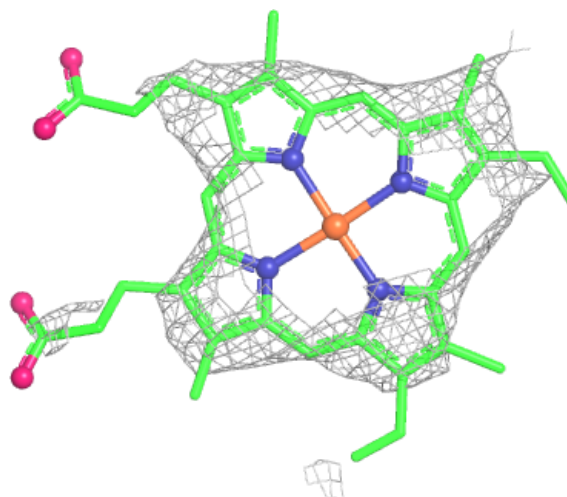
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	867	6/6	0.85	0.10	98,121,134,139	0
4	GOL	B	867	6/6	0.87	0.17	72,94,110,114	0
4	GOL	B	870	6/6	0.91	0.20	51,71,96,107	0
5	HEM	D	200	43/43	0.96	0.14	92,118,162,199	0
5	HEM	C	200	43/43	0.97	0.11	72,117,151,157	43

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around HEM C 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.