



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:25 AM GMT

PDB ID : 3OZW
Title : The Crystal Structure of flavohemoglobin from *R. eutrophus* in complex with ketoconazole
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Deposited on : 2010-09-27
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

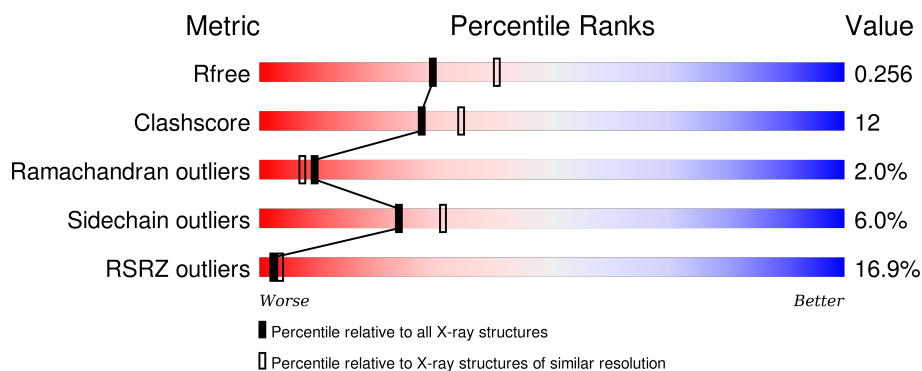
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	403	<div> <div>11%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	B	403	<div> <div>23%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	KKK	A	413	X	-	-	-
4	KKK	B	413	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6795 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 Flavohemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3156	2011	543	588	14			
1	B	403	Total	C	N	O	S	0	2	0
			3170	2020	546	590	14			

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



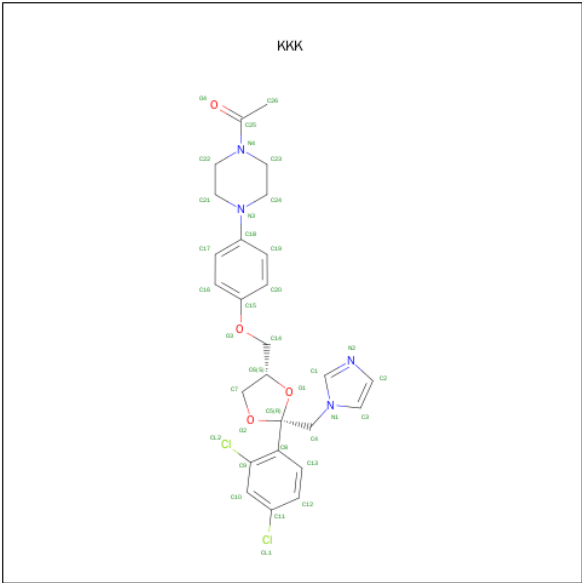
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 1-ACETYL-4-(4-{[(2R,4S)-2-(2,4-DICHLOROPHENYL)-2-(1H-IMIDAZOL-1-YLMETHYL)-1,3-DIOXOLAN-4-YL]METHOXY}PHENYL)PIPERAZINE (three-letter code: KKK) (formula: C₂₆H₂₈Cl₂N₄O₄).



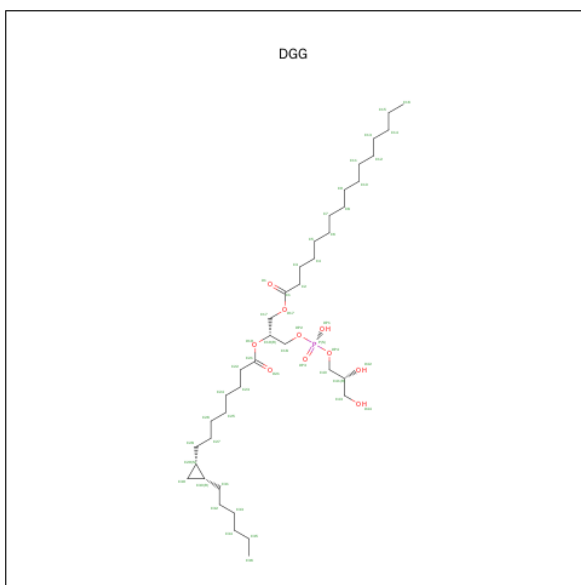
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			36	26	2	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	N	O	
4	B	1	36	26	2	4	4	0

- Molecule 5 is 1-[GLYCEROLYLPHOSPHONYL]-2-[8-(2-HEXYL-CYCLOPROPYL)-OCTANAL-1-YL]-3-[HEXADECANAL-1-YL]-GLYCEROL (three-letter code: DGG) (formula: $C_{39}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	19	17	2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

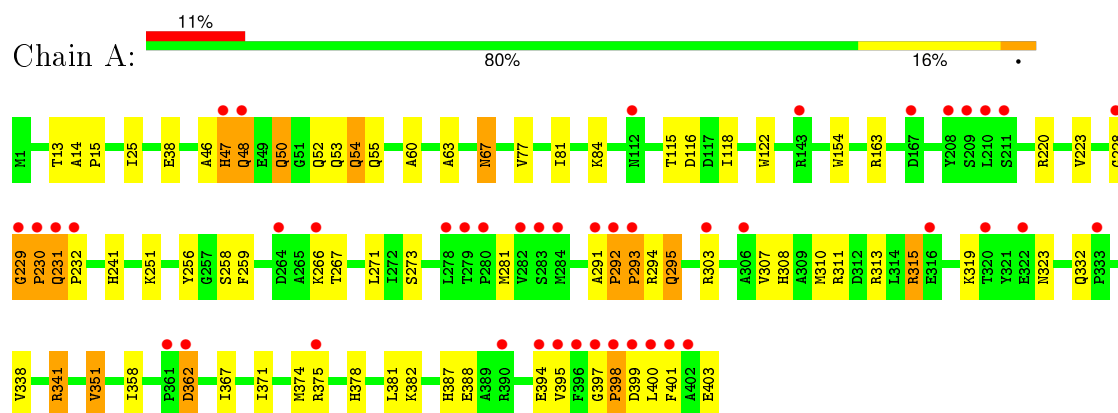
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total	O	0	0
			94	94		
7	B	87	Total	O	0	0
			87	87		

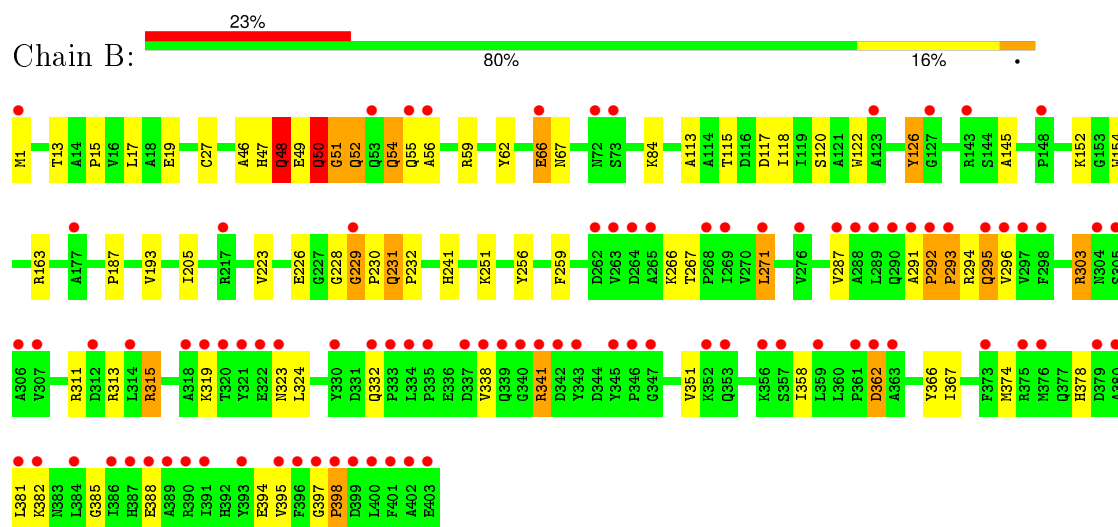
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Flavohemoglobin



• Molecule 1: Flavohemoglobin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.12Å 87.12Å 292.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.30) 92.8 (29.37-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.205 , 0.241 0.227 , 0.256	Depositor DCC
R_{free} test set	2573 reflections (5.71%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 47432 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6795	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, PO4, DGG, KKK, FAD

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	0.76	3/3233 (0.1%)	0.74	0/4393
1	B	0.76	2/3253 (0.1%)	0.73	0/4419
All	All	0.76	5/6486 (0.1%)	0.74	0/8812

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	TYR	CD1-CE1	9.80	1.54	1.39
1	A	256	TYR	CE1-CZ	-6.25	1.30	1.38
1	A	256	TYR	CE2-CZ	-6.09	1.30	1.38
1	A	256	TYR	CG-CD1	-5.69	1.31	1.39
1	B	256	TYR	CE1-CZ	-5.29	1.31	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	226	GLU	Peptide

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	3156	0	3112	80	0
1	B	3170	0	3131	68	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	53	0	31	4	0
3	B	53	0	31	1	0
4	A	36	0	28	6	0
4	B	36	0	28	13	0
5	A	19	0	30	11	0
6	A	5	0	0	0	0
7	A	94	0	0	17	0
7	B	87	0	0	10	0
All	All	6795	0	6451	154	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 12.

All (154) 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:B:117:ASP:HB2	7:B:473:HOH:O	1.17	1.30
1:A:116:ASP:HB2	7:A:496:HOH:O	1.32	1.24
1:B:27:CYS:SG	7:B:491:HOH:O	2.05	1.14
1:B:49:GLU:O	1:B:50:GLN:HB2	1.42	1.10
1:A:341:ARG:HG2	1:A:341:ARG:HH21	1.14	1.03
1:B:341:ARG:HG2	1:B:341:ARG:HH21	1.19	1.02
1:B:27:CYS:CB	7:B:491:HOH:O	2.08	1.02
1:B:54:GLN:HE21	1:B:55:GLN:HE21	1.09	1.00
1:B:27:CYS:HB2	7:B:491:HOH:O	1.62	0.99
1:A:291:ALA:HA	1:A:292:PRO:C	1.86	0.96
1:B:48:GLN:HG3	7:B:440:HOH:O	1.65	0.95
1:A:230:PRO:HG3	1:B:59:ARG:HG2	1.45	0.95
1:B:291:ALA:HA	1:B:292:PRO:C	1.91	0.91
1:A:54:GLN:HE21	1:A:55:GLN:HE21	0.94	0.89
1:A:54:GLN:NE2	1:A:55:GLN:HE21	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLN:HE21	1:A:55:GLN:NE2	1.73	0.85
1:A:77:VAL:HG21	5:A:416:DGG:H251	1.60	0.83
1:A:232:PRO:HG2	3:A:405:FAD:C5A	2.07	0.83
1:B:341:ARG:NH2	1:B:341:ARG:HG2	1.95	0.81
1:A:341:ARG:HG2	1:A:341:ARG:NH2	1.89	0.80
1:A:394:GLU:HA	7:A:408:HOH:O	1.82	0.78
1:A:399:ASP:HB3	7:A:415:HOH:O	1.85	0.76
1:A:303:ARG:HG3	1:A:332:GLN:HB2	1.67	0.75
1:A:13:THR:HG21	1:A:118:ILE:HG12	1.70	0.73
1:B:54:GLN:HE21	1:B:55:GLN:NE2	1.86	0.73
1:B:47:HIS:ND1	4:B:413:KKK:H19	2.04	0.72
1:A:230:PRO:CG	1:B:59:ARG:HG2	2.20	0.71
1:B:47:HIS:CE1	4:B:413:KKK:H21A	2.24	0.71
1:A:351:VAL:HG22	1:A:358:ILE:HD13	1.73	0.71
1:B:367:ILE:HG22	1:B:374:MET:HG2	1.71	0.70
1:A:60:ALA:HB1	5:A:416:DGG:H391	1.74	0.70
1:B:51:GLY:HA3	1:B:52:GLN:HB2	1.74	0.69
1:A:54:GLN:NE2	1:A:55:GLN:NE2	2.37	0.69
3:A:405:FAD:H2A	1:B:62:TYR:HE1	1.57	0.68
1:A:400:LEU:HD23	7:A:415:HOH:O	1.93	0.68
1:A:67:ASN:OD1	5:A:416:DGG:H232	1.93	0.68
1:A:367:ILE:HG22	1:A:374:MET:HG2	1.76	0.66
1:A:46:ALA:C	1:A:48:GLN:H	1.98	0.66
1:B:54:GLN:NE2	1:B:55:GLN:HE21	1.90	0.62
1:A:55:GLN:NE2	1:B:113:ALA:HB1	2.14	0.61
1:B:230:PRO:HD2	1:B:231:GLN:HE21	1.65	0.61
1:A:294:ARG:O	1:A:295:GLN:HB2	2.00	0.61
3:A:405:FAD:H2A	1:B:62:TYR:CE1	2.35	0.61
1:A:400:LEU:CD2	7:A:415:HOH:O	2.47	0.61
1:B:51:GLY:CA	1:B:52:GLN:HB2	2.30	0.60
1:A:259:PHE:CG	1:A:394:GLU:HB2	2.37	0.60
1:A:232:PRO:HG2	3:A:405:FAD:N7A	2.14	0.60
1:B:294:ARG:O	1:B:295:GLN:HB2	2.00	0.60
1:A:398:PRO:HG2	7:A:440:HOH:O	2.02	0.59
1:A:259:PHE:CD2	1:A:394:GLU:HB2	2.36	0.59
1:B:66:GLU:HB3	7:B:484:HOH:O	2.01	0.59
1:B:259:PHE:CD2	1:B:394:GLU:HB2	2.38	0.59
1:A:230:PRO:HD2	1:A:231:GLN:HE21	1.66	0.59
1:A:122:TRP:HZ3	5:A:416:DGG:H332	1.67	0.59
1:A:394:GLU:CA	7:A:408:HOH:O	2.48	0.59
1:A:399:ASP:OD1	7:A:408:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ALA:HB1	5:A:416:DGG:H242	1.86	0.57
1:B:13:THR:HG21	1:B:118:ILE:HG12	1.86	0.57
1:A:163:ARG:NH1	1:A:313:ARG:HH22	2.02	0.57
1:B:56:ALA:CB	4:B:413:KKK:H16	2.33	0.57
1:B:228:GLY:O	1:B:229:GLY:C	2.43	0.56
1:A:77:VAL:CG2	5:A:416:DGG:H251	2.33	0.56
1:A:291:ALA:HA	1:A:293:PRO:N	2.20	0.56
1:B:49:GLU:O	1:B:50:GLN:CB	2.31	0.56
1:A:294:ARG:O	1:A:295:GLN:CB	2.54	0.56
4:A:413:KKK:CL1	5:A:416:DGG:H322	2.42	0.56
1:A:220:ARG:NH2	1:A:310:MET:CE	2.69	0.56
1:A:220:ARG:HH22	1:A:310:MET:CE	2.19	0.55
1:B:351:VAL:HG22	1:B:358:ILE:HD13	1.89	0.55
1:A:77:VAL:HG11	5:A:416:DGG:H231	1.88	0.55
4:A:413:KKK:CL1	5:A:416:DGG:H352	2.44	0.55
1:B:259:PHE:CG	1:B:394:GLU:HB2	2.42	0.55
1:A:228:GLY:O	1:A:229:GLY:C	2.46	0.54
1:B:223:VAL:O	1:B:241:HIS:HE1	1.90	0.54
1:B:46:ALA:O	1:B:49:GLU:HG2	2.08	0.53
1:A:52:GLN:HE22	1:B:19[A]:GLU:HG3	1.74	0.53
1:B:126:TYR:CE1	2:B:404:HEM:HAB	2.44	0.53
1:B:67:ASN:ND2	7:B:484:HOH:O	2.41	0.53
1:A:267:THR:OG1	1:A:362:ASP:O	2.26	0.53
1:A:46:ALA:C	1:A:48:GLN:N	2.62	0.52
1:B:47:HIS:CE1	4:B:413:KKK:C21	2.91	0.52
1:B:294:ARG:O	1:B:295:GLN:CB	2.58	0.52
1:B:291:ALA:HA	1:B:293:PRO:N	2.25	0.51
1:A:311:ARG:HD2	1:A:315:ARG:HD3	1.92	0.51
1:B:395:VAL:HG12	1:B:397:GLY:H	1.75	0.51
1:B:303:ARG:HG3	1:B:332:GLN:HB2	1.93	0.51
1:A:308:HIS:CE1	1:A:311:ARG:HG2	2.46	0.51
1:A:220:ARG:NH2	1:A:310:MET:HE1	2.27	0.50
1:A:50:GLN:HG3	1:B:15:PRO:HG2	1.94	0.50
1:A:122:TRP:CZ3	5:A:416:DGG:H332	2.46	0.49
1:A:398:PRO:HB3	7:A:485:HOH:O	2.11	0.49
1:B:385:GLY:HA2	7:B:488:HOH:O	2.12	0.49
1:B:398:PRO:HG3	4:B:413:KKK:H21	1.93	0.49
1:B:232:PRO:HG2	3:B:405:FAD:C5A	2.43	0.49
1:A:351:VAL:HB	7:A:459:HOH:O	2.12	0.49
1:B:398:PRO:CG	4:B:413:KKK:H21	2.42	0.49
1:A:53:GLN:HG2	4:A:413:KKK:C20	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:VAL:HG13	1:B:358:ILE:HD11	1.95	0.49
1:B:311:ARG:HD2	1:B:315:ARG:HD3	1.95	0.49
1:B:115:THR:OG1	1:B:118:ILE:HD12	2.13	0.48
1:B:398:PRO:CD	4:B:413:KKK:H21	2.43	0.48
1:A:341:ARG:HH21	1:A:341:ARG:CG	2.03	0.48
2:A:404:HEM:HMB2	2:A:404:HEM:HBB2	1.96	0.48
4:A:413:KKK:H13	4:A:413:KKK:C6	2.44	0.48
1:A:378:HIS:CD2	1:A:382:LYS:HD2	2.48	0.47
2:A:404:HEM:HHD	2:A:404:HEM:HBC2	1.96	0.47
1:B:145:ALA:HB2	1:B:152:LYS:HG3	1.96	0.47
4:A:413:KKK:C13	4:A:413:KKK:C6	2.91	0.47
1:A:395:VAL:HG12	1:A:397:GLY:H	1.79	0.47
1:B:193:VAL:O	1:B:205:ILE:HA	2.14	0.47
1:A:223:VAL:O	1:A:241:HIS:HE1	1.97	0.47
1:A:273:SER:HB3	1:A:281:MET:HG3	1.97	0.47
1:B:267:THR:OG1	1:B:362:ASP:O	2.32	0.47
1:A:401:PHE:HD2	7:A:440:HOH:O	1.97	0.47
2:A:404:HEM:CMB	2:A:404:HEM:HBB2	2.45	0.47
1:A:231:GLN:H	1:A:231:GLN:HE21	1.60	0.47
1:A:115:THR:OG1	1:A:118:ILE:HD12	2.14	0.47
1:A:77:VAL:HG21	5:A:416:DGG:C25	2.41	0.46
1:A:400:LEU:HD22	1:A:403:GLU:OE2	2.14	0.46
4:A:413:KKK:C3	4:A:413:KKK:C8	2.93	0.46
1:A:395:VAL:N	7:A:408:HOH:O	2.48	0.46
2:A:404:HEM:CBC	2:A:404:HEM:HHD	2.45	0.46
1:B:47:HIS:C	1:B:49:GLU:H	2.18	0.46
1:B:154:TRP:HB3	1:B:251:LYS:HB3	1.98	0.46
2:B:404:HEM:HBD2	4:B:413:KKK:H20	1.98	0.46
1:A:231:GLN:NE2	1:A:231:GLN:H	2.14	0.46
1:A:38:GLU:HB2	7:A:486:HOH:O	2.17	0.45
1:A:375:ARG:HG2	7:B:406:HOH:O	2.17	0.45
1:B:49:GLU:OE2	7:B:451:HOH:O	2.21	0.44
1:A:14:ALA:N	1:A:15:PRO:CD	2.80	0.44
4:B:413:KKK:H17	4:B:413:KKK:H24A	1.74	0.44
1:A:292:PRO:HA	1:A:293:PRO:HD2	1.75	0.44
1:A:398:PRO:CB	7:A:485:HOH:O	2.66	0.44
1:A:154:TRP:HB3	1:A:251:LYS:HB3	2.00	0.43
1:A:308:HIS:ND1	1:A:311:ARG:HG2	2.33	0.43
1:B:378:HIS:CD2	1:B:382:LYS:HD2	2.53	0.43
1:A:230:PRO:HG3	1:B:59:ARG:CG	2.33	0.43
1:A:81:ILE:HD13	2:A:404:HEM:HMA1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:NH1	1:B:313:ARG:HH22	2.17	0.42
1:A:387:HIS:HB3	7:A:439:HOH:O	2.19	0.42
1:B:17:LEU:HD22	1:B:122:TRP:CE2	2.55	0.42
1:B:56:ALA:HB3	4:B:413:KKK:H16	1.99	0.42
1:B:187:PRO:HG3	1:B:287:VAL:HG21	2.02	0.42
1:A:371:ILE:HG21	1:A:401:PHE:HD1	1.85	0.41
1:A:399:ASP:N	7:A:468:HOH:O	2.52	0.41
1:B:398:PRO:HD3	4:B:413:KKK:C22	2.50	0.41
1:A:293:PRO:HB2	1:A:294:ARG:HA	2.02	0.41
1:B:292:PRO:HA	1:B:293:PRO:HD2	1.77	0.41
1:B:271:LEU:HD12	1:B:366:TYR:HB2	2.03	0.41
1:A:395:VAL:HG23	7:A:408:HOH:O	2.20	0.41
2:B:404:HEM:C4D	4:B:413:KKK:H1	2.56	0.40
1:B:296:VAL:O	1:B:324:LEU:HA	2.21	0.40
1:B:398:PRO:HD3	4:B:413:KKK:N4	2.36	0.40
1:A:48:GLN:C	1:A:48:GLN:HE21	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	401/403 (100%)	379 (94%)	15 (4%)	7 (2%)	11	10
1	B	403/403 (100%)	382 (95%)	12 (3%)	9 (2%)	8	6
All	All	804/806 (100%)	761 (95%)	27 (3%)	16 (2%)	9	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	292	PRO

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Mol	Chain	Res	Type
1	A	293	PRO
1	A	295	GLN
1	B	48	GLN
1	B	50	GLN
1	B	292	PRO
1	B	293	PRO
1	B	295	GLN
1	A	229	GLY
1	B	51	GLY
1	B	52	GLN
1	B	229	GLY
1	A	398	PRO
1	B	398	PRO
1	A	230	PRO

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	334/334 (100%)	313 (94%)	21 (6%)	22	29
1	B	336/334 (101%)	317 (94%)	19 (6%)	25	34
All	All	670/668 (100%)	630 (94%)	40 (6%)	24	31

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	47	HIS
1	A	48	GLN
1	A	50	GLN
1	A	54	GLN
1	A	67	ASN
1	A	84	LYS
1	A	231	GLN
1	A	258	SER

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Mol	Chain	Res	Type
1	A	266	LYS
1	A	271	LEU
1	A	307	VAL
1	A	315	ARG
1	A	319	LYS
1	A	323	ASN
1	A	338	VAL
1	A	341	ARG
1	A	351	VAL
1	A	362	ASP
1	A	381	LEU
1	A	388	GLU
1	B	1	MET
1	B	48	GLN
1	B	50	GLN
1	B	54	GLN
1	B	66	GLU
1	B	84	LYS
1	B	120	SER
1	B	231	GLN
1	B	266	LYS
1	B	271	LEU
1	B	303	ARG
1	B	315	ARG
1	B	319	LYS
1	B	323	ASN
1	B	338	VAL
1	B	341	ARG
1	B	362	ASP
1	B	381	LEU
1	B	388	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	47	HIS
1	A	48	GLN
1	A	50	GLN
1	A	54	GLN
1	A	231	GLN
1	A	241	HIS

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Mol	Chain	Res	Type
1	A	339	GLN
1	A	377	GLN
1	B	4	GLN
1	B	48	GLN
1	B	50	GLN
1	B	53	GLN
1	B	55	GLN
1	B	67	ASN
1	B	231	GLN
1	B	241	HIS
1	B	339	GLN
1	B	378	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	HEM	A	404	1,4	30,50,50	1.94	6 (20%)	24,82,82	2.77	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	405	-	48,58,58	1.37	6 (12%)	54,89,89	2.19	9 (16%)
6	PO4	A	406	-	4,4,4	0.26	0	6,6,6	0.28	0
4	KKK	A	413	2	39,40,40	1.32	4 (10%)	49,57,57	2.18	14 (28%)
5	DGG	A	416	-	15,19,50	0.44	0	14,22,59	4.18	2 (14%)
2	HEM	B	404	1,4	30,50,50	2.20	10 (33%)	24,82,82	3.17	11 (45%)
3	FAD	B	405	-	48,58,58	1.37	5 (10%)	54,89,89	2.28	9 (16%)
4	KKK	B	413	2	39,40,40	1.70	7 (17%)	49,57,57	2.79	12 (24%)

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	404	1,4	-	0/10/54/54	0/0/8/8
3	FAD	A	405	-	-	0/30/50/50	0/6/6/6
6	PO4	A	406	-	-	0/0/0/0	0/0/0/0
4	KKK	A	413	2	2/2/5/5	1/24/45/45	0/5/5/5
5	DGG	A	416	-	-	0/14/21/59	0/0/1/1
2	HEM	B	404	1,4	-	0/10/54/54	0/0/8/8
3	FAD	B	405	-	-	0/30/50/50	0/6/6/6
4	KKK	B	413	2	2/2/5/5	1/24/45/45	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	HEM	C3B-C4B	-5.53	1.46	1.51
2	A	404	HEM	C3D-C4D	-5.45	1.44	1.51
2	B	404	HEM	C3B-C4B	-4.93	1.47	1.51
4	B	413	KKK	C5-C8	-4.55	1.50	1.53
4	A	413	KKK	C5-C8	-4.51	1.50	1.53
2	B	404	HEM	C3D-C4D	-3.99	1.46	1.51
2	B	404	HEM	C2C-C1C	-3.55	1.45	1.52
2	A	404	HEM	C2C-C1C	-3.54	1.45	1.52
4	B	413	KKK	C3-N1	-2.61	1.32	1.37
4	A	413	KKK	C3-N1	-2.34	1.33	1.37
3	A	405	FAD	C6-C5X	-2.08	1.38	1.41
2	A	404	HEM	C2A-C3A	-2.06	1.31	1.37
2	A	404	HEM	C2B-C1B	-2.01	1.45	1.51
4	A	413	KKK	C25-N4	2.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	413	KKK	O1-C5	2.15	1.45	1.42
2	B	404	HEM	C4C-NC	2.28	1.38	1.36
3	A	405	FAD	C1'-N10	2.33	1.50	1.48
4	B	413	KKK	C11-CL1	2.34	1.79	1.74
4	B	413	KKK	C25-N4	2.34	1.43	1.35
2	B	404	HEM	CMA-C3A	2.44	1.56	1.51
3	B	405	FAD	C2A-N1A	2.62	1.38	1.33
3	A	405	FAD	C2A-N1A	2.68	1.39	1.33
3	A	405	FAD	C10-N1	2.68	1.40	1.35
2	B	404	HEM	C3C-CAC	2.74	1.56	1.51
2	B	404	HEM	CAA-C2A	2.77	1.56	1.52
3	B	405	FAD	C4-N3	2.87	1.38	1.33
2	A	404	HEM	FE-NC	3.13	2.08	1.95
3	B	405	FAD	C2A-N3A	3.35	1.38	1.32
2	B	404	HEM	FE-ND	3.53	2.16	1.97
3	B	405	FAD	C4X-N5	3.68	1.39	1.33
4	A	413	KKK	C4-C5	3.76	1.56	1.52
4	B	413	KKK	C9-CL2	3.80	1.82	1.73
2	B	404	HEM	C1C-NC	3.82	1.40	1.36
3	A	405	FAD	C2A-N3A	3.87	1.39	1.32
3	B	405	FAD	C1'-N10	4.10	1.52	1.48
2	B	404	HEM	FE-NB	4.23	2.19	1.97
3	A	405	FAD	C4X-N5	4.94	1.41	1.33
4	B	413	KKK	C4-C5	5.85	1.58	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	413	KKK	C13-C8-C5	-15.06	111.58	119.13
3	A	405	FAD	N3A-C2A-N1A	-11.86	119.81	128.89
5	A	416	DGG	C39-C30-C29	-10.90	44.76	59.49
3	B	405	FAD	N3A-C2A-N1A	-10.89	120.56	128.89
5	A	416	DGG	C39-C29-C30	-10.83	44.86	59.49
2	B	404	HEM	CBA-CAA-C2A	-6.59	100.72	112.53
4	A	413	KKK	C13-C8-C5	-6.54	115.85	119.13
4	A	413	KKK	C23-N4-C25	-5.22	109.10	122.92
2	A	404	HEM	CBA-CAA-C2A	-4.70	104.10	112.53
4	A	413	KKK	C22-N4-C25	-4.55	110.87	122.92
4	A	413	KKK	C24-N3-C18	-4.54	105.74	117.92
4	B	413	KKK	C22-N4-C25	-4.48	111.05	122.92
4	A	413	KKK	C19-C18-N3	-4.36	115.51	121.38
4	B	413	KKK	C10-C9-C8	-3.95	116.88	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	HEM	CBD-CAD-C3D	-3.94	102.10	113.55
2	B	404	HEM	C3C-CAC-CBC	-3.86	118.54	124.46
3	B	405	FAD	C4X-C4-N3	-3.76	118.45	123.59
3	A	405	FAD	P-O3P-PA	-3.50	122.89	132.73
4	B	413	KKK	C21-N3-C18	-3.45	108.67	117.92
4	A	413	KKK	O2-C5-O1	-3.39	103.68	106.13
4	B	413	KKK	C23-N4-C25	-3.33	114.09	122.92
4	B	413	KKK	C23-N4-C22	-3.14	106.73	112.56
4	A	413	KKK	O3-C14-C6	-2.83	101.22	108.17
4	A	413	KKK	O4-C25-N4	-2.67	117.24	121.03
2	A	404	HEM	CBD-CAD-C3D	-2.56	106.09	113.55
2	A	404	HEM	CMA-C3A-C4A	-2.49	124.24	128.36
4	A	413	KKK	C21-N3-C18	-2.39	111.52	117.92
4	A	413	KKK	O1-C6-C14	-2.33	105.51	109.49
3	A	405	FAD	C2B-C1B-N9A	-2.22	110.91	114.29
2	A	404	HEM	CAA-C2A-C1A	-2.15	124.67	127.01
3	B	405	FAD	C1B-N9A-C4A	-2.08	123.80	126.94
3	B	405	FAD	P-O3P-PA	-2.07	126.91	132.73
4	B	413	KKK	C24-N3-C18	-2.07	112.38	117.92
3	A	405	FAD	C1'-C2'-C3'	2.05	115.68	109.82
4	B	413	KKK	C9-C10-C11	2.15	121.09	118.69
3	B	405	FAD	C5X-C9A-N10	2.20	119.29	117.62
3	A	405	FAD	C6-C5X-C9A	2.20	121.88	118.98
4	B	413	KKK	O3-C14-C6	2.23	113.64	108.17
4	A	413	KKK	C13-C8-C9	2.36	119.74	116.72
2	B	404	HEM	C2D-C3D-C4D	2.44	105.64	101.50
2	A	404	HEM	C4B-CHC-C1C	2.47	129.94	125.82
3	A	405	FAD	C4X-N5-C5X	2.60	119.75	116.76
3	B	405	FAD	C4B-O4B-C1B	2.90	112.90	109.72
2	B	404	HEM	CAA-CBA-CGA	2.90	118.07	112.75
2	A	404	HEM	CMD-C2D-C3D	2.92	127.28	114.35
4	A	413	KKK	O2-C5-C4	3.04	114.14	109.48
4	A	413	KKK	C14-O3-C15	3.06	124.47	117.89
3	A	405	FAD	C5X-C9A-N10	3.27	120.10	117.62
2	B	404	HEM	CAD-C3D-C4D	3.30	124.10	112.47
2	B	404	HEM	CMC-C2C-C3C	3.33	124.83	116.53
3	A	405	FAD	C1'-N10-C9A	3.42	122.70	118.86
3	B	405	FAD	C1'-N10-C9A	3.44	122.73	118.86
4	B	413	KKK	C5-O1-C6	3.51	112.16	107.66
2	B	404	HEM	CMD-C2D-C3D	3.55	130.04	114.35
4	A	413	KKK	O2-C5-C8	3.60	116.79	111.62
4	B	413	KKK	C8-C9-CL2	3.75	126.82	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	413	KKK	C13-C8-C9	4.02	121.87	116.72
2	A	404	HEM	CAD-C3D-C4D	4.27	127.54	112.47
3	B	405	FAD	C4X-C10-N10	4.46	123.15	120.52
2	B	404	HEM	C3B-C4B-CHC	4.92	130.10	123.16
2	A	404	HEM	CAD-C3D-C2D	5.05	127.72	113.22
3	A	405	FAD	C4-N3-C2	5.47	119.97	115.25
2	A	404	HEM	CMC-C2C-C3C	5.54	130.36	116.53
2	B	404	HEM	CAD-C3D-C2D	5.88	130.11	113.22
2	A	404	HEM	CMB-C2B-C3B	5.91	131.29	116.53
2	B	404	HEM	CMB-C2B-C3B	6.61	133.03	116.53
3	B	405	FAD	C4-N3-C2	7.04	121.33	115.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	413	KKK	C5
4	A	413	KKK	C6
4	B	413	KKK	C5
4	B	413	KKK	C6

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	413	KKK	O2-C5-C4-N1
4	B	413	KKK	O2-C5-C4-N1

There are no ring outliers.

7 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	HEM	5	0
3	A	405	FAD	4	0
4	A	413	KKK	6	0
5	A	416	DGG	11	0
2	B	404	HEM	3	0
3	B	405	FAD	1	0
4	B	413	KKK	13	0

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	403/403 (100%)	0.61	44 (10%) 7 11	29, 54, 105, 198	0
1	B	403/403 (100%)	1.13	92 (22%) 1 1	26, 57, 126, 174	0
All	All	806/806 (100%)	0.87	136 (16%) 2 3	26, 55, 117, 198	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	PHE	13.5
1	B	339	GLN	9.7
1	A	395	VAL	9.7
1	B	403	GLU	9.2
1	B	401	PHE	8.6
1	A	396	PHE	8.6
1	A	398	PRO	8.4
1	B	338	VAL	7.9
1	B	319	LYS	7.3
1	A	402	ALA	7.3
1	B	399	ASP	7.2
1	B	341	ARG	6.9
1	B	343	TYR	6.8
1	B	393	TYR	6.2
1	B	381	LEU	6.1
1	B	293	PRO	6.0
1	A	400	LEU	6.0
1	B	263	VAL	5.8
1	B	397	GLY	5.8
1	B	288	ALA	5.8
1	B	340	GLY	5.8
1	A	266	LYS	5.8
1	A	292	PRO	5.6
1	B	321	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	397	GLY	5.3
1	B	73	SER	5.3
1	B	356	LYS	5.2
1	B	391	ILE	5.2
1	A	228	GLY	5.1
1	A	362	ASP	4.8
1	B	292	PRO	4.8
1	B	387	HIS	4.7
1	B	291	ALA	4.5
1	B	342	ASP	4.4
1	B	386	ILE	4.4
1	B	345	TYR	4.3
1	B	289	LEU	4.3
1	A	47	HIS	4.2
1	B	363	ALA	4.2
1	B	362	ASP	4.2
1	B	398	PRO	4.1
1	B	382	LYS	4.1
1	B	400	LEU	4.1
1	B	388	GLU	4.0
1	B	322	GLU	4.0
1	B	265	ALA	4.0
1	A	399	ASP	3.9
1	B	375	ARG	3.9
1	A	282	VAL	3.8
1	A	291	ALA	3.8
1	B	306	ALA	3.8
1	A	167	ASP	3.8
1	B	264	ASP	3.8
1	B	320	THR	3.7
1	B	335	PRO	3.6
1	B	333	PRO	3.5
1	A	230	PRO	3.5
1	B	359	LEU	3.5
1	B	72	ASN	3.5
1	B	296	VAL	3.5
1	B	361	PRO	3.4
1	B	376	MET	3.4
1	B	346	PRO	3.4
1	A	279	THR	3.4
1	B	269	ILE	3.4
1	B	290	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	3.3
1	B	390	ARG	3.3
1	B	380	ALA	3.3
1	B	389	ALA	3.3
1	B	66	GLU	3.3
1	B	347	GLY	3.2
1	B	357	SER	3.2
1	B	295	GLN	3.1
1	B	353	GLN	3.1
1	B	337	ASP	3.1
1	B	396	PHE	3.0
1	B	56	ALA	2.9
1	B	304	ASN	2.9
1	B	298	PHE	2.9
1	A	112	ASN	2.9
1	B	268	PRO	2.8
1	B	402	ALA	2.8
1	B	148	PRO	2.8
1	A	264	ASP	2.8
1	B	332	GLN	2.8
1	A	210	LEU	2.8
1	A	375	ARG	2.8
1	A	280	PRO	2.8
1	B	55	GLN	2.7
1	B	229	GLY	2.5
1	B	177	ALA	2.5
1	A	231	GLN	2.5
1	A	48	GLN	2.5
1	B	323	ASN	2.5
1	B	287	VAL	2.5
1	A	278	LEU	2.4
1	B	262	ASP	2.4
1	B	217[A]	ARG	2.4
1	A	229	GLY	2.4
1	A	293	PRO	2.4
1	B	1	MET	2.4
1	A	211	SER	2.4
1	A	394	GLU	2.4
1	B	318	ALA	2.4
1	B	271	LEU	2.3
1	A	208	TYR	2.3
1	B	305	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	ARG	2.3
1	B	297	VAL	2.3
1	B	352	LYS	2.3
1	B	127	GLY	2.3
1	B	330	TYR	2.2
1	A	322	GLU	2.2
1	A	303	ARG	2.2
1	A	284	MET	2.2
1	B	307	VAL	2.2
1	A	209	SER	2.2
1	B	312	ASP	2.2
1	B	314	LEU	2.1
1	B	379	ASP	2.1
1	A	306	ALA	2.1
1	A	283	SER	2.1
1	A	361	PRO	2.1
1	B	395	VAL	2.1
1	A	232	PRO	2.1
1	A	320	THR	2.1
1	B	53	GLN	2.1
1	B	373	PHE	2.0
1	A	316	GLU	2.0
1	B	276	VAL	2.0
1	B	123	ALA	2.0
1	B	384	LEU	2.0
1	A	333	PRO	2.0
1	A	390	ARG	2.0
1	B	143	ARG	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	DGG	A	416	19/50	0.74	0.29	1.49	44,55,96,100	0
4	KKK	B	413	36/36	0.92	0.28	0.46	32,108,265,275	0
4	KKK	A	413	36/36	0.91	0.23	0.01	36,62,124,132	0
2	HEM	A	404	43/43	0.98	0.17	-0.40	22,29,62,69	0
2	HEM	B	404	43/43	0.98	0.14	-0.62	22,29,48,76	0
3	FAD	B	405	53/53	0.96	0.14	-0.64	26,33,60,64	0
3	FAD	A	405	53/53	0.96	0.12	-0.86	22,36,82,90	0
6	PO4	A	406	5/5	0.94	0.11	-1.13	46,65,72,75	0

6.5 Other polymers

There are no such residues in this entry.