



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QM4  
Title : Human Cytochrome P450 (CYP) 2D6 - Prinomastat Complex  
Authors : Wang, A.; Stout, C.D.; Johnson, E.F.  
Deposited on : 2011-02-03  
Resolution : 2.85 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](mailto: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.

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

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

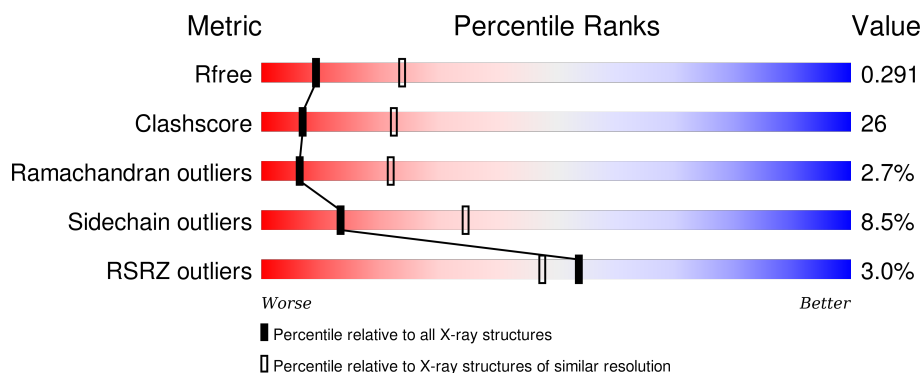
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	<div> <div>3%</div> <div>52%</div> <div>39%</div> <div>6%</div> <div>•</div> </div>
1	B	479	<div> <div>3%</div> <div>51%</div> <div>39%</div> <div>6%</div> <div>5%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7445 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 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3677	2359	651	653	14			
1	B	457	Total	C	N	O	S	0	0	0
			3618	2318	641	645	14			

There are 30 discrepancies between the modelled and reference sequences:

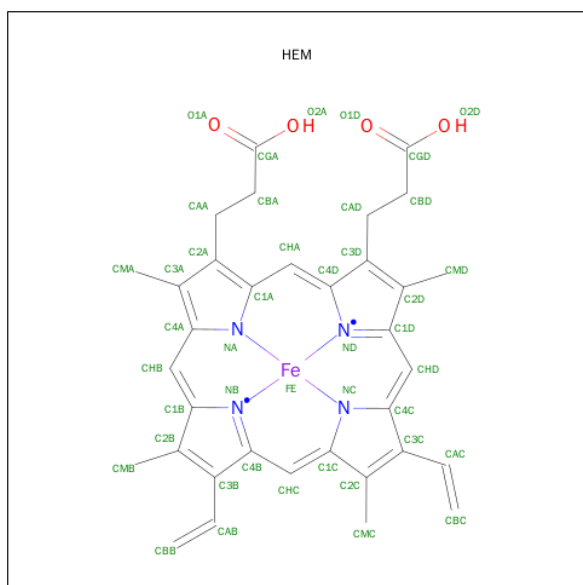
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP P10635
A	24	ALA	-	EXPRESSION TAG	UNP P10635
A	25	LYS	-	EXPRESSION TAG	UNP P10635
A	26	LYS	-	EXPRESSION TAG	UNP P10635
A	27	THR	-	EXPRESSION TAG	UNP P10635
A	28	SER	-	EXPRESSION TAG	UNP P10635
A	29	SER	-	EXPRESSION TAG	UNP P10635
A	30	LYS	-	EXPRESSION TAG	UNP P10635
A	31	GLY	-	EXPRESSION TAG	UNP P10635
A	32	LYS	-	EXPRESSION TAG	UNP P10635
A	33	LEU	-	EXPRESSION TAG	UNP P10635
A	498	HIS	-	EXPRESSION TAG	UNP P10635
A	499	HIS	-	EXPRESSION TAG	UNP P10635
A	500	HIS	-	EXPRESSION TAG	UNP P10635
A	501	HIS	-	EXPRESSION TAG	UNP P10635
B	23	MET	-	EXPRESSION TAG	UNP P10635
B	24	ALA	-	EXPRESSION TAG	UNP P10635
B	25	LYS	-	EXPRESSION TAG	UNP P10635
B	26	LYS	-	EXPRESSION TAG	UNP P10635
B	27	THR	-	EXPRESSION TAG	UNP P10635
B	28	SER	-	EXPRESSION TAG	UNP P10635
B	29	SER	-	EXPRESSION TAG	UNP P10635
B	30	LYS	-	EXPRESSION TAG	UNP P10635
B	31	GLY	-	EXPRESSION TAG	UNP P10635
B	32	LYS	-	EXPRESSION TAG	UNP P10635

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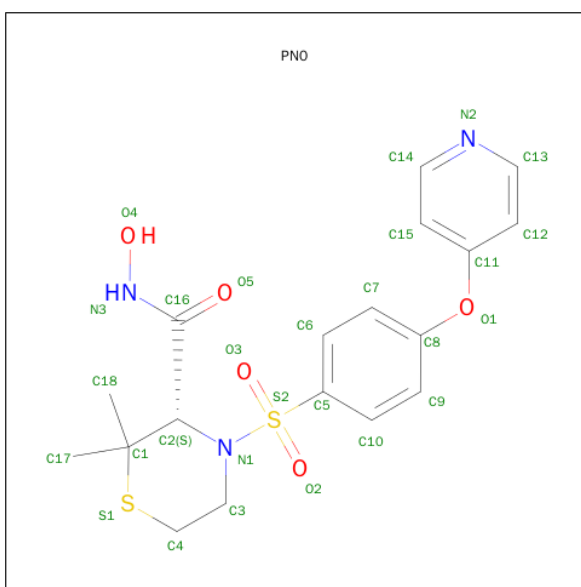
Chain	Residue	Modelled	Actual	Comment	Reference
B	33	LEU	-	EXPRESSION TAG	UNP P10635
B	498	HIS	-	EXPRESSION TAG	UNP P10635
B	499	HIS	-	EXPRESSION TAG	UNP P10635
B	500	HIS	-	EXPRESSION TAG	UNP P10635
B	501	HIS	-	EXPRESSION TAG	UNP P10635

- 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		

- Molecule 3 is PRINOMASTAT (three-letter code: PN0) (formula:  $C_{18}H_{21}N_3O_5S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	18	3	5	2		
3	B	1	Total	C	N	O	S	0	0
			28	18	3	5	2		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		

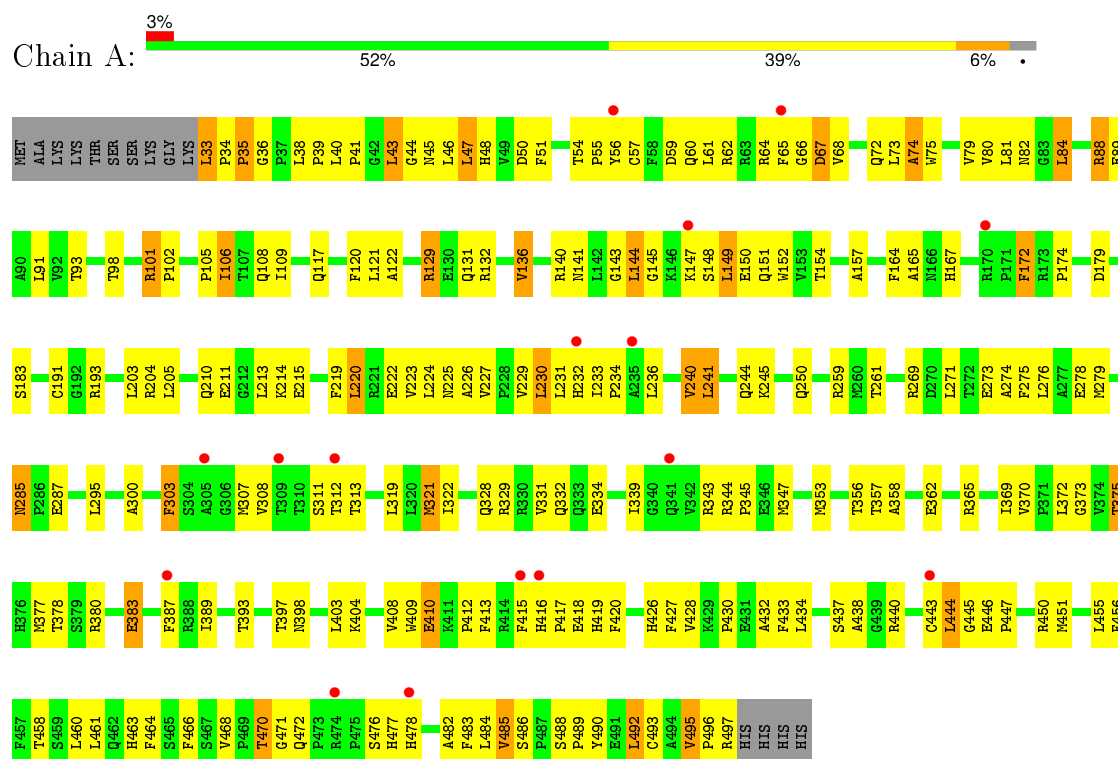
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	4	Total	O	0	0
			4	4		

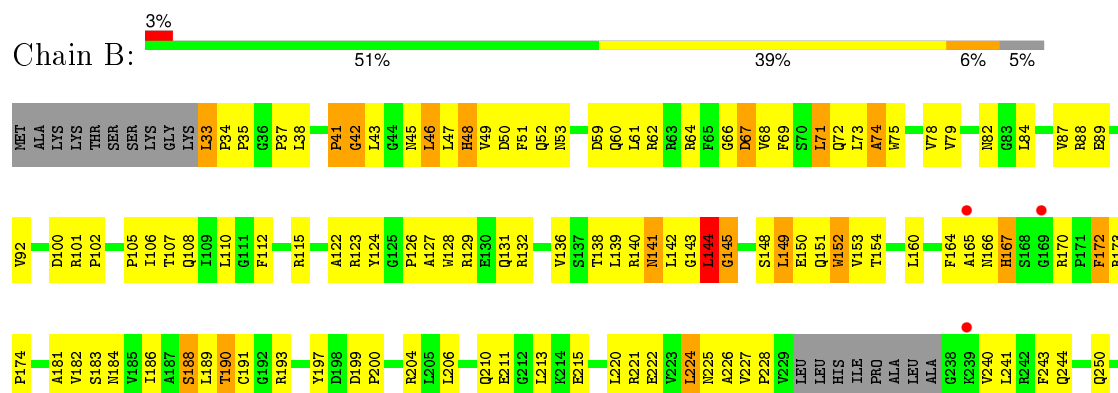
### 3 Residue-property plots

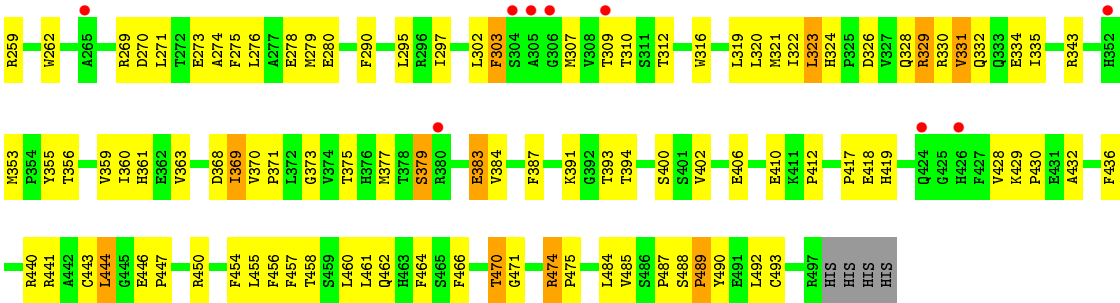
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Cytochrome P450 2D6



#### • Molecule 1: Cytochrome P450 2D6





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.54Å 55.07Å 145.87Å 90.00° 134.97° 90.00°	Depositor
Resolution (Å)	41.00 – 2.85 36.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.00-2.85) 98.8 (36.41-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.68Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.243 , 0.288 0.239 , 0.291	Depositor DCC
$R_{free}$ test set	1314 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30136 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PN0, HEM, NI

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	0.45	0/3777	0.67	0/5139
1	B	0.42	0/3715	0.65	0/5051
All	All	0.44	0/7492	0.66	0/10190

There are no bond length outliers.

There are no bond angle outliers.

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	3677	0	3663	199	0
1	B	3618	0	3594	201	0
2	A	43	0	30	6	0
2	B	43	0	30	3	0
3	A	28	0	21	2	0
3	B	28	0	21	1	0
4	B	1	0	0	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
All	All	7445	0	7359	392	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 26.

All (392) 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:A:72:GLN:HG2	1:B:38:LEU:HD22	1.36	1.06
1:A:40:LEU:HD21	1:A:47:LEU:HD11	1.49	0.93
1:B:429:LYS:HZ2	1:B:450:ARG:HH12	1.17	0.92
1:A:79:VAL:HG11	1:A:389:ILE:HD11	1.54	0.89
1:B:474:ARG:HH11	1:B:474:ARG:HG2	1.37	0.88
1:A:132:ARG:O	1:A:136:VAL:HG12	1.73	0.87
1:B:312:THR:HB	1:B:369:ILE:HD11	1.55	0.87
1:A:47:LEU:H	1:A:47:LEU:HD23	1.42	0.83
1:B:110:LEU:HD12	1:B:112:PHE:HE2	1.43	0.82
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.44	0.81
1:A:149:LEU:HB3	1:A:451:MET:HE1	1.63	0.80
1:A:276:LEU:HD23	1:A:279:MET:CE	2.12	0.80
1:A:444:LEU:C	1:A:444:LEU:HD23	2.03	0.79
1:B:410:GLU:O	1:B:412:PRO:HD3	1.84	0.78
1:A:369:ILE:HG22	1:A:370:VAL:HG23	1.66	0.77
1:A:213:LEU:HD21	1:A:484:LEU:HD22	1.67	0.77
1:B:173:ARG:NH1	1:B:489:PRO:HA	1.99	0.76
1:B:107:THR:HB	1:B:112:PHE:CD2	2.21	0.75
1:B:173:ARG:HH11	1:B:490:TYR:H	1.32	0.75
1:A:105:PRO:HG3	1:B:60:GLN:OE1	1.86	0.75
1:B:211:GLU:HB3	1:B:243:PHE:HD2	1.52	0.74
1:B:474:ARG:NH1	1:B:474:ARG:HG2	1.99	0.73
1:B:102:PRO:HG3	1:B:394:THR:HG23	1.70	0.73
1:A:276:LEU:HD23	1:A:279:MET:HE1	1.69	0.73
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.53	0.73
1:B:429:LYS:NZ	1:B:450:ARG:HH12	1.85	0.73
1:B:220:LEU:HD13	1:B:220:LEU:O	1.88	0.73
1:A:105:PRO:O	1:A:108:GLN:HG3	1.90	0.72
1:B:359:VAL:O	1:B:363:VAL:HG23	1.88	0.72
1:B:67:ASP:HA	1:B:82:ASN:HB2	1.71	0.72
1:B:174:PRO:HD3	1:B:492:LEU:HD22	1.72	0.72
1:B:186:ILE:O	1:B:190:THR:HG23	1.89	0.72
1:B:211:GLU:CB	1:B:243:PHE:HD2	2.04	0.71
1:B:312:THR:CB	1:B:369:ILE:HD11	2.21	0.71
1:B:129:ARG:CZ	1:B:129:ARG:HB2	2.20	0.71
1:A:410:GLU:O	1:A:412:PRO:HD3	1.91	0.71
1:A:412:PRO:HB2	1:A:413:PHE:CD1	2.25	0.71
1:A:62:ARG:O	1:A:66:GLY:HA2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLU:OE1	1:B:384:VAL:HA	1.91	0.70
1:A:380:ARG:NH1	1:A:380:ARG:HB2	2.04	0.70
1:B:321:MET:HE2	1:B:457:PHE:HZ	1.56	0.70
1:A:321:MET:CE	1:A:328:GLN:HA	2.21	0.70
1:A:34:PRO:HA	1:A:387:PHE:CD2	2.26	0.70
1:B:211:GLU:HB3	1:B:243:PHE:CD2	2.27	0.70
1:B:215:GLU:OE2	1:B:244:GLN:HG3	1.91	0.70
1:A:39:PRO:CG	1:A:45:ASN:HB2	2.20	0.70
1:A:43:LEU:O	1:A:46:LEU:HB2	1.93	0.69
1:B:173:ARG:HD2	1:B:490:TYR:O	1.93	0.69
1:B:220:LEU:HD13	1:B:224:LEU:HG	1.74	0.69
1:A:79:VAL:HG11	1:A:389:ILE:CD1	2.22	0.68
1:B:62:ARG:O	1:B:66:GLY:HA2	1.94	0.68
1:B:87:VAL:HG21	1:B:402:VAL:CG2	2.23	0.68
1:A:75:TRP:HE1	1:A:226:ALA:HA	1.59	0.68
1:A:312:THR:HG22	1:A:369:ILE:HD11	1.76	0.68
1:A:179:ASP:OD1	1:A:311:SER:HB2	1.94	0.68
1:B:279:MET:HG2	1:B:290:PHE:O	1.95	0.67
1:A:244:GLN:NE2	3:A:503:PN0:H3	2.10	0.67
1:B:444:LEU:C	1:B:444:LEU:HD23	2.14	0.67
1:A:339:ILE:HD11	1:A:353:MET:SD	2.35	0.67
1:A:47:LEU:H	1:A:47:LEU:CD2	2.06	0.66
1:B:182:VAL:HG11	1:B:310:THR:HB	1.77	0.66
1:A:33:LEU:O	1:A:387:PHE:HD2	1.77	0.66
1:A:408:VAL:HG11	1:A:432:ALA:CB	2.26	0.66
1:A:285:ASN:HD22	1:A:285:ASN:H	1.44	0.66
1:A:319:LEU:HB2	1:A:490:TYR:CE2	2.31	0.65
1:A:275:PHE:CD2	1:A:295:LEU:HD13	2.31	0.65
1:A:132:ARG:O	1:A:136:VAL:CG1	2.43	0.65
1:A:59:ASP:HA	1:A:62:ARG:HG2	1.79	0.64
1:B:441:ARG:HD2	2:B:502:HEM:O2D	1.96	0.64
1:B:150:GLU:O	1:B:154:THR:HG23	1.97	0.64
1:B:151:GLN:HA	1:B:154:THR:HG23	1.81	0.63
1:B:303:PHE:HE1	1:B:307:MET:CE	2.12	0.63
1:A:203:LEU:HD23	1:A:203:LEU:O	1.99	0.63
1:A:370:VAL:HG12	1:A:373:GLY:HA2	1.80	0.63
1:B:369:ILE:HG22	1:B:370:VAL:HG23	1.80	0.63
1:A:213:LEU:HD22	1:A:308:VAL:HG21	1.80	0.63
1:B:174:PRO:HD3	1:B:492:LEU:CD2	2.28	0.62
1:B:213:LEU:HD21	1:B:484:LEU:HD22	1.80	0.62
1:A:39:PRO:HG2	1:A:45:ASN:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:HG23	1:A:471:GLY:N	2.15	0.62
1:A:91:LEU:HD11	1:A:397:THR:HG21	1.79	0.62
1:B:206:LEU:O	1:B:210:GLN:HG2	2.00	0.61
1:B:204:ARG:HG2	1:B:204:ARG:HH11	1.66	0.61
1:B:331:VAL:HG11	1:B:461:LEU:HD12	1.83	0.61
1:A:73:LEU:HD12	1:A:73:LEU:O	2.01	0.60
1:B:149:LEU:HD11	1:B:189:LEU:HD11	1.81	0.60
1:B:454:PHE:HD1	1:B:455:LEU:HD23	1.65	0.60
1:B:316:TRP:CD2	1:B:487:PRO:HG3	2.37	0.60
1:A:274:ALA:O	1:A:278:GLU:HG2	2.00	0.60
1:B:122:ALA:O	1:B:441:ARG:NH2	2.25	0.60
1:A:321:MET:HE3	1:A:328:GLN:HA	1.83	0.60
1:B:124:TYR:HE1	1:B:440:ARG:HE	1.46	0.60
1:B:206:LEU:HD23	1:B:307:MET:HE2	1.83	0.60
1:B:429:LYS:NZ	1:B:450:ARG:NH1	2.49	0.60
1:B:312:THR:CG2	1:B:369:ILE:HD11	2.32	0.60
1:B:129:ARG:NH1	1:B:129:ARG:HB2	2.17	0.60
1:B:49:VAL:HG23	1:B:49:VAL:O	2.01	0.59
1:A:428:VAL:O	1:A:430:PRO:HD3	2.02	0.59
1:A:321:MET:HE1	1:A:328:GLN:HA	1.84	0.59
1:A:365:ARG:HH22	1:A:404:LYS:HG2	1.67	0.59
1:A:440:ARG:HG3	1:A:440:ARG:HH21	1.67	0.59
1:A:443:CYS:HB2	2:A:502:HEM:C4A	2.37	0.59
1:A:236:LEU:O	1:A:240:VAL:HG23	2.03	0.59
1:B:259:ARG:HD3	1:B:276:LEU:HD21	1.83	0.59
1:A:84:LEU:HD12	1:A:84:LEU:O	2.02	0.59
1:A:191:CYS:HG	1:A:303:PHE:HE2	1.51	0.59
1:B:128:TRP:NE1	1:B:441:ARG:NE	2.51	0.59
1:A:446:GLU:HB3	1:A:447:PRO:HD3	1.84	0.58
1:B:35:PRO:HD3	1:B:387:PHE:CE2	2.38	0.58
1:B:460:LEU:O	1:B:464:PHE:HB2	2.04	0.58
1:B:278:GLU:HA	1:B:278:GLU:OE2	2.03	0.58
1:A:380:ARG:NH1	1:A:380:ARG:CB	2.67	0.58
1:B:470:THR:HG23	1:B:471:GLY:H	1.68	0.58
1:B:167:HIS:ND1	1:B:172:PHE:CD1	2.71	0.57
1:A:67:ASP:HA	1:A:82:ASN:HB2	1.85	0.57
1:B:330:ARG:HB2	1:B:355:TYR:CE2	2.38	0.57
1:A:444:LEU:HD22	2:A:502:HEM:HMD3	1.85	0.57
1:B:140:ARG:HA	1:B:144:LEU:HB3	1.86	0.57
1:B:303:PHE:HE1	1:B:307:MET:HE3	1.68	0.57
1:A:211:GLU:O	1:A:215:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLN:O	1:A:332:GLN:HG3	2.05	0.57
1:B:440:ARG:HG2	1:B:440:ARG:HH21	1.68	0.57
1:A:334:GLU:OE2	1:A:353:MET:HB3	2.05	0.57
1:B:446:GLU:O	1:B:450:ARG:HG2	2.05	0.57
1:A:129:ARG:HH11	1:A:129:ARG:CG	2.17	0.56
1:B:101:ARG:HD2	1:B:375:THR:O	2.05	0.56
1:B:361:HIS:NE2	1:B:450:ARG:NH1	2.52	0.56
1:A:259:ARG:HD3	1:A:276:LEU:CD2	2.35	0.56
1:A:285:ASN:OD1	1:A:287:GLU:HB2	2.05	0.56
1:A:233:ILE:N	1:A:234:PRO:HD3	2.20	0.56
1:A:117:GLN:HB3	1:A:122:ALA:HA	1.88	0.56
1:A:229:VAL:HG22	1:A:229:VAL:O	2.05	0.56
1:B:276:LEU:HD23	1:B:279:MET:CE	2.35	0.56
1:B:66:GLY:O	1:B:68:VAL:N	2.38	0.56
1:B:132:ARG:O	1:B:136:VAL:HG12	2.06	0.56
1:A:72:GLN:CG	1:B:38:LEU:HD22	2.25	0.56
1:B:79:VAL:HG23	1:B:393:THR:HG21	1.86	0.55
1:B:410:GLU:C	1:B:412:PRO:HD3	2.27	0.55
1:B:227:VAL:HG12	1:B:227:VAL:O	2.07	0.55
1:A:383:GLU:HG3	1:A:383:GLU:O	2.07	0.55
1:A:41:PRO:CB	1:B:42:GLY:H	2.20	0.55
1:B:138:THR:CG2	1:B:271:LEU:HD12	2.37	0.55
1:A:174:PRO:HD3	1:A:492:LEU:HD22	1.88	0.54
1:B:269:ARG:HB2	1:B:273:GLU:OE2	2.07	0.54
1:A:219:PHE:O	1:A:223:VAL:HG23	2.07	0.54
1:A:66:GLY:O	1:A:68:VAL:N	2.40	0.54
1:B:142:LEU:HD11	1:B:271:LEU:N	2.22	0.54
1:B:84:LEU:HD22	1:B:432:ALA:HB2	1.89	0.54
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.71	0.54
1:A:463:HIS:CG	1:A:463:HIS:O	2.61	0.54
1:B:276:LEU:HA	1:B:279:MET:CE	2.37	0.54
1:B:126:PRO:HG2	1:B:127:ALA:H	1.73	0.54
1:B:224:LEU:N	1:B:224:LEU:HD23	2.23	0.54
1:A:408:VAL:HG11	1:A:432:ALA:HB3	1.90	0.54
1:B:165:ALA:C	1:B:167:HIS:H	2.11	0.54
1:A:39:PRO:HG3	1:A:45:ASN:OD1	2.08	0.53
1:B:275:PHE:CD2	1:B:295:LEU:HD13	2.43	0.53
1:A:84:LEU:HD12	1:A:84:LEU:C	2.29	0.53
1:B:183:SER:O	1:B:186:ILE:HG22	2.08	0.53
1:B:456:PHE:O	1:B:460:LEU:HG	2.08	0.53
1:A:41:PRO:HB3	1:B:42:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:O	1:A:233:ILE:HD13	2.08	0.53
1:A:470:THR:HG23	1:A:471:GLY:H	1.74	0.53
1:A:233:ILE:HG21	1:A:236:LEU:HD12	1.90	0.53
1:A:215:GLU:OE1	1:A:241:LEU:HA	2.08	0.53
1:A:313:THR:OG1	1:A:369:ILE:HD12	2.09	0.53
1:A:369:ILE:HG22	1:A:370:VAL:CG2	2.37	0.53
1:A:332:GLN:NE2	1:A:497:ARG:HD2	2.24	0.53
1:A:151:GLN:HA	1:A:154:THR:OG1	2.08	0.52
1:B:274:ALA:O	1:B:278:GLU:HG2	2.09	0.52
1:A:416:HIS:CE1	1:A:418:GLU:HB2	2.45	0.52
1:A:38:LEU:N	1:A:39:PRO:HD3	2.24	0.52
1:B:138:THR:HG21	1:B:271:LEU:HD12	1.90	0.52
1:B:370:VAL:HG12	1:B:373:GLY:HA2	1.91	0.52
1:A:51:PHE:CD2	1:A:222:GLU:HG3	2.45	0.52
1:B:271:LEU:CD2	1:B:302:LEU:HD12	2.38	0.52
1:A:437:SER:OG	1:A:438:ALA:N	2.41	0.52
1:B:446:GLU:HB3	1:B:447:PRO:HD3	1.92	0.52
1:A:443:CYS:HB2	2:A:502:HEM:NA	2.25	0.51
1:A:224:LEU:HD12	1:A:240:VAL:HG21	1.92	0.51
1:A:147:LYS:HA	1:A:151:GLN:NE2	2.25	0.51
1:B:330:ARG:CB	1:B:355:TYR:CE2	2.94	0.51
1:B:123:ARG:NH2	1:B:377:MET:CE	2.73	0.51
1:A:140:ARG:HA	1:A:144:LEU:HB3	1.91	0.51
1:A:428:VAL:HG23	1:A:428:VAL:O	2.11	0.51
1:B:184:ASN:ND2	1:B:197:TYR:HE2	2.09	0.51
1:A:64:ARG:HD2	1:A:65:PHE:CE1	2.46	0.51
1:B:141:ASN:C	1:B:143:GLY:H	2.14	0.51
1:B:369:ILE:O	1:B:371:PRO:HD3	2.10	0.51
1:A:412:PRO:HB2	1:A:413:PHE:HD1	1.71	0.51
1:A:259:ARG:HD3	1:A:276:LEU:HD22	1.91	0.50
1:B:417:PRO:C	1:B:419:HIS:H	2.14	0.50
1:B:356:THR:O	1:B:360:ILE:HG13	2.11	0.50
1:B:444:LEU:O	1:B:444:LEU:HD23	2.12	0.50
1:B:191:CYS:HG	1:B:303:PHE:HE2	1.58	0.50
1:B:100:ASP:HA	1:B:124:TYR:HB2	1.94	0.50
1:B:172:PHE:N	1:B:172:PHE:CD2	2.80	0.50
1:A:51:PHE:CE2	1:A:222:GLU:HG3	2.45	0.50
1:B:319:LEU:O	1:B:322:ILE:HG12	2.11	0.50
1:B:141:ASN:ND2	1:B:141:ASN:O	2.45	0.50
1:B:244:GLN:NE2	3:B:503:PN0:H3	2.27	0.50
1:B:332:GLN:NE2	1:B:464:PHE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLN:HE21	1:A:497:ARG:HH11	1.59	0.49
1:A:241:LEU:O	1:A:245:LYS:HD3	2.13	0.49
1:B:59:ASP:HA	1:B:62:ARG:HG2	1.94	0.49
1:B:383:GLU:O	1:B:383:GLU:HG3	2.12	0.49
1:B:33:LEU:O	1:B:387:PHE:HD2	1.96	0.49
1:B:139:LEU:HB3	1:B:144:LEU:HD12	1.94	0.49
1:A:227:VAL:O	1:A:229:VAL:N	2.39	0.49
1:B:73:LEU:O	1:B:74:ALA:HB3	2.12	0.49
1:A:36:GLY:C	1:A:65:PHE:CE2	2.86	0.49
1:A:120:PHE:HD2	1:A:121:LEU:HG	1.78	0.49
1:A:440:ARG:NH2	1:A:440:ARG:HG3	2.28	0.48
1:A:231:LEU:O	1:A:232:HIS:HB2	2.12	0.48
1:B:34:PRO:HA	1:B:387:PHE:CD2	2.47	0.48
1:A:444:LEU:HD22	2:A:502:HEM:CMD	2.43	0.48
1:A:220:LEU:HD12	1:A:240:VAL:CG1	2.42	0.48
1:A:106:ILE:HG22	1:A:225:ASN:OD1	2.14	0.48
1:A:150:GLU:OE1	1:A:347:MET:N	2.44	0.48
1:A:476:SER:OG	1:A:478:HIS:ND1	2.47	0.48
1:A:165:ALA:C	1:A:167:HIS:H	2.17	0.48
1:B:428:VAL:O	1:B:430:PRO:HD3	2.14	0.48
1:A:276:LEU:HA	1:A:279:MET:CE	2.44	0.48
1:A:444:LEU:HD23	1:A:445:GLY:N	2.28	0.48
1:B:428:VAL:O	1:B:428:VAL:HG23	2.14	0.48
1:A:89:GLU:HA	1:A:93:THR:OG1	2.13	0.48
1:B:128:TRP:CE2	1:B:441:ARG:NE	2.81	0.48
1:A:80:VAL:C	1:A:81:LEU:HD23	2.34	0.48
1:B:334:GLU:OE2	1:B:353:MET:HB3	2.14	0.48
1:B:87:VAL:HG21	1:B:402:VAL:HG21	1.93	0.47
1:A:357:THR:HG22	1:A:427:PHE:CD1	2.50	0.47
1:B:172:PHE:N	1:B:172:PHE:HD2	2.11	0.47
1:A:74:ALA:CB	1:A:226:ALA:HB1	2.44	0.47
1:A:370:VAL:HG12	1:A:373:GLY:CA	2.45	0.47
1:B:331:VAL:CG1	1:B:461:LEU:HD12	2.44	0.47
1:A:230:LEU:HD23	1:A:231:LEU:N	2.29	0.47
1:B:164:PHE:O	1:B:167:HIS:HB2	2.14	0.47
1:B:123:ARG:NH2	1:B:377:MET:HE1	2.30	0.47
1:B:131:GLN:OE1	1:B:131:GLN:HA	2.13	0.47
1:A:362:GLU:OE1	1:A:420:PHE:HE1	1.98	0.47
1:B:328:GLN:O	1:B:332:GLN:HG3	2.15	0.47
1:A:39:PRO:HG3	1:A:45:ASN:CG	2.35	0.47
1:A:39:PRO:HG3	1:A:45:ASN:HB2	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TRP:CE3	1:B:276:LEU:HD13	2.50	0.47
1:A:48:HIS:NE2	1:A:61:LEU:HD21	2.30	0.47
1:B:173:ARG:NH1	1:B:490:TYR:H	2.05	0.46
1:A:232:HIS:C	1:A:234:PRO:HD3	2.36	0.46
1:B:335:ILE:HD13	1:B:462:GLN:HB2	1.96	0.46
1:A:433:PHE:O	1:A:434:LEU:HD23	2.15	0.46
1:A:39:PRO:HG3	1:A:45:ASN:CB	2.45	0.46
1:A:75:TRP:CD1	1:A:75:TRP:N	2.82	0.46
1:B:343:ARG:O	1:B:343:ARG:HG3	2.15	0.46
1:B:129:ARG:CB	1:B:129:ARG:NH1	2.79	0.46
1:A:75:TRP:CZ3	1:B:61:LEU:HD21	2.49	0.46
1:A:231:LEU:CD2	1:B:52:GLN:HB2	2.45	0.46
1:A:477:HIS:N	1:A:477:HIS:ND1	2.61	0.46
1:B:276:LEU:HA	1:B:279:MET:HE2	1.95	0.46
1:B:220:LEU:CD1	1:B:224:LEU:HG	2.43	0.46
1:A:485:VAL:O	1:A:485:VAL:HG22	2.16	0.46
1:B:356:THR:HG21	1:B:458:THR:HG22	1.97	0.46
1:A:466:PHE:HA	1:A:493:CYS:O	2.16	0.46
1:A:84:LEU:HD22	1:A:432:ALA:HA	1.97	0.46
1:A:106:ILE:HG12	1:A:106:ILE:O	2.16	0.46
1:A:141:ASN:C	1:A:143:GLY:H	2.19	0.46
1:B:224:LEU:HD12	1:B:240:VAL:HG21	1.98	0.46
1:A:413:PHE:N	1:A:413:PHE:CD1	2.84	0.46
1:A:75:TRP:HD1	1:A:75:TRP:H	1.63	0.46
1:B:221:ARG:O	1:B:225:ASN:HB2	2.16	0.46
1:A:482:ALA:O	1:A:483:PHE:HB3	2.15	0.45
1:B:224:LEU:H	1:B:224:LEU:HD23	1.81	0.45
1:B:276:LEU:HD23	1:B:279:MET:HE3	1.98	0.45
1:A:358:ALA:HB1	1:A:420:PHE:HB2	1.98	0.45
1:B:126:PRO:HG2	1:B:127:ALA:N	2.31	0.45
1:A:269:ARG:HG2	1:A:273:GLU:OE2	2.14	0.45
1:B:444:LEU:HD22	2:B:502:HEM:HMD2	1.99	0.45
1:A:461:LEU:HD23	1:A:466:PHE:HE1	1.82	0.45
1:B:443:CYS:HB2	2:B:502:HEM:NA	2.31	0.45
1:B:115:ARG:HG2	1:B:115:ARG:HH11	1.82	0.45
1:B:470:THR:HG23	1:B:471:GLY:N	2.32	0.45
1:B:440:ARG:NH2	1:B:440:ARG:HG2	2.31	0.45
1:B:74:ALA:HB3	1:B:226:ALA:HB1	1.99	0.45
1:A:120:PHE:CD2	1:A:121:LEU:HG	2.52	0.45
1:A:331:VAL:HG11	1:A:461:LEU:HD12	1.99	0.45
1:A:39:PRO:CG	1:A:45:ASN:CB	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:CG	1:A:88:ARG:HH11	2.31	0.44
1:B:323:LEU:HD11	1:B:475:PRO:O	2.17	0.44
1:A:40:LEU:HB2	1:A:41:PRO:HD2	2.00	0.44
1:A:490:TYR:CD1	1:A:490:TYR:C	2.91	0.44
1:B:45:ASN:HA	1:B:48:HIS:CE1	2.53	0.44
1:A:210:GLN:O	1:A:214:LYS:HG3	2.18	0.44
1:B:320:LEU:O	1:B:324:HIS:HB2	2.18	0.44
1:B:370:VAL:HG12	1:B:373:GLY:CA	2.48	0.44
1:A:39:PRO:HB3	1:A:45:ASN:CA	2.48	0.44
1:A:357:THR:HG22	1:A:427:PHE:CE1	2.53	0.44
1:B:466:PHE:HA	1:B:493:CYS:O	2.18	0.44
1:A:56:TYR:O	1:A:60:GLN:HG2	2.17	0.44
1:A:39:PRO:HB3	1:A:44:GLY:C	2.38	0.44
1:B:101:ARG:NH1	1:B:441:ARG:HH11	2.16	0.44
1:B:370:VAL:CG1	1:B:373:GLY:HA2	2.48	0.44
1:A:308:VAL:O	1:A:308:VAL:HG23	2.18	0.44
1:B:68:VAL:O	1:B:68:VAL:HG12	2.17	0.44
1:B:43:LEU:O	1:B:74:ALA:HA	2.18	0.44
1:A:33:LEU:HD12	1:A:387:PHE:HA	2.00	0.43
1:B:188:SER:OG	1:B:189:LEU:N	2.50	0.43
1:A:365:ARG:HD2	1:A:409:TRP:CE2	2.52	0.43
1:B:270:ASP:OD2	1:B:273:GLU:HG3	2.18	0.43
1:A:444:LEU:CD2	2:A:502:HEM:HHD	2.48	0.43
1:A:444:LEU:HD22	2:A:502:HEM:C2D	2.53	0.43
1:A:451:MET:HG2	1:A:455:LEU:HD12	2.01	0.43
1:B:262:TRP:CZ3	1:B:276:LEU:HB3	2.52	0.43
1:B:43:LEU:HG	1:B:46:LEU:HD22	1.99	0.43
1:B:160:LEU:HD13	1:B:181:ALA:HB2	2.01	0.43
1:A:172:PHE:N	1:A:172:PHE:HD2	2.16	0.43
1:A:172:PHE:N	1:A:172:PHE:CD2	2.85	0.43
1:B:112:PHE:CD1	1:B:297:ILE:HD13	2.52	0.43
1:A:102:PRO:HB2	1:B:64:ARG:HH22	1.83	0.43
1:B:316:TRP:CG	1:B:487:PRO:HG3	2.54	0.43
1:B:276:LEU:HA	1:B:279:MET:HE3	2.00	0.43
1:B:45:ASN:HA	1:B:48:HIS:HE1	1.83	0.43
1:A:460:LEU:O	1:A:464:PHE:HB2	2.17	0.43
1:A:300:ALA:HB1	3:A:503:PN0:H17	2.01	0.43
1:B:143:GLY:O	1:B:145:GLY:N	2.51	0.43
1:B:368:ASP:OD1	1:B:400:SER:HA	2.18	0.43
1:B:69:PHE:CE1	1:B:71:LEU:HD21	2.53	0.43
1:B:41:PRO:O	1:B:42:GLY:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:N	1:B:34:PRO:CD	2.82	0.43
1:A:131:GLN:HA	1:A:131:GLN:OE1	2.19	0.43
1:A:109:ILE:HG22	1:A:109:ILE:O	2.19	0.43
1:B:33:LEU:N	1:B:34:PRO:HD3	2.34	0.43
1:B:241:LEU:CD1	1:B:241:LEU:N	2.81	0.43
1:A:276:LEU:HA	1:A:279:MET:HE2	2.00	0.42
1:B:379:SER:O	1:B:391:LYS:HE3	2.19	0.42
1:A:450:ARG:HH11	1:A:450:ARG:HG3	1.84	0.42
1:B:276:LEU:HD23	1:B:279:MET:HE1	2.00	0.42
1:A:470:THR:CG2	1:A:471:GLY:N	2.82	0.42
1:B:279:MET:O	1:B:280:GLU:C	2.56	0.42
1:A:495:VAL:HA	1:A:496:PRO:HD3	1.72	0.42
1:B:105:PRO:O	1:B:108:GLN:HG3	2.19	0.42
1:B:316:TRP:CE2	1:B:487:PRO:HG3	2.53	0.42
1:B:226:ALA:O	1:B:227:VAL:HG23	2.20	0.42
1:A:50:ASP:HB3	1:A:57:CYS:SG	2.59	0.42
1:B:406:GLU:HG2	1:B:406:GLU:H	1.67	0.42
1:A:98:THR:HG22	1:A:378:THR:HG22	2.00	0.42
1:A:54:THR:HB	1:A:55:PRO:HD3	2.02	0.42
1:B:436:PHE:CE1	1:B:446:GLU:HG3	2.54	0.42
1:A:417:PRO:C	1:A:419:HIS:H	2.23	0.42
1:B:152:TRP:O	1:B:152:TRP:HE3	2.03	0.42
1:A:344:ARG:HA	1:A:345:PRO:HD3	1.93	0.42
1:B:488:SER:O	1:B:489:PRO:C	2.58	0.42
1:B:309:THR:OG1	1:B:310:THR:N	2.52	0.42
1:A:102:PRO:HA	1:A:377:MET:SD	2.60	0.42
1:A:372:LEU:HA	1:A:398:ASN:HA	2.02	0.42
1:B:321:MET:HE2	1:B:457:PHE:CZ	2.45	0.42
1:A:65:PHE:N	1:A:65:PHE:CD1	2.88	0.42
1:A:205:LEU:HA	1:A:205:LEU:HD12	1.78	0.42
1:A:157:ALA:HA	1:A:456:PHE:HE1	1.85	0.41
1:A:389:ILE:HG23	1:A:393:THR:HG21	2.01	0.41
1:B:149:LEU:O	1:B:153:VAL:HG23	2.20	0.41
1:A:233:ILE:N	1:A:234:PRO:CD	2.80	0.41
1:B:199:ASP:HA	1:B:200:PRO:HD3	1.91	0.41
1:A:410:GLU:C	1:A:412:PRO:HD3	2.41	0.41
1:B:123:ARG:HE	1:B:123:ARG:HB3	1.59	0.41
1:A:220:LEU:HA	1:A:220:LEU:HD22	1.87	0.41
1:B:269:ARG:HH11	1:B:269:ARG:HG2	1.85	0.41
1:B:329:ARG:NH1	1:B:329:ARG:HG3	2.36	0.41
1:B:51:PHE:CZ	1:B:222:GLU:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:CG1	1:A:373:GLY:HA2	2.48	0.41
1:B:164:PHE:CE2	1:B:460:LEU:HD22	2.56	0.41
1:A:81:LEU:HD23	1:A:81:LEU:N	2.35	0.41
1:A:183:SER:OG	1:A:307:MET:HG3	2.21	0.41
1:A:483:PHE:CD2	1:A:484:LEU:HD13	2.56	0.41
1:B:78:VAL:HG12	1:B:79:VAL:N	2.36	0.41
1:B:271:LEU:HD22	1:B:302:LEU:HD12	2.03	0.41
1:A:356:THR:HG21	1:A:458:THR:CG2	2.50	0.41
1:B:303:PHE:CE1	1:B:307:MET:HE1	2.55	0.41
1:B:79:VAL:CG2	1:B:393:THR:HG21	2.51	0.41
1:B:417:PRO:O	1:B:419:HIS:N	2.54	0.41
1:A:47:LEU:N	1:A:47:LEU:CD2	2.76	0.41
1:A:147:LYS:HA	1:A:151:GLN:HE21	1.85	0.41
1:B:417:PRO:C	1:B:419:HIS:N	2.74	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.95	0.41
1:B:170:ARG:HA	1:B:170:ARG:HD2	1.96	0.41
1:B:88:ARG:O	1:B:92:VAL:HB	2.21	0.41
1:B:107:THR:O	1:B:112:PHE:HD2	2.04	0.41
1:A:319:LEU:O	1:A:322:ILE:HG12	2.20	0.41
1:B:204:ARG:HG2	1:B:204:ARG:NH1	2.35	0.40
1:A:426:HIS:CD2	1:A:426:HIS:N	2.89	0.40
1:A:101:ARG:HD2	1:A:375:THR:O	2.21	0.40
1:A:35:PRO:HD3	1:A:387:PHE:CE2	2.57	0.40
1:A:40:LEU:HD12	1:A:40:LEU:C	2.42	0.40
1:B:444:LEU:CD2	1:B:444:LEU:C	2.86	0.40
1:A:362:GLU:HG3	1:A:415:PHE:CE1	2.56	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	463/479 (97%)	396 (86%)	58 (12%)	9 (2%)	10	32
1	B	453/479 (95%)	382 (84%)	55 (12%)	16 (4%)	4	16
All	All	916/958 (96%)	778 (85%)	113 (12%)	25 (3%)	6	22

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	470	THR
1	B	67	ASP
1	B	470	THR
1	B	42	GLY
1	A	74	ALA
1	B	37	PRO
1	B	144	LEU
1	B	418	GLU
1	B	489	PRO
1	A	35	PRO
1	B	74	ALA
1	A	148	SER
1	B	46	LEU
1	B	50	ASP
1	B	148	SER
1	B	166	ASN
1	A	410	GLU
1	B	41	PRO
1	B	106	ILE
1	B	228	PRO
1	A	106	ILE
1	A	145	GLY
1	B	145	GLY
1	A	489	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/409 (97%)	359 (90%)	38 (10%)	10	28
1	B	391/409 (96%)	362 (93%)	29 (7%)	17	42
All	All	788/818 (96%)	721 (92%)	67 (8%)	13	34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	43	LEU
1	A	47	LEU
1	A	84	LEU
1	A	88	ARG
1	A	101	ARG
1	A	129	ARG
1	A	136	VAL
1	A	144	LEU
1	A	149	LEU
1	A	152	TRP
1	A	164	PHE
1	A	172	PHE
1	A	193	ARG
1	A	204	ARG
1	A	220	LEU
1	A	230	LEU
1	A	240	VAL
1	A	241	LEU
1	A	250	GLN
1	A	261	THR
1	A	271	LEU
1	A	285	ASN
1	A	303	PHE
1	A	321	MET
1	A	329	ARG
1	A	343	ARG
1	A	375	THR
1	A	383	GLU
1	A	403	LEU
1	A	444	LEU
1	A	468	VAL
1	A	472	GLN
1	A	485	VAL
1	A	486	SER

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Mol	Chain	Res	Type
1	A	488	SER
1	A	492	LEU
1	A	495	VAL
1	B	33	LEU
1	B	47	LEU
1	B	48	HIS
1	B	53	ASN
1	B	71	LEU
1	B	72	GLN
1	B	75	TRP
1	B	141	ASN
1	B	144	LEU
1	B	149	LEU
1	B	152	TRP
1	B	167	HIS
1	B	172	PHE
1	B	188	SER
1	B	190	THR
1	B	193	ARG
1	B	224	LEU
1	B	250	GLN
1	B	303	PHE
1	B	323	LEU
1	B	326	ASP
1	B	329	ARG
1	B	331	VAL
1	B	369	ILE
1	B	379	SER
1	B	383	GLU
1	B	444	LEU
1	B	474	ARG
1	B	485	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	141	ASN
1	A	151	GLN
1	A	250	GLN
1	A	332	GLN
1	A	426	HIS

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Mol	Chain	Res	Type
1	B	48	HIS
1	B	53	ASN
1	B	72	GLN
1	B	141	ASN
1	B	151	GLN
1	B	210	GLN
1	B	332	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	502	1,3	30,50,50	3.53	13 (43%)	24,82,82	2.58	10 (41%)
3	PN0	A	503	2	28,30,30	1.75	7 (25%)	36,44,44	1.55	8 (22%)
2	HEM	B	502	1,3	30,50,50	3.67	12 (40%)	24,82,82	2.68	9 (37%)
3	PN0	B	503	2	28,30,30	1.77	6 (21%)	36,44,44	1.63	9 (25%)

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	502	1,3	-	0/10/54/54	0/0/8/8
3	PN0	A	503	2	-	0/21/39/39	0/2/3/3
2	HEM	B	502	1,3	-	0/10/54/54	0/0/8/8
3	PN0	B	503	2	-	0/21/39/39	0/2/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEM	C3B-C4B	-9.72	1.43	1.51
2	A	502	HEM	C3B-C4B	-8.35	1.44	1.51
2	B	502	HEM	C3D-C4D	-8.02	1.41	1.51
2	B	502	HEM	C3C-CAC	-7.86	1.36	1.51
2	A	502	HEM	C3C-CAC	-7.32	1.37	1.51
2	A	502	HEM	C3D-C4D	-7.26	1.42	1.51
2	B	502	HEM	C2C-C1C	-7.10	1.39	1.52
2	A	502	HEM	C2C-C1C	-6.84	1.39	1.52
2	A	502	HEM	C2D-C3D	-5.88	1.36	1.54
2	B	502	HEM	C2D-C3D	-5.50	1.38	1.54
2	A	502	HEM	C3B-CAB	-5.48	1.41	1.51
2	B	502	HEM	C3B-CAB	-4.98	1.42	1.51
3	B	503	PN0	C1-S1	-4.52	1.80	1.84
2	A	502	HEM	C1C-NC	-3.90	1.31	1.36
3	A	503	PN0	C1-S1	-3.88	1.80	1.84
2	B	502	HEM	C2D-C1D	-3.61	1.40	1.51
2	A	502	HEM	C2D-C1D	-3.58	1.40	1.51
2	B	502	HEM	C1C-NC	-3.46	1.31	1.36
2	A	502	HEM	C2B-C1B	-3.15	1.41	1.51
3	A	503	PN0	C5-S2	-2.88	1.72	1.76
2	B	502	HEM	C2B-C1B	-2.67	1.43	1.51
3	B	503	PN0	C5-S2	-2.57	1.72	1.76
2	B	502	HEM	CBC-CAC	2.13	1.41	1.29
2	A	502	HEM	FE-NC	2.14	2.04	1.95
3	A	503	PN0	C7-C8	2.16	1.43	1.38
3	B	503	PN0	C10-C5	2.28	1.42	1.38
2	A	502	HEM	CBC-CAC	2.32	1.42	1.29
3	A	503	PN0	C9-C8	2.38	1.43	1.38
3	B	503	PN0	C6-C5	2.45	1.42	1.38
3	A	503	PN0	C6-C5	2.54	1.43	1.38
3	B	503	PN0	C9-C8	2.75	1.44	1.38
2	B	502	HEM	CMA-C3A	2.82	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	PN0	C15-C11	3.05	1.44	1.38
2	A	502	HEM	CMA-C3A	3.12	1.58	1.51
3	A	503	PN0	C2-C16	3.15	1.58	1.52
2	B	502	HEM	CBB-CAB	3.20	1.47	1.29
2	A	502	HEM	CBB-CAB	3.25	1.48	1.29
3	B	503	PN0	C15-C11	3.65	1.46	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	PN0	C18-C1-C17	-3.80	105.15	109.63
3	B	503	PN0	C18-C1-C17	-3.74	105.22	109.63
3	A	503	PN0	O2-S2-C5	-3.44	103.54	108.00
3	B	503	PN0	C6-C5-S2	-2.67	116.84	119.79
3	B	503	PN0	O3-S2-O2	-2.55	115.06	119.47
3	B	503	PN0	O2-S2-C5	-2.53	104.72	108.00
3	B	503	PN0	O1-C11-C12	-2.35	110.99	119.42
3	A	503	PN0	O1-C11-C12	-2.03	112.15	119.42
3	A	503	PN0	O3-S2-O2	-2.00	116.01	119.47
3	A	503	PN0	C5-S2-N1	2.03	110.70	107.38
2	A	502	HEM	C3B-C4B-CHC	2.21	126.28	123.16
2	A	502	HEM	C1D-CHD-C4C	2.25	129.58	125.82
3	B	503	PN0	C10-C5-S2	2.28	122.31	119.79
3	A	503	PN0	O1-C11-C15	2.33	127.75	119.42
3	B	503	PN0	O4-N3-C16	2.34	123.18	119.86
3	A	503	PN0	O4-N3-C16	2.41	123.28	119.86
2	A	502	HEM	CMD-C2D-C3D	2.57	125.70	114.35
3	B	503	PN0	O1-C11-C15	2.59	128.68	119.42
2	B	502	HEM	CMD-C2D-C3D	2.68	126.18	114.35
2	B	502	HEM	C1D-CHD-C4C	2.69	130.32	125.82
2	A	502	HEM	C4B-CHC-C1C	2.91	130.69	125.82
3	A	503	PN0	C11-O1-C8	2.93	126.12	118.81
2	B	502	HEM	C4B-CHC-C1C	3.37	131.46	125.82
2	A	502	HEM	C3C-CAC-CBC	3.49	129.80	124.46
2	B	502	HEM	C3C-CAC-CBC	3.52	129.85	124.46
2	A	502	HEM	C3B-CAB-CBB	3.67	130.08	124.46
3	B	503	PN0	C11-O1-C8	3.77	128.21	118.81
2	B	502	HEM	C3B-CAB-CBB	3.89	130.43	124.46
2	A	502	HEM	CMC-C2C-C3C	4.22	127.06	116.53
2	B	502	HEM	CAD-C3D-C4D	4.24	127.44	112.47
2	A	502	HEM	CAD-C3D-C4D	4.37	127.87	112.47
2	B	502	HEM	CMC-C2C-C3C	4.48	127.71	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	HEM	CAD-C3D-C2D	4.90	127.30	113.22
2	B	502	HEM	CAD-C3D-C2D	5.24	128.28	113.22
2	B	502	HEM	CMB-C2B-C3B	5.59	130.47	116.53
2	A	502	HEM	CMB-C2B-C3B	5.64	130.61	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	HEM	6	0
3	A	503	PN0	2	0
2	B	502	HEM	3	0
3	B	503	PN0	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	465/479 (97%)	0.08	16 (3%) 49 41	43, 77, 101, 111	0
1	B	457/479 (95%)	0.09	12 (2%) 59 54	53, 79, 99, 111	0
All	All	922/958 (96%)	0.09	28 (3%) 54 47	43, 78, 100, 111	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	HIS	4.8
1	B	309	THR	3.2
1	A	341	GLN	3.1
1	B	352	HIS	3.1
1	A	474	ARG	2.9
1	A	309	THR	2.8
1	A	305	ALA	2.7
1	B	239	LYS	2.6
1	B	306	GLY	2.5
1	A	65	PHE	2.5
1	A	170	ARG	2.5
1	B	169	GLY	2.4
1	B	305	ALA	2.4
1	A	478	HIS	2.4
1	B	380	ARG	2.4
1	A	416	HIS	2.4
1	B	426	HIS	2.4
1	B	304	SER	2.3
1	A	147	LYS	2.3
1	B	424	GLN	2.2
1	B	165	ALA	2.2
1	A	443	CYS	2.2
1	A	387	PHE	2.1
1	A	56	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	312	THR	2.1
1	A	235	ALA	2.0
1	A	415	PHE	2.0
1	B	265	ALA	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	HEM	B	502	43/43	0.97	0.28	0.46	52,59,61,62	0
3	PN0	B	503	28/28	0.95	0.26	0.09	46,72,83,83	0
2	HEM	A	502	43/43	0.98	0.23	-0.15	33,41,45,50	0
3	PN0	A	503	28/28	0.95	0.23	-0.27	57,70,80,84	0
4	NI	B	600	1/1	0.98	0.07	-2.12	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.