



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 AM GMT

PDB ID : 3CSL  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

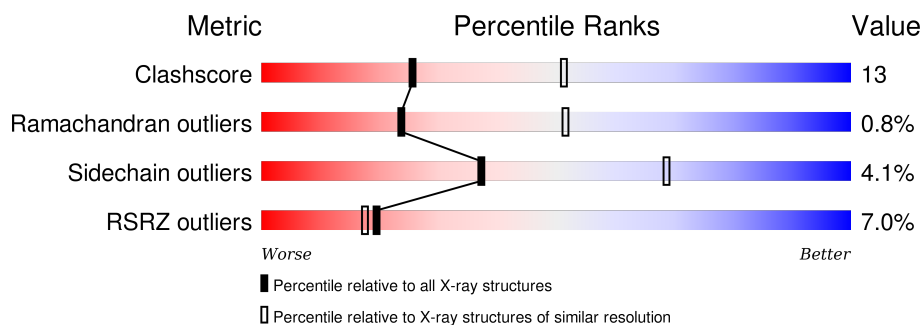
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	865	<div> <div>6%</div> <div> <div>62%</div> <div>23%</div> <div>13%</div> </div> </div>
1	B	865	<div> <div>7%</div> <div> <div>62%</div> <div>23%</div> <div>13%</div> </div> </div>
2	C	206	<div> <div>4%</div> <div> <div>66%</div> <div>13%</div> <div>21%</div> </div> </div>
2	D	206	<div> <div>5%</div> <div> <div>67%</div> <div>11%</div> <div>21%</div> </div> </div>

## 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 (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

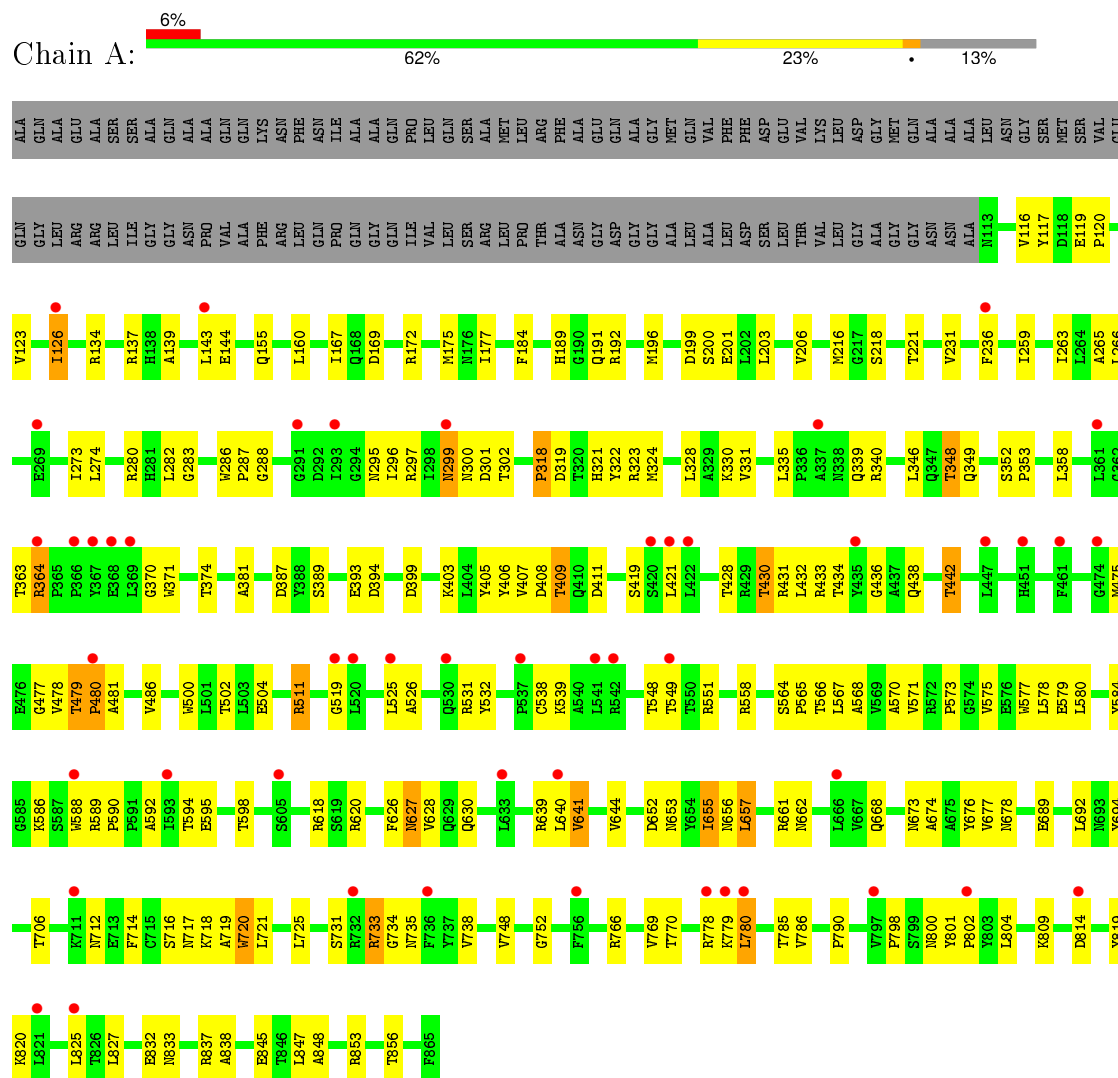
- Molecule 5 is water.

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

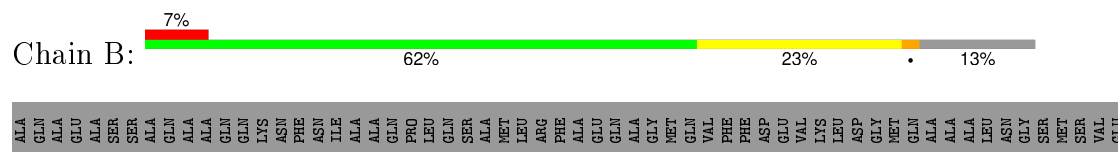
### 3 Residue-property plots

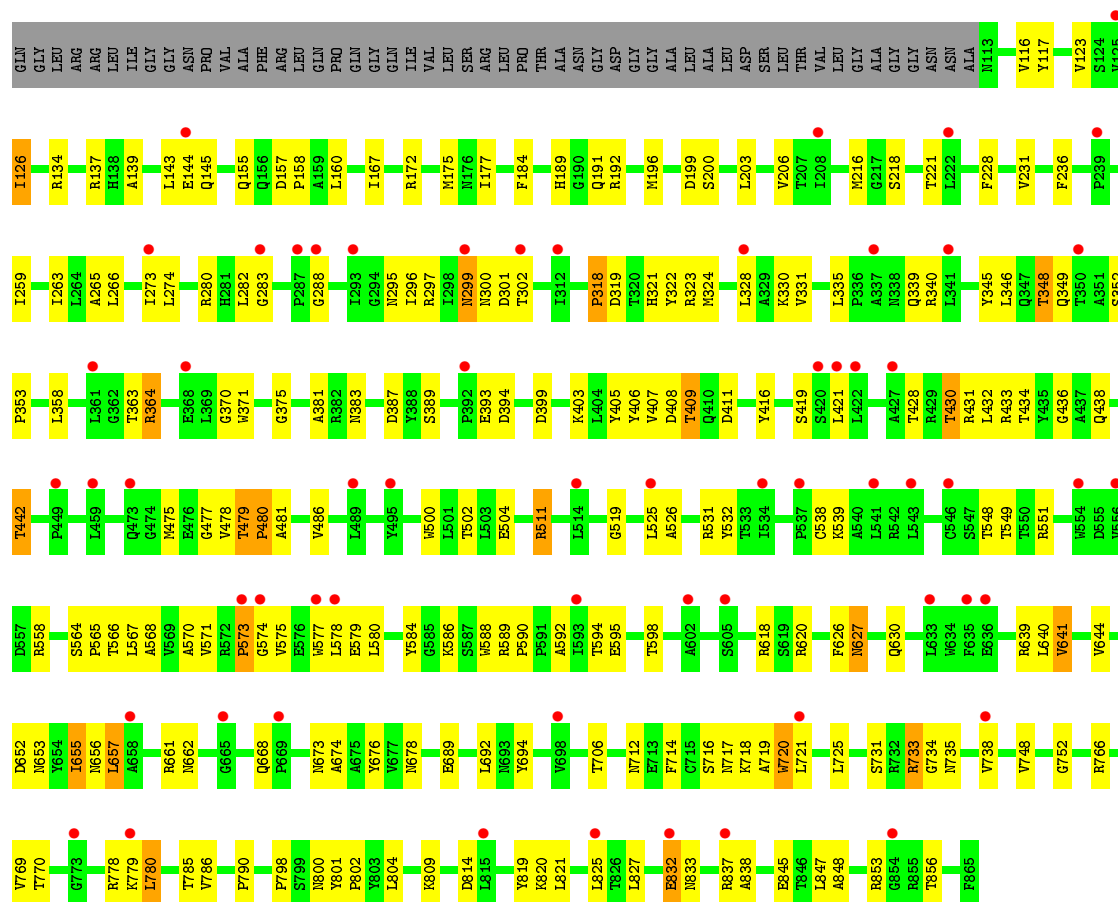
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: HasR protein

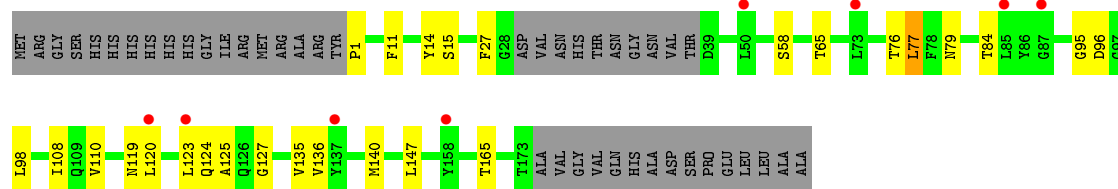


#### • Molecule 1: HasR protein

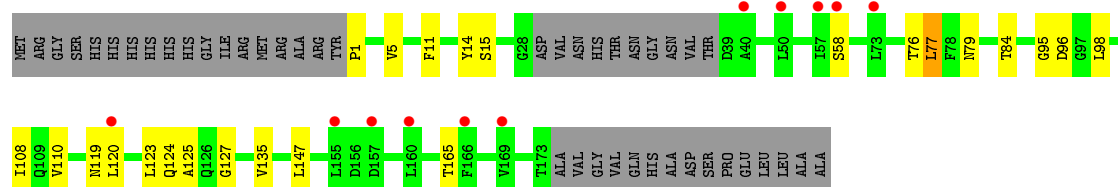




### • Molecule 2: Hemophore HasA



### • Molecule 2: Hemophore HasA





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 86.9 (49.17-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.239 , 0.274 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 99334 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEM

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	0.21	0/6027	0.38	0/8188
1	B	0.21	0/6027	0.38	0/8188
2	C	0.21	0/1211	0.33	0/1649
2	D	0.21	0/1211	0.33	0/1649
All	All	0.21	0/14476	0.37	0/19674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	152	0
1	B	5889	0	5597	150	0
2	C	1184	0	1078	18	0
2	D	1184	0	1078	17	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	16	0	0	0	0
5	D	1	0	0	0	0
All	All	14317	0	13466	347	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 13.

All (347) 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	1.30	0.96
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:HBB2	3:A:866:HEM:HHC	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	1.36	0.90
1:A:477:GLY:HA2	1:A:480:PRO:HB3	1.57	0.85
1:B:477:GLY:HA2	1:B:480:PRO:HB3	1.58	0.83
1:A:175:MET:HE1	1:A:196:MET:HG2	1.60	0.83
1:B:175:MET:HE1	1:B:196:MET:HG2	1.60	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
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:H	2:D:123:LEU:HD23	1.50	0.77
3:B:866:HEM:HMC2	3:B:866:HEM:HBC2	1.68	0.76
2:C:123:LEU:H	2:C:123:LEU:HD23	1.50	0.75
3:A:866:HEM:HBC2	3:A:866:HEM:HMC2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:TRP:CD1	1:A:721:LEU:HD13	2.26	0.70
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
1:B:302:THR:HB	2:D:125:ALA:HB2	1.73	0.69
2:C:76:THR:HG23	2:C:79:ASN:HB3	1.73	0.69
3:B:866:HEM:CBD	3:B:866:HEM:HHA	2.23	0.68
3:A:866:HEM:CBD	3:A:866:HEM:HHA	2.23	0.68
1:B:668:GLN:HG3	2:D:58:SER:HB3	1.75	0.67
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:B:191:GLN:HG2	1:B:845:GLU:CD	2.19	0.63
1:A:191:GLN:HG2	1:A:845:GLU:CD	2.19	0.62
1:B:411:ASP:HB3	1:B:430:THR:HG23	1.81	0.62
1:A:177:ILE:HD12	1:A:346:LEU:HD23	1.79	0.62
1:B:778:ARG:HG3	1:B:778:ARG:O	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
2:C:96:ASP:HB2	2:C:110:VAL:HG13	1.82	0.60
1:A:411:ASP:HB3	1:A:430:THR:HG23	1.81	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:124:GLN:O	2:C:125:ALA:HB3	2.02	0.60
2:C:1:PRO:HB3	2:C:119:ASN:HD21	1.67	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
3:B:866:HEM:CMC	3:B:866:HEM:HBC2	2.32	0.59
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:CMC	3:A:866:HEM:HBC2	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:B:720:TRP:O	1:B:721:LEU:HB2	2.03	0.58
1:A:407:VAL:HB	1:A:434:THR:HB	1.85	0.58
1:B:780:LEU:HD23	1:B:819:TYR:HD1	1.68	0.58
1:B:144:GLU:HA	1:B:766:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:LEU:HD23	1:A:827:LEU:H	1.69	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: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:B:477:GLY:CA	1:B:480:PRO:HB3	2.33	0.57
1:A:364:ARG:HD2	1:A:364:ARG:O	2.05	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:725:LEU:HB3	1:B:738:VAL:HG11	1.87	0.56
1:B:475:MET:HA	1:B:478:VAL:HG23	1.87	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: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
1:B:265:ALA:HB2	1:B:274:LEU:HD23	1.88	0.55
1:A:526:ALA:HB2	1:A:531:ARG:HA	1.89	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:B:827:LEU:H	1:B:827:LEU:HD23	1.70	0.55
2:C:95:GLY:HA3	2:C:108:ILE:HG21	1.88	0.55
1:A:502:THR:HB	1:A:570:ALA:HB3	1.88	0.55
1:A:216:MET:SD	1:A:438:GLN:HB2	2.47	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:O	1:A:780:LEU:HD13	2.08	0.54
2:D:1:PRO:CB	2:D:119:ASN:HD21	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:THR:HG22	1:B:549:THR:N	2.22	0.54
1:B:526:ALA:HB2	1:B:531:ARG:HA	1.90	0.53
1:A:328:LEU:HD21	1:A:330:LYS:HE3	1.90	0.53
2:C:1:PRO:CB	2:C:119:ASN:HD21	2.21	0.53
1:B:475:MET:SD	1:B:478:VAL:HG21	2.48	0.53
1:A:348:THR:HG23	1:A:381:ALA:HB3	1.89	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:HBD1	3:B:866:HEM:HHA	1.89	0.53
3:A:866:HEM:HBD1	3:A:866:HEM:HHA	1.90	0.52
1:B:640:LEU:HD23	1:B:694:TYR:HB2	1.91	0.52
1:B:328:LEU:HD21	1:B:330:LYS:HE3	1.90	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:B:297:ARG:NH2	1:B:847:LEU:HA	2.22	0.52
1:A:231:VAL:HG13	1:A:236:PHE:HE2	1.75	0.52
1:B:319:ASP:HB3	1:B:353:PRO:HB2	1.92	0.51
1:A:319:ASP:HB3	1:A:353:PRO:HB2	1.92	0.51
1:B:577:TRP:CZ3	1:B:630:GLN:HG2	2.46	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:321:HIS:CE1	1:B:353:PRO:HG2	2.46	0.51
1:B:566:THR:C	1:B:567:LEU:HD12	2.31	0.51
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
3:A:866:HEM:HBD2	3:A:866:HEM:HHA	1.92	0.50
1:A:280:ARG:HD3	1:A:322:TYR:OH	2.11	0.50
1:A:640:LEU:HD23	1:A:694:TYR:HB2	1.92	0.50
1:B:589:ARG:HG3	1:B:589:ARG:O	2.12	0.50
1:A:566:THR:C	1:A:567:LEU:HD12	2.32	0.50
1:A:116:VAL:HG13	1:A:123:VAL:HG13	1.94	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:B:845:GLU:HG2	1:B:848:ALA:H	1.77	0.49
1:B:655:ILE:HG22	1:B:678:ASN:ND2	2.27	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
3:B:866:HEM:HBD2	3:B:866:HEM:HHA	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:SER:HB2	2:D:98:LEU:HD12	1.95	0.49
1:B:280:ARG:HD3	1:B:322:TYR:OH	2.12	0.49
1:A:126:ILE:CG2	1:A:206:VAL:HB	2.42	0.49
1:B:589:ARG:HH12	1:B:655:ILE:CD1	2.25	0.49
1:A:769:VAL:HG13	1:A:786:VAL:HB	1.93	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:189:HIS:HB2	1:B:191:GLN:NE2	2.29	0.48
1:B:116:VAL:HG13	1:B:123:VAL:HG13	1.95	0.48
1:A:716:SER:O	1:A:748:VAL:HG23	2.14	0.48
1:A:779:LYS:NZ	1:A:820:LYS:HG3	2.15	0.48
1:B:725:LEU:HB3	1:B:738:VAL:CG1	2.44	0.48
1:A:798:PRO:HB2	1:A:800:ASN:OD1	2.14	0.48
1:A:579:GLU:HB3	1:A:627:ASN:ND2	2.29	0.48
1:B:579:GLU:HB3	1:B:627:ASN:ND2	2.29	0.48
2:C:58:SER:HB2	2:C:98:LEU:HD12	1.95	0.48
1:B:716:SER:O	1:B:748:VAL:HG23	2.14	0.48
1:B:405:TYR:CZ	1:B:436:GLY:HA3	2.49	0.48
1:B:199:ASP:O	1:B:200:SER:HB3	2.14	0.47
1:B:731:SER:OG	1:B:733:ARG:HG2	2.14	0.47
1:B:564:SER:HB3	1:B:586:LYS:O	2.13	0.47
2:C:84:THR:HG21	2:C:127:GLY:HA2	1.95	0.47
1:A:731:SER:OG	1:A:733:ARG:HG2	2.14	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: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:B:363:THR:HG23	1:B:364:ARG:HG3	1.97	0.47
1:A:519:GLY:HA3	1:A:551:ARG:NH1	2.30	0.47
2:C:15:SER:HA	2:C:165:THR:HA	1.97	0.47
1:B:511:ARG:O	1:B:511:ARG:HG3	2.14	0.47
1:A:139:ALA:HB1	1:A:160:LEU:HD22	1.97	0.47
1:A:363:THR:HG23	1:A:364:ARG:HG3	1.97	0.47
1:A:564:SER:HB3	1:A:586:LYS:O	2.13	0.47
1:A:335:LEU:HB2	1:A:339:GLN:HB2	1.96	0.47
1:A:405:TYR:CZ	1:A:436:GLY:HA3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:C	1:B:302:THR:H	2.18	0.47
1:A:661:ARG:HD3	1:A:718:LYS:HA	1.97	0.47
1:A:300:ASN:C	1:A:302:THR:H	2.19	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:798:PRO:HD2	1:B:801:TYR:CE1	2.50	0.46
2:D:124:GLN:O	2:D:125:ALA:CB	2.64	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
1:B:661:ARG:HD3	1:B:718:LYS:HA	1.97	0.46
3:B:866:HEM:HBD1	3:B:866:HEM:CHA	2.46	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
1:A:580:LEU:HD23	1:A:626:PHE:HB3	1.98	0.46
1:B:779:LYS:HG2	1:B:820:LYS:HZ3	1.81	0.46
1:A:661:ARG:O	1:A:673:ASN:HB2	2.15	0.46
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:A:324:MET:HA	1:A:349:GLN:O	2.16	0.46
1:B:479:THR:O	1:B:594:THR:HA	2.16	0.46
1:B:393:GLU:O	1:B:394:ASP:HB2	2.16	0.45
1:A:137:ARG:NH1	1:A:155:GLN:HB3	2.26	0.45
1:A:117:TYR:CG	1:A:641:VAL:HG22	2.51	0.45
1:A:779:LYS:HG2	1:A:820:LYS:HZ3	1.80	0.45
1:A:374:THR:HG21	3:A:866:HEM:HAA2	1.97	0.45
1:B:780:LEU:HD23	1:B:819:TYR:CD1	2.51	0.45
1:B:500:TRP:O	1:B:571:VAL:HA	2.17	0.45
1:A:500:TRP:O	1:A:571:VAL:HA	2.17	0.45
1:B:117:TYR:CG	1:B:641:VAL:HG22	2.52	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:B:137:ARG:NH1	1:B:155:GLN:HB3	2.26	0.45
2:C:124:GLN:O	2:C:125:ALA:CB	2.64	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
1:A:779:LYS:HA	1:A:779:LYS:HD2	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HG3	1:A:598:THR:HA	1.99	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:479:THR:O	1:A:594:THR:HA	2.16	0.44
1:A:387:ASP:OD2	1:A:403:LYS:HD3	2.16	0.44
1:B:733:ARG:HG3	1:B:735:ASN:H	1.82	0.44
1:A:589:ARG:HA	1:A:590:PRO:HD3	1.84	0.44
1:A:579:GLU:HB3	1:A:627:ASN:HD21	1.81	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:579:GLU:HB3	1:B:627:ASN:HD21	1.81	0.44
1:B:339:GLN:HA	1:B:389:SER:O	2.18	0.44
1:B:139:ALA:HB1	1:B:160:LEU:HD22	1.98	0.44
1:A:733:ARG:HG3	1:A:735:ASN:HB2	2.00	0.44
1:B:480:PRO:HG3	1:B:598:THR:HA	1.99	0.44
1:A:231:VAL:HG11	1:A:263:ILE:HD13	1.99	0.44
1:B:644:VAL:HA	1:B:689:GLU:O	2.18	0.44
1:A:733:ARG:HG3	1:A:735:ASN:H	1.82	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:837:ARG:NH2	1:A:837:ARG:HB2	2.32	0.44
1:A:853:ARG:HH11	1:A:856:THR:CG2	2.26	0.43
1:A:644:VAL:HA	1:A:689:GLU:O	2.18	0.43
1:A:592:ALA:HB3	1:A:595:GLU:HG2	2.00	0.43
1:B:657:LEU:HD21	1:B:674:ALA:HB1	2.00	0.43
1:A:218:SER:O	1:A:221:THR:HB	2.18	0.43
1:A:480:PRO:HB2	1:A:481:ALA:H	1.43	0.43
1:A:119:GLU:HA	1:A:120:PRO:HD3	1.80	0.43
1:A:656:ASN:HB2	1:A:714:PHE:CE1	2.53	0.43
1:B:588:TRP:CH2	1:B:590:PRO:HG3	2.54	0.43
1:A:339:GLN:HA	1:A:389:SER:O	2.18	0.43
1:B:662:ASN:ND2	1:B:718:LYS:HE3	2.34	0.43
1:B:652:ASP:O	1:B:653:ASN:HB2	2.17	0.43
1:A:778:ARG:HG3	1:A:778:ARG:O	2.19	0.43
1:A:595:GLU:HA	1:A:676:TYR:CD1	2.52	0.43
1:B:589:ARG:HA	1:B:590:PRO:HD3	1.84	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:231:VAL:HG11	1:B:263:ILE:HD13	2.00	0.43
1:B:656:ASN:HB2	1:B:714:PHE:CE1	2.53	0.43
1:B:595:GLU:HA	1:B:676:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:THR:HG22	1:B:549:THR:H	1.82	0.43
3:A:866:HEM:HHC	3:A:866:HEM:CBB	2.34	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
1:B:577:TRP:CD1	1:B:578:LEU:HB2	2.54	0.42
1:B:592:ALA:HB3	1:B:595:GLU:HG2	2.00	0.42
3:B:866:HEM:CHA	3:B:866:HEM:CBD	2.92	0.42
1:A:407:VAL:O	1:A:433:ARG:HA	2.19	0.42
1:A:299:ASN:C	1:A:301:ASP:H	2.23	0.42
1:B:405:TYR:CE2	1:B:436:GLY:HA3	2.53	0.42
1:B:733:ARG:HG3	1:B:735:ASN:HB2	2.00	0.42
1:A:662:ASN:ND2	1:A:718:LYS:HE3	2.34	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:B:299:ASN:C	1:B:301:ASP:H	2.23	0.42
1:A:286:TRP:HA	1:A:287:PRO:HD3	1.87	0.42
1:A:479:THR:O	1:A:594:THR:HG23	2.20	0.42
1:B:145:GLN:HB3	1:B:145:GLN:HE21	1.72	0.42
1:B:640:LEU:HD22	1:B:641:VAL:H	1.84	0.42
1:A:419:SER:OG	1:A:421:LEU:HD23	2.19	0.42
1:A:532:TYR:CE1	1:A:538:CYS:HA	2.55	0.42
1:A:296:ILE:HG22	1:A:804:LEU:HD13	2.02	0.42
1:B:296:ILE:HG22	1:B:804:LEU:HD13	2.02	0.42
1:B:273:ILE:HD13	1:B:331:VAL:HG22	2.01	0.42
1:B:564:SER:HA	1:B:565:PRO:HD3	1.76	0.42
1:B:779:LYS:HA	1:B:779:LYS:HD2	1.67	0.41
1:A:358:LEU:HD12	1:A:370:GLY:O	2.20	0.41
1:A:169:ASP:O	1:A:172:ARG:HD2	2.20	0.41
1:B:790:PRO:O	1:B:809:LYS:HB3	2.20	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:358:LEU:HD12	1:B:370:GLY:O	2.20	0.41
1:A:847:LEU:HA	1:A:847:LEU:HD12	1.89	0.41
1:B:300:ASN:C	1:B:302:THR:N	2.74	0.41
1:A:640:LEU:HD22	1:A:641:VAL:H	1.85	0.41
1:B:584:TYR:HE2	1:B:620:ARG:HD3	1.85	0.41
1:B:479:THR:O	1:B:594:THR:HG23	2.21	0.41
1:A:288:GLY:HA3	1:A:838:ALA:CA	2.49	0.41
2:D:11:PHE:HA	2:D:14:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:VAL:O	1:A:641:VAL:HA	2.20	0.41
2:C:27:PHE:HD1	2:C:65:THR:HG22	1.86	0.41
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
1:B:407:VAL:O	1:B:433:ARG:HA	2.20	0.41
1:A:717:ASN:O	1:A:719:ALA:N	2.48	0.41
2:C:136:VAL:O	2:C:140:MET:HG3	2.21	0.41
1:B:538:CYS:O	1:B:539:LYS:HB2	2.20	0.41
1:A:538:CYS:O	1:A:539:LYS:HB2	2.20	0.41
2:D:76:THR:CG2	2:D:79:ASN:HB3	2.48	0.41
1:A:199:ASP:C	1:A:201:GLU:H	2.24	0.41
1:A:564:SER:HA	1:A:565:PRO:HD3	1.76	0.41
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.93	0.41
1:B:717:ASN:O	1:B:719:ALA:N	2.48	0.41
1:A:802:PRO:HG3	2:C:77:LEU:CD2	2.51	0.41
2:C:11:PHE:HA	2:C:14:TYR:HD2	1.86	0.40
1:B:692:LEU:HD23	1:B:692:LEU:C	2.42	0.40
1:A:134:ARG:HD2	1:A:814:ASP:OD2	2.21	0.40
1:B:832:GLU:HB2	1:B:856:THR:HB	2.03	0.40
1:B:375:GLY:HA2	1:B:416:TYR:CD1	2.57	0.40
1:B:345:TYR:HA	1:B:383:ASN:O	2.21	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:B:177:ILE:HA	1:B:228:PHE:O	2.22	0.40
1:A:692:LEU:HD23	1:A:692:LEU:C	2.42	0.40
1:B:157:ASP:HA	1:B:158:PRO:HD3	1.93	0.40
1:A:655:ILE:HA	1:A:677:VAL:O	2.21	0.40
1:A:300:ASN:C	1:A:302:THR:N	2.74	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%)	24	51
1	B	751/865 (87%)	679 (90%)	66 (9%)	6 (1%)	24	51
2	C	159/206 (77%)	150 (94%)	8 (5%)	1 (1%)	30	59
2	D	159/206 (77%)	150 (94%)	7 (4%)	2 (1%)	15	37
All	All	1820/2142 (85%)	1657 (91%)	148 (8%)	15 (1%)	24	51

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%)	587 (95%)	29 (5%)	32	63
1	B	616/695 (89%)	587 (95%)	29 (5%)	32	63
2	C	124/158 (78%)	123 (99%)	1 (1%)	86	96
2	D	124/158 (78%)	123 (99%)	1 (1%)	86	96
All	All	1480/1706 (87%)	1420 (96%)	60 (4%)	37	69

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ILE
1	A	143	LEU
1	A	192	ARG
1	A	266	LEU
1	A	323	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	618	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	780	LEU
1	A	825	LEU
1	A	833	ASN
1	B	126	ILE
1	B	143	LEU
1	B	192	ARG
1	B	266	LEU
1	B	323	ARG
1	B	340	ARG
1	B	348	THR
1	B	364	ARG
1	B	409	THR
1	B	428	THR
1	B	430	THR
1	B	442	THR
1	B	479	THR

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Mol	Chain	Res	Type
1	B	486	VAL
1	B	511	ARG
1	B	525	LEU
1	B	558	ARG
1	B	618	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	780	LEU
1	B	825	LEU
1	B	833	ASN
2	C	120	LEU
2	D	120	LEU

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

Mol	Chain	Res	Type
1	A	300	ASN
1	A	608	GLN
1	A	627	ASN
1	B	193	ASN
1	B	608	GLN
1	B	627	ASN
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 carbohydrates 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$
3	HEM	A	866	1	30,50,50	2.10	8 (26%)	24,82,82	2.29	10 (41%)
4	GOL	A	867	-	5,5,5	0.32	0	5,5,5	0.12	0
4	GOL	A	868	-	5,5,5	0.35	0	5,5,5	0.12	0
4	GOL	A	869	-	5,5,5	0.35	0	5,5,5	0.21	0
4	GOL	A	870	-	5,5,5	0.34	0	5,5,5	0.19	0
4	GOL	A	871	-	5,5,5	0.34	0	5,5,5	0.21	0
3	HEM	B	866	1	30,50,50	2.09	7 (23%)	24,82,82	2.28	10 (41%)
4	GOL	B	867	-	5,5,5	0.35	0	5,5,5	0.23	0
4	GOL	B	868	-	5,5,5	0.34	0	5,5,5	0.20	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
3	HEM	A	866	1	-	0/10/54/54	0/0/8/8
4	GOL	A	867	-	-	0/4/4/4	0/0/0/0
4	GOL	A	868	-	-	0/4/4/4	0/0/0/0
4	GOL	A	869	-	-	0/4/4/4	0/0/0/0
4	GOL	A	870	-	-	0/4/4/4	0/0/0/0
4	GOL	A	871	-	-	0/4/4/4	0/0/0/0
3	HEM	B	866	1	-	0/10/54/54	0/0/8/8
4	GOL	B	867	-	-	0/4/4/4	0/0/0/0
4	GOL	B	868	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	866	HEM	C3B-C4B	-6.90	1.45	1.51
3	B	866	HEM	C3B-C4B	-6.86	1.45	1.51
3	A	866	HEM	C3D-C4D	-4.68	1.45	1.51
3	B	866	HEM	C3D-C4D	-4.65	1.45	1.51
3	A	866	HEM	C2C-C1C	-3.71	1.45	1.52
3	B	866	HEM	C2C-C1C	-3.70	1.45	1.52
3	B	866	HEM	C2D-C1D	-2.06	1.45	1.51
3	A	866	HEM	C2D-C1D	-2.05	1.45	1.51
3	A	866	HEM	C4C-NC	2.00	1.38	1.36
3	A	866	HEM	FE-NB	2.01	2.08	1.97
3	A	866	HEM	C3C-CAC	2.04	1.55	1.51
3	B	866	HEM	C3C-CAC	2.04	1.55	1.51
3	B	866	HEM	C1C-NC	2.19	1.38	1.36
3	B	866	HEM	FE-NC	2.27	2.04	1.95
3	A	866	HEM	FE-NC	2.34	2.05	1.95

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	866	HEM	CAA-C2A-C1A	-2.50	124.29	127.01
3	A	866	HEM	CAA-C2A-C1A	-2.49	124.30	127.01
3	B	866	HEM	C3B-CAB-CBB	-2.32	120.90	124.46
3	A	866	HEM	C3B-CAB-CBB	-2.27	120.97	124.46
3	A	866	HEM	C3B-C4B-NB	-2.07	107.67	111.63
3	B	866	HEM	CBA-CAA-C2A	-2.01	108.92	112.53
3	B	866	HEM	C2D-C3D-C4D	2.04	104.96	101.50
3	A	866	HEM	C2D-C3D-C4D	2.08	105.02	101.50
3	B	866	HEM	C3B-C4B-CHC	2.19	126.25	123.16
3	A	866	HEM	C3B-C4B-CHC	2.35	126.47	123.16
3	A	866	HEM	CMD-C2D-C3D	2.90	127.17	114.35
3	B	866	HEM	CMD-C2D-C3D	2.90	127.19	114.35
3	A	866	HEM	CMB-C2B-C3B	3.59	125.48	116.53
3	B	866	HEM	CMB-C2B-C3B	3.60	125.52	116.53
3	A	866	HEM	CMC-C2C-C3C	4.31	127.28	116.53
3	B	866	HEM	CMC-C2C-C3C	4.35	127.38	116.53
3	A	866	HEM	CAD-C3D-C4D	4.57	128.59	112.47
3	A	866	HEM	CAD-C3D-C2D	4.58	126.38	113.22
3	B	866	HEM	CAD-C3D-C2D	4.58	126.39	113.22
3	B	866	HEM	CAD-C3D-C4D	4.59	128.65	112.47

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	866	HEM	9	0
3	B	866	HEM	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	753/865 (87%)	0.85	49 (6%)	22 20	53, 91, 133, 199	0
1	B	753/865 (87%)	0.98	61 (8%)	15 12	61, 91, 134, 196	0
2	C	163/206 (79%)	0.44	8 (4%)	33 32	82, 109, 141, 179	0
2	D	163/206 (79%)	0.40	11 (6%)	21 19	82, 109, 141, 179	0
All	All	1832/2142 (85%)	0.83	129 (7%)	19 17	53, 94, 138, 199	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	LEU	7.1
1	A	422	LEU	7.1
1	A	420	SER	6.2
1	A	447	LEU	5.4
1	A	541	LEU	4.7
2	C	50	LEU	4.6
1	A	421	LEU	4.2
2	C	120	LEU	4.2
2	C	137	TYR	4.1
1	A	711	LYS	4.0
1	B	449	PRO	3.9
1	B	636	GLU	3.8
1	B	287	PRO	3.8
2	D	40	ALA	3.8
1	A	825	LEU	3.7
1	B	420	SER	3.7
1	A	480	PRO	3.6
1	B	422	LEU	3.5
2	D	120	LEU	3.5
1	B	361	LEU	3.4
2	D	160	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	605	SER	3.4
1	A	821	LEU	3.4
1	B	541	LEU	3.4
1	B	854	GLY	3.3
1	A	549	THR	3.3
1	B	573	PRO	3.2
1	A	361	LEU	3.2
1	B	473	GLN	3.1
2	D	157	ASP	3.1
1	B	602	ALA	3.0
2	C	158	TYR	3.0
1	B	368	GLU	3.0
1	A	537	PRO	3.0
1	B	779	LYS	2.9
1	A	530	GLN	2.9
1	B	577	TRP	2.9
1	A	778	ARG	2.8
1	B	293	ILE	2.8
1	B	312	ILE	2.8
1	A	368	GLU	2.8
1	A	666	LEU	2.8
1	B	832	GLU	2.8
1	B	288	GLY	2.8
1	A	369	LEU	2.7
1	B	222	LEU	2.7
1	B	302	THR	2.7
1	A	525	LEU	2.7
1	B	341	LEU	2.7
1	B	525	LEU	2.6
1	B	633	LEU	2.6
1	A	519	GLY	2.6
1	A	814	ASP	2.6
1	B	543	LEU	2.6
1	B	546	CYS	2.6
1	A	367	TYR	2.6
1	A	293	ILE	2.6
1	B	658	ALA	2.5
1	A	451	HIS	2.5
1	B	337	ALA	2.4
1	B	208	ILE	2.4
2	D	58	SER	2.4
1	A	364	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	593	ILE	2.4
1	A	366	PRO	2.3
1	A	756	PHE	2.3
1	B	299	ASN	2.3
1	B	773	GLY	2.3
2	D	166	PHE	2.3
1	A	143	LEU	2.3
1	B	239	PRO	2.3
1	B	514	LEU	2.3
1	A	588	TRP	2.3
1	B	593	ILE	2.3
1	A	780	LEU	2.3
1	B	669	PRO	2.3
1	A	269	GLU	2.3
1	B	489	LEU	2.3
1	B	537	PRO	2.3
1	A	435	TYR	2.3
1	B	283	GLY	2.3
1	B	427	ALA	2.3
1	B	665	GLY	2.3
1	A	640	LEU	2.2
1	B	825	LEU	2.2
1	A	337	ALA	2.2
1	A	291	GLY	2.2
1	B	459	LEU	2.2
2	C	123	LEU	2.2
2	D	73	LEU	2.2
1	B	556	VAL	2.2
1	A	520	LEU	2.2
1	A	299	ASN	2.2
1	B	721	LEU	2.2
2	C	87	GLY	2.2
1	A	797	VAL	2.2
1	B	350	THR	2.2
1	B	534	ILE	2.2
2	D	169	VAL	2.2
1	B	273	ILE	2.1
2	C	73	LEU	2.1
1	A	542	ARG	2.1
1	A	779	LYS	2.1
1	A	474	GLY	2.1
1	A	236	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	392	PRO	2.1
1	B	635	PHE	2.1
2	D	155	LEU	2.1
1	A	736	PHE	2.1
1	B	125	VAL	2.1
1	B	554	TRP	2.1
1	B	328	LEU	2.1
1	B	815	LEU	2.1
2	C	85	LEU	2.1
1	A	802	PRO	2.1
1	B	837	ARG	2.1
1	A	126	ILE	2.0
1	B	574	GLY	2.0
1	A	633	LEU	2.0
1	B	605	SER	2.0
2	D	57	ILE	2.0
2	D	50	LEU	2.0
1	B	698	VAL	2.0
1	B	738	VAL	2.0
1	A	461	PHE	2.0
1	B	495	TYR	2.0
1	B	578	LEU	2.0
1	A	732	ARG	2.0
1	B	144	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEM	B	866	43/43	0.96	0.32	1.46	38,80,148,169	0
4	GOL	A	869	6/6	0.87	0.23	0.70	105,119,128,128	0
4	GOL	A	868	6/6	0.92	0.25	0.49	49,82,113,137	0
3	HEM	A	866	43/43	0.97	0.26	0.21	42,79,148,171	0
4	GOL	B	867	6/6	0.77	0.25	-0.10	65,89,122,123	0
4	GOL	B	868	6/6	0.90	0.21	-0.85	73,109,123,124	0
4	GOL	A	870	6/6	0.81	0.29	-	101,122,137,144	0
4	GOL	A	867	6/6	0.88	0.22	-	68,74,118,119	0
4	GOL	A	871	6/6	0.69	0.50	-	60,120,142,145	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.