Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:33 AM GMT

PDB ID	:	3ME6
Title	:	Crystal structure of cytochrome 2B4 in complex with the anti-platelet drug clopidogrel
Authors	:	Gay, S.C.; Roberts, A.G.; Maekawa, K.; Talakad, J.C.; Hong, W.X.; Zhang, Q.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2010-03-31
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

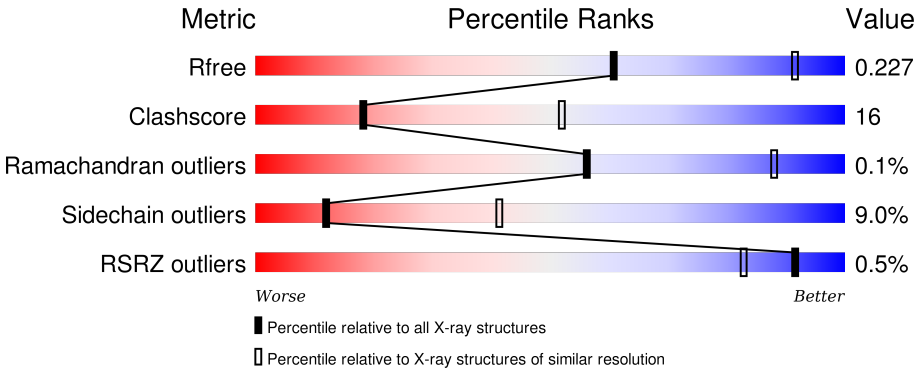
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	476	67% 26%
1	B	476	66% 28%
1	C	476	% 67% 28%
1	D	476	68% 25% 5%

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	CGE	A	501	-	-	-	X
3	CGE	B	501	-	-	X	X
3	CGE	C	501	-	-	X	X
3	CGE	D	501	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15302 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3723	2402	643	667	11			
1	B	465	Total	C	N	O	S	0	1	0
			3729	2405	646	667	11			
1	C	465	Total	C	N	O	S	0	1	0
			3729	2405	646	667	11			
1	D	465	Total	C	N	O	S	0	1	0
			3733	2407	646	669	11			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	SER	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	GLY	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	ARG	DELETION	UNP P00178
A	22	LYS	GLY	ENGINEERED	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	ENGINEERED	UNP P00178
A	24	THR	PRO	ENGINEERED	UNP P00178
A	25	SER	LYS	ENGINEERED	UNP P00178
A	26	SER	ALA	ENGINEERED	UNP P00178
A	27	LYS	HIS	ENGINEERED	UNP P00178
A	29	LYS	ARG	ENGINEERED	UNP P00178
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	ENGINEERED	UNP P00178
A	492	HIS	-	EXPRESSION TAG	UNP P00178
A	493	HIS	-	EXPRESSION TAG	UNP P00178
A	494	HIS	-	EXPRESSION TAG	UNP P00178
A	495	HIS	-	EXPRESSION TAG	UNP P00178
B	21	ALA	GLU	ENGINEERED	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	SER	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	GLY	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	ARG	DELETION	UNP P00178
B	22	LYS	GLY	ENGINEERED	UNP P00178
B	23	LYS	HIS	ENGINEERED	UNP P00178
B	24	THR	PRO	ENGINEERED	UNP P00178
B	25	SER	LYS	ENGINEERED	UNP P00178
B	26	SER	ALA	ENGINEERED	UNP P00178
B	27	LYS	HIS	ENGINEERED	UNP P00178
B	29	LYS	ARG	ENGINEERED	UNP P00178
B	221	SER	PRO	SEE REMARK 999	UNP P00178
B	226	TYR	HIS	ENGINEERED	UNP P00178
B	492	HIS	-	EXPRESSION TAG	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	EXPRESSION TAG	UNP P00178
B	494	HIS	-	EXPRESSION TAG	UNP P00178
B	495	HIS	-	EXPRESSION TAG	UNP P00178
C	21	ALA	GLU	ENGINEERED	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	SER	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	GLY	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	ARG	DELETION	UNP P00178
C	22	LYS	GLY	ENGINEERED	UNP P00178
C	23	LYS	HIS	ENGINEERED	UNP P00178
C	24	THR	PRO	ENGINEERED	UNP P00178
C	25	SER	LYS	ENGINEERED	UNP P00178
C	26	SER	ALA	ENGINEERED	UNP P00178
C	27	LYS	HIS	ENGINEERED	UNP P00178
C	29	LYS	ARG	ENGINEERED	UNP P00178
C	221	SER	PRO	SEE REMARK 999	UNP P00178
C	226	TYR	HIS	ENGINEERED	UNP P00178
C	492	HIS	-	EXPRESSION TAG	UNP P00178
C	493	HIS	-	EXPRESSION TAG	UNP P00178
C	494	HIS	-	EXPRESSION TAG	UNP P00178
C	495	HIS	-	EXPRESSION TAG	UNP P00178
D	21	ALA	GLU	ENGINEERED	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	SER	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178

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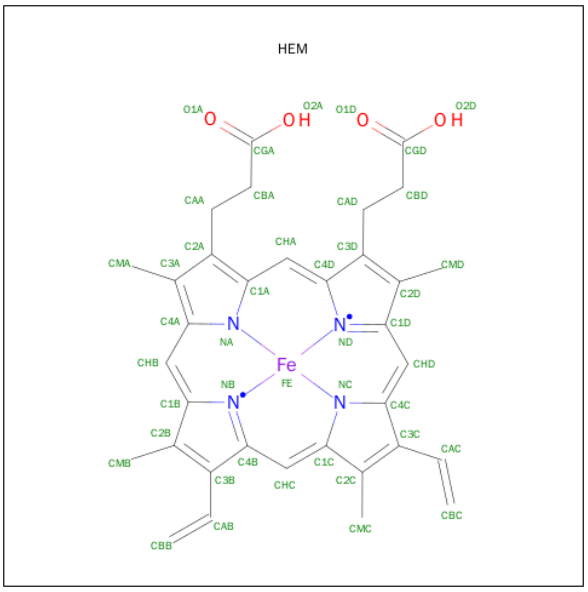
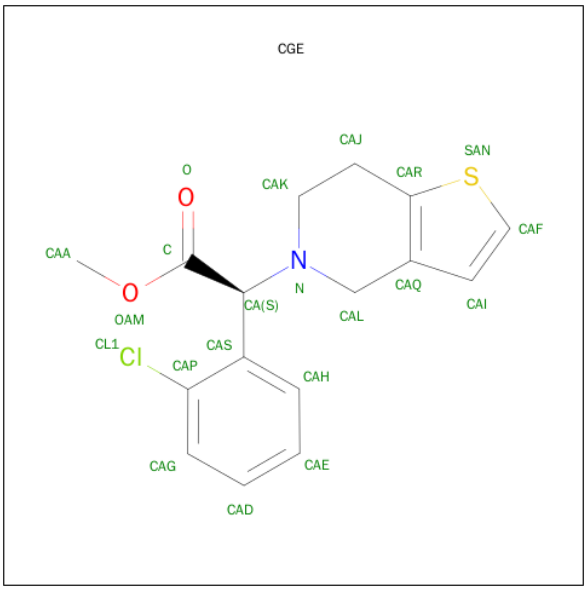
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	GLY	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	ARG	DELETION	UNP P00178
D	22	LYS	GLY	ENGINEERED	UNP P00178
D	23	LYS	HIS	ENGINEERED	UNP P00178
D	24	THR	PRO	ENGINEERED	UNP P00178
D	25	SER	LYS	ENGINEERED	UNP P00178
D	26	SER	ALA	ENGINEERED	UNP P00178
D	27	LYS	HIS	ENGINEERED	UNP P00178
D	29	LYS	ARG	ENGINEERED	UNP P00178
D	221	SER	PRO	SEE REMARK 999	UNP P00178
D	226	TYR	HIS	ENGINEERED	UNP P00178
D	492	HIS	-	EXPRESSION TAG	UNP P00178
D	493	HIS	-	EXPRESSION TAG	UNP P00178
D	494	HIS	-	EXPRESSION TAG	UNP P00178
D	495	HIS	-	EXPRESSION TAG	UNP P00178

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



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

- Molecule 3 is CLOPIDOGREL (three-letter code: CGE) (formula: $C_{16}H_{16}ClNO_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			21	16	1	1	2	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			21	16	1	1	2	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			21	16	1	1	2	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			21	16	1	1	2	1		

- Molecule 4 is water.

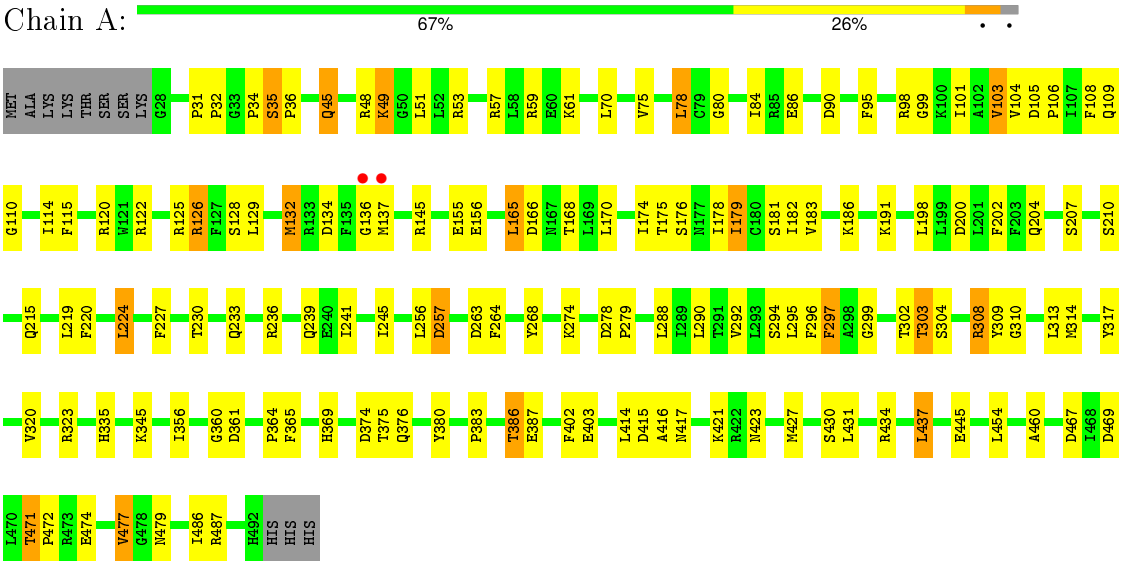
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	35	Total	O	0	0
			35	35		
4	C	32	Total	O	0	0
			32	32		
4	D	35	Total	O	0	0
			35	35		

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.

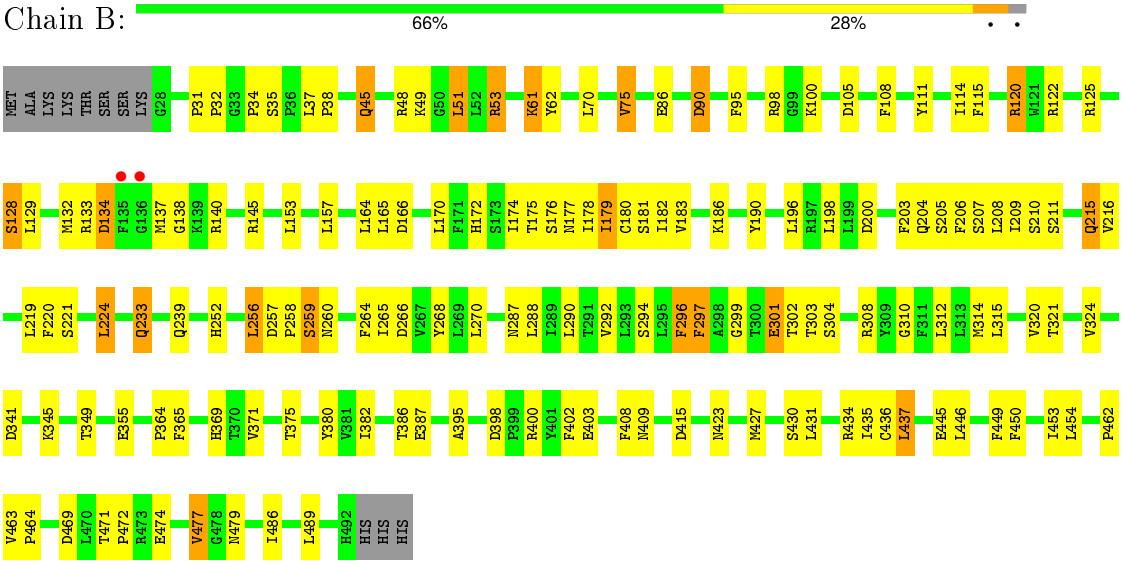
- Molecule 1: Cytochrome P450 2B4

Chain A:



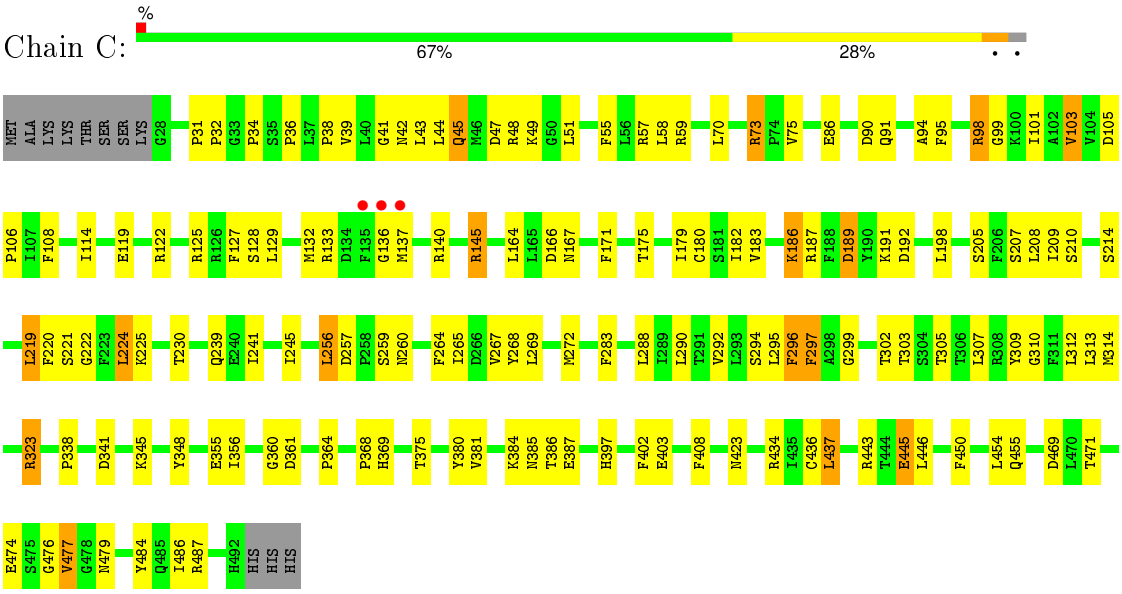
- Molecule 1: Cytochrome P450 2B4

Chain B:



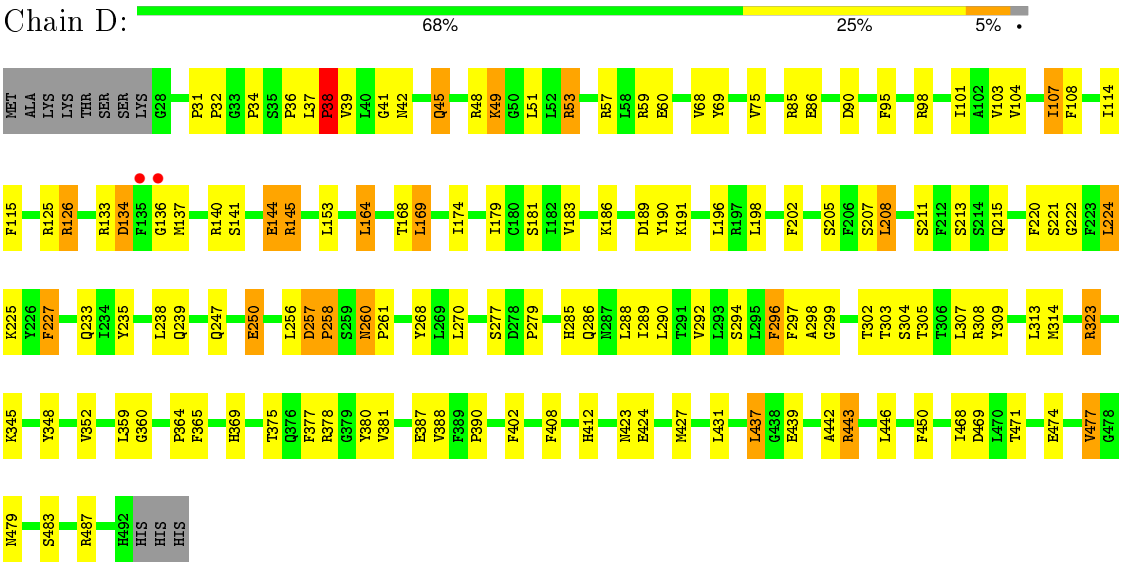
- Molecule 1: Cytochrome P450 2B4

Chain C:



• Molecule 1: Cytochrome P450 2B4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	234.49Å 234.49Å 57.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.75 – 3.10 76.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (76.75-3.10) 97.7 (76.75-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.178 , 0.234 0.178 , 0.227	Depositor DCC
R_{free} test set	3169 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.459 for -h,-k,l 0.467 for h,-h-k,-l 0.460 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 62520 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15302	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: HEM, CGE

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	0.91	0/3820	0.96	8/5173 (0.2%)
1	B	0.91	0/3826	0.97	8/5180 (0.2%)
1	C	0.94	1/3826 (0.0%)	0.96	7/5180 (0.1%)
1	D	0.95	2/3830 (0.1%)	0.96	6/5185 (0.1%)
All	All	0.93	3/15302 (0.0%)	0.96	29/20718 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	38	PRO	N-CD	5.31	1.55	1.47
1	D	258	PRO	N-CD	5.22	1.55	1.47
1	C	119	GLU	CG-CD	5.09	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	445	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	D	134	ASP	N-CA-C	5.88	126.88	111.00
1	B	400	ARG	CB-CA-C	5.87	122.15	110.40
1	C	259	SER	CB-CA-C	5.86	121.23	110.10
1	D	164	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	259	SER	CB-CA-C	5.76	121.05	110.10
1	C	323	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	313	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	B	260	ASN	N-CA-CB	-5.65	100.43	110.60
1	D	443	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	323	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	443	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	120	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	134	ASP	N-CA-C	5.50	125.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	260	ASN	N-CA-CB	-5.46	100.77	110.60
1	A	263	ASP	N-CA-CB	-5.41	100.87	110.60
1	D	323	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	257	ASP	CB-CA-C	5.33	121.06	110.40
1	A	78	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	165	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	A	308	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	90	ASP	CB-CA-C	-5.18	100.03	110.40
1	C	58	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	133	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	256	LEU	CB-CA-C	-5.15	100.42	110.20
1	A	134	ASP	N-CA-C	5.10	124.76	111.00
1	A	323	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	308	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	256	LEU	CA-CB-CG	5.00	126.80	115.30

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	3723	0	3722	113	0
1	B	3729	0	3733	109	0
1	C	3729	0	3733	117	0
1	D	3733	0	3737	121	0
2	A	43	0	30	6	0
2	B	43	0	30	9	0
2	C	43	0	30	5	0
2	D	43	0	30	7	0
3	A	21	0	16	6	0
3	B	21	0	16	8	0
3	C	21	0	16	8	0
3	D	21	0	16	8	0
4	A	30	0	0	2	0
4	B	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	32	0	0	1	0
4	D	35	0	0	5	0
All	All	15302	0	15109	472	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 16.

All (472) 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:D:307:LEU:HD23	1:D:450[A]:PHE:CE2	1.52	1.45
1:C:307:LEU:HD23	1:C:450[A]:PHE:CE1	1.59	1.38
1:C:122:ARG:HD2	4:C:1160:HOH:O	1.35	1.27
1:D:75:VAL:HG12	1:D:387:GLU:HB3	1.16	1.14
1:A:297:PHE:HB3	3:A:501:CGE:HAJA	1.30	1.11
1:B:297:PHE:HB3	3:B:501:CGE:HAJA	1.33	1.10
1:B:75:VAL:HG12	1:B:387:GLU:HB3	1.28	1.08
1:D:125:ARG:HG3	1:D:437:LEU:HD11	1.39	1.03
1:A:137:MET:N	1:A:145:ARG:HH12	1.56	1.03
1:C:307:LEU:HD23	1:C:450[A]:PHE:CD1	1.91	1.03
1:D:126:ARG:HG3	1:D:126:ARG:HH11	1.20	1.02
1:D:307:LEU:CD2	1:D:450[A]:PHE:CE2	2.44	1.01
1:D:220:PHE:HB2	1:D:224:LEU:HD12	1.44	0.99
1:C:220:PHE:HB2	1:C:224:LEU:HD12	1.44	0.97
1:D:137:MET:H	1:D:145:ARG:HH12	1.06	0.96
1:A:31:PRO:HA	1:A:380:TYR:CE1	2.01	0.96
1:C:297:PHE:HB3	3:C:501:CGE:HAJA	1.47	0.95
1:B:31:PRO:HA	1:B:380:TYR:CE1	2.02	0.94
1:A:256:LEU:HD12	1:A:257:ASP:H	1.33	0.94
1:C:256:LEU:HD12	1:C:257:ASP:H	1.29	0.94
1:D:137:MET:N	1:D:145:ARG:HH12	1.67	0.93
1:B:137:MET:N	1:B:145:ARG:HH12	1.67	0.93
1:A:75:VAL:HG12	1:A:387:GLU:HB3	1.50	0.92
1:D:305:THR:HG22	4:D:1095:HOH:O	1.68	0.92
1:C:307:LEU:CD2	1:C:450[A]:PHE:CE1	2.53	0.90
1:A:183:VAL:HG11	1:A:292:VAL:HG13	1.52	0.90
2:D:500:HEM:HBB2	2:D:500:HEM:HMB1	1.52	0.90
1:D:31:PRO:HA	1:D:380:TYR:CE1	2.06	0.90
1:D:86:GLU:HA	1:D:90:ASP:OD2	1.71	0.90
1:B:220:PHE:HB2	1:B:224:LEU:HD12	1.52	0.89
1:C:75:VAL:HG12	1:C:387:GLU:HB3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:HD23	1:D:450[A]:PHE:CD2	2.05	0.88
1:C:307:LEU:CD2	1:C:450[A]:PHE:CD1	2.57	0.88
1:A:220:PHE:HB2	1:A:224:LEU:HD12	1.53	0.87
1:D:297:PHE:HB3	3:D:501:CGE:HAJA	1.56	0.87
1:C:307:LEU:HD23	1:C:450[A]:PHE:HE1	1.04	0.86
1:D:220:PHE:HB2	1:D:224:LEU:CD1	2.03	0.86
1:B:210:SER:HA	4:B:1078:HOH:O	1.74	0.86
1:A:137:MET:H	1:A:145:ARG:HH12	1.18	0.85
1:A:210:SER:HA	4:A:1071:HOH:O	1.74	0.85
1:D:49:LYS:HE2	1:D:53:ARG:HD2	1.58	0.85
1:B:75:VAL:CG1	1:B:387:GLU:HB3	2.07	0.84
1:D:125:ARG:HG3	1:D:437:LEU:CD1	2.08	0.84
1:D:286:GLN:HG3	4:D:1168:HOH:O	1.76	0.83
1:C:179:ILE:HG21	1:C:296:PHE:HA	1.59	0.83
1:D:75:VAL:HG12	1:D:387:GLU:CB	2.04	0.83
1:C:314:MET:HE2	1:C:314:MET:HA	1.59	0.83
1:B:86:GLU:HA	1:B:90:ASP:OD2	1.78	0.83
1:D:307:LEU:HD23	1:D:450[A]:PHE:HE2	0.99	0.83
1:C:31:PRO:HA	1:C:380:TYR:CE1	2.15	0.82
1:A:477:VAL:HG13	3:A:501:CGE:HAA	1.63	0.81
1:C:137:MET:N	1:C:145:ARG:HH12	1.78	0.80
1:D:256:LEU:HD12	1:D:257:ASP:H	1.45	0.80
1:A:145:ARG:HD3	1:A:181:SER:OG	1.82	0.79
1:D:307:LEU:CD2	1:D:450[A]:PHE:CD2	2.64	0.79
1:A:86:GLU:O	1:A:90:ASP:HB2	1.83	0.79
1:C:86:GLU:HA	1:C:90:ASP:OD2	1.81	0.79
1:D:51:LEU:HD12	1:D:215:GLN:HG2	1.63	0.78
1:C:477:VAL:HG13	3:C:501:CGE:HAA	1.62	0.78
2:C:500:HEM:ND	3:C:501:CGE:HAD	1.99	0.78
1:D:307:LEU:CD2	1:D:450[A]:PHE:HE2	1.89	0.78
1:B:125:ARG:HG3	1:B:437:LEU:HD11	1.64	0.77
1:B:120:ARG:HD3	1:B:287:ASN:HD21	1.49	0.77
1:A:86:GLU:HA	1:A:90:ASP:OD2	1.85	0.76
1:D:179:ILE:HG21	1:D:296:PHE:HA	1.67	0.76
1:C:314:MET:CE	1:C:314:MET:HA	2.16	0.76
1:B:206:PHE:CD2	1:B:301:GLU:HG2	2.20	0.76
1:A:125:ARG:CZ	1:A:437:LEU:HD12	2.17	0.74
1:A:122:ARG:HD2	4:A:1130:HOH:O	1.88	0.74
1:D:126:ARG:NH1	1:D:126:ARG:HG3	1.98	0.73
1:D:227:PHE:N	1:D:227:PHE:HD1	1.85	0.73
2:D:500:HEM:HBB2	2:D:500:HEM:CMB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:LEU:O	1:C:450[A]:PHE:HB2	1.89	0.72
1:A:137:MET:N	1:A:145:ARG:NH1	2.33	0.72
1:D:220:PHE:CB	1:D:224:LEU:HD12	2.18	0.72
2:B:500:HEM:C4D	3:B:501:CGE:HAD	2.24	0.72
3:D:501:CGE:HAK	3:D:501:CGE:CAH	2.20	0.71
1:B:402:PHE:CE1	1:B:423:ASN:ND2	2.58	0.71
1:C:268:TYR:CE1	1:C:288:LEU:HB2	2.26	0.71
1:D:137:MET:H	1:D:145:ARG:NH1	1.84	0.71
1:B:449:PHE:O	1:B:453:ILE:HG13	1.91	0.71
1:A:80:GLY:O	1:A:84:ILE:HD12	1.91	0.70
1:D:126:ARG:CG	1:D:126:ARG:HH11	2.01	0.70
1:B:125:ARG:CZ	1:B:437:LEU:HD12	2.22	0.70
1:A:70:LEU:HB3	1:A:219:LEU:HD12	1.72	0.70
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.27	0.70
1:D:227:PHE:CD1	1:D:227:PHE:N	2.58	0.69
1:B:137:MET:H	1:B:145:ARG:HH12	1.38	0.69
1:D:125:ARG:CG	1:D:437:LEU:HD11	2.21	0.69
1:B:114:ILE:HD12	1:B:294:SER:HB3	1.73	0.69
1:A:125:ARG:HG3	1:A:437:LEU:HD11	1.75	0.69
1:B:469:ASP:OD2	1:B:471:THR:HB	1.93	0.69
1:A:125:ARG:HG3	1:A:437:LEU:CD1	2.24	0.68
1:C:86:GLU:O	1:C:90:ASP:HB2	1.94	0.68
1:A:402:PHE:CE1	1:A:423:ASN:ND2	2.61	0.68
1:C:70:LEU:HD22	1:C:219:LEU:HD11	1.76	0.68
1:C:469:ASP:OD2	1:C:471:THR:HB	1.94	0.68
2:A:500:HEM:ND	3:A:501:CGE:HAD	2.09	0.67
1:B:49:LYS:HB3	1:B:53:ARG:HG2	1.76	0.67
1:B:86:GLU:O	1:B:90:ASP:HB2	1.94	0.67
1:A:469:ASP:OD2	1:A:471:THR:HB	1.95	0.67
1:D:57:ARG:O	1:D:60:GLU:HG2	1.95	0.67
1:C:307:LEU:CD2	1:C:450[A]:PHE:HD1	2.08	0.66
1:D:75:VAL:CG1	1:D:387:GLU:HB3	2.10	0.66
2:C:500:HEM:C4D	3:C:501:CGE:HAD	2.29	0.66
1:D:31:PRO:HA	1:D:380:TYR:CD1	2.31	0.66
1:B:98:ARG:HG2	1:B:115:PHE:HA	1.77	0.66
1:A:80:GLY:O	1:A:84:ILE:CD1	2.44	0.66
1:B:369:HIS:HE1	2:B:500:HEM:O2A	1.78	0.65
1:D:32:PRO:HD3	1:D:380:TYR:CE1	2.31	0.65
1:C:136:GLY:C	1:C:145:ARG:HH12	1.99	0.65
1:A:137:MET:H	1:A:145:ARG:NH1	1.92	0.65
1:B:233:GLN:OE1	1:B:233:GLN:HA	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:MET:N	1:C:145:ARG:NH1	2.45	0.64
1:D:183:VAL:HG11	1:D:292:VAL:HG13	1.80	0.63
1:B:239:GLN:OE1	1:B:239:GLN:HA	1.96	0.63
1:C:220:PHE:HB2	1:C:224:LEU:CD1	2.23	0.63
1:B:427:MET:HE2	1:B:431:LEU:HD11	1.80	0.63
1:A:374:ASP:OD1	1:A:383:PRO:HA	1.99	0.63
1:D:250:GLU:HA	1:D:250:GLU:OE2	1.99	0.63
1:A:132:MET:HG2	1:A:182:ILE:HG21	1.79	0.62
1:D:137:MET:N	1:D:145:ARG:NH1	2.43	0.62
3:C:501:CGE:CAH	3:C:501:CGE:HAK	2.29	0.62
1:C:179:ILE:HG13	1:C:299:GLY:HA3	1.81	0.62
1:B:129:LEU:HD23	1:B:437:LEU:HG	1.80	0.62
1:D:134:ASP:C	1:D:134:ASP:OD1	2.38	0.61
1:C:32:PRO:HD3	1:C:380:TYR:CE1	2.35	0.61
1:D:169:LEU:HB2	4:D:1055:HOH:O	2.01	0.61
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.36	0.61
1:A:314:MET:HA	1:A:314:MET:HE2	1.83	0.60
1:B:179:ILE:HG21	1:B:296:PHE:HA	1.82	0.60
1:B:114:ILE:HD12	1:B:294:SER:CB	2.31	0.60
1:B:128:SER:HB3	1:B:437:LEU:HD21	1.82	0.60
1:B:183:VAL:HG11	1:B:292:VAL:HG13	1.83	0.60
1:C:114:ILE:HD12	1:C:294:SER:HB3	1.83	0.60
1:B:179:ILE:HG22	1:B:180:CYS:N	2.16	0.60
1:C:222:GLY:HA2	1:C:225:LYS:HE3	1.84	0.59
1:A:101:ILE:HG22	1:A:103:VAL:HG23	1.85	0.59
1:D:427:MET:HE2	1:D:431:LEU:HD11	1.84	0.59
1:D:314:MET:HE2	1:D:450[B]:PHE:HZ	1.67	0.59
1:D:95:PHE:O	1:D:369:HIS:HD2	1.86	0.59
1:A:175:THR:HG22	1:A:445:GLU:OE1	2.03	0.58
1:D:323:ARG:HB2	1:D:348:TYR:CE2	2.37	0.58
1:A:314:MET:HA	1:A:314:MET:CE	2.33	0.58
1:D:164:LEU:HD23	1:D:487:ARG:HB3	1.86	0.58
1:D:446:LEU:O	1:D:450[A]:PHE:HB2	2.04	0.58
2:B:500:HEM:ND	3:B:501:CGE:HAD	2.19	0.58
1:B:61:LYS:HB3	1:B:62:TYR:CD2	2.39	0.58
1:C:132:MET:HG2	1:C:182:ILE:HG21	1.85	0.58
1:D:369:HIS:HE1	2:D:500:HEM:O2A	1.86	0.58
1:C:183:VAL:HG11	1:C:292:VAL:HG13	1.84	0.58
1:D:34:PRO:HB2	1:D:45:GLN:OE1	2.04	0.58
1:C:256:LEU:HD12	1:C:257:ASP:N	2.12	0.57
2:D:500:HEM:ND	3:D:501:CGE:HAD	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:HA	1:C:290:LEU:HD13	1.85	0.57
1:D:469:ASP:OD2	1:D:471:THR:HB	2.03	0.57
1:C:114:ILE:CD1	1:C:294:SER:HB3	2.34	0.57
1:C:36:PRO:HA	1:C:41:GLY:O	2.05	0.57
1:C:205:SER:O	1:C:209:ILE:HG13	2.04	0.57
1:C:34:PRO:HG2	1:C:42:ASN:ND2	2.20	0.57
3:A:501:CGE:HAK	3:A:501:CGE:CAH	2.35	0.57
1:D:126:ARG:NH1	1:D:126:ARG:CG	2.62	0.57
1:D:309:TYR:CE2	1:D:360:GLY:HA2	2.39	0.57
1:B:98:ARG:NH2	2:B:500:HEM:O2D	2.32	0.57
1:A:256:LEU:HD12	1:A:257:ASP:N	2.13	0.57
1:D:297:PHE:HD1	3:D:501:CGE:HAKA	1.69	0.57
1:C:95:PHE:O	1:C:369:HIS:HD2	1.87	0.57
1:B:205:SER:O	1:B:209:ILE:HG13	2.05	0.56
1:A:309:TYR:CE2	1:A:360:GLY:HA2	2.40	0.56
1:C:164:LEU:HD23	1:C:487:ARG:HB3	1.87	0.56
1:B:31:PRO:HA	1:B:380:TYR:CD1	2.41	0.56
1:B:175:THR:HG22	1:B:445:GLU:OE1	2.04	0.56
1:A:49:LYS:HE3	1:A:53:ARG:HG2	1.88	0.56
1:A:434:ARG:HB3	2:A:500:HEM:O1A	2.06	0.56
3:B:501:CGE:HAK	3:B:501:CGE:CAH	2.36	0.56
1:D:140:ARG:NH2	1:D:145:ARG:HG2	2.20	0.56
1:D:36:PRO:HA	1:D:41:GLY:O	2.05	0.56
1:B:111:TYR:HB2	1:B:290:LEU:HD12	1.88	0.56
1:C:114:ILE:HD12	1:C:294:SER:CB	2.35	0.56
1:A:179:ILE:HG21	1:A:296:PHE:HA	1.88	0.56
1:B:125:ARG:HG3	1:B:437:LEU:CD1	2.35	0.55
1:C:314:MET:CE	1:C:314:MET:CA	2.85	0.55
1:B:355:GLU:HG3	1:B:408:PHE:CE1	2.41	0.55
1:A:32:PRO:HD3	1:A:380:TYR:OH	2.07	0.55
1:C:38:PRO:O	1:C:39:VAL:HB	2.06	0.55
1:C:307:LEU:HA	1:C:450[A]:PHE:HE1	1.70	0.55
1:D:86:GLU:O	1:D:90:ASP:HB2	2.07	0.55
1:B:220:PHE:HB2	1:B:224:LEU:CD1	2.31	0.55
1:D:98:ARG:HG2	1:D:115:PHE:HA	1.87	0.55
1:B:446:LEU:O	1:B:450[A]:PHE:HD2	1.90	0.55
1:A:51:LEU:HD12	1:A:215:GLN:HG2	1.89	0.55
1:D:314:MET:HE1	1:D:352:VAL:HG11	1.89	0.55
1:D:258:PRO:HA	1:D:270:LEU:HD21	1.89	0.54
1:A:125:ARG:CG	1:A:437:LEU:HD11	2.37	0.54
1:C:31:PRO:HA	1:C:380:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:PHE:CE1	1:C:423:ASN:ND2	2.76	0.54
1:C:136:GLY:CA	1:C:145:ARG:HH12	2.21	0.54
1:C:103:VAL:HG21	1:C:214:SER:HB3	1.88	0.54
1:C:477:VAL:CG1	3:C:501:CGE:HAA	2.35	0.53
1:D:37:LEU:O	1:D:38:PRO:C	2.47	0.53
1:C:297:PHE:HD2	1:C:297:PHE:O	1.92	0.53
1:D:107:ILE:HD12	1:D:238:LEU:HB2	1.90	0.53
1:C:73:ARG:HH11	1:C:73:ARG:HG3	1.72	0.53
1:C:384:LYS:HG2	1:C:385:ASN:HD22	1.74	0.53
1:A:34:PRO:HB2	1:A:45:GLN:OE1	2.09	0.53
1:A:361:ASP:CG	1:A:361:ASP:O	2.46	0.53
1:D:323:ARG:HD3	4:D:1112:HOH:O	2.09	0.53
1:A:297:PHE:CB	3:A:501:CGE:HAJA	2.21	0.53
1:B:145:ARG:HD3	1:B:181:SER:OG	2.08	0.53
1:A:178:ILE:O	1:A:182:ILE:HG13	2.09	0.53
1:A:403:GLU:HG3	1:B:403:GLU:HG3	1.91	0.53
1:A:241:ILE:O	1:A:245:ILE:HG13	2.09	0.53
1:C:297:PHE:CB	3:C:501:CGE:HAJA	2.29	0.52
1:A:460:ALA:HB3	1:A:487:ARG:HG2	1.92	0.52
1:A:31:PRO:HA	1:A:380:TYR:HE1	1.71	0.52
1:A:70:LEU:HB3	1:A:219:LEU:CD1	2.38	0.52
1:C:125:ARG:HG3	1:C:437:LEU:CD1	2.39	0.52
1:A:32:PRO:HD3	1:A:380:TYR:CE1	2.45	0.52
1:A:220:PHE:HB2	1:A:224:LEU:CD1	2.32	0.52
1:C:136:GLY:HA3	1:C:145:ARG:HH12	1.74	0.52
1:B:98:ARG:HB2	1:B:434:ARG:NH1	2.24	0.52
1:C:140:ARG:HH21	1:C:145:ARG:HG2	1.74	0.52
1:B:427:MET:CE	1:B:431:LEU:HD11	2.39	0.52
1:A:98:ARG:HG3	1:A:99:GLY:O	2.09	0.52
1:C:129:LEU:HD23	1:C:437:LEU:HG	1.92	0.52
1:B:172:HIS:HE1	1:B:203:PHE:CD1	2.27	0.52
1:D:314:MET:CE	1:D:352:VAL:HG11	2.41	0.51
1:D:314:MET:CE	1:D:450[B]:PHE:HZ	2.22	0.51
1:A:98:ARG:HG2	1:A:115:PHE:HA	1.92	0.51
1:B:114:ILE:CD1	1:B:294:SER:HB3	2.40	0.50
1:B:51:LEU:HB2	1:B:215:GLN:HG2	1.93	0.50
1:D:314:MET:HE2	1:D:450[B]:PHE:CZ	2.45	0.50
1:A:129:LEU:CD2	1:A:437:LEU:HG	2.40	0.50
1:D:168:THR:HA	1:D:308:ARG:HD2	1.94	0.50
1:C:51:LEU:HD22	1:C:55:PHE:CZ	2.46	0.50
1:A:430:SER:CB	2:A:500:HEM:HBA1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASP:OD1	1:A:204:GLN:HG3	2.11	0.50
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.11	0.50
1:D:314:MET:HE1	1:D:352:VAL:CG1	2.42	0.50
1:D:285:HIS:O	1:D:289:ILE:HG12	2.12	0.50
1:B:430:SER:HB3	2:B:500:HEM:HBA1	1.94	0.50
1:D:477:VAL:HG13	3:D:501:CGE:HAA	1.94	0.50
1:D:298:ALA:HA	3:D:501:CGE:HAK	1.92	0.49
1:C:256:LEU:CD1	1:C:257:ASP:H	2.14	0.49
1:B:268:TYR:CZ	1:B:288:LEU:HB2	2.47	0.49
1:A:98:ARG:HB2	1:A:434:ARG:NH1	2.27	0.49
1:D:107:ILE:HD11	1:D:235:TYR:HA	1.95	0.49
1:D:101:ILE:HB	1:D:104:VAL:HG22	1.94	0.49
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.48	0.49
1:C:310:GLY:O	1:C:314:MET:HG2	2.13	0.49
1:A:233:GLN:OE1	1:A:233:GLN:HA	2.12	0.49
1:A:415:ASP:O	1:A:416:ALA:C	2.51	0.49
1:C:32:PRO:HD3	1:C:380:TYR:CZ	2.48	0.49
1:A:95:PHE:O	1:A:369:HIS:HD2	1.96	0.49
1:B:100:LYS:HD2	1:B:105:ASP:CG	2.32	0.49
1:A:125:ARG:CZ	1:A:437:LEU:CD1	2.90	0.48
1:C:98:ARG:HG3	1:C:99:GLY:O	2.13	0.48
1:B:206:PHE:CD2	1:B:301:GLU:CG	2.94	0.48
1:B:132:MET:HG2	1:B:182:ILE:HG21	1.94	0.48
2:D:500:HEM:HMB1	2:D:500:HEM:CBB	2.35	0.48
1:A:430:SER:HB3	2:A:500:HEM:HBA1	1.94	0.48
1:C:208:LEU:HD22	1:C:230:THR:HB	1.95	0.48
1:C:361:ASP:O	1:C:361:ASP:CG	2.51	0.48
1:C:307:LEU:HD21	1:C:450[A]:PHE:HD1	1.79	0.48
1:A:299:GLY:HA2	2:A:500:HEM:HMC3	1.96	0.48
1:A:376:GLN:HA	1:A:380:TYR:O	2.12	0.48
1:A:168:THR:HA	1:A:308:ARG:HD2	1.95	0.48
1:D:402:PHE:CE1	1:D:423:ASN:ND2	2.82	0.48
1:B:364:PRO:HG3	1:B:479:ASN:ND2	2.28	0.48
1:A:183:VAL:HA	1:A:264:PHE:HB3	1.96	0.48
1:B:179:ILE:HG21	1:B:296:PHE:CD1	2.49	0.48
1:B:34:PRO:HB2	1:B:45:GLN:OE1	2.14	0.48
1:A:317:TYR:HB3	1:A:320:VAL:HG23	1.96	0.48
1:D:299:GLY:HA2	2:D:500:HEM:HMC3	1.96	0.47
1:A:471:THR:HA	1:A:472:PRO:HD3	1.72	0.47
1:A:310:GLY:O	1:A:314:MET:HG2	2.15	0.47
1:C:183:VAL:HA	1:C:264:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASN:ND2	1:C:171:PHE:CE2	2.80	0.47
1:D:134:ASP:O	1:D:134:ASP:OD1	2.33	0.47
1:C:91:GLN:HB3	1:C:94:ALA:HB3	1.96	0.47
1:B:95:PHE:O	1:B:369:HIS:HD2	1.97	0.47
1:C:299:GLY:HA2	2:C:500:HEM:HMC2	1.95	0.47
1:B:128:SER:HB3	1:B:437:LEU:CD2	2.44	0.47
1:B:108:PHE:HA	1:B:290:LEU:HD13	1.96	0.47
1:D:38:PRO:O	1:D:39:VAL:HB	2.14	0.47
1:D:313:LEU:HD13	1:D:408:PHE:CD1	2.50	0.47
1:D:239:GLN:OE1	1:D:239:GLN:HA	2.14	0.47
1:A:114:ILE:CD1	1:A:294:SER:HB3	2.44	0.47
1:B:355:GLU:CD	1:B:409:ASN:O	2.54	0.47
1:C:128:SER:HB2	1:C:437:LEU:HD21	1.96	0.47
1:B:45:GLN:HE21	1:B:45:GLN:N	2.13	0.47
1:B:137:MET:HB3	1:B:145:ARG:NH1	2.30	0.46
1:D:49:LYS:CE	1:D:53:ARG:HD2	2.38	0.46
1:A:174:ILE:O	1:A:178:ILE:HG12	2.15	0.46
1:A:364:PRO:HG3	1:A:479:ASN:ND2	2.31	0.46
1:A:335:HIS:HB2	1:C:341:ASP:OD2	2.15	0.46
1:D:45:GLN:N	1:D:45:GLN:HE21	2.13	0.46
1:D:364:PRO:HG3	1:D:479:ASN:ND2	2.30	0.46
1:C:283:PHE:N	1:C:283:PHE:CD1	2.83	0.46
2:B:500:HEM:CHA	3:B:501:CGE:HAD	2.46	0.46
1:C:323:ARG:HB2	1:C:348:TYR:CE2	2.51	0.46
1:D:85:ARG:NH2	1:D:424:GLU:O	2.46	0.46
1:B:190:TYR:O	1:B:196:LEU:HD21	2.15	0.46
1:D:114:ILE:HD12	1:D:294:SER:HB3	1.97	0.46
1:B:209:ILE:HD13	3:B:501:CGE:HAI	1.98	0.46
1:B:153:LEU:HD22	1:B:174:ILE:HD13	1.98	0.46
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.70	0.46
1:B:200:ASP:CG	1:B:204:GLN:HE21	2.19	0.46
1:A:129:LEU:HD23	1:A:437:LEU:HG	1.97	0.46
1:A:179:ILE:HG21	1:A:296:PHE:HD1	1.80	0.46
1:C:338:PRO:HD3	1:C:455:GLN:OE1	2.16	0.46
1:B:164:LEU:HD21	1:B:462:PRO:HD3	1.98	0.46
1:C:47:ASP:OD2	1:C:57:ARG:HD3	2.16	0.46
1:A:136:GLY:HA3	1:A:145:ARG:HH22	1.81	0.46
1:D:365:PHE:CE1	1:D:477:VAL:HG23	2.51	0.46
1:B:320:VAL:O	1:B:321:THR:C	2.52	0.46
1:D:323:ARG:CD	4:D:1112:HOH:O	2.63	0.46
1:C:132:MET:HE1	1:C:437:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:HA	1:A:290:LEU:HD13	1.97	0.46
1:C:127:PHE:CZ	1:C:267:VAL:HG12	2.51	0.46
1:B:415:ASP:C	1:B:415:ASP:OD1	2.55	0.46
1:C:189:ASP:OD2	1:C:189:ASP:C	2.54	0.45
1:D:307:LEU:HD21	1:D:450[A]:PHE:CD2	2.48	0.45
1:B:175:THR:OG1	1:B:304:SER:HB3	2.17	0.45
1:C:210:SER:HB2	1:C:476:GLY:HA3	1.97	0.45
1:C:137:MET:H	1:C:145:ARG:HH12	1.63	0.45
1:D:205:SER:HA	1:D:208:LEU:HD12	1.97	0.45
2:A:500:HEM:C4D	3:A:501:CGE:HAD	2.51	0.45
1:D:423:ASN:OD1	1:D:423:ASN:C	2.55	0.45
1:A:49:LYS:HB2	1:A:49:LYS:HE3	1.64	0.45
1:C:355:GLU:HG3	1:C:408:PHE:CD1	2.52	0.45
1:D:108:PHE:HA	1:D:290:LEU:HD13	1.99	0.45
1:D:179:ILE:HD12	1:D:179:ILE:HG23	1.81	0.45
1:D:179:ILE:HG13	1:D:299:GLY:HA3	1.98	0.45
1:D:256:LEU:CD1	1:D:257:ASP:H	2.21	0.45
1:A:423:ASN:C	1:A:423:ASN:OD1	2.55	0.45
1:B:435:ILE:O	1:B:436:CYS:C	2.54	0.45
1:C:186:LYS:HG2	1:C:187:ARG:N	2.32	0.45
1:B:134:ASP:C	1:B:134:ASP:OD2	2.55	0.45
1:C:241:ILE:O	1:C:245:ILE:HG13	2.17	0.45
1:B:395:ALA:HA	1:B:398:ASP:HB2	1.98	0.45
1:A:156:GLU:HG2	1:A:170:LEU:HD21	1.98	0.45
1:D:359:LEU:HA	1:D:359:LEU:HD12	1.80	0.45
1:C:309:TYR:CE2	1:C:360:GLY:HA2	2.52	0.45
1:C:486:ILE:HG23	1:C:486:ILE:O	2.17	0.45
1:B:310:GLY:O	1:B:314:MET:HG2	2.17	0.45
1:B:324:VAL:HG13	1:B:349:THR:OG1	2.17	0.45
1:C:179:ILE:HG23	1:C:179:ILE:HD12	1.71	0.44
1:B:32:PRO:HD3	1:B:380:TYR:OH	2.17	0.44
1:B:365:PHE:CE1	1:B:477:VAL:HG23	2.52	0.44
1:B:477:VAL:HG13	3:B:501:CGE:HAA	1.99	0.44
1:C:477:VAL:HG13	3:C:501:CGE:CAA	2.40	0.44
1:D:202:PHE:CE1	1:D:297:PHE:CD2	3.05	0.44
1:B:252:HIS:CB	1:B:265:ILE:HG21	2.47	0.44
1:D:277:SER:O	1:D:279:PRO:HD3	2.18	0.44
1:C:101:ILE:HD11	1:C:368:PRO:HD3	1.99	0.44
1:A:101:ILE:HB	1:A:104:VAL:HG22	1.99	0.44
1:B:174:ILE:O	1:B:178:ILE:HG12	2.18	0.44
1:B:178:ILE:O	1:B:182:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HD12	1:A:294:SER:CB	2.47	0.44
1:D:260:ASN:HA	1:D:261:PRO:HD2	1.69	0.44
1:B:371:VAL:HG21	1:B:382:ILE:HG22	1.98	0.44
1:A:427:MET:HE2	1:A:431:LEU:HD11	2.00	0.44
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.81	0.44
1:C:105:ASP:N	1:C:106:PRO:HD2	2.32	0.44
1:D:268:TYR:CZ	1:D:288:LEU:HB2	2.52	0.44
1:C:133:ARG:H	1:C:133:ARG:HG3	1.52	0.44
1:D:307:LEU:HA	1:D:450[A]:PHE:HE2	1.83	0.44
1:D:297:PHE:CD1	3:D:501:CGE:HAKA	2.52	0.44
1:D:31:PRO:HA	1:D:380:TYR:HE1	1.73	0.44
1:B:183:VAL:HA	1:B:264:PHE:HB3	2.00	0.44
1:B:204:GLN:O	1:B:208:LEU:HG	2.18	0.44
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.84	0.44
1:C:239:GLN:HA	1:C:239:GLN:OE1	2.18	0.43
1:C:140:ARG:HH21	1:C:145:ARG:CG	2.31	0.43
1:B:471:THR:HA	1:B:472:PRO:HD3	1.83	0.43
1:A:114:ILE:HD12	1:A:294:SER:HB3	2.00	0.43
1:C:364:PRO:HG3	1:C:479:ASN:ND2	2.33	0.43
1:C:310:GLY:HA3	1:C:450[A]:PHE:HZ	1.84	0.43
1:A:365:PHE:CE1	1:A:477:VAL:HG23	2.52	0.43
1:B:179:ILE:HG21	1:B:296:PHE:HD1	1.84	0.43
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.53	0.43
1:C:45:GLN:N	1:C:45:GLN:HE21	2.16	0.43
1:B:256:LEU:HG	1:B:257:ASP:N	2.33	0.43
1:D:222:GLY:HA2	1:D:225:LYS:HE3	2.01	0.43
1:C:192:ASP:OD1	1:C:192:ASP:C	2.56	0.43
1:B:297:PHE:CB	3:B:501:CGE:HAJA	2.24	0.43
2:D:500:HEM:C4D	3:D:501:CGE:HAD	2.54	0.43
1:A:132:MET:HE2	1:A:132:MET:HB2	1.59	0.43
1:A:179:ILE:CG2	1:A:296:PHE:HD1	2.31	0.43
1:C:356:ILE:O	1:C:360:GLY:N	2.52	0.43
1:B:37:LEU:O	1:B:38:PRO:C	2.57	0.43
1:D:190:TYR:O	1:D:196:LEU:HD21	2.18	0.43
1:D:268:TYR:CG	1:D:288:LEU:HD13	2.54	0.43
1:B:172:HIS:HD2	1:B:304:SER:OG	2.02	0.42
1:A:278:ASP:HA	1:A:279:PRO:HD2	1.85	0.42
1:D:68:VAL:HG22	1:D:69:TYR:H	1.83	0.42
1:B:53:ARG:HB2	1:B:53:ARG:HE	1.65	0.42
1:D:95:PHE:HE1	1:D:388:VAL:HG21	1.83	0.42
1:D:141:SER:OG	1:D:144:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.78	0.42
1:A:179:ILE:HD13	1:A:179:ILE:HA	1.48	0.42
1:C:125:ARG:HG3	1:C:437:LEU:HD13	2.00	0.42
1:A:35:SER:HA	1:A:36:PRO:HD3	1.93	0.42
1:B:265:ILE:HG22	1:B:266:ASP:N	2.35	0.42
1:C:269:LEU:O	1:C:272:MET:HB2	2.19	0.42
1:B:341:ASP:C	1:B:341:ASP:OD1	2.58	0.42
1:B:70:LEU:HB3	1:B:219:LEU:HD12	2.02	0.42
1:D:32:PRO:HD3	1:D:380:TYR:HE1	1.78	0.42
1:B:312:LEU:O	1:B:315:LEU:HB2	2.19	0.42
1:B:299:GLY:HA2	2:B:500:HEM:HMC3	2.02	0.42
1:B:125:ARG:CZ	1:B:437:LEU:CD1	2.94	0.42
1:A:310:GLY:HA2	1:A:356:ILE:HD13	2.01	0.42
1:A:415:ASP:O	1:A:417:ASN:N	2.53	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.79	0.42
1:B:434:ARG:HB3	2:B:500:HEM:O1A	2.20	0.42
1:A:70:LEU:HD22	1:A:219:LEU:HD11	2.01	0.42
1:C:403:GLU:OE2	1:D:412:HIS:HD2	2.03	0.42
1:A:314:MET:CE	1:A:314:MET:CA	2.98	0.41
1:C:183:VAL:O	1:C:265:ILE:HG12	2.20	0.41
1:A:200:ASP:O	1:A:204:GLN:HB2	2.19	0.41
1:C:434:ARG:HB3	2:C:500:HEM:O1A	2.20	0.41
1:C:70:LEU:HB3	1:C:219:LEU:HD12	2.02	0.41
1:A:403:GLU:N	1:B:403:GLU:OE2	2.47	0.41
1:D:307:LEU:HD21	1:D:450[A]:PHE:HD2	1.84	0.41
1:A:365:PHE:HE1	1:A:477:VAL:HG23	1.85	0.41
1:C:220:PHE:O	1:C:224:LEU:HD12	2.20	0.41
1:A:32:PRO:HD3	1:A:380:TYR:CZ	2.55	0.41
1:B:355:GLU:HG3	1:B:408:PHE:CD1	2.55	0.41
1:B:369:HIS:CE1	2:B:500:HEM:O2A	2.67	0.41
1:D:439:GLU:HG3	1:D:443:ARG:HD3	2.03	0.41
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.90	0.41
1:B:138:GLY:O	1:B:140:ARG:HG3	2.20	0.41
1:D:307:LEU:HA	1:D:450[A]:PHE:CE2	2.56	0.41
1:C:297:PHE:C	1:C:297:PHE:CD2	2.94	0.41
1:D:95:PHE:CE1	1:D:388:VAL:HG21	2.56	0.41
1:A:268:TYR:CZ	1:A:288:LEU:HB2	2.54	0.41
1:A:175:THR:OG1	1:A:304:SER:HB3	2.20	0.41
1:D:153:LEU:HD22	1:D:174:ILE:HD13	2.02	0.41
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.56	0.41
1:A:125:ARG:HG3	1:A:437:LEU:HD13	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:HG21	1:A:445:GLU:CD	2.41	0.41
1:C:313:LEU:HD23	1:C:313:LEU:HA	1.87	0.41
1:D:37:LEU:O	1:D:38:PRO:O	2.39	0.41
1:C:175:THR:HG22	1:C:445:GLU:OE1	2.19	0.41
1:C:180:CYS:SG	1:C:296:PHE:CE1	3.14	0.41
1:D:179:ILE:HA	1:D:179:ILE:HD13	1.65	0.41
1:D:202:PHE:HE1	1:D:297:PHE:CD2	2.38	0.41
1:C:136:GLY:HA3	1:C:145:ARG:NH1	2.35	0.41
1:C:313:LEU:HD13	1:C:408:PHE:CD1	2.56	0.41
1:A:179:ILE:CG2	1:A:296:PHE:CD1	3.04	0.41
1:C:44:LEU:C	1:C:45:GLN:HE21	2.25	0.41
1:C:295:LEU:HA	1:C:295:LEU:HD23	1.81	0.41
1:A:414:LEU:O	1:A:421:LYS:HE2	2.20	0.41
1:A:80:GLY:O	1:A:84:ILE:HD13	2.18	0.40
1:A:427:MET:O	1:A:427:MET:HG3	2.22	0.40
1:D:377:PHE:O	1:D:378:ARG:HB2	2.21	0.40
1:D:140:ARG:NH2	1:D:145:ARG:CG	2.84	0.40
1:D:145:ARG:HD3	1:D:181:SER:OG	2.21	0.40
1:C:436:CYS:HB2	2:C:500:HEM:NA	2.35	0.40
1:C:105:ASP:O	1:C:106:PRO:C	2.60	0.40
1:B:463:VAL:HA	1:B:464:PRO:HD3	1.92	0.40
1:D:136:GLY:HA3	1:D:145:ARG:HH22	1.86	0.40
1:A:383:PRO:HG2	1:A:386:THR:OG1	2.21	0.40
1:B:216:VAL:O	1:B:219:LEU:HB2	2.21	0.40
1:B:258:PRO:HA	1:B:270:LEU:HD21	2.02	0.40
1:C:312:LEU:HD13	1:C:484:TYR:CD1	2.56	0.40
1:C:355:GLU:HG3	1:C:408:PHE:CE1	2.56	0.40
1:B:176:SER:O	1:B:177:ASN:C	2.58	0.40
1:D:442:ALA:O	1:D:446:LEU:HG	2.22	0.40
1:A:105:ASP:N	1:A:106:PRO:HD2	2.37	0.40
1:A:110:GLY:O	1:A:120:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	464/476 (98%)	434 (94%)	30 (6%)	0	100 100
1	B	464/476 (98%)	430 (93%)	34 (7%)	0	100 100
1	C	464/476 (98%)	432 (93%)	31 (7%)	1 (0%)	52 84
1	D	464/476 (98%)	431 (93%)	33 (7%)	0	100 100
All	All	1856/1904 (98%)	1727 (93%)	128 (7%)	1 (0%)	56 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	LEU

5.3.2 Protein sidechains (i)

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	408/421 (97%)	368 (90%)	40 (10%)	10 36
1	B	409/421 (97%)	374 (91%)	35 (9%)	13 45
1	C	409/421 (97%)	379 (93%)	30 (7%)	17 52
1	D	410/421 (97%)	368 (90%)	42 (10%)	9 33
All	All	1636/1684 (97%)	1489 (91%)	147 (9%)	12 41

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	45	GLN
1	A	48	ARG
1	A	49	LYS
1	A	57	ARG
1	A	59	ARG
1	A	61	LYS

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	103	VAL
1	A	109	GLN
1	A	126	ARG
1	A	128	SER
1	A	132	MET
1	A	155	GLU
1	A	165	LEU
1	A	166	ASP
1	A	176	SER
1	A	179	ILE
1	A	186	LYS
1	A	191	LYS
1	A	198	LEU
1	A	202	PHE
1	A	207	SER
1	A	224	LEU
1	A	227	PHE
1	A	230	THR
1	A	236	ARG
1	A	274	LYS
1	A	297	PHE
1	A	302	THR
1	A	303	THR
1	A	345	LYS
1	A	375	THR
1	A	386	THR
1	A	437	LEU
1	A	467	ASP
1	A	471	THR
1	A	474	GLU
1	A	477	VAL
1	A	486	ILE
1	B	35	SER
1	B	45	GLN
1	B	48	ARG
1	B	51	LEU
1	B	53	ARG
1	B	61	LYS
1	B	75	VAL
1	B	122	ARG
1	B	128	SER

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Mol	Chain	Res	Type
1	B	133	ARG
1	B	165	LEU
1	B	166	ASP
1	B	179	ILE
1	B	186	LYS
1	B	198	LEU
1	B	207	SER
1	B	211	SER
1	B	215	GLN
1	B	221	SER
1	B	224	LEU
1	B	233	GLN
1	B	259	SER
1	B	296	PHE
1	B	297	PHE
1	B	301	GLU
1	B	302	THR
1	B	303	THR
1	B	345	LYS
1	B	375	THR
1	B	386	THR
1	B	437	LEU
1	B	474	GLU
1	B	477	VAL
1	B	486	ILE
1	B	489	LEU
1	C	45	GLN
1	C	48	ARG
1	C	49	LYS
1	C	59	ARG
1	C	73	ARG
1	C	98	ARG
1	C	103	VAL
1	C	145	ARG
1	C	166	ASP
1	C	186	LYS
1	C	189	ASP
1	C	191	LYS
1	C	198	LEU
1	C	207	SER
1	C	219	LEU
1	C	221	SER

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Mol	Chain	Res	Type
1	C	224	LEU
1	C	296	PHE
1	C	297	PHE
1	C	302	THR
1	C	303	THR
1	C	305	THR
1	C	345	LYS
1	C	375	THR
1	C	381	VAL
1	C	386	THR
1	C	397	HIS
1	C	437	LEU
1	C	474	GLU
1	C	477	VAL
1	D	38	PRO
1	D	42	ASN
1	D	45	GLN
1	D	48	ARG
1	D	49	LYS
1	D	53	ARG
1	D	59	ARG
1	D	103	VAL
1	D	107	ILE
1	D	126	ARG
1	D	144	GLU
1	D	145	ARG
1	D	169	LEU
1	D	186	LYS
1	D	189	ASP
1	D	191	LYS
1	D	198	LEU
1	D	207	SER
1	D	208	LEU
1	D	211	SER
1	D	213	SER
1	D	221	SER
1	D	224	LEU
1	D	227	PHE
1	D	233	GLN
1	D	247	GLN
1	D	250	GLU
1	D	257	ASP

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Mol	Chain	Res	Type
1	D	260	ASN
1	D	296	PHE
1	D	302	THR
1	D	303	THR
1	D	304	SER
1	D	345	LYS
1	D	375	THR
1	D	381	VAL
1	D	390	PRO
1	D	437	LEU
1	D	468	ILE
1	D	474	GLU
1	D	477	VAL
1	D	483	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	369	HIS
1	B	172	HIS
1	B	204	GLN
1	B	260	ASN
1	B	369	HIS
1	C	369	HIS
1	C	385	ASN
1	D	172	HIS
1	D	260	ASN
1	D	369	HIS
1	D	385	ASN

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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	500	1	30,50,50	2.46	8 (26%)	24,82,82	2.46	13 (54%)
3	CGE	A	501	-	19,23,23	1.77	3 (15%)	19,32,32	4.22	11 (57%)
2	HEM	B	500	1	30,50,50	2.33	11 (36%)	24,82,82	2.53	11 (45%)
3	CGE	B	501	-	19,23,23	1.75	5 (26%)	19,32,32	4.16	11 (57%)
2	HEM	C	500	1	30,50,50	2.45	9 (30%)	24,82,82	2.28	9 (37%)
3	CGE	C	501	-	19,23,23	1.74	3 (15%)	19,32,32	4.28	10 (52%)
2	HEM	D	500	1	30,50,50	2.47	10 (33%)	24,82,82	2.46	10 (41%)
3	CGE	D	501	-	19,23,23	1.73	3 (15%)	19,32,32	4.58	12 (63%)

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	500	1	-	0/10/54/54	0/0/8/8
3	CGE	A	501	-	-	0/14/23/23	0/3/3/3
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
3	CGE	B	501	-	-	0/14/23/23	0/3/3/3
2	HEM	C	500	1	-	0/10/54/54	0/0/8/8
3	CGE	C	501	-	-	0/14/23/23	0/3/3/3
2	HEM	D	500	1	-	0/10/54/54	0/0/8/8
3	CGE	D	501	-	-	0/14/23/23	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C4B	-8.95	1.43	1.51
2	C	500	HEM	C3B-C4B	-8.31	1.44	1.51
2	D	500	HEM	C3B-C4B	-8.16	1.44	1.51
2	B	500	HEM	C3B-C4B	-6.72	1.45	1.51
2	D	500	HEM	C3D-C4D	-5.96	1.43	1.51
2	B	500	HEM	C3D-C4D	-5.72	1.44	1.51
2	A	500	HEM	C3D-C4D	-5.36	1.44	1.51
2	C	500	HEM	C3D-C4D	-5.00	1.45	1.51
2	D	500	HEM	C2C-C1C	-4.34	1.44	1.52
2	A	500	HEM	C2C-C1C	-3.99	1.45	1.52
2	B	500	HEM	C2C-C1C	-3.69	1.45	1.52
3	D	501	CGE	CAS-CA	-3.62	1.48	1.52
3	C	501	CGE	CAS-CA	-3.26	1.48	1.52
2	C	500	HEM	C2C-C1C	-3.25	1.46	1.52
3	A	501	CGE	CAS-CA	-2.74	1.49	1.52
2	C	500	HEM	C2D-C1D	-2.70	1.43	1.51
2	A	500	HEM	C2D-C1D	-2.54	1.43	1.51
2	B	500	HEM	C2D-C1D	-2.44	1.43	1.51
2	C	500	HEM	C2B-C1B	-2.40	1.44	1.51
2	A	500	HEM	C2B-C1B	-2.33	1.44	1.51
2	D	500	HEM	C2B-C1B	-2.23	1.44	1.51
3	B	501	CGE	CAS-CA	-2.21	1.49	1.52
2	D	500	HEM	C2D-C1D	-2.17	1.44	1.51
2	B	500	HEM	C2B-C1B	-2.10	1.45	1.51
2	D	500	HEM	CAA-C2A	2.04	1.55	1.52
2	D	500	HEM	C3B-CAB	2.04	1.55	1.51
3	B	501	CGE	CAK-CAJ	2.16	1.55	1.51
3	B	501	CGE	CAJ-CAR	2.18	1.52	1.50
2	A	500	HEM	FE-ND	2.25	2.09	1.97
2	B	500	HEM	FE-NC	2.27	2.04	1.95
2	B	500	HEM	FE-NB	2.52	2.10	1.97
3	B	501	CGE	CAP-CL1	2.58	1.79	1.73
2	B	500	HEM	CAA-C2A	2.58	1.56	1.52
2	C	500	HEM	CAA-C2A	2.59	1.56	1.52
2	D	500	HEM	C1C-NC	2.60	1.39	1.36
3	D	501	CGE	CAP-CL1	2.62	1.80	1.73
2	B	500	HEM	FE-ND	2.62	2.11	1.97
3	A	501	CGE	CAP-CL1	2.63	1.80	1.73
3	C	501	CGE	CAP-CL1	2.70	1.80	1.73
2	C	500	HEM	C1C-NC	2.71	1.39	1.36
2	B	500	HEM	C1C-NC	2.77	1.39	1.36
2	A	500	HEM	C4C-NC	2.85	1.39	1.36
2	D	500	HEM	FE-NC	2.99	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	FE-NC	3.36	2.09	1.95
2	C	500	HEM	C4C-NC	3.52	1.40	1.36
2	D	500	HEM	C4C-NC	3.66	1.40	1.36
2	B	500	HEM	C4C-NC	3.70	1.40	1.36
2	C	500	HEM	FE-NC	4.17	2.12	1.95
3	D	501	CGE	OAM-C	5.46	1.47	1.33
3	C	501	CGE	OAM-C	5.50	1.47	1.33
3	B	501	CGE	OAM-C	5.77	1.47	1.33
3	A	501	CGE	OAM-C	5.80	1.48	1.33

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	CGE	CAQ-CAL-N	-7.84	100.62	113.62
3	D	501	CGE	CAQ-CAL-N	-7.19	101.70	113.62
3	B	501	CGE	CAQ-CAL-N	-7.12	101.81	113.62
3	A	501	CGE	CAQ-CAL-N	-6.84	102.29	113.62
3	D	501	CGE	CAS-CAP-CL1	-3.73	116.31	120.42
2	B	500	HEM	C3C-CAC-CBC	-3.43	119.20	124.46
2	C	500	HEM	CBA-CAA-C2A	-3.36	106.51	112.53
3	D	501	CGE	CAK-CAJ-CAR	-3.30	106.48	111.66
3	A	501	CGE	OAM-C-O	-3.18	117.22	123.79
3	A	501	CGE	CAK-CAJ-CAR	-3.15	106.70	111.66
3	B	501	CGE	O-C-CA	-3.12	121.12	125.30
3	B	501	CGE	CAS-CAP-CL1	-3.09	117.01	120.42
2	D	500	HEM	C3C-CAC-CBC	-3.07	119.75	124.46
3	A	501	CGE	CAS-CAP-CL1	-3.03	117.08	120.42
3	C	501	CGE	OAM-C-O	-2.97	117.66	123.79
2	B	500	HEM	CMA-C3A-C4A	-2.89	123.58	128.36
3	B	501	CGE	OAM-C-O	-2.77	118.07	123.79
2	D	500	HEM	C3B-CAB-CBB	-2.77	120.20	124.46
2	A	500	HEM	CBA-CAA-C2A	-2.77	107.57	112.53
3	D	501	CGE	OAM-C-O	-2.75	118.11	123.79
2	B	500	HEM	C3B-CAB-CBB	-2.73	120.27	124.46
2	A	500	HEM	C3B-CAB-CBB	-2.71	120.29	124.46
3	C	501	CGE	CAG-CAP-CAS	-2.68	119.51	121.97
3	C	501	CGE	CAK-CAJ-CAR	-2.65	107.49	111.66
2	A	500	HEM	C3C-CAC-CBC	-2.62	120.43	124.46
3	D	501	CGE	O-C-CA	-2.58	121.84	125.30
2	A	500	HEM	CMA-C3A-C4A	-2.54	124.15	128.36
3	D	501	CGE	CAG-CAP-CAS	-2.45	119.73	121.97
2	D	500	HEM	CBD-CAD-C3D	-2.41	106.54	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	CBA-CAA-C2A	-2.37	108.28	112.53
2	A	500	HEM	CAD-CBD-CGD	-2.28	103.72	113.02
3	A	501	CGE	CAG-CAP-CAS	-2.28	119.88	121.97
2	C	500	HEM	C3B-CAB-CBB	-2.14	121.17	124.46
2	C	500	HEM	CAD-CBD-CGD	-2.12	104.36	113.02
2	A	500	HEM	CAA-CBA-CGA	-2.11	108.88	112.75
2	A	500	HEM	CBD-CAD-C3D	-2.11	107.42	113.55
3	C	501	CGE	CAJ-CAK-N	-2.09	105.86	110.64
2	D	500	HEM	CAA-CBA-CGA	-2.06	108.97	112.75
3	B	501	CGE	CAG-CAP-CL1	2.02	122.57	118.39
3	C	501	CGE	CAL-CAQ-CAI	2.05	129.40	127.31
3	D	501	CGE	CAH-CAS-CA	2.13	124.27	120.62
3	A	501	CGE	CAH-CAS-CA	2.14	124.29	120.62
3	B	501	CGE	CAH-CAS-CA	2.17	124.35	120.62
3	A	501	CGE	CAG-CAP-CL1	2.25	123.03	118.39
2	C	500	HEM	C2D-C3D-C4D	2.47	105.69	101.50
2	D	500	HEM	C2D-C3D-C4D	2.57	105.85	101.50
3	B	501	CGE	CAL-CAQ-CAI	2.69	130.06	127.31
3	D	501	CGE	CAG-CAP-CL1	2.69	123.96	118.39
2	A	500	HEM	C2D-C3D-C4D	2.87	106.36	101.50
2	B	500	HEM	C2D-C3D-C4D	2.89	106.41	101.50
2	B	500	HEM	CMD-C2D-C3D	3.03	127.73	114.35
2	D	500	HEM	CMD-C2D-C3D	3.08	127.98	114.35
3	D	501	CGE	CAA-OAM-C	3.08	123.22	115.99
3	C	501	CGE	CAA-OAM-C	3.09	123.24	115.99
2	C	500	HEM	CMD-C2D-C3D	3.28	128.84	114.35
3	A	501	CGE	CAA-OAM-C	3.38	123.91	115.99
2	A	500	HEM	CMD-C2D-C3D	3.38	129.32	114.35
2	B	500	HEM	C3B-C4B-CHC	3.46	128.04	123.16
3	B	501	CGE	CAA-OAM-C	3.50	124.19	115.99
2	C	500	HEM	CMC-C2C-C3C	3.61	125.54	116.53
3	B	501	CGE	CAH-CAS-CAP	3.66	120.75	116.79
2	D	500	HEM	CAD-C3D-C4D	3.83	125.97	112.47
2	A	500	HEM	CAD-C3D-C4D	3.86	126.07	112.47
2	C	500	HEM	CMB-C2B-C3B	3.89	126.25	116.53
2	A	500	HEM	CMC-C2C-C3C	4.00	126.52	116.53
2	B	500	HEM	CMC-C2C-C3C	4.06	126.66	116.53
2	A	500	HEM	CMB-C2B-C3B	4.10	126.76	116.53
2	B	500	HEM	CAD-C3D-C4D	4.11	126.96	112.47
2	B	500	HEM	CMB-C2B-C3B	4.15	126.89	116.53
2	D	500	HEM	CMB-C2B-C3B	4.16	126.90	116.53
2	C	500	HEM	CAD-C3D-C4D	4.38	127.92	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	CGE	CAH-CAS-CAP	4.52	121.67	116.79
2	C	500	HEM	CAD-C3D-C2D	4.58	126.38	113.22
2	B	500	HEM	CAD-C3D-C2D	4.67	126.63	113.22
3	D	501	CGE	CAH-CAS-CAP	4.77	121.94	116.79
2	A	500	HEM	CAD-C3D-C2D	4.99	127.57	113.22
3	C	501	CGE	CAH-CAS-CAP	5.01	122.20	116.79
2	D	500	HEM	CMC-C2C-C3C	5.09	129.24	116.53
2	D	500	HEM	CAD-C3D-C2D	5.20	128.17	113.22
3	C	501	CGE	OAM-C-CA	5.49	119.65	110.83
3	D	501	CGE	OAM-C-CA	5.74	120.05	110.83
3	A	501	CGE	OAM-C-CA	5.77	120.11	110.83
3	B	501	CGE	OAM-C-CA	6.21	120.81	110.83
3	B	501	CGE	CAL-N-CAK	12.50	123.17	110.02
3	A	501	CGE	CAL-N-CAK	12.86	123.54	110.02
3	C	501	CGE	CAL-N-CAK	12.99	123.68	110.02
3	D	501	CGE	CAL-N-CAK	14.62	125.40	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	6	0
3	A	501	CGE	6	0
2	B	500	HEM	9	0
3	B	501	CGE	8	0
2	C	500	HEM	5	0
3	C	501	CGE	8	0
2	D	500	HEM	7	0
3	D	501	CGE	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	465/476 (97%)	0.08	2 (0%)	93	85	10, 41, 72, 87	7 (1%)
1	B	465/476 (97%)	0.07	2 (0%)	93	85	9, 41, 72, 86	2 (0%)
1	C	465/476 (97%)	0.10	3 (0%)	90	80	10, 41, 72, 84	2 (0%)
1	D	465/476 (97%)	0.06	2 (0%)	93	85	9, 41, 72, 84	2 (0%)
All	All	1860/1904 (97%)	0.08	9 (0%)	91	83	9, 41, 72, 87	13 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	GLY	4.9
1	A	136	GLY	4.7
1	C	136	GLY	4.5
1	B	136	GLY	3.7
1	C	135	PHE	2.3
1	A	137	MET	2.3
1	B	135	PHE	2.3
1	D	135	PHE	2.1
1	C	137	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	CGE	D	501	21/21	0.92	0.58	5.00	108,111,111,111	0
3	CGE	B	501	21/21	0.90	0.53	4.77	96,101,102,103	0
3	CGE	C	501	21/21	0.92	0.49	4.41	96,101,101,103	0
3	CGE	A	501	21/21	0.93	0.53	3.80	93,97,98,99	0
2	HEM	B	500	43/43	0.99	0.27	0.30	24,28,32,40	0
2	HEM	A	500	43/43	0.99	0.25	0.02	24,31,34,41	0
2	HEM	D	500	43/43	0.99	0.25	-0.07	11,26,33,37	0
2	HEM	C	500	43/43	0.99	0.25	-0.16	20,26,37,42	0

6.5 Other polymers

There are no such residues in this entry.