Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:26 AM GMT

PDB ID	:	3OZV
Title	:	The Crystal Structure of flavohemoglobin from R. eutrophus in complex with econazole
Authors	:	El Hammi, E.; Warkentin, E.; Demmer, U.; Ermler, U.; Baciou, L.
Deposited on	:	2010-09-27
Resolution	:	2.40 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:

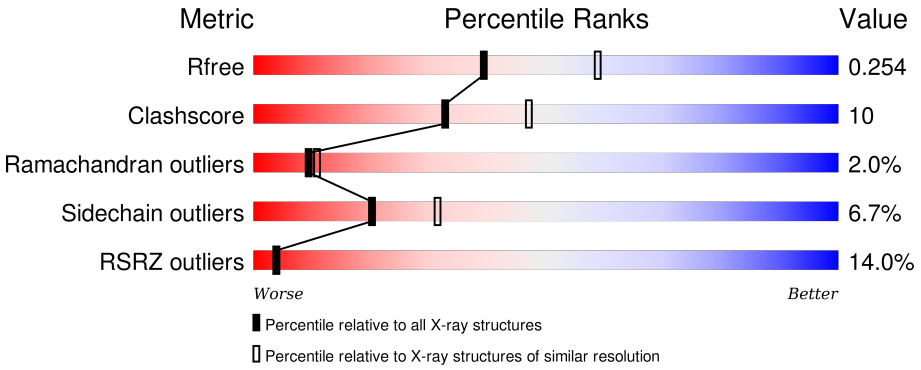
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	6% 81% 15%
1	B	403	22% 79% 19%

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	DGG	B	406	-	-	-	X
5	ECN	A	411	X	-	X	-
5	ECN	B	411	X	-	X	-

2 Entry composition

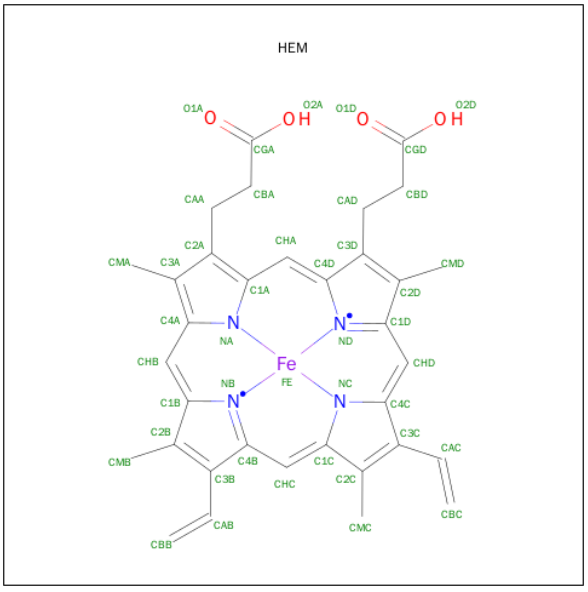
There are 7 unique types of molecules in this entry. The entry contains 6722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

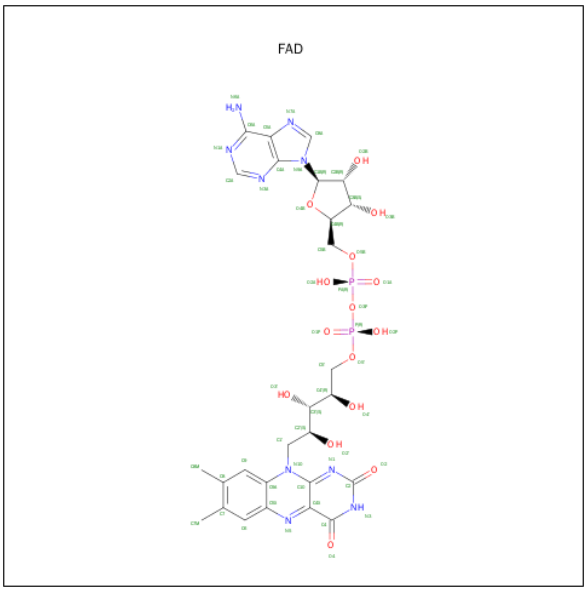
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	403	Total	C	N	O	S	0	1	0
			3162	2015	543	590	14			
1	A	403	Total	C	N	O	S	0	0	0
			3156	2011	543	588	14			

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



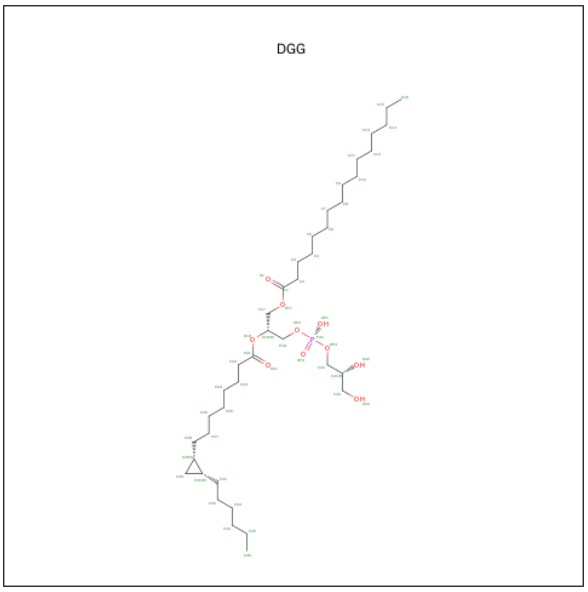
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 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
4	B	1	Total	C	O	0	0
			19	17	2		

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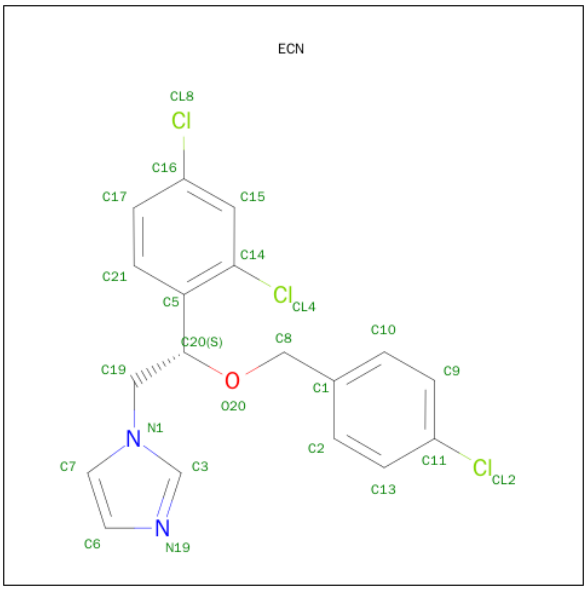
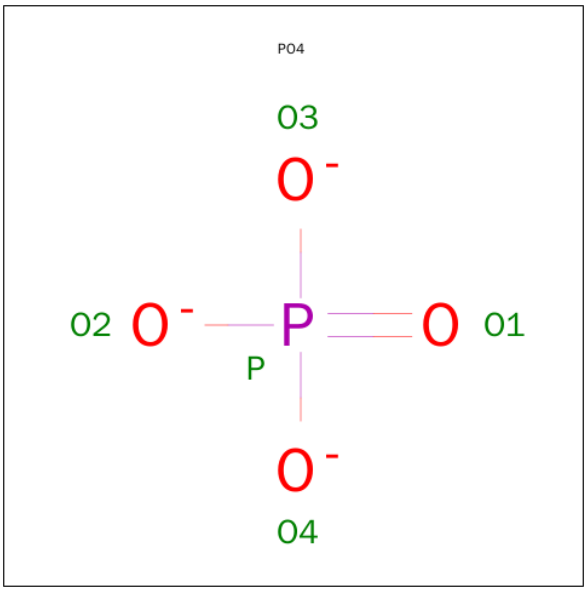
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 19 17 2	0	0

- Molecule 5 is 1-[(2S)-2-[(4-CHLOROBENZYL)OXY]-2-(2,4-DICHLOROPHENYL)ETHYL]-1H-IMIDAZOLE (three-letter code: ECN) (formula: $C_{18}H_{15}Cl_3N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C Cl N O 24 18 3 2 1	0	0
5	A	1	Total C Cl N O 24 18 3 2 1	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 5 4 1	0	0

- Molecule 7 is water.

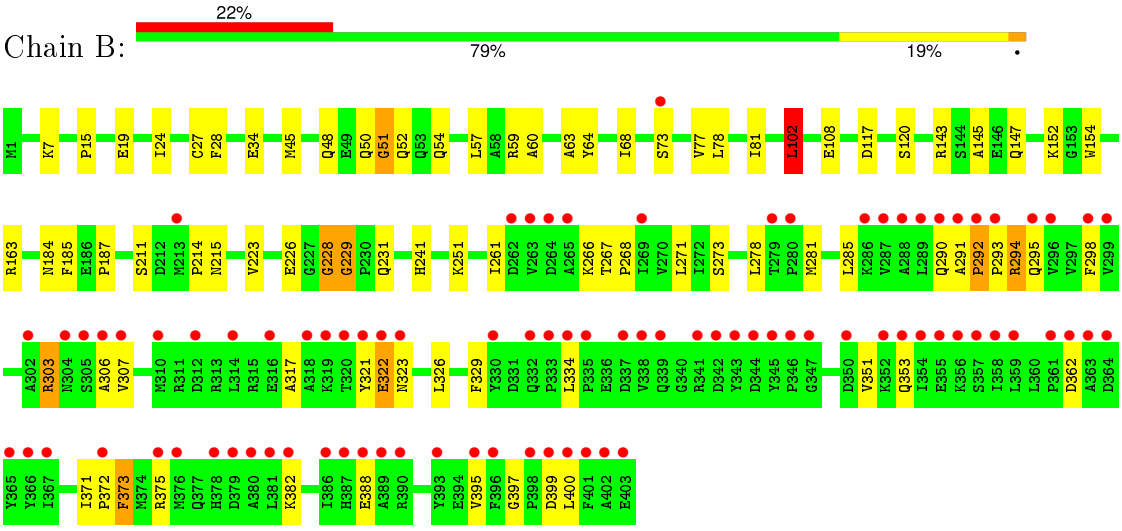
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	58	Total O 58 58	0	0
7	A	63	Total O 63 63	0	0

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 (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.

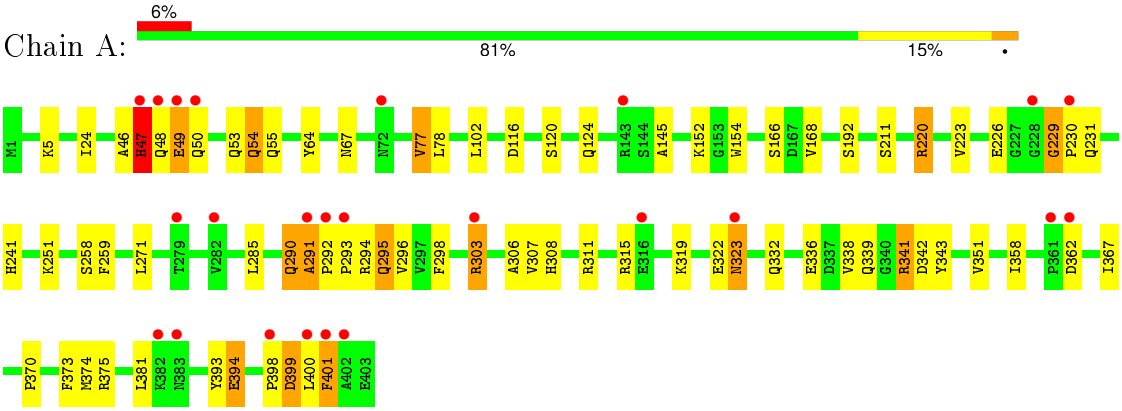
- Molecule 1: Flavohemoglobin

Chain B:



- Molecule 1: Flavohemoglobin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.22Å 87.22Å 291.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.40) 99.1 (29.13-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.210 , 0.248 0.227 , 0.254	Depositor DCC
R_{free} test set	2269 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 44752 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6722	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ECN, PO4, DGG, FAD, 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	0.63	0/3233	0.71	0/4393
1	B	0.64	0/3242	0.70	2/4405 (0.0%)
All	All	0.64	0/6475	0.71	2/8798 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	228	GLY	N-CA-C	-5.17	100.17	113.10

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	60	0
1	B	3162	0	3118	52	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	53	0	31	4	0
3	B	53	0	31	0	0
4	A	19	0	31	6	0
4	B	19	0	31	6	0
5	A	24	0	15	15	0
5	B	24	0	15	18	0
6	A	5	0	0	0	0
7	A	63	0	0	0	0
7	B	58	0	0	0	0
All	All	6722	0	6444	135	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 10.

All (135) 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:24:ILE:HG22	5:B:411:ECN:CL2	1.41	1.57
5:A:411:ECN:H10	5:A:411:ECN:C20	1.70	1.21
1:B:24:ILE:CG2	5:B:411:ECN:CL2	2.26	1.19
5:A:411:ECN:C10	5:A:411:ECN:H20	1.53	1.16
5:B:411:ECN:C10	5:B:411:ECN:H20	1.38	1.15
1:A:399:ASP:HA	1:A:400:LEU:HB2	1.28	1.13
1:A:24:ILE:HG21	5:A:411:ECN:CL2	1.85	1.13
5:B:411:ECN:C10	5:B:411:ECN:C20	2.27	1.12
4:A:406:DGG:H352	5:A:411:ECN:H2	1.30	1.11
1:B:77:VAL:HG11	4:B:406:DGG:H241	1.21	1.11
5:B:411:ECN:C20	5:B:411:ECN:H10	1.81	1.10
5:B:411:ECN:H10	5:B:411:ECN:H20	1.18	1.08
1:A:341:ARG:HG2	1:A:341:ARG:HH21	1.21	1.01
1:A:220:ARG:HH21	1:A:220:ARG:HG2	1.32	0.94
1:B:102:LEU:HD13	5:B:411:ECN:C9	2.04	0.87
4:B:406:DGG:H341	5:B:411:ECN:H8C2	1.56	0.85
1:B:371:ILE:HD11	1:B:395:VAL:HG13	1.58	0.84
1:B:63:ALA:HB1	4:B:406:DGG:H242	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:411:ECN:C19	5:B:411:ECN:H10	2.09	0.82
1:A:54:GLN:HE21	1:A:55:GLN:NE2	1.78	0.81
4:A:406:DGG:H352	5:A:411:ECN:C2	2.09	0.81
1:A:398:PRO:O	1:A:399:ASP:HB2	1.82	0.80
1:A:48:GLN:N	1:A:49:GLU:HA	1.95	0.79
1:B:77:VAL:CG1	4:B:406:DGG:H241	2.09	0.78
1:B:371:ILE:HD11	1:B:395:VAL:CG1	2.12	0.78
5:A:411:ECN:H20	5:A:411:ECN:H10	0.79	0.76
1:A:399:ASP:CA	1:A:400:LEU:HB2	2.12	0.75
5:A:411:ECN:C10	5:A:411:ECN:C20	2.41	0.74
5:A:411:ECN:CL4	5:A:411:ECN:H10	2.26	0.72
1:B:59:ARG:HG3	1:B:59:ARG:HH21	1.55	0.71
1:B:102:LEU:HD13	5:B:411:ECN:C11	2.21	0.70
1:A:211:SER:OG	1:A:220:ARG:NH2	2.26	0.69
1:B:57:LEU:HD11	5:B:411:ECN:H2	1.75	0.68
1:A:374:MET:CE	1:A:393:TYR:HB2	2.24	0.67
1:A:399:ASP:HB3	1:A:401:PHE:N	2.10	0.67
1:A:102:LEU:HD11	5:A:411:ECN:C9	2.25	0.66
1:A:54:GLN:NE2	1:A:55:GLN:NE2	2.43	0.66
4:A:406:DGG:C35	5:A:411:ECN:H2	2.18	0.65
1:A:341:ARG:NH2	1:A:342:ASP:OD1	2.29	0.65
1:B:295:GLN:HB2	1:B:323:ASN:O	1.96	0.64
1:A:220:ARG:NH2	1:A:220:ARG:HG2	2.06	0.64
1:A:303:ARG:HB3	1:A:307:VAL:HG11	1.79	0.64
1:A:341:ARG:HG2	1:A:341:ARG:NH2	1.95	0.63
1:A:24:ILE:CG2	5:A:411:ECN:CL2	2.75	0.63
1:A:47:HIS:CD2	1:A:53:GLN:OE1	2.51	0.62
1:A:399:ASP:HA	1:A:400:LEU:CB	2.16	0.62
1:A:226:GLU:HG2	3:A:405:FAD:O3B	2.00	0.62
1:B:63:ALA:HB1	4:B:406:DGG:C24	2.29	0.62
1:B:77:VAL:HG21	4:B:406:DGG:H261	1.81	0.61
1:A:54:GLN:HE21	1:A:55:GLN:HE21	1.46	0.61
1:B:102:LEU:HD22	5:B:411:ECN:C10	2.30	0.60
1:A:67:ASN:ND2	4:A:406:DGG:H232	2.16	0.60
1:A:398:PRO:O	1:A:399:ASP:CB	2.50	0.60
1:B:59:ARG:HD3	1:B:400:LEU:O	2.03	0.59
1:A:168:VAL:CG2	1:A:307:VAL:HG23	2.32	0.58
2:A:404:HEM:HMB2	2:A:404:HEM:HBB2	1.85	0.58
1:A:120:SER:O	1:A:124:GLN:HG3	2.04	0.58
1:B:329:PHE:HE1	1:B:353:GLN:HE22	1.52	0.58
1:A:48:GLN:N	1:A:49:GLU:CA	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:MET:O	1:B:48:GLN:HB2	2.04	0.57
1:A:211:SER:OG	1:A:220:ARG:HG2	2.05	0.57
1:B:223:VAL:O	1:B:241:HIS:HE1	1.86	0.57
1:B:64:TYR:CZ	1:B:68:ILE:HD12	2.40	0.56
1:B:27:CYS:SG	1:B:108:GLU:OE2	2.63	0.56
1:B:372:PRO:O	1:B:373:PHE:HB2	2.06	0.56
2:A:404:HEM:NB	5:A:411:ECN:H3	2.21	0.56
1:A:168:VAL:HG22	1:A:307:VAL:HG23	1.88	0.55
1:B:102:LEU:HD22	5:B:411:ECN:H10	1.89	0.55
2:B:404:HEM:HBB2	2:B:404:HEM:HMB2	1.89	0.55
1:A:293:PRO:N	1:A:294:ARG:HA	2.22	0.55
1:A:229:GLY:O	1:A:231:GLN:N	2.41	0.53
1:A:154:TRP:HB3	1:A:251:LYS:HB3	1.91	0.53
1:B:143:ARG:O	1:B:147:GLN:HG3	2.07	0.53
1:B:397:GLY:O	1:B:399:ASP:OD1	2.27	0.53
1:A:303:ARG:HB3	1:A:307:VAL:CG1	2.39	0.52
1:A:290:GLN:O	1:A:291:ALA:HB3	2.10	0.51
1:B:102:LEU:HD13	5:B:411:ECN:C10	2.41	0.51
1:B:291:ALA:HA	1:B:292:PRO:C	2.31	0.51
1:B:15:PRO:HG3	3:A:405:FAD:C2A	2.41	0.51
1:B:185:PHE:CE2	1:B:214:PRO:HA	2.46	0.51
1:A:285:LEU:HD12	1:A:296:VAL:HG11	1.91	0.51
1:B:371:ILE:CD1	1:B:395:VAL:HG13	2.36	0.50
2:A:404:HEM:CMB	2:A:404:HEM:HBB2	2.42	0.50
1:A:351:VAL:HG22	1:A:358:ILE:HG12	1.92	0.50
1:A:367:ILE:HG22	1:A:374:MET:HG2	1.93	0.50
1:B:28:PHE:HB2	5:B:411:ECN:CL2	2.49	0.49
1:A:285:LEU:HD13	1:A:298:PHE:CD1	2.48	0.49
1:B:382:LYS:HE3	1:B:388:GLU:OE1	2.13	0.49
1:A:77:VAL:CG2	4:A:406:DGG:H271	2.44	0.48
1:B:371:ILE:HD11	1:B:395:VAL:HG11	1.95	0.47
2:B:404:HEM:HHD	2:B:404:HEM:HBC2	1.96	0.47
1:B:145:ALA:HB2	1:B:152:LYS:HG3	1.96	0.47
5:B:411:ECN:C9	5:B:411:ECN:CL4	3.00	0.47
2:B:404:HEM:CMB	2:B:404:HEM:HBB2	2.45	0.47
2:A:404:HEM:C4B	5:A:411:ECN:H3	2.50	0.47
1:A:339:GLN:HB3	1:A:343:TYR:CZ	2.50	0.47
1:B:154:TRP:HB3	1:B:251:LYS:HB3	1.97	0.46
1:B:321:TYR:O	1:B:322:GLU:CB	2.64	0.46
1:A:370:PRO:O	1:A:373:PHE:HB3	2.16	0.46
1:B:329:PHE:HE1	1:B:353:GLN:NE2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLY:O	1:B:229:GLY:C	2.54	0.46
2:B:404:HEM:NB	5:B:411:ECN:H3	2.30	0.46
1:B:7:LYS:HG2	1:B:68:ILE:HG12	1.97	0.46
1:B:268:PRO:HA	1:B:294:ARG:HG3	1.98	0.45
1:B:60:ALA:HB2	1:B:400:LEU:HD13	1.99	0.45
1:A:24:ILE:HD13	5:A:411:ECN:CL2	2.54	0.45
1:B:298:PHE:HB3	1:B:326:LEU:HD12	1.99	0.44
1:A:64:TYR:HB2	4:A:406:DGG:H281	2.00	0.44
1:A:374:MET:HE3	1:A:393:TYR:HB2	1.97	0.44
1:A:294:ARG:O	1:A:295:GLN:HB2	2.18	0.44
1:A:102:LEU:HD11	5:A:411:ECN:C11	2.48	0.43
1:B:59:ARG:NH2	1:B:59:ARG:HG3	2.28	0.43
1:A:145:ALA:HB2	1:A:152:LYS:HG3	2.00	0.43
1:A:47:HIS:HD2	1:A:53:GLN:OE1	1.98	0.43
1:B:303:ARG:HB3	1:B:307:VAL:HG21	1.99	0.43
1:A:46:ALA:C	1:A:48:GLN:H	2.22	0.43
1:A:223:VAL:O	1:A:241:HIS:HE1	2.01	0.43
1:B:317:ALA:O	1:B:321:TYR:HD2	2.02	0.42
1:A:166:SER:HB2	1:A:306:ALA:O	2.19	0.42
1:A:168:VAL:HG21	1:A:307:VAL:HG23	2.01	0.42
1:B:273:SER:HB3	1:B:281:MET:HG3	2.02	0.42
1:B:78:LEU:HD23	1:B:81:ILE:HD12	2.01	0.42
1:B:163:ARG:HB3	1:B:163:ARG:HE	1.72	0.42
1:A:292:PRO:HA	1:A:293:PRO:HA	1.73	0.41
1:A:308:HIS:CE1	1:A:311:ARG:HG3	2.55	0.41
1:B:57:LEU:HD11	5:B:411:ECN:C2	2.46	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.93	0.41
1:A:259:PHE:CG	1:A:394:GLU:HB2	2.55	0.41
1:B:50:GLN:O	1:B:51:GLY:C	2.60	0.41
1:A:323:ASN:ND2	1:A:323:ASN:H	2.18	0.41
1:B:187:PRO:HG2	1:B:261:ILE:HD11	2.02	0.40
1:A:48:GLN:H	1:A:49:GLU:HA	1.83	0.40
1:B:306:ALA:HB2	1:B:334:LEU:HD11	2.03	0.40
1:A:48:GLN:HG2	3:A:405:FAD:C4A	2.51	0.40
1:A:226:GLU:CG	3:A:405:FAD:O3B	2.68	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	401/403 (100%)	379 (94%)	15 (4%)	7 (2%)	11 14
1	B	402/403 (100%)	382 (95%)	11 (3%)	9 (2%)	8 9
All	All	803/806 (100%)	761 (95%)	26 (3%)	16 (2%)	9 11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	PRO
1	B	373	PHE
1	A	47	HIS
1	A	230	PRO
1	B	51	GLY
1	B	52	GLN
1	B	215	ASN
1	B	229	GLY
1	A	295	GLN
1	A	399	ASP
1	B	184	ASN
1	B	322	GLU
1	A	50	GLN
1	A	291	ALA
1	A	229	GLY
1	B	292	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%)	309 (92%)	25 (8%)	17 26
1	B	335/334 (100%)	314 (94%)	21 (6%)	22 35
All	All	669/668 (100%)	623 (93%)	46 (7%)	20 30

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19[A]	GLU
1	B	19[B]	GLU
1	B	34	GLU
1	B	54	GLN
1	B	73	SER
1	B	102	LEU
1	B	117	ASP
1	B	120	SER
1	B	211	SER
1	B	231	GLN
1	B	266	LYS
1	B	267	THR
1	B	271	LEU
1	B	278	LEU
1	B	285	LEU
1	B	290	GLN
1	B	294	ARG
1	B	303	ARG
1	B	351	VAL
1	B	362	ASP
1	B	375	ARG
1	A	5	LYS
1	A	47	HIS
1	A	49	GLU
1	A	54	GLN
1	A	77	VAL
1	A	116	ASP
1	A	192	SER
1	A	220	ARG
1	A	258	SER
1	A	271	LEU
1	A	290	GLN
1	A	303	ARG
1	A	315	ARG
1	A	319	LYS

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Mol	Chain	Res	Type
1	A	322	GLU
1	A	323	ASN
1	A	332	GLN
1	A	336	GLU
1	A	338	VAL
1	A	341	ARG
1	A	362	ASP
1	A	375	ARG
1	A	381	LEU
1	A	394	GLU
1	A	401	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	47	HIS
1	B	50	GLN
1	B	53	GLN
1	B	67	ASN
1	B	231	GLN
1	B	241	HIS
1	B	339	GLN
1	B	353	GLN
1	B	392	HIS
1	A	47	HIS
1	A	55	GLN
1	A	241	HIS
1	A	290	GLN
1	A	339	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	HEM	A	404	1,5	30,50,50	2.35	7 (23%)	24,82,82	2.75	9 (37%)
3	FAD	A	405	-	48,58,58	1.43	5 (10%)	54,89,89	2.14	10 (18%)
4	DGG	A	406	-	15,19,50	0.46	0	14,22,59	0.58	0
6	PO4	A	407	-	4,4,4	0.34	0	6,6,6	0.28	0
5	ECN	A	411	2	24,26,26	1.46	4 (16%)	31,35,35	2.67	11 (35%)
2	HEM	B	404	1,5	30,50,50	2.17	7 (23%)	24,82,82	2.72	8 (33%)
3	FAD	B	405	-	48,58,58	1.45	6 (12%)	54,89,89	2.43	10 (18%)
4	DGG	B	406	-	15,19,50	0.54	0	14,22,59	0.55	0
5	ECN	B	411	2	24,26,26	1.15	1 (4%)	31,35,35	2.07	7 (22%)

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	1,5	-	0/10/54/54	0/0/8/8
3	FAD	A	405	-	-	0/30/50/50	0/6/6/6
4	DGG	A	406	-	-	0/14/21/59	0/0/1/1
6	PO4	A	407	-	-	0/0/0/0	0/0/0/0
5	ECN	A	411	2	1/1/1/1	0/13/13/13	0/3/3/3
2	HEM	B	404	1,5	-	0/10/54/54	0/0/8/8
3	FAD	B	405	-	-	0/30/50/50	0/6/6/6
4	DGG	B	406	-	-	0/14/21/59	0/0/1/1
5	ECN	B	411	2	1/1/1/1	0/13/13/13	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	HEM	C3B-C4B	-9.02	1.43	1.51
2	B	404	HEM	C3B-C4B	-7.06	1.45	1.51
2	A	404	HEM	C3D-C4D	-5.28	1.44	1.51
2	B	404	HEM	C2C-C1C	-4.29	1.44	1.52
2	A	404	HEM	C2C-C1C	-4.02	1.45	1.52
2	B	404	HEM	C3D-C4D	-3.72	1.46	1.51
2	A	404	HEM	C2B-C1B	-2.46	1.43	1.51
2	A	404	HEM	C2D-C1D	-2.02	1.45	1.51
2	B	404	HEM	C1C-NC	2.05	1.38	1.36
3	B	405	FAD	C5X-N5	2.12	1.38	1.35
2	B	404	HEM	C3C-CAC	2.21	1.55	1.51
2	B	404	HEM	FE-NB	2.40	2.10	1.97
3	B	405	FAD	C2A-N1A	2.49	1.38	1.33
5	A	411	ECN	C15-C14	2.53	1.42	1.38
5	A	411	ECN	C15-C16	2.56	1.42	1.38
2	A	404	HEM	FE-NC	2.57	2.05	1.95
3	A	405	FAD	C4-N3	2.60	1.37	1.33
2	A	404	HEM	C3B-CAB	2.61	1.56	1.51
3	A	405	FAD	C2A-N1A	2.72	1.39	1.33
3	A	405	FAD	C5X-N5	2.96	1.40	1.35
3	B	405	FAD	C2A-N3A	3.09	1.37	1.32
3	B	405	FAD	C4-N3	3.32	1.39	1.33
5	B	411	ECN	C14-CL4	3.33	1.81	1.73
5	A	411	ECN	C16-CL8	3.38	1.82	1.74
2	B	404	HEM	FE-ND	3.42	2.15	1.97
3	B	405	FAD	C4X-N5	3.66	1.39	1.33
5	A	411	ECN	C14-CL4	3.78	1.82	1.73
3	A	405	FAD	C2A-N3A	4.16	1.39	1.32
3	A	405	FAD	C4X-N5	4.84	1.40	1.33
3	B	405	FAD	C1'-N10	5.46	1.54	1.48

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	405	FAD	N3A-C2A-N1A	-12.53	119.30	128.89
3	A	405	FAD	N3A-C2A-N1A	-11.22	120.30	128.89
5	A	411	ECN	O20-C20-C5	-7.30	101.35	112.41
2	B	404	HEM	CBA-CAA-C2A	-6.16	101.48	112.53
2	A	404	HEM	CBA-CAA-C2A	-5.33	102.97	112.53
5	A	411	ECN	C5-C14-CL4	-5.19	114.70	120.42
5	B	411	ECN	O20-C20-C5	-3.76	106.72	112.41
5	B	411	ECN	C14-C5-C20	-3.43	117.84	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	405	FAD	P-O3P-PA	-3.38	123.23	132.73
5	B	411	ECN	C15-C14-C5	-3.23	118.28	122.46
3	B	405	FAD	C4X-C4-N3	-3.20	119.22	123.59
5	A	411	ECN	C15-C14-C5	-3.15	118.37	122.46
2	A	404	HEM	CAA-C2A-C1A	-3.00	123.75	127.01
2	A	404	HEM	C3B-CAB-CBB	-2.89	120.02	124.46
2	A	404	HEM	CMA-C3A-C4A	-2.70	123.90	128.36
2	B	404	HEM	C3B-CAB-CBB	-2.69	120.32	124.46
3	A	405	FAD	P-O3P-PA	-2.67	125.22	132.73
3	A	405	FAD	C4-C4X-C10	-2.61	118.27	119.94
5	A	411	ECN	C14-C5-C20	-2.60	118.89	122.20
5	B	411	ECN	C9-C11-CL2	-2.51	115.24	119.35
5	A	411	ECN	C17-C16-CL8	-2.39	115.43	119.35
3	B	405	FAD	C1B-N9A-C4A	-2.19	123.63	126.94
5	A	411	ECN	C8-C1-C2	-2.01	115.83	120.66
3	A	405	FAD	C5X-C9A-N10	2.25	119.33	117.62
3	A	405	FAD	C1'-C2'-C3'	2.35	116.55	109.82
3	B	405	FAD	C4X-N5-C5X	2.50	119.64	116.76
2	A	404	HEM	CMD-C2D-C3D	2.56	125.66	114.35
3	A	405	FAD	C4X-N5-C5X	2.61	119.77	116.76
3	B	405	FAD	C1'-C2'-C3'	2.63	117.33	109.82
5	A	411	ECN	O20-C8-C1	2.66	116.32	109.99
3	A	405	FAD	C4-C4X-N5	2.72	122.02	118.72
5	B	411	ECN	C13-C11-CL2	2.74	123.84	119.35
2	B	404	HEM	CMD-C2D-C3D	2.74	126.48	114.35
3	B	405	FAD	C4B-O4B-C1B	2.77	112.76	109.72
3	A	405	FAD	C4B-O4B-C1B	2.87	112.87	109.72
5	A	411	ECN	O20-C20-C19	2.95	113.65	106.40
3	A	405	FAD	C1'-N10-C9A	3.39	122.67	118.86
2	B	404	HEM	CMC-C2C-C3C	3.48	125.22	116.53
2	B	404	HEM	C3B-C4B-CHC	3.80	128.51	123.16
3	B	405	FAD	C5X-C9A-N10	3.85	120.54	117.62
3	B	405	FAD	C1'-N10-C9A	4.48	123.89	118.86
2	A	404	HEM	CAD-C3D-C4D	4.51	128.39	112.47
2	B	404	HEM	CAD-C3D-C4D	4.75	129.21	112.47
5	A	411	ECN	C21-C5-C14	4.80	121.97	116.79
2	B	404	HEM	CAD-C3D-C2D	4.83	127.10	113.22
5	B	411	ECN	O20-C20-C19	5.02	118.72	106.40
2	A	404	HEM	CAD-C3D-C2D	5.09	127.84	113.22
5	A	411	ECN	C15-C16-CL8	5.13	125.51	119.14
2	A	404	HEM	CMC-C2C-C3C	5.25	129.63	116.53
5	A	411	ECN	C15-C14-CL4	5.47	126.93	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	404	HEM	CMB-C2B-C3B	5.73	130.84	116.53
5	B	411	ECN	C21-C5-C14	5.77	123.02	116.79
3	A	405	FAD	C4-N3-C2	5.92	120.36	115.25
2	B	404	HEM	CMB-C2B-C3B	5.98	131.46	116.53
3	B	405	FAD	C4-N3-C2	6.58	120.93	115.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	411	ECN	C20
5	B	411	ECN	C20

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	HEM	4	0
3	A	405	FAD	4	0
4	A	406	DGG	6	0
5	A	411	ECN	15	0
2	B	404	HEM	4	0
4	B	406	DGG	6	0
5	B	411	ECN	18	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^{th} 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%)	0.21	24 (5%) 25 25	28, 55, 102, 170	0
1	B	403/403 (100%)	0.99	89 (22%) 1 1	27, 62, 145, 185	0
All	All	806/806 (100%)	0.60	113 (14%) 4 4	27, 57, 134, 185	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	ALA	10.6
1	B	292	PRO	9.8
1	A	292	PRO	8.0
1	B	381	LEU	7.9
1	B	293	PRO	7.4
1	B	335	PRO	6.5
1	A	293	PRO	6.4
1	B	386	ILE	6.1
1	B	319	LYS	6.1
1	B	334	LEU	6.1
1	B	321	TYR	6.0
1	B	402	ALA	5.7
1	B	380	ALA	5.6
1	A	400	LEU	5.6
1	B	362	ASP	5.6
1	B	320	THR	5.6
1	B	343	TYR	5.3
1	B	356	LYS	5.2
1	B	318	ALA	5.2
1	A	228	GLY	4.9
1	B	400	LEU	4.9
1	B	403	GLU	4.8
1	B	291	ALA	4.7
1	B	295	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	337	ASP	4.6
1	B	305	SER	4.6
1	B	263	VAL	4.6
1	B	341	ARG	4.5
1	B	269	ILE	4.5
1	B	287	VAL	4.5
1	B	289	LEU	4.5
1	A	230	PRO	4.4
1	B	379	ASP	4.3
1	B	339	GLN	4.2
1	B	352	LYS	4.2
1	B	399	ASP	4.1
1	B	322	GLU	4.1
1	B	389	ALA	4.0
1	B	288	ALA	4.0
1	B	290	GLN	4.0
1	B	347	GLY	3.9
1	B	265	ALA	3.9
1	A	401	PHE	3.9
1	B	332	GLN	3.8
1	B	357	SER	3.7
1	B	307	VAL	3.7
1	B	363	ALA	3.7
1	B	382	LYS	3.6
1	B	306	ALA	3.6
1	B	346	PRO	3.6
1	B	342	ASP	3.5
1	B	264	ASP	3.5
1	B	361	PRO	3.5
1	B	330	TYR	3.5
1	B	314	LEU	3.5
1	B	304	ASN	3.4
1	B	376	MET	3.4
1	A	362	ASP	3.4
1	B	350	ASP	3.4
1	B	387	HIS	3.4
1	B	354	ILE	3.3
1	B	262	ASP	3.3
1	B	388	GLU	3.3
1	B	296	VAL	3.2
1	B	390	ARG	3.2
1	A	382	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	333	PRO	3.1
1	B	372	PRO	2.9
1	B	355	GLU	2.9
1	B	393	TYR	2.9
1	B	323	ASN	2.9
1	B	401	PHE	2.8
1	A	279	THR	2.8
1	A	282	VAL	2.8
1	B	298	PHE	2.7
1	B	344	ASP	2.7
1	B	398	PRO	2.7
1	B	395	VAL	2.7
1	B	353	GLN	2.6
1	A	48	GLN	2.6
1	B	364	ASP	2.6
1	B	345	TYR	2.5
1	B	312	ASP	2.5
1	A	383	ASN	2.4
1	B	279	THR	2.4
1	B	73	SER	2.4
1	B	213	MET	2.4
1	B	378	HIS	2.4
1	B	302	ALA	2.3
1	A	398	PRO	2.3
1	B	396	PHE	2.3
1	A	47	HIS	2.3
1	B	280	PRO	2.3
1	B	375	ARG	2.3
1	A	72	ASN	2.3
1	B	299	VAL	2.3
1	B	366	TYR	2.2
1	A	50	GLN	2.2
1	A	143	ARG	2.2
1	B	286	LYS	2.2
1	B	338	VAL	2.2
1	A	316	GLU	2.2
1	B	358	ILE	2.2
1	B	316	GLU	2.2
1	A	49	GLU	2.2
1	A	323	ASN	2.2
1	A	291	ALA	2.2
1	B	359	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	310	MET	2.1
1	B	367	ILE	2.1
1	A	303	ARG	2.1
1	B	365	TYR	2.0
1	A	361	PRO	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^{th} 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
4	DGG	B	406	19/50	0.70	0.48	2.24	28,71,191,193	0
5	ECN	A	411	24/24	0.89	0.24	1.79	29,73,99,139	0
5	ECN	B	411	24/24	0.95	0.20	1.55	31,53,239,322	0
4	DGG	A	406	19/50	0.68	0.31	1.54	45,58,95,97	0
2	HEM	A	404	43/43	0.98	0.16	-0.34	21,29,66,82	0
2	HEM	B	404	43/43	0.98	0.15	-0.40	19,32,56,80	0
3	FAD	B	405	53/53	0.95	0.15	-0.64	24,35,55,63	0
3	FAD	A	405	53/53	0.96	0.13	-0.65	23,33,80,88	0
6	PO4	A	407	5/5	0.97	0.15	-0.85	58,70,73,88	0

6.5 Other polymers (i)

There are no such residues in this entry.