Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:49 AM GMT

PDB ID	:	3G5N
Title	:	Triple ligand occupancy crystal structure of cytochrome P450 2B4 in complex with the inhibitor 1-biphenyl-4-methyl-1H-imidazole
Authors	:	Gay, S.C.; Sun, L.; Maekawa, K.; Halpert, J.R.; Stout, C.D.
Deposited on	:	2009-02-05
Resolution	:	2.50 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:

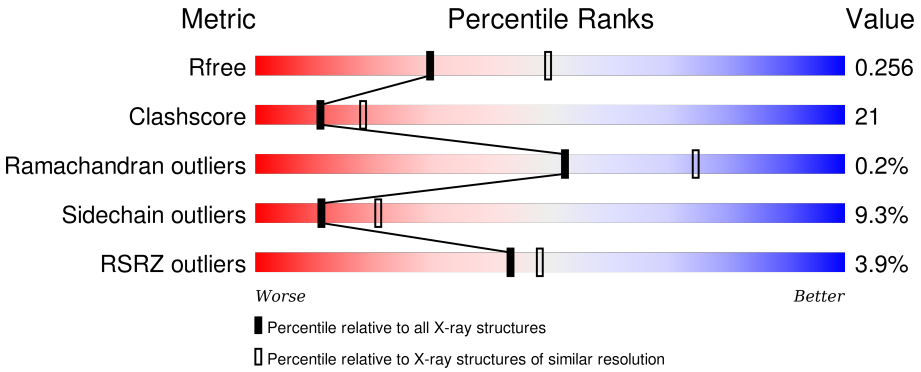
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	4% 67% 24% 5% •
1	B	476	2% 65% 25% • 5%
1	C	476	5% 61% 29% 5% 5%
1	D	476	4% 64% 27% • 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	PB2	A	503	-	-	X	X
3	PB2	B	502	-	-	X	-
3	PB2	B	503	-	-	X	-
3	PB2	C	502	-	-	X	X
3	PB2	C	503	-	-	X	X
3	PB2	D	502	-	-	X	-
3	PB2	D	503	-	-	X	X
4	CM5	A	504	-	-	-	X
4	CM5	B	504	-	-	-	X
4	CM5	C	504	-	-	-	X
4	CM5	D	504	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14746 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	456	Total	C	N	O	S	0	0	0
			3573	2310	607	646	10			
1	B	451	Total	C	N	O	S	0	1	0
			3511	2269	596	637	9			
1	C	452	Total	C	N	O	S	0	1	0
			3504	2265	599	631	9			
1	D	451	Total	C	N	O	S	0	0	0
			3526	2277	600	639	10			

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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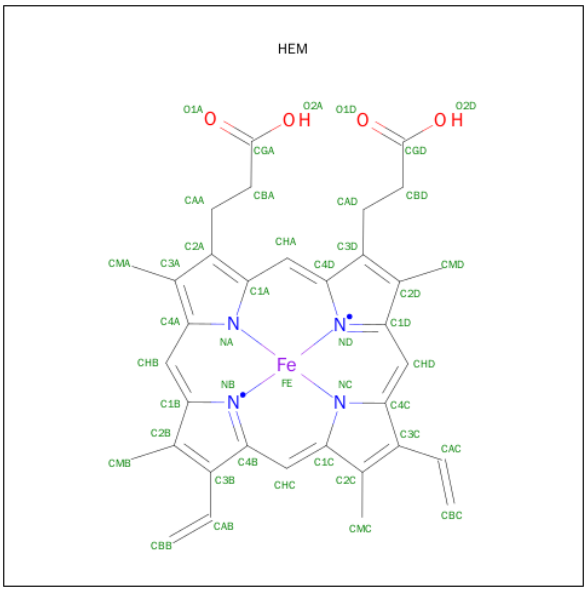
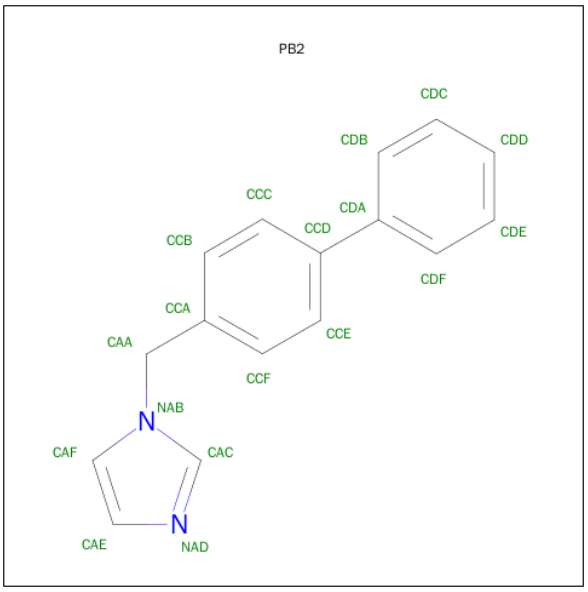
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	GLY	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	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: $C_{34}H_{32}FeN_4O_4$).



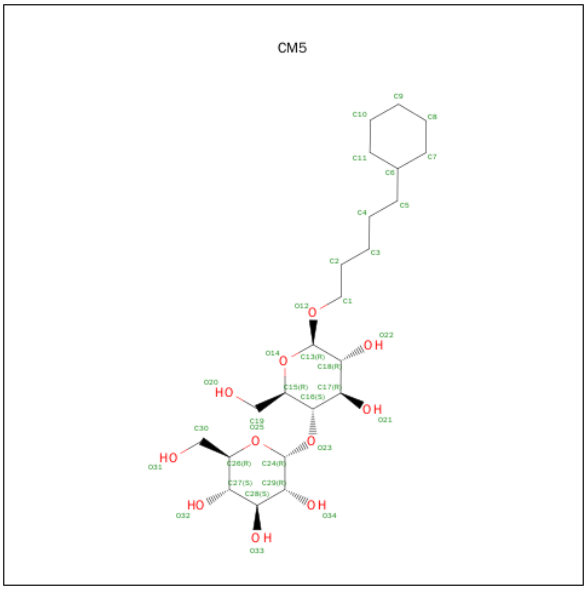
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-(BIPHENYL-4-YLMETHYL)-1H-IMIDAZOLE (three-letter code: PB2) (formula: $C_{16}H_{14}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 18 16 2	0	0
3	A	1	Total C 12 12	0	0
3	B	1	Total C N 18 16 2	0	0
3	B	1	Total C N 18 16 2	0	0
3	B	1	Total C N 18 16 2	0	0
3	B	1	Total C 12 12	0	0
3	C	1	Total C N 18 16 2	0	0
3	C	1	Total C N 18 16 2	0	0
3	C	1	Total C 12 12	0	0
3	D	1	Total C N 18 16 2	0	0
3	D	1	Total C N 18 16 2	0	0
3	D	1	Total C 12 12	0	0

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 17 5	0	0
4	B	1	Total C O 22 17 5	0	0
4	C	1	Total C O 22 17 5	0	0
4	D	1	Total C O 22 17 5	0	0

- Molecule 5 is water.

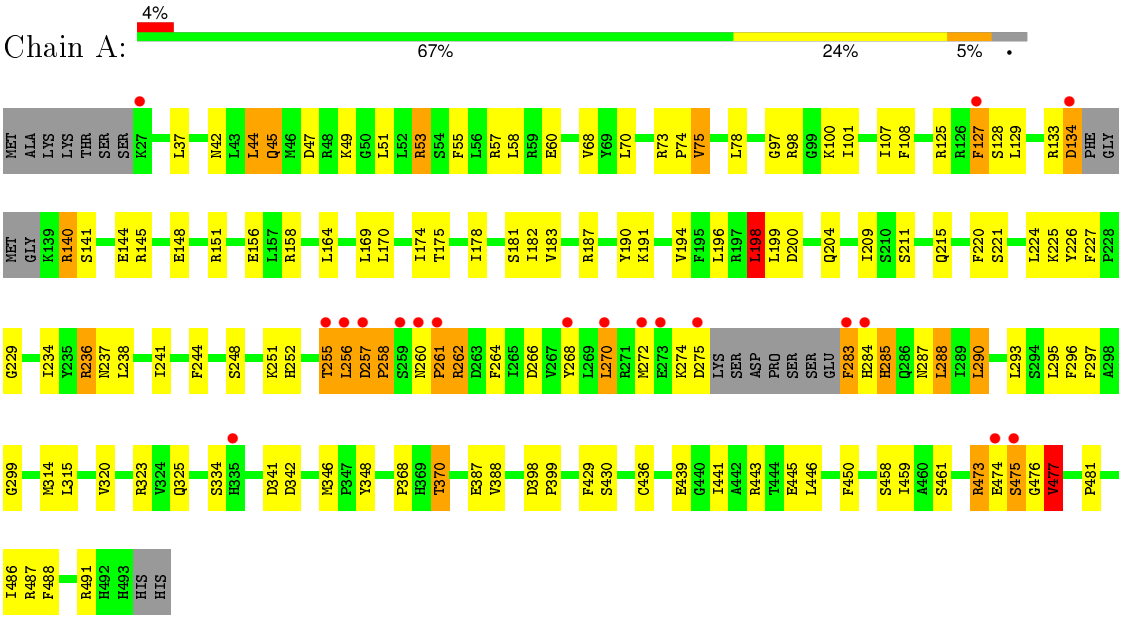
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	B	40	Total O 40 40	0	0
5	C	30	Total O 30 30	0	0
5	D	54	Total O 54 54	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

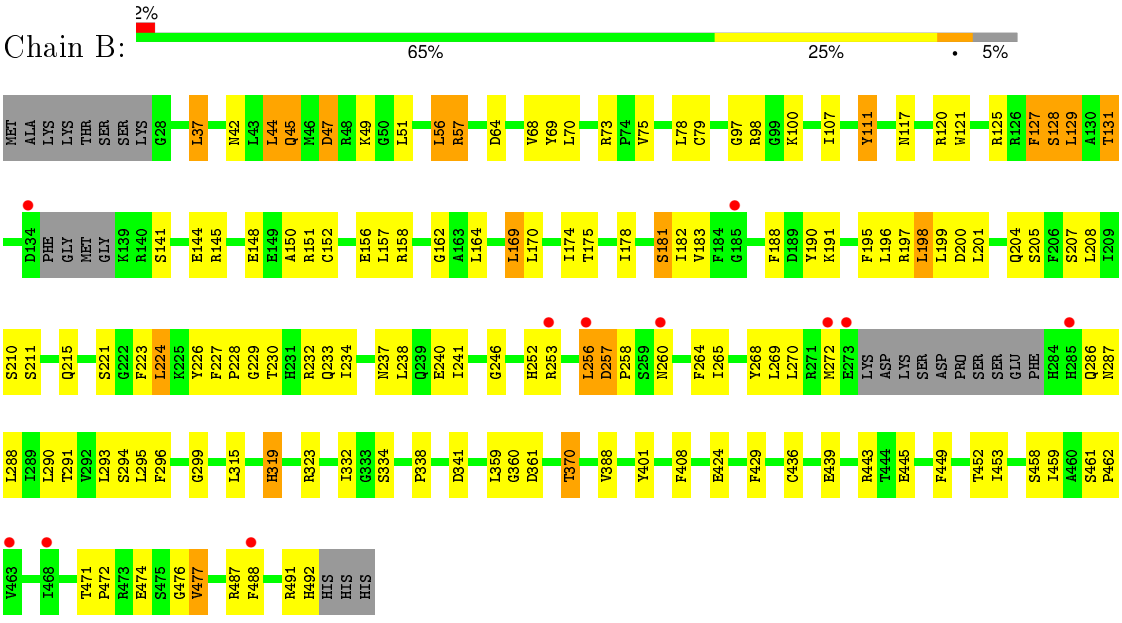
- Molecule 1: Cytochrome P450 2B4

Chain A:



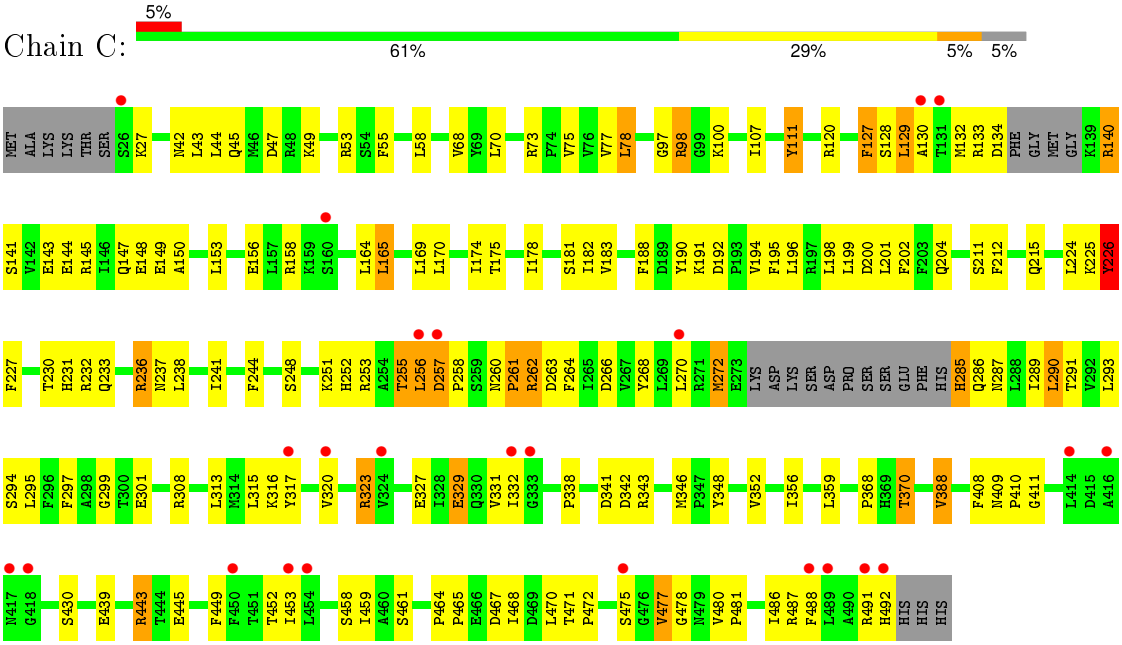
- Molecule 1: Cytochrome P450 2B4

Chain B:



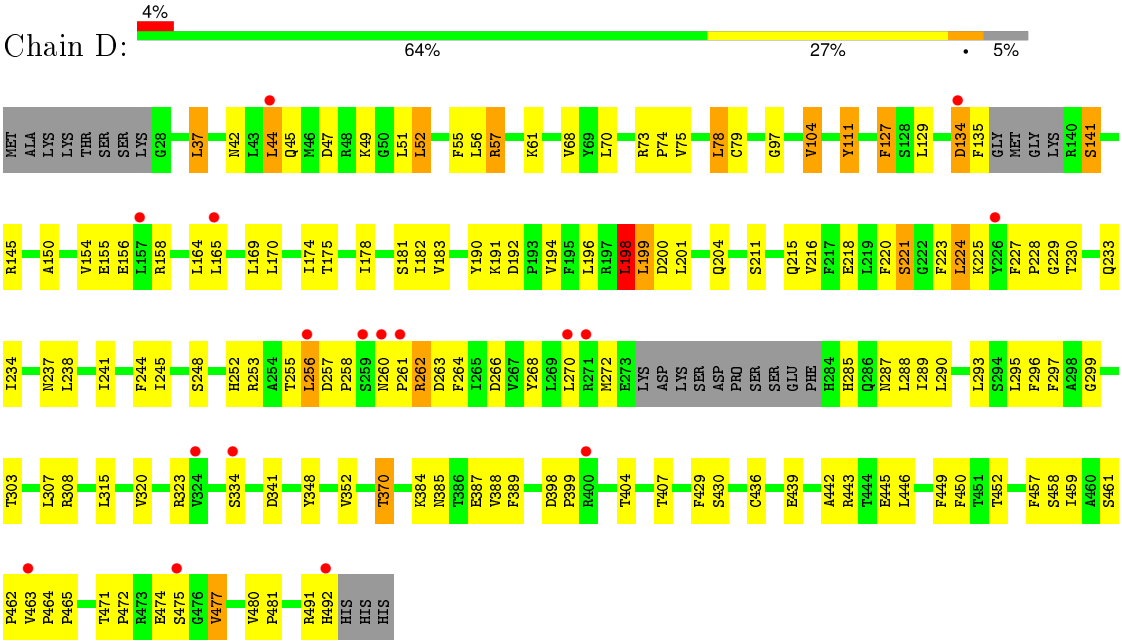
• Molecule 1: Cytochrome P450 2B4

Chain C:



• Molecule 1: Cytochrome P450 2B4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.70Å 152.53Å 181.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.48 – 2.50 45.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.48-2.50) 97.0 (45.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.218 , 0.247 0.230 , 0.256	Depositor DCC
R_{free} test set	4089 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 81677 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14746	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, CM5, PB2

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	0.95	2/3661 (0.1%)	0.92	3/4974 (0.1%)
1	B	0.90	1/3598 (0.0%)	0.86	2/4893 (0.0%)
1	C	0.90	2/3592 (0.1%)	0.91	4/4888 (0.1%)
1	D	0.90	2/3613 (0.1%)	0.88	3/4912 (0.1%)
All	All	0.91	7/14464 (0.0%)	0.89	12/19667 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	VAL	CB-CG1	-5.96	1.40	1.52
1	D	79	CYS	CB-SG	-5.94	1.72	1.81
1	A	388	VAL	CB-CG1	-5.76	1.40	1.52
1	B	388	VAL	CB-CG1	-5.56	1.41	1.52
1	C	388	VAL	CB-CG1	-5.25	1.41	1.52
1	C	226	TYR	CB-CG	5.20	1.59	1.51
1	D	104	VAL	CB-CG1	-5.17	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	111	TYR	N-CA-C	-5.81	95.32	111.00
1	D	198	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	98	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	D	111	TYR	N-CA-C	-5.68	95.67	111.00
1	C	443	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	198	LEU	CA-CB-CG	5.49	127.92	115.30
1	D	111	TYR	C-N-CA	-5.43	110.89	122.30
1	A	285	HIS	N-CA-C	5.37	125.51	111.00
1	B	111	TYR	N-CA-C	-5.19	96.98	111.00
1	B	111	TYR	C-N-CA	-5.10	111.58	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	PRO	N-CA-C	-5.05	98.98	112.10
1	C	120	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	3573	0	3494	146	0
1	B	3511	0	3429	139	0
1	C	3504	0	3407	183	0
1	D	3526	0	3440	139	0
2	A	43	0	30	9	0
2	B	43	0	30	11	0
2	C	43	0	30	5	0
2	D	43	0	30	12	0
3	A	30	0	23	11	0
3	B	66	0	51	22	0
3	C	48	0	37	19	0
3	D	48	0	37	18	0
4	A	22	0	30	1	0
4	B	22	0	30	4	0
4	C	22	0	30	7	0
4	D	22	0	30	1	0
5	A	56	0	0	3	0
5	B	40	0	0	6	0
5	C	30	0	0	0	0
5	D	54	0	0	3	0
All	All	14746	0	14158	600	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 21.

All (600) 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:141:SER:OG	1:C:144:GLU:HG3	1.33	1.26
1:B:56:LEU:O	1:B:56:LEU:HD12	1.35	1.21
1:C:164:LEU:HD23	1:C:487:ARG:CG	1.72	1.19
1:A:141:SER:OG	1:A:144:GLU:HG3	1.42	1.19
1:C:327:GLU:O	1:C:331:VAL:HG23	1.43	1.18
1:C:164:LEU:CD2	1:C:487:ARG:HG3	1.75	1.16
1:B:198:LEU:HD23	1:B:241:ILE:HD12	1.29	1.13
1:C:231:HIS:CE1	1:C:233[B]:GLN:HG2	1.86	1.09
1:C:165:LEU:O	1:C:165:LEU:HD12	1.51	1.08
1:C:256:LEU:O	1:C:256:LEU:HD13	1.52	1.08
1:D:474:GLU:HA	1:D:474:GLU:OE1	1.47	1.06
1:C:164:LEU:CD2	1:C:487:ARG:CG	2.32	1.03
1:C:164:LEU:HD23	1:C:487:ARG:HG2	1.39	1.03
1:C:164:LEU:HD21	1:C:487:ARG:NE	1.75	1.01
2:D:500:HEM:HBC2	2:D:500:HEM:HHD	1.39	1.01
3:C:503:PB2:HDD	1:D:224:LEU:O	1.59	1.01
1:C:231:HIS:CE1	1:C:233[B]:GLN:CG	2.44	1.00
1:B:73:ARG:HB2	3:B:503:PB2:HCB	1.42	1.00
1:A:314:MET:CE	1:A:450:PHE:CZ	2.47	0.98
1:A:44:LEU:HD23	1:B:287:ASN:HD22	1.28	0.97
1:C:165:LEU:HD12	1:C:165:LEU:C	1.82	0.96
1:A:258:PRO:HA	1:A:260:ASN:H	1.29	0.95
1:C:129:LEU:N	1:C:129:LEU:CD1	2.30	0.95
1:A:314:MET:HE1	1:A:450:PHE:CZ	2.04	0.92
3:A:503:PB2:HDF	5:B:525:HOH:O	1.66	0.92
1:A:283:PHE:O	1:A:287:ASN:HB2	1.68	0.92
1:D:266:ASP:O	1:D:270:LEU:HD13	1.70	0.91
1:C:129:LEU:HD13	1:C:129:LEU:N	1.86	0.90
1:B:164:LEU:HD23	1:B:487:ARG:HG3	1.54	0.89
1:A:97:GLY:HA3	1:A:370:THR:HG22	1.52	0.89
1:B:97:GLY:HA3	1:B:370:THR:HG22	1.54	0.89
1:A:145:ARG:HD3	1:A:181:SER:OG	1.74	0.88
1:C:231:HIS:HE1	1:C:233[B]:GLN:CG	1.87	0.87
1:C:129:LEU:HD13	1:C:129:LEU:H	1.37	0.87
1:C:47:ASP:HB3	1:C:49:LYS:H	1.41	0.85
1:D:134:ASP:HB3	1:D:135:PHE:CB	2.06	0.85
1:C:477:VAL:O	1:C:477:VAL:HG13	1.77	0.85
1:B:197:ARG:HG2	1:B:237:ASN:OD1	1.76	0.85
1:C:301:GLU:HG3	5:D:507:HOH:O	1.75	0.84
1:A:314:MET:CE	1:A:450:PHE:HZ	1.90	0.84
1:B:319:HIS:CD2	1:B:319:HIS:H	1.94	0.84
1:B:47:ASP:CG	1:B:57:ARG:NH1	2.31	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:H	1:D:256:LEU:HD12	1.40	0.84
1:C:231:HIS:ND1	1:C:233[B]:GLN:HG2	1.93	0.83
2:A:500:HEM:HMB2	2:A:500:HEM:HBB2	1.59	0.83
1:B:258:PRO:HA	1:B:260:ASN:H	1.43	0.83
1:C:165:LEU:CD1	1:C:165:LEU:C	2.47	0.82
1:B:200:ASP:O	1:B:204:GLN:HB3	1.79	0.82
1:B:230:THR:CG2	3:B:502:PB2:CCE	2.58	0.82
1:D:56:LEU:O	1:D:56:LEU:HD12	1.80	0.82
1:B:117:ASN:HB3	4:B:504:CM5:H32A	1.59	0.81
1:A:44:LEU:HD23	1:B:287:ASN:ND2	1.93	0.81
1:A:200:ASP:O	1:A:204:GLN:HB3	1.81	0.81
1:A:133:ARG:HA	1:A:141:SER:HB2	1.63	0.81
1:D:97:GLY:HA3	1:D:370:THR:HG22	1.61	0.81
1:B:56:LEU:HD12	1:B:56:LEU:C	1.97	0.80
1:A:283:PHE:CD2	1:A:285:HIS:CB	2.64	0.80
1:A:226:TYR:CD2	1:B:226:TYR:HB3	2.16	0.80
1:B:127:PHE:O	1:B:131:THR:CG2	2.30	0.80
1:B:269:LEU:O	1:B:272:MET:CB	2.30	0.80
1:C:251:LYS:O	1:C:255:THR:HG23	1.82	0.80
1:B:258:PRO:HA	1:B:260:ASN:N	1.96	0.79
1:C:257:ASP:OD1	1:C:258:PRO:CD	2.30	0.79
1:C:129:LEU:O	1:C:132:MET:CB	2.30	0.79
1:A:258:PRO:CG	1:A:258:PRO:O	2.30	0.79
1:B:73:ARG:HG3	3:B:503:PB2:CCA	2.12	0.79
1:D:477:VAL:O	1:D:477:VAL:CG1	2.30	0.79
1:B:230:THR:CG2	3:B:502:PB2:HCE	2.12	0.78
1:A:387:GLU:OE1	3:A:503:PB2:CCE	2.31	0.78
1:B:491:ARG:O	1:B:492:HIS:CB	2.29	0.78
1:C:141:SER:O	1:C:145:ARG:HG3	1.84	0.78
1:A:258:PRO:HG2	1:A:258:PRO:O	1.82	0.77
1:A:258:PRO:CA	1:A:260:ASN:H	1.96	0.77
1:C:97:GLY:HA3	1:C:370:THR:HG22	1.67	0.77
1:C:327:GLU:O	1:C:331:VAL:CG2	2.30	0.77
1:C:200:ASP:O	1:C:204:GLN:HB3	1.85	0.76
3:C:503:PB2:CDD	1:D:224:LEU:O	2.33	0.76
1:A:227:PHE:CE1	1:B:70:LEU:HB3	2.21	0.76
1:D:42:ASN:HD22	1:D:45:GLN:NE2	1.84	0.76
1:A:283:PHE:N	1:A:283:PHE:CD1	2.52	0.76
1:C:133:ARG:O	1:C:134:ASP:CB	2.34	0.76
1:C:231:HIS:CE1	1:C:233[B]:GLN:HG3	2.19	0.76
1:A:474:GLU:O	1:A:475:SER:HB3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD23	1:B:487:ARG:CG	2.17	0.75
2:A:500:HEM:CMB	2:A:500:HEM:HBB2	2.16	0.75
1:A:288:LEU:CD2	1:A:288:LEU:N	2.47	0.75
1:B:288:LEU:HD13	4:B:504:CM5:H92	1.67	0.75
1:A:258:PRO:HA	1:A:260:ASN:N	2.01	0.74
1:C:475:SER:HA	1:C:478:GLY:O	1.87	0.74
1:D:200:ASP:O	1:D:204:GLN:HB3	1.88	0.74
1:C:449:PHE:O	1:C:453:ILE:HG13	1.87	0.73
1:A:474:GLU:O	1:A:475:SER:CB	2.36	0.73
3:C:502:PB2:CDE	3:C:503:PB2:HDC	2.19	0.73
1:B:73:ARG:CB	3:B:503:PB2:HCB	2.16	0.73
1:B:47:ASP:HB3	1:B:49:LYS:H	1.54	0.73
1:A:288:LEU:HD23	1:A:288:LEU:N	2.04	0.72
1:C:257:ASP:OD1	1:C:258:PRO:HD3	1.88	0.72
1:C:262:ARG:HG3	1:C:266:ASP:OD1	1.90	0.72
1:A:47:ASP:HB3	1:A:49:LYS:H	1.54	0.72
1:C:164:LEU:HD21	1:C:487:ARG:HE	1.53	0.72
1:A:44:LEU:CD2	1:B:287:ASN:HD22	2.01	0.72
1:A:53:ARG:HH11	1:A:53:ARG:HB3	1.55	0.72
1:B:170:LEU:O	1:B:174:ILE:HG23	1.89	0.72
1:B:246:GLY:HA2	1:B:286:GLN:OE1	1.91	0.71
1:B:230:THR:HG23	3:B:502:PB2:HCF	1.71	0.71
1:C:227:PHE:CE1	1:D:70:LEU:HB3	2.26	0.70
1:A:164:LEU:HD23	1:A:487:ARG:HG3	1.73	0.70
1:D:477:VAL:O	1:D:477:VAL:HG13	1.90	0.70
1:C:251:LYS:O	1:C:255:THR:CG2	2.39	0.70
1:A:283:PHE:HD2	1:A:285:HIS:CB	2.04	0.69
1:B:258:PRO:CA	1:B:260:ASN:H	2.05	0.69
1:C:226:TYR:CD2	1:C:226:TYR:C	2.66	0.69
1:C:70:LEU:HB3	1:D:227:PHE:CE1	2.27	0.69
1:C:332:ILE:O	1:C:332:ILE:HG22	1.92	0.69
1:C:253:ARG:O	1:C:256:LEU:CD1	2.41	0.69
1:C:257:ASP:OD1	1:C:258:PRO:HD2	1.90	0.69
1:B:47:ASP:CG	1:B:57:ARG:HH12	1.96	0.69
1:C:164:LEU:CD2	1:C:487:ARG:NE	2.54	0.69
1:A:387:GLU:OE1	3:A:503:PB2:HCE	1.92	0.69
1:D:253:ARG:O	1:D:256:LEU:HD12	1.93	0.69
1:D:150:ALA:O	1:D:154:VAL:HG23	1.93	0.68
1:A:225:LYS:HG2	1:B:477:VAL:HG11	1.75	0.68
1:B:152:CYS:HB3	5:B:498:HOH:O	1.94	0.68
1:C:253:ARG:O	1:C:256:LEU:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD12	3:A:503:PB2:HDC	1.75	0.68
1:D:134:ASP:CB	1:D:135:PHE:CB	2.71	0.68
1:A:446:LEU:O	1:A:450:PHE:HB2	1.94	0.68
1:A:258:PRO:CD	1:A:258:PRO:O	2.41	0.68
1:C:332:ILE:O	1:C:332:ILE:CG2	2.40	0.68
1:A:476:GLY:O	1:A:477:VAL:HG12	1.93	0.68
1:B:230:THR:CG2	3:B:502:PB2:CCF	2.72	0.67
1:A:73:ARG:HG3	3:A:503:PB2:CCF	2.24	0.67
1:D:256:LEU:N	1:D:256:LEU:HD12	2.10	0.67
2:C:500:HEM:HBB2	2:C:500:HEM:HMB2	1.75	0.67
1:C:475:SER:CA	1:C:478:GLY:O	2.42	0.67
1:B:237:ASN:O	1:B:241:ILE:HG12	1.95	0.67
1:D:73:ARG:HG3	3:D:503:PB2:HCB	1.77	0.67
3:C:502:PB2:CCC	1:D:230:THR:CG2	2.73	0.66
1:D:73:ARG:CB	3:D:503:PB2:HCB	2.25	0.66
1:C:164:LEU:HD21	1:C:487:ARG:CG	2.23	0.66
1:B:127:PHE:O	1:B:131:THR:HG23	1.93	0.66
1:C:141:SER:HG	1:C:144:GLU:HG3	1.56	0.66
1:C:477:VAL:O	1:C:477:VAL:CG1	2.42	0.66
1:D:446:LEU:O	1:D:450:PHE:HB2	1.95	0.66
1:B:230:THR:HG23	3:B:502:PB2:CCF	2.26	0.66
1:C:128:SER:OG	1:C:129:LEU:HD13	1.96	0.66
3:A:503:PB2:CDF	5:B:525:HOH:O	2.32	0.66
1:B:127:PHE:O	1:B:131:THR:HG22	1.95	0.66
1:C:315:LEU:HD23	1:C:459:ILE:HD12	1.78	0.66
1:B:230:THR:HG22	3:B:502:PB2:CCE	2.25	0.66
1:D:73:ARG:HG3	3:D:503:PB2:CCB	2.24	0.66
1:C:140:ARG:NH2	1:C:148:GLU:OE2	2.29	0.65
1:A:476:GLY:O	1:A:477:VAL:CB	2.44	0.65
3:C:503:PB2:HDE	1:D:224:LEU:N	2.12	0.65
1:C:258:PRO:HA	1:C:260:ASN:H	1.61	0.65
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.77	0.65
1:D:47:ASP:OD2	1:D:57:ARG:NH2	2.30	0.65
3:C:502:PB2:CCC	1:D:230:THR:HG23	2.26	0.65
1:A:140:ARG:NH2	1:A:148:GLU:OE2	2.30	0.65
1:B:439:GLU:O	1:B:443:ARG:HG3	1.96	0.65
1:B:150:ALA:HB1	1:B:452:THR:HG21	1.79	0.65
1:A:204:GLN:HE21	1:A:236:ARG:HH12	1.45	0.65
1:C:129:LEU:N	1:C:129:LEU:HD12	2.12	0.65
1:C:320:VAL:HG13	1:C:348:TYR:OH	1.97	0.65
3:C:502:PB2:HCC	1:D:230:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:CD1	1:D:256:LEU:H	2.10	0.64
1:C:129:LEU:O	1:C:132:MET:N	2.31	0.64
1:C:256:LEU:O	1:C:256:LEU:CD1	2.39	0.64
1:D:255:THR:OG1	1:D:262:ARG:NH2	2.31	0.64
1:D:145:ARG:HD3	1:D:181:SER:OG	1.98	0.64
1:C:70:LEU:HD22	3:C:502:PB2:CAC	2.28	0.64
1:B:208:LEU:HD22	1:B:226:TYR:HD1	1.63	0.64
1:C:143:GLU:O	1:C:147:GLN:HG3	1.98	0.64
3:C:503:PB2:HDE	1:D:224:LEU:H	1.61	0.64
1:C:204:GLN:HE21	1:C:236:ARG:HH12	1.46	0.63
1:C:129:LEU:O	1:C:132:MET:CA	2.45	0.63
1:A:475:SER:HB3	1:B:232:ARG:NH1	2.14	0.63
1:B:121:TRP:HZ2	2:B:500:HEM:O1D	1.81	0.63
1:A:42:ASN:HD22	1:A:45:GLN:NE2	1.96	0.63
1:C:178:ILE:O	1:C:182:ILE:HG13	1.99	0.63
1:D:154:VAL:HG13	1:D:457:PHE:HE2	1.62	0.63
1:C:491:ARG:O	1:C:492:HIS:CB	2.45	0.63
1:B:56:LEU:O	1:B:56:LEU:CD1	2.30	0.63
1:C:129:LEU:O	1:C:133:ARG:N	2.31	0.63
1:A:125:ARG:O	1:A:129:LEU:HD13	1.99	0.63
1:D:258:PRO:HA	1:D:260:ASN:H	1.64	0.63
1:B:145:ARG:HD3	1:B:181:SER:OG	1.99	0.63
1:D:387:GLU:OE1	3:D:503:PB2:CCC	2.47	0.63
1:C:255:THR:OG1	1:C:262:ARG:NH1	2.32	0.63
1:A:164:LEU:HD23	1:A:487:ARG:CG	2.28	0.62
1:C:127:PHE:C	1:C:127:PHE:CD1	2.72	0.62
1:D:268:TYR:CD1	1:D:289:ILE:HD11	2.34	0.62
1:C:198:LEU:CD2	1:C:202:PHE:HD1	2.10	0.62
1:C:128:SER:OG	1:C:129:LEU:CD1	2.47	0.62
1:B:125:ARG:O	1:B:129:LEU:HD22	2.00	0.62
1:A:141:SER:OG	1:A:144:GLU:CG	2.35	0.62
1:A:266:ASP:O	1:A:270:LEU:HD22	1.99	0.62
1:B:198:LEU:HD23	1:B:241:ILE:CD1	2.20	0.62
1:C:226:TYR:HD2	1:C:226:TYR:C	2.02	0.62
1:C:308:ARG:NH2	1:C:481:PRO:O	2.32	0.62
1:A:255:THR:OG1	1:A:262:ARG:NH2	2.30	0.62
2:D:500:HEM:ND	3:D:501:PB2:HAE	2.14	0.61
3:C:502:PB2:CCB	1:D:230:THR:HG23	2.30	0.61
3:C:502:PB2:HDE	3:C:503:PB2:HDD	1.82	0.61
1:C:439:GLU:O	1:C:443:ARG:HG3	1.99	0.61
1:C:164:LEU:HD21	1:C:487:ARG:HG3	1.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:O	1:D:174:ILE:HG23	2.00	0.61
1:B:257:ASP:OD1	1:B:258:PRO:HD2	2.01	0.61
1:B:164:LEU:HD21	1:B:462:PRO:HD3	1.82	0.60
1:A:133:ARG:HA	1:A:141:SER:CB	2.30	0.60
1:A:486:ILE:HD13	1:A:488:PHE:CZ	2.36	0.60
1:C:164:LEU:HD23	1:C:487:ARG:HG3	1.45	0.60
1:D:253:ARG:O	1:D:256:LEU:CD1	2.49	0.60
3:D:502:PB2:CDE	3:D:503:PB2:HDD	2.32	0.60
1:C:170:LEU:O	1:C:174:ILE:HG23	2.01	0.60
1:C:342:ASP:O	1:C:346:MET:HG3	2.01	0.59
1:B:256:LEU:O	1:B:256:LEU:HD13	2.02	0.59
1:C:164:LEU:HD21	1:C:487:ARG:CD	2.33	0.59
2:D:500:HEM:HBD1	2:D:500:HEM:HHA	1.84	0.59
2:B:500:HEM:ND	3:B:501:PB2:HAE	2.16	0.59
1:D:481:PRO:HA	5:D:543:HOH:O	2.02	0.59
1:C:42:ASN:HD22	1:C:45:GLN:NE2	2.00	0.59
1:D:127:PHE:C	1:D:127:PHE:CD1	2.74	0.59
1:A:314:MET:SD	1:A:450:PHE:CZ	2.94	0.59
1:A:314:MET:HE2	1:A:450:PHE:HZ	1.66	0.59
3:C:502:PB2:HCC	1:D:230:THR:HG23	1.85	0.59
1:D:270:LEU:N	1:D:270:LEU:HD12	2.17	0.59
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	2.33	0.59
2:B:500:HEM:HBC2	2:B:500:HEM:HHD	1.83	0.59
1:B:162:GLY:HA2	1:B:488:PHE:O	2.03	0.59
1:B:449:PHE:O	1:B:453:ILE:HG13	2.02	0.59
1:B:42:ASN:HD22	1:B:45:GLN:NE2	2.00	0.58
1:D:268:TYR:CE1	1:D:289:ILE:HD11	2.38	0.58
1:A:314:MET:SD	1:A:450:PHE:CE1	2.96	0.58
1:B:141:SER:OG	1:B:144:GLU:HG3	2.02	0.58
1:A:283:PHE:N	1:A:283:PHE:HD1	2.01	0.58
1:A:175:THR:HG22	1:A:445:GLU:OE1	2.04	0.58
1:C:237:ASN:O	1:C:241:ILE:HG12	2.03	0.58
1:B:201:LEU:HD22	1:B:241:ILE:HG13	1.86	0.58
1:A:284:HIS:O	1:A:288:LEU:HD23	2.04	0.58
1:D:320:VAL:HG13	1:D:348:TYR:OH	2.03	0.58
1:A:439:GLU:O	1:A:443:ARG:HG3	2.03	0.57
1:C:145:ARG:HD3	1:C:181:SER:OG	2.04	0.57
1:C:230:THR:CG2	3:D:502:PB2:CCE	2.81	0.57
1:D:296:PHE:CD1	2:D:500:HEM:HBC1	2.39	0.57
1:C:198:LEU:CD2	1:C:202:PHE:CD1	2.87	0.57
4:C:504:CM5:H191	4:C:504:CM5:H11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HA	1:A:196:LEU:HD21	1.85	0.57
1:C:368:PRO:HB2	1:D:223:PHE:CD2	2.40	0.57
1:B:198:LEU:CD2	1:B:241:ILE:HD12	2.21	0.57
1:A:476:GLY:O	1:A:477:VAL:CG1	2.53	0.57
1:A:441:ILE:HG13	5:A:522:HOH:O	2.05	0.57
1:C:464:PRO:HD2	1:C:467:ASP:HB2	1.87	0.57
1:B:47:ASP:OD1	1:B:57:ARG:NH1	2.38	0.57
1:D:73:ARG:HB3	3:D:503:PB2:HCB	1.87	0.57
1:B:56:LEU:CD1	1:B:56:LEU:C	2.69	0.56
1:A:476:GLY:O	1:A:477:VAL:HB	2.03	0.56
1:B:315:LEU:HD23	1:B:459:ILE:HD12	1.86	0.56
1:A:315:LEU:HD23	1:A:459:ILE:HD12	1.87	0.56
1:D:308:ARG:NH2	1:D:481:PRO:O	2.38	0.56
1:A:475:SER:CB	1:B:232:ARG:NH1	2.69	0.56
2:C:500:HEM:CMB	2:C:500:HEM:HBB2	2.36	0.56
1:D:141:SER:O	1:D:145:ARG:HG3	2.05	0.56
1:C:293:LEU:HG	1:C:297:PHE:HE2	1.70	0.56
1:B:121:TRP:CZ2	2:B:500:HEM:O1D	2.59	0.56
1:C:198:LEU:HD21	1:C:202:PHE:CD1	2.41	0.56
1:A:299:GLY:HA3	2:A:500:HEM:C1C	2.41	0.56
1:A:53:ARG:HB3	1:A:53:ARG:NH1	2.19	0.56
1:A:70:LEU:HD12	3:A:503:PB2:CDC	2.36	0.55
1:C:331:VAL:HG21	1:C:346:MET:HG2	1.87	0.55
1:A:215:GLN:HB3	1:B:228:PRO:HB3	1.88	0.55
1:C:198:LEU:HD23	1:C:202:PHE:HD1	1.71	0.55
1:D:73:ARG:CG	3:D:503:PB2:HCB	2.36	0.55
1:A:98:ARG:NH2	4:A:504:CM5:O20	2.40	0.55
1:C:253:ARG:C	1:C:256:LEU:HD12	2.27	0.55
1:A:287:ASN:HB2	1:B:37:LEU:HD21	1.88	0.55
1:A:148:GLU:HG3	1:A:151:ARG:NH2	2.22	0.55
1:C:198:LEU:C	1:C:198:LEU:HD23	2.27	0.55
1:D:293:LEU:HG	1:D:297:PHE:HE2	1.71	0.55
1:C:231:HIS:ND1	1:C:233[A]:GLN:HB2	2.21	0.55
1:B:73:ARG:CG	3:B:503:PB2:CCA	2.84	0.55
1:C:55:PHE:HE2	1:C:77:VAL:HG21	1.72	0.55
1:D:262:ARG:NH1	1:D:266:ASP:OD1	2.39	0.54
3:C:502:PB2:HDE	3:C:503:PB2:CDD	2.36	0.54
1:A:477:VAL:HG13	1:A:477:VAL:O	2.07	0.54
2:B:500:HEM:C1D	3:B:501:PB2:HAE	2.42	0.54
1:A:148:GLU:HG3	1:A:151:ARG:HH22	1.73	0.54
1:B:230:THR:HG22	3:B:502:PB2:CCF	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:O	1:C:198:LEU:HD23	2.07	0.54
1:A:283:PHE:O	1:B:37:LEU:HD21	2.06	0.54
1:A:314:MET:HE2	1:A:450:PHE:CZ	2.40	0.54
1:B:211:SER:O	1:B:215:GLN:HG3	2.08	0.54
1:B:141:SER:O	1:B:145:ARG:HG3	2.08	0.54
1:B:191:LYS:HA	1:B:196:LEU:HD21	1.90	0.54
1:D:439:GLU:O	1:D:443:ARG:HG3	2.08	0.54
1:B:299:GLY:HA3	2:B:500:HEM:C1C	2.43	0.53
1:B:183:VAL:HA	1:B:264:PHE:HB3	1.89	0.53
3:B:496:PB2:CDC	3:B:503:PB2:HDD	2.39	0.53
1:B:97:GLY:CA	1:B:370:THR:HG22	2.34	0.53
1:C:294:SER:HB3	1:D:216:VAL:HG11	1.90	0.53
1:B:111:TYR:OH	1:C:107:ILE:HD13	2.09	0.53
1:C:149:GLU:OE1	1:C:190:TYR:OH	2.23	0.53
1:C:480:VAL:O	1:C:480:VAL:HG12	2.08	0.53
1:D:183:VAL:HA	1:D:264:PHE:HB3	1.90	0.53
1:A:194:VAL:HG11	1:A:244:PHE:CD2	2.44	0.53
1:A:170:LEU:O	1:A:174:ILE:HG23	2.08	0.53
1:A:51:LEU:O	1:A:55:PHE:HD1	1.91	0.53
1:A:134:ASP:H	1:A:141:SER:CB	2.22	0.52
1:B:51:LEU:HD13	3:B:496:PB2:CCB	2.39	0.52
1:B:230:THR:HG23	3:B:502:PB2:CCE	2.39	0.52
1:C:262:ARG:CG	1:C:266:ASP:OD1	2.56	0.52
1:B:253:ARG:O	1:B:256:LEU:HD12	2.08	0.52
1:A:178:ILE:O	1:A:182:ILE:HG13	2.09	0.52
2:D:500:HEM:HBC2	2:D:500:HEM:CHD	2.17	0.52
1:D:134:ASP:CA	1:D:135:PHE:CB	2.87	0.52
1:C:43:LEU:CD1	1:D:229:GLY:HA3	2.40	0.52
1:D:178:ILE:O	1:D:182:ILE:HG13	2.09	0.52
2:A:500:HEM:CBB	2:A:500:HEM:HMB2	2.35	0.52
1:D:256:LEU:CD1	1:D:256:LEU:N	2.70	0.52
1:C:191:LYS:HA	1:C:196:LEU:HD21	1.92	0.52
1:C:268:TYR:O	1:C:272:MET:HB2	2.10	0.52
1:B:319:HIS:HD2	1:B:319:HIS:H	1.53	0.51
1:C:98:ARG:HD2	4:C:504:CM5:H18	1.91	0.51
1:D:293:LEU:HG	1:D:297:PHE:CE2	2.45	0.51
1:C:268:TYR:CD1	1:C:289:ILE:HD11	2.45	0.51
1:D:474:GLU:OE1	1:D:474:GLU:CA	2.30	0.51
1:D:201:LEU:HD22	1:D:241:ILE:HG13	1.93	0.51
1:D:164:LEU:HD21	1:D:462:PRO:HD3	1.91	0.51
1:D:237:ASN:O	1:D:241:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:HIS:CE1	1:C:233[A]:GLN:HB2	2.45	0.51
1:A:73:ARG:HG3	3:A:503:PB2:CCA	2.41	0.51
1:C:150:ALA:HB1	1:C:452:THR:HG21	1.92	0.51
3:C:502:PB2:HCB	1:D:230:THR:HG23	1.93	0.51
1:B:265:ILE:O	1:B:268:TYR:HB3	2.10	0.51
1:B:47:ASP:HB3	1:B:49:LYS:N	2.22	0.51
1:C:430:SER:CB	2:C:500:HEM:HBA1	2.41	0.51
1:D:73:ARG:HG3	3:D:503:PB2:CCA	2.41	0.51
1:B:47:ASP:CB	1:B:57:ARG:HH12	2.24	0.50
1:C:317:TYR:HB3	1:C:320:VAL:HG23	1.93	0.50
1:A:198:LEU:C	1:A:198:LEU:HD12	2.32	0.50
1:B:230:THR:HG21	3:B:502:PB2:HCE	1.93	0.50
1:A:293:LEU:HG	1:A:297:PHE:HE2	1.76	0.50
1:B:70:LEU:HD22	3:B:496:PB2:CAE	2.41	0.50
1:C:475:SER:O	1:C:478:GLY:O	2.30	0.50
1:A:274:LYS:O	1:A:275:ASP:O	2.30	0.50
1:D:165:LEU:HD12	1:D:165:LEU:O	2.11	0.50
1:D:491:ARG:O	1:D:492:HIS:O	2.30	0.50
3:C:502:PB2:CDE	3:C:503:PB2:CDC	2.90	0.50
1:D:477:VAL:O	1:D:477:VAL:HG12	2.10	0.50
1:C:293:LEU:HG	1:C:297:PHE:CE2	2.46	0.50
1:C:174:ILE:HD12	1:C:449:PHE:CD1	2.47	0.50
1:A:194:VAL:HG11	1:A:244:PHE:CE2	2.47	0.50
1:D:303:THR:HA	2:D:500:HEM:CBB	2.42	0.50
1:A:262:ARG:HG3	1:A:266:ASP:OD1	2.11	0.50
1:D:288:LEU:HD13	4:D:504:CM5:H92	1.92	0.50
1:C:255:THR:OG1	1:C:256:LEU:N	2.45	0.50
3:B:496:PB2:HDC	3:B:503:PB2:HDD	1.94	0.50
1:B:319:HIS:CD2	1:B:319:HIS:N	2.69	0.50
1:A:299:GLY:HA3	2:A:500:HEM:C2C	2.46	0.50
1:D:348:TYR:O	1:D:352:VAL:HG23	2.12	0.50
1:A:134:ASP:H	1:A:141:SER:HB3	1.77	0.50
1:C:256:LEU:O	1:C:257:ASP:OD2	2.30	0.50
1:D:198:LEU:C	1:D:198:LEU:HD12	2.32	0.50
1:C:78:LEU:HD22	1:C:388:VAL:CG1	2.42	0.50
1:C:477:VAL:HG11	1:D:225:LYS:HG2	1.93	0.49
1:C:226:TYR:O	1:C:226:TYR:HD2	1.94	0.49
1:A:133:ARG:O	1:A:134:ASP:O	2.30	0.49
2:A:500:HEM:HBD1	2:A:500:HEM:HHA	1.95	0.49
1:D:78:LEU:HD22	1:D:388:VAL:CG1	2.42	0.49
1:D:270:LEU:N	1:D:270:LEU:CD1	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:PHE:CD2	1:B:488:PHE:N	2.79	0.49
2:D:500:HEM:CBC	2:D:500:HEM:HHD	2.25	0.49
1:C:194:VAL:HG11	1:C:244:PHE:CD2	2.48	0.49
1:D:47:ASP:HB3	1:D:49:LYS:H	1.77	0.49
1:C:194:VAL:HG11	1:C:244:PHE:CE2	2.48	0.49
1:C:252:HIS:NE2	1:C:263:ASP:OD2	2.34	0.49
1:A:107:ILE:HD13	1:D:111:TYR:OH	2.13	0.49
1:C:258:PRO:HA	1:C:260:ASN:N	2.27	0.49
1:A:237:ASN:O	1:A:241:ILE:HG12	2.13	0.49
1:C:248:SER:O	1:C:252:HIS:ND1	2.45	0.49
1:C:268:TYR:CE1	1:C:289:ILE:HD11	2.47	0.49
1:A:145:ARG:NH1	1:A:181:SER:OG	2.36	0.48
1:A:314:MET:HE1	1:A:450:PHE:CE1	2.44	0.48
1:B:175:THR:HG22	1:B:445:GLU:OE1	2.13	0.48
1:B:291:THR:O	1:B:294:SER:HB2	2.14	0.48
1:B:70:LEU:HD22	3:B:496:PB2:CAF	2.43	0.48
1:A:288:LEU:HD23	1:A:288:LEU:H	1.78	0.48
1:D:204:GLN:HG3	1:D:233:GLN:HE22	1.78	0.48
1:A:70:LEU:HB3	1:B:227:PHE:CZ	2.49	0.48
1:A:209:ILE:HD12	1:B:474:GLU:OE1	2.12	0.48
1:D:200:ASP:O	1:D:204:GLN:CB	2.61	0.48
4:C:504:CM5:C19	4:C:504:CM5:H11	2.44	0.48
1:A:473:ARG:NH2	1:A:481:PRO:O	2.46	0.48
1:D:47:ASP:C	1:D:49:LYS:N	2.66	0.48
1:C:348:TYR:O	1:C:352:VAL:HG23	2.14	0.48
1:C:127:PHE:O	1:C:127:PHE:CD1	2.66	0.48
1:D:252:HIS:NE2	1:D:263:ASP:OD2	2.34	0.48
1:D:47:ASP:C	1:D:49:LYS:H	2.17	0.48
1:A:251:LYS:HB2	1:A:251:LYS:HE3	1.52	0.48
1:D:303:THR:HA	2:D:500:HEM:HBB1	1.96	0.47
2:D:500:HEM:C1D	3:D:501:PB2:HAE	2.48	0.47
1:C:316:LYS:HB2	1:C:468:ILE:HB	1.95	0.47
1:C:290:LEU:HD12	1:D:44:LEU:HD21	1.95	0.47
1:D:471:THR:HA	1:D:472:PRO:HD3	1.78	0.47
1:B:229:GLY:HA2	1:B:234:ILE:HD13	1.96	0.47
1:C:256:LEU:HD22	1:C:256:LEU:C	2.34	0.47
1:A:257:ASP:O	1:A:258:PRO:C	2.48	0.47
1:D:429:PHE:CD2	1:D:439:GLU:HG3	2.49	0.47
1:A:293:LEU:HG	1:A:297:PHE:CE2	2.49	0.47
1:A:211:SER:O	1:A:215:GLN:HG3	2.14	0.47
1:D:307:LEU:HD23	1:D:450:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:SER:O	1:D:252:HIS:ND1	2.48	0.47
1:C:164:LEU:CD2	1:C:487:ARG:CD	2.91	0.47
1:C:260:ASN:N	1:C:261:PRO:CD	2.77	0.47
1:C:230:THR:HG23	3:D:502:PB2:CCF	2.45	0.47
1:C:299:GLY:HA3	2:C:500:HEM:C1C	2.50	0.47
4:C:504:CM5:H20	4:C:504:CM5:C13	2.28	0.47
1:B:183:VAL:HG11	1:B:293:LEU:HD21	1.97	0.47
1:A:227:PHE:CZ	1:B:70:LEU:HB3	2.48	0.47
1:A:226:TYR:HB3	1:B:226:TYR:CD2	2.49	0.47
1:B:252:HIS:O	1:B:256:LEU:HB3	2.15	0.47
1:A:368:PRO:HB2	1:B:223:PHE:CD2	2.49	0.47
1:A:187:ARG:NH1	5:A:508:HOH:O	2.47	0.47
1:D:404:THR:HB	1:D:407:THR:HB	1.97	0.47
1:D:429:PHE:HB3	1:D:436:CYS:HB3	1.96	0.46
1:A:57:ARG:NH1	1:A:60:GLU:OE1	2.48	0.46
1:C:329:GLU:OE2	1:C:329:GLU:CA	2.61	0.46
1:A:314:MET:SD	1:A:450:PHE:HZ	2.35	0.46
1:C:329:GLU:OE2	1:C:329:GLU:HA	2.16	0.46
3:C:502:PB2:HDE	3:C:503:PB2:CDC	2.45	0.46
1:B:73:ARG:CB	3:B:503:PB2:CCB	2.91	0.46
1:B:178:ILE:O	1:B:182:ILE:HG13	2.15	0.46
1:C:183:VAL:HA	1:C:264:PHE:HB3	1.97	0.46
1:C:475:SER:C	1:C:478:GLY:O	2.54	0.46
1:D:51:LEU:O	1:D:55:PHE:HD1	1.99	0.46
1:A:342:ASP:O	1:A:346:MET:HG3	2.15	0.46
1:D:57:ARG:HE	1:D:57:ARG:HB3	1.47	0.46
1:D:211:SER:O	1:D:215:GLN:HG3	2.15	0.46
1:C:252:HIS:O	1:C:256:LEU:HB3	2.16	0.46
1:B:227:PHE:CD1	1:B:228:PRO:HD2	2.51	0.46
1:D:174:ILE:HD12	1:D:449:PHE:CD1	2.51	0.46
1:A:70:LEU:CD1	3:A:503:PB2:HDC	2.43	0.46
1:B:477:VAL:HG13	1:B:477:VAL:O	2.15	0.46
1:D:229:GLY:HA2	1:D:234:ILE:CD1	2.45	0.46
1:D:285:HIS:C	1:D:287:ASN:N	2.68	0.46
1:A:70:LEU:HB3	1:B:227:PHE:CE1	2.52	0.45
1:B:188:PHE:CG	1:B:195:PHE:HB2	2.51	0.45
1:D:442:ALA:HB2	2:D:500:HEM:HMC2	1.98	0.45
1:B:107:ILE:HD13	1:C:111:TYR:OH	2.16	0.45
1:D:253:ARG:HH11	1:D:253:ARG:HG3	1.80	0.45
1:B:148:GLU:HG3	1:B:151:ARG:HH22	1.81	0.45
1:C:408:PHE:CE1	1:C:410:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:HEM:CBB	2:B:500:HEM:HMB2	2.46	0.45
1:C:192:ASP:O	1:C:196:LEU:HD23	2.16	0.45
1:D:194:VAL:HG11	1:D:244:PHE:CD2	2.51	0.45
1:C:253:ARG:O	1:C:256:LEU:HD11	2.15	0.45
1:B:156:GLU:HG3	1:B:190:TYR:CD2	2.51	0.45
1:D:429:PHE:O	1:D:430:SER:HB3	2.16	0.45
1:C:285:HIS:C	1:C:287:ASN:N	2.70	0.45
1:B:257:ASP:OD1	1:B:258:PRO:CD	2.63	0.45
1:A:183:VAL:HA	1:A:264:PHE:HB3	1.97	0.45
1:D:389:PHE:CZ	3:D:503:PB2:HDE	2.51	0.45
4:C:504:CM5:O12	4:C:504:CM5:O20	2.30	0.45
1:B:183:VAL:HG21	1:B:293:LEU:CD2	2.47	0.45
1:C:156:GLU:HG3	1:C:190:TYR:CD2	2.52	0.45
1:A:73:ARG:HD3	1:B:100:LYS:O	2.17	0.45
1:A:156:GLU:HG3	1:A:190:TYR:CD2	2.52	0.45
1:B:258:PRO:C	1:B:260:ASN:H	2.19	0.44
1:A:255:THR:CB	1:A:262:ARG:NH2	2.79	0.44
1:B:476:GLY:CA	5:B:527:HOH:O	2.64	0.44
1:A:429:PHE:O	1:A:430:SER:HB3	2.17	0.44
1:B:229:GLY:HA2	1:B:234:ILE:CD1	2.48	0.44
1:C:215:GLN:HB3	1:D:228:PRO:HB3	2.00	0.44
1:D:156:GLU:HG3	1:D:190:TYR:CE2	2.53	0.44
1:C:73:ARG:HG3	3:C:503:PB2:CCA	2.47	0.44
1:A:475:SER:OG	1:A:475:SER:O	2.30	0.44
1:D:191:LYS:HA	1:D:196:LEU:HD21	1.99	0.44
1:C:257:ASP:CB	1:C:258:PRO:CD	2.95	0.44
1:D:296:PHE:CD1	2:D:500:HEM:CBC	3.01	0.44
1:A:296:PHE:CD1	2:A:500:HEM:CBC	3.01	0.44
1:A:296:PHE:CD1	2:A:500:HEM:HBC1	2.53	0.44
1:B:401:TYR:CE2	1:B:424:GLU:HB2	2.53	0.44
1:B:270:LEU:C	1:B:272:MET:N	2.70	0.44
1:C:227:PHE:CZ	1:D:70:LEU:HB3	2.53	0.44
1:C:98:ARG:NH1	1:D:220:PHE:CE2	2.86	0.44
1:A:288:LEU:HD22	1:A:288:LEU:N	2.25	0.43
1:A:272:MET:O	1:A:275:ASP:CB	2.66	0.43
1:C:244:PHE:CD1	1:C:244:PHE:C	2.92	0.43
1:D:218:GLU:O	1:D:221:SER:HB2	2.17	0.43
1:C:188:PHE:CG	1:C:195:PHE:HB2	2.53	0.43
1:C:464:PRO:O	1:C:465:PRO:C	2.57	0.43
1:C:98:ARG:HD2	4:C:504:CM5:C18	2.49	0.43
1:D:389:PHE:HZ	3:D:503:PB2:HDE	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ASN:N	1:D:261:PRO:HD3	2.32	0.43
1:C:287:ASN:HB2	1:D:37:LEU:HD21	1.99	0.43
1:C:486:ILE:HG12	1:C:487:ARG:N	2.34	0.43
1:C:294:SER:CB	1:D:216:VAL:HG11	2.47	0.43
1:B:429:PHE:HB3	1:B:436:CYS:HB3	2.00	0.43
1:C:130:ALA:O	1:C:134:ASP:C	2.57	0.43
1:B:332:ILE:HD13	1:B:338:PRO:HB3	2.00	0.43
4:B:504:CM5:H71	4:B:504:CM5:H41	1.24	0.43
1:D:192:ASP:O	1:D:196:LEU:HD23	2.19	0.43
1:C:232:ARG:HB3	1:C:232:ARG:HH21	1.84	0.43
1:B:64:ASP:HB3	1:B:79:CYS:O	2.19	0.43
1:A:100:LYS:O	1:B:73:ARG:HD3	2.19	0.43
1:B:164:LEU:HG	1:B:487:ARG:CZ	2.49	0.43
1:A:229:GLY:HA2	1:A:234:ILE:CD1	2.48	0.43
4:C:504:CM5:C1	4:C:504:CM5:C19	2.97	0.42
1:C:323:ARG:HB3	1:C:323:ARG:HE	1.26	0.42
1:C:27:LYS:H	1:C:27:LYS:HG2	1.46	0.42
1:B:120:ARG:HD2	4:B:504:CM5:H82	2.00	0.42
1:C:153:LEU:CD1	1:C:170:LEU:HD21	2.49	0.42
1:D:464:PRO:O	1:D:465:PRO:C	2.56	0.42
1:C:313:LEU:HD23	1:C:470:LEU:HD11	2.00	0.42
1:A:73:ARG:HG3	3:A:503:PB2:HCF	1.98	0.42
1:D:150:ALA:HB1	1:D:452:THR:HG21	2.01	0.42
1:D:165:LEU:HD12	1:D:165:LEU:C	2.39	0.42
1:A:133:ARG:C	1:A:134:ASP:O	2.57	0.42
1:C:260:ASN:N	1:C:261:PRO:HD3	2.35	0.42
3:A:503:PB2:CDE	5:B:525:HOH:O	2.64	0.42
1:C:230:THR:CG2	3:D:502:PB2:CCF	2.98	0.42
1:D:480:VAL:HA	1:D:481:PRO:HD3	1.81	0.42
1:C:200:ASP:O	1:C:204:GLN:CB	2.61	0.42
1:A:288:LEU:HD22	1:A:288:LEU:HA	1.54	0.42
1:C:149:GLU:OE1	1:C:190:TYR:CE1	2.73	0.42
1:C:359:LEU:HD11	1:C:408:PHE:HA	1.99	0.42
1:A:314:MET:SD	1:A:450:PHE:HE1	2.41	0.42
2:C:500:HEM:C1B	3:C:501:PB2:HAC	2.54	0.42
1:C:211:SER:O	1:C:215:GLN:HG3	2.20	0.42
1:D:175:THR:HG22	1:D:445:GLU:OE1	2.19	0.42
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.94	0.42
1:B:169:LEU:O	1:B:169:LEU:HD12	2.19	0.42
1:C:471:THR:HA	1:C:472:PRO:HD3	1.74	0.42
1:A:476:GLY:CA	5:A:539:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:VAL:HG11	1:D:244:PHE:CE2	2.55	0.42
1:C:175:THR:HG22	1:C:445:GLU:OE1	2.19	0.42
1:B:471:THR:HA	1:B:472:PRO:HD3	1.79	0.42
1:C:486:ILE:HD13	1:C:488:PHE:CZ	2.55	0.42
1:A:226:TYR:CE2	1:B:226:TYR:HB3	2.54	0.42
1:A:220:PHE:CE2	1:B:98:ARG:NH2	2.88	0.42
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.75	0.42
1:D:155:GLU:OE1	5:D:512:HOH:O	2.22	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.84	0.41
1:A:101:ILE:HD13	1:B:224:LEU:HD13	2.02	0.41
1:C:70:LEU:HB3	1:D:227:PHE:CZ	2.55	0.41
1:C:70:LEU:HD22	3:C:502:PB2:NAD	2.35	0.41
1:B:296:PHE:CD1	2:B:500:HEM:HBC1	2.54	0.41
1:B:128:SER:OG	1:B:129:LEU:HD13	2.20	0.41
1:D:244:PHE:C	1:D:244:PHE:CD1	2.94	0.41
1:A:256:LEU:HG	1:A:256:LEU:H	1.59	0.41
1:D:70:LEU:HD22	3:D:502:PB2:CAF	2.50	0.41
1:C:313:LEU:HD12	1:C:356:ILE:HG12	2.02	0.41
1:A:108:PHE:HB3	1:B:69:TYR:OH	2.20	0.41
1:A:287:ASN:HA	1:A:287:ASN:HD22	1.59	0.41
1:C:212:PHE:CD2	1:D:234:ILE:HG23	2.55	0.41
1:A:248:SER:O	1:A:252:HIS:ND1	2.43	0.41
1:A:436:CYS:HA	2:A:500:HEM:CHA	2.50	0.41
1:D:398:ASP:HA	1:D:399:PRO:HD3	1.89	0.41
1:A:283:PHE:CE2	1:A:285:HIS:CB	3.03	0.41
1:B:230:THR:CG2	3:B:502:PB2:HCF	2.40	0.41
1:D:70:LEU:HD22	3:D:502:PB2:CAE	2.51	0.41
1:B:360:GLY:O	1:B:361:ASP:C	2.59	0.41
1:C:262:ARG:CD	1:C:266:ASP:OD1	2.68	0.41
1:D:262:ARG:HG2	1:D:266:ASP:OD1	2.20	0.41
1:B:246:GLY:CA	1:B:286:GLN:OE1	2.66	0.41
1:A:209:ILE:HG23	1:B:205:SER:HB3	2.03	0.41
1:A:320:VAL:HG13	1:A:348:TYR:OH	2.21	0.41
1:C:409:ASN:C	1:C:411:GLY:H	2.23	0.41
1:C:409:ASN:C	1:C:411:GLY:N	2.73	0.41
1:C:230:THR:HG22	3:D:502:PB2:CCE	2.51	0.41
1:D:73:ARG:HA	1:D:74:PRO:HD3	1.94	0.41
1:A:128:SER:OG	1:A:129:LEU:HD12	2.20	0.41
1:A:323:ARG:HE	1:A:323:ARG:HB3	1.39	0.41
2:B:500:HEM:HBC2	2:B:500:HEM:CHD	2.50	0.41
1:C:201:LEU:HD22	1:C:241:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:THR:O	1:C:294:SER:HB2	2.21	0.41
1:C:338:PRO:HD2	1:C:452:THR:OG1	2.21	0.41
1:D:323:ARG:HB3	1:D:323:ARG:HE	1.32	0.41
1:D:315:LEU:HD23	1:D:459:ILE:HD12	2.02	0.41
1:A:141:SER:O	1:A:145:ARG:HG3	2.21	0.41
1:A:260:ASN:N	1:A:261:PRO:HD3	2.36	0.41
1:D:463:VAL:HA	1:D:464:PRO:HD3	1.76	0.41
1:D:199:LEU:HA	1:D:199:LEU:HD12	1.92	0.41
1:B:157:LEU:HA	1:B:157:LEU:HD23	1.95	0.40
1:D:299:GLY:HA3	2:D:500:HEM:C1C	2.56	0.40
1:C:100:LYS:O	1:D:73:ARG:HD3	2.21	0.40
1:B:152:CYS:CB	5:B:498:HOH:O	2.62	0.40
1:D:241:ILE:O	1:D:245:ILE:HG13	2.22	0.40
1:A:127:PHE:CZ	1:A:264:PHE:HD2	2.39	0.40
1:B:359:LEU:HD11	1:B:408:PHE:HA	2.02	0.40
1:A:290:LEU:HD12	1:B:44:LEU:HD21	2.03	0.40
1:C:58:LEU:HA	1:C:58:LEU:HD23	1.86	0.40
1:C:257:ASP:CB	1:C:258:PRO:HD2	2.52	0.40
1:C:225:LYS:HG2	1:D:477:VAL:HG11	2.02	0.40
1:A:156:GLU:HG3	1:A:190:TYR:CE2	2.56	0.40
1:A:325:GLN:HG2	1:A:491:ARG:NH1	2.37	0.40
1:D:384:LYS:O	1:D:385:ASN:HB2	2.22	0.40
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.86	0.40
1:B:323:ARG:HB3	1:B:323:ARG:HE	1.39	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	450/476 (94%)	427 (95%)	21 (5%)	2 (0%)	39 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	446/476 (94%)	417 (94%)	29 (6%)	0	100 100
1	C	447/476 (94%)	418 (94%)	27 (6%)	2 (0%)	39 61
1	D	445/476 (94%)	417 (94%)	28 (6%)	0	100 100
All	All	1788/1904 (94%)	1679 (94%)	105 (6%)	4 (0%)	52 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	VAL
1	C	286	GLN
1	C	261	PRO
1	A	261	PRO

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	381/421 (90%)	344 (90%)	37 (10%)	10 19
1	B	372/421 (88%)	336 (90%)	36 (10%)	10 19
1	C	368/421 (87%)	335 (91%)	33 (9%)	12 22
1	D	376/421 (89%)	343 (91%)	33 (9%)	12 23
All	All	1497/1684 (89%)	1358 (91%)	139 (9%)	11 21

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	LEU
1	A	45	GLN
1	A	53	ARG
1	A	68	VAL
1	A	74	PRO
1	A	75	VAL

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	127	PHE
1	A	134	ASP
1	A	140	ARG
1	A	158	ARG
1	A	169	LEU
1	A	198	LEU
1	A	199	LEU
1	A	221	SER
1	A	224	LEU
1	A	236	ARG
1	A	238	LEU
1	A	255	THR
1	A	256	LEU
1	A	257	ASP
1	A	262	ARG
1	A	268	TYR
1	A	270	LEU
1	A	283	PHE
1	A	288	LEU
1	A	290	LEU
1	A	295	LEU
1	A	334	SER
1	A	341	ASP
1	A	370	THR
1	A	458	SER
1	A	461	SER
1	A	473	ARG
1	A	475	SER
1	A	477	VAL
1	B	37	LEU
1	B	44	LEU
1	B	45	GLN
1	B	47	ASP
1	B	56	LEU
1	B	57	ARG
1	B	68	VAL
1	B	75	VAL
1	B	78	LEU
1	B	127	PHE
1	B	128	SER
1	B	129	LEU

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Mol	Chain	Res	Type
1	B	131	THR
1	B	158	ARG
1	B	169	LEU
1	B	181	SER
1	B	198	LEU
1	B	199	LEU
1	B	207	SER
1	B	210	SER
1	B	221	SER
1	B	224	LEU
1	B	233	GLN
1	B	238	LEU
1	B	240	GLU
1	B	256	LEU
1	B	257	ASP
1	B	290	LEU
1	B	295	LEU
1	B	319	HIS
1	B	334	SER
1	B	341	ASP
1	B	370	THR
1	B	458	SER
1	B	461	SER
1	B	477	VAL
1	C	44	LEU
1	C	53	ARG
1	C	68	VAL
1	C	75	VAL
1	C	78	LEU
1	C	127	PHE
1	C	129	LEU
1	C	140	ARG
1	C	158	ARG
1	C	165	LEU
1	C	169	LEU
1	C	199	LEU
1	C	224	LEU
1	C	226	TYR
1	C	236	ARG
1	C	238	LEU
1	C	255	THR
1	C	256	LEU

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Mol	Chain	Res	Type
1	C	257	ASP
1	C	262	ARG
1	C	270	LEU
1	C	272	MET
1	C	285	HIS
1	C	290	LEU
1	C	295	LEU
1	C	323	ARG
1	C	329	GLU
1	C	341	ASP
1	C	343	ARG
1	C	370	THR
1	C	458	SER
1	C	461	SER
1	C	477	VAL
1	D	37	LEU
1	D	44	LEU
1	D	52	LEU
1	D	57	ARG
1	D	61	LYS
1	D	68	VAL
1	D	75	VAL
1	D	78	LEU
1	D	104	VAL
1	D	127	PHE
1	D	129	LEU
1	D	134	ASP
1	D	141	SER
1	D	158	ARG
1	D	169	LEU
1	D	198	LEU
1	D	199	LEU
1	D	221	SER
1	D	224	LEU
1	D	238	LEU
1	D	256	LEU
1	D	257	ASP
1	D	262	ARG
1	D	272	MET
1	D	290	LEU
1	D	295	LEU
1	D	334	SER

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Mol	Chain	Res	Type
1	D	341	ASP
1	D	370	THR
1	D	458	SER
1	D	461	SER
1	D	475	SER
1	D	477	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	204	GLN
1	A	233	GLN
1	A	385	ASN
1	B	45	GLN
1	B	233	GLN
1	B	287	ASN
1	B	319	HIS
1	B	456	ASN
1	C	45	GLN
1	C	204	GLN
1	C	287	ASN
1	D	45	GLN
1	D	233	GLN
1	D	287	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

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

20 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	1,3	30,50,50	3.05	9 (30%)	24,82,82	2.17	9 (37%)
3	PB2	A	501	2	19,20,20	2.14	6 (31%)	24,26,26	0.80	0
3	PB2	A	503	-	13,13,20	1.88	4 (30%)	16,16,26	0.93	0
4	CM5	A	504	-	23,23,36	0.49	0	29,29,49	2.18	8 (27%)
3	PB2	B	496	-	19,20,20	2.01	6 (31%)	24,26,26	1.29	4 (16%)
2	HEM	B	500	1,3	30,50,50	3.13	7 (23%)	24,82,82	2.25	9 (37%)
3	PB2	B	501	2	19,20,20	2.37	7 (36%)	24,26,26	0.98	1 (4%)
3	PB2	B	502	-	19,20,20	1.99	4 (21%)	24,26,26	0.87	0
3	PB2	B	503	-	13,13,20	1.92	3 (23%)	16,16,26	0.97	0
4	CM5	B	504	-	23,23,36	0.53	0	29,29,49	2.30	11 (37%)
2	HEM	C	500	1,3	30,50,50	3.21	8 (26%)	24,82,82	2.28	9 (37%)
3	PB2	C	501	2	19,20,20	2.10	7 (36%)	24,26,26	1.44	2 (8%)
3	PB2	C	502	-	19,20,20	2.01	4 (21%)	24,26,26	0.94	0
3	PB2	C	503	-	13,13,20	1.97	3 (23%)	16,16,26	1.21	2 (12%)
4	CM5	C	504	-	23,23,36	0.49	0	29,29,49	1.82	5 (17%)
2	HEM	D	500	1,3	30,50,50	2.65	10 (33%)	24,82,82	2.18	10 (41%)
3	PB2	D	501	2	19,20,20	2.17	7 (36%)	24,26,26	1.45	4 (16%)
3	PB2	D	502	-	19,20,20	2.00	4 (21%)	24,26,26	0.70	0
3	PB2	D	503	-	13,13,20	2.01	4 (30%)	16,16,26	0.99	0
4	CM5	D	504	-	23,23,36	0.49	0	29,29,49	2.51	10 (34%)

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	1,3	-	0/10/54/54	0/0/8/8
3	PB2	A	501	2	-	0/8/8/8	0/3/3/3
3	PB2	A	503	-	-	0/4/4/8	0/2/2/3
4	CM5	A	504	-	-	0/11/35/65	0/2/2/3
3	PB2	B	496	-	-	0/8/8/8	0/3/3/3
2	HEM	B	500	1,3	-	0/10/54/54	0/0/8/8
3	PB2	B	501	2	-	0/8/8/8	0/3/3/3
3	PB2	B	502	-	-	0/8/8/8	0/3/3/3
3	PB2	B	503	-	-	0/4/4/8	0/2/2/3
4	CM5	B	504	-	-	0/11/35/65	0/2/2/3
2	HEM	C	500	1,3	-	0/10/54/54	0/0/8/8
3	PB2	C	501	2	-	0/8/8/8	0/3/3/3
3	PB2	C	502	-	-	0/8/8/8	0/3/3/3
3	PB2	C	503	-	-	0/4/4/8	0/2/2/3
4	CM5	C	504	-	-	0/11/35/65	1/2/2/3
2	HEM	D	500	1,3	-	0/10/54/54	0/0/8/8
3	PB2	D	501	2	-	0/8/8/8	0/3/3/3
3	PB2	D	502	-	-	0/8/8/8	0/3/3/3
3	PB2	D	503	-	-	0/4/4/8	0/2/2/3
4	CM5	D	504	-	-	0/11/35/65	0/2/2/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C3B-C4B	-12.27	1.40	1.51
2	A	500	HEM	C3B-C4B	-11.65	1.41	1.51
2	B	500	HEM	C3B-C4B	-11.47	1.41	1.51
2	D	500	HEM	C3B-C4B	-8.50	1.44	1.51
2	B	500	HEM	C3D-C4D	-7.72	1.41	1.51
2	D	500	HEM	C3D-C4D	-7.51	1.41	1.51
2	A	500	HEM	C3D-C4D	-7.07	1.42	1.51
2	C	500	HEM	C3D-C4D	-6.97	1.42	1.51
2	B	500	HEM	C2C-C1C	-6.05	1.41	1.52
2	C	500	HEM	C2C-C1C	-5.85	1.41	1.52
2	A	500	HEM	C2C-C1C	-5.78	1.41	1.52
2	C	500	HEM	FE-NB	-4.96	1.71	1.97
2	D	500	HEM	C2C-C1C	-4.85	1.43	1.52
2	B	500	HEM	FE-NC	-4.38	1.78	1.95
3	C	502	PB2	CAF-NAB	-4.34	1.29	1.37
3	B	502	PB2	CAF-NAB	-4.22	1.29	1.37
3	B	501	PB2	CAF-NAB	-3.87	1.30	1.37
2	A	500	HEM	C2D-C1D	-3.29	1.41	1.51
2	D	500	HEM	C2B-C1B	-3.06	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	FE-NC	-2.94	1.84	1.95
2	A	500	HEM	FE-NB	-2.86	1.82	1.97
3	A	501	PB2	CAF-NAB	-2.83	1.32	1.37
2	B	500	HEM	C2B-C1B	-2.81	1.42	1.51
2	C	500	HEM	C2D-C1D	-2.79	1.42	1.51
2	A	500	HEM	C2B-C1B	-2.78	1.42	1.51
2	C	500	HEM	C2B-C1B	-2.77	1.42	1.51
2	B	500	HEM	C2D-C1D	-2.65	1.43	1.51
2	D	500	HEM	C2A-C3A	-2.64	1.29	1.37
3	B	502	PB2	CAA-NAB	-2.59	1.43	1.49
3	C	502	PB2	CAA-NAB	-2.58	1.43	1.49
2	A	500	HEM	C2A-C3A	-2.56	1.30	1.37
2	D	500	HEM	C2D-C1D	-2.56	1.43	1.51
3	B	496	PB2	CAF-NAB	-2.55	1.32	1.37
3	B	503	PB2	CDF-CDA	-2.47	1.33	1.39
3	D	501	PB2	CAF-NAB	-2.44	1.33	1.37
3	C	501	PB2	CAF-NAB	-2.38	1.33	1.37
2	C	500	HEM	C2A-C3A	-2.31	1.30	1.37
3	D	503	PB2	CDF-CDA	-2.27	1.34	1.39
2	B	500	HEM	C2A-C3A	-2.27	1.30	1.37
2	D	500	HEM	C4A-CHB	-2.21	1.33	1.39
3	C	501	PB2	CAA-NAB	-2.18	1.44	1.49
3	B	496	PB2	CAA-NAB	-2.16	1.44	1.49
3	A	503	PB2	CCE-CCD	-2.16	1.34	1.39
2	A	500	HEM	C2D-C3D	-2.13	1.48	1.54
3	A	503	PB2	CCA-CCF	2.02	1.43	1.38
2	A	500	HEM	C4C-NC	2.05	1.38	1.36
3	C	501	PB2	CCB-CCA	2.07	1.43	1.38
3	A	501	PB2	CDE-CDD	2.09	1.43	1.38
3	D	503	PB2	CCA-CCF	2.11	1.43	1.38
3	D	502	PB2	CDE-CDD	2.12	1.43	1.38
3	A	501	PB2	CAA-CCA	2.15	1.56	1.51
3	B	496	PB2	CDE-CDD	2.18	1.43	1.38
2	C	500	HEM	FE-ND	2.21	2.09	1.97
3	C	503	PB2	CDE-CDD	2.22	1.43	1.38
3	B	501	PB2	CCB-CCA	2.23	1.43	1.38
2	D	500	HEM	C4C-NC	2.30	1.38	1.36
3	B	501	PB2	CDE-CDD	2.31	1.44	1.38
3	D	502	PB2	CCF-CCA	2.36	1.43	1.38
2	D	500	HEM	C1C-NC	2.42	1.39	1.36
3	C	501	PB2	CCF-CCE	2.52	1.43	1.38
3	B	496	PB2	CCF-CCA	2.60	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PB2	CCF-CCA	2.60	1.44	1.38
3	D	501	PB2	CCF-CCE	2.63	1.43	1.38
3	D	501	PB2	CCF-CCA	2.67	1.44	1.38
3	B	501	PB2	CCF-CCA	2.74	1.44	1.38
3	D	501	PB2	CCB-CCA	2.75	1.44	1.38
3	B	501	PB2	CCF-CCE	2.83	1.43	1.38
3	C	501	PB2	CCF-CCA	2.98	1.45	1.38
3	D	501	PB2	CDE-CDD	3.02	1.45	1.38
3	B	503	PB2	CCC-CCD	3.17	1.46	1.39
3	A	503	PB2	CDB-CDA	3.35	1.46	1.39
3	C	503	PB2	CCC-CCD	3.44	1.46	1.39
3	C	502	PB2	CCC-CCD	3.49	1.46	1.39
3	B	502	PB2	CCC-CCD	3.56	1.47	1.39
3	D	503	PB2	CCC-CCD	3.60	1.47	1.39
3	C	503	PB2	CDB-CDA	3.69	1.47	1.39
3	B	502	PB2	CDB-CDA	3.71	1.47	1.39
3	B	503	PB2	CDB-CDA	3.77	1.47	1.39
3	C	501	PB2	CDB-CDA	3.78	1.47	1.39
3	A	503	PB2	CCC-CCD	3.79	1.47	1.39
3	D	503	PB2	CDB-CDA	3.81	1.47	1.39
3	C	502	PB2	CDB-CDA	3.82	1.47	1.39
3	A	501	PB2	CCC-CCD	3.99	1.47	1.39
3	D	501	PB2	CCC-CCD	4.05	1.48	1.39
3	B	496	PB2	CDB-CDA	4.14	1.48	1.39
3	D	502	PB2	CDB-CDA	4.43	1.48	1.39
3	B	496	PB2	CCC-CCD	4.54	1.49	1.39
3	C	501	PB2	CCC-CCD	4.58	1.49	1.39
3	D	502	PB2	CCC-CCD	4.73	1.49	1.39
3	D	501	PB2	CDB-CDA	4.81	1.49	1.39
3	B	501	PB2	CCC-CCD	4.92	1.49	1.39
3	A	501	PB2	CDB-CDA	5.16	1.50	1.39
3	B	501	PB2	CDB-CDA	5.35	1.50	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	504	CM5	C13-O14-C15	-7.80	105.30	113.15
4	B	504	CM5	C13-O14-C15	-5.37	107.75	113.15
4	A	504	CM5	C13-O14-C15	-5.01	108.11	113.15
4	A	504	CM5	C1-O12-C13	-4.36	106.33	113.94
3	C	501	PB2	CCC-CCD-CDA	-4.15	113.96	121.39
4	D	504	CM5	C1-O12-C13	-4.12	106.75	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	CM5	C16-C17-C18	-4.10	104.97	110.56
4	C	504	CM5	C17-C16-C15	-3.59	104.13	111.40
2	D	500	HEM	C3C-CAC-CBC	-3.53	119.05	124.46
3	D	501	PB2	CCE-CCF-CCA	-3.49	116.26	121.04
4	D	504	CM5	O14-C15-C16	-3.42	103.60	109.97
4	B	504	CM5	C5-C6-C7	-3.29	105.14	112.10
4	D	504	CM5	O22-C18-C17	-3.27	104.08	110.00
4	A	504	CM5	C17-C16-C15	-3.23	104.85	111.40
2	A	500	HEM	C3B-CAB-CBB	-3.21	119.53	124.46
2	C	500	HEM	C3B-C4B-CHC	-3.17	118.71	123.16
4	C	504	CM5	C13-C18-C17	-3.11	103.84	109.97
4	D	504	CM5	C17-C16-C15	-3.07	105.18	111.40
2	B	500	HEM	C4B-CHC-C1C	-2.99	120.82	125.82
4	D	504	CM5	C11-C6-C7	-2.94	101.87	109.26
2	B	500	HEM	C3C-CAC-CBC	-2.93	119.96	124.46
4	C	504	CM5	C1-O12-C13	-2.92	108.84	113.94
2	C	500	HEM	C3C-CAC-CBC	-2.88	120.04	124.46
4	D	504	CM5	C10-C11-C6	-2.83	107.65	112.22
2	B	500	HEM	CMA-C3A-C4A	-2.73	123.84	128.36
3	B	501	PB2	CDC-CDB-CDA	-2.71	116.98	120.56
4	B	504	CM5	C1-O12-C13	-2.67	109.28	113.94
3	B	496	PB2	CCC-CCD-CDA	-2.66	116.61	121.39
3	D	501	PB2	CCC-CCD-CDA	-2.63	116.67	121.39
4	B	504	CM5	C17-C16-C15	-2.60	106.13	111.40
4	A	504	CM5	C10-C11-C6	-2.55	108.10	112.22
4	B	504	CM5	C13-C18-C17	-2.52	105.02	109.97
4	A	504	CM5	C5-C6-C7	-2.50	106.80	112.10
2	C	500	HEM	C4B-CHC-C1C	-2.49	121.66	125.82
2	D	500	HEM	CAA-CBA-CGA	-2.48	108.21	112.75
2	D	500	HEM	C4B-CHC-C1C	-2.40	121.81	125.82
2	A	500	HEM	C1D-CHD-C4C	-2.36	121.87	125.82
3	B	496	PB2	CDF-CDA-CCD	-2.33	117.21	121.39
3	D	501	PB2	CDD-CDE-CDF	-2.22	116.93	120.19
4	B	504	CM5	C10-C9-C8	-2.22	104.15	111.27
2	C	500	HEM	CMA-C3A-C4A	-2.20	124.72	128.36
4	A	504	CM5	C3-C4-C5	-2.19	105.89	113.66
3	B	496	PB2	CCF-CCE-CCD	-2.19	117.95	121.14
3	D	501	PB2	CCB-CCC-CCD	-2.17	117.97	121.14
2	A	500	HEM	C4B-CHC-C1C	-2.14	122.24	125.82
4	B	504	CM5	C8-C7-C6	-2.14	108.77	112.22
3	B	496	PB2	CCC-CCB-CCA	-2.13	118.12	121.04
4	B	504	CM5	C9-C8-C7	-2.09	107.06	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	CM5	C4-C5-C6	-2.03	104.67	115.51
3	C	503	PB2	CCC-CCD-CCE	2.00	121.34	117.55
2	D	500	HEM	CAA-C2A-C1A	2.04	129.22	127.01
2	B	500	HEM	C2D-C3D-C4D	2.07	105.01	101.50
2	A	500	HEM	C2D-C3D-C4D	2.13	105.10	101.50
3	C	501	PB2	CCE-CCD-CDA	2.27	125.46	121.39
2	D	500	HEM	CMD-C2D-C3D	2.29	124.47	114.35
2	A	500	HEM	CMD-C2D-C3D	2.31	124.55	114.35
2	C	500	HEM	CMD-C2D-C3D	2.31	124.56	114.35
2	D	500	HEM	CMC-C2C-C3C	2.48	122.71	116.53
3	C	503	PB2	CDF-CDA-CDB	2.49	122.26	117.55
2	B	500	HEM	CMD-C2D-C3D	2.50	125.41	114.35
2	A	500	HEM	CMC-C2C-C3C	2.52	122.83	116.53
4	D	504	CM5	O14-C13-C18	2.54	115.49	110.28
2	D	500	HEM	C3B-C4B-CHC	2.61	126.84	123.16
4	D	504	CM5	C13-C18-C17	2.82	115.52	109.97
2	D	500	HEM	CMB-C2B-C3B	2.90	123.78	116.53
4	B	504	CM5	O12-C13-C18	3.23	112.12	108.04
2	C	500	HEM	CMC-C2C-C3C	3.32	124.81	116.53
2	A	500	HEM	CAD-C3D-C2D	3.59	123.55	113.22
2	B	500	HEM	CMC-C2C-C3C	3.67	125.70	116.53
4	C	504	CM5	C13-O14-C15	3.78	116.96	113.15
2	B	500	HEM	CMB-C2B-C3B	3.88	126.22	116.53
2	A	500	HEM	CMB-C2B-C3B	3.97	126.44	116.53
2	C	500	HEM	CMB-C2B-C3B	4.01	126.53	116.53
2	C	500	HEM	CAD-C3D-C2D	4.10	125.00	113.22
2	B	500	HEM	CAD-C3D-C2D	4.42	125.92	113.22
2	D	500	HEM	CAD-C3D-C2D	4.47	126.08	113.22
2	B	500	HEM	CAD-C3D-C4D	4.70	129.06	112.47
4	C	504	CM5	O14-C15-C19	4.74	112.42	106.62
2	D	500	HEM	CAD-C3D-C4D	4.76	129.25	112.47
4	D	504	CM5	O14-C15-C19	4.81	112.51	106.62
4	B	504	CM5	O14-C15-C19	5.03	112.78	106.62
2	C	500	HEM	CAD-C3D-C4D	5.23	130.92	112.47
2	A	500	HEM	CAD-C3D-C4D	5.34	131.32	112.47
4	A	504	CM5	O14-C15-C19	6.07	114.06	106.62

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	504	CM5	C13-C15-C16-C17-C18-O14

19 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	9	0
3	A	503	PB2	11	0
4	A	504	CM5	1	0
3	B	496	PB2	5	0
2	B	500	HEM	11	0
3	B	501	PB2	2	0
3	B	502	PB2	10	0
3	B	503	PB2	7	0
4	B	504	CM5	4	0
2	C	500	HEM	5	0
3	C	501	PB2	1	0
3	C	502	PB2	13	0
3	C	503	PB2	10	0
4	C	504	CM5	7	0
2	D	500	HEM	12	0
3	D	501	PB2	2	0
3	D	502	PB2	7	0
3	D	503	PB2	10	0
4	D	504	CM5	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	456/476 (95%)	0.12	19 (4%)	40	45	34, 59, 97, 128	0
1	B	451/476 (94%)	0.05	11 (2%)	62	66	27, 61, 98, 125	0
1	C	452/476 (94%)	0.20	24 (5%)	30	34	31, 62, 100, 123	0
1	D	451/476 (94%)	0.10	17 (3%)	44	49	27, 60, 96, 121	0
All	All	1810/1904 (95%)	0.12	71 (3%)	43	48	27, 61, 98, 128	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	SER	6.9
1	C	416	ALA	6.5
1	A	283	PHE	6.1
1	C	130	ALA	5.0
1	A	256	LEU	5.0
1	C	26	SER	4.9
1	A	127	PHE	4.8
1	A	273	GLU	3.9
1	D	260	ASN	3.8
1	D	259	SER	3.6
1	B	272	MET	3.6
1	A	474	GLU	3.5
1	A	260	ASN	3.5
1	C	418	GLY	3.4
1	A	268	TYR	3.4
1	C	324	VAL	3.4
1	B	256	LEU	3.4
1	C	454	LEU	3.3
1	A	335	HIS	3.2
1	D	270	LEU	3.1
1	C	332	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	468	ILE	3.0
1	D	492	HIS	3.0
1	A	257	ASP	3.0
1	C	488	PHE	2.9
1	D	226	TYR	2.9
1	A	255	THR	2.9
1	B	134	ASP	2.9
1	C	317	TYR	2.9
1	B	285	HIS	2.9
1	D	261	PRO	2.8
1	C	492	HIS	2.8
1	A	270	LEU	2.8
1	B	488	PHE	2.8
1	D	256	LEU	2.7
1	C	417	ASN	2.7
1	D	475	SER	2.7
1	D	324	VAL	2.7
1	C	453	ILE	2.6
1	C	257	ASP	2.6
1	C	131	THR	2.6
1	A	134	ASP	2.6
1	D	165	LEU	2.6
1	B	463	VAL	2.5
1	B	260	ASN	2.5
1	C	160	SER	2.5
1	C	414	LEU	2.5
1	C	450	PHE	2.4
1	A	259	SER	2.4
1	D	134	ASP	2.4
1	C	489	LEU	2.4
1	D	400	ARG	2.3
1	C	333	GLY	2.3
1	D	157	LEU	2.3
1	A	284	HIS	2.3
1	A	27	LYS	2.2
1	C	475	SER	2.2
1	C	491	ARG	2.2
1	C	256	LEU	2.2
1	D	334	SER	2.1
1	A	272	MET	2.1
1	D	271	ARG	2.1
1	C	320	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	44	LEU	2.1
1	C	270	LEU	2.1
1	A	275	ASP	2.1
1	D	463	VAL	2.1
1	B	253	ARG	2.0
1	B	273	GLU	2.0
1	B	185	GLY	2.0
1	A	261	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CM5	C	504	22/34	0.86	0.45	16.21	20,20,20,20	0
3	PB2	D	503	12/18	0.82	0.45	13.80	62,69,83,85	12
4	CM5	D	504	22/34	0.91	0.37	9.02	20,20,20,20	0
3	PB2	C	503	12/18	0.78	0.40	6.89	57,66,72,72	12
3	PB2	A	503	12/18	0.87	0.37	5.97	53,63,77,78	12
4	CM5	A	504	22/34	0.88	0.28	5.93	20,20,20,20	0
4	CM5	B	504	22/34	0.86	0.35	5.86	20,20,20,20	0
3	PB2	C	502	18/18	0.90	0.29	3.79	54,78,87,89	0
3	PB2	B	503	12/18	0.90	0.24	1.66	61,73,81,85	12
3	PB2	B	496	18/18	0.95	0.21	0.97	53,60,74,76	0
3	PB2	D	502	18/18	0.93	0.17	0.12	43,65,73,74	0
3	PB2	D	501	18/18	0.97	0.19	0.03	27,39,50,51	0
3	PB2	B	502	18/18	0.94	0.18	-0.01	53,68,82,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	D	500	43/43	0.98	0.17	-0.05	36,51,59,63	0
3	PB2	C	501	18/18	0.97	0.15	-0.24	30,46,52,52	0
2	HEM	C	500	43/43	0.98	0.14	-0.44	32,51,61,66	0
3	PB2	B	501	18/18	0.98	0.16	-0.58	30,40,46,51	0
2	HEM	B	500	43/43	0.99	0.13	-0.63	31,43,58,63	0
3	PB2	A	501	18/18	0.99	0.15	-0.88	32,35,47,49	0
2	HEM	A	500	43/43	0.98	0.13	-0.89	31,42,51,63	0

6.5 Other polymers (i)

There are no such residues in this entry.