Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 PM GMT

PDB ID	:	4RUI
Title	:	Crystal structure of a cytochrome P450 2A6 in complex with a monoterpene - sabinene.
Authors	:	Shah, M.B.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2014-11-19
Resolution	:	2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

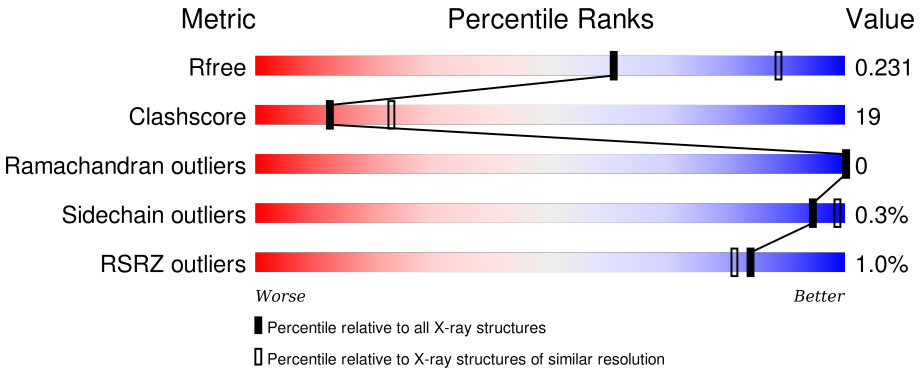
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	65% 32%
1	B	476	68% 29%
1	C	476	63% 34%
1	D	476	75% 22%
1	E	476	66% 32%

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Mol	Chain	Length	Quality of chain
1	F	476	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SNE	A	501	-	-	-	X
3	SNE	B	502	-	-	-	X
3	SNE	C	502	-	-	X	X
3	SNE	D	502	-	-	-	X
3	SNE	E	502	-	-	-	X
3	SNE	F	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22515 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 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	465	Total	C	N	O	S	0	0	0
			3688	2368	628	674	18			
1	A	464	Total	C	N	O	S	0	0	0
			3687	2369	627	673	18			
1	B	465	Total	C	N	O	S	0	0	0
			3692	2374	631	669	18			
1	C	464	Total	C	N	O	S	0	0	0
			3594	2313	598	665	18			
1	E	465	Total	C	N	O	S	0	0	0
			3627	2327	613	669	18			
1	F	465	Total	C	N	O	S	0	0	0
			3597	2320	593	666	18			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	23	MET	-	EXPRESSION TAG	UNP P11509
D	24	ALA	-	EXPRESSION TAG	UNP P11509
D	25	LYS	-	EXPRESSION TAG	UNP P11509
D	26	LYS	-	EXPRESSION TAG	UNP P11509
D	27	THR	-	EXPRESSION TAG	UNP P11509
D	28	SER	-	EXPRESSION TAG	UNP P11509
D	392	TYR	PHE	Natural Variant	UNP P11509
D	495	HIS	-	EXPRESSION TAG	UNP P11509
D	496	HIS	-	EXPRESSION TAG	UNP P11509
D	497	HIS	-	EXPRESSION TAG	UNP P11509
D	498	HIS	-	EXPRESSION TAG	UNP P11509
A	23	MET	-	EXPRESSION TAG	UNP P11509
A	24	ALA	-	EXPRESSION TAG	UNP P11509
A	25	LYS	-	EXPRESSION TAG	UNP P11509
A	26	LYS	-	EXPRESSION TAG	UNP P11509
A	27	THR	-	EXPRESSION TAG	UNP P11509
A	28	SER	-	EXPRESSION TAG	UNP P11509

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Chain	Residue	Modelled	Actual	Comment	Reference
A	392	TYR	PHE	Natural Variant	UNP P11509
A	495	HIS	-	EXPRESSION TAG	UNP P11509
A	496	HIS	-	EXPRESSION TAG	UNP P11509
A	497	HIS	-	EXPRESSION TAG	UNP P11509
A	498	HIS	-	EXPRESSION TAG	UNP P11509
B	23	MET	-	EXPRESSION TAG	UNP P11509
B	24	ALA	-	EXPRESSION TAG	UNP P11509
B	25	LYS	-	EXPRESSION TAG	UNP P11509
B	26	LYS	-	EXPRESSION TAG	UNP P11509
B	27	THR	-	EXPRESSION TAG	UNP P11509
B	28	SER	-	EXPRESSION TAG	UNP P11509
B	392	TYR	PHE	Natural Variant	UNP P11509
B	495	HIS	-	EXPRESSION TAG	UNP P11509
B	496	HIS	-	EXPRESSION TAG	UNP P11509
B	497	HIS	-	EXPRESSION TAG	UNP P11509
B	498	HIS	-	EXPRESSION TAG	UNP P11509
C	23	MET	-	EXPRESSION TAG	UNP P11509
C	24	ALA	-	EXPRESSION TAG	UNP P11509
C	25	LYS	-	EXPRESSION TAG	UNP P11509
C	26	LYS	-	EXPRESSION TAG	UNP P11509
C	27	THR	-	EXPRESSION TAG	UNP P11509
C	28	SER	-	EXPRESSION TAG	UNP P11509
C	392	TYR	PHE	Natural Variant	UNP P11509
C	495	HIS	-	EXPRESSION TAG	UNP P11509
C	496	HIS	-	EXPRESSION TAG	UNP P11509
C	497	HIS	-	EXPRESSION TAG	UNP P11509
C	498	HIS	-	EXPRESSION TAG	UNP P11509
E	23	MET	-	EXPRESSION TAG	UNP P11509
E	24	ALA	-	EXPRESSION TAG	UNP P11509
E	25	LYS	-	EXPRESSION TAG	UNP P11509
E	26	LYS	-	EXPRESSION TAG	UNP P11509
E	27	THR	-	EXPRESSION TAG	UNP P11509
E	28	SER	-	EXPRESSION TAG	UNP P11509
E	392	TYR	PHE	Natural Variant	UNP P11509
E	495	HIS	-	EXPRESSION TAG	UNP P11509
E	496	HIS	-	EXPRESSION TAG	UNP P11509
E	497	HIS	-	EXPRESSION TAG	UNP P11509
E	498	HIS	-	EXPRESSION TAG	UNP P11509
F	23	MET	-	EXPRESSION TAG	UNP P11509
F	24	ALA	-	EXPRESSION TAG	UNP P11509
F	25	LYS	-	EXPRESSION TAG	UNP P11509
F	26	LYS	-	EXPRESSION TAG	UNP P11509

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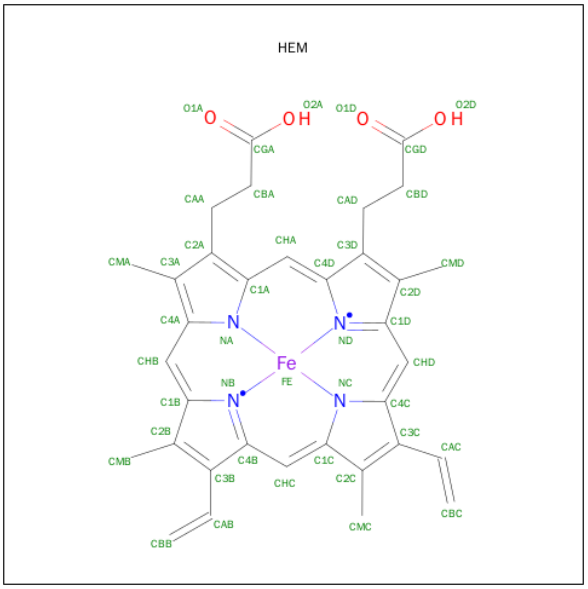
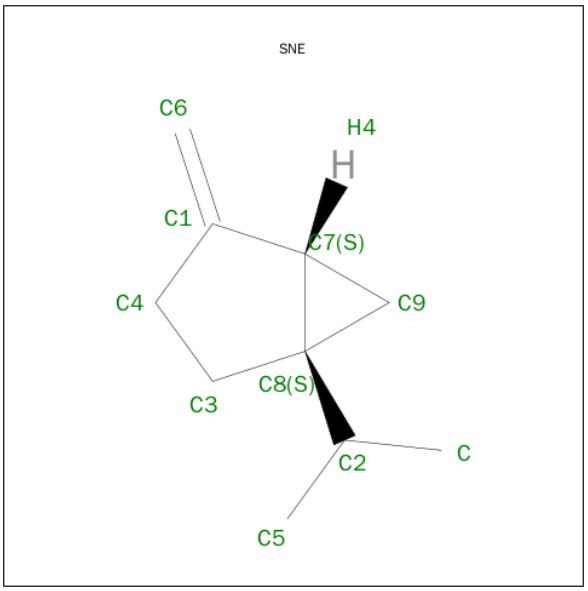
Chain	Residue	Modelled	Actual	Comment	Reference
F	27	THR	-	EXPRESSION TAG	UNP P11509
F	28	SER	-	EXPRESSION TAG	UNP P11509
F	392	TYR	PHE	Natural Variant	UNP P11509
F	495	HIS	-	EXPRESSION TAG	UNP P11509
F	496	HIS	-	EXPRESSION TAG	UNP P11509
F	497	HIS	-	EXPRESSION TAG	UNP P11509
F	498	HIS	-	EXPRESSION TAG	UNP P11509

- 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	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
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	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SABINENE (three-letter code: SNE) (formula: $C_{10}H_{16}$).



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

- Molecule 4 is water.

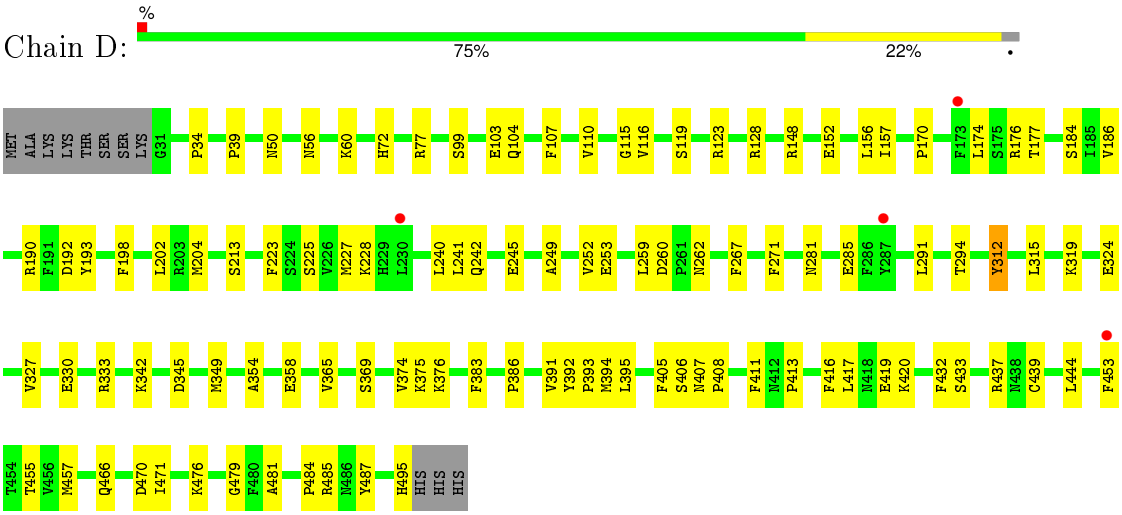
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	53	Total O 53 53	0	0
4	A	74	Total O 74 74	0	0
4	B	65	Total O 65 65	0	0
4	C	36	Total O 36 36	0	0
4	E	46	Total O 46 46	0	0
4	F	38	Total O 38 38	0	0

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.

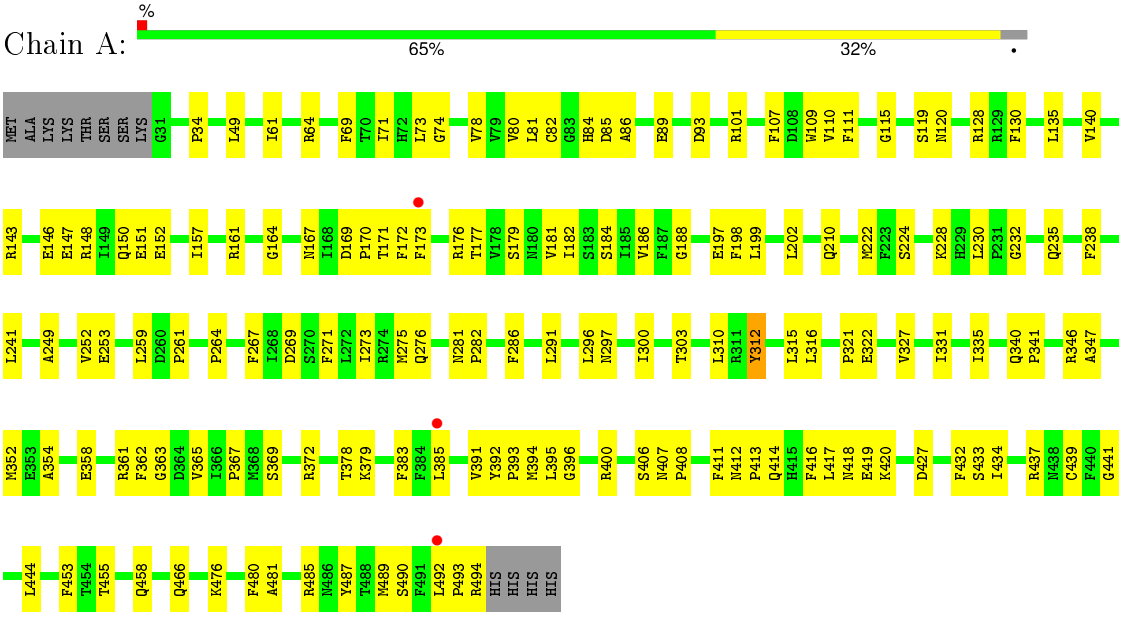
- Molecule 1: Cytochrome P450 2A6

Chain D:



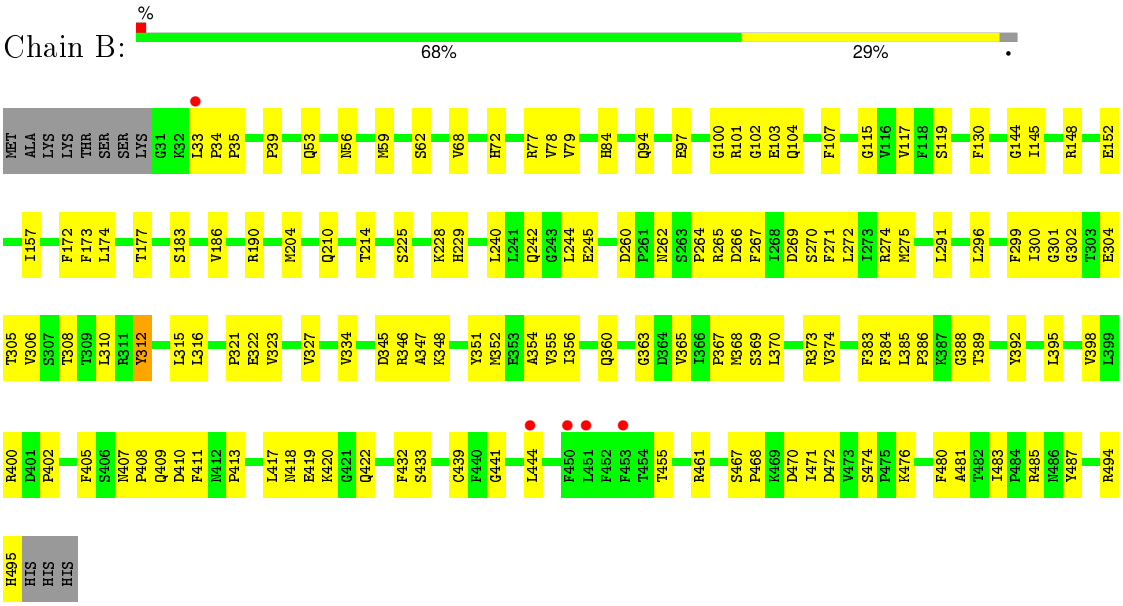
- Molecule 1: Cytochrome P450 2A6

Chain A:



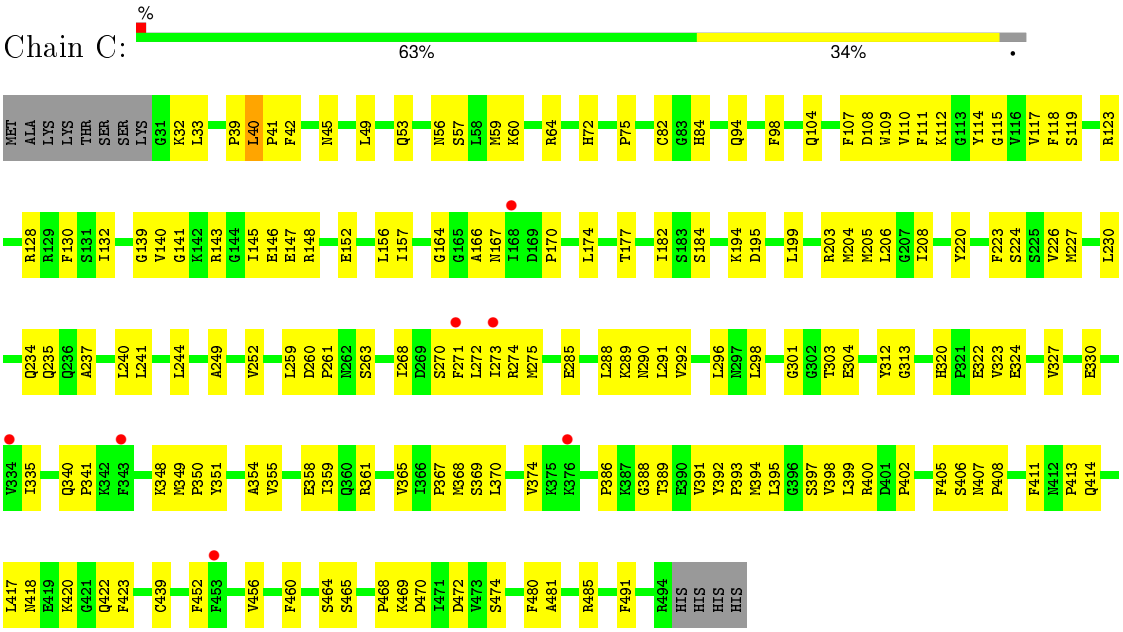
- Molecule 1: Cytochrome P450 2A6

Chain B:



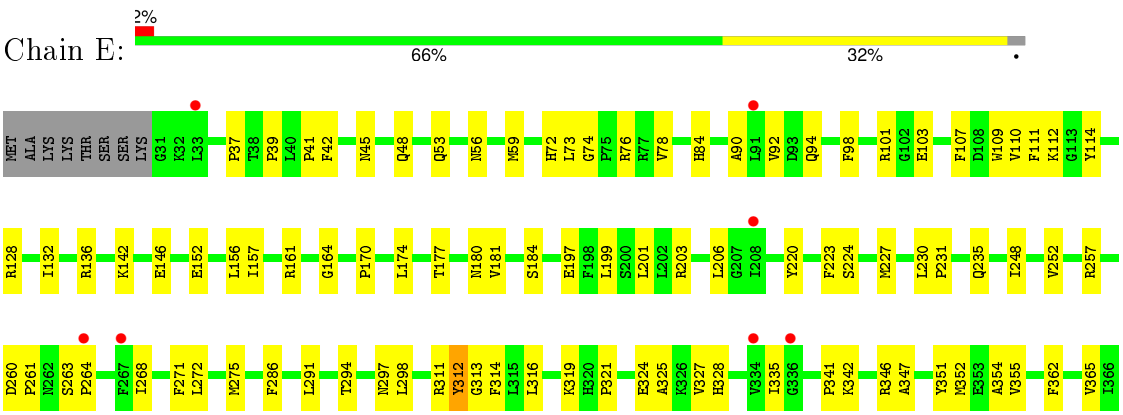
• Molecule 1: Cytochrome P450 2A6

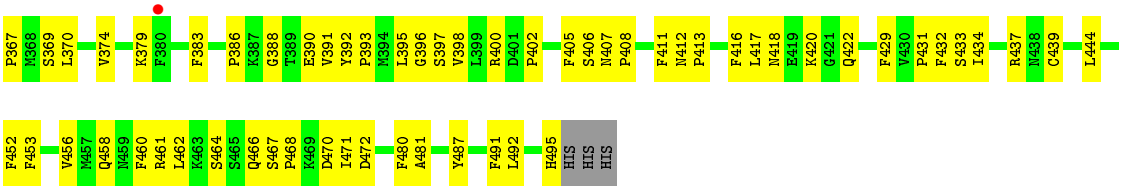
Chain C:



• Molecule 1: Cytochrome P450 2A6

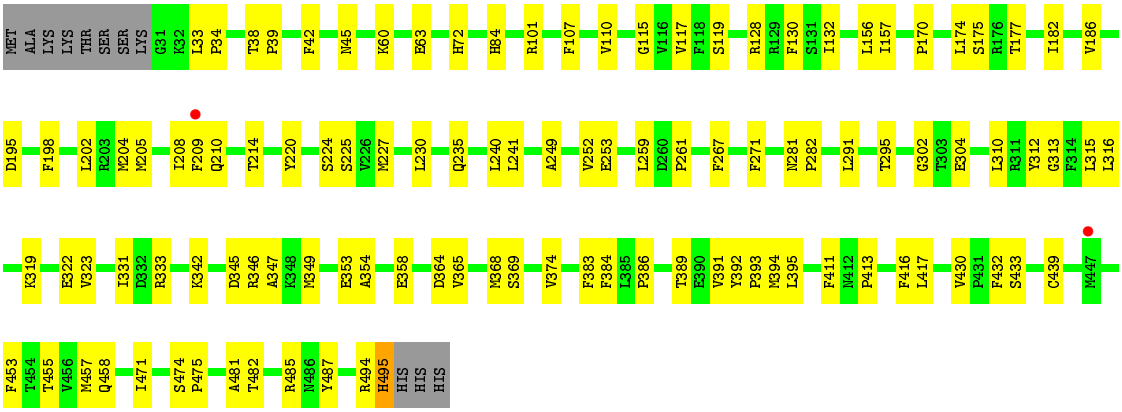
Chain E:





- Molecule 1: Cytochrome P450 2A6

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.74Å 132.97Å 133.03Å 62.40° 99.06° 80.93°	Depositor
Resolution (Å)	50.00 – 2.61 38.75 – 2.61	Depositor EDS
% Data completeness (in resolution range)	90.2 (50.00-2.61) 75.4 (38.75-2.61)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.197 , 0.261 0.207 , 0.231	Depositor DCC
R_{free} test set	5000 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.2	EDS
Estimated twinning fraction	0.417 for h,-l,-h+k-l 0.417 for h,h-k+l,-k 0.032 for -h,-h+k-l,-l 0.029 for -h,l,k 0.030 for -h,-k,h-k+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 99609 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22515	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, SNE

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	0.70	0/3778	0.73	0/5105
1	B	0.68	0/3784	0.73	0/5113
1	C	0.68	0/3684	0.73	1/4997 (0.0%)
1	D	0.66	0/3780	0.69	0/5112
1	E	0.65	0/3717	0.70	0/5034
1	F	0.67	0/3689	0.68	0/5005
All	All	0.68	0/22432	0.71	1/30366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	40	LEU	CA-CB-CG	-5.25	103.23	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	3687	0	3585	157	0
1	B	3692	0	3591	115	0
1	C	3594	0	3388	179	0
1	D	3688	0	3560	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3627	0	3441	162	0
1	F	3597	0	3372	111	0
2	A	43	0	30	15	0
2	B	43	0	30	17	0
2	C	43	0	30	3	0
2	D	43	0	30	15	0
2	E	43	0	30	10	0
2	F	43	0	30	14	0
3	A	10	0	16	1	0
3	B	10	0	16	2	0
3	C	10	0	16	6	0
3	D	10	0	16	1	0
3	E	10	0	16	4	0
3	F	10	0	16	3	0
4	A	74	0	0	11	0
4	B	65	0	0	8	0
4	C	36	0	0	1	0
4	D	53	0	0	7	0
4	E	46	0	0	4	0
4	F	38	0	0	1	0
All	All	22515	0	21213	841	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 19.

All (841) 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:F:354:ALA:CB	1:F:417:LEU:HD21	1.62	1.30
1:C:40:LEU:HB3	1:C:41:PRO:CD	1.66	1.26
1:E:107:PHE:O	1:E:110:VAL:HG12	1.30	1.25
1:A:439:CYS:HB2	2:A:502:HEM:NA	1.57	1.17
1:E:354:ALA:CB	1:E:417:LEU:HD21	1.77	1.15
1:C:330:GLU:OE2	1:C:351:TYR:HB3	1.43	1.14
1:C:139:GLY:HA3	1:C:145:ILE:HG23	1.24	1.14
1:C:140:VAL:HA	1:C:145:ILE:HD13	1.21	1.11
1:D:354:ALA:CB	1:D:417:LEU:CD1	2.29	1.11
1:A:49:LEU:HD21	1:A:71:ILE:HD11	1.18	1.10
1:F:354:ALA:CB	1:F:417:LEU:CD2	2.31	1.08
1:D:354:ALA:CB	1:D:417:LEU:HD11	1.83	1.08
1:A:111:PHE:CZ	1:A:296:LEU:HD12	1.88	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:HG13	1:B:352:MET:HE2	1.23	1.07
1:A:115:GLY:O	1:A:119:SER:HB3	1.53	1.06
1:A:439:CYS:HB2	2:A:502:HEM:C1A	1.90	1.06
1:F:354:ALA:HB1	1:F:417:LEU:CD2	1.85	1.05
1:C:40:LEU:HB3	1:C:41:PRO:HD2	1.09	1.05
1:B:419:GLU:HA	4:B:613:HOH:O	1.54	1.05
1:E:230:LEU:HD22	1:E:231:PRO:HD2	1.37	1.05
1:F:209:PHE:CE2	1:F:304:GLU:HB3	1.92	1.05
1:E:223:PHE:O	1:E:227:MET:HG3	1.59	1.03
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.39	1.02
1:D:39:PRO:HG3	1:D:72:HIS:CE1	1.94	1.02
1:D:312:TYR:CD2	1:D:484:PRO:HB3	1.95	1.01
1:B:439:CYS:HB2	2:B:501:HEM:NA	1.75	0.99
1:A:49:LEU:HD21	1:A:71:ILE:CD1	1.93	0.99
1:C:249:ALA:O	1:C:252:VAL:HG12	1.62	0.99
1:C:206:LEU:O	1:C:206:LEU:HD13	1.62	0.99
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.41	0.98
1:E:206:LEU:O	1:E:206:LEU:HD13	1.64	0.96
1:C:439:CYS:HB2	2:C:501:HEM:NA	1.79	0.96
1:A:157:ILE:HD11	1:A:455:THR:HG22	1.47	0.96
1:E:110:VAL:HG13	1:E:111:PHE:CD1	2.01	0.96
1:C:139:GLY:CA	1:C:145:ILE:HG23	1.95	0.96
1:A:249:ALA:O	1:A:252:VAL:HG12	1.64	0.95
1:A:354:ALA:CB	1:A:417:LEU:HD21	1.96	0.95
1:E:110:VAL:CG1	1:E:111:PHE:CD1	2.51	0.94
1:A:86:ALA:HB3	4:A:658:HOH:O	1.67	0.94
1:B:327:VAL:HG13	1:B:352:MET:CE	1.98	0.93
1:B:115:GLY:O	1:B:119:SER:HB3	1.69	0.93
1:A:378:THR:CG2	1:A:385:LEU:HB2	1.98	0.93
1:E:354:ALA:CB	1:E:417:LEU:CD2	2.47	0.93
1:A:413:PRO:O	1:A:417:LEU:HD23	1.70	0.92
1:D:354:ALA:HB1	1:D:417:LEU:CD1	1.98	0.91
1:E:110:VAL:HG13	1:E:111:PHE:N	1.82	0.91
1:D:192:ASP:HA	4:D:633:HOH:O	1.70	0.91
1:E:37:PRO:HB2	1:E:48:GLN:OE1	1.71	0.91
1:E:354:ALA:HB1	1:E:417:LEU:CD2	2.01	0.90
1:C:301:GLY:HA2	3:C:502:SNE:H12	1.53	0.90
1:F:354:ALA:HB1	1:F:417:LEU:HD21	1.43	0.90
1:C:237:ALA:O	1:C:241:LEU:HD23	1.71	0.89
1:A:327:VAL:HG13	1:A:352:MET:CE	2.02	0.89
1:D:342:LYS:O	1:D:345:ASP:HB2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HZ	1:A:296:LEU:HD12	1.35	0.89
2:D:501:HEM:HBB2	2:D:501:HEM:HMB1	1.52	0.89
1:B:439:CYS:HB2	2:B:501:HEM:C1A	2.07	0.89
1:B:225:SER:HA	1:B:228:LYS:HE3	1.55	0.89
1:C:40:LEU:CB	1:C:41:PRO:CD	2.49	0.88
1:E:92:VAL:HG23	1:E:434:ILE:HD12	1.54	0.88
1:C:170:PRO:HB2	1:C:174:LEU:HD23	1.55	0.88
1:B:461:ARG:HD3	4:B:616:HOH:O	1.72	0.87
1:E:107:PHE:CE2	3:E:502:SNE:H7	2.09	0.87
1:D:354:ALA:HB2	1:D:417:LEU:CD1	2.02	0.87
1:E:439:CYS:HB2	2:E:501:HEM:NA	1.89	0.86
1:C:140:VAL:HA	1:C:145:ILE:CD1	2.04	0.86
1:D:345:ASP:O	1:D:349:MET:HG3	1.76	0.85
1:E:492:LEU:HD12	1:E:492:LEU:N	1.90	0.85
1:A:109:TRP:CE3	1:A:110:VAL:HG23	2.11	0.85
1:F:209:PHE:CD2	1:F:304:GLU:HG3	2.11	0.85
1:F:413:PRO:O	1:F:417:LEU:HD23	1.77	0.85
1:A:354:ALA:CB	1:A:417:LEU:CD2	2.54	0.85
1:E:354:ALA:HB1	1:E:417:LEU:HD21	1.57	0.84
1:C:354:ALA:CB	1:C:417:LEU:CD2	2.56	0.84
1:E:109:TRP:O	1:E:109:TRP:CE3	2.30	0.84
1:A:181:VAL:O	1:A:184:SER:HB2	1.76	0.84
1:B:413:PRO:O	1:B:417:LEU:HD23	1.78	0.84
1:F:495:HIS:CD2	1:F:495:HIS:O	2.30	0.84
1:A:111:PHE:CE2	1:A:296:LEU:HD12	2.12	0.83
1:E:206:LEU:C	1:E:206:LEU:HD13	1.98	0.83
1:C:370:LEU:HD21	3:C:502:SNE:H5	1.60	0.83
1:F:249:ALA:O	1:F:252:VAL:HG12	1.77	0.83
1:D:312:TYR:CE2	1:D:484:PRO:HB3	2.14	0.83
1:C:140:VAL:CA	1:C:145:ILE:HD13	2.05	0.83
1:C:354:ALA:CB	1:C:417:LEU:HD21	2.08	0.83
1:A:354:ALA:HB1	1:A:417:LEU:CD2	2.10	0.82
1:C:117:VAL:HG12	1:C:118:PHE:CD1	2.15	0.81
1:F:110:VAL:HG11	1:F:241:LEU:HD22	1.62	0.81
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.10	0.81
1:C:109:TRP:HE3	1:C:110:VAL:CG2	1.94	0.81
1:C:206:LEU:C	1:C:206:LEU:HD13	2.01	0.80
1:A:86:ALA:CB	4:A:658:HOH:O	2.26	0.80
1:E:354:ALA:HB2	1:E:417:LEU:HD21	1.62	0.80
1:B:327:VAL:CG1	1:B:352:MET:HE2	2.10	0.79
1:A:327:VAL:HG13	1:A:352:MET:HE1	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.65	0.79
1:E:107:PHE:O	1:E:110:VAL:CG1	2.23	0.79
1:F:354:ALA:HB2	1:F:417:LEU:HD21	1.62	0.78
2:D:501:HEM:CMB	2:D:501:HEM:HBB2	2.13	0.78
1:A:249:ALA:O	1:A:252:VAL:CG1	2.30	0.78
1:C:204:MET:HA	1:C:240:LEU:HD22	1.65	0.78
1:A:111:PHE:CZ	1:A:296:LEU:CD1	2.66	0.78
1:F:374:VAL:HG21	1:F:386:PRO:O	1.84	0.78
1:C:330:GLU:OE2	1:C:351:TYR:CB	2.27	0.77
1:B:444:LEU:HD23	2:B:501:HEM:HBC2	1.64	0.77
1:B:354:ALA:CB	1:B:417:LEU:HD21	2.15	0.77
1:D:354:ALA:HB1	1:D:417:LEU:HD13	1.65	0.77
1:F:474:SER:HB3	1:F:485:ARG:HH21	1.50	0.77
1:F:392:TYR:HB3	1:F:394:MET:HE3	1.67	0.77
1:F:354:ALA:HB2	1:F:417:LEU:CD2	2.14	0.77
1:A:111:PHE:HZ	1:A:296:LEU:CD1	1.96	0.77
1:B:327:VAL:CG1	1:B:352:MET:CE	2.63	0.77
1:E:391:VAL:O	1:E:393:PRO:HD3	1.84	0.77
1:E:152:GLU:HG3	1:E:177:THR:HG23	1.66	0.77
1:E:170:PRO:HB2	1:E:174:LEU:HD23	1.67	0.76
1:A:249:ALA:HA	1:A:252:VAL:HG12	1.67	0.76
1:A:109:TRP:HE3	1:A:110:VAL:HG23	1.48	0.76
1:B:244:LEU:HB3	1:B:296:LEU:HD11	1.66	0.76
1:E:73:LEU:O	1:E:76:ARG:HG3	1.85	0.76
1:E:37:PRO:CB	1:E:48:GLN:OE1	2.34	0.76
1:F:175:SER:HB3	1:F:202:LEU:HD22	1.67	0.76
1:D:439:CYS:HB2	2:D:501:HEM:NA	1.99	0.76
1:F:358:GLU:HG3	1:F:411:PHE:CE1	2.20	0.76
1:C:32:LYS:HG3	1:C:33:LEU:H	1.50	0.76
1:E:374:VAL:HG21	1:E:386:PRO:O	1.85	0.76
1:F:271:PHE:CE2	1:F:291:LEU:HB2	2.20	0.76
1:C:139:GLY:O	1:C:145:ILE:HG12	1.86	0.75
1:C:139:GLY:HA3	1:C:145:ILE:CG2	2.12	0.75
1:D:374:VAL:HG22	1:D:376:LYS:O	1.86	0.75
1:D:444:LEU:HD23	2:D:501:HEM:CBC	2.17	0.75
1:D:416:PHE:O	1:D:417:LEU:HD12	1.86	0.74
1:C:40:LEU:CB	1:C:41:PRO:HD2	2.04	0.74
1:C:130:PHE:CE2	1:C:274:ARG:HD3	2.22	0.74
1:C:109:TRP:CE3	1:C:110:VAL:HG22	2.23	0.74
1:C:199:LEU:C	1:C:199:LEU:HD13	2.07	0.74
1:F:209:PHE:CD2	1:F:304:GLU:CG	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:PHE:HA	4:E:613:HOH:O	1.86	0.73
1:C:39:PRO:HG3	1:C:72:HIS:ND1	2.02	0.73
1:A:249:ALA:C	1:A:252:VAL:HG12	2.08	0.72
1:C:348:LYS:O	1:C:350:PRO:HD2	1.89	0.72
1:C:109:TRP:HE3	1:C:110:VAL:HG23	1.52	0.72
1:C:330:GLU:OE1	1:C:349:MET:CA	2.38	0.72
1:A:392:TYR:HB3	1:A:394:MET:CE	2.20	0.72
1:E:110:VAL:CG1	1:E:111:PHE:N	2.52	0.72
1:D:39:PRO:HB3	1:D:72:HIS:ND1	2.05	0.72
1:D:407:ASN:N	1:D:408:PRO:HD3	2.04	0.71
1:E:313:GLY:HA3	1:E:453:PHE:HZ	1.56	0.71
1:C:199:LEU:HD11	1:C:203:ARG:NE	2.05	0.71
1:A:176:ARG:HG2	1:A:198:PHE:CE2	2.25	0.71
1:E:491:PHE:C	1:E:492:LEU:HD12	2.10	0.71
1:A:458:GLN:HA	1:A:494:ARG:HH12	1.54	0.71
1:C:40:LEU:HD12	1:C:41:PRO:HD3	1.73	0.70
1:F:182:ILE:HD13	2:F:501:HEM:HBC1	1.72	0.70
1:D:312:TYR:CD2	1:D:484:PRO:CB	2.74	0.70
1:F:230:LEU:O	1:F:235:GLN:NE2	2.20	0.70
1:F:494:ARG:O	1:F:495:HIS:C	2.30	0.70
1:E:109:TRP:O	1:E:109:TRP:CD2	2.45	0.70
1:A:378:THR:HG23	1:A:385:LEU:HB2	1.70	0.69
1:B:444:LEU:HD23	2:B:501:HEM:CBC	2.22	0.69
2:F:501:HEM:HBB2	2:F:501:HEM:CMB	2.22	0.69
1:C:109:TRP:CE3	1:C:110:VAL:CG2	2.75	0.69
1:A:148:ARG:NH2	1:A:152:GLU:OE2	2.26	0.69
1:C:208:ILE:HG12	1:C:241:LEU:HD22	1.75	0.69
1:C:354:ALA:HB2	1:C:417:LEU:CD2	2.22	0.69
2:F:501:HEM:HBB2	2:F:501:HEM:HMB2	1.74	0.69
1:E:76:ARG:NH2	1:E:390:GLU:OE2	2.25	0.68
1:F:107:PHE:O	1:F:110:VAL:HG12	1.92	0.68
1:E:374:VAL:HG23	1:E:388:GLY:H	1.57	0.68
1:E:128:ARG:O	1:E:132:ILE:HG13	1.93	0.68
1:E:432:PHE:CE1	2:E:501:HEM:HBB2	2.28	0.68
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.74	0.68
1:E:492:LEU:CD1	1:E:492:LEU:N	2.55	0.68
1:B:345:ASP:HA	1:B:348:LYS:HE2	1.76	0.68
1:A:249:ALA:CA	1:A:252:VAL:HG12	2.23	0.68
1:C:128:ARG:O	1:C:132:ILE:HG13	1.93	0.68
1:E:406:SER:O	1:E:407:ASN:HB2	1.93	0.68
1:F:209:PHE:HD2	1:F:304:GLU:HG3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PRO:HB2	1:D:174:LEU:HD23	1.75	0.67
1:B:354:ALA:HB1	1:B:417:LEU:CD2	2.24	0.67
1:C:330:GLU:OE1	1:C:349:MET:HA	1.94	0.67
1:E:206:LEU:CD1	1:E:206:LEU:C	2.63	0.67
1:B:368:MET:HB2	4:B:664:HOH:O	1.94	0.67
1:D:34:PRO:HD3	1:D:383:PHE:HB3	1.76	0.67
1:A:327:VAL:HG13	1:A:352:MET:HE2	1.77	0.66
1:F:439:CYS:HB2	2:F:501:HEM:NA	2.10	0.66
1:C:439:CYS:HB2	2:C:501:HEM:C1A	2.29	0.66
1:C:110:VAL:HG21	1:C:241:LEU:HB3	1.76	0.66
1:A:458:GLN:HA	1:A:494:ARG:NH1	2.10	0.66
1:E:354:ALA:HB2	1:E:417:LEU:CD2	2.22	0.66
1:C:139:GLY:C	1:C:145:ILE:HG23	2.15	0.66
1:C:418:ASN:OD1	1:C:418:ASN:C	2.31	0.66
1:B:210:GLN:O	1:B:214:THR:HG23	1.95	0.66
1:C:117:VAL:CG1	1:C:118:PHE:CD1	2.78	0.66
1:C:350:PRO:HB3	1:C:423:PHE:HB2	1.77	0.66
1:E:197:GLU:O	1:E:201:LEU:HD13	1.96	0.66
1:D:354:ALA:HB3	1:D:417:LEU:HD11	1.76	0.65
1:A:249:ALA:HA	1:A:252:VAL:CG1	2.26	0.65
1:F:33:LEU:HD23	1:F:384:PHE:O	1.95	0.65
1:D:405:PHE:O	1:D:408:PRO:HG3	1.97	0.65
1:A:167:ASN:ND2	1:A:490:SER:OG	2.30	0.65
1:A:143:ARG:NH2	1:A:147:GLU:HG3	2.11	0.65
1:D:444:LEU:HD23	2:D:501:HEM:HBC2	1.77	0.65
1:F:354:ALA:HB3	1:F:417:LEU:HD21	1.72	0.65
1:A:172:PHE:O	1:A:176:ARG:HB2	1.97	0.64
1:D:249:ALA:O	1:D:252:VAL:HG12	1.96	0.64
1:E:413:PRO:O	1:E:417:LEU:HD23	1.97	0.64
1:D:354:ALA:HB2	1:D:417:LEU:HD12	1.77	0.64
1:A:354:ALA:HB3	1:A:417:LEU:HD21	1.79	0.64
1:F:374:VAL:CG2	1:F:386:PRO:O	2.44	0.64
1:E:39:PRO:HG3	1:E:72:HIS:CE1	2.33	0.64
1:B:33:LEU:HD23	1:B:384:PHE:O	1.97	0.64
1:D:374:VAL:CG2	1:D:376:LYS:O	2.45	0.64
1:E:248:ILE:O	1:E:252:VAL:HG23	1.98	0.64
1:D:157:ILE:HD11	1:D:455:THR:HG22	1.78	0.64
1:D:39:PRO:HG3	1:D:72:HIS:ND1	2.12	0.64
1:C:104:GLN:HB3	1:C:118:PHE:HE2	1.62	0.64
1:F:42:PHE:HA	4:F:616:HOH:O	1.96	0.64
1:A:135:LEU:O	1:A:140:VAL:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ARG:NH2	1:D:386:PRO:HG2	2.12	0.64
1:A:378:THR:HG22	1:A:385:LEU:HB2	1.80	0.64
1:D:391:VAL:O	1:D:393:PRO:HD3	1.98	0.63
1:B:420:LYS:HD2	1:B:422:GLN:OE1	1.98	0.63
1:B:354:ALA:HB1	1:B:417:LEU:HD21	1.79	0.63
1:E:405:PHE:O	1:E:408:PRO:HG3	1.98	0.63
1:B:79:VAL:HG21	1:B:385:LEU:CD2	2.29	0.63
1:A:230:LEU:O	1:A:235:GLN:NE2	2.29	0.63
1:D:107:PHE:O	1:D:110:VAL:HG12	1.99	0.62
1:F:271:PHE:CD2	1:F:291:LEU:HB2	2.34	0.62
1:E:128:ARG:NH1	2:E:501:HEM:O1D	2.29	0.62
1:C:223:PHE:O	1:C:227:MET:HG3	1.99	0.62
1:F:156:LEU:HD13	1:F:177:THR:OG1	1.98	0.62
1:A:416:PHE:O	1:A:417:LEU:HD22	1.99	0.62
1:F:170:PRO:HB2	1:F:174:LEU:HD23	1.82	0.62
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.81	0.62
1:B:476:LYS:HB2	1:B:485:ARG:HA	1.81	0.62
1:F:107:PHE:CE2	3:F:502:SNE:H7	2.35	0.62
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.82	0.61
1:A:110:VAL:HG21	1:A:241:LEU:HB3	1.81	0.61
1:C:82:CYS:SG	1:C:394:MET:HG3	2.40	0.61
1:C:104:GLN:HG3	1:C:107:PHE:HD1	1.65	0.61
1:A:275:MET:HG2	1:A:286:PHE:O	2.01	0.61
1:E:111:PHE:CE2	1:E:297:ASN:OD1	2.53	0.61
1:C:354:ALA:HB1	1:C:417:LEU:CD2	2.30	0.61
1:E:199:LEU:HG	1:E:203:ARG:HH21	1.65	0.61
1:E:73:LEU:HB2	1:E:76:ARG:HD3	1.82	0.61
1:D:259:LEU:HD12	4:D:635:HOH:O	2.01	0.61
1:E:257:ARG:HG3	4:E:631:HOH:O	1.99	0.61
1:C:234:GLN:OE1	1:C:234:GLN:N	2.33	0.61
1:C:139:GLY:C	1:C:145:ILE:CG2	2.69	0.61
1:C:472:ASP:C	1:C:472:ASP:OD1	2.38	0.61
1:E:72:HIS:HA	1:E:76:ARG:O	2.00	0.60
1:C:206:LEU:CD1	1:C:206:LEU:C	2.69	0.60
1:D:419:GLU:HG2	1:D:420:LYS:N	2.16	0.60
1:C:413:PRO:O	1:C:417:LEU:HD23	2.01	0.60
1:B:354:ALA:CB	1:B:417:LEU:CD2	2.78	0.60
1:E:365:VAL:O	1:E:481:ALA:HA	2.01	0.60
1:C:141:GLY:H	1:C:145:ILE:HD11	1.65	0.60
1:C:195:ASP:OD1	1:C:195:ASP:C	2.38	0.60
1:F:39:PRO:HG3	1:F:72:HIS:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLN:OE1	1:D:471:ILE:HA	2.02	0.60
1:D:148:ARG:HH11	1:D:148:ARG:HA	1.64	0.60
1:B:346:ARG:HG3	1:B:347:ALA:N	2.16	0.60
1:C:148:ARG:NH1	1:C:184:SER:OG	2.35	0.60
1:C:224:SER:C	1:C:226:VAL:H	2.04	0.60
1:D:285:GLU:HA	1:D:285:GLU:OE1	2.01	0.59
1:E:351:TYR:O	1:E:355:VAL:HG23	2.02	0.59
1:F:495:HIS:HD2	1:F:495:HIS:O	1.84	0.59
1:B:94:GLN:HB3	1:B:97:GLU:OE2	2.02	0.59
1:F:346:ARG:HB2	1:F:353:GLU:OE1	2.02	0.59
1:E:452:PHE:O	1:E:456:VAL:HG23	2.02	0.59
1:C:118:PHE:HE1	3:C:502:SNE:H1	1.66	0.59
1:C:117:VAL:HG11	1:C:118:PHE:CE1	2.37	0.59
1:B:225:SER:HA	1:B:228:LYS:CE	2.30	0.59
1:B:130:PHE:HD2	1:B:274:ARG:HH11	1.49	0.59
1:F:259:LEU:O	1:F:261:PRO:HD3	2.01	0.59
1:C:303:THR:HG22	1:C:304:GLU:N	2.16	0.59
1:D:128:ARG:HD2	2:D:501:HEM:O1D	2.02	0.59
1:E:335:ILE:HD13	1:E:341:PRO:HB3	1.85	0.59
1:F:157:ILE:HD11	1:F:455:THR:HG22	1.85	0.59
1:C:268:ILE:HG23	1:C:291:LEU:HD11	1.84	0.59
1:B:94:GLN:HG2	1:B:97:GLU:OE2	2.02	0.59
1:D:312:TYR:CE2	1:D:484:PRO:CB	2.86	0.58
1:B:316:LEU:HD13	1:B:411:PHE:CE1	2.38	0.58
1:F:316:LEU:O	1:F:319:LYS:N	2.35	0.58
1:A:82:CYS:N	4:A:658:HOH:O	2.35	0.58
1:B:152:GLU:HG3	1:B:177:THR:HG23	1.84	0.58
2:A:502:HEM:HBC2	2:A:502:HEM:CMC	2.33	0.58
1:B:174:LEU:HD12	1:B:310:LEU:HD13	1.85	0.58
1:A:143:ARG:HH21	1:A:147:GLU:HG3	1.67	0.58
1:A:61:ILE:O	1:A:64:ARG:HB3	2.04	0.58
1:B:97:GLU:O	1:B:374:VAL:HA	2.04	0.58
1:F:453:PHE:O	1:F:457:MET:HG2	2.04	0.58
1:A:252:VAL:HG13	1:A:253:GLU:N	2.19	0.58
2:B:501:HEM:CMC	2:B:501:HEM:HBC2	2.34	0.57
1:C:130:PHE:CE2	1:C:274:ARG:CD	2.87	0.57
1:B:148:ARG:NH2	1:B:190:ARG:HD2	2.19	0.57
1:E:110:VAL:CG1	1:E:111:PHE:CE1	2.88	0.57
1:C:330:GLU:OE1	1:C:349:MET:C	2.43	0.57
1:E:312:TYR:HH	1:E:362:PHE:HE2	1.51	0.57
1:D:433:SER:CB	2:D:501:HEM:HBA1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:SER:HB2	1:D:395:LEU:HG	1.87	0.57
1:D:354:ALA:HB2	1:D:417:LEU:HD11	1.68	0.57
1:C:322:GLU:HG3	1:C:323:VAL:HG23	1.87	0.57
1:C:107:PHE:CE2	3:C:502:SNE:H7	2.39	0.57
1:E:146:GLU:OE1	1:E:342:LYS:HG3	2.04	0.57
1:C:40:LEU:HB3	1:C:41:PRO:HD3	1.78	0.57
1:B:79:VAL:HG21	1:B:385:LEU:HD23	1.85	0.57
1:A:416:PHE:C	1:A:417:LEU:HD22	2.25	0.57
1:E:374:VAL:HG23	1:E:388:GLY:N	2.19	0.57
1:E:294:THR:O	1:E:298:LEU:HD23	2.05	0.57
1:E:444:LEU:HD23	2:E:501:HEM:CBC	2.35	0.56
2:D:501:HEM:HMC2	2:D:501:HEM:CBC	2.25	0.56
1:F:346:ARG:CG	1:F:347:ALA:N	2.67	0.56
1:C:94:GLN:O	1:C:98:PHE:HD1	1.88	0.56
1:B:144:GLY:HA3	4:B:622:HOH:O	2.04	0.56
1:F:209:PHE:CE2	1:F:304:GLU:CB	2.79	0.56
1:E:223:PHE:O	1:E:227:MET:CG	2.44	0.56
1:D:107:PHE:CE2	3:D:502:SNE:H7	2.40	0.56
1:F:291:LEU:O	1:F:295:THR:OG1	2.20	0.56
1:D:374:VAL:HG11	1:D:386:PRO:O	2.06	0.56
1:C:368:MET:HB3	1:C:394:MET:HE2	1.88	0.56
1:E:379:LYS:HA	1:E:383:PHE:O	2.04	0.56
1:C:474:SER:O	1:C:485:ARG:NE	2.39	0.56
1:C:117:VAL:CG1	1:C:118:PHE:CE1	2.89	0.56
1:B:369:SER:HB2	1:B:395:LEU:HG	1.88	0.56
1:C:391:VAL:O	1:C:393:PRO:HD3	2.05	0.56
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.41	0.56
1:C:367:PRO:HD2	1:C:480:PHE:O	2.04	0.56
1:F:495:HIS:O	1:F:495:HIS:CG	2.58	0.56
1:C:205:MET:SD	1:C:303:THR:HG21	2.46	0.56
1:B:367:PRO:HD2	1:B:480:PHE:O	2.06	0.56
1:C:354:ALA:HB2	1:C:417:LEU:HD22	1.87	0.56
1:C:199:LEU:O	1:C:199:LEU:HD13	2.06	0.56
1:C:170:PRO:HB2	1:C:174:LEU:CD2	2.32	0.56
1:E:369:SER:HB2	1:E:395:LEU:HG	1.86	0.56
1:C:374:VAL:HG21	1:C:386:PRO:O	2.06	0.55
1:E:235:GLN:HB2	4:E:630:HOH:O	2.05	0.55
2:D:501:HEM:CBB	2:D:501:HEM:HMB1	2.30	0.55
1:C:104:GLN:HG3	1:C:104:GLN:O	2.06	0.55
1:A:199:LEU:HD13	1:C:164:GLY:O	2.06	0.55
1:B:94:GLN:CB	1:B:97:GLU:OE2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:ALA:CB	1:F:417:LEU:HD22	2.35	0.55
1:E:76:ARG:NH2	1:E:103:GLU:HB3	2.22	0.55
1:E:110:VAL:HG11	1:E:111:PHE:CE1	2.42	0.55
1:C:452:PHE:O	1:C:456:VAL:HG23	2.07	0.55
1:A:232:GLY:HA2	4:A:633:HOH:O	2.07	0.55
1:A:433:SER:CB	2:A:502:HEM:HBA1	2.37	0.55
1:D:437:ARG:O	2:D:501:HEM:O2A	2.25	0.54
1:A:392:TYR:HB3	1:A:394:MET:HE3	1.87	0.54
1:B:494:ARG:HB3	4:B:646:HOH:O	2.07	0.54
1:C:40:LEU:N	1:C:40:LEU:HD22	2.22	0.54
1:C:139:GLY:CA	1:C:145:ILE:CG2	2.77	0.54
1:E:201:LEU:N	1:E:201:LEU:HD12	2.22	0.54
1:E:468:PRO:HA	1:E:471:ILE:HD12	1.89	0.54
1:B:386:PRO:HD2	1:B:389:THR:HG21	1.88	0.54
1:E:39:PRO:HG3	1:E:72:HIS:ND1	2.22	0.54
1:F:34:PRO:HD3	1:F:383:PHE:HB3	1.89	0.54
1:E:170:PRO:HB2	1:E:174:LEU:CD2	2.36	0.54
1:F:369:SER:HB2	1:F:395:LEU:HG	1.89	0.54
1:A:441:GLY:HA3	2:A:502:HEM:C3C	2.43	0.54
1:D:39:PRO:CB	1:D:72:HIS:ND1	2.71	0.54
1:B:101:ARG:HG3	1:B:102:GLY:O	2.07	0.54
1:C:354:ALA:HB2	1:C:417:LEU:HD21	1.83	0.54
1:C:199:LEU:C	1:C:199:LEU:CD1	2.75	0.54
1:F:433:SER:CB	2:F:501:HEM:HBA1	2.38	0.54
1:F:101:ARG:NH2	2:F:501:HEM:O2A	2.39	0.54
1:C:109:TRP:CZ3	1:C:110:VAL:HG22	2.42	0.54
1:D:148:ARG:HD3	1:D:184:SER:OG	2.08	0.54
1:B:327:VAL:CG1	1:B:352:MET:HE1	2.34	0.53
1:B:407:ASN:HB3	1:B:410:ASP:OD1	2.08	0.53
1:A:281:ASN:C	1:A:281:ASN:OD1	2.47	0.53
1:E:370:LEU:HD13	1:E:480:PHE:HE1	1.73	0.53
1:A:109:TRP:CH2	1:A:238:PHE:HB3	2.43	0.53
1:F:209:PHE:HZ	3:F:502:SNE:H9	1.73	0.53
1:A:176:ARG:HG3	1:A:202:LEU:CD1	2.38	0.53
1:F:186:VAL:HA	1:F:267:PHE:HB3	1.90	0.53
1:A:365:VAL:O	1:A:481:ALA:HA	2.07	0.53
1:E:110:VAL:HG13	1:E:111:PHE:H	1.66	0.53
1:E:402:PRO:HA	1:E:405:PHE:O	2.08	0.53
1:C:420:LYS:O	1:C:422:GLN:HG3	2.08	0.53
1:A:101:ARG:HB3	1:A:120:ASN:OD1	2.09	0.53
1:A:296:LEU:HD11	1:A:300:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:CG	1:C:33:LEU:H	2.18	0.53
1:C:368:MET:HB3	1:C:394:MET:CE	2.39	0.53
1:E:157:ILE:CD1	1:E:460:PHE:HE2	2.22	0.53
1:A:476:LYS:HB2	1:A:485:ARG:HA	1.90	0.53
1:B:186:VAL:HA	1:B:267:PHE:HB3	1.91	0.53
1:D:176:ARG:HG2	1:D:198:PHE:CE2	2.43	0.53
1:E:157:ILE:HD12	1:E:460:PHE:HE2	1.74	0.53
1:E:197:GLU:O	1:E:201:LEU:CD1	2.57	0.53
1:A:361:ARG:HH12	1:A:408:PRO:HA	1.73	0.53
1:C:480:PHE:HZ	3:C:502:SNE:C9	2.21	0.53
1:B:183:SER:OG	1:B:299:PHE:HE1	1.91	0.52
1:E:374:VAL:O	1:E:374:VAL:HG23	2.09	0.52
1:E:252:VAL:HG22	1:E:268:ILE:HD13	1.92	0.52
1:E:199:LEU:HD23	1:E:203:ARG:NH2	2.24	0.52
1:E:107:PHE:O	1:E:111:PHE:HD1	1.92	0.52
1:B:157:ILE:HD11	1:B:455:THR:HG22	1.90	0.52
1:C:358:GLU:HG3	1:C:411:PHE:CE1	2.45	0.52
1:E:324:GLU:O	1:E:327:VAL:HB	2.08	0.52
1:E:432:PHE:HB3	1:E:439:CYS:HB3	1.91	0.52
1:D:56:ASN:O	1:D:60:LYS:HG2	2.10	0.52
2:F:501:HEM:CBB	2:F:501:HEM:HMB2	2.39	0.52
1:E:235:GLN:HA	1:E:235:GLN:OE1	2.10	0.52
1:C:301:GLY:CA	3:C:502:SNE:H12	2.31	0.52
1:E:107:PHE:CZ	3:E:502:SNE:H7	2.44	0.52
1:D:99:SER:OG	1:D:375:LYS:HE2	2.10	0.52
1:A:432:PHE:O	1:A:433:SER:HB3	2.10	0.51
1:C:53:GLN:HB3	1:C:56:ASN:HB2	1.92	0.51
1:E:367:PRO:HD2	1:E:480:PHE:O	2.11	0.51
1:C:289:LYS:O	1:C:291:LEU:N	2.44	0.51
1:C:143:ARG:HH21	1:C:147:GLU:CG	2.23	0.51
1:A:34:PRO:HD3	1:A:383:PHE:HB3	1.91	0.51
1:B:323:VAL:O	1:B:327:VAL:HG23	2.11	0.51
1:A:101:ARG:HB3	1:A:120:ASN:ND2	2.26	0.51
1:C:324:GLU:O	1:C:327:VAL:HB	2.10	0.51
1:E:230:LEU:HD13	1:E:231:PRO:O	2.09	0.51
1:F:209:PHE:CZ	3:F:502:SNE:H9	2.45	0.51
1:C:237:ALA:O	1:C:241:LEU:CD2	2.54	0.51
1:E:199:LEU:CD2	1:E:203:ARG:HH21	2.24	0.51
1:A:161:ARG:HB3	1:C:194:LYS:HD3	1.91	0.51
1:B:78:VAL:HG11	1:B:392:TYR:CD2	2.46	0.51
1:F:391:VAL:O	1:F:393:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ARG:O	1:E:487:TYR:OH	2.24	0.51
1:C:320:HIS:ND1	1:C:322:GLU:OE1	2.38	0.51
1:A:276:GLN:HG2	4:A:664:HOH:O	2.11	0.51
1:B:266:ASP:O	1:B:269:ASP:HB2	2.11	0.51
1:E:417:LEU:HA	1:E:422:GLN:O	2.11	0.51
1:B:420:LYS:HG3	1:B:422:GLN:HG3	1.92	0.51
1:F:346:ARG:O	1:F:349:MET:N	2.27	0.51
1:E:464:SER:HB3	1:E:466:GLN:O	2.11	0.51
1:E:458:GLN:O	1:E:458:GLN:HG2	2.10	0.51
1:D:213:SER:HA	1:D:479:GLY:HA3	1.92	0.51
1:E:439:CYS:HB2	2:E:501:HEM:C1A	2.45	0.51
1:C:59:MET:HE1	1:C:397:SER:HB3	1.92	0.51
1:D:470:ASP:O	1:D:471:ILE:C	2.49	0.51
1:F:33:LEU:HD22	1:F:34:PRO:HD2	1.93	0.51
1:B:467:SER:O	1:B:470:ASP:HB2	2.11	0.51
1:A:439:CYS:HB2	2:A:502:HEM:CHA	2.39	0.51
1:B:356:ILE:O	1:B:360:GLN:HG3	2.11	0.51
1:C:84:HIS:HA	1:C:398:VAL:HG13	1.93	0.51
1:D:365:VAL:O	1:D:481:ALA:HA	2.11	0.50
1:A:378:THR:HG23	1:A:385:LEU:HD13	1.93	0.50
1:A:199:LEU:HB2	4:A:649:HOH:O	2.11	0.50
1:B:408:PRO:HD2	1:B:409:GLN:OE1	2.11	0.50
1:E:275:MET:HG2	1:E:286:PHE:O	2.12	0.50
1:F:474:SER:O	1:F:485:ARG:NE	2.43	0.50
1:A:264:PRO:HG3	1:A:273:ILE:HD13	1.93	0.50
1:F:430:VAL:O	1:F:430:VAL:HG23	2.12	0.50
1:C:64:ARG:HD2	4:C:623:HOH:O	2.12	0.50
1:B:315:LEU:HD13	1:B:487:TYR:CD2	2.46	0.50
1:F:195:ASP:HB3	1:F:198:PHE:HB3	1.94	0.50
1:E:325:ALA:O	1:E:328:HIS:N	2.45	0.50
1:B:107:PHE:CE2	3:B:502:SNE:H7	2.47	0.50
1:E:110:VAL:CG1	1:E:111:PHE:H	2.21	0.50
1:A:170:PRO:HG3	1:A:489:MET:SD	2.52	0.50
1:D:439:CYS:HB2	2:D:501:HEM:C1A	2.47	0.50
1:A:296:LEU:HD13	1:A:300:ILE:HG13	1.94	0.50
1:B:296:LEU:HG	1:B:300:ILE:HD11	1.93	0.50
1:B:183:SER:OG	1:B:299:PHE:CE1	2.65	0.50
1:A:396:GLY:O	1:A:400:ARG:HG3	2.12	0.50
1:D:433:SER:HB3	2:D:501:HEM:HBA1	1.94	0.49
1:E:199:LEU:CG	1:E:203:ARG:HH21	2.24	0.49
1:A:315:LEU:HB2	1:A:487:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:HB3	1:C:167:ASN:HB3	1.93	0.49
1:B:433:SER:CB	2:B:501:HEM:HBA1	2.42	0.49
1:D:186:VAL:HA	1:D:267:PHE:HB3	1.94	0.49
1:A:109:TRP:CZ3	1:A:110:VAL:HG23	2.45	0.49
1:A:310:LEU:HD23	1:A:453:PHE:CE1	2.47	0.49
1:C:220:TYR:HA	1:C:227:MET:SD	2.53	0.49
1:B:39:PRO:HG3	1:B:72:HIS:CE1	2.47	0.49
1:E:74:GLY:HA2	1:E:223:PHE:HE2	1.77	0.49
1:A:412:ASN:OD1	1:A:414:GLN:HG2	2.12	0.49
1:C:369:SER:HB2	1:C:395:LEU:HG	1.94	0.49
1:C:104:GLN:CG	1:C:107:PHE:HD1	2.25	0.49
1:A:354:ALA:CB	1:A:417:LEU:HD22	2.38	0.49
1:E:45:ASN:HD22	1:E:48:GLN:HE22	1.59	0.49
1:B:301:GLY:HA2	3:B:502:SNE:H12	1.95	0.49
1:A:182:ILE:O	1:A:186:VAL:HG22	2.13	0.49
1:C:224:SER:C	1:C:226:VAL:N	2.65	0.49
1:F:342:LYS:O	1:F:345:ASP:HB2	2.12	0.49
1:A:89:GLU:O	1:A:93:ASP:HB2	2.12	0.48
1:C:42:PHE:CD1	1:C:75:PRO:HB3	2.48	0.48
1:D:252:VAL:CG1	1:D:253:GLU:N	2.76	0.48
1:C:259:LEU:O	1:C:261:PRO:HD3	2.12	0.48
1:F:60:LYS:O	1:F:63:GLU:HB2	2.13	0.48
1:E:316:LEU:HD13	1:E:411:PHE:CE1	2.48	0.48
1:F:416:PHE:C	1:F:417:LEU:HD22	2.34	0.48
1:B:59:MET:O	1:B:62:SER:OG	2.30	0.48
1:E:271:PHE:CE2	1:E:291:LEU:HB2	2.49	0.48
1:A:407:ASN:N	1:A:408:PRO:HD3	2.28	0.48
1:D:407:ASN:N	1:D:408:PRO:CD	2.76	0.48
1:D:115:GLY:O	1:D:119:SER:HB3	2.14	0.48
1:E:396:GLY:O	1:E:400:ARG:HG3	2.14	0.48
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.49	0.48
1:B:265:ARG:CZ	4:B:610:HOH:O	2.61	0.48
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.95	0.48
1:D:193:TYR:N	4:D:633:HOH:O	2.34	0.48
1:A:184:SER:O	1:A:188:GLY:HA2	2.14	0.48
1:E:170:PRO:O	1:E:174:LEU:HD23	2.14	0.48
1:D:39:PRO:CG	1:D:72:HIS:ND1	2.76	0.48
1:F:346:ARG:HG2	1:F:347:ALA:H	1.79	0.48
1:F:333:ARG:HH11	1:F:333:ARG:HG2	1.79	0.48
1:B:334:VAL:CG1	1:B:334:VAL:O	2.62	0.48
1:F:45:ASN:OD1	1:F:72:HIS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:O	1:A:261:PRO:HD3	2.14	0.48
1:F:354:ALA:HB2	1:F:417:LEU:HD22	1.92	0.47
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.96	0.47
1:C:104:GLN:CG	1:C:104:GLN:O	2.62	0.47
1:F:495:HIS:C	1:F:495:HIS:CD2	2.88	0.47
1:F:182:ILE:HD13	2:F:501:HEM:CBC	2.44	0.47
1:A:312:TYR:CE2	1:A:363:GLY:HA2	2.49	0.47
1:E:418:ASN:ND2	1:E:422:GLN:HB2	2.29	0.47
1:D:190:ARG:NH2	4:D:622:HOH:O	2.36	0.47
1:A:444:LEU:HD23	2:A:502:HEM:HMC1	1.96	0.47
1:A:327:VAL:CG1	1:A:352:MET:HE1	2.40	0.47
1:F:365:VAL:O	1:F:481:ALA:HA	2.14	0.47
2:A:502:HEM:HMC1	2:A:502:HEM:HBC2	1.95	0.47
1:D:374:VAL:CG1	1:D:386:PRO:O	2.62	0.47
1:F:302:GLY:CA	2:F:501:HEM:HBC2	2.45	0.47
1:C:374:VAL:HG23	1:C:388:GLY:N	2.30	0.47
1:B:468:PRO:C	1:B:470:ASP:N	2.66	0.47
1:C:114:TYR:CD1	1:C:114:TYR:N	2.82	0.47
1:A:224:SER:O	1:A:228:LYS:HE2	2.13	0.47
1:B:306:VAL:CG2	2:B:501:HEM:HAB	2.44	0.47
1:E:444:LEU:HD23	2:E:501:HEM:HBC2	1.97	0.47
1:F:392:TYR:HB3	1:F:394:MET:CE	2.40	0.47
1:E:78:VAL:HG11	1:E:392:TYR:CD2	2.50	0.47
1:C:400:ARG:HA	1:C:408:PRO:HB3	1.96	0.47
1:C:460:PHE:CD1	1:C:491:PHE:HB3	2.49	0.47
1:C:270:SER:HA	1:C:273:ILE:HD12	1.97	0.47
1:B:441:GLY:HA3	2:B:501:HEM:C3C	2.49	0.47
1:E:199:LEU:CD2	1:E:203:ARG:NH2	2.78	0.47
1:F:345:ASP:O	1:F:349:MET:HG3	2.15	0.47
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.45	0.47
1:F:101:ARG:NH1	2:F:501:HEM:O2A	2.47	0.47
1:E:327:VAL:HG13	1:E:352:MET:HE2	1.97	0.47
1:B:365:VAL:O	1:B:481:ALA:HA	2.15	0.47
1:A:74:GLY:HA3	1:A:222:MET:O	2.15	0.47
1:C:108:ASP:OD1	1:C:112:LYS:O	2.33	0.47
1:E:370:LEU:HD13	1:E:480:PHE:CE1	2.49	0.46
1:E:230:LEU:HD13	1:E:231:PRO:N	2.30	0.46
1:F:322:GLU:HG2	1:F:323:VAL:N	2.29	0.46
1:C:156:LEU:HD22	1:C:177:THR:HG21	1.97	0.46
1:F:315:LEU:HD13	1:F:487:TYR:CD2	2.50	0.46
1:E:346:ARG:HG3	1:E:347:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:ASP:O	1:E:261:PRO:C	2.53	0.46
1:C:291:LEU:HD12	1:C:291:LEU:O	2.15	0.46
1:E:467:SER:O	1:E:470:ASP:N	2.48	0.46
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.97	0.46
1:B:260:ASP:O	1:B:262:ASN:N	2.49	0.46
1:A:418:ASN:HB2	1:A:419:GLU:OE1	2.15	0.46
1:F:433:SER:HB2	2:F:501:HEM:HBA1	1.96	0.46
1:E:201:LEU:N	1:E:201:LEU:CD1	2.78	0.46
1:E:53:GLN:HB3	1:E:56:ASN:HB2	1.97	0.46
1:A:367:PRO:HD2	1:A:480:PHE:O	2.16	0.46
1:D:358:GLU:HG3	1:D:411:PHE:CE1	2.50	0.46
1:F:331:ILE:HG21	1:F:458:GLN:HB2	1.96	0.46
1:E:110:VAL:CG1	1:E:111:PHE:HD1	2.20	0.46
1:A:296:LEU:HD11	1:A:300:ILE:HD11	1.95	0.46
1:E:92:VAL:HG23	1:E:434:ILE:CD1	2.38	0.46
1:D:271:PHE:CE2	1:D:291:LEU:HB2	2.51	0.46
1:A:439:CYS:HA	2:A:502:HEM:C4D	2.50	0.46
1:E:416:PHE:C	1:E:417:LEU:HD22	2.35	0.46
1:E:432:PHE:CZ	2:E:501:HEM:HBB2	2.51	0.46
1:F:117:VAL:HG22	2:F:501:HEM:HAD1	1.98	0.46
1:B:402:PRO:HA	1:B:405:PHE:O	2.16	0.46
1:E:461:ARG:NH1	1:E:495:HIS:ND1	2.64	0.46
1:A:73:LEU:HD12	1:A:78:VAL:HG21	1.96	0.46
1:C:45:ASN:OD1	1:C:72:HIS:N	2.44	0.46
1:A:101:ARG:N	1:A:120:ASN:OD1	2.49	0.46
1:B:264:PRO:HB3	1:B:269:ASP:HB3	1.98	0.46
1:D:260:ASP:O	1:D:262:ASN:N	2.48	0.46
1:A:354:ALA:HB1	1:A:417:LEU:HD21	1.76	0.46
1:B:472:ASP:OD1	1:B:474:SER:OG	2.32	0.46
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.97	0.46
1:A:101:ARG:HB3	1:A:120:ASN:HD21	1.80	0.46
1:C:40:LEU:CD1	1:C:41:PRO:HD3	2.45	0.46
1:F:252:VAL:HG13	1:F:253:GLU:N	2.31	0.46
1:A:210:GLN:NE2	4:A:672:HOH:O	2.48	0.46
1:C:406:SER:O	1:C:407:ASN:HB2	2.16	0.45
1:B:351:TYR:O	1:B:355:VAL:HG23	2.16	0.45
1:E:370:LEU:CD2	3:E:502:SNE:H5	2.46	0.45
1:D:252:VAL:HG13	1:D:253:GLU:N	2.31	0.45
1:B:77:ARG:NH2	1:B:386:PRO:HG2	2.32	0.45
1:B:373:ARG:NH1	1:B:388:GLY:O	2.49	0.45
1:A:69:PHE:O	1:A:80:VAL:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:SER:OG	1:C:465:SER:N	2.49	0.45
1:C:117:VAL:HG12	1:C:118:PHE:N	2.31	0.45
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.81	0.45
1:A:161:ARG:O	1:A:164:GLY:N	2.49	0.45
1:D:260:ASP:C	1:D:262:ASN:H	2.19	0.45
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.51	0.45
1:F:130:PHE:CE1	1:F:271:PHE:HD1	2.34	0.45
1:C:130:PHE:CD2	1:C:274:ARG:HD3	2.52	0.45
1:C:199:LEU:CD1	1:C:203:ARG:NE	2.78	0.45
1:A:85:ASP:O	1:A:89:GLU:HG3	2.16	0.45
1:A:335:ILE:HD13	1:A:341:PRO:HB3	1.97	0.45
1:A:433:SER:O	1:A:434:ILE:HG23	2.17	0.45
1:F:374:VAL:HG23	1:F:374:VAL:O	2.15	0.45
1:A:130:PHE:CE1	1:A:271:PHE:HD1	2.34	0.45
1:D:453:PHE:O	1:D:457:MET:HG2	2.16	0.45
1:A:379:LYS:HE2	1:A:379:LYS:HB2	1.79	0.45
1:E:437:ARG:HE	2:E:501:HEM:CGD	2.29	0.45
1:D:406:SER:O	1:D:407:ASN:HB2	2.17	0.45
1:B:468:PRO:HA	1:B:471:ILE:HG13	1.98	0.45
1:A:369:SER:HB2	1:A:395:LEU:HG	1.99	0.45
1:E:314:PHE:CD2	1:E:462:LEU:HD21	2.51	0.45
1:E:136:ARG:O	1:E:142:LYS:NZ	2.32	0.45
1:C:145:ILE:HG13	1:C:146:GLU:N	2.32	0.45
1:E:460:PHE:CD1	1:E:491:PHE:HB3	2.51	0.45
1:C:392:TYR:HB3	1:C:394:MET:CE	2.46	0.45
1:D:242:GLN:NE2	1:D:245:GLU:OE1	2.46	0.45
1:B:204:MET:HG2	1:B:240:LEU:HD22	1.99	0.45
1:D:413:PRO:O	1:D:417:LEU:HD13	2.17	0.45
1:D:312:TYR:CD2	1:D:484:PRO:CG	3.00	0.45
1:B:101:ARG:NH1	2:B:501:HEM:O2A	2.40	0.45
1:C:130:PHE:CD2	1:C:274:ARG:CD	3.00	0.45
1:A:148:ARG:NH1	1:A:151:GLU:HB3	2.32	0.45
1:B:94:GLN:CG	1:B:97:GLU:OE2	2.64	0.45
1:F:115:GLY:O	1:F:119:SER:HB3	2.17	0.45
1:C:289:LYS:O	1:C:292:VAL:N	2.50	0.45
1:F:235:GLN:OE1	1:F:235:GLN:HA	2.16	0.45
1:A:419:GLU:HG2	1:A:420:LYS:H	1.81	0.45
1:A:419:GLU:HG2	1:A:420:LYS:N	2.32	0.45
1:E:94:GLN:O	1:E:98:PHE:HD1	1.99	0.45
1:C:288:LEU:O	1:C:289:LYS:C	2.56	0.44
1:E:59:MET:CE	1:E:397:SER:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:HIS:HA	1:B:398:VAL:HG13	2.00	0.44
1:B:103:GLU:HG3	1:B:104:GLN:N	2.31	0.44
1:E:420:LYS:HG3	1:E:422:GLN:HG3	1.99	0.44
1:D:148:ARG:NH2	1:D:190:ARG:HD2	2.31	0.44
1:B:174:LEU:HA	1:B:174:LEU:HD13	1.87	0.44
1:E:319:LYS:HD3	1:E:471:ILE:HB	1.99	0.44
1:C:468:PRO:O	1:C:469:LYS:C	2.55	0.44
1:E:412:ASN:HA	1:E:413:PRO:HD3	1.70	0.44
1:A:331:ILE:HG21	1:A:458:GLN:HB2	1.99	0.44
1:C:157:ILE:HD13	1:C:460:PHE:HE2	1.82	0.44
1:E:429:PHE:CZ	1:E:431:PRO:HG3	2.52	0.44
1:C:115:GLY:O	1:C:119:SER:HB3	2.17	0.44
3:E:502:SNE:H6	3:E:502:SNE:H1	1.16	0.44
1:B:242:GLN:NE2	1:B:245:GLU:OE1	2.50	0.44
1:D:315:LEU:HD13	1:D:487:TYR:CD2	2.51	0.44
1:C:40:LEU:HA	1:C:40:LEU:HD13	1.40	0.44
1:B:296:LEU:O	1:B:300:ILE:HG13	2.17	0.44
1:A:264:PRO:HB3	1:A:269:ASP:HB3	1.99	0.44
1:A:391:VAL:O	1:A:393:PRO:HD3	2.17	0.44
1:E:418:ASN:HD21	1:E:422:GLN:HB2	1.82	0.44
1:B:370:LEU:HD12	4:B:653:HOH:O	2.16	0.44
2:A:502:HEM:HMC1	2:A:502:HEM:CBC	2.48	0.44
1:D:439:CYS:HB2	2:D:501:HEM:C4A	2.51	0.44
1:F:358:GLU:HG3	1:F:411:PHE:CD1	2.50	0.44
1:C:39:PRO:CG	1:C:72:HIS:ND1	2.78	0.44
1:A:458:GLN:O	1:A:494:ARG:NH1	2.50	0.44
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.82	0.44
1:E:220:TYR:HA	1:E:227:MET:SD	2.58	0.44
1:F:128:ARG:O	1:F:132:ILE:HG13	2.18	0.44
1:B:35:PRO:HD2	1:B:383:PHE:CE2	2.52	0.44
1:A:128:ARG:HD2	2:A:502:HEM:O1D	2.18	0.44
1:C:289:LYS:O	1:C:290:ASN:C	2.56	0.44
1:E:41:PRO:O	1:E:42:PHE:HB3	2.18	0.44
2:B:501:HEM:HMC2	2:B:501:HEM:CBC	2.48	0.43
1:F:368:MET:HB3	1:F:394:MET:HE2	2.00	0.43
1:C:118:PHE:CD1	1:C:118:PHE:N	2.86	0.43
1:A:186:VAL:HA	1:A:267:PHE:HB3	2.01	0.43
1:C:407:ASN:N	1:C:408:PRO:HD3	2.33	0.43
1:E:161:ARG:O	1:E:164:GLY:N	2.40	0.43
1:A:146:GLU:O	1:A:150:GLN:HG3	2.19	0.43
1:A:437:ARG:NH1	2:A:502:HEM:O2D	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:PHE:O	1:D:433:SER:HB3	2.17	0.43
1:D:345:ASP:O	1:D:349:MET:CG	2.59	0.43
1:B:468:PRO:C	1:B:470:ASP:H	2.20	0.43
1:E:272:LEU:O	1:E:275:MET:HB2	2.18	0.43
1:B:100:GLY:HA3	1:B:373:ARG:HB3	2.00	0.43
1:D:392:TYR:HB3	1:D:394:MET:HE3	2.00	0.43
1:A:107:PHE:CZ	3:A:501:SNE:H7	2.52	0.43
1:A:433:SER:C	1:A:434:ILE:HG23	2.39	0.43
1:A:433:SER:OG	1:A:434:ILE:N	2.49	0.43
1:E:230:LEU:O	1:E:235:GLN:NE2	2.40	0.43
1:F:302:GLY:HA2	2:F:501:HEM:HBC2	2.00	0.43
1:A:358:GLU:HG3	1:A:411:PHE:CD1	2.53	0.43
1:A:321:PRO:O	1:A:322:GLU:C	2.57	0.43
1:E:230:LEU:CD2	1:E:231:PRO:HD2	2.28	0.43
1:C:374:VAL:CG2	1:C:389:THR:H	2.32	0.43
1:B:272:LEU:O	1:B:275:MET:HB2	2.18	0.43
1:B:400:ARG:NH1	4:B:639:HOH:O	2.48	0.43
1:C:42:PHE:CE1	1:C:75:PRO:HB3	2.54	0.43
1:F:374:VAL:HG22	1:F:389:THR:H	1.83	0.43
1:D:419:GLU:H	1:D:419:GLU:CD	2.22	0.43
1:D:176:ARG:HA	1:D:202:LEU:HD11	2.00	0.43
1:C:60:LYS:HG3	1:C:64:ARG:HH21	1.83	0.43
1:A:179:SER:HA	1:A:303:THR:OG1	2.18	0.43
1:D:319:LYS:HD3	1:D:471:ILE:HB	2.01	0.43
1:C:59:MET:CE	1:C:397:SER:HB3	2.49	0.43
1:F:195:ASP:HB3	1:F:198:PHE:CB	2.49	0.43
1:A:169:ASP:CB	1:C:167:ASN:HB3	2.48	0.43
1:D:103:GLU:HG3	1:D:104:GLN:N	2.34	0.43
1:F:205:MET:HA	1:F:208:ILE:HD12	2.00	0.43
1:E:181:VAL:O	1:E:184:SER:HB2	2.18	0.43
1:B:306:VAL:HG22	2:B:501:HEM:HAB	1.99	0.43
1:A:81:LEU:CA	4:A:658:HOH:O	2.67	0.43
1:F:474:SER:HA	1:F:475:PRO:HD3	1.92	0.43
1:F:346:ARG:HG3	1:F:347:ALA:N	2.34	0.43
1:B:432:PHE:O	1:B:433:SER:HB3	2.19	0.43
1:A:458:GLN:C	1:A:494:ARG:HH11	2.21	0.43
1:A:433:SER:HB2	2:A:502:HEM:HBA1	2.00	0.42
1:A:296:LEU:CD1	1:A:300:ILE:CD1	2.97	0.42
1:F:209:PHE:CD2	1:F:304:GLU:HB3	2.49	0.42
1:A:252:VAL:CG1	1:A:253:GLU:N	2.82	0.42
1:F:174:LEU:HD12	1:F:310:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:PHE:O	1:D:227:MET:SD	2.77	0.42
1:F:84:HIS:C	1:F:84:HIS:ND1	2.72	0.42
1:F:209:PHE:HE2	1:F:304:GLU:HB3	1.66	0.42
1:C:271:PHE:CG	1:C:291:LEU:HD13	2.54	0.42
1:F:313:GLY:HA3	1:F:453:PHE:HZ	1.84	0.42
1:E:458:GLN:CG	1:E:458:GLN:O	2.67	0.42
1:C:335:ILE:HD13	1:C:341:PRO:HB3	2.01	0.42
1:B:302:GLY:HA2	2:B:501:HEM:C2C	2.54	0.42
1:C:439:CYS:HB2	2:C:501:HEM:C4A	2.51	0.42
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.85	0.42
1:C:139:GLY:O	1:C:145:ILE:CG1	2.62	0.42
1:E:312:TYR:HD1	1:E:312:TYR:O	2.02	0.42
1:B:269:ASP:O	1:B:270:SER:C	2.57	0.42
1:A:372:ARG:NH1	4:A:606:HOH:O	2.50	0.42
1:B:439:CYS:HB2	2:B:501:HEM:C4A	2.48	0.42
1:E:312:TYR:OH	1:E:362:PHE:HE2	2.02	0.42
1:A:281:ASN:HA	1:A:282:PRO:HD3	1.91	0.42
1:C:402:PRO:HA	1:C:405:PHE:O	2.20	0.42
1:E:224:SER:HB3	4:E:608:HOH:O	2.19	0.42
1:A:148:ARG:HH12	1:A:151:GLU:HB3	1.85	0.42
1:E:45:ASN:HD22	1:E:48:GLN:NE2	2.18	0.42
1:E:109:TRP:O	1:E:109:TRP:CG	2.72	0.42
1:A:101:ARG:HB3	1:A:120:ASN:CG	2.40	0.42
1:E:316:LEU:HD13	1:E:411:PHE:CD1	2.54	0.42
1:D:116:VAL:HG12	1:D:294:THR:HG23	1.99	0.42
1:F:364:ASP:O	1:F:482:THR:OG1	2.33	0.42
1:E:74:GLY:CA	1:E:223:PHE:HE2	2.33	0.42
1:E:109:TRP:CE3	1:E:109:TRP:C	2.91	0.42
1:E:73:LEU:HB2	1:E:76:ARG:CD	2.48	0.42
1:F:432:PHE:HB3	1:F:439:CYS:HB3	2.01	0.42
1:A:427:ASP:HA	4:A:637:HOH:O	2.19	0.42
1:E:263:SER:HA	1:E:264:PRO:HD3	1.88	0.42
1:C:361:ARG:HG3	1:C:399:LEU:HB3	2.01	0.42
1:B:418:ASN:HD21	1:B:422:GLN:HB2	1.84	0.42
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.55	0.42
1:C:143:ARG:HH21	1:C:147:GLU:HG2	1.84	0.42
1:A:466:GLN:NE2	4:A:638:HOH:O	2.52	0.42
1:C:355:VAL:O	1:C:359:ILE:HG13	2.19	0.42
2:A:502:HEM:CBC	2:A:502:HEM:CMC	2.97	0.42
1:B:476:LYS:N	1:B:483:ILE:O	2.51	0.42
1:B:190:ARG:HH11	1:B:190:ARG:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PHE:CE1	1:C:166:ALA:CB	3.02	0.42
1:F:220:TYR:HA	1:F:227:MET:SD	2.60	0.42
1:B:304:GLU:O	1:B:308:THR:OG1	2.24	0.42
1:D:312:TYR:HD2	1:D:484:PRO:CG	2.33	0.41
1:C:107:PHE:HB3	1:C:111:PHE:HE1	1.85	0.41
1:E:156:LEU:HD13	1:E:177:THR:OG1	2.20	0.41
1:D:156:LEU:HD13	1:D:177:THR:OG1	2.20	0.41
1:A:84:HIS:ND1	1:A:85:ASP:OD1	2.53	0.41
1:C:313:GLY:HA2	1:C:359:ILE:HD13	2.02	0.41
1:B:321:PRO:O	1:B:322:GLU:C	2.58	0.41
1:C:182:ILE:HG12	1:C:298:LEU:O	2.19	0.41
1:B:305:THR:OG1	1:B:306:VAL:N	2.53	0.41
1:B:228:LYS:HG3	1:B:229:HIS:CE1	2.54	0.41
1:C:230:LEU:O	1:C:235:GLN:NE2	2.38	0.41
1:F:224:SER:OG	1:F:225:SER:N	2.52	0.41
1:C:365:VAL:O	1:C:481:ALA:HA	2.20	0.41
1:E:439:CYS:HB2	2:E:501:HEM:C4A	2.51	0.41
1:C:60:LYS:HG3	1:C:64:ARG:NH2	2.36	0.41
1:B:172:PHE:O	1:B:173:PHE:C	2.59	0.41
1:C:40:LEU:N	1:C:40:LEU:CD2	2.83	0.41
1:C:252:VAL:HG23	1:C:268:ILE:CG2	2.51	0.41
1:A:354:ALA:HB2	1:A:417:LEU:CD2	2.49	0.41
1:A:176:ARG:HA	1:A:202:LEU:HD11	2.01	0.41
1:C:123:ARG:HG3	1:C:285:GLU:OE2	2.20	0.41
1:F:33:LEU:CD2	1:F:34:PRO:HD2	2.51	0.41
1:E:319:LYS:HD2	1:E:468:PRO:O	2.19	0.41
1:D:330:GLU:HG3	1:D:333:ARG:NH2	2.36	0.41
1:B:34:PRO:HB3	1:B:68:VAL:O	2.20	0.41
1:C:49:LEU:HD23	1:C:57:SER:HB3	2.01	0.41
1:A:340:GLN:HA	1:A:341:PRO:HD3	1.87	0.41
1:C:340:GLN:HA	1:C:341:PRO:HD3	1.90	0.41
1:E:84:HIS:HA	1:E:398:VAL:HG13	2.02	0.41
1:E:112:LYS:HB2	1:E:114:TYR:CD1	2.56	0.41
1:C:272:LEU:O	1:C:275:MET:N	2.54	0.41
1:D:281:ASN:OD1	1:D:281:ASN:C	2.58	0.41
1:E:157:ILE:HD12	1:E:460:PHE:CE2	2.52	0.41
1:F:38:THR:HA	1:F:39:PRO:HD3	1.83	0.41
1:B:190:ARG:NH1	1:B:190:ARG:HG3	2.35	0.41
1:A:419:GLU:H	1:A:419:GLU:CD	2.23	0.41
1:C:468:PRO:O	1:C:470:ASP:N	2.53	0.41
1:F:204:MET:HA	1:F:240:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLN:HB3	1:B:56:ASN:HB2	2.02	0.41
1:E:199:LEU:HD23	1:E:203:ARG:HH21	1.85	0.41
1:C:152:GLU:HG3	1:C:177:THR:HG23	2.02	0.41
1:C:260:ASP:HB3	1:C:263:SER:O	2.21	0.41
1:F:210:GLN:O	1:F:214:THR:HG23	2.21	0.41
1:A:271:PHE:CE1	1:A:286:PHE:CD1	3.09	0.41
1:E:321:PRO:HA	1:E:324:GLU:HB3	2.02	0.41
1:A:492:LEU:HA	1:A:493:PRO:HD2	1.76	0.41
1:F:252:VAL:CG1	1:F:253:GLU:N	2.83	0.41
1:B:494:ARG:O	1:B:495:HIS:HB2	2.20	0.41
1:B:370:LEU:HA	1:B:370:LEU:HD12	1.76	0.41
1:A:346:ARG:HG3	1:A:347:ALA:N	2.36	0.41
1:B:312:TYR:CE1	1:B:363:GLY:HA2	2.56	0.41
1:D:204:MET:HA	1:D:240:LEU:HD22	2.03	0.41
1:F:281:ASN:HA	1:F:282:PRO:HD3	1.97	0.41
1:A:439:CYS:HA	2:A:502:HEM:CHA	2.51	0.41
1:D:312:TYR:CE2	1:D:484:PRO:CA	3.04	0.41
1:A:412:ASN:HA	1:A:413:PRO:HD3	1.93	0.41
1:C:208:ILE:HG12	1:C:241:LEU:CD2	2.45	0.41
1:E:101:ARG:NH1	2:E:501:HEM:O2A	2.53	0.41
1:A:197:GLU:O	1:A:198:PHE:C	2.58	0.41
1:A:406:SER:O	1:A:407:ASN:HB2	2.20	0.41
1:A:170:PRO:O	1:A:171:THR:C	2.58	0.41
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.87	0.41
1:D:50:ASN:OD1	1:D:50:ASN:C	2.59	0.41
1:B:117:VAL:HG22	2:B:501:HEM:HAD1	2.04	0.40
1:D:192:ASP:CA	4:D:633:HOH:O	2.48	0.40
1:E:433:SER:OG	1:E:434:ILE:N	2.54	0.40
1:E:152:GLU:CD	1:E:180:ASN:HD22	2.24	0.40
1:D:495:HIS:HE1	4:D:646:HOH:O	2.03	0.40
1:D:225:SER:HA	1:D:228:LYS:HE3	2.02	0.40
1:F:39:PRO:HG3	1:F:72:HIS:ND1	2.35	0.40
1:E:472:ASP:OD1	1:E:472:ASP:C	2.60	0.40
1:B:260:ASP:C	1:B:262:ASN:N	2.74	0.40
1:A:316:LEU:HD11	1:A:362:PHE:CD2	2.56	0.40
1:D:324:GLU:O	1:D:327:VAL:HB	2.21	0.40
1:C:40:LEU:O	1:C:42:PHE:N	2.54	0.40
1:C:330:GLU:OE1	1:C:349:MET:HB3	2.21	0.40
1:A:111:PHE:CE2	1:A:297:ASN:ND2	2.89	0.40
1:F:271:PHE:CD2	1:F:291:LEU:HD13	2.57	0.40
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLN:HB2	4:D:642:HOH:O	2.21	0.40
1:F:319:LYS:HD3	1:F:471:ILE:HB	2.03	0.40
1:E:90:ALA:O	1:E:98:PHE:CD1	2.74	0.40
2:B:501:HEM:CMC	2:B:501:HEM:CBC	2.98	0.40
1:F:368:MET:HB3	1:F:394:MET:CE	2.51	0.40
1:A:152:GLU:HG3	1:A:177:THR:HG23	2.03	0.40
1:C:418:ASN:OD1	1:C:420:LYS:N	2.54	0.40
1:C:414:GLN:OE1	1:C:414:GLN:HA	2.22	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	462/476 (97%)	408 (88%)	54 (12%)	0	100	100
1	B	463/476 (97%)	405 (88%)	58 (12%)	0	100	100
1	C	462/476 (97%)	407 (88%)	55 (12%)	0	100	100
1	D	463/476 (97%)	423 (91%)	40 (9%)	0	100	100
1	E	463/476 (97%)	395 (85%)	68 (15%)	0	100	100
1	F	463/476 (97%)	410 (89%)	53 (11%)	0	100	100
All	All	2776/2856 (97%)	2448 (88%)	328 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	394/422 (93%)	393 (100%)	1 (0%)	94	99
1	B	393/422 (93%)	392 (100%)	1 (0%)	94	99
1	C	371/422 (88%)	370 (100%)	1 (0%)	94	99
1	D	392/422 (93%)	391 (100%)	1 (0%)	94	99
1	E	376/422 (89%)	375 (100%)	1 (0%)	94	99
1	F	369/422 (87%)	367 (100%)	2 (0%)	92	98
All	All	2295/2532 (91%)	2288 (100%)	7 (0%)	94	99

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	312	TYR
1	A	312	TYR
1	B	312	TYR
1	C	312	TYR
1	E	312	TYR
1	F	312	TYR
1	F	495	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	255	ASN
1	E	254	HIS
1	E	255	ASN
1	F	236	GLN
1	F	466	GLN
1	F	495	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
3	SNE	A	501	-	9,11,11	0.73	0	7,18,18	1.71	2 (28%)
2	HEM	A	502	1	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
2	HEM	B	501	1	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
3	SNE	B	502	-	9,11,11	0.73	0	7,18,18	1.72	2 (28%)
2	HEM	C	501	1	30,50,50	2.21	8 (26%)	24,82,82	2.30	9 (37%)
3	SNE	C	502	-	9,11,11	0.74	0	7,18,18	1.72	2 (28%)
2	HEM	D	501	1	30,50,50	2.20	8 (26%)	24,82,82	2.31	9 (37%)
3	SNE	D	502	-	9,11,11	0.74	0	7,18,18	1.71	2 (28%)
2	HEM	E	501	1	30,50,50	2.20	8 (26%)	24,82,82	2.31	9 (37%)
3	SNE	E	502	-	9,11,11	3.63	1 (11%)	7,18,18	16.08	2 (28%)
2	HEM	F	501	1	30,50,50	2.20	8 (26%)	24,82,82	2.31	9 (37%)
3	SNE	F	502	-	9,11,11	0.73	0	7,18,18	1.71	2 (28%)

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
3	SNE	A	501	-	-	0/6/24/24	0/1/2/2
2	HEM	A	502	1	-	0/10/54/54	0/0/8/8
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	SNE	B	502	-	-	0/6/24/24	0/1/2/2
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8
3	SNE	C	502	-	-	0/6/24/24	0/1/2/2
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8
3	SNE	D	502	-	-	0/6/24/24	0/1/2/2
2	HEM	E	501	1	-	0/10/54/54	0/0/8/8
3	SNE	E	502	-	-	0/6/24/24	0/1/2/2
2	HEM	F	501	1	-	0/10/54/54	0/0/8/8
3	SNE	F	502	-	-	0/6/24/24	0/1/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	HEM	C3B-C4B	-7.31	1.45	1.51
2	D	501	HEM	C3B-C4B	-7.30	1.45	1.51
2	B	501	HEM	C3B-C4B	-7.28	1.45	1.51
2	C	501	HEM	C3B-C4B	-7.25	1.45	1.51
2	E	501	HEM	C3B-C4B	-7.23	1.45	1.51
2	F	501	HEM	C3B-C4B	-7.19	1.45	1.51
2	C	501	HEM	C3D-C4D	-5.10	1.45	1.51
2	B	501	HEM	C3D-C4D	-5.08	1.45	1.51
2	E	501	HEM	C3D-C4D	-5.08	1.45	1.51
2	D	501	HEM	C3D-C4D	-5.08	1.45	1.51
2	F	501	HEM	C3D-C4D	-5.07	1.45	1.51
2	A	502	HEM	C3D-C4D	-5.06	1.45	1.51
2	F	501	HEM	C2C-C1C	-3.81	1.45	1.52
2	B	501	HEM	C2C-C1C	-3.79	1.45	1.52
2	D	501	HEM	C2C-C1C	-3.79	1.45	1.52
2	C	501	HEM	C2C-C1C	-3.79	1.45	1.52
2	E	501	HEM	C2C-C1C	-3.78	1.45	1.52
2	A	502	HEM	C2C-C1C	-3.77	1.45	1.52
2	E	501	HEM	C2D-C1D	-2.09	1.45	1.51
2	A	502	HEM	C2D-C1D	-2.08	1.45	1.51
2	F	501	HEM	C2D-C1D	-2.07	1.45	1.51
2	C	501	HEM	C2D-C1D	-2.06	1.45	1.51
2	B	501	HEM	C2D-C1D	-2.05	1.45	1.51
2	D	501	HEM	C2D-C1D	-2.04	1.45	1.51
2	D	501	HEM	FE-ND	2.13	2.08	1.97
2	F	501	HEM	FE-ND	2.13	2.08	1.97
2	C	501	HEM	FE-ND	2.14	2.08	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	FE-ND	2.14	2.08	1.97
2	A	502	HEM	FE-ND	2.15	2.08	1.97
2	C	501	HEM	C4C-NC	2.15	1.38	1.36
2	B	501	HEM	FE-ND	2.16	2.08	1.97
2	A	502	HEM	C4C-NC	2.17	1.38	1.36
2	D	501	HEM	C4C-NC	2.17	1.38	1.36
2	F	501	HEM	C4C-NC	2.18	1.38	1.36
2	D	501	HEM	C1C-NC	2.20	1.38	1.36
2	B	501	HEM	C4C-NC	2.22	1.38	1.36
2	B	501	HEM	C1C-NC	2.23	1.38	1.36
2	E	501	HEM	C1C-NC	2.25	1.38	1.36
2	E	501	HEM	C4C-NC	2.27	1.38	1.36
2	C	501	HEM	C1C-NC	2.29	1.38	1.36
2	A	502	HEM	C1C-NC	2.29	1.38	1.36
2	F	501	HEM	C1C-NC	2.30	1.38	1.36
2	A	502	HEM	FE-NC	2.78	2.06	1.95
2	F	501	HEM	FE-NC	2.78	2.06	1.95
2	D	501	HEM	FE-NC	2.79	2.06	1.95
2	B	501	HEM	FE-NC	2.79	2.06	1.95
2	C	501	HEM	FE-NC	2.80	2.06	1.95
2	E	501	HEM	FE-NC	2.80	2.06	1.95
3	E	502	SNE	C6-C1	10.66	1.58	1.32

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	SNE	C7-C1-C6	-34.41	88.83	126.14
3	E	502	SNE	C4-C1-C6	-24.98	98.33	125.39
3	C	502	SNE	C7-C1-C6	-3.44	122.41	126.14
3	B	502	SNE	C7-C1-C6	-3.41	122.44	126.14
3	A	501	SNE	C7-C1-C6	-3.39	122.47	126.14
3	F	502	SNE	C7-C1-C6	-3.38	122.47	126.14
3	D	502	SNE	C7-C1-C6	-3.35	122.50	126.14
2	B	501	HEM	C3B-CAB-CBB	-2.92	119.98	124.46
2	A	502	HEM	C3C-CAC-CBC	-2.92	119.98	124.46
2	B	501	HEM	C3C-CAC-CBC	-2.92	119.98	124.46
2	D	501	HEM	C3C-CAC-CBC	-2.92	119.98	124.46
2	F	501	HEM	C3C-CAC-CBC	-2.92	119.98	124.46
2	E	501	HEM	C3B-CAB-CBB	-2.90	120.00	124.46
2	F	501	HEM	C3B-CAB-CBB	-2.90	120.01	124.46
2	E	501	HEM	C3C-CAC-CBC	-2.90	120.01	124.46
2	C	501	HEM	C3B-CAB-CBB	-2.90	120.01	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	HEM	C3B-CAB-CBB	-2.89	120.02	124.46
2	C	501	HEM	C3C-CAC-CBC	-2.88	120.04	124.46
2	D	501	HEM	C3B-CAB-CBB	-2.88	120.04	124.46
3	D	502	SNE	C4-C1-C6	-2.71	122.46	125.39
3	A	501	SNE	C4-C1-C6	-2.69	122.47	125.39
3	F	502	SNE	C4-C1-C6	-2.67	122.49	125.39
3	B	502	SNE	C4-C1-C6	-2.67	122.50	125.39
3	C	502	SNE	C4-C1-C6	-2.64	122.53	125.39
2	C	501	HEM	C3B-C4B-CHC	2.15	126.19	123.16
2	A	502	HEM	C3B-C4B-CHC	2.16	126.21	123.16
2	B	501	HEM	C3B-C4B-CHC	2.18	126.23	123.16
2	D	501	HEM	C3B-C4B-CHC	2.18	126.23	123.16
2	E	501	HEM	C3B-C4B-CHC	2.19	126.24	123.16
2	F	501	HEM	C3B-C4B-CHC	2.19	126.25	123.16
2	E	501	HEM	C2D-C3D-C4D	2.31	105.41	101.50
2	B	501	HEM	C2D-C3D-C4D	2.32	105.43	101.50
2	D	501	HEM	C2D-C3D-C4D	2.32	105.43	101.50
2	C	501	HEM	C2D-C3D-C4D	2.33	105.44	101.50
2	F	501	HEM	C2D-C3D-C4D	2.33	105.45	101.50
2	A	502	HEM	C2D-C3D-C4D	2.34	105.46	101.50
2	E	501	HEM	CMD-C2D-C3D	2.91	127.24	114.35
2	D	501	HEM	CMD-C2D-C3D	2.92	127.27	114.35
2	A	502	HEM	CMD-C2D-C3D	2.92	127.27	114.35
2	B	501	HEM	CMD-C2D-C3D	2.93	127.29	114.35
2	C	501	HEM	CMD-C2D-C3D	2.93	127.30	114.35
2	F	501	HEM	CMD-C2D-C3D	2.93	127.31	114.35
2	C	501	HEM	CMB-C2B-C3B	3.74	125.88	116.53
2	D	501	HEM	CMB-C2B-C3B	3.76	125.91	116.53
2	E	501	HEM	CMB-C2B-C3B	3.76	125.91	116.53
2	B	501	HEM	CMB-C2B-C3B	3.76	125.92	116.53
2	B	501	HEM	CMC-C2C-C3C	3.76	125.92	116.53
2	F	501	HEM	CMC-C2C-C3C	3.77	125.95	116.53
2	A	502	HEM	CMB-C2B-C3B	3.78	125.96	116.53
2	E	501	HEM	CMC-C2C-C3C	3.78	125.96	116.53
2	A	502	HEM	CMC-C2C-C3C	3.79	125.98	116.53
2	F	501	HEM	CMB-C2B-C3B	3.79	125.98	116.53
2	C	501	HEM	CMC-C2C-C3C	3.79	125.99	116.53
2	D	501	HEM	CMC-C2C-C3C	3.79	126.00	116.53
2	F	501	HEM	CAD-C3D-C4D	4.19	127.27	112.47
2	A	502	HEM	CAD-C3D-C4D	4.20	127.27	112.47
2	E	501	HEM	CAD-C3D-C4D	4.20	127.28	112.47
2	B	501	HEM	CAD-C3D-C4D	4.21	127.30	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	CAD-C3D-C4D	4.21	127.30	112.47
2	C	501	HEM	CAD-C3D-C4D	4.21	127.31	112.47
2	C	501	HEM	CAD-C3D-C2D	4.88	127.25	113.22
2	D	501	HEM	CAD-C3D-C2D	4.89	127.26	113.22
2	B	501	HEM	CAD-C3D-C2D	4.89	127.27	113.22
2	A	502	HEM	CAD-C3D-C2D	4.89	127.27	113.22
2	F	501	HEM	CAD-C3D-C2D	4.89	127.28	113.22
2	E	501	HEM	CAD-C3D-C2D	4.90	127.31	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SNE	1	0
2	A	502	HEM	15	0
2	B	501	HEM	17	0
3	B	502	SNE	2	0
2	C	501	HEM	3	0
3	C	502	SNE	6	0
2	D	501	HEM	15	0
3	D	502	SNE	1	0
2	E	501	HEM	10	0
3	E	502	SNE	4	0
2	F	501	HEM	14	0
3	F	502	SNE	3	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	464/476 (97%)	-0.05	3 (0%)	90 88	32, 57, 74, 86	0
1	B	465/476 (97%)	-0.05	5 (1%)	82 79	25, 59, 75, 95	0
1	C	464/476 (97%)	0.08	7 (1%)	76 71	40, 69, 92, 102	0
1	D	465/476 (97%)	-0.04	4 (0%)	85 83	39, 62, 81, 93	0
1	E	465/476 (97%)	0.01	8 (1%)	73 68	41, 70, 96, 106	0
1	F	465/476 (97%)	-0.14	2 (0%)	93 91	39, 62, 81, 92	0
All	All	2788/2856 (97%)	-0.03	29 (1%)	84 81	25, 63, 86, 106	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	209	PHE	3.1
1	E	91	LEU	3.0
1	B	33	LEU	3.0
1	E	33	LEU	2.9
1	A	385	LEU	2.8
1	C	273	ILE	2.8
1	E	264	PRO	2.8
1	E	334	VAL	2.8
1	C	334	VAL	2.7
1	E	208	ILE	2.7
1	E	380	PHE	2.7
1	E	336	GLY	2.5
1	D	287	TYR	2.5
1	B	444	LEU	2.4
1	B	451	LEU	2.4
1	F	447	MET	2.4
1	D	230	LEU	2.3
1	D	173	PHE	2.2
1	B	453	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	2.1
1	D	453	PHE	2.1
1	A	173	PHE	2.1
1	B	450	PHE	2.1
1	C	343	PHE	2.1
1	C	376	LYS	2.1
1	C	168	ILE	2.0
1	C	271	PHE	2.0
1	E	267	PHE	2.0
1	C	453	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	SNE	C	502	10/10	0.72	0.58	10.12	89,90,90,90	0
3	SNE	A	501	10/10	0.81	0.49	9.08	63,64,64,65	0
3	SNE	E	502	10/10	0.59	0.57	8.87	83,83,84,84	0
3	SNE	B	502	10/10	0.77	0.51	6.58	63,64,65,65	0
3	SNE	F	502	10/10	0.68	0.51	4.56	94,95,96,96	0
3	SNE	D	502	10/10	0.81	0.30	2.99	54,58,58,59	0
2	HEM	A	502	43/43	0.96	0.20	0.61	42,46,48,49	0
2	HEM	E	501	43/43	0.96	0.21	0.59	49,55,62,65	0
2	HEM	F	501	43/43	0.95	0.20	0.54	55,60,62,62	0
2	HEM	B	501	43/43	0.97	0.21	0.50	36,43,47,49	0
2	HEM	D	501	43/43	0.97	0.19	0.40	32,44,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	C	501	43/43	0.96	0.18	0.10	51,59,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.