



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:22 PM GMT

PDB ID : 4EJH
Title : Human Cytochrome P450 2A13 in complex with 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2012-04-06
Resolution : 2.35 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

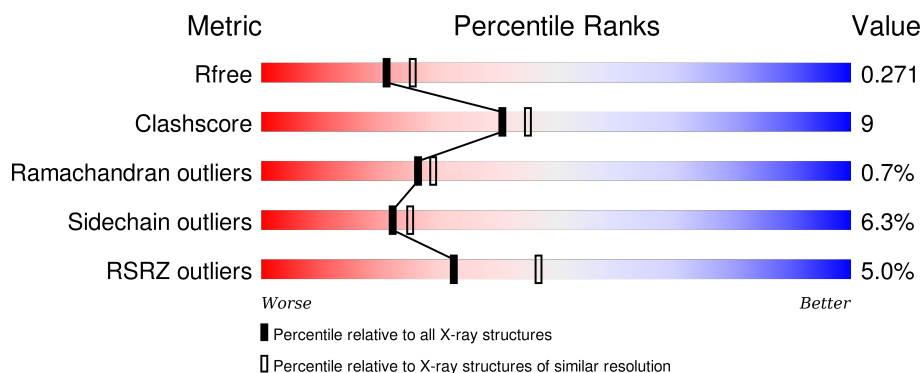
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	476	 82% 13% . .
1	B	476	 79% 17% . .
1	C	476	 82% 14% . .
1	D	476	 81% 15% . .
1	E	476	 3% 76% 20% . .

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Mol	Chain	Length	Quality of chain
1	F	476	
1	G	476	
1	H	476	

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
3	0QA	A	502	-	-	-	X
3	0QA	B	502	-	-	-	X
3	0QA	C	502	-	-	-	X
3	0QA	D	502	-	-	-	X
3	0QA	E	502	-	-	-	X
3	0QA	F	502	-	-	X	X
4	GOL	H	502	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30804 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 Cytochrome P450 2A13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	8	2	0
			3777	2430	653	676	18			
1	B	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	C	464	Total	C	N	O	S	0	2	0
			3776	2429	653	676	18			
1	D	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	E	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	F	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	G	463	Total	C	N	O	S	0	0	0
			3737	2404	642	673	18			
1	H	459	Total	C	N	O	S	0	1	0
			3723	2396	640	669	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	INITIATING METHIONINE	UNP Q16696
A	24	ALA	-	EXPRESSION TAG	UNP Q16696
A	25	LYS	-	EXPRESSION TAG	UNP Q16696
A	26	LYS	-	EXPRESSION TAG	UNP Q16696
A	27	THR	-	EXPRESSION TAG	UNP Q16696
A	28	SER	-	EXPRESSION TAG	UNP Q16696
A	29	SER	-	EXPRESSION TAG	UNP Q16696
A	30	LYS	-	EXPRESSION TAG	UNP Q16696
A	495	HIS	-	EXPRESSION TAG	UNP Q16696
A	496	HIS	-	EXPRESSION TAG	UNP Q16696
A	497	HIS	-	EXPRESSION TAG	UNP Q16696
A	498	HIS	-	EXPRESSION TAG	UNP Q16696
B	23	MET	-	INITIATING METHIONINE	UNP Q16696

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	-	EXPRESSION TAG	UNP Q16696
B	25	LYS	-	EXPRESSION TAG	UNP Q16696
B	26	LYS	-	EXPRESSION TAG	UNP Q16696
B	27	THR	-	EXPRESSION TAG	UNP Q16696
B	28	SER	-	EXPRESSION TAG	UNP Q16696
B	29	SER	-	EXPRESSION TAG	UNP Q16696
B	30	LYS	-	EXPRESSION TAG	UNP Q16696
B	495	HIS	-	EXPRESSION TAG	UNP Q16696
B	496	HIS	-	EXPRESSION TAG	UNP Q16696
B	497	HIS	-	EXPRESSION TAG	UNP Q16696
B	498	HIS	-	EXPRESSION TAG	UNP Q16696
C	23	MET	-	INITIATING METHIONINE	UNP Q16696
C	24	ALA	-	EXPRESSION TAG	UNP Q16696
C	25	LYS	-	EXPRESSION TAG	UNP Q16696
C	26	LYS	-	EXPRESSION TAG	UNP Q16696
C	27	THR	-	EXPRESSION TAG	UNP Q16696
C	28	SER	-	EXPRESSION TAG	UNP Q16696
C	29	SER	-	EXPRESSION TAG	UNP Q16696
C	30	LYS	-	EXPRESSION TAG	UNP Q16696
C	495	HIS	-	EXPRESSION TAG	UNP Q16696
C	496	HIS	-	EXPRESSION TAG	UNP Q16696
C	497	HIS	-	EXPRESSION TAG	UNP Q16696
C	498	HIS	-	EXPRESSION TAG	UNP Q16696
D	23	MET	-	INITIATING METHIONINE	UNP Q16696
D	24	ALA	-	EXPRESSION TAG	UNP Q16696
D	25	LYS	-	EXPRESSION TAG	UNP Q16696
D	26	LYS	-	EXPRESSION TAG	UNP Q16696
D	27	THR	-	EXPRESSION TAG	UNP Q16696
D	28	SER	-	EXPRESSION TAG	UNP Q16696
D	29	SER	-	EXPRESSION TAG	UNP Q16696
D	30	LYS	-	EXPRESSION TAG	UNP Q16696
D	495	HIS	-	EXPRESSION TAG	UNP Q16696
D	496	HIS	-	EXPRESSION TAG	UNP Q16696
D	497	HIS	-	EXPRESSION TAG	UNP Q16696
D	498	HIS	-	EXPRESSION TAG	UNP Q16696
E	23	MET	-	INITIATING METHIONINE	UNP Q16696
E	24	ALA	-	EXPRESSION TAG	UNP Q16696
E	25	LYS	-	EXPRESSION TAG	UNP Q16696
E	26	LYS	-	EXPRESSION TAG	UNP Q16696
E	27	THR	-	EXPRESSION TAG	UNP Q16696
E	28	SER	-	EXPRESSION TAG	UNP Q16696
E	29	SER	-	EXPRESSION TAG	UNP Q16696

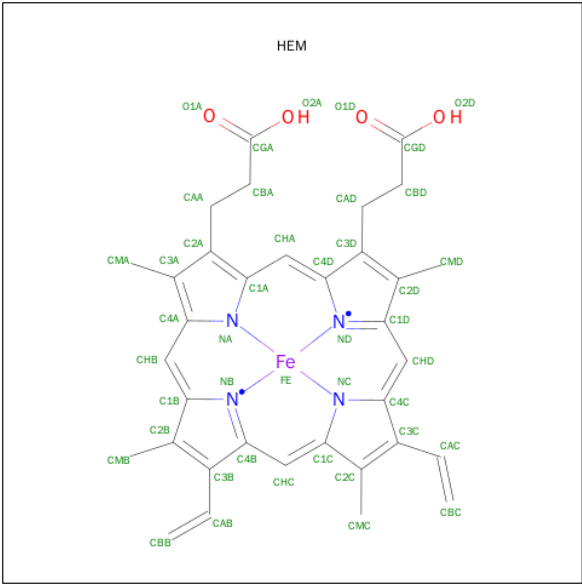
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Chain	Residue	Modelled	Actual	Comment	Reference
E	30	LYS	-	EXPRESSION TAG	UNP Q16696
E	495	HIS	-	EXPRESSION TAG	UNP Q16696
E	496	HIS	-	EXPRESSION TAG	UNP Q16696
E	497	HIS	-	EXPRESSION TAG	UNP Q16696
E	498	HIS	-	EXPRESSION TAG	UNP Q16696
F	23	MET	-	INITIATING METHIONINE	UNP Q16696
F	24	ALA	-	EXPRESSION TAG	UNP Q16696
F	25	LYS	-	EXPRESSION TAG	UNP Q16696
F	26	LYS	-	EXPRESSION TAG	UNP Q16696
F	27	THR	-	EXPRESSION TAG	UNP Q16696
F	28	SER	-	EXPRESSION TAG	UNP Q16696
F	29	SER	-	EXPRESSION TAG	UNP Q16696
F	30	LYS	-	EXPRESSION TAG	UNP Q16696
F	495	HIS	-	EXPRESSION TAG	UNP Q16696
F	496	HIS	-	EXPRESSION TAG	UNP Q16696
F	497	HIS	-	EXPRESSION TAG	UNP Q16696
F	498	HIS	-	EXPRESSION TAG	UNP Q16696
G	23	MET	-	INITIATING METHIONINE	UNP Q16696
G	24	ALA	-	EXPRESSION TAG	UNP Q16696
G	25	LYS	-	EXPRESSION TAG	UNP Q16696
G	26	LYS	-	EXPRESSION TAG	UNP Q16696
G	27	THR	-	EXPRESSION TAG	UNP Q16696
G	28	SER	-	EXPRESSION TAG	UNP Q16696
G	29	SER	-	EXPRESSION TAG	UNP Q16696
G	30	LYS	-	EXPRESSION TAG	UNP Q16696
G	495	HIS	-	EXPRESSION TAG	UNP Q16696
G	496	HIS	-	EXPRESSION TAG	UNP Q16696
G	497	HIS	-	EXPRESSION TAG	UNP Q16696
G	498	HIS	-	EXPRESSION TAG	UNP Q16696
H	23	MET	-	INITIATING METHIONINE	UNP Q16696
H	24	ALA	-	EXPRESSION TAG	UNP Q16696
H	25	LYS	-	EXPRESSION TAG	UNP Q16696
H	26	LYS	-	EXPRESSION TAG	UNP Q16696
H	27	THR	-	EXPRESSION TAG	UNP Q16696
H	28	SER	-	EXPRESSION TAG	UNP Q16696
H	29	SER	-	EXPRESSION TAG	UNP Q16696
H	30	LYS	-	EXPRESSION TAG	UNP Q16696
H	495	HIS	-	EXPRESSION TAG	UNP Q16696
H	496	HIS	-	EXPRESSION TAG	UNP Q16696
H	497	HIS	-	EXPRESSION TAG	UNP Q16696
H	498	HIS	-	EXPRESSION TAG	UNP Q16696

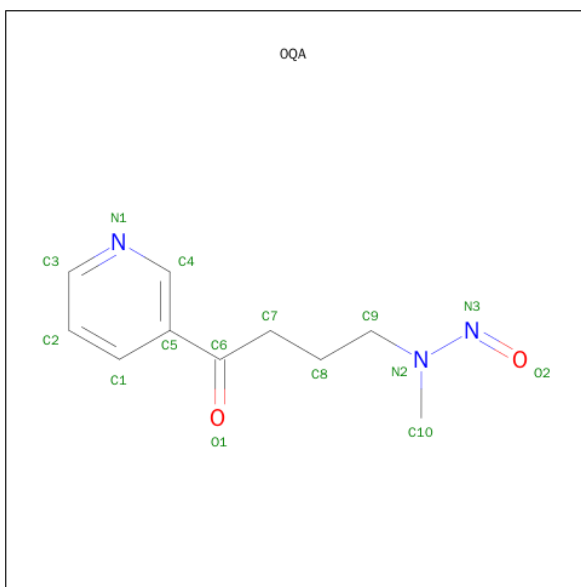
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-[METHYL(NITROSO)AMINO]-1-(PYRIDIN-3-YL)BUTAN-1-ONE (three-letter code: 0QA) (formula: C₁₀H₁₃N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	3	2		
3	B	1	Total	C	N	O	0	0
			15	10	3	2		
3	C	1	Total	C	N	O	0	0
			15	10	3	2		
3	D	1	Total	C	N	O	0	0
			15	10	3	2		
3	E	1	Total	C	N	O	0	0
			15	10	3	2		
3	F	1	Total	C	N	O	0	0
			15	10	3	2		

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



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

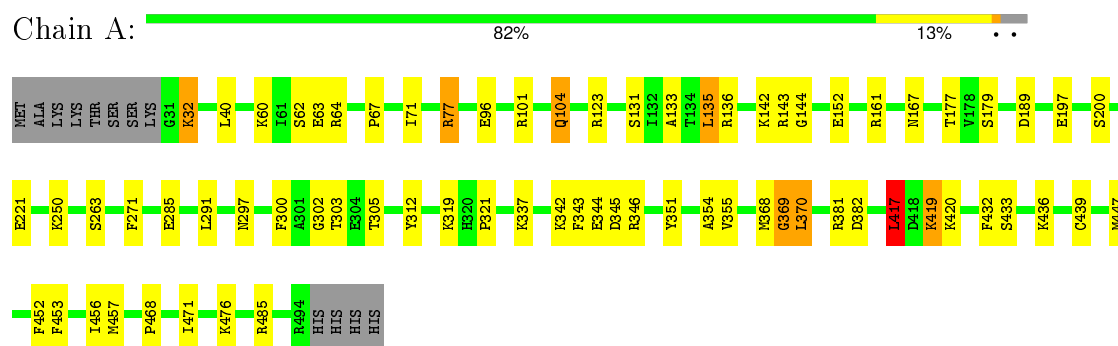
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	39	Total	O	0	0
			39	39		
5	C	71	Total	O	0	0
			71	71		
5	D	49	Total	O	0	0
			49	49		
5	E	13	Total	O	0	0
			13	13		
5	F	11	Total	O	0	0
			11	11		
5	G	12	Total	O	0	0
			12	12		
5	H	10	Total	O	0	0
			10	10		

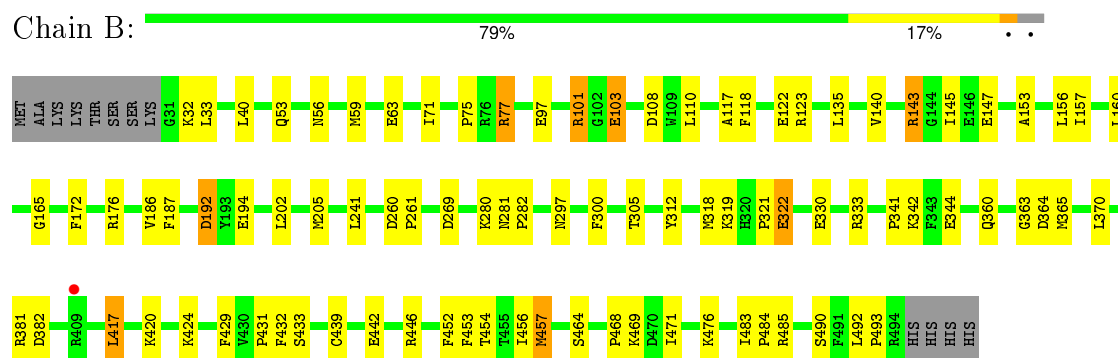
3 Residue-property plots

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.

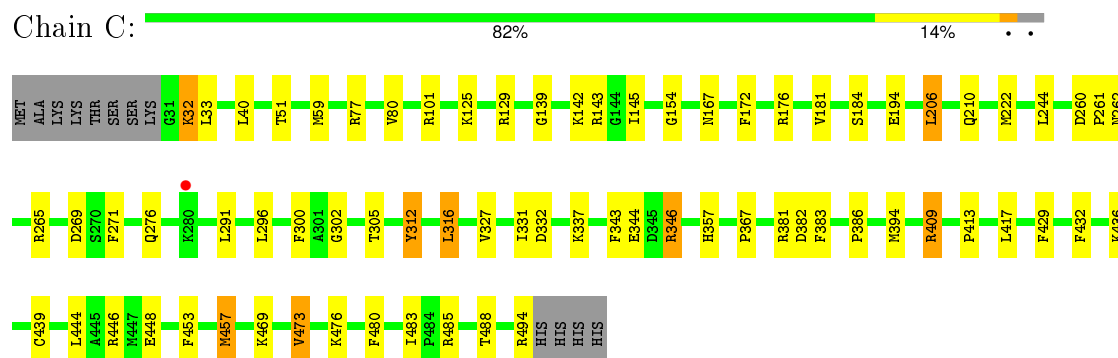
• Molecule 1: Cytochrome P450 2A13




• Molecule 1: Cytochrome P450 2A13

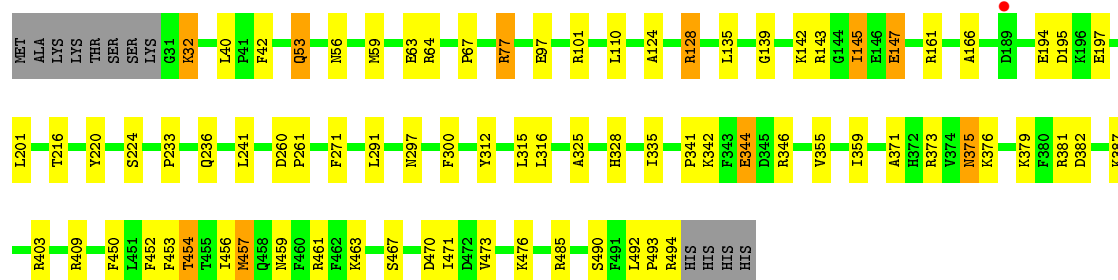


• Molecule 1: Cytochrome P450 2A13




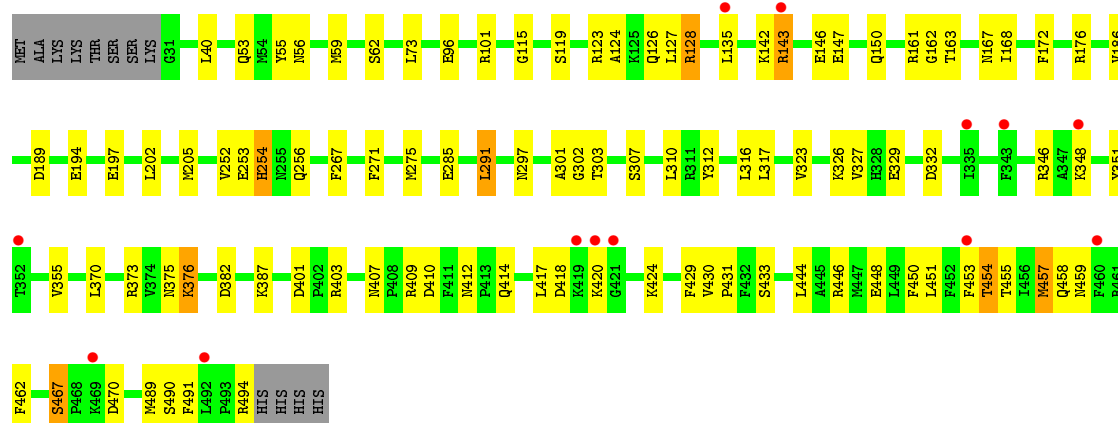
• Molecule 1: Cytochrome P450 2A13

Chain D:  81% 15% . .



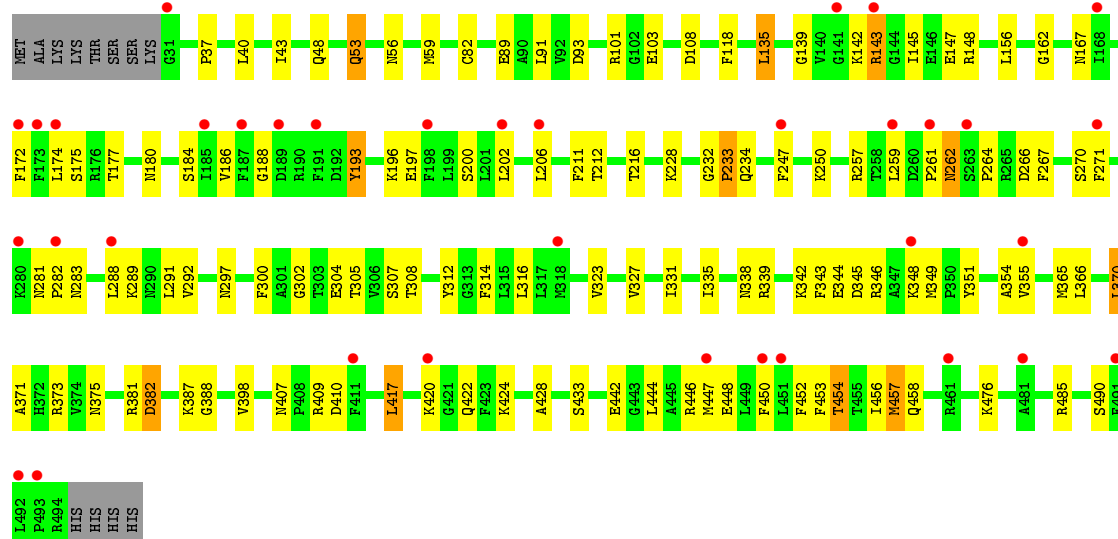
• Molecule 1: Cytochrome P450 2A13

Chain E:  3% 76% 20% . .

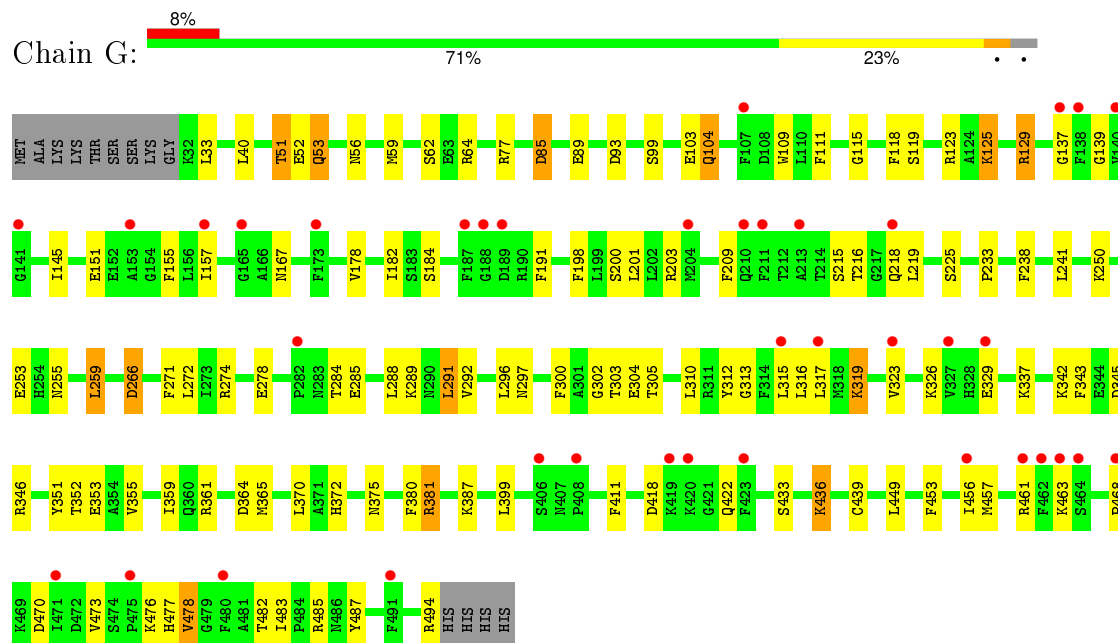


• Molecule 1: Cytochrome P450 2A13

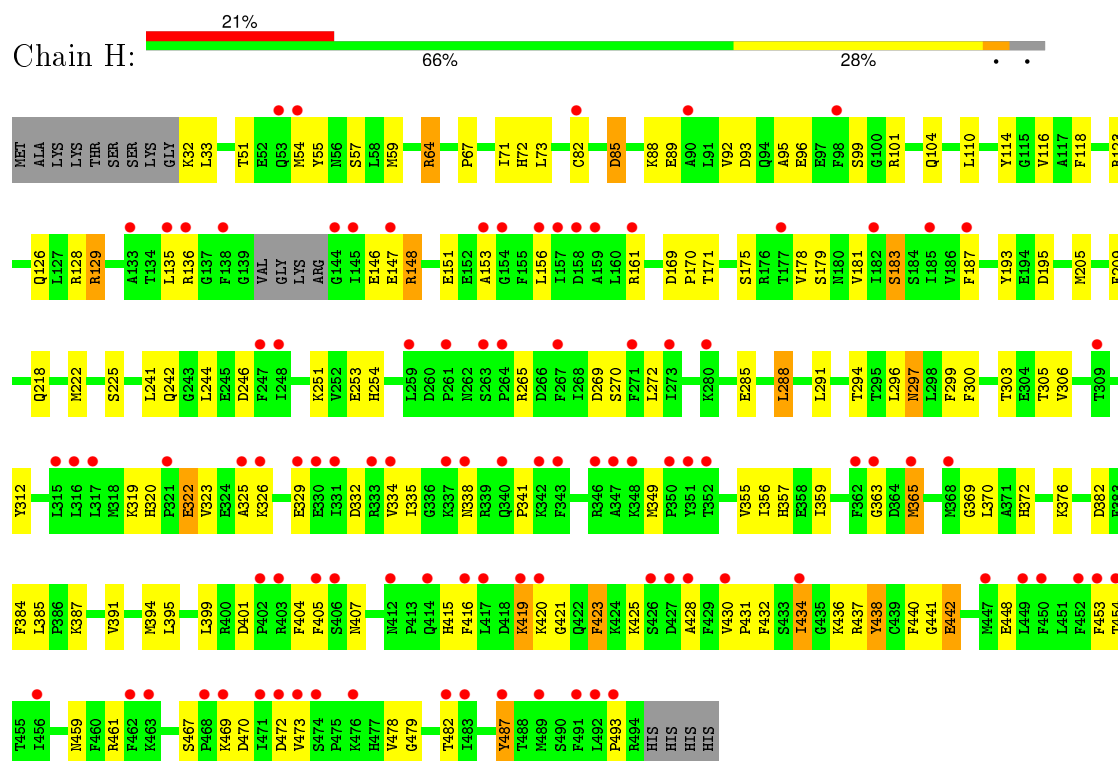
Chain F:  7% 71% 24% . .



• Molecule 1: Cytochrome P450 2A13



• Molecule 1: Cytochrome P450 2A13



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.68Å 119.27Å 153.66Å 100.59° 101.86° 93.56°	Depositor
Resolution (Å)	69.77 – 2.35 69.77 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (69.77-2.35) 91.0 (69.77-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.34Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.214 , 0.273 0.214 , 0.271	Depositor DCC
R_{free} test set	10209 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 197861 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30804	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% 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: GOL, 0QA, 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	1.01	2/3880 (0.1%)	0.90	1/5224 (0.0%)
1	B	0.99	3/3871 (0.1%)	0.88	4/5212 (0.1%)
1	C	1.04	4/3879 (0.1%)	0.89	2/5223 (0.0%)
1	D	0.99	1/3871 (0.0%)	0.87	1/5212 (0.0%)
1	E	0.85	0/3871	0.79	0/5212
1	F	0.80	0/3871	0.76	1/5212 (0.0%)
1	G	0.82	0/3834	0.81	0/5170
1	H	0.77	0/3822	0.75	1/5149 (0.0%)
All	All	0.92	10/30899 (0.0%)	0.83	10/41614 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	473	VAL	CB-CG2	5.94	1.65	1.52
1	C	383	PHE	CE2-CZ	5.37	1.47	1.37
1	B	63	GLU	CG-CD	5.28	1.59	1.51
1	B	322	GLU	CG-CD	5.24	1.59	1.51
1	A	133	ALA	CA-CB	5.20	1.63	1.52
1	C	429	PHE	CE1-CZ	5.20	1.47	1.37
1	C	80	VAL	CB-CG2	5.09	1.63	1.52
1	D	97	GLU	CD-OE1	5.06	1.31	1.25
1	A	104	GLN	CG-CD	5.05	1.62	1.51
1	B	103	GLU	CB-CG	-5.01	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	C	143	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	H	288	LEU	CA-CB-CG	5.86	128.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	F	316	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	417	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	33	LEU	CA-CB-CG	5.29	127.45	115.30
1	B	417	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	269	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	195	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3777	0	3747	50	0
1	B	3771	0	3741	47	0
1	C	3776	0	3745	53	0
1	D	3771	0	3741	56	0
1	E	3771	0	3741	55	0
1	F	3771	0	3741	78	0
1	G	3737	0	3670	85	0
1	H	3723	0	3668	81	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
2	E	43	0	30	3	0
2	F	43	0	30	9	0
2	G	43	0	30	6	0
2	H	43	0	30	6	0
3	A	15	0	13	4	0
3	B	15	0	13	5	0
3	C	15	0	13	4	0
3	D	15	0	13	5	0
3	E	15	0	13	3	0
3	F	15	0	13	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	6	0	8	2	0
4	H	6	0	8	0	0
5	A	56	0	0	0	0
5	B	39	0	0	3	0
5	C	71	0	0	4	0
5	D	49	0	0	3	0
5	E	13	0	0	0	0
5	F	11	0	0	0	0
5	G	12	0	0	1	0
5	H	10	0	0	0	0
All	All	30804	0	30128	524	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 9.

All (524) 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:C:32:LYS:HD2	1:C:33:LEU:H	1.09	1.07
1:D:381:ARG:O	1:D:382:ASP:HB2	1.55	1.03
1:D:143:ARG:HH12	1:D:147:GLU:HB2	1.22	1.03
3:B:502:OQA:O1	3:B:502:OQA:H5	1.58	0.99
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.26	0.98
3:F:502:OQA:O1	3:F:502:OQA:H1	1.64	0.97
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.31	0.95
1:C:59:MET:CE	1:C:394:MET:HE2	1.99	0.91
1:D:341:PRO:HG3	1:D:454:THR:HG22	1.54	0.90
1:E:172:PHE:O	1:E:176:ARG:HG3	1.72	0.89
1:C:32:LYS:HD2	1:C:33:LEU:N	1.89	0.86
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.40	0.86
1:D:143:ARG:NH1	1:D:147:GLU:HB2	1.91	0.85
1:C:125:LYS:HE2	1:C:129:ARG:HH22	1.39	0.85
1:G:216:THR:HG21	1:G:233:PRO:HG2	1.56	0.85
1:C:59:MET:CE	1:C:394:MET:CE	2.56	0.84
1:A:381:ARG:O	1:A:382:ASP:HB2	1.79	0.83
1:G:53:GLN:OE1	1:G:53:GLN:HA	1.77	0.82
1:A:342:LYS:HE3	1:A:344:GLU:OE1	1.80	0.81
1:F:139:GLY:O	1:F:145:ILE:HB	1.81	0.81
1:E:450:PHE:O	1:E:454:THR:HB	1.82	0.80
1:F:433:SER:HB3	2:F:501:HEM:HBA1	1.64	0.79
1:B:165:GLY:O	1:B:490:SER:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:476:LYS:HG3	1:G:477:HIS:H	1.47	0.78
1:H:187:PHE:CE1	1:H:251:LYS:HB3	2.20	0.77
1:F:271:PHE:CD2	1:F:291:LEU:HB2	2.19	0.77
1:C:327:VAL:HG11	1:C:457:MET:CE	2.15	0.76
1:C:305:THR:HG21	3:C:502:0QA:O2	1.86	0.75
1:F:262:ASN:O	1:F:264:PRO:HD3	1.85	0.75
1:H:73:LEU:HB3	1:H:222:MET:HG2	1.67	0.75
1:D:452:PHE:O	1:D:456:ILE:HD12	1.87	0.74
1:A:77:ARG:HH11	1:A:77:ARG:CG	1.99	0.74
1:C:327:VAL:HG11	1:C:457:MET:HE2	1.70	0.73
3:D:502:0QA:O1	3:D:502:0QA:H5	1.88	0.73
1:G:182:ILE:HD11	1:G:302:GLY:HA3	1.70	0.73
1:D:143:ARG:HH12	1:D:147:GLU:CB	2.00	0.73
1:C:32:LYS:CD	1:C:33:LEU:H	1.96	0.72
1:A:142:LYS:HG3	1:A:143:ARG:N	2.04	0.72
1:D:381:ARG:O	1:D:382:ASP:CB	2.27	0.72
1:C:59:MET:HE1	1:C:394:MET:CE	2.19	0.72
3:C:502:0QA:O1	3:C:502:0QA:H5	1.88	0.72
1:H:320:HIS:HB3	1:H:323:VAL:HG22	1.72	0.71
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.00	0.71
1:A:433:SER:HB3	2:A:501:HEM:HBA1	1.73	0.70
1:H:114:TYR:CE1	1:H:123:ARG:NH1	2.59	0.70
1:F:174:LEU:HD21	1:F:314:PHE:HE1	1.56	0.70
1:F:271:PHE:CE2	1:F:291:LEU:HB2	2.27	0.70
3:A:502:0QA:O1	3:A:502:0QA:H5	1.89	0.69
1:E:376:LYS:HA	1:E:387:LYS:HG3	1.73	0.69
1:A:342:LYS:HG3	1:A:344:GLU:HG3	1.74	0.69
1:H:178:VAL:HG11	1:H:306:VAL:HB	1.74	0.69
1:H:407:ASN:O	1:H:415:HIS:NE2	2.25	0.69
1:B:143:ARG:O	1:B:147:GLU:HG2	1.92	0.69
2:H:501:HEM:HBB2	2:H:501:HEM:HMB1	1.75	0.68
1:H:441:GLY:HA3	2:H:501:HEM:C3C	2.29	0.68
1:G:109:TRP:CH2	1:G:238:PHE:HB3	2.28	0.68
1:H:372:HIS:O	1:H:391:VAL:N	2.23	0.68
1:E:205:MET:HE1	1:E:303:THR:HG21	1.76	0.67
1:H:92:VAL:HG23	1:H:434:ILE:HG13	1.76	0.67
1:G:315:LEU:HB2	1:G:487:TYR:CE2	2.29	0.67
1:C:59:MET:HE1	1:C:394:MET:HE2	1.73	0.67
1:F:302:GLY:HA2	2:F:501:HEM:HMC2	1.77	0.67
1:C:453:PHE:O	1:C:457:MET:HG2	1.93	0.67
1:G:478:VAL:O	1:G:478:VAL:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ARG:HB2	1:C:269:ASP:OD1	1.94	0.67
1:C:125:LYS:CE	1:C:129:ARG:HH22	2.08	0.67
1:A:60:LYS:HG3	1:D:403:ARG:NH2	2.10	0.66
1:H:54:MET:HB2	1:H:479:GLY:HA2	1.78	0.66
1:F:407:ASN:HB3	1:F:410:ASP:HB2	1.77	0.66
1:F:297:ASN:HA	3:F:502:OQA:N1	2.11	0.66
2:D:501:HEM:C4D	3:D:502:OQA:H1	2.28	0.66
1:D:341:PRO:CG	1:D:454:THR:HG22	2.26	0.66
1:B:122:GLU:OE2	1:B:122:GLU:HA	1.97	0.65
1:E:302:GLY:HA2	2:E:501:HEM:HMC2	1.79	0.65
1:F:323:VAL:O	1:F:327:VAL:HG23	1.96	0.65
1:F:433:SER:CB	2:F:501:HEM:HBA1	2.26	0.65
1:F:450:PHE:O	1:F:454:THR:HB	1.96	0.65
1:H:179:SER:O	1:H:183:SER:HB2	1.97	0.65
1:C:139:GLY:HA2	1:C:142:LYS:HD2	1.78	0.64
1:F:288:LEU:O	1:F:292:VAL:HG23	1.97	0.64
1:A:381:ARG:O	1:A:382:ASP:CB	2.42	0.64
1:D:409:ARG:HG2	5:D:631:HOH:O	1.98	0.64
1:E:453:PHE:O	1:E:457:MET:HB2	1.97	0.64
1:D:166:ALA:O	1:D:490:SER:HB3	1.98	0.64
1:E:297:ASN:HA	3:E:502:OQA:N1	2.13	0.64
1:D:53:GLN:HG3	1:D:56:ASN:HB2	1.80	0.64
1:C:453:PHE:O	1:C:457:MET:CG	2.46	0.64
2:G:501:HEM:HBB2	2:G:501:HEM:HMB2	1.78	0.64
1:E:301:ALA:HA	3:E:502:OQA:H3	1.80	0.63
1:C:77:ARG:NH2	1:C:386:PRO:HG2	2.13	0.63
1:F:118:PHE:HE2	1:F:370:LEU:HD11	1.63	0.63
1:E:332:ASP:OD2	1:E:494:ARG:NH2	2.28	0.63
1:F:345:ASP:O	1:F:349:MET:HG3	1.98	0.63
1:F:145:ILE:HD12	1:F:148:ARG:HB3	1.81	0.63
2:E:501:HEM:HMB1	2:E:501:HEM:HBB2	1.81	0.63
1:G:355:VAL:O	1:G:359:ILE:HG12	1.98	0.63
1:D:143:ARG:HH11	1:D:143:ARG:HG3	1.64	0.62
1:H:372:HIS:NE2	2:H:501:HEM:O1A	2.29	0.62
1:F:448:GLU:O	1:F:452:PHE:CD2	2.51	0.62
1:D:77:ARG:CG	1:D:77:ARG:HH11	2.11	0.62
1:C:77:ARG:HH22	1:C:386:PRO:HG2	1.64	0.62
1:F:216:THR:HG21	1:F:233:PRO:HG2	1.81	0.62
1:A:342:LYS:HG3	1:A:344:GLU:CG	2.30	0.61
1:G:476:LYS:HG3	1:G:477:HIS:N	2.15	0.61
1:D:375:ASN:O	1:D:387:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:GLN:NE2	1:H:118:PHE:CE1	2.69	0.61
1:E:53:GLN:HG3	1:E:56:ASN:HB2	1.81	0.61
1:G:33:LEU:HD21	1:G:77:ARG:HD2	1.82	0.61
3:C:502:OQA:O1	3:C:502:OQA:C9	2.48	0.61
3:D:502:OQA:C9	3:D:502:OQA:O1	2.48	0.61
1:E:205:MET:CE	1:E:303:THR:HG21	2.30	0.61
1:H:146:GLU:C	1:H:148:ARG:H	2.05	0.61
1:C:59:MET:HE3	1:C:394:MET:CE	2.31	0.60
1:H:363:GLY:O	1:H:365:MET:CE	2.49	0.60
1:G:365:MET:HA	1:G:365:MET:CE	2.32	0.60
1:F:343:PHE:CE1	1:F:447:MET:HA	2.37	0.60
1:F:174:LEU:HD21	1:F:314:PHE:CE1	2.37	0.59
1:F:308:THR:HB	1:F:365:MET:CE	2.32	0.59
1:D:379:LYS:HD3	5:D:640:HOH:O	2.02	0.59
1:D:341:PRO:HG3	1:D:454:THR:CG2	2.30	0.59
1:A:179:SER:HB2	1:A:303:THR:HG23	1.83	0.59
1:H:432:PHE:CG	1:H:442:GLU:HG3	2.37	0.59
1:D:342:LYS:HE2	1:D:344:GLU:OE1	2.02	0.59
1:F:375:ASN:O	1:F:387:LYS:HG3	2.02	0.59
1:F:40:LEU:HD22	1:F:43:ILE:HD11	1.85	0.59
1:C:172:PHE:O	1:C:176:ARG:HG3	2.02	0.59
1:G:215:SER:N	4:G:502:GOL:O3	2.28	0.59
1:B:77:ARG:NH1	5:B:612:HOH:O	2.35	0.58
1:G:285:GLU:HA	1:G:285:GLU:OE1	2.03	0.58
1:A:297:ASN:HA	3:A:502:OQA:N1	2.18	0.58
1:G:123:ARG:HA	1:G:285:GLU:HG3	1.86	0.58
1:A:142:LYS:HG3	1:A:144:GLY:H	1.68	0.58
1:D:220:TYR:CZ	1:D:224:SER:HB2	2.39	0.58
1:F:420:LYS:HE2	1:F:422:GLN:HE21	1.68	0.58
1:A:197:GLU:O	1:A:200:SER:HB3	2.04	0.57
1:H:129:ARG:HG3	1:H:129:ARG:HH11	1.68	0.57
1:G:125:LYS:O	1:G:129:ARG:HB2	2.05	0.57
1:F:305:THR:HA	1:F:365:MET:CE	2.34	0.57
1:H:363:GLY:O	1:H:365:MET:HE2	2.05	0.57
1:F:308:THR:HB	1:F:365:MET:HE1	1.86	0.57
1:G:209:PHE:HE2	1:G:300:PHE:HD1	1.52	0.57
1:B:77:ARG:HG2	1:B:77:ARG:NH1	2.11	0.57
1:G:178:VAL:HG11	1:G:303:THR:O	2.05	0.57
1:C:332:ASP:CG	1:C:494:ARG:HH22	2.08	0.57
2:C:501:HEM:C4D	3:C:502:OQA:H1	2.33	0.56
1:C:210:GLN:HG3	1:C:483:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:ARG:HD3	1:F:388:GLY:HA2	1.86	0.56
1:E:142:LYS:HG2	1:E:143:ARG:HH22	1.70	0.56
1:G:315:LEU:HB2	1:G:487:TYR:HE2	1.68	0.56
1:F:143:ARG:O	1:F:147:GLU:HG2	2.05	0.56
1:G:375:ASN:O	1:G:387:LYS:HG3	2.06	0.56
1:H:51:THR:HG23	1:H:218:GLN:HB2	1.88	0.56
1:H:372:HIS:HE1	1:H:437:ARG:HB2	1.70	0.56
1:D:476:LYS:NZ	5:D:604:HOH:O	2.38	0.56
1:F:381:ARG:O	1:F:382:ASP:HB2	2.04	0.56
1:G:151:GLU:O	1:G:155:PHE:HD2	1.88	0.56
1:D:124:ALA:O	1:D:128:ARG:HB2	2.06	0.56
1:A:468:PRO:HA	1:A:471:ILE:HD12	1.87	0.56
1:H:382:ASP:OD1	1:H:382:ASP:N	2.39	0.56
1:H:114:TYR:HE1	1:H:123:ARG:NH1	2.03	0.56
1:G:278:GLU:HG2	1:G:284:THR:OG1	2.05	0.55
1:F:476:LYS:HB2	1:F:485:ARG:HA	1.87	0.55
1:G:178:VAL:CG1	1:G:303:THR:HA	2.36	0.55
1:B:453:PHE:O	1:B:457:MET:HB2	2.06	0.55
1:H:401:ASP:HB3	1:H:404:PHE:HB2	1.88	0.55
1:H:104:GLN:NE2	1:H:118:PHE:HE1	2.04	0.55
1:G:319:LYS:HE2	1:G:473:VAL:HG22	1.88	0.55
1:G:215:SER:HB3	4:G:502:GOL:O3	2.05	0.55
1:E:142:LYS:HG2	1:E:143:ARG:NH2	2.22	0.55
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.08	0.54
1:H:95:ALA:O	1:H:99:SER:HB3	2.07	0.54
1:G:361:ARG:NH1	1:G:399:LEU:O	2.37	0.54
1:A:142:LYS:CG	1:A:144:GLY:H	2.21	0.54
1:D:355:VAL:O	1:D:359:ILE:HG13	2.08	0.54
1:H:355:VAL:O	1:H:359:ILE:HG12	2.08	0.54
1:F:448:GLU:O	1:F:452:PHE:HD2	1.91	0.54
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.89	0.54
1:C:59:MET:CE	1:C:394:MET:HE3	2.37	0.54
1:F:103:GLU:HB2	1:F:108:ASP:OD2	2.08	0.54
1:B:101:ARG:HD2	1:B:117:ALA:O	2.08	0.54
1:F:89:GLU:O	1:F:93:ASP:HB2	2.08	0.54
1:G:139:GLY:CA	1:G:145:ILE:HG12	2.38	0.54
1:G:478:VAL:HG22	1:G:482:THR:HG23	1.89	0.53
1:G:453:PHE:O	1:G:457:MET:HG3	2.08	0.53
1:E:253:GLU:HA	1:E:256:GLN:HG3	1.90	0.53
1:E:101:ARG:CZ	1:E:370:LEU:HD23	2.38	0.53
1:E:254:HIS:C	1:E:254:HIS:ND1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:LEU:O	1:E:448:GLU:HG3	2.09	0.53
1:F:354:ALA:HB2	1:F:417:LEU:HD13	1.90	0.53
1:H:407:ASN:H	1:H:415:HIS:HE1	1.56	0.53
1:A:419:LYS:HB2	1:A:420:LYS:HE2	1.89	0.53
1:F:259:LEU:O	1:F:261:PRO:HD3	2.08	0.53
1:G:139:GLY:HA2	1:G:145:ILE:HG12	1.90	0.53
1:A:67:PRO:HG3	1:D:63:GLU:O	2.09	0.53
2:F:501:HEM:ND	3:F:502:OQA:C10	2.71	0.53
1:H:101:ARG:NH1	2:H:501:HEM:O2A	2.42	0.53
1:F:53:GLN:HG3	1:F:56:ASN:OD1	2.09	0.52
1:G:433:SER:HB3	2:G:501:HEM:HBA1	1.91	0.52
1:A:104:GLN:NE2	1:A:221:GLU:OE2	2.43	0.52
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.92	0.52
3:B:502:OQA:O1	3:B:502:OQA:C9	2.44	0.52
1:G:288:LEU:O	1:G:292:VAL:HG23	2.09	0.52
1:G:461:ARG:HB3	1:G:494:ARG:HD3	1.91	0.52
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.90	0.52
1:F:373:ARG:NH1	1:F:388:GLY:O	2.43	0.52
1:B:321:PRO:HD2	1:B:322:GLU:OE2	2.10	0.52
1:G:316:LEU:O	1:G:317:LEU:HB2	2.10	0.52
1:E:123:ARG:O	1:E:127:LEU:HG	2.08	0.52
1:D:110:LEU:HD22	1:D:241:LEU:HB3	1.92	0.52
3:F:502:OQA:O1	3:F:502:OQA:C10	2.49	0.52
1:H:265:ARG:HB2	1:H:269:ASP:OD2	2.09	0.52
1:C:181:VAL:O	1:C:184:SER:HB2	2.09	0.52
1:G:439:CYS:HB2	2:G:501:HEM:NA	2.25	0.51
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.45	0.51
1:A:381:ARG:HB3	1:D:64[B]:ARG:HH21	1.74	0.51
1:H:322:GLU:O	1:H:325:ALA:HB3	2.10	0.51
1:G:99:SER:HB2	1:G:436:LYS:HB3	1.92	0.51
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.45	0.51
1:H:96:GLU:HA	1:H:96:GLU:OE1	2.10	0.51
1:H:469:LYS:HG3	1:H:469:LYS:O	2.10	0.51
1:F:118:PHE:CE2	1:F:370:LEU:HD11	2.44	0.51
2:H:501:HEM:HBB2	2:H:501:HEM:CMB	2.38	0.51
1:F:327:VAL:O	1:F:331:ILE:HG13	2.11	0.51
1:B:432:PHE:HB3	1:B:439:CYS:HB3	1.93	0.51
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.92	0.51
1:A:342:LYS:HG2	1:A:345:ASP:OD2	2.11	0.51
1:H:341:PRO:HG2	1:H:454:THR:HG22	1.92	0.51
1:B:442:GLU:OE1	1:B:446:ARG:NE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ASN:ND2	1:F:193:TYR:HE1	2.09	0.51
1:H:305:THR:HA	1:H:365:MET:HG3	1.92	0.51
1:E:462:PHE:HB3	1:E:489:MET:HE3	1.93	0.51
1:B:305:THR:HG21	3:B:502:OQA:O2	2.11	0.50
1:G:259:LEU:HD21	1:G:272:LEU:HB3	1.94	0.50
1:A:161:ARG:HG2	1:A:161:ARG:HH11	1.76	0.50
1:F:142:LYS:HE3	1:F:143:ARG:NH2	2.25	0.50
2:D:501:HEM:HMB2	2:D:501:HEM:HBB2	1.93	0.50
1:F:180:ASN:HD22	1:F:193:TYR:HE1	1.58	0.50
1:C:332:ASP:OD2	1:C:494:ARG:NH2	2.38	0.50
1:G:104:GLN:HE21	1:G:104:GLN:N	2.10	0.50
1:C:327:VAL:HG11	1:C:457:MET:HE3	1.94	0.50
1:F:211:PHE:CE1	1:F:233:PRO:HB2	2.47	0.50
1:C:59:MET:HE1	1:C:394:MET:HE3	1.90	0.50
1:G:476:LYS:CG	1:G:477:HIS:H	2.17	0.50
1:F:211:PHE:HE1	1:F:233:PRO:HB2	1.77	0.50
1:E:161:ARG:O	1:E:163:THR:N	2.45	0.49
1:E:412:ASN:OD1	1:E:414:GLN:HB2	2.11	0.49
1:B:452:PHE:O	1:B:456:ILE:HD12	2.12	0.49
1:H:187:PHE:CE1	1:H:251:LYS:CB	2.94	0.49
1:H:55:TYR:CE2	1:H:59:MET:HG2	2.47	0.49
1:B:297:ASN:HD22	3:B:502:OQA:C4	2.25	0.49
1:H:55:TYR:CE2	1:H:59:MET:CG	2.95	0.49
1:E:375:ASN:O	1:E:387:LYS:HE2	2.13	0.49
1:B:318:MET:SD	1:B:464:SER:HB3	2.52	0.49
1:D:161:ARG:NH2	1:D:459:ASN:OD1	2.44	0.49
3:A:502:OQA:C9	3:A:502:OQA:O1	2.49	0.49
1:B:172:PHE:O	1:B:176:ARG:HG3	2.12	0.49
1:C:51:THR:HG22	1:C:222:MET:CE	2.43	0.49
1:E:124:ALA:O	1:E:128:ARG:HB2	2.12	0.49
1:H:244:LEU:HB3	1:H:296:LEU:HD11	1.95	0.49
1:B:110:LEU:HD22	1:B:241:LEU:HB3	1.95	0.48
2:F:501:HEM:ND	3:F:502:OQA:H3	2.28	0.48
1:A:60:LYS:HG3	1:D:403:ARG:HH21	1.75	0.48
1:G:313:GLY:HA2	1:G:359:ILE:HD12	1.96	0.48
1:A:453:PHE:HD2	1:A:457:MET:CE	2.25	0.48
1:H:288:LEU:O	1:H:291:LEU:HB3	2.12	0.48
1:A:101:ARG:NH1	1:A:370:LEU:HB3	2.27	0.48
1:G:255:ASN:ND2	1:G:266:ASP:OD1	2.46	0.48
1:E:375:ASN:O	1:E:387:LYS:HG3	2.13	0.48
1:E:332:ASP:CG	1:E:494:ARG:HH22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LEU:O	1:C:210:GLN:HB2	2.12	0.48
1:A:131:SER:O	1:A:135:LEU:HB2	2.13	0.48
1:C:453:PHE:O	1:C:457:MET:HG3	2.14	0.48
1:F:381:ARG:O	1:F:382:ASP:CB	2.61	0.48
1:D:197:GLU:O	1:D:201:LEU:HG	2.14	0.48
1:G:317:LEU:HD23	1:G:323:VAL:HG23	1.96	0.48
1:F:351:TYR:O	1:F:355:VAL:HG23	2.14	0.48
1:A:63:GLU:O	1:D:67:PRO:HG3	2.14	0.47
1:H:51:THR:HG23	1:H:218:GLN:CB	2.44	0.47
1:B:360:GLN:HG2	5:B:633:HOH:O	2.13	0.47
1:A:319:LYS:C	1:A:321:PRO:HD3	2.33	0.47
1:H:175:SER:O	1:H:179:SER:HB3	2.14	0.47
1:F:188:GLY:N	1:F:266:ASP:HB3	2.29	0.47
1:B:381:ARG:O	1:B:382:ASP:HB2	2.14	0.47
1:D:101:ARG:O	1:D:373:ARG:HG2	2.15	0.47
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.52	0.47
1:F:398:VAL:HG12	1:F:428:ALA:HB1	1.97	0.47
1:H:187:PHE:CE1	1:H:251:LYS:HD3	2.50	0.47
1:H:187:PHE:HE1	1:H:251:LYS:HB3	1.73	0.47
1:H:363:GLY:O	1:H:365:MET:HE1	2.13	0.47
1:D:315:LEU:HG	1:D:473:VAL:HG12	1.97	0.47
1:A:432:PHE:HB3	1:A:439:CYS:HB3	1.96	0.47
1:E:418:ASP:OD1	1:E:420:LYS:HB2	2.14	0.47
1:G:418:ASP:OD1	1:G:422:GLN:HB2	2.14	0.47
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.18	0.47
1:G:104:GLN:OE1	1:G:118:PHE:CE1	2.68	0.47
1:A:152:GLU:HG3	1:A:177:THR:HG23	1.96	0.47
1:D:297:ASN:HA	3:D:502:OQA:N1	2.30	0.47
1:A:161:ARG:HG2	1:A:161:ARG:NH1	2.30	0.47
1:D:467:SER:HB3	1:D:470:ASP:OD2	2.15	0.47
1:C:302:GLY:HA2	2:C:501:HEM:HMC2	1.97	0.47
1:G:111:PHE:CG	1:G:118:PHE:CD2	3.03	0.47
1:F:206:LEU:HD13	1:F:304:GLU:OE1	2.15	0.47
1:E:401:ASP:OD2	1:E:403:ARG:HG2	2.15	0.47
1:E:348:LYS:HB2	1:E:348:LYS:HE2	1.61	0.47
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.50	0.46
1:H:369:GLY:O	1:H:370:LEU:HD12	2.15	0.46
1:H:405:PHE:HB3	1:H:415:HIS:CE1	2.50	0.46
1:F:424:LYS:HE2	1:F:424:LYS:HB3	1.54	0.46
1:B:118:PHE:HE2	1:B:370:LEU:HD11	1.79	0.46
1:G:209:PHE:CE1	1:G:304:GLU:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:THR:HA	1:F:365:MET:HE1	1.96	0.46
1:B:140:VAL:HA	1:B:145:ILE:HG21	1.97	0.46
1:D:143:ARG:HG3	1:D:143:ARG:NH1	2.27	0.46
1:H:357:HIS:HB3	1:H:416:PHE:CZ	2.49	0.46
1:A:351:TYR:O	1:A:355:VAL:HG23	2.16	0.46
1:D:145:ILE:HA	1:D:145:ILE:HD12	1.75	0.46
1:H:209:PHE:CZ	1:H:300:PHE:HD1	2.34	0.46
1:C:473:VAL:HG22	5:C:605:HOH:O	2.15	0.46
1:G:64:ARG:HB3	1:G:64:ARG:NH2	2.30	0.46
1:F:156:LEU:HB2	1:F:177:THR:HG21	1.97	0.46
1:H:73:LEU:CB	1:H:222:MET:HG2	2.42	0.46
1:G:182:ILE:HD11	1:G:302:GLY:CA	2.43	0.46
1:F:37:PRO:HB2	1:F:48:GLN:NE2	2.30	0.46
1:F:59:MET:HE1	1:F:82:CYS:SG	2.55	0.46
1:B:281:ASN:HA	1:B:282:PRO:HD2	1.79	0.46
1:A:305:THR:HG23	3:A:502:OQA:H3	1.97	0.46
1:F:197:GLU:O	1:F:200:SER:HB3	2.15	0.46
1:D:341:PRO:CB	1:D:454:THR:HG21	2.46	0.46
1:E:302:GLY:HA2	2:E:501:HEM:CMC	2.45	0.46
1:G:111:PHE:CD2	1:G:118:PHE:HD2	2.33	0.46
1:F:305:THR:HG22	1:F:365:MET:HE2	1.98	0.46
1:H:430:VAL:N	1:H:431:PRO:HD3	2.31	0.46
1:C:343:PHE:O	1:C:346:ARG:HB2	2.16	0.46
1:F:331:ILE:HG23	1:F:335:ILE:HD12	1.97	0.45
1:H:175:SER:O	1:H:179:SER:CB	2.64	0.45
1:H:423:PHE:CE1	1:H:425:LYS:HG3	2.52	0.45
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.98	0.45
1:G:103:GLU:C	1:G:104:GLN:HE21	2.19	0.45
1:B:330:GLU:HG2	1:B:333:ARG:NH2	2.31	0.45
1:G:64:ARG:CZ	1:G:64:ARG:HB3	2.46	0.45
1:H:399:LEU:HD23	1:H:428:ALA:O	2.17	0.45
1:B:341:PRO:HG2	1:B:454:THR:HG22	1.98	0.45
1:E:454:THR:HG22	1:E:455:THR:N	2.32	0.45
1:E:59:MET:O	1:E:62:SER:HB3	2.17	0.45
1:E:326:LYS:HD2	1:E:351:TYR:CZ	2.52	0.45
2:F:501:HEM:NA	3:F:502:OQA:H2	2.32	0.45
1:G:145:ILE:HD13	1:G:145:ILE:HA	1.83	0.45
1:G:111:PHE:CG	1:G:118:PHE:HD2	2.35	0.45
1:C:409:ARG:HB3	1:C:409:ARG:HE	1.68	0.45
1:B:433:SER:HB3	2:B:501:HEM:HBA1	1.99	0.45
1:D:32:LYS:HA	1:D:32:LYS:HD2	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:GLU:O	1:F:446:ARG:HG3	2.17	0.45
1:A:136:ARG:O	1:A:142:LYS:HE3	2.17	0.45
1:G:271:PHE:CE1	1:G:291:LEU:HB2	2.51	0.45
1:C:409:ARG:HG2	5:C:630:HOH:O	2.15	0.45
1:G:51:THR:HG23	1:G:218:GLN:HB2	1.99	0.45
1:E:168:ILE:HD11	1:E:491:PHE:CD1	2.52	0.45
1:E:252:VAL:O	1:E:256:GLN:HG3	2.17	0.45
1:B:342:LYS:HE2	1:B:344:GLU:OE1	2.16	0.45
1:A:368:MET:O	1:A:369:GLY:C	2.55	0.45
1:H:461:ARG:NH1	1:H:493:PRO:O	2.47	0.45
1:H:423:PHE:C	1:H:423:PHE:CD1	2.90	0.45
1:G:370:LEU:HD12	1:G:370:LEU:HA	1.81	0.44
1:H:67:PRO:HA	1:H:82:CYS:HB2	1.99	0.44
1:D:335:ILE:HD13	1:D:341:PRO:HB3	1.99	0.44
1:B:53:GLN:HG2	1:B:56:ASN:OD1	2.16	0.44
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.51	0.44
1:F:172:PHE:HA	1:F:175:SER:OG	2.16	0.44
1:H:123:ARG:HA	1:H:285:GLU:HG3	1.99	0.44
1:G:365:MET:HA	1:G:365:MET:HE2	1.99	0.44
1:A:452:PHE:O	1:A:456:ILE:HD12	2.17	0.44
1:A:142:LYS:HG3	1:A:143:ARG:H	1.79	0.44
1:G:310:LEU:HD23	1:G:453:PHE:CE2	2.53	0.44
1:D:139:GLY:O	1:D:145:ILE:HB	2.18	0.44
1:G:157:ILE:HD11	1:G:456:ILE:HA	1.98	0.44
1:B:260:ASP:HA	1:B:261:PRO:HD2	1.81	0.44
1:H:89:GLU:O	1:H:93:ASP:HB2	2.17	0.44
1:E:202:LEU:HA	1:E:205:MET:HE2	1.98	0.44
1:G:478:VAL:O	1:G:478:VAL:CG1	2.65	0.44
1:H:487:TYR:C	1:H:487:TYR:CD1	2.91	0.44
1:C:367:PRO:HD2	1:C:480:PHE:O	2.18	0.44
1:F:186:VAL:HA	1:F:267:PHE:CB	2.48	0.44
1:F:302:GLY:HA2	2:F:501:HEM:CMC	2.47	0.44
1:C:271:PHE:CG	1:C:291:LEU:HD13	2.52	0.44
1:C:312:TYR:O	1:C:316:LEU:HD22	2.18	0.44
1:G:380:PHE:O	1:G:381:ARG:C	2.56	0.44
1:G:85:ASP:HB3	1:G:381:ARG:HH12	1.83	0.44
1:G:365:MET:CA	1:G:365:MET:HE2	2.45	0.44
1:G:271:PHE:CD1	1:G:291:LEU:HB2	2.52	0.44
1:F:232:GLY:O	1:F:234:GLN:N	2.51	0.44
1:G:191:PHE:CD2	1:G:198:PHE:CD1	3.06	0.44
1:F:197:GLU:OE1	1:F:247:PHE:CE1	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:HB2	1:B:108:ASP:OD2	2.18	0.44
1:H:441:GLY:HA3	2:H:501:HEM:CAC	2.48	0.43
1:E:101:ARG:NH2	1:E:370:LEU:HD23	2.33	0.43
1:H:128:ARG:NH2	1:H:438:TYR:CD2	2.85	0.43
1:B:192:ASP:C	1:B:194:GLU:H	2.20	0.43
1:E:291:LEU:O	1:E:291:LEU:HD12	2.18	0.43
1:A:476:LYS:HB2	1:A:485:ARG:HA	2.01	0.43
1:E:451:LEU:HD23	1:E:451:LEU:HA	1.86	0.43
1:C:444:LEU:O	1:C:448:GLU:HG3	2.19	0.43
1:G:449:LEU:O	1:G:453:PHE:HB2	2.17	0.43
1:A:343:PHE:CE1	1:A:447:MET:HA	2.53	0.43
1:E:115:GLY:O	1:E:119:SER:HB3	2.19	0.43
1:H:116:VAL:HG12	1:H:294:THR:HG23	2.01	0.43
1:H:116:VAL:CG1	1:H:294:THR:HG23	2.47	0.43
1:E:351:TYR:O	1:E:355:VAL:HG23	2.18	0.43
1:H:161:ARG:HH22	1:H:459:ASN:HD22	1.65	0.43
1:B:202:LEU:HD23	1:B:205:MET:CE	2.48	0.43
1:H:64:ARG:HB2	1:H:64:ARG:HE	1.70	0.43
1:F:135:LEU:HA	1:F:135:LEU:HD12	1.82	0.43
1:H:55:TYR:CE2	1:H:59:MET:HG3	2.53	0.43
1:C:154:GLY:HA3	5:C:650:HOH:O	2.18	0.43
1:D:453:PHE:O	1:D:457:MET:HB2	2.19	0.43
1:F:175:SER:HB2	1:F:202:LEU:HD22	2.01	0.43
1:C:432:PHE:HB3	1:C:439:CYS:HB3	2.00	0.43
1:E:407:ASN:HB3	1:E:410:ASP:HB2	2.01	0.43
1:H:440:PHE:CD1	1:H:440:PHE:C	2.92	0.43
1:C:51:THR:HG22	1:C:222:MET:HE3	2.00	0.42
1:C:260:ASP:HA	1:C:261:PRO:HD2	1.92	0.42
1:G:296:LEU:HD12	1:G:296:LEU:HA	1.81	0.42
1:F:452:PHE:O	1:F:456:ILE:HG13	2.20	0.42
1:D:471:ILE:HG22	1:D:473:VAL:HG13	2.01	0.42
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.72	0.42
1:B:186:VAL:HG23	1:B:187:PHE:CD1	2.54	0.42
1:C:357:HIS:NE2	1:C:446:ARG:NH2	2.67	0.42
1:G:53:GLN:HB3	1:G:56:ASN:HB2	2.01	0.42
1:E:317:LEU:HD13	1:E:457:MET:CE	2.49	0.42
1:E:467:SER:O	1:E:470:ASP:HB2	2.20	0.42
1:D:492:LEU:HA	1:D:493:PRO:HD3	1.81	0.42
1:D:325:ALA:O	1:D:328:HIS:HB2	2.19	0.42
1:B:59:MET:CE	1:B:59:MET:HA	2.50	0.42
1:G:305:THR:HG22	1:G:365:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:MET:CE	1:F:82:CYS:SG	3.08	0.42
1:H:394:MET:O	1:H:395:LEU:C	2.57	0.42
1:G:411:PHE:O	1:G:411:PHE:CD2	2.72	0.42
1:A:436:LYS:HE2	1:C:262:ASN:OD1	2.19	0.42
1:H:153:ALA:HA	1:H:156:LEU:HB3	2.02	0.42
1:D:216:THR:HG21	1:D:233:PRO:HG2	2.01	0.42
1:B:476:LYS:HB2	1:B:485:ARG:HA	2.01	0.42
1:C:381:ARG:O	1:C:382:ASP:HB2	2.20	0.42
1:G:89:GLU:O	1:G:93:ASP:HB2	2.19	0.42
1:F:344:GLU:C	1:F:346:ARG:H	2.22	0.42
1:B:319:LYS:HD2	1:B:468:PRO:O	2.19	0.42
1:F:300:PHE:CD2	3:F:502:0QA:C2	3.02	0.42
1:D:341:PRO:CB	1:D:454:THR:CG2	2.98	0.42
1:G:487:TYR:CD1	1:G:487:TYR:C	2.93	0.42
1:G:323:VAL:HG21	1:G:411:PHE:HE2	1.84	0.42
1:B:429:PHE:CZ	1:B:431:PRO:HG3	2.55	0.42
1:H:356:ILE:HG12	1:H:453:PHE:HD2	1.85	0.42
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.73	0.42
1:E:310:LEU:HD23	1:E:453:PHE:CE1	2.55	0.42
3:E:502:0QA:H6	3:E:502:0QA:H2	1.63	0.42
1:B:363:GLY:O	1:B:364:ASP:C	2.58	0.42
1:G:59:MET:O	1:G:62:SER:HB3	2.20	0.42
1:B:71:ILE:HA	1:B:71:ILE:HD12	1.92	0.42
1:E:96:GLU:O	1:E:375:ASN:ND2	2.52	0.42
1:G:343:PHE:CE2	1:G:346:ARG:NH2	2.88	0.42
1:A:71:ILE:HA	1:A:71:ILE:HD12	1.93	0.42
2:F:501:HEM:C4D	3:F:502:0QA:C10	3.03	0.42
1:G:302:GLY:HA2	2:G:501:HEM:CMC	2.50	0.42
1:F:281:ASN:OD1	1:F:282:PRO:HD2	2.20	0.42
1:H:73:LEU:HB3	1:H:222:MET:CG	2.44	0.41
1:G:288:LEU:O	1:G:291:LEU:HB3	2.20	0.41
1:D:59:MET:HA	1:D:59:MET:CE	2.50	0.41
1:H:71:ILE:HG13	1:H:72:HIS:N	2.35	0.41
1:E:271:PHE:O	1:E:275:MET:HG3	2.21	0.41
2:F:501:HEM:C1A	3:F:502:0QA:H2	2.55	0.41
1:G:477:HIS:HB2	1:G:483:ILE:HD12	2.02	0.41
1:E:146:GLU:O	1:E:150:GLN:HG3	2.19	0.41
1:C:167:ASN:ND2	1:C:488:THR:OG1	2.45	0.41
1:E:143:ARG:O	1:E:147:GLU:HG2	2.20	0.41
1:F:143:ARG:H	1:F:143:ARG:NE	2.18	0.41
1:B:153:ALA:O	1:B:157:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LYS:HB3	1:B:424:LYS:HE3	1.90	0.41
1:H:299:PHE:O	1:H:303:THR:HB	2.20	0.41
1:B:75:PRO:HA	5:B:603:HOH:O	2.20	0.41
1:E:186:VAL:HA	1:E:267:PHE:HB3	2.03	0.41
1:C:101:ARG:NH1	2:C:501:HEM:O2A	2.48	0.41
1:A:453:PHE:CD2	1:A:457:MET:CE	3.03	0.41
1:B:341:PRO:CG	1:B:454:THR:HG22	2.50	0.41
1:B:483:ILE:HA	1:B:484:PRO:HD2	1.90	0.41
1:C:331:ILE:CD1	1:C:457:MET:HB2	2.50	0.41
1:F:420:LYS:HE2	1:F:422:GLN:NE2	2.34	0.41
1:D:291:LEU:O	1:D:291:LEU:HD12	2.20	0.41
1:H:116:VAL:HB	1:H:294:THR:HG23	2.03	0.41
1:E:429:PHE:CZ	1:E:431:PRO:HG3	2.56	0.41
1:E:55:TYR:CD2	1:E:55:TYR:C	2.93	0.41
1:A:302:GLY:HA2	2:A:501:HEM:HMC2	2.02	0.41
1:H:146:GLU:C	1:H:148:ARG:N	2.73	0.41
1:D:101:ARG:HD3	1:D:371:ALA:O	2.20	0.41
1:C:436:LYS:NZ	5:C:631:HOH:O	2.52	0.41
1:G:250:LYS:CE	5:G:605:HOH:O	2.69	0.41
1:B:492:LEU:HA	1:B:493:PRO:HD3	1.92	0.41
3:D:502:0QA:H10	3:D:502:0QA:H8	1.78	0.41
1:H:178:VAL:CG1	1:H:306:VAL:HB	2.47	0.41
1:F:335:ILE:HA	1:F:339:ARG:NH2	2.36	0.41
1:E:430:VAL:N	1:E:431:PRO:CD	2.83	0.41
1:E:323:VAL:O	1:E:327:VAL:HG23	2.21	0.41
1:D:461:ARG:HB3	1:D:494:ARG:HD2	2.03	0.41
1:H:169:ASP:HA	1:H:170:PRO:HD3	1.89	0.41
1:A:354:ALA:HB2	1:A:417:LEU:HD13	2.03	0.41
1:G:433:SER:CB	2:G:501:HEM:HBA1	2.51	0.40
1:G:351:TYR:O	1:G:355:VAL:HG23	2.21	0.40
1:F:453:PHE:O	1:F:457:MET:HB2	2.20	0.40
1:H:110:LEU:HD22	1:H:241:LEU:HB3	2.03	0.40
1:G:297:ASN:HA	1:G:297:ASN:HD22	1.66	0.40
1:H:297:ASN:HA	1:H:297:ASN:HD22	1.58	0.40
3:B:502:0QA:H1	3:B:502:0QA:H6	1.62	0.40
1:D:341:PRO:CG	1:D:454:THR:CG2	2.96	0.40
1:G:372:HIS:NE2	2:G:501:HEM:O1A	2.49	0.40
1:F:444:LEU:O	1:F:448:GLU:HG3	2.21	0.40
1:G:352:THR:O	1:G:353:GLU:C	2.58	0.40
1:B:156:LEU:O	1:B:160:LEU:HG	2.21	0.40
1:H:384:PHE:C	1:H:385:LEU:HD23	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ASP:HA	1:D:261:PRO:HD3	1.87	0.40
1:F:53:GLN:CG	1:F:56:ASN:OD1	2.69	0.40
1:E:123:ARG:HA	1:E:285:GLU:HG3	2.03	0.40
1:G:200:SER:O	1:G:203:ARG:HB3	2.20	0.40
1:G:115:GLY:O	1:G:119:SER:HB3	2.21	0.40
1:D:450:PHE:O	1:D:454:THR:HB	2.21	0.40
1:F:101:ARG:HD3	1:F:371:ALA:O	2.21	0.40
1:H:181:VAL:HG11	1:H:448:GLU:OE2	2.21	0.40
1:E:458:GLN:OE1	1:E:459:ASN:ND2	2.54	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	464/476 (98%)	439 (95%)	24 (5%)	1 (0%)	52	63
1	B	463/476 (97%)	445 (96%)	18 (4%)	0	100	100
1	C	464/476 (98%)	443 (96%)	20 (4%)	1 (0%)	52	63
1	D	463/476 (97%)	444 (96%)	18 (4%)	1 (0%)	52	63
1	E	463/476 (97%)	434 (94%)	28 (6%)	1 (0%)	52	63
1	F	463/476 (97%)	413 (89%)	44 (10%)	6 (1%)	15	13
1	G	461/476 (97%)	417 (90%)	36 (8%)	8 (2%)	11	9
1	H	456/476 (96%)	396 (87%)	53 (12%)	7 (2%)	13	11
All	All	3697/3808 (97%)	3431 (93%)	241 (6%)	25 (1%)	26	29

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	346	ARG

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Mol	Chain	Res	Type
1	G	364	ASP
1	G	468	PRO
1	A	369	GLY
1	E	162	GLY
1	F	338	ASN
1	G	137	GLY
1	G	225	SER
1	G	337	LYS
1	H	85	ASP
1	H	419	LYS
1	G	345	ASP
1	G	381	ARG
1	H	147	GLU
1	H	193	TYR
1	D	42	PHE
1	F	212	THR
1	F	382	ASP
1	H	171	THR
1	H	322	GLU
1	F	162	GLY
1	F	193	TYR
1	H	421	GLY
1	F	233	PRO
1	G	478	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	410/419 (98%)	391 (95%)	19 (5%)	33	42
1	B	409/419 (98%)	392 (96%)	17 (4%)	36	46
1	C	410/419 (98%)	394 (96%)	16 (4%)	39	51
1	D	409/419 (98%)	388 (95%)	21 (5%)	29	36
1	E	409/419 (98%)	380 (93%)	29 (7%)	18	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	409/419 (98%)	383 (94%)	26 (6%)	22	24
1	G	403/419 (96%)	375 (93%)	28 (7%)	19	21
1	H	403/419 (96%)	354 (88%)	49 (12%)	6	5
All	All	3262/3352 (97%)	3057 (94%)	205 (6%)	22	25

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	40	LEU
1	A	62	SER
1	A	64[A]	ARG
1	A	64[B]	ARG
1	A	77	ARG
1	A	96	GLU
1	A	135	LEU
1	A	167	ASN
1	A	189	ASP
1	A	250	LYS
1	A	263	SER
1	A	300	PHE
1	A	312	TYR
1	A	337	LYS
1	A	346	ARG
1	A	370	LEU
1	A	417	LEU
1	A	419	LYS
1	B	32	LYS
1	B	40	LEU
1	B	77	ARG
1	B	97	GLU
1	B	101	ARG
1	B	135	LEU
1	B	143	ARG
1	B	192	ASP
1	B	280	LYS
1	B	300	PHE
1	B	312	TYR
1	B	365	MET
1	B	417	LEU
1	B	420	LYS

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Mol	Chain	Res	Type
1	B	457	MET
1	B	469	LYS
1	B	471	ILE
1	C	32	LYS
1	C	40	LEU
1	C	145	ILE
1	C	194	GLU
1	C	206	LEU
1	C	276	GLN
1	C	300	PHE
1	C	312	TYR
1	C	316	LEU
1	C	337	LYS
1	C	344	GLU
1	C	409	ARG
1	C	413	PRO
1	C	417	LEU
1	C	457	MET
1	C	469	LYS
1	D	32	LYS
1	D	40	LEU
1	D	53	GLN
1	D	77	ARG
1	D	128	ARG
1	D	135	LEU
1	D	142	LYS
1	D	145	ILE
1	D	147	GLU
1	D	194	GLU
1	D	236	GLN
1	D	300	PHE
1	D	312	TYR
1	D	316	LEU
1	D	344	GLU
1	D	346	ARG
1	D	375	ASN
1	D	376	LYS
1	D	454	THR
1	D	457	MET
1	D	463	LYS
1	E	40	LEU
1	E	73	LEU

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Mol	Chain	Res	Type
1	E	126	GLN
1	E	128	ARG
1	E	135	LEU
1	E	143	ARG
1	E	167	ASN
1	E	189	ASP
1	E	194	GLU
1	E	197	GLU
1	E	254	HIS
1	E	291	LEU
1	E	307	SER
1	E	312	TYR
1	E	316	LEU
1	E	329	GLU
1	E	346	ARG
1	E	373	ARG
1	E	376	LYS
1	E	382	ASP
1	E	409	ARG
1	E	417	LEU
1	E	424	LYS
1	E	433	SER
1	E	446	ARG
1	E	454	THR
1	E	457	MET
1	E	467	SER
1	E	490	SER
1	F	53	GLN
1	F	91	LEU
1	F	135	LEU
1	F	143	ARG
1	F	167	ASN
1	F	184	SER
1	F	196	LYS
1	F	228	LYS
1	F	250	LYS
1	F	257	ARG
1	F	262	ASN
1	F	270	SER
1	F	283	ASN
1	F	289	LYS
1	F	307	SER

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Mol	Chain	Res	Type
1	F	312	TYR
1	F	342	LYS
1	F	348	LYS
1	F	366	LEU
1	F	370	LEU
1	F	409	ARG
1	F	417	LEU
1	F	454	THR
1	F	457	MET
1	F	458	GLN
1	F	490	SER
1	G	40	LEU
1	G	51	THR
1	G	52	GLU
1	G	53	GLN
1	G	85	ASP
1	G	104	GLN
1	G	125	LYS
1	G	129	ARG
1	G	167	ASN
1	G	184	SER
1	G	201	LEU
1	G	219	LEU
1	G	241	LEU
1	G	253	GLU
1	G	259	LEU
1	G	266	ASP
1	G	274	ARG
1	G	289	LYS
1	G	291	LEU
1	G	312	TYR
1	G	319	LYS
1	G	326	LYS
1	G	329	GLU
1	G	342	LYS
1	G	436	LYS
1	G	463	LYS
1	G	470	ASP
1	G	485	ARG
1	H	32	LYS
1	H	33	LEU
1	H	57	SER

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Mol	Chain	Res	Type
1	H	64	ARG
1	H	85	ASP
1	H	88	LYS
1	H	126	GLN
1	H	129	ARG
1	H	135	LEU
1	H	136	ARG
1	H	148	ARG
1	H	151	GLU
1	H	183	SER
1	H	195	ASP
1	H	205	MET
1	H	225	SER
1	H	242	GLN
1	H	246	ASP
1	H	253	GLU
1	H	254	HIS
1	H	270	SER
1	H	272	LEU
1	H	297	ASN
1	H	312	TYR
1	H	319	LYS
1	H	326	LYS
1	H	329	GLU
1	H	332	ASP
1	H	334	VAL
1	H	335	ILE
1	H	338	ASN
1	H	349	MET
1	H	365	MET
1	H	376	LYS
1	H	387	LYS
1	H	419	LYS
1	H	420	LYS
1	H	423	PHE
1	H	434	ILE
1	H	436	LYS
1	H	438	TYR
1	H	442	GLU
1	H	467	SER
1	H	470	ASP
1	H	472	ASP

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Mol	Chain	Res	Type
1	H	473	VAL
1	H	478	VAL
1	H	482	THR
1	H	487	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	ASN
1	D	236	GLN
1	E	210	GLN
1	F	283	ASN
1	F	422	GLN
1	G	104	GLN
1	G	126	GLN
1	G	255	ASN

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](#)

16 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	501	1,3	30,50,50	2.17	8 (26%)	24,82,82	2.60	9 (37%)
3	0QA	A	502	2	13,15,15	0.43	0	14,18,18	2.48	5 (35%)
2	HEM	B	501	1	30,50,50	2.61	7 (23%)	24,82,82	2.24	10 (41%)
3	0QA	B	502	-	13,15,15	0.61	0	14,18,18	2.11	6 (42%)
2	HEM	C	501	1,3	30,50,50	2.29	8 (26%)	24,82,82	2.55	8 (33%)
3	0QA	C	502	2	13,15,15	0.62	0	14,18,18	1.72	5 (35%)
2	HEM	D	501	1	30,50,50	2.25	9 (30%)	24,82,82	2.32	8 (33%)
3	0QA	D	502	-	13,15,15	0.62	0	14,18,18	1.72	5 (35%)
2	HEM	E	501	1,3	30,50,50	2.19	6 (20%)	24,82,82	2.33	6 (25%)
3	0QA	E	502	2	13,15,15	0.69	0	14,18,18	1.56	4 (28%)
2	HEM	F	501	1,3	30,50,50	2.14	11 (36%)	24,82,82	2.44	10 (41%)
3	0QA	F	502	2	13,15,15	0.52	0	14,18,18	1.42	3 (21%)
2	HEM	G	501	1	30,50,50	2.10	10 (33%)	24,82,82	2.43	9 (37%)
4	GOL	G	502	-	5,5,5	0.61	0	5,5,5	0.48	0
2	HEM	H	501	1	30,50,50	1.82	8 (26%)	24,82,82	2.69	11 (45%)
4	GOL	H	502	-	5,5,5	1.32	1 (20%)	5,5,5	2.47	2 (40%)

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	501	1,3	-	0/10/54/54	0/0/8/8
3	0QA	A	502	2	-	0/12/12/12	0/1/1/1
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	0QA	B	502	-	-	0/12/12/12	0/1/1/1
2	HEM	C	501	1,3	-	0/10/54/54	0/0/8/8
3	0QA	C	502	2	-	0/12/12/12	0/1/1/1
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8
3	0QA	D	502	-	-	0/12/12/12	0/1/1/1
2	HEM	E	501	1,3	-	0/10/54/54	0/0/8/8
3	0QA	E	502	2	-	1/12/12/12	0/1/1/1
2	HEM	F	501	1,3	-	0/10/54/54	0/0/8/8
3	0QA	F	502	2	-	0/12/12/12	0/1/1/1
2	HEM	G	501	1	-	0/10/54/54	0/0/8/8
4	GOL	G	502	-	-	0/4/4/4	0/0/0/0
2	HEM	H	501	1	-	0/10/54/54	0/0/8/8
4	GOL	H	502	-	-	0/4/4/4	0/0/0/0

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C4B	-10.33	1.42	1.51
2	C	501	HEM	C3B-C4B	-7.33	1.45	1.51
2	E	501	HEM	C3B-C4B	-7.14	1.45	1.51
2	F	501	HEM	C3B-C4B	-6.80	1.45	1.51
2	D	501	HEM	C3B-C4B	-6.73	1.45	1.51
2	A	501	HEM	C3B-C4B	-6.15	1.46	1.51
2	G	501	HEM	C3B-C4B	-5.52	1.46	1.51
2	A	501	HEM	C3D-C4D	-5.47	1.44	1.51
2	E	501	HEM	C3D-C4D	-5.39	1.44	1.51
2	C	501	HEM	C3D-C4D	-4.89	1.45	1.51
2	D	501	HEM	C3D-C4D	-4.80	1.45	1.51
2	C	501	HEM	C2C-C1C	-4.71	1.43	1.52
2	H	501	HEM	C3B-C4B	-4.70	1.47	1.51
2	A	501	HEM	C2C-C1C	-4.49	1.44	1.52
2	B	501	HEM	C3D-C4D	-4.30	1.46	1.51
2	E	501	HEM	C2C-C1C	-4.17	1.44	1.52
2	H	501	HEM	C3D-C4D	-4.06	1.46	1.51
2	G	501	HEM	C3D-C4D	-4.04	1.46	1.51
2	F	501	HEM	C3D-C4D	-3.96	1.46	1.51
2	F	501	HEM	C2C-C1C	-3.74	1.45	1.52
2	B	501	HEM	C2C-C1C	-3.73	1.45	1.52
2	G	501	HEM	C2C-C1C	-3.60	1.45	1.52
2	H	501	HEM	C2C-C1C	-3.04	1.46	1.52
2	D	501	HEM	C2C-C1C	-2.74	1.47	1.52
2	H	501	HEM	C2D-C1D	-2.42	1.43	1.51
2	D	501	HEM	C2D-C1D	-2.33	1.44	1.51
2	H	501	HEM	C2B-C1B	-2.20	1.44	1.51
2	F	501	HEM	C2B-C1B	-2.20	1.44	1.51
4	H	502	GOL	O2-C2	-2.20	1.36	1.43
2	C	501	HEM	C2B-C1B	-2.16	1.44	1.51
2	F	501	HEM	C2D-C1D	-2.05	1.45	1.51
2	A	501	HEM	C2B-C1B	-2.00	1.45	1.51
2	B	501	HEM	FE-ND	2.02	2.08	1.97
2	F	501	HEM	C1C-NC	2.09	1.38	1.36
2	F	501	HEM	FE-NB	2.11	2.08	1.97
2	G	501	HEM	C3B-CAB	2.16	1.55	1.51
2	G	501	HEM	C3C-CAC	2.16	1.55	1.51
2	E	501	HEM	CMA-C3A	2.17	1.56	1.51
2	G	501	HEM	C1C-NC	2.17	1.38	1.36
2	A	501	HEM	FE-ND	2.20	2.09	1.97
2	C	501	HEM	C3B-CAB	2.22	1.55	1.51
2	D	501	HEM	FE-ND	2.23	2.09	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	HEM	FE-NC	2.25	2.04	1.95
2	F	501	HEM	C3C-CAC	2.37	1.55	1.51
2	F	501	HEM	C4C-NC	2.38	1.38	1.36
2	B	501	HEM	CMD-C2D	2.41	1.58	1.53
2	D	501	HEM	C3B-CAB	2.45	1.55	1.51
2	E	501	HEM	C3B-CAB	2.45	1.55	1.51
2	C	501	HEM	CMA-C3A	2.46	1.56	1.51
2	B	501	HEM	C3C-CAC	2.47	1.55	1.51
2	H	501	HEM	FE-ND	2.47	2.10	1.97
2	H	501	HEM	C3B-CAB	2.48	1.56	1.51
2	A	501	HEM	C3C-CAC	2.49	1.56	1.51
2	G	501	HEM	CAA-C2A	2.68	1.56	1.52
2	F	501	HEM	FE-ND	2.69	2.11	1.97
2	D	501	HEM	FE-NC	2.71	2.06	1.95
2	C	501	HEM	FE-ND	2.73	2.12	1.97
2	G	501	HEM	FE-ND	2.78	2.12	1.97
2	F	501	HEM	CAA-C2A	2.81	1.56	1.52
2	A	501	HEM	CMA-C3A	2.89	1.57	1.51
2	G	501	HEM	C4C-NC	2.92	1.39	1.36
2	A	501	HEM	FE-NC	2.92	2.07	1.95
2	D	501	HEM	CAA-C2A	3.02	1.57	1.52
2	E	501	HEM	C3C-CAC	3.05	1.57	1.51
2	C	501	HEM	C3C-CAC	3.19	1.57	1.51
2	B	501	HEM	CAA-C2A	3.38	1.57	1.52
2	G	501	HEM	FE-NB	3.43	2.15	1.97
2	D	501	HEM	CMA-C3A	3.95	1.59	1.51

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	0QA	C9-N2-N3	-5.59	98.39	119.29
2	C	501	HEM	C3C-CAC-CBC	-5.24	116.41	124.46
2	H	501	HEM	CAA-CBA-CGA	-5.05	103.50	112.75
2	A	501	HEM	C3C-CAC-CBC	-4.62	117.38	124.46
4	H	502	GOL	O3-C3-C2	-4.46	88.56	110.18
3	A	502	0QA	C8-C7-C6	-4.34	104.99	113.53
3	B	502	0QA	C8-C7-C6	-4.32	105.04	113.53
3	A	502	0QA	C9-C8-C7	-4.22	100.96	111.94
2	A	501	HEM	CAA-CBA-CGA	-4.14	105.16	112.75
2	E	501	HEM	CAA-CBA-CGA	-3.66	106.03	112.75
2	B	501	HEM	CBD-CAD-C3D	-3.64	102.97	113.55
3	B	502	0QA	C9-N2-N3	-3.62	105.77	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	CAA-CBA-CGA	-3.57	106.20	112.75
3	D	502	0QA	C9-N2-N3	-3.48	106.28	119.29
3	C	502	0QA	C9-N2-N3	-3.47	106.32	119.29
3	D	502	0QA	C8-C7-C6	-3.33	106.99	113.53
3	C	502	0QA	C8-C7-C6	-3.32	107.00	113.53
2	D	501	HEM	C3C-CAC-CBC	-3.30	119.39	124.46
2	F	501	HEM	C3C-CAC-CBC	-3.14	119.64	124.46
3	E	502	0QA	C5-C4-N1	-3.10	119.05	123.52
2	H	501	HEM	CBD-CAD-C3D	-2.94	104.98	113.55
3	B	502	0QA	C9-C8-C7	-2.91	104.36	111.94
4	H	502	GOL	O2-C2-C3	-2.91	95.33	108.65
2	G	501	HEM	CMA-C3A-C4A	-2.79	123.75	128.36
3	E	502	0QA	C8-C7-C6	-2.58	108.46	113.53
3	A	502	0QA	C5-C4-N1	-2.53	119.88	123.52
2	A	501	HEM	CMA-C3A-C4A	-2.52	124.19	128.36
3	B	502	0QA	C5-C4-N1	-2.50	119.91	123.52
3	F	502	0QA	C8-C7-C6	-2.43	108.75	113.53
2	F	501	HEM	C3B-CAB-CBB	-2.43	120.73	124.46
3	F	502	0QA	C9-N2-N3	-2.26	110.84	119.29
2	B	501	HEM	CAA-CBA-CGA	-2.26	108.61	112.75
3	E	502	0QA	C9-N2-N3	-2.26	110.86	119.29
2	B	501	HEM	C3B-CAB-CBB	-2.23	121.04	124.46
3	C	502	0QA	C5-C4-N1	-2.17	120.39	123.52
3	D	502	0QA	C5-C4-N1	-2.17	120.39	123.52
2	G	501	HEM	C2C-C1C-NC	-2.13	106.61	110.21
2	C	501	HEM	CBD-CAD-C3D	-2.12	107.39	113.55
2	B	501	HEM	C3C-CAC-CBC	-2.11	121.22	124.46
2	H	501	HEM	C3B-C4B-NB	-2.06	107.69	111.63
2	F	501	HEM	CBD-CAD-C3D	-2.06	107.57	113.55
2	G	501	HEM	CBA-CAA-C2A	2.06	116.23	112.53
3	B	502	0QA	C3-N1-C4	2.15	120.81	116.84
3	D	502	0QA	C3-N1-C4	2.18	120.85	116.84
3	C	502	0QA	C3-N1-C4	2.18	120.86	116.84
2	D	501	HEM	C4B-CHC-C1C	2.22	129.54	125.82
3	C	502	0QA	C1-C5-C4	2.23	120.29	117.67
3	D	502	0QA	C1-C5-C4	2.26	120.31	117.67
2	A	501	HEM	C3B-C4B-CHC	2.28	126.38	123.16
2	B	501	HEM	CMD-C2D-C3D	2.29	124.48	114.35
3	B	502	0QA	C1-C5-C4	2.30	120.37	117.67
2	H	501	HEM	C2D-C3D-C4D	2.37	105.52	101.50
2	C	501	HEM	C3B-CAB-CBB	2.40	128.14	124.46
3	F	502	0QA	C3-N1-C4	2.60	121.62	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	0QA	C3-N1-C4	2.60	121.63	116.84
2	E	501	HEM	CMD-C2D-C3D	2.76	126.58	114.35
3	E	502	0QA	C3-N1-C4	2.78	121.96	116.84
2	B	501	HEM	C2D-C3D-C4D	2.78	106.21	101.50
2	D	501	HEM	CMD-C2D-C3D	2.81	126.76	114.35
2	H	501	HEM	C2C-C1C-CHC	2.88	128.06	123.68
2	H	501	HEM	C3B-C4B-CHC	2.89	127.23	123.16
2	A	501	HEM	CMD-C2D-C3D	2.92	127.27	114.35
2	F	501	HEM	C3B-C4B-CHC	2.93	127.28	123.16
2	G	501	HEM	CMC-C2C-C3C	2.94	123.88	116.53
2	F	501	HEM	CMD-C2D-C3D	2.98	127.53	114.35
2	G	501	HEM	CMD-C2D-C3D	3.08	127.99	114.35
2	D	501	HEM	C2C-C1C-CHC	3.19	128.54	123.68
2	H	501	HEM	CMD-C2D-C3D	3.33	129.10	114.35
2	D	501	HEM	CMC-C2C-C3C	3.38	124.96	116.53
2	C	501	HEM	CAD-C3D-C4D	3.43	124.56	112.47
2	C	501	HEM	CMD-C2D-C3D	3.51	129.87	114.35
2	F	501	HEM	CMC-C2C-C3C	3.57	125.44	116.53
2	C	501	HEM	CMC-C2C-C3C	3.63	125.59	116.53
2	B	501	HEM	CMC-C2C-C3C	3.80	126.02	116.53
2	H	501	HEM	CMC-C2C-C3C	3.85	126.15	116.53
2	A	501	HEM	CAD-C3D-C4D	3.87	126.12	112.47
2	E	501	HEM	CMC-C2C-C3C	4.12	126.82	116.53
2	F	501	HEM	CAD-C3D-C2D	4.15	125.14	113.22
2	G	501	HEM	C3B-C4B-CHC	4.22	129.10	123.16
2	A	501	HEM	CMC-C2C-C3C	4.24	127.13	116.53
2	B	501	HEM	CAD-C3D-C2D	4.28	125.51	113.22
2	B	501	HEM	CMB-C2B-C3B	4.37	127.43	116.53
2	F	501	HEM	CMB-C2B-C3B	4.41	127.55	116.53
2	D	501	HEM	CAD-C3D-C4D	4.41	128.03	112.47
2	H	501	HEM	CAD-C3D-C2D	4.48	126.08	113.22
2	B	501	HEM	CAD-C3D-C4D	4.48	128.26	112.47
2	H	501	HEM	CAD-C3D-C4D	4.51	128.37	112.47
2	D	501	HEM	CMB-C2B-C3B	4.53	127.83	116.53
2	A	501	HEM	CMB-C2B-C3B	4.57	127.94	116.53
2	E	501	HEM	CAD-C3D-C4D	4.68	128.98	112.47
2	G	501	HEM	CAD-C3D-C2D	4.69	126.71	113.22
2	C	501	HEM	CMB-C2B-C3B	4.87	128.69	116.53
2	G	501	HEM	CAD-C3D-C4D	4.92	129.83	112.47
2	E	501	HEM	CAD-C3D-C2D	4.94	127.42	113.22
2	E	501	HEM	CMB-C2B-C3B	4.94	128.87	116.53
2	D	501	HEM	CAD-C3D-C2D	5.02	127.65	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	CAD-C3D-C4D	5.04	130.24	112.47
2	G	501	HEM	CMB-C2B-C3B	5.15	129.38	116.53
2	A	501	HEM	CAD-C3D-C2D	5.52	129.08	113.22
2	H	501	HEM	CMB-C2B-C3B	5.83	131.09	116.53
2	C	501	HEM	CAD-C3D-C2D	6.04	130.59	113.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	0QA	O2-N3-N2-C10

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
3	A	502	0QA	4	0
2	B	501	HEM	1	0
3	B	502	0QA	5	0
2	C	501	HEM	3	0
3	C	502	0QA	4	0
2	D	501	HEM	2	0
3	D	502	0QA	5	0
2	E	501	HEM	3	0
3	E	502	0QA	3	0
2	F	501	HEM	9	0
3	F	502	0QA	9	0
2	G	501	HEM	6	0
4	G	502	GOL	2	0
2	H	501	HEM	6	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, 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	464/476 (97%)	0.28	0 100 100	20, 35, 53, 63	0
1	B	464/476 (97%)	0.28	1 (0%) 95 98	19, 35, 54, 62	0
1	C	464/476 (97%)	0.23	1 (0%) 95 98	19, 33, 48, 58	0
1	D	464/476 (97%)	0.26	1 (0%) 95 98	17, 35, 55, 63	0
1	E	464/476 (97%)	0.32	13 (2%) 56 69	27, 48, 70, 78	0
1	F	464/476 (97%)	0.70	35 (7%) 17 26	27, 60, 85, 91	0
1	G	463/476 (97%)	0.73	38 (8%) 14 23	29, 59, 78, 88	0
1	H	459/476 (96%)	1.09	98 (21%) 1 2	28, 71, 92, 96	0
All	All	3706/3808 (97%)	0.48	187 (5%) 32 47	17, 44, 81, 96	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	141	GLY	6.6
1	H	491	PHE	6.2
1	F	491	PHE	5.4
1	H	468	PRO	5.1
1	H	453	PHE	5.0
1	G	419	LYS	4.8
1	F	141	GLY	4.8
1	G	491	PHE	4.7
1	F	168	ILE	4.6
1	H	273	ILE	4.6
1	F	172	PHE	4.5
1	H	416	PHE	4.5
1	H	343	PHE	4.4
1	F	206	LEU	4.4
1	H	420	LYS	4.3
1	H	434	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	317	LEU	4.2
1	E	420	LYS	4.1
1	G	456	ILE	4.1
1	H	454	THR	3.9
1	H	489	MET	3.9
1	H	133	ALA	3.9
1	H	452	PHE	3.8
1	H	156	LEU	3.8
1	G	165	GLY	3.6
1	H	153	ALA	3.6
1	H	428	ALA	3.6
1	H	406	SER	3.6
1	H	450	PHE	3.6
1	H	154	GLY	3.6
1	H	259	LEU	3.6
1	G	317	LEU	3.6
1	G	471	ILE	3.5
1	H	449	LEU	3.5
1	H	347	ALA	3.4
1	H	267	PHE	3.4
1	F	355	VAL	3.4
1	F	247	PHE	3.3
1	G	157	ILE	3.3
1	H	316	LEU	3.3
1	G	282	PRO	3.3
1	G	420	LYS	3.2
1	H	462	PHE	3.2
1	H	136	ARG	3.2
1	F	492	LEU	3.2
1	G	468	PRO	3.2
1	H	159	ALA	3.2
1	E	343	PHE	3.1
1	H	261	PRO	3.1
1	H	426	SER	3.1
1	G	462	PHE	3.1
1	F	143	ARG	3.1
1	H	315	LEU	3.1
1	F	451	LEU	3.1
1	H	53	GLN	3.0
1	H	352	THR	3.0
1	H	350	PRO	3.0
1	E	135	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	143	ARG	3.0
1	H	362	PHE	3.0
1	G	323	VAL	3.0
1	H	405	PHE	3.0
1	H	330	GLU	3.0
1	F	288	LEU	3.0
1	G	173	PHE	2.9
1	G	188	GLY	2.9
1	H	427	ASP	2.9
1	H	351	TYR	2.9
1	F	261	PRO	2.9
1	H	334	VAL	2.9
1	H	430	VAL	2.9
1	H	98	PHE	2.9
1	H	271	PHE	2.9
1	H	412	ASN	2.9
1	G	464	SER	2.9
1	H	447	MET	2.8
1	H	263	SER	2.8
1	F	191	PHE	2.8
1	H	161	ARG	2.8
1	H	333	ARG	2.8
1	H	483	ILE	2.8
1	G	140	VAL	2.7
1	H	326	LYS	2.7
1	G	408	PRO	2.7
1	F	461	ARG	2.7
1	F	189	ASP	2.7
1	H	417	LEU	2.7
1	G	213	ALA	2.7
1	H	340	GLN	2.6
1	H	329	GLU	2.6
1	H	138	PHE	2.6
1	F	282	PRO	2.6
1	H	463	LYS	2.6
1	G	211	PHE	2.6
1	H	476	LYS	2.6
1	H	135	LEU	2.6
1	H	338	ASN	2.6
1	H	185	ILE	2.6
1	F	173	PHE	2.5
1	G	138	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	280	LYS	2.5
1	H	348	LYS	2.5
1	F	202	LEU	2.5
1	G	218	GLN	2.5
1	H	363	GLY	2.5
1	H	325	ALA	2.5
1	H	469	LYS	2.5
1	F	263	SER	2.5
1	F	280	LYS	2.5
1	G	475	PRO	2.5
1	H	145	ILE	2.5
1	E	352	THR	2.5
1	H	157	ILE	2.5
1	H	472	ASP	2.5
1	F	447	MET	2.4
1	H	187	PHE	2.4
1	H	177	THR	2.4
1	F	174	LEU	2.4
1	F	259	LEU	2.4
1	H	493	PRO	2.4
1	H	456	ILE	2.4
1	D	189	ASP	2.4
1	G	480	PHE	2.4
1	H	264	PRO	2.4
1	G	327	VAL	2.4
1	F	450	PHE	2.4
1	H	280	LYS	2.3
1	G	153	ALA	2.3
1	G	423	PHE	2.3
1	H	402	PRO	2.3
1	F	411	PHE	2.3
1	E	335	ILE	2.3
1	G	137	GLY	2.3
1	H	158	ASP	2.3
1	H	419	LYS	2.3
1	G	461	ARG	2.3
1	H	144	GLY	2.3
1	H	182	ILE	2.3
1	H	471	ILE	2.3
1	F	198	PHE	2.3
1	E	348	LYS	2.3
1	G	204	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	403	ARG	2.3
1	F	420	LYS	2.2
1	E	460	PHE	2.2
1	G	463	LYS	2.2
1	H	309	THR	2.2
1	H	473	VAL	2.2
1	E	453	PHE	2.2
1	F	187	PHE	2.2
1	F	348	LYS	2.2
1	H	487	TYR	2.2
1	F	318	MET	2.2
1	G	315	LEU	2.2
1	H	368	MET	2.2
1	E	421	GLY	2.1
1	H	147	GLU	2.1
1	G	187	PHE	2.1
1	H	365	MET	2.1
1	H	414	GLN	2.1
1	E	469	LYS	2.1
1	H	346	ARG	2.1
1	G	210	GLN	2.1
1	H	90	ALA	2.1
1	F	493	PRO	2.1
1	H	474	SER	2.1
1	F	185	ILE	2.1
1	H	248	ILE	2.1
1	E	419	LYS	2.1
1	F	31	GLY	2.1
1	G	189	ASP	2.1
1	G	406	SER	2.1
1	H	321	PRO	2.1
1	H	337	LYS	2.1
1	H	247	PHE	2.1
1	B	409	ARG	2.0
1	H	54	MET	2.0
1	F	481	ALA	2.0
1	H	331	ILE	2.0
1	H	482	THR	2.0
1	F	271	PHE	2.0
1	H	492	LEU	2.0
1	H	82	CYS	2.0
1	H	342	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	329	GLU	2.0
1	E	492	LEU	2.0
1	G	107	PHE	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
4	GOL	H	502	6/6	0.94	0.27	6.75	33,36,42,50	0
3	0QA	F	502	15/15	0.90	0.36	5.32	84,85,86,87	0
3	0QA	C	502	15/15	0.91	0.22	4.88	48,55,58,67	0
3	0QA	E	502	15/15	0.90	0.29	4.57	71,74,76,78	0
3	0QA	A	502	15/15	0.94	0.24	4.08	57,62,71,72	0
3	0QA	B	502	15/15	0.91	0.21	2.20	42,51,59,59	0
3	0QA	D	502	15/15	0.94	0.21	2.17	48,55,58,67	0
2	HEM	A	501	43/43	0.98	0.17	0.74	21,27,31,36	0
2	HEM	B	501	43/43	0.98	0.17	0.44	18,25,29,32	0
2	HEM	D	501	43/43	0.98	0.16	0.24	18,26,29,30	0
2	HEM	G	501	43/43	0.98	0.15	-0.09	33,38,43,47	0
2	HEM	E	501	43/43	0.98	0.15	-0.10	30,35,37,39	0
2	HEM	C	501	43/43	0.98	0.15	-0.18	12,22,27,28	0
2	HEM	F	501	43/43	0.97	0.16	-0.20	37,49,54,59	0
4	GOL	G	502	6/6	0.92	0.16	-0.31	54,56,58,58	0
2	HEM	H	501	43/43	0.96	0.16	-0.43	47,52,60,63	0

6.5 Other polymers

There are no such residues in this entry.