



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:35 AM GMT

PDB ID : 3VEC
Title : Rhodococcus jostii RHA1 DypB D153A variant in complex with heme
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Deposited on : 2012-01-07
Resolution : 2.60 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>

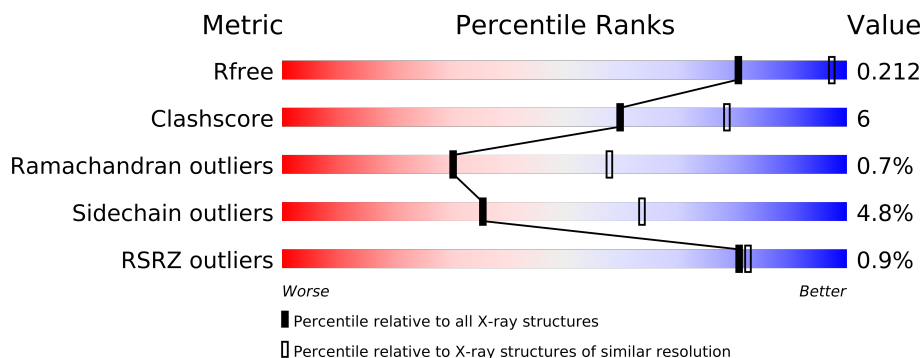
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	353	
1	B	353	
1	C	353	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	404	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7565 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 DypB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	6	0
			2389	1499	409	473	8			
1	B	309	Total	C	N	O	S	0	5	0
			2383	1494	406	475	8			
1	C	309	Total	C	N	O	S	0	3	0
			2369	1487	404	471	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q0SE24
A	-1	SER	-	EXPRESSION TAG	UNP Q0SE24
A	0	HIS	-	EXPRESSION TAG	UNP Q0SE24
A	153	ALA	ASP	ENGINEERED MUTATION	UNP Q0SE24
B	-2	GLY	-	EXPRESSION TAG	UNP Q0SE24
B	-1	SER	-	EXPRESSION TAG	UNP Q0SE24
B	0	HIS	-	EXPRESSION TAG	UNP Q0SE24
B	153	ALA	ASP	ENGINEERED MUTATION	UNP Q0SE24
C	-2	GLY	-	EXPRESSION TAG	UNP Q0SE24
C	-1	SER	-	EXPRESSION TAG	UNP Q0SE24
C	0	HIS	-	EXPRESSION TAG	UNP Q0SE24
C	153	ALA	ASP	ENGINEERED MUTATION	UNP Q0SE24

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



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		
3	C	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	112	Total	O	0	0
			112	112		
5	C	50	Total	O	0	0
			50	50		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.43Å 132.43Å 160.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 41.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 99.0 (41.85-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.166 , 0.212 0.166 , 0.212	Depositor DCC
R_{free} test set	2559 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.7	EDS
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 50346 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7565	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, CL, 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	0.74	1/2440 (0.0%)	0.88	6/3321 (0.2%)
1	B	0.74	1/2434 (0.0%)	0.82	1/3313 (0.0%)
1	C	0.71	1/2420 (0.0%)	0.81	0/3294
All	All	0.73	3/7294 (0.0%)	0.84	7/9928 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	TRP	CD2-CE2	5.41	1.47	1.41
1	C	72	TRP	CD2-CE2	5.39	1.47	1.41
1	A	72	TRP	CD2-CE2	5.00	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	A	55	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	B	141	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	A	141	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	190	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	55	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	236	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2389	0	2297	33	1
1	B	2383	0	2283	23	1
1	C	2369	0	2276	32	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	6	0	8	1	0
5	A	121	0	0	0	0
5	B	112	0	0	0	0
5	C	50	0	0	1	0
All	All	7565	0	6954	85	1

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 6.

All (85) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:289[B]:ARG:HH11	1:C:289[B]:ARG:HG2	1.24	0.99
1:C:289[B]:ARG:HG2	1:C:289[B]:ARG:NH1	1.93	0.81
1:A:289[A]:ARG:CG	1:A:289[A]:ARG:HH11	1.94	0.81
1:C:100:THR:HB	1:C:101:PRO:HD2	1.64	0.79
1:A:277[A]:ARG:HH11	1:A:277[A]:ARG:HG2	1.52	0.75
1:B:199:THR:O	1:B:203:GLU:HG3	1.89	0.73
1:C:229:LEU:HD12	1:C:288:ASP:HB2	1.76	0.68
1:C:137:VAL:HG21	1:C:260:TYR:CD2	2.32	0.65
1:B:10:PRO:HD2	1:B:307:ARG:HD3	1.79	0.63
1:B:301:LEU:HD23	1:B:302:PHE:N	2.15	0.62
1:A:289[A]:ARG:HH11	1:A:289[A]:ARG:HG3	1.64	0.61
1:C:204[A]:ARG:NH1	1:C:289[A]:ARG:HH12	1.98	0.61
1:A:35[B]:ARG:HB2	1:A:74:ARG:HH21	1.67	0.60
1:A:7:ARG:HG2	1:C:159:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39[B]:CYS:SG	1:A:313:LEU:O	2.61	0.58
1:A:39[B]:CYS:SG	1:A:313:LEU:C	2.81	0.57
1:C:137:VAL:HG21	1:C:260:TYR:HD2	1.70	0.57
1:A:10:PRO:CG	1:A:46:ASP:HB3	2.36	0.56
1:C:45:ILE:O	1:C:48:PRO:HD2	2.06	0.56
1:B:220:ALA:O	1:B:222:PRO:HD3	2.07	0.55
1:B:301:LEU:C	1:B:301:LEU:HD23	2.27	0.54
1:A:289[A]:ARG:HG2	1:A:289[A]:ARG:HH11	1.71	0.54
1:A:277[A]:ARG:CG	1:A:277[A]:ARG:HH11	2.19	0.53
1:A:35[B]:ARG:HB2	1:A:74:ARG:NH2	2.23	0.52
1:C:301:LEU:HD23	1:C:302:PHE:N	2.24	0.52
1:A:39[A]:CYS:SG	1:A:75:VAL:HG11	2.50	0.52
1:A:189:HIS:HA	1:A:293:PHE:O	2.09	0.52
1:A:85:HIS:HD2	1:A:86:PRO:O	1.91	0.52
1:A:35[A]:ARG:HB2	1:A:74:ARG:HH21	1.74	0.52
1:C:100:THR:HB	1:C:101:PRO:CD	2.38	0.52
1:B:187:TYR:CG	2:B:401:HEM:HBB1	2.45	0.52
1:B:307:ARG:HH11	1:B:307:ARG:HG3	1.75	0.50
1:B:218:ASP:N	1:B:218:ASP:OD2	2.44	0.50
1:C:189:HIS:ND1	1:C:294:SER:HB3	2.26	0.50
1:A:185:GLN:NE2	1:A:187:TYR:OH	2.44	0.50
1:A:230:ASN:HD22	1:A:274:MET:HG2	1.77	0.49
1:C:185:GLN:NE2	1:C:275:LEU:HD21	2.28	0.49
1:C:29:GLY:HA3	1:C:34:ASP:OD2	2.12	0.49
1:A:254:GLU:HB2	1:A:256:GLU:HG3	1.94	0.49
1:C:289[B]:ARG:CG	1:C:289[B]:ARG:NH1	2.71	0.49
1:C:185:GLN:HE22	1:C:275:LEU:HD21	1.77	0.49
1:A:35[A]:ARG:HB2	1:A:74:ARG:NH2	2.28	0.47
1:C:69:ALA:HA	1:C:84:LEU:HD21	1.96	0.47
1:A:113:LYS:H	4:A:404:GOL:H32	1.78	0.47
1:B:289[B]:ARG:HG3	1:B:292:ASP:OD2	2.15	0.47
1:A:257:TYR:CE1	1:B:121:ARG:HG3	2.51	0.46
1:A:52:VAL:HG22	1:A:61:LEU:CD2	2.46	0.46
1:C:212:GLU:HB2	5:C:517:HOH:O	2.16	0.45
1:B:89:PRO:O	1:B:90:LEU:HD23	2.16	0.45
1:B:239:GLU:OE1	1:B:241:ASP:OD1	2.35	0.45
1:C:249:PHE:CE1	1:C:258:GLY:HA3	2.51	0.45
1:A:10:PRO:HG3	1:A:46:ASP:HB3	1.98	0.45
1:C:229:LEU:O	1:C:277:ARG:HD3	2.17	0.45
1:A:289[A]:ARG:NH1	1:A:292:ASP:OD2	2.49	0.45
1:B:187:TYR:CE1	1:B:296:ALA:HB2	2.52	0.44
1:A:192:SER:O	1:A:196:THR:HG23	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:262:ILE:O	1:B:262:ILE:HG23	2.16	0.44
1:B:181:TYR:CD2	1:B:268:PRO:HD3	2.53	0.44
1:A:139:GLY:HA2	1:A:248:ALA:O	2.18	0.43
1:B:221:GLN:NE2	1:B:225:SER:OG	2.51	0.43
1:A:181:TYR:CD1	1:A:268:PRO:HD3	2.52	0.43
1:C:146:ARG:HA	1:C:151:PHE:O	2.18	0.43
1:B:136:GLU:OE2	1:B:138:HIS:CE1	2.72	0.43
1:B:142:TYR:HB3	1:B:146:ARG:O	2.19	0.43
1:C:171:ASP:OD1	1:C:177:ARG:NH1	2.51	0.43
1:C:38:VAL:HG11	1:C:71:PHE:CZ	2.54	0.42
1:C:160:ASP:HB3	1:C:161:ASP:H	1.46	0.42
1:A:7:ARG:HG2	1:C:159:THR:CG2	2.49	0.42
1:A:189:HIS:HE1	2:A:401:HEM:HBB2	1.85	0.42
1:A:74:ARG:HE	1:A:74:ARG:HB3	1.71	0.42
1:C:189:HIS:CE1	1:C:294:SER:HB3	2.55	0.41
1:C:205:VAL:HG22	1:C:289[A]:ARG:HB2	2.03	0.41
1:A:185:GLN:NE2	1:A:275:LEU:HD21	2.35	0.41
1:B:78:SER:O	1:B:79:SER:HB2	2.21	0.41
1:A:52:VAL:O	1:A:55:ARG:HB2	2.21	0.41
1:A:277[A]:ARG:NH1	1:A:277[A]:ARG:CG	2.84	0.41
1:B:91:SER:HA	1:B:96:SER:OG	2.20	0.41
1:C:84:LEU:HD13	1:C:303:PHE:HB2	2.03	0.41
1:C:182:VAL:O	1:C:182:VAL:HG13	2.21	0.41
1:C:80:LYS:HA	1:C:81:PRO:HD3	1.98	0.41
1:B:189:HIS:HA	1:B:293:PHE:O	2.20	0.41
1:B:185:GLN:HE22	1:B:275:LEU:HD21	1.86	0.40
1:C:204[A]:ARG:NH2	1:C:289[A]:ARG:HH22	2.20	0.40
1:B:187:TYR:CD1	2:B:401:HEM:HBB1	2.55	0.40
1:C:45:ILE:HA	1:C:45:ILE:HD12	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212[A]:GLU:OE2	1:B:121:ARG:NH2[5_555]	2.12	0.08

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	312/353 (88%)	301 (96%)	10 (3%)	1 (0%)	50	77
1	B	312/353 (88%)	295 (95%)	16 (5%)	1 (0%)	50	77
1	C	310/353 (88%)	288 (93%)	18 (6%)	4 (1%)	18	35
All	All	934/1059 (88%)	884 (95%)	44 (5%)	6 (1%)	30	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	70	GLN
1	B	79	SER
1	C	31	SER
1	C	262	ILE
1	C	306	SER
1	A	76	SER

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	258/283 (91%)	242 (94%)	16 (6%)	26	49
1	B	257/283 (91%)	245 (95%)	12 (5%)	36	65
1	C	255/283 (90%)	241 (94%)	14 (6%)	30	56
All	All	770/849 (91%)	728 (94%)	42 (6%)	35	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	32	ASP
1	A	33	ASP
1	A	35[A]	ARG
1	A	35[B]	ARG
1	A	78	SER

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Mol	Chain	Res	Type
1	A	80	LYS
1	A	134	VAL
1	A	137[A]	VAL
1	A	137[B]	VAL
1	A	192	SER
1	A	216	LEU
1	A	221	GLN
1	A	289[A]	ARG
1	A	289[B]	ARG
1	A	311	GLU
1	B	14	LEU
1	B	31	SER
1	B	39[A]	CYS
1	B	39[B]	CYS
1	B	46[A]	ASP
1	B	46[B]	ASP
1	B	75	VAL
1	B	91	SER
1	B	145	SER
1	B	218	ASP
1	B	219	ASP
1	B	235	ASP
1	C	7	ARG
1	C	21	SER
1	C	30	ASP
1	C	79	SER
1	C	80	LYS
1	C	145	SER
1	C	211	LEU
1	C	218	ASP
1	C	228	THR
1	C	289[A]	ARG
1	C	289[B]	ARG
1	C	294	SER
1	C	295	THR
1	C	313	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	213	ASN

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Mol	Chain	Res	Type
1	A	221	GLN
1	A	230	ASN
1	B	185	GLN
1	B	221	GLN
1	C	185	GLN
1	C	221	GLN
1	C	230	ASN

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 ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	401	1	49,50,50	5.13	25 (51%)	46,82,82	2.56	18 (39%)
4	GOL	A	404	-	5,5,5	0.28	0	5,5,5	1.42	1 (20%)
2	HEM	B	401	1	49,50,50	5.06	24 (48%)	46,82,82	2.79	17 (36%)
2	HEM	C	401	1	49,50,50	5.40	23 (46%)	46,82,82	2.78	20 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	401	1	-	0/14/114/114	0/0/8/8
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0
2	HEM	B	401	1	-	0/14/114/114	0/0/8/8
2	HEM	C	401	1	-	0/14/114/114	0/0/8/8

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C3D-C4D	21.11	1.49	1.44
2	C	401	HEM	C2B-C1B	20.45	1.49	1.44
2	A	401	HEM	C2B-C1B	19.20	1.49	1.44
2	C	401	HEM	C3D-C4D	18.80	1.49	1.44
2	A	401	HEM	C3D-C4D	15.91	1.48	1.44
2	B	401	HEM	C2B-C1B	15.88	1.48	1.44
2	C	401	HEM	C2D-C1D	14.99	1.48	1.44
2	A	401	HEM	C2D-C1D	14.32	1.48	1.44
2	B	401	HEM	C2D-C1D	10.44	1.47	1.44
2	A	401	HEM	CHB-C1B	7.81	1.46	1.35
2	B	401	HEM	C4A-C3A	7.69	1.49	1.40
2	A	401	HEM	C4A-C3A	7.64	1.49	1.40
2	A	401	HEM	CHA-C4D	7.33	1.46	1.35
2	C	401	HEM	CHA-C4D	7.10	1.45	1.35
2	C	401	HEM	C4A-C3A	6.66	1.48	1.40
2	C	401	HEM	CHB-C1B	6.61	1.45	1.35
2	B	401	HEM	CHC-C1C	6.48	1.48	1.36
2	B	401	HEM	CHA-C4D	6.27	1.44	1.35
2	B	401	HEM	C1C-NC	6.16	1.46	1.38
2	B	401	HEM	CHB-C1B	6.11	1.44	1.35
2	C	401	HEM	C4C-NC	5.87	1.46	1.38
2	C	401	HEM	C1A-NA	5.74	1.47	1.36
2	C	401	HEM	C1C-NC	5.64	1.46	1.38
2	A	401	HEM	C1A-NA	5.57	1.47	1.36
2	A	401	HEM	C1C-NC	5.31	1.45	1.38
2	A	401	HEM	C4A-NA	5.10	1.46	1.36
2	B	401	HEM	C1A-NA	5.06	1.46	1.36
2	A	401	HEM	CHD-C4C	4.94	1.45	1.36
2	B	401	HEM	C4A-NA	4.86	1.46	1.36
2	A	401	HEM	C4C-NC	4.85	1.44	1.38
2	C	401	HEM	CHD-C4C	4.84	1.45	1.36
2	B	401	HEM	C4C-NC	4.78	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	CHC-C1C	4.55	1.44	1.36
2	A	401	HEM	CHC-C1C	4.54	1.44	1.36
2	C	401	HEM	C4A-NA	4.50	1.45	1.36
2	B	401	HEM	C3B-C4B	4.08	1.49	1.44
2	B	401	HEM	CHD-C4C	4.02	1.43	1.36
2	B	401	HEM	C1A-C2A	3.84	1.50	1.43
2	B	401	HEM	FE-ND	3.81	2.11	1.97
2	A	401	HEM	FE-NB	3.80	2.11	1.97
2	B	401	HEM	CHC-C4B	3.67	1.47	1.39
2	A	401	HEM	C3C-CAC	3.63	1.51	1.40
2	A	401	HEM	C1A-C2A	3.53	1.49	1.43
2	C	401	HEM	C1A-C2A	3.47	1.49	1.43
2	C	401	HEM	C1A-CHA	3.41	1.49	1.39
2	C	401	HEM	CHD-C1D	3.37	1.47	1.39
2	C	401	HEM	FE-NB	3.36	2.10	1.97
2	C	401	HEM	FE-ND	3.34	2.10	1.97
2	A	401	HEM	FE-ND	3.33	2.10	1.97
2	B	401	HEM	C2A-C3A	3.20	1.47	1.37
2	A	401	HEM	C2A-C3A	3.11	1.46	1.37
2	C	401	HEM	C2A-C3A	3.05	1.46	1.37
2	B	401	HEM	C3C-CAC	2.86	1.49	1.40
2	C	401	HEM	CHC-C4B	2.83	1.46	1.39
2	C	401	HEM	C3C-CAC	2.81	1.49	1.40
2	A	401	HEM	C1A-CHA	2.78	1.47	1.39
2	A	401	HEM	C4D-ND	-2.72	1.34	1.39
2	A	401	HEM	CHC-C4B	2.70	1.45	1.39
2	A	401	HEM	C3B-CAB	2.69	1.48	1.40
2	A	401	HEM	CHD-C1D	2.64	1.45	1.39
2	B	401	HEM	FE-NB	2.60	2.07	1.97
2	B	401	HEM	C4D-ND	-2.52	1.34	1.39
2	B	401	HEM	C3B-C2B	2.38	1.47	1.43
2	A	401	HEM	C3B-C4B	2.35	1.47	1.44
2	B	401	HEM	C4A-CHB	2.34	1.46	1.39
2	B	401	HEM	C2C-C1C	2.33	1.50	1.43
2	C	401	HEM	C2C-C1C	2.24	1.49	1.43
2	A	401	HEM	C4A-CHB	2.23	1.46	1.39
2	C	401	HEM	C3B-CAB	2.21	1.47	1.40
2	C	401	HEM	C3B-C4B	2.12	1.47	1.44
2	A	401	HEM	C2C-C1C	2.04	1.49	1.43
2	B	401	HEM	C3C-C2C	2.03	1.47	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	HEM	C3A-C4A-NA	8.47	115.81	109.41
2	B	401	HEM	C3A-C4A-NA	7.15	114.81	109.41
2	A	401	HEM	C3A-C4A-NA	6.99	114.69	109.41
2	B	401	HEM	C2D-C1D-ND	6.35	120.43	112.93
2	A	401	HEM	CBD-CAD-C3D	-6.25	100.74	114.37
2	B	401	HEM	C4D-ND-C1D	-6.11	98.91	105.16
2	B	401	HEM	C1A-CHA-C4D	-5.91	119.69	127.47
2	C	401	HEM	C4A-NA-C1A	-5.68	99.28	106.76
2	B	401	HEM	C4A-NA-C1A	-5.63	99.34	106.76
2	A	401	HEM	C4C-NC-C1C	-5.47	99.85	105.53
2	A	401	HEM	C4A-NA-C1A	-5.41	99.64	106.76
2	B	401	HEM	CBD-CAD-C3D	-5.18	103.06	114.37
2	C	401	HEM	C4C-NC-C1C	-5.17	100.16	105.53
2	C	401	HEM	CBD-CAD-C3D	-4.58	104.39	114.37
2	C	401	HEM	C4A-CHB-C1B	-4.44	121.62	127.47
2	B	401	HEM	C2A-C1A-NA	4.40	115.85	109.73
2	C	401	HEM	C1B-NB-C4B	-4.09	100.97	105.16
2	C	401	HEM	C1A-CHA-C4D	-4.07	122.11	127.47
2	B	401	HEM	C4C-NC-C1C	-3.99	101.38	105.53
2	C	401	HEM	C4D-ND-C1D	-3.95	101.12	105.16
2	C	401	HEM	C2D-C1D-ND	3.81	117.42	112.93
2	A	401	HEM	C2D-C1D-ND	3.77	117.38	112.93
2	C	401	HEM	C3A-C4A-CHB	-3.67	119.04	126.00
2	B	401	HEM	C3A-C4A-CHB	-3.63	119.12	126.00
2	A	401	HEM	C2A-C1A-NA	3.47	114.55	109.73
2	A	401	HEM	C4D-ND-C1D	-3.46	101.62	105.16
2	A	401	HEM	C1B-NB-C4B	-3.45	101.63	105.16
2	C	401	HEM	C2A-C1A-NA	3.32	114.34	109.73
2	C	401	HEM	CHC-C1C-NC	-3.30	121.86	124.73
2	C	401	HEM	C4A-C3A-C2A	-3.28	104.71	107.00
2	C	401	HEM	C2A-C1A-CHA	-3.21	119.91	126.00
2	B	401	HEM	C1A-C2A-C3A	-3.17	103.64	106.92
2	B	401	HEM	C2A-C1A-CHA	-3.06	120.19	126.00
2	C	401	HEM	CAD-C3D-C4D	2.97	129.87	124.53
2	B	401	HEM	CAD-C3D-C4D	2.94	129.81	124.53
2	A	401	HEM	CHC-C1C-NC	-2.90	122.21	124.73
2	A	401	HEM	C4A-CHB-C1B	-2.87	123.69	127.47
4	A	404	GOL	O1-C1-C2	-2.82	95.94	109.71
2	A	401	HEM	C4A-C3A-C2A	-2.79	105.06	107.00
2	C	401	HEM	C3B-C4B-NB	2.67	115.91	114.00
2	A	401	HEM	C3A-C4A-CHB	-2.50	121.27	126.00
2	B	401	HEM	C4A-CHB-C1B	-2.50	124.19	127.47
2	A	401	HEM	C3B-C4B-NB	2.40	115.72	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C1A-CHA-C4D	-2.38	124.34	127.47
2	A	401	HEM	C2A-C1A-CHA	-2.37	121.51	126.00
2	A	401	HEM	CAD-CBD-CGD	-2.33	106.22	113.48
2	A	401	HEM	CAD-C3D-C4D	2.30	128.67	124.53
2	B	401	HEM	CMB-C2B-C3B	2.30	131.57	126.16
2	C	401	HEM	CHA-C4D-ND	-2.20	121.28	124.31
2	C	401	HEM	CMD-C2D-C3D	2.19	130.57	125.60
2	A	401	HEM	CMD-C2D-C3D	2.15	130.46	125.60
2	B	401	HEM	C3B-C4B-NB	-2.10	112.50	114.00
2	C	401	HEM	CHC-C4B-NB	2.07	126.31	124.58
2	C	401	HEM	CMB-C2B-C3B	2.04	130.96	126.16
2	B	401	HEM	CHC-C1C-NC	-2.03	122.97	124.73
2	B	401	HEM	O2A-CGA-O1A	-2.01	118.18	123.30

There are no chirality outliers.

There are no torsion outliers.

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	308/353 (87%)	-0.53	1 (0%) 91 92	28, 43, 70, 106	0
1	B	309/353 (87%)	-0.52	2 (0%) 86 89	28, 46, 74, 94	0
1	C	309/353 (87%)	-0.31	5 (1%) 68 69	38, 60, 85, 112	0
All	All	926/1059 (87%)	-0.45	8 (0%) 81 82	28, 49, 82, 112	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	78	SER	2.8
1	C	77	ALA	2.6
1	C	36	ALA	2.5
1	C	314	GLY	2.3
1	B	78	SER	2.3
1	B	77	ALA	2.1
1	C	171	ASP	2.1
1	A	35[A]	ARG	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	404	6/6	0.20	4.39	52,54,70,74	0
2	HEM	C	401	43/43	0.14	0.83	44,49,53,55	0
2	HEM	B	401	43/43	0.12	0.74	32,40,47,52	0
2	HEM	A	401	43/43	0.12	0.19	31,38,41,48	0
3	CL	A	403	1/1	0.11	-0.08	46,46,46,46	0
3	CL	B	402	1/1	0.13	-0.52	41,41,41,41	0
3	CL	C	402	1/1	0.10	-1.99	50,50,50,50	0
3	CL	C	403	1/1	0.11	-2.13	67,67,67,67	0
3	CL	B	403	1/1	0.08	-2.59	59,59,59,59	0
3	CL	A	402	1/1	0.07	-2.97	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.