



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:55 PM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

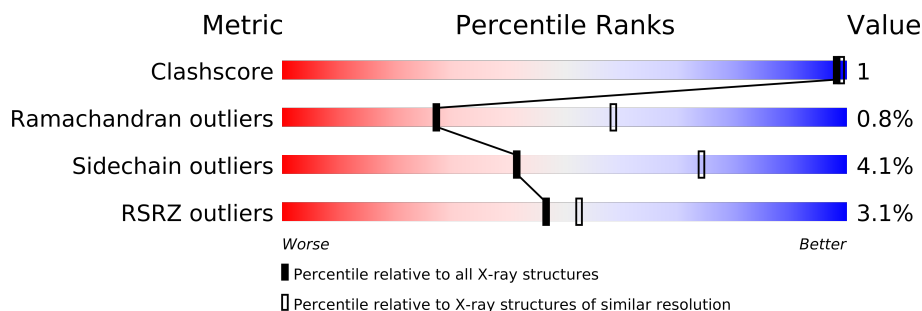
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	865	
1	B	865	
2	C	206	
2	D	206	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	HEM	B	866	-	X
4	GOL	A	868	-	X
4	GOL	A	871	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14317 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

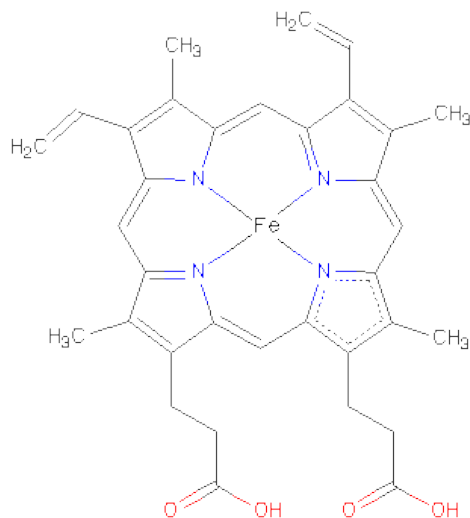
Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	EXPRESSION TAG	UNP Q54450
C	-16	ARG	-	EXPRESSION TAG	UNP Q54450
C	-15	GLY	-	EXPRESSION TAG	UNP Q54450
C	-14	SER	-	EXPRESSION TAG	UNP Q54450
C	-13	HIS	-	EXPRESSION TAG	UNP Q54450
C	-12	HIS	-	EXPRESSION TAG	UNP Q54450
C	-11	HIS	-	EXPRESSION TAG	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: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

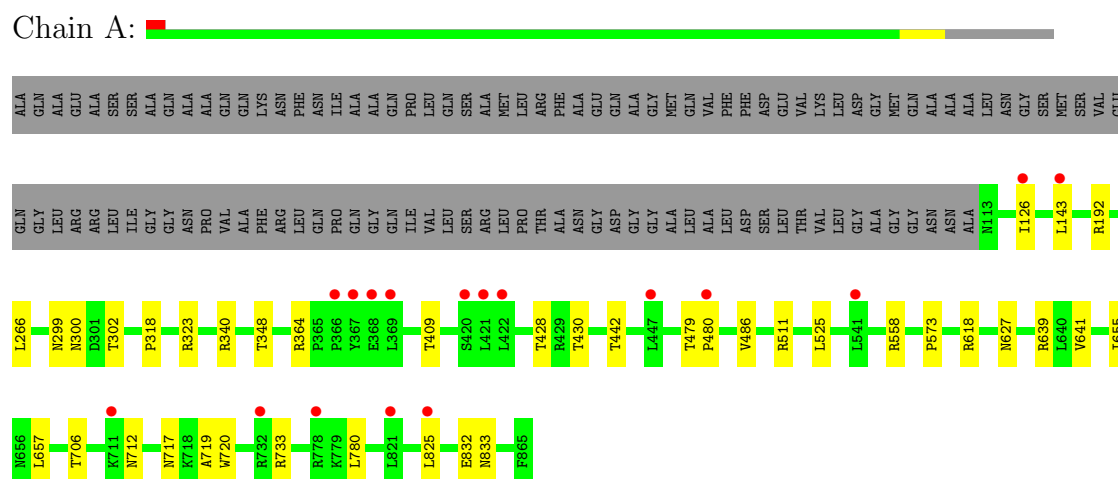
- Molecule 5 is water.

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

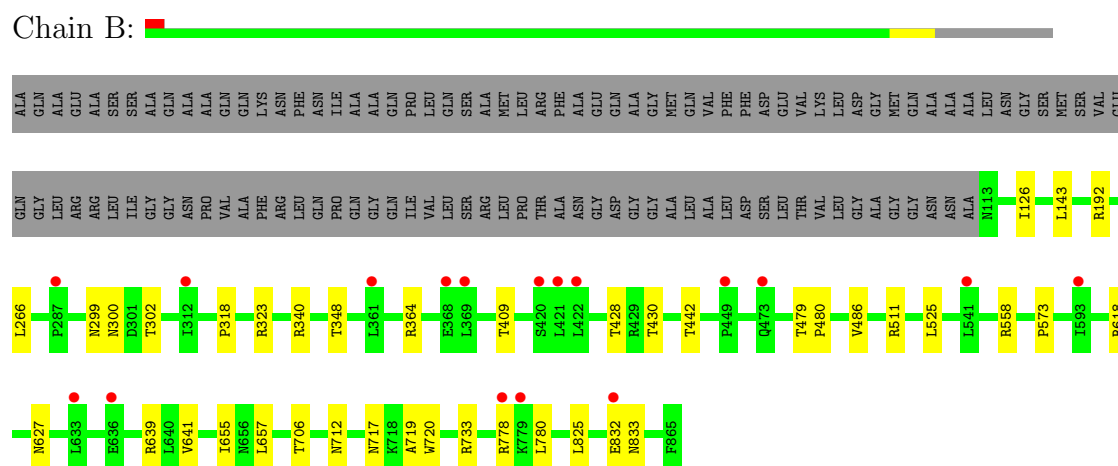
3 Residue-property plots

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.

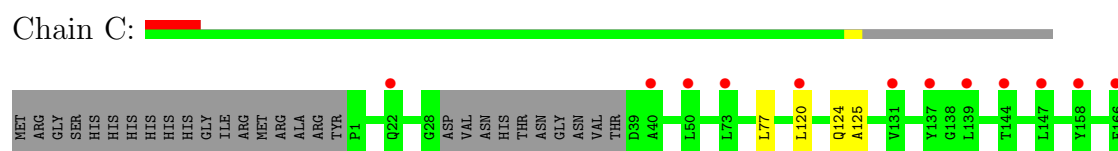
• Molecule 1: HasR protein



• Molecule 1: HasR protein



• Molecule 2: Hemophore HasA



T173
ALA
VAL
GLY
VAL
GLN
HIS
ALA
ASP
SER
PRO
GLU
LEU
ALA
ALA

● Molecule 2: Hemophore HasA

Chain D:

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	ILE	ARG	MET	ARG	ARG	TYR	P1	V5	G28	ASP	VAL	ASN	HIS	THR	ASN	GLY	ASN	VAL	THR	D39	A40	L50	L57	L73	L77	L85	L120	Q124	A125	Y137	L155	Y158	G159	L160	V169
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T173
ALA
VAL
GLY
VAL
GLN
HIS
ALA
ASP
SER
PRO
GLU
LEU
ALA
ALA

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 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
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 , 53.5	EDS
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 99334 reflections	Xtriage
F_o, F_c correlation	0.92	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.

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

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5889	0	0	2	0
1	B	5889	0	0	3	0
2	C	1184	0	0	1	0
2	D	1184	0	0	1	0
3	A	43	0	0	1	0
3	B	43	0	0	1	0
4	A	30	0	40	0	0
4	B	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	56	9	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:866:HEM:CBD	3:B:866:HEM:CHA	2.92	0.48
3:A:866:HEM:CBD	3:A:866:HEM:CHA	2.92	0.47
1:A:717:ASN:O	1:A:719:ALA:N	2.48	0.47
1:B:717:ASN:O	1:B:719:ALA:N	2.48	0.46
2:D:124:GLN:O	2:D:125:ALA:CB	2.64	0.46
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	0.41
1:A:300:ASN:C	1:A:302:THR:N	2.74	0.40
1:B:778:ARG:CG	1:B:778:ARG:O	2.70	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%)	27 58
1	B	751/865 (87%)	679 (90%)	66 (9%)	6 (1%)	27 58
2	C	159/206 (77%)	150 (94%)	8 (5%)	1 (1%)	33 66
2	D	159/206 (77%)	150 (94%)	7 (4%)	2 (1%)	18 43
All	All	1820/2142 (85%)	1657 (91%)	148 (8%)	15 (1%)	27 58

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%)	36	69
1	B	616/695 (89%)	587 (95%)	29 (5%)	36	69
2	C	124/158 (78%)	123 (99%)	1 (1%)	89	98
2	D	124/158 (78%)	123 (99%)	1 (1%)	89	98
All	All	1480/1706 (87%)	1420 (96%)	60 (4%)	41	74

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	49,50,50	2.30	15 (30%)	46,82,82	2.04	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	867	-	5,5,5	0.31	0	5,5,5	0.18	0
4	GOL	A	868	-	5,5,5	0.34	0	5,5,5	0.14	0
4	GOL	A	869	-	5,5,5	0.34	0	5,5,5	0.22	0
4	GOL	A	870	-	5,5,5	0.33	0	5,5,5	0.23	0
4	GOL	A	871	-	5,5,5	0.33	0	5,5,5	0.26	0
3	HEM	B	866	1	49,50,50	2.30	15 (30%)	46,82,82	1.97	7 (15%)
4	GOL	B	867	-	5,5,5	0.33	0	5,5,5	0.27	0
4	GOL	B	868	-	5,5,5	0.33	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
3	HEM	A	866	1	-	1/14/114/114	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	-	1/14/114/114	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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	866	HEM	C3D-C2D	5.74	1.53	1.43
3	A	866	HEM	C3D-C2D	5.69	1.53	1.43
3	B	866	HEM	C3B-C2B	-5.68	1.33	1.43
3	A	866	HEM	C3B-C2B	-5.68	1.33	1.43
3	A	866	HEM	C3C-C2C	-5.30	1.34	1.43
3	B	866	HEM	C3C-C2C	-5.29	1.34	1.43
3	B	866	HEM	C3C-CAC	4.68	1.55	1.40
3	A	866	HEM	C3C-CAC	4.68	1.55	1.40
3	A	866	HEM	C3B-CAB	4.63	1.55	1.40
3	B	866	HEM	C3B-CAB	4.60	1.54	1.40
3	B	866	HEM	C4A-C3A	4.27	1.45	1.40
3	B	866	HEM	C3D-C4D	4.21	1.45	1.44
3	A	866	HEM	C4A-C3A	4.20	1.45	1.40
3	A	866	HEM	C3D-C4D	4.04	1.45	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	866	HEM	C2B-C1B	3.31	1.45	1.44
3	B	866	HEM	C2B-C1B	3.28	1.45	1.44
3	A	866	HEM	FE-NB	2.82	2.08	1.97
3	A	866	HEM	FE-ND	2.79	2.08	1.97
3	A	866	HEM	FE-NA	2.78	2.04	1.92
3	B	866	HEM	FE-NA	2.75	2.04	1.92
3	B	866	HEM	FE-NB	2.71	2.07	1.97
3	B	866	HEM	FE-ND	2.58	2.07	1.97
3	B	866	HEM	CMB-C2B	2.47	1.55	1.47
3	B	866	HEM	CMC-C2C	2.44	1.55	1.47
3	A	866	HEM	CMC-C2C	2.44	1.55	1.47
3	A	866	HEM	CMB-C2B	2.43	1.54	1.47
3	A	866	HEM	CMD-C2D	2.41	1.54	1.47
3	B	866	HEM	CMD-C2D	2.40	1.54	1.47
3	A	866	HEM	C2D-C1D	2.35	1.45	1.44
3	B	866	HEM	C2D-C1D	2.23	1.45	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	866	HEM	C3B-C4B-NB	-8.85	107.67	114.00
3	B	866	HEM	C3B-C4B-NB	-8.41	107.98	114.00
3	A	866	HEM	C4D-ND-C1D	6.07	111.37	105.16
3	B	866	HEM	C4D-ND-C1D	5.94	111.24	105.16
3	A	866	HEM	C2D-C1D-ND	-3.42	108.89	112.93
3	B	866	HEM	C2D-C1D-ND	-3.30	109.04	112.93
3	A	866	HEM	C1B-NB-C4B	2.84	108.07	105.16
3	B	866	HEM	C1B-NB-C4B	2.48	107.70	105.16
3	B	866	HEM	CAD-C3D-C4D	2.29	128.65	124.53
3	A	866	HEM	CAD-C3D-C4D	2.26	128.59	124.53
3	A	866	HEM	C4C-NC-C1C	2.20	107.82	105.53
3	B	866	HEM	C4C-NC-C1C	2.15	107.77	105.53
3	B	866	HEM	CBA-CAA-C2A	-2.14	108.92	112.69
3	A	866	HEM	CBA-CAA-C2A	-2.10	108.99	112.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	866	HEM	C2D-C3D-CAD-CBD
3	A	866	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.57	17 (2%) 57 64	53, 91, 133, 199	0
1	B	753/865 (87%)	0.60	17 (2%) 57 64	61, 91, 134, 196	0
2	C	163/206 (79%)	0.60	12 (7%) 14 15	82, 109, 141, 179	0
2	D	163/206 (79%)	0.59	11 (6%) 17 19	82, 109, 141, 179	0
All	All	1832/2142 (85%)	0.59	57 (3%) 47 52	53, 94, 138, 199	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	LEU	7.3
1	B	421	LEU	5.3
1	B	422	LEU	4.9
1	A	541	LEU	4.8
1	A	447	LEU	4.8
1	A	421	LEU	4.7
2	C	40	ALA	4.1
2	C	50	LEU	3.8
1	B	636	GLU	3.7
2	D	120	LEU	3.5
2	C	137	TYR	3.4
2	C	120	LEU	3.2
2	D	169	VAL	3.1
1	A	480	PRO	3.0
1	A	825	LEU	2.9
1	A	711	LYS	2.9
2	D	137	TYR	2.9
1	B	361	LEU	2.8
2	D	50	LEU	2.8
1	B	449	PRO	2.8
2	D	40	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	73	LEU	2.7
2	C	158	TYR	2.6
1	B	593	ILE	2.6
1	A	367	TYR	2.6
2	D	160	LEU	2.5
1	A	420	SER	2.5
2	D	155	LEU	2.5
1	B	779	LYS	2.5
2	C	147	LEU	2.5
1	B	312	ILE	2.5
1	B	420	SER	2.5
1	A	821	LEU	2.4
2	D	158	TYR	2.4
2	C	139	LEU	2.4
1	B	778	ARG	2.3
1	A	366	PRO	2.3
1	B	287	PRO	2.3
2	C	73	LEU	2.3
1	A	778	ARG	2.3
2	D	85	LEU	2.2
1	A	126	ILE	2.2
2	D	57	ILE	2.2
1	A	368	GLU	2.2
1	B	368	GLU	2.1
1	B	832	GLU	2.1
2	C	166	PHE	2.1
1	B	633	LEU	2.1
2	C	131	VAL	2.1
1	A	143	LEU	2.1
1	B	541	LEU	2.1
2	C	22	GLN	2.1
1	B	369	LEU	2.1
1	B	473	GLN	2.0
1	A	732	ARG	2.0
1	A	369	LEU	2.0
2	C	144	THR	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	871	6/6	0.40	36.63	60,120,142,145	0
3	HEM	B	866	43/43	0.35	2.86	38,80,148,169	0
4	GOL	A	868	6/6	0.26	2.59	49,82,113,137	0
3	HEM	A	866	43/43	0.29	1.53	42,79,148,171	0
4	GOL	A	869	6/6	0.21	0.71	105,119,128,128	0
4	GOL	A	870	6/6	0.19	-0.27	101,122,137,144	0
4	GOL	B	867	6/6	0.20	-0.63	65,89,122,123	0
4	GOL	A	867	6/6	0.22	-0.71	68,74,118,119	0
4	GOL	B	868	6/6	0.14	-2.05	73,109,123,124	0

6.5 Other polymers ⓘ

There are no such residues in this entry.