



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:46 AM UTC

PDB ID : 3CSL / pdb_00003csl
Title : Structure of the Serratia marcescens hemophore receptor HasR in complex with its hemophore HasA and heme
Authors : Krieg, S.; Diederichs, K.
Deposited on : 2008-04-10
Resolution : 2.70 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

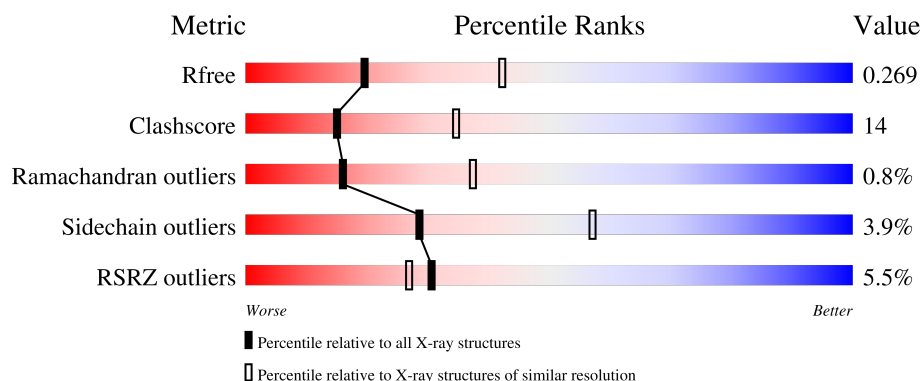
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	 4% 61% 24% 13%
1	B	865	 5% 61% 24% 13%
2	C	206	 5% 66% 13% 21%
2	D	206	 4% 67% 12% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14317 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
			5889	3674	1043	1159	13			
1	B	753	Total	C	N	O	S	0	0	0
			5889	3674	1043	1159	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	ALA	GLY	SEE REMARK 999	UNP Q79AD2
B	645	ALA	GLY	SEE REMARK 999	UNP Q79AD2

- Molecule 2 is a protein called Hemophore HasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	S	0	0	0
			1184	743	189	251	1			
2	D	163	Total	C	N	O	S	0	0	0
			1184	743	189	251	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

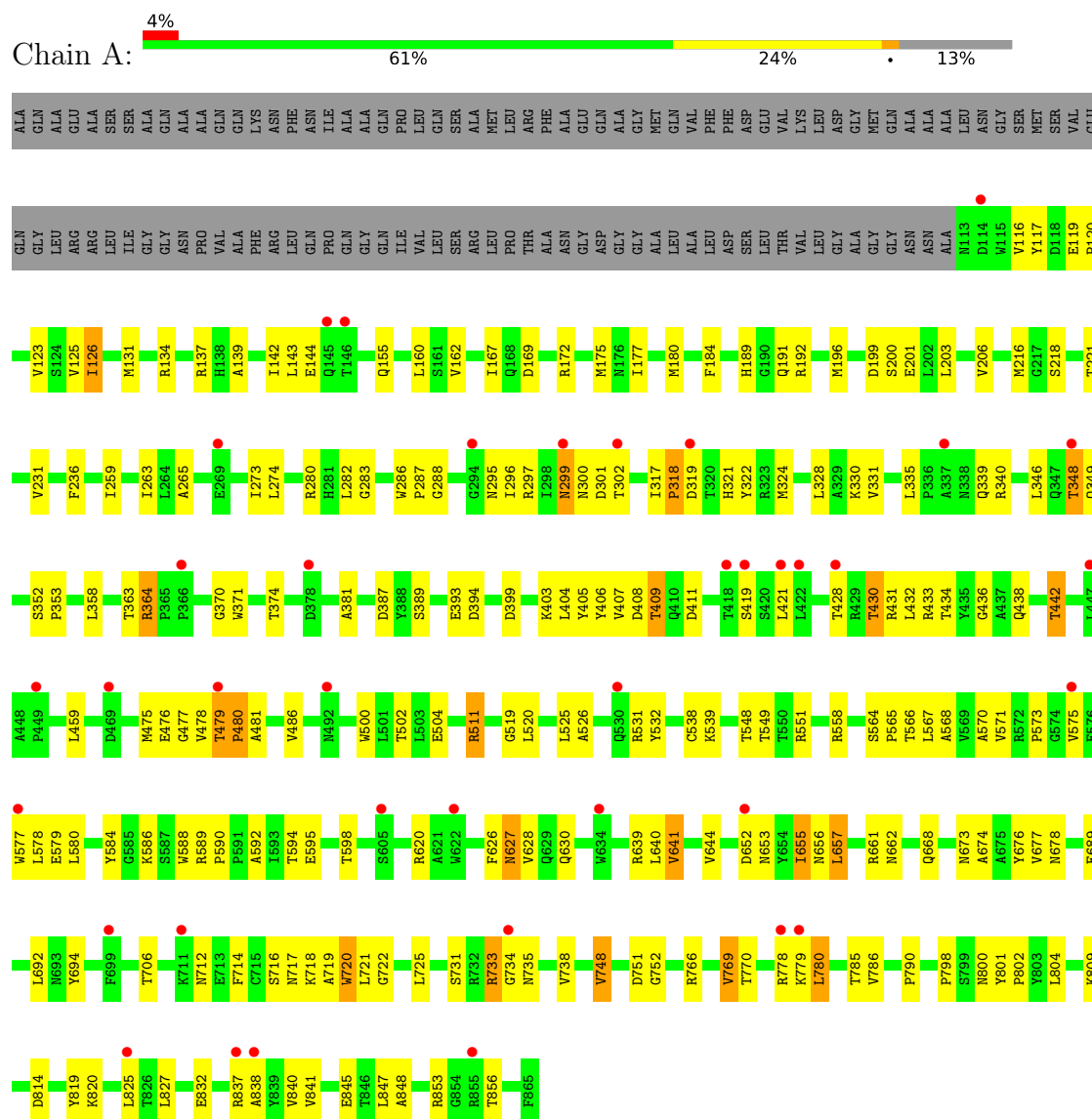
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total 26	O 26	0	0
5	B	16	Total 16	O 16	0	0
5	D	1	Total 1	O 1	0	0

3 Residue-property plots

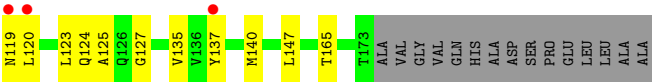
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.02Å 163.40Å 595.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 2.70 49.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.17-2.70) 95.0 (49.17-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.274 0.235 , 0.269	Depositor DCC
R_{free} test set	4959 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14317	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: HEM, GOL

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	0.25	0/6027	0.68	3/8188 (0.0%)
1	B	0.25	0/6027	0.68	3/8188 (0.0%)
2	C	0.24	0/1211	0.65	2/1649 (0.1%)
2	D	0.24	0/1211	0.65	2/1649 (0.1%)
All	All	0.25	0/14476	0.68	10/19674 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	751	ASP	CB-CA-C	-5.51	110.23	116.63
1	A	751	ASP	CB-CA-C	-5.49	110.27	116.63
2	C	110	VAL	CA-C-N	5.48	125.42	119.78
2	C	110	VAL	C-N-CA	5.48	125.42	119.78
1	A	317	ILE	CA-C-N	5.38	126.56	119.84
1	A	317	ILE	C-N-CA	5.38	126.56	119.84
2	D	110	VAL	CA-C-N	5.37	125.31	119.78
2	D	110	VAL	C-N-CA	5.37	125.31	119.78
1	B	317	ILE	CA-C-N	5.36	126.54	119.84
1	B	317	ILE	C-N-CA	5.36	126.54	119.84

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	5889	0	5597	167	0
1	B	5889	0	5597	165	0
2	C	1184	0	1078	19	0
2	D	1184	0	1078	18	0
3	A	43	0	30	9	0
3	B	43	0	30	8	0
4	A	30	0	40	0	0
4	B	12	0	16	0	0
5	A	26	0	0	0	0
5	B	16	0	0	0	0
5	D	1	0	0	0	0
All	All	14317	0	13466	379	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 14.

All (379) 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	1.40	1.03
1:B:137:ARG:HD3	1:B:853:ARG:HD2	1.41	1.01
1:A:779:LYS:HZ3	1:A:820:LYS:HG3	1.31	0.95
1:A:318:PRO:HG2	1:A:371:TRP:HB2	1.48	0.95
3:B:866:HEM:HHC	3:B:866:HEM:HBB2	1.48	0.93
3:A:866:HEM:HHC	3:A:866:HEM:HBB2	1.48	0.93
1:B:318:PRO:HG2	1:B:371:TRP:HB2	1.48	0.91
1:B:779:LYS:HZ3	1:B:820:LYS:HG3	1.34	0.91
1:B:162:VAL:HG23	1:B:175:MET:HE3	1.57	0.85
1:A:477:GLY:HA2	1:A:480:PRO:HB3	1.57	0.85
1:A:162:VAL:HG23	1:A:175:MET:HE3	1.57	0.85
3:B:866:HEM:HMC1	3:B:866:HEM:HBC2	1.59	0.84
1:B:477:GLY:HA2	1:B:480:PRO:HB3	1.58	0.83
1:B:539:LYS:HA	1:B:734:GLY:HA2	1.61	0.83
1:A:539:LYS:HA	1:A:734:GLY:HA2	1.61	0.82
1:A:575:VAL:HG22	1:A:577:TRP:H	1.44	0.81
1:B:575:VAL:HG22	1:B:577:TRP:H	1.44	0.80
1:A:144:GLU:HA	1:A:766:ARG:HH12	1.48	0.79
1:B:853:ARG:HH11	1:B:856:THR:HG21	1.46	0.79
1:A:302:THR:HB	2:C:125:ALA:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ARG:HH11	1:A:856:THR:HG21	1.47	0.77
1:B:144:GLU:HA	1:B:766:ARG:HH12	1.48	0.77
2:D:123:LEU:HD23	2:D:123:LEU:H	1.50	0.77
2:C:123:LEU:H	2:C:123:LEU:HD23	1.50	0.75
3:A:866:HEM:HMC2	3:A:866:HEM:HBC2	1.68	0.75
1:A:137:ARG:HH11	1:A:155:GLN:HB3	1.53	0.74
1:B:137:ARG:HH11	1:B:155:GLN:HB3	1.53	0.73
1:B:504:GLU:HB3	1:B:568:ALA:HB3	1.71	0.72
1:A:297:ARG:HH22	1:A:847:LEU:HA	1.55	0.72
1:B:297:ARG:HH22	1:B:847:LEU:HA	1.55	0.71
1:A:504:GLU:HB3	1:A:568:ALA:HB3	1.73	0.70
1:A:720:TRP:CD1	1:A:721:LEU:HD13	2.26	0.70
1:B:302:THR:HB	2:D:125:ALA:HB2	1.73	0.69
1:B:720:TRP:CD1	1:B:721:LEU:HD13	2.26	0.69
2:D:76:THR:HG23	2:D:79:ASN:HB3	1.73	0.69
2:C:76:THR:HG23	2:C:79:ASN:HB3	1.73	0.69
3:B:866:HEM:HHA	3:B:866:HEM:CBD	2.23	0.68
3:A:866:HEM:HHA	3:A:866:HEM:CBD	2.23	0.68
1:B:191:GLN:HG2	1:B:845:GLU:CD	2.19	0.67
1:B:668:GLN:HG3	2:D:58:SER:HB3	1.75	0.67
1:A:191:GLN:HG2	1:A:845:GLU:CD	2.19	0.67
1:B:180:MET:HE3	1:B:405:TYR:HB2	1.77	0.66
1:A:180:MET:HE3	1:A:405:TYR:HB2	1.78	0.64
1:B:177:ILE:HD12	1:B:346:LEU:HD23	1.80	0.64
1:A:668:GLN:HG3	2:C:58:SER:HB3	1.80	0.63
1:A:177:ILE:HD12	1:A:346:LEU:HD23	1.79	0.62
1:B:411:ASP:HB3	1:B:430:THR:HG23	1.81	0.62
1:B:778:ARG:O	1:B:778:ARG:HG3	1.99	0.62
1:A:322:TYR:HB2	1:A:352:SER:HB2	1.81	0.62
1:B:200:SER:HA	1:B:203:LEU:HD12	1.82	0.61
2:D:96:ASP:HB2	2:D:110:VAL:HG13	1.83	0.61
1:B:172:ARG:NH1	1:B:655:ILE:HD13	2.16	0.60
1:A:411:ASP:HB3	1:A:430:THR:HG23	1.81	0.60
2:C:96:ASP:HB2	2:C:110:VAL:HG13	1.82	0.60
1:A:172:ARG:NH1	1:A:655:ILE:HD13	2.16	0.60
1:B:322:TYR:HB2	1:B:352:SER:HB2	1.82	0.60
2:C:1:PRO:HB3	2:C:119:ASN:HD21	1.67	0.60
2:C:124:GLN:O	2:C:125:ALA:HB3	2.02	0.60
1:B:288:GLY:HA3	1:B:838:ALA:HA	1.84	0.60
1:B:283:GLY:HA2	1:B:321:HIS:HB2	1.84	0.59
1:A:200:SER:HA	1:A:203:LEU:HD12	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLY:HA3	1:A:838:ALA:HA	1.83	0.59
1:B:259:ILE:HD11	1:B:282:LEU:HD21	1.84	0.59
3:A:866:HEM:HBC2	3:A:866:HEM:CMC	2.33	0.59
2:D:124:GLN:O	2:D:125:ALA:HB3	2.02	0.59
1:A:259:ILE:HD11	1:A:282:LEU:HD21	1.84	0.59
1:A:720:TRP:O	1:A:721:LEU:HB2	2.03	0.58
1:A:144:GLU:HA	1:A:766:ARG:NH1	2.18	0.58
1:B:184:PHE:HA	1:B:432:LEU:HD23	1.85	0.58
1:A:407:VAL:HB	1:A:434:THR:HB	1.85	0.58
1:B:720:TRP:O	1:B:721:LEU:HB2	2.03	0.58
1:B:780:LEU:HD23	1:B:819:TYR:HD1	1.68	0.58
1:A:827:LEU:HD23	1:A:827:LEU:H	1.69	0.58
1:B:144:GLU:HA	1:B:766:ARG:NH1	2.18	0.58
1:A:184:PHE:HA	1:A:432:LEU:HD23	1.84	0.58
1:A:283:GLY:HA2	1:A:321:HIS:HB2	1.85	0.58
1:A:780:LEU:HD23	1:A:819:TYR:HD1	1.68	0.58
1:A:589:ARG:HH12	1:A:655:ILE:HD12	1.69	0.57
1:B:407:VAL:HB	1:B:434:THR:HB	1.86	0.57
1:B:502:THR:HB	1:B:570:ALA:HB3	1.86	0.57
1:B:779:LYS:NZ	1:B:820:LYS:HG3	2.15	0.57
1:A:175:MET:HE2	1:A:196:MET:HG2	1.85	0.57
1:B:175:MET:HE2	1:B:196:MET:HG2	1.87	0.57
1:B:589:ARG:HH12	1:B:655:ILE:HD12	1.69	0.57
1:A:477:GLY:CA	1:A:480:PRO:HB3	2.32	0.57
1:A:475:MET:HA	1:A:478:VAL:HG23	1.86	0.57
2:D:1:PRO:HB3	2:D:119:ASN:HD21	1.69	0.57
1:A:364:ARG:HD2	1:A:364:ARG:O	2.05	0.57
1:B:477:GLY:CA	1:B:480:PRO:HB3	2.33	0.57
1:B:167:ILE:CG2	1:B:172:ARG:HB3	2.35	0.56
1:A:126:ILE:HG23	1:A:206:VAL:HB	1.87	0.56
1:A:167:ILE:CG2	1:A:172:ARG:HB3	2.36	0.56
1:B:475:MET:HA	1:B:478:VAL:HG23	1.87	0.56
1:B:725:LEU:HB3	1:B:738:VAL:HG11	1.87	0.56
3:B:866:HEM:HBC2	3:B:866:HEM:CMC	2.32	0.56
1:B:431:ARG:HD3	1:B:433:ARG:HE	1.70	0.56
1:A:725:LEU:HB3	1:A:738:VAL:HG11	1.88	0.56
1:B:216:MET:SD	1:B:438:GLN:HB2	2.46	0.56
1:B:566:THR:C	1:B:567:LEU:HD12	2.31	0.56
1:A:431:ARG:HD3	1:A:433:ARG:HE	1.70	0.55
1:B:126:ILE:HG23	1:B:206:VAL:HB	1.87	0.55
2:D:95:GLY:HA3	2:D:108:ILE:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ALA:HB2	1:A:531:ARG:HA	1.89	0.55
1:B:265:ALA:HB2	1:B:274:LEU:HD23	1.88	0.55
1:B:364:ARG:HD2	1:B:364:ARG:O	2.05	0.55
1:A:297:ARG:NH2	1:A:847:LEU:HA	2.22	0.55
1:A:475:MET:SD	1:A:478:VAL:HG21	2.46	0.55
1:A:502:THR:HB	1:A:570:ALA:HB3	1.88	0.55
1:B:827:LEU:HD23	1:B:827:LEU:H	1.70	0.55
2:C:95:GLY:HA3	2:C:108:ILE:HG21	1.88	0.55
1:A:216:MET:SD	1:A:438:GLN:HB2	2.47	0.55
1:A:566:THR:C	1:A:567:LEU:HD12	2.32	0.55
1:B:539:LYS:HA	1:B:734:GLY:CA	2.36	0.55
1:A:265:ALA:HB2	1:A:274:LEU:HD23	1.88	0.54
1:A:548:THR:HG22	1:A:549:THR:N	2.22	0.54
1:B:348:THR:HG23	1:B:381:ALA:HB3	1.89	0.54
1:B:780:LEU:O	1:B:780:LEU:HD13	2.08	0.54
1:A:780:LEU:HD13	1:A:780:LEU:O	2.08	0.54
2:D:1:PRO:CB	2:D:119:ASN:HD21	2.21	0.54
1:B:548:THR:HG22	1:B:549:THR:N	2.22	0.54
1:A:328:LEU:HD21	1:A:330:LYS:HE3	1.90	0.53
1:A:779:LYS:NZ	1:A:820:LYS:HG3	2.15	0.53
1:B:526:ALA:HB2	1:B:531:ARG:HA	1.90	0.53
1:A:348:THR:HG23	1:A:381:ALA:HB3	1.89	0.53
1:B:475:MET:SD	1:B:478:VAL:HG21	2.48	0.53
2:C:1:PRO:CB	2:C:119:ASN:HD21	2.21	0.53
2:D:135:VAL:HG23	2:D:147:LEU:HB2	1.91	0.53
1:A:539:LYS:HA	1:A:734:GLY:CA	2.36	0.53
3:B:866:HEM:HHA	3:B:866:HEM:HBD1	1.89	0.53
3:A:866:HEM:HHA	3:A:866:HEM:HBD1	1.90	0.52
1:B:328:LEU:HD21	1:B:330:LYS:HE3	1.90	0.52
1:B:640:LEU:HD23	1:B:694:TYR:HB2	1.91	0.52
2:C:135:VAL:HG23	2:C:147:LEU:HB2	1.90	0.52
1:B:770:THR:HG22	1:B:785:THR:HG23	1.91	0.52
1:A:231:VAL:HG13	1:A:236:PHE:HE2	1.75	0.52
1:B:297:ARG:NH2	1:B:847:LEU:HA	2.22	0.52
1:A:319:ASP:HB3	1:A:353:PRO:HB2	1.92	0.51
1:B:300:ASN:C	1:B:302:THR:H	2.18	0.51
1:B:319:ASP:HB3	1:B:353:PRO:HB2	1.92	0.51
1:A:321:HIS:CE1	1:A:353:PRO:HG2	2.45	0.51
1:A:770:THR:HG22	1:A:785:THR:HG23	1.91	0.51
1:B:577:TRP:CZ3	1:B:630:GLN:HG2	2.46	0.51
1:B:321:HIS:CE1	1:B:353:PRO:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:VAL:HG13	1:B:236:PHE:HE2	1.76	0.51
1:A:577:TRP:CZ3	1:A:630:GLN:HG2	2.46	0.51
1:B:131:MET:HE3	1:B:142:ILE:HG21	1.91	0.50
1:A:280:ARG:HD3	1:A:322:TYR:OH	2.11	0.50
3:A:866:HEM:HH A	3:A:866:HEM:HBD2	1.92	0.50
1:A:300:ASN:C	1:A:302:THR:H	2.19	0.50
1:A:640:LEU:HD23	1:A:694:TYR:HB2	1.92	0.50
1:A:116:VAL:HG13	1:A:123:VAL:HG13	1.94	0.50
1:A:131:MET:HE3	1:A:142:ILE:HG21	1.92	0.50
1:B:589:ARG:O	1:B:589:ARG:HG3	2.12	0.50
1:B:769:VAL:HG13	1:B:786:VAL:HB	1.93	0.50
1:A:589:ARG:HG3	1:A:589:ARG:O	2.12	0.50
1:B:406:TYR:CE1	1:B:408:ASP:HB2	2.47	0.50
1:A:845:GLU:HG2	1:A:848:ALA:H	1.77	0.49
1:A:589:ARG:HH12	1:A:655:ILE:CD1	2.25	0.49
1:A:655:ILE:HG22	1:A:678:ASN:ND2	2.27	0.49
1:B:126:ILE:CG2	1:B:206:VAL:HB	2.42	0.49
1:B:655:ILE:HG22	1:B:678:ASN:ND2	2.27	0.49
1:B:845:GLU:HG2	1:B:848:ALA:H	1.77	0.49
1:A:126:ILE:CG2	1:A:206:VAL:HB	2.42	0.49
1:B:280:ARG:HD3	1:B:322:TYR:OH	2.12	0.49
3:B:866:HEM:HH A	3:B:866:HEM:HBD2	1.92	0.49
2:D:58:SER:HB2	2:D:98:LEU:HD12	1.95	0.49
1:A:769:VAL:HG13	1:A:786:VAL:HB	1.93	0.49
1:B:589:ARG:HH12	1:B:655:ILE:CD1	2.25	0.49
2:C:137:TYR:HA	2:C:140:MET:HE2	1.95	0.49
2:D:137:TYR:HA	2:D:140:MET:HE2	1.94	0.49
1:B:295:ASN:O	1:B:299:ASN:HB3	2.13	0.49
1:A:406:TYR:CE1	1:A:408:ASP:HB2	2.47	0.49
2:D:84:THR:HG21	2:D:127:GLY:HA2	1.95	0.48
1:A:189:HIS:HB2	1:A:191:GLN:NE2	2.29	0.48
1:B:116:VAL:HG13	1:B:123:VAL:HG13	1.95	0.48
1:B:189:HIS:HB2	1:B:191:GLN:NE2	2.29	0.48
1:A:716:SER:O	1:A:748:VAL:HG23	2.14	0.48
1:A:579:GLU:HB3	1:A:627:ASN:ND2	2.29	0.48
1:A:798:PRO:HB2	1:A:800:ASN:OD1	2.14	0.48
1:B:579:GLU:HB3	1:B:627:ASN:ND2	2.29	0.48
1:B:725:LEU:HB3	1:B:738:VAL:CG1	2.44	0.48
1:B:405:TYR:CZ	1:B:436:GLY:HA3	2.49	0.48
1:B:716:SER:O	1:B:748:VAL:HG23	2.14	0.48
2:C:58:SER:HB2	2:C:98:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:O	1:B:200:SER:HB3	2.14	0.47
1:B:564:SER:HB3	1:B:586:LYS:O	2.13	0.47
1:B:731:SER:OG	1:B:733:ARG:HG2	2.14	0.47
2:C:84:THR:HG21	2:C:127:GLY:HA2	1.95	0.47
1:A:295:ASN:O	1:A:299:ASN:HB3	2.13	0.47
1:A:511:ARG:O	1:A:511:ARG:HG3	2.14	0.47
1:A:731:SER:OG	1:A:733:ARG:HG2	2.14	0.47
1:B:519:GLY:HA3	1:B:551:ARG:NH1	2.29	0.47
1:A:399:ASP:HB3	1:A:442:THR:HG23	1.96	0.47
1:B:399:ASP:HB3	1:B:442:THR:HG23	1.96	0.47
1:A:139:ALA:HB1	1:A:160:LEU:HD22	1.97	0.47
1:A:160:LEU:O	1:A:175:MET:HE1	2.15	0.47
1:A:519:GLY:HA3	1:A:551:ARG:NH1	2.30	0.47
1:B:363:THR:HG23	1:B:364:ARG:HG3	1.97	0.47
1:B:511:ARG:O	1:B:511:ARG:HG3	2.14	0.47
2:C:15:SER:HA	2:C:165:THR:HA	1.97	0.47
1:A:299:ASN:C	1:A:301:ASP:H	2.23	0.47
1:A:335:LEU:HB2	1:A:339:GLN:HB2	1.96	0.47
1:A:363:THR:HG23	1:A:364:ARG:HG3	1.97	0.47
1:A:405:TYR:CZ	1:A:436:GLY:HA3	2.50	0.47
1:A:564:SER:HB3	1:A:586:LYS:O	2.13	0.47
1:A:322:TYR:CB	1:A:352:SER:HB2	2.45	0.47
1:B:661:ARG:O	1:B:673:ASN:HB2	2.15	0.47
1:A:661:ARG:HD3	1:A:718:LYS:HA	1.97	0.47
1:A:199:ASP:O	1:A:200:SER:HB3	2.15	0.47
1:B:335:LEU:HB2	1:B:339:GLN:HB2	1.96	0.47
1:A:798:PRO:HD2	1:A:801:TYR:CE1	2.50	0.46
1:B:798:PRO:HB2	1:B:800:ASN:OD1	2.14	0.46
1:A:725:LEU:HB3	1:A:738:VAL:CG1	2.44	0.46
1:B:299:ASN:C	1:B:301:ASP:H	2.23	0.46
1:B:798:PRO:HD2	1:B:801:TYR:CE1	2.50	0.46
1:A:393:GLU:O	1:A:394:ASP:HB2	2.16	0.46
2:D:15:SER:HA	2:D:165:THR:HA	1.97	0.46
2:D:124:GLN:O	2:D:125:ALA:CB	2.64	0.46
1:B:661:ARG:HD3	1:B:718:LYS:HA	1.97	0.46
1:A:580:LEU:HD23	1:A:626:PHE:HB3	1.98	0.46
3:A:866:HEM:HBD1	3:A:866:HEM:CHA	2.46	0.46
1:B:322:TYR:CB	1:B:352:SER:HB2	2.46	0.46
3:B:866:HEM:HBD1	3:B:866:HEM:CHA	2.46	0.46
1:A:324:MET:HA	1:A:349:GLN:O	2.16	0.46
1:A:661:ARG:O	1:A:673:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASP:OD2	1:B:403:LYS:HD3	2.16	0.46
1:B:580:LEU:HD23	1:B:626:PHE:HB3	1.97	0.46
1:B:779:LYS:HG2	1:B:820:LYS:HZ3	1.81	0.46
1:B:479:THR:O	1:B:594:THR:HA	2.16	0.46
1:A:199:ASP:C	1:A:201:GLU:H	2.24	0.45
1:B:393:GLU:O	1:B:394:ASP:HB2	2.16	0.45
1:A:117:TYR:CG	1:A:641:VAL:HG22	2.51	0.45
1:A:137:ARG:NH1	1:A:155:GLN:HB3	2.26	0.45
1:A:374:THR:HG21	3:A:866:HEM:HAA2	1.97	0.45
1:B:500:TRP:O	1:B:571:VAL:HA	2.17	0.45
1:B:780:LEU:HD23	1:B:819:TYR:CD1	2.51	0.45
1:A:300:ASN:C	1:A:302:THR:N	2.74	0.45
1:A:500:TRP:O	1:A:571:VAL:HA	2.17	0.45
1:A:779:LYS:HG2	1:A:820:LYS:HZ3	1.80	0.45
1:B:117:TYR:CG	1:B:641:VAL:HG22	2.52	0.45
1:B:160:LEU:O	1:B:175:MET:HE1	2.16	0.45
1:B:324:MET:HA	1:B:349:GLN:O	2.16	0.45
1:A:752:GLY:HA2	1:A:801:TYR:OH	2.17	0.45
1:B:802:PRO:HG3	2:D:77:LEU:CD2	2.46	0.45
1:A:692:LEU:C	1:A:692:LEU:HD23	2.42	0.45
1:B:137:ARG:NH1	1:B:155:GLN:HB3	2.26	0.45
1:B:283:GLY:HA2	1:B:321:HIS:CB	2.47	0.45
1:B:752:GLY:HA2	1:B:801:TYR:OH	2.17	0.45
1:B:837:ARG:NH2	1:B:837:ARG:HB2	2.32	0.45
2:C:124:GLN:O	2:C:125:ALA:CB	2.64	0.45
1:B:300:ASN:C	1:B:302:THR:N	2.74	0.45
1:A:480:PRO:HG3	1:A:598:THR:HA	1.99	0.45
1:A:779:LYS:HA	1:A:779:LYS:HD2	1.67	0.45
1:B:479:THR:OG1	1:B:480:PRO:HA	2.17	0.45
1:A:283:GLY:HA2	1:A:321:HIS:CB	2.47	0.45
1:A:387:ASP:OD2	1:A:403:LYS:HD3	2.16	0.44
1:A:479:THR:O	1:A:594:THR:HA	2.16	0.44
1:B:520:LEU:C	1:B:520:LEU:HD23	2.42	0.44
1:B:733:ARG:HG3	1:B:735:ASN:H	1.82	0.44
1:A:579:GLU:HB3	1:A:627:ASN:HD21	1.81	0.44
1:A:589:ARG:HA	1:A:590:PRO:HD3	1.84	0.44
1:A:479:THR:OG1	1:A:480:PRO:HA	2.17	0.44
1:A:548:THR:HG22	1:A:549:THR:H	1.82	0.44
1:B:139:ALA:HB1	1:B:160:LEU:HD22	1.98	0.44
1:B:339:GLN:HA	1:B:389:SER:O	2.18	0.44
1:B:579:GLU:HB3	1:B:627:ASN:HD21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:C	1:A:274:LEU:HD13	2.43	0.44
1:A:520:LEU:C	1:A:520:LEU:HD23	2.42	0.44
1:A:733:ARG:HG3	1:A:735:ASN:HB2	2.00	0.44
1:B:692:LEU:HD23	1:B:692:LEU:C	2.42	0.44
1:A:231:VAL:HG11	1:A:263:ILE:HD13	1.99	0.44
1:B:199:ASP:C	1:B:201:GLU:H	2.25	0.44
1:B:480:PRO:HG3	1:B:598:THR:HA	1.99	0.44
1:B:644:VAL:HA	1:B:689:GLU:O	2.18	0.44
1:A:652:ASP:O	1:A:653:ASN:HB2	2.18	0.44
1:A:657:LEU:HD21	1:A:674:ALA:HB1	2.00	0.44
1:A:733:ARG:HG3	1:A:735:ASN:H	1.82	0.44
1:A:837:ARG:NH2	1:A:837:ARG:HB2	2.32	0.44
1:A:175:MET:CE	1:A:196:MET:HG2	2.48	0.43
1:A:218:SER:O	1:A:221:THR:HB	2.18	0.43
1:A:592:ALA:HB3	1:A:595:GLU:HG2	2.00	0.43
1:A:644:VAL:HA	1:A:689:GLU:O	2.18	0.43
1:A:853:ARG:HH11	1:A:856:THR:CG2	2.26	0.43
1:B:657:LEU:HD21	1:B:674:ALA:HB1	2.00	0.43
1:A:119:GLU:HA	1:A:120:PRO:HD3	1.80	0.43
1:A:480:PRO:HB2	1:A:481:ALA:H	1.43	0.43
1:B:274:LEU:HD13	1:B:274:LEU:C	2.43	0.43
1:A:656:ASN:HB2	1:A:714:PHE:CE1	2.53	0.43
1:A:339:GLN:HA	1:A:389:SER:O	2.18	0.43
1:A:778:ARG:O	1:A:778:ARG:HG3	2.19	0.43
1:B:364:ARG:HD2	1:B:364:ARG:C	2.43	0.43
1:B:588:TRP:CH2	1:B:590:PRO:HG3	2.54	0.43
1:B:652:ASP:O	1:B:653:ASN:HB2	2.17	0.43
1:B:662:ASN:ND2	1:B:718:LYS:HE3	2.34	0.43
1:A:595:GLU:HA	1:A:676:TYR:CD1	2.52	0.43
1:A:405:TYR:CE2	1:A:436:GLY:HA3	2.53	0.43
1:B:218:SER:O	1:B:221:THR:HB	2.18	0.43
1:B:589:ARG:HA	1:B:590:PRO:HD3	1.84	0.43
1:B:231:VAL:HG11	1:B:263:ILE:HD13	2.00	0.43
1:B:595:GLU:HA	1:B:676:TYR:CD1	2.53	0.43
1:B:656:ASN:HB2	1:B:714:PHE:CE1	2.53	0.43
1:B:548:THR:HG22	1:B:549:THR:H	1.82	0.43
1:A:364:ARG:HD2	1:A:364:ARG:C	2.43	0.43
1:A:577:TRP:CD1	1:A:578:LEU:HB2	2.54	0.43
1:A:588:TRP:CH2	1:A:590:PRO:HG3	2.54	0.43
3:A:866:HEM:HHC	3:A:866:HEM:CBB	2.34	0.43
1:B:577:TRP:CD1	1:B:578:LEU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:ALA:HB3	1:B:595:GLU:HG2	2.00	0.42
1:A:407:VAL:O	1:A:433:ARG:HA	2.19	0.42
3:B:866:HEM:CBD	3:B:866:HEM:CHA	2.92	0.42
1:A:662:ASN:ND2	1:A:718:LYS:HE3	2.34	0.42
1:B:405:TYR:CE2	1:B:436:GLY:HA3	2.53	0.42
1:B:459:LEU:C	1:B:459:LEU:HD12	2.45	0.42
1:B:733:ARG:HG3	1:B:735:ASN:HB2	2.00	0.42
1:B:184:PHE:HB2	1:B:409:THR:HG21	2.02	0.42
1:B:419:SER:OG	1:B:421:LEU:HD23	2.19	0.42
1:A:184:PHE:HB2	1:A:409:THR:HG21	2.01	0.42
1:A:273:ILE:HD13	1:A:331:VAL:HG22	2.01	0.42
1:A:286:TRP:HA	1:A:287:PRO:HD3	1.87	0.42
1:A:717:ASN:C	1:A:719:ALA:H	2.27	0.42
1:A:479:THR:O	1:A:594:THR:HG23	2.20	0.42
1:B:145:GLN:HE21	1:B:145:GLN:HB3	1.72	0.42
1:A:419:SER:OG	1:A:421:LEU:HD23	2.19	0.42
1:B:476:GLU:CD	1:B:476:GLU:H	2.28	0.42
1:B:640:LEU:HD22	1:B:641:VAL:H	1.84	0.42
1:A:296:ILE:HG22	1:A:804:LEU:HD13	2.02	0.42
1:A:532:TYR:CE1	1:A:538:CYS:HA	2.55	0.42
1:A:840:VAL:O	1:A:841:VAL:C	2.63	0.42
1:B:273:ILE:HD13	1:B:331:VAL:HG22	2.01	0.42
1:B:296:ILE:HG22	1:B:804:LEU:HD13	2.02	0.42
1:B:564:SER:HA	1:B:565:PRO:HD3	1.76	0.42
1:A:358:LEU:HD12	1:A:370:GLY:O	2.20	0.41
1:B:779:LYS:HA	1:B:779:LYS:HD2	1.67	0.41
1:A:169:ASP:O	1:A:172:ARG:HD2	2.20	0.41
1:A:459:LEU:C	1:A:459:LEU:HD12	2.45	0.41
1:A:584:TYR:HE2	1:A:620:ARG:HD3	1.85	0.41
1:B:573:PRO:HB2	1:B:574:GLY:H	1.74	0.41
1:B:790:PRO:O	1:B:809:LYS:HB3	2.20	0.41
1:A:720:TRP:C	1:A:722:GLY:H	2.29	0.41
1:B:358:LEU:HD12	1:B:370:GLY:O	2.20	0.41
1:A:476:GLU:H	1:A:476:GLU:CD	2.29	0.41
1:A:640:LEU:HD22	1:A:641:VAL:H	1.85	0.41
1:A:847:LEU:HA	1:A:847:LEU:HD12	1.89	0.41
1:B:584:TYR:HE2	1:B:620:ARG:HD3	1.85	0.41
1:A:288:GLY:HA3	1:A:838:ALA:CA	2.49	0.41
1:B:479:THR:O	1:B:594:THR:HG23	2.21	0.41
2:D:11:PHE:HA	2:D:14:TYR:HD2	1.86	0.41
1:A:628:VAL:O	1:A:641:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PRO:O	1:A:809:LYS:HB3	2.20	0.41
1:B:134:ARG:HD2	1:B:814:ASP:OD2	2.21	0.41
2:C:27:PHE:HD1	2:C:65:THR:HG22	1.86	0.41
1:A:717:ASN:O	1:A:719:ALA:N	2.48	0.41
1:B:175:MET:CE	1:B:196:MET:HG2	2.49	0.41
1:B:407:VAL:O	1:B:433:ARG:HA	2.20	0.41
2:C:136:VAL:O	2:C:140:MET:HG3	2.21	0.41
1:A:538:CYS:O	1:A:539:LYS:HB2	2.20	0.41
1:A:564:SER:HA	1:A:565:PRO:HD3	1.76	0.41
1:B:538:CYS:O	1:B:539:LYS:HB2	2.20	0.41
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.93	0.41
1:B:840:VAL:O	1:B:841:VAL:C	2.63	0.41
2:D:76:THR:CG2	2:D:79:ASN:HB3	2.48	0.41
1:A:802:PRO:HG3	2:C:77:LEU:CD2	2.51	0.41
1:B:717:ASN:O	1:B:719:ALA:N	2.48	0.41
1:A:134:ARG:HD2	1:A:814:ASP:OD2	2.21	0.40
1:A:403:LYS:C	1:A:404:LEU:HD12	2.45	0.40
1:B:717:ASN:C	1:B:719:ALA:H	2.27	0.40
1:B:720:TRP:C	1:B:722:GLY:H	2.29	0.40
2:C:11:PHE:HA	2:C:14:TYR:HD2	1.86	0.40
1:B:345:TYR:HA	1:B:383:ASN:O	2.21	0.40
1:B:375:GLY:HA2	1:B:416:TYR:CD1	2.57	0.40
1:B:403:LYS:C	1:B:404:LEU:HD12	2.46	0.40
1:B:832:GLU:HB2	1:B:856:THR:HB	2.03	0.40
1:B:157:ASP:HA	1:B:158:PRO:HD3	1.93	0.40
1:B:177:ILE:HA	1:B:228:PHE:O	2.22	0.40
1:B:480:PRO:HB2	1:B:481:ALA:H	1.43	0.40
1:B:532:TYR:CE1	1:B:538:CYS:HA	2.55	0.40
1:A:655:ILE:HA	1:A:677:VAL:O	2.21	0.40
1:A:175:MET:HE2	1:A:196:MET:SD	2.61	0.40
1:A:780:LEU:HD23	1:A:819:TYR:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	751/865 (87%)	678 (90%)	67 (9%)	6 (1%)	16	37
1	B	751/865 (87%)	679 (90%)	66 (9%)	6 (1%)	16	37
2	C	159/206 (77%)	150 (94%)	8 (5%)	1 (1%)	21	44
2	D	159/206 (77%)	150 (94%)	7 (4%)	2 (1%)	9	25
All	All	1820/2142 (85%)	1657 (91%)	148 (8%)	15 (1%)	16	37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	PRO
1	A	480	PRO
1	A	573	PRO
1	B	318	PRO
1	B	480	PRO
1	B	573	PRO
1	A	733	ARG
1	A	832	GLU
1	B	733	ARG
1	B	832	GLU
2	C	77	LEU
2	D	77	LEU
1	A	299	ASN
1	B	299	ASN
2	D	5	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	616/695 (89%)	588 (96%)	28 (4%)	24	52
1	B	616/695 (89%)	588 (96%)	28 (4%)	24	52
2	C	124/158 (78%)	123 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	124/158 (78%)	123 (99%)	1 (1%)	73	88
All	All	1480/1706 (87%)	1422 (96%)	58 (4%)	28	57

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	A	126	ILE
1	A	143	LEU
1	A	192	ARG
1	A	340	ARG
1	A	348	THR
1	A	364	ARG
1	A	409	THR
1	A	428	THR
1	A	430	THR
1	A	442	THR
1	A	479	THR
1	A	486	VAL
1	A	511	ARG
1	A	525	LEU
1	A	558	ARG
1	A	627	ASN
1	A	639	ARG
1	A	641	VAL
1	A	655	ILE
1	A	657	LEU
1	A	706	THR
1	A	712	ASN
1	A	720	TRP
1	A	748	VAL
1	A	769	VAL
1	A	780	LEU
1	A	825	LEU
1	B	125	VAL
1	B	126	ILE
1	B	143	LEU
1	B	192	ARG
1	B	340	ARG
1	B	348	THR
1	B	364	ARG
1	B	409	THR

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Mol	Chain	Res	Type
1	B	428	THR
1	B	430	THR
1	B	442	THR
1	B	479	THR
1	B	486	VAL
1	B	511	ARG
1	B	525	LEU
1	B	558	ARG
1	B	627	ASN
1	B	639	ARG
1	B	641	VAL
1	B	655	ILE
1	B	657	LEU
1	B	706	THR
1	B	712	ASN
1	B	720	TRP
1	B	748	VAL
1	B	769	VAL
1	B	780	LEU
1	B	825	LEU
2	C	120	LEU
2	D	120	LEU

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

Mol	Chain	Res	Type
1	A	182	GLN
1	A	229	ASN
1	A	314	ASN
1	A	342	GLN
1	A	608	GLN
1	A	627	ASN
1	A	629	GLN
1	A	712	ASN
1	A	793	GLN
1	B	182	GLN
1	B	229	ASN
1	B	314	ASN
1	B	339	GLN
1	B	342	GLN
1	B	608	GLN
1	B	627	ASN

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Mol	Chain	Res	Type
1	B	629	GLN
2	C	119	ASN
2	C	126	GLN
2	D	119	ASN
2	D	126	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands 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	$\# Z > 2$
4	GOL	A	869	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	B	868	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	A	867	-	5,5,5	0.36	0	5,5,5	0.17	0
4	GOL	A	870	-	5,5,5	0.37	0	5,5,5	0.25	0
3	HEM	B	866	1	50,50,50	1.85	10 (20%)	67,82,82	1.25	5 (7%)
4	GOL	A	868	-	5,5,5	0.38	0	5,5,5	0.22	0
4	GOL	B	867	-	5,5,5	0.38	0	5,5,5	0.29	0
3	HEM	A	866	1	50,50,50	1.87	11 (22%)	67,82,82	1.28	5 (7%)
4	GOL	A	871	-	5,5,5	0.37	0	5,5,5	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	869	-	-	2/4/4/4	-
4	GOL	B	868	-	-	2/4/4/4	-
4	GOL	A	867	-	-	2/4/4/4	-
4	GOL	A	870	-	-	2/4/4/4	-
3	HEM	B	866	1	-	5/14/54/54	-
4	GOL	A	868	-	-	3/4/4/4	-
4	GOL	B	867	-	-	2/4/4/4	-
3	HEM	A	866	1	-	5/14/54/54	-
4	GOL	A	871	-	-	2/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	866	HEM	C3D-C2D	7.90	1.53	1.36
3	A	866	HEM	C3D-C2D	7.86	1.53	1.36
3	A	866	HEM	FE-NB	4.30	2.08	1.94
3	A	866	HEM	FE-ND	4.26	2.08	1.94
3	B	866	HEM	FE-NB	4.16	2.07	1.94
3	B	866	HEM	FE-ND	4.01	2.07	1.94
3	A	866	HEM	FE-NC	2.99	2.05	1.95
3	B	866	HEM	CAC-C3C	2.91	1.55	1.47
3	B	866	HEM	FE-NC	2.91	2.04	1.95
3	A	866	HEM	CAC-C3C	2.91	1.55	1.47
3	A	866	HEM	CAB-C3B	2.85	1.55	1.47
3	B	866	HEM	CAB-C3B	2.82	1.54	1.47
3	A	866	HEM	FE-NA	2.78	2.04	1.95
3	B	866	HEM	FE-NA	2.74	2.04	1.95
3	B	866	HEM	CMB-C2B	2.10	1.55	1.50
3	B	866	HEM	CMC-C2C	2.06	1.55	1.50
3	A	866	HEM	CMC-C2C	2.05	1.55	1.50
3	A	866	HEM	CMB-C2B	2.04	1.54	1.50
3	A	866	HEM	CMA-C3A	2.02	1.54	1.50
3	A	866	HEM	CMD-C2D	2.01	1.54	1.50
3	B	866	HEM	CMA-C3A	2.01	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	866	HEM	C4D-ND-C1D	5.21	111.37	105.21
3	B	866	HEM	C4D-ND-C1D	5.10	111.24	105.21
3	A	866	HEM	C3B-C4B-NB	-2.50	107.67	109.47
3	A	866	HEM	C1B-NB-C4B	2.42	108.07	105.21
3	B	866	HEM	C3B-C2B-C1B	2.30	108.14	106.41
3	A	866	HEM	C3B-C2B-C1B	2.28	108.12	106.41
3	B	866	HEM	CAD-C3D-C4D	2.27	128.65	124.70
3	A	866	HEM	CAD-C3D-C4D	2.23	128.59	124.70
3	B	866	HEM	C1B-NB-C4B	2.11	107.70	105.21
3	B	866	HEM	C3B-C4B-NB	-2.07	107.98	109.47

There are no chirality outliers.

All (25) torsion outliers are listed below:

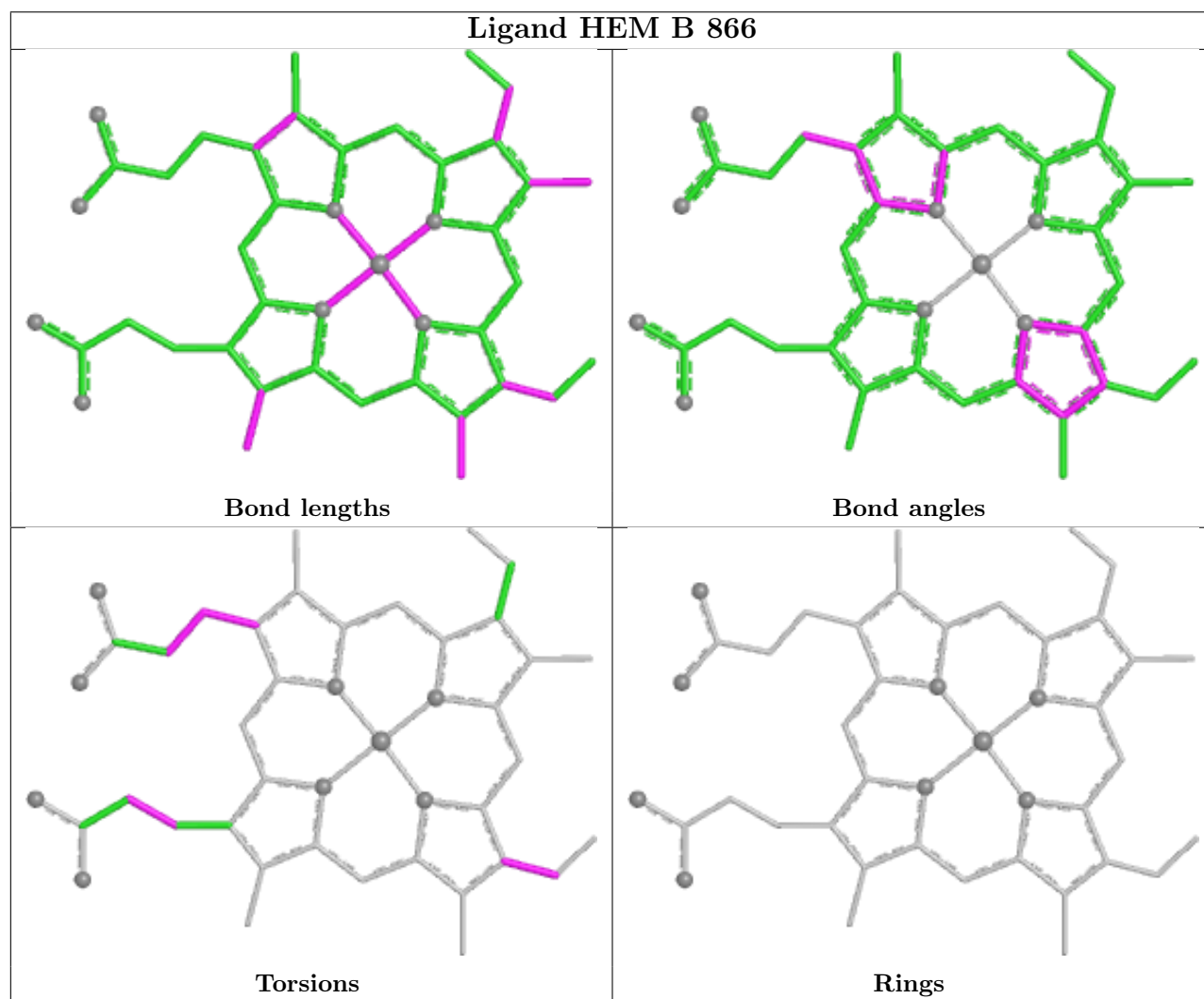
Mol	Chain	Res	Type	Atoms
3	A	866	HEM	C2D-C3D-CAD-CBD
3	A	866	HEM	C4D-C3D-CAD-CBD
3	B	866	HEM	C2D-C3D-CAD-CBD
3	B	866	HEM	C4D-C3D-CAD-CBD
4	A	867	GOL	O1-C1-C2-C3
4	A	868	GOL	O1-C1-C2-C3
4	A	869	GOL	O1-C1-C2-C3
4	A	871	GOL	O1-C1-C2-C3
4	B	867	GOL	O1-C1-C2-C3
4	B	868	GOL	O1-C1-C2-C3
4	A	868	GOL	O1-C1-C2-O2
4	B	868	GOL	O1-C1-C2-O2
4	A	870	GOL	O1-C1-C2-C3
4	A	867	GOL	O1-C1-C2-O2
4	A	869	GOL	O1-C1-C2-O2
4	A	871	GOL	O1-C1-C2-O2
4	B	867	GOL	O1-C1-C2-O2
3	A	866	HEM	C2A-CAA-CBA-CGA
3	B	866	HEM	C2A-CAA-CBA-CGA
4	A	870	GOL	O1-C1-C2-O2
3	A	866	HEM	C4B-C3B-CAB-CBB
3	B	866	HEM	C4B-C3B-CAB-CBB
3	A	866	HEM	C3D-CAD-CBD-CGD
3	B	866	HEM	C3D-CAD-CBD-CGD
4	A	868	GOL	O2-C2-C3-O3

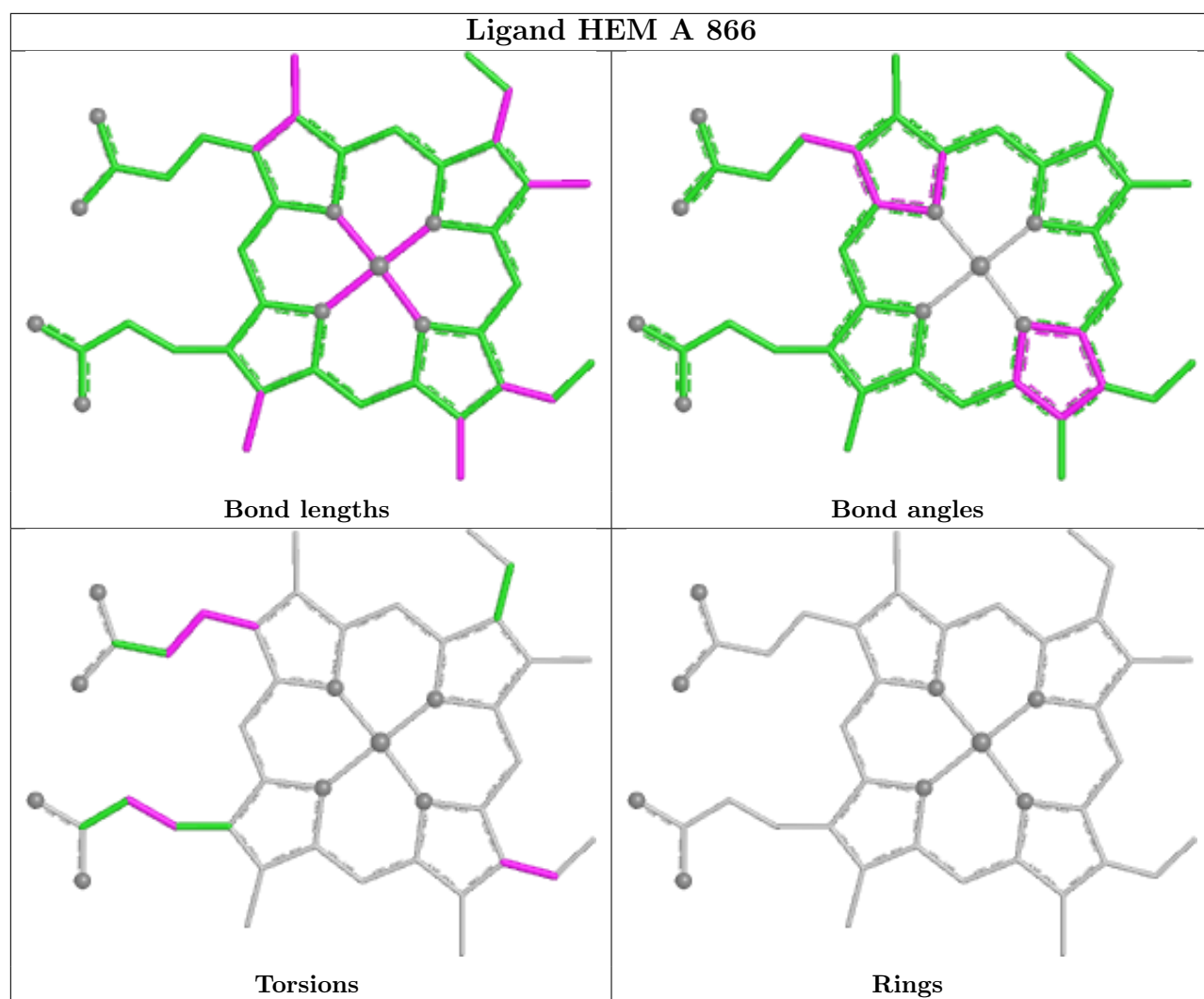
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	866	HEM	8	0
3	A	866	HEM	9	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%)	0.61	38 (5%) 34 30	53, 91, 133, 199	0
1	B	753/865 (87%)	0.59	43 (5%) 29 26	61, 91, 134, 196	0
2	C	163/206 (79%)	0.67	10 (6%) 27 24	82, 109, 141, 179	0
2	D	163/206 (79%)	0.58	9 (5%) 30 27	82, 109, 141, 179	0
All	All	1832/2142 (85%)	0.60	100 (5%) 30 27	53, 94, 138, 199	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	PRO	5.3
1	B	421	LEU	5.2
2	C	40	ALA	4.8
1	A	418	THR	4.4
2	D	1	PRO	4.4
1	B	418	THR	4.4
2	D	137	TYR	4.3
2	D	120	LEU	4.2
2	C	137	TYR	4.2
1	A	577	TRP	4.2
2	C	28	GLY	4.0
1	A	422	LEU	4.0
2	D	40	ALA	4.0
1	A	605	SER	4.0
1	A	634	TRP	4.0
2	D	39	ASP	3.8
2	C	120	LEU	3.7
1	B	302	THR	3.7
1	B	577	TRP	3.6
1	A	575	VAL	3.5
1	B	428	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	422	LEU	3.3
1	B	294	GLY	3.3
2	C	39	ASP	3.3
1	B	837	ARG	3.3
1	B	575	VAL	3.3
1	A	421	LEU	3.3
1	B	734	GLY	3.3
1	A	299	ASN	3.2
1	B	449	PRO	3.1
1	A	779	LYS	3.1
1	B	634	TRP	3.0
1	B	292	ASP	2.9
1	A	449	PRO	2.9
2	D	41	ASN	2.9
1	B	779	LYS	2.8
1	A	302	THR	2.8
1	B	299	ASN	2.8
1	A	469	ASP	2.8
2	D	76	THR	2.8
1	B	337	ALA	2.7
1	A	778	ARG	2.7
1	A	530	GLN	2.7
1	A	447	LEU	2.7
1	A	734	GLY	2.7
1	B	269	GLU	2.6
1	A	337	ALA	2.6
1	A	378	ASP	2.5
1	A	492	ASN	2.5
2	C	173	THR	2.5
1	B	711	LYS	2.5
1	B	291	GLY	2.5
1	A	711	LYS	2.5
2	D	28	GLY	2.5
1	B	239	PRO	2.5
1	B	419	SER	2.5
1	B	605	SER	2.5
1	A	294	GLY	2.5
1	A	855	ARG	2.4
1	A	366	PRO	2.4
1	A	319	ASP	2.4
1	B	368	GLU	2.4
1	B	542	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	114	ASP	2.4
1	B	361	LEU	2.4
1	B	319	ASP	2.4
1	A	622	TRP	2.4
1	A	837	ARG	2.4
1	B	778	ARG	2.4
2	C	41	ASN	2.3
1	B	420	SER	2.3
2	C	123	LEU	2.3
1	B	492	ASN	2.3
1	A	838	ALA	2.3
2	C	2	ALA	2.3
1	B	753	GLY	2.3
1	A	825	LEU	2.3
1	B	304	ASN	2.3
1	B	686	ARG	2.3
1	A	145	GLN	2.3
1	A	146	THR	2.2
1	A	479	THR	2.2
1	A	419	SER	2.2
1	B	699	PHE	2.2
1	A	348	THR	2.2
1	B	303	GLY	2.2
1	B	255	GLY	2.2
1	B	283	GLY	2.2
1	B	199	ASP	2.2
1	A	699	PHE	2.2
1	A	269	GLU	2.1
1	B	357	THR	2.1
1	B	854	GLY	2.1
1	A	652	ASP	2.1
1	B	114	ASP	2.1
1	B	366	PRO	2.1
1	A	428	THR	2.0
2	D	119	ASN	2.0
1	B	660	ASP	2.0
1	B	113	ASN	2.0

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

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](#)

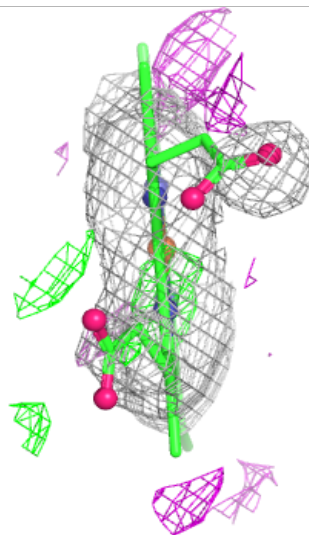
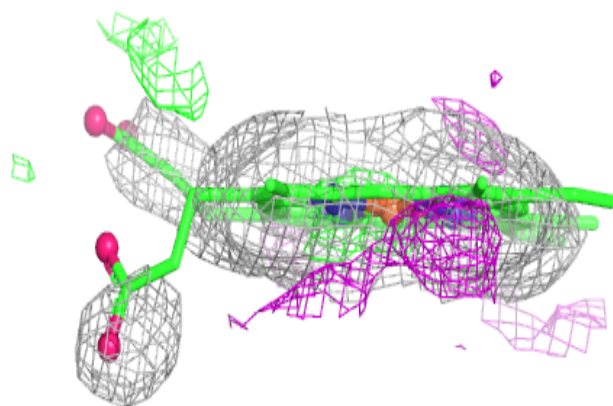
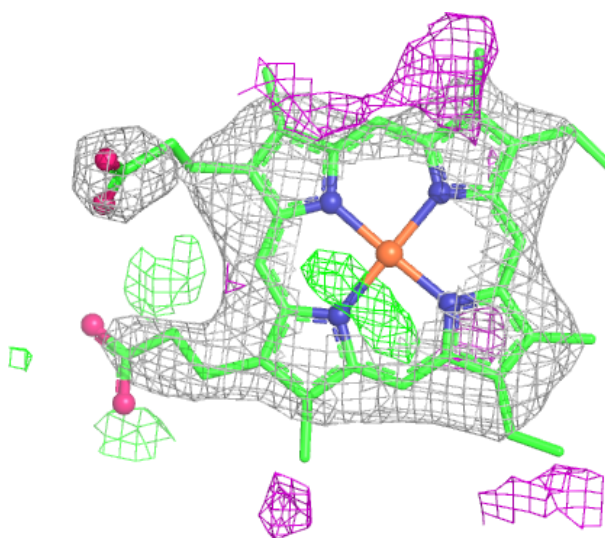
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

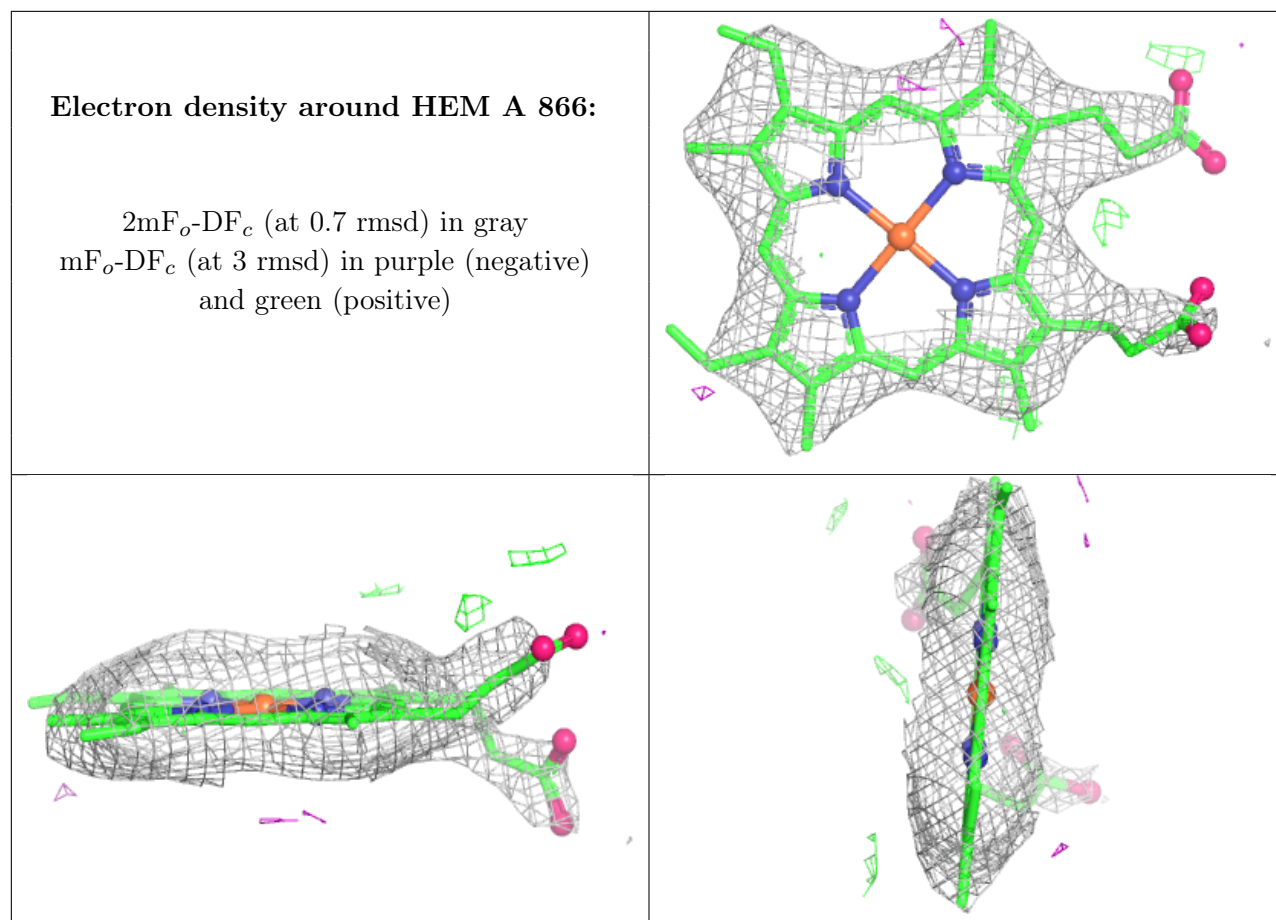
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	871	6/6	0.80	0.22	60,120,142,145	0
4	GOL	A	867	6/6	0.82	0.15	68,74,118,119	0
4	GOL	A	868	6/6	0.88	0.16	49,82,113,137	0
4	GOL	B	868	6/6	0.91	0.18	73,109,123,124	0
4	GOL	A	869	6/6	0.92	0.15	105,119,128,128	0
4	GOL	B	867	6/6	0.93	0.14	65,89,122,123	0
4	GOL	A	870	6/6	0.93	0.12	101,122,137,144	0
3	HEM	B	866	43/43	0.97	0.14	38,80,148,169	0
3	HEM	A	866	43/43	0.98	0.11	42,79,148,171	0

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 B 866:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.