



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 PM GMT

PDB ID : 3TDA  
Title : Competitive replacement of thioridazine by prinomastat in crystals of cytochrome P450 2D6  
Authors : Wang, A; Stout, C.D.; Johnson, E.F.  
Deposited on : 2011-08-10  
Resolution : 2.67 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

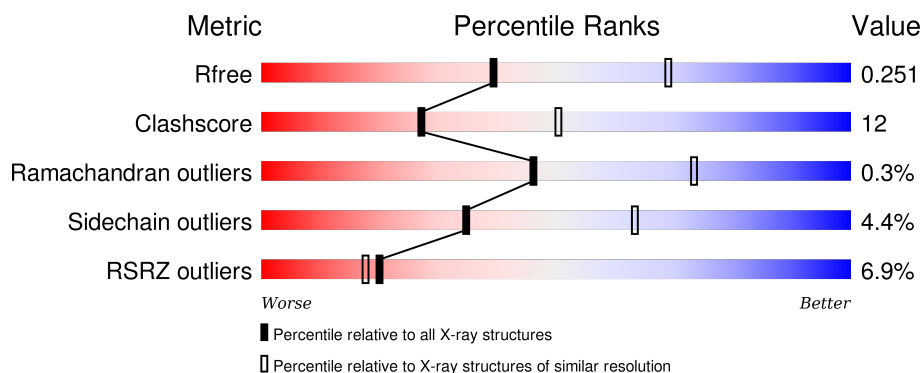
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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>5%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	479	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• 5%</div> </div> </div>
1	C	479	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>• •</div> </div> </div>
1	D	479	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15106 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	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	B	456	Total	C	N	O	S	0	0	0
			3614	2317	640	643	14			
1	C	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	D	456	Total	C	N	O	S	0	0	0
			3614	2317	640	643	14			

There are 60 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

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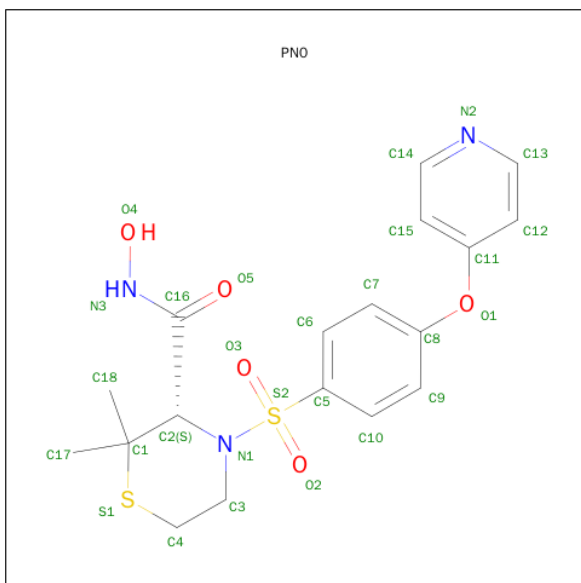
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	EXPRESSION TAG	UNP P10635
B	30	LYS	-	EXPRESSION TAG	UNP P10635
B	31	GLY	-	EXPRESSION TAG	UNP P10635
B	32	LYS	-	EXPRESSION TAG	UNP P10635
B	33	LEU	-	EXPRESSION TAG	UNP P10635
B	498	HIS	-	EXPRESSION TAG	UNP P10635
B	499	HIS	-	EXPRESSION TAG	UNP P10635
B	500	HIS	-	EXPRESSION TAG	UNP P10635
B	501	HIS	-	EXPRESSION TAG	UNP P10635
C	23	MET	-	EXPRESSION TAG	UNP P10635
C	24	ALA	-	EXPRESSION TAG	UNP P10635
C	25	LYS	-	EXPRESSION TAG	UNP P10635
C	26	LYS	-	EXPRESSION TAG	UNP P10635
C	27	THR	-	EXPRESSION TAG	UNP P10635
C	28	SER	-	EXPRESSION TAG	UNP P10635
C	29	SER	-	EXPRESSION TAG	UNP P10635
C	30	LYS	-	EXPRESSION TAG	UNP P10635
C	31	GLY	-	EXPRESSION TAG	UNP P10635
C	32	LYS	-	EXPRESSION TAG	UNP P10635
C	33	LEU	-	EXPRESSION TAG	UNP P10635
C	498	HIS	-	EXPRESSION TAG	UNP P10635
C	499	HIS	-	EXPRESSION TAG	UNP P10635
C	500	HIS	-	EXPRESSION TAG	UNP P10635
C	501	HIS	-	EXPRESSION TAG	UNP P10635
D	23	MET	-	EXPRESSION TAG	UNP P10635
D	24	ALA	-	EXPRESSION TAG	UNP P10635
D	25	LYS	-	EXPRESSION TAG	UNP P10635
D	26	LYS	-	EXPRESSION TAG	UNP P10635
D	27	THR	-	EXPRESSION TAG	UNP P10635
D	28	SER	-	EXPRESSION TAG	UNP P10635
D	29	SER	-	EXPRESSION TAG	UNP P10635
D	30	LYS	-	EXPRESSION TAG	UNP P10635
D	31	GLY	-	EXPRESSION TAG	UNP P10635
D	32	LYS	-	EXPRESSION TAG	UNP P10635
D	33	LEU	-	EXPRESSION TAG	UNP P10635
D	498	HIS	-	EXPRESSION TAG	UNP P10635
D	499	HIS	-	EXPRESSION TAG	UNP P10635
D	500	HIS	-	EXPRESSION TAG	UNP P10635
D	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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is PRINOMASTAT (three-letter code: PN0) (formula:  $\text{C}_{18}\text{H}_{21}\text{N}_3\text{O}_5\text{S}_2$ ).



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		
3	C	1	Total	C	N	O	S	0	0
			28	18	3	5	2		
3	D	1	Total	C	N	O	S	0	0
			28	18	3	5	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	2	Total	Zn	0	0
			2	2		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

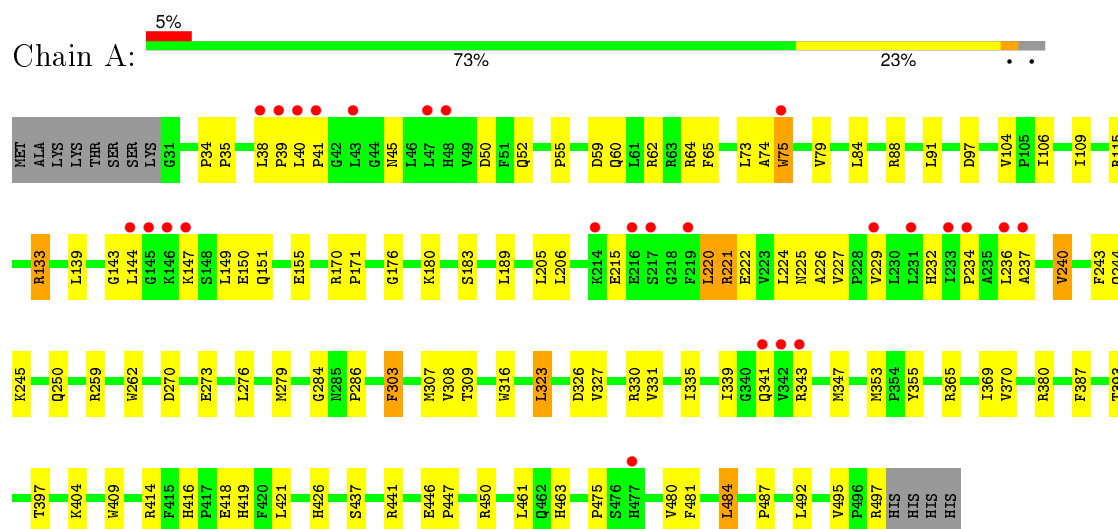
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	48	Total	O	0	0
			48	48		
5	C	63	Total	O	0	0
			63	63		
5	D	37	Total	O	0	0
			37	37		

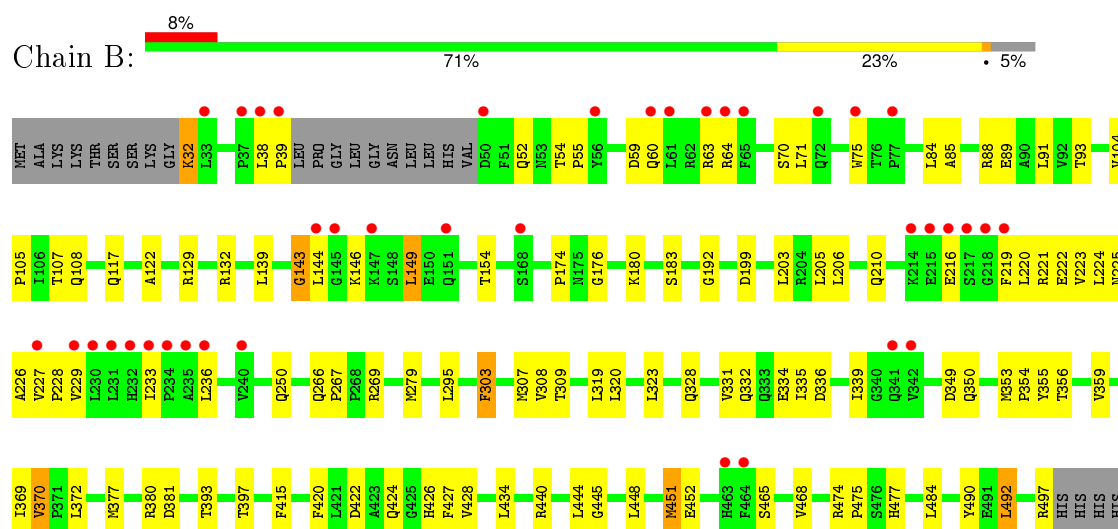
### 3 Residue-property plots [i](#)

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 2D6

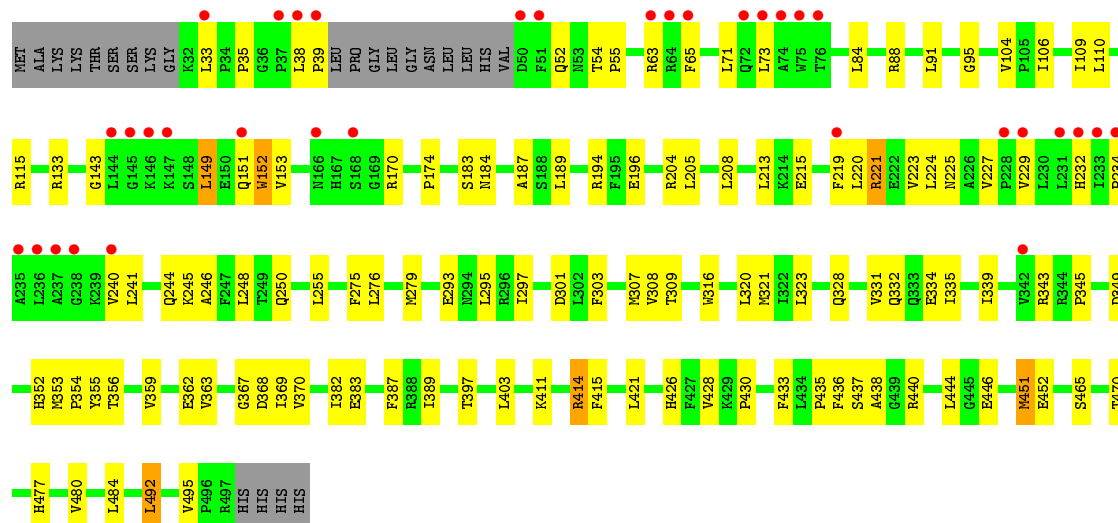


#### • Molecule 1: Cytochrome P450 2D6



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.05Å 192.74Å 247.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.04 – 2.67 42.19 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.04-2.67) 99.8 (42.19-2.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.18 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.217 , 0.255 0.212 , 0.251	Depositor DCC
$R_{free}$ test set	3907 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	10 of 78918 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3835e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/3790	0.64	0/5155
1	B	0.44	0/3711	0.62	0/5045
1	C	0.47	0/3790	0.65	0/5155
1	D	0.43	0/3711	0.61	0/5045
All	All	0.45	0/15002	0.63	0/20400

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 [i](#)

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	3690	0	3679	80	0
1	B	3614	0	3596	81	0
1	C	3690	0	3679	93	0
1	D	3614	0	3596	101	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	6	0
2	D	43	0	30	3	0
3	A	28	0	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	21	0	0
3	C	28	0	21	1	0
3	D	28	0	21	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	61	0	0	4	0
5	B	48	0	0	2	0
5	C	63	0	0	2	0
5	D	37	0	0	0	0
All	All	15106	0	14754	357	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 12.

All (357) 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:B:32:LYS:HA	1:B:32:LYS:NZ	1.80	0.94
1:A:133:ARG:HA	1:A:133:ARG:HH11	1.36	0.90
1:D:440:ARG:HG3	1:D:440:ARG:HH21	1.36	0.89
1:D:220:LEU:HB3	1:D:240:VAL:HG12	1.61	0.83
1:B:303:PHE:CD1	1:B:307:MET:CE	2.63	0.82
1:A:40:LEU:HB3	1:A:41:PRO:HD2	1.63	0.81
1:A:369:ILE:HG13	1:A:370:VAL:HG23	1.63	0.78
1:B:38:LEU:HD12	1:B:39:PRO:HD2	1.66	0.78
1:B:32:LYS:HA	1:B:32:LYS:HZ2	1.48	0.76
1:C:221:ARG:HH11	1:C:221:ARG:HG2	1.52	0.75
1:B:143:GLY:O	1:B:146:LYS:HG2	1.88	0.74
1:B:32:LYS:HA	1:B:32:LYS:HZ3	1.50	0.73
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.70	0.73
1:B:440:ARG:HG3	1:B:440:ARG:HH21	1.51	0.73
1:D:440:ARG:HG3	1:D:440:ARG:NH2	2.04	0.72
1:C:55:PRO:HD3	1:C:481:PHE:CE1	2.24	0.72
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.69	0.72
1:A:183:SER:OG	1:A:307:MET:HB2	1.90	0.71
1:D:309:THR:HB	2:D:800:HEM:HAB	1.73	0.71
1:C:55:PRO:CG	1:C:481:PHE:CE1	2.74	0.70
1:A:276:LEU:HD23	1:A:279:MET:HE1	1.72	0.70
1:C:224:LEU:HD22	1:C:240:VAL:HG11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HD23	1:C:279:MET:HE1	1.73	0.70
1:A:224:LEU:HD21	1:A:236:LEU:HD13	1.72	0.70
1:D:110:LEU:HD22	1:D:248:LEU:HD12	1.74	0.69
1:D:54:THR:HB	1:D:55:PRO:HD3	1.74	0.69
1:A:38:LEU:HD12	1:A:39:PRO:HD2	1.73	0.69
1:D:35:PRO:HD3	1:D:387:PHE:CE1	2.28	0.69
1:C:40:LEU:HG	1:C:41:PRO:HD2	1.76	0.68
1:A:262:TRP:CD1	1:A:273:GLU:HG2	2.27	0.68
1:C:219:PHE:O	1:C:223:VAL:HG23	1.94	0.67
1:C:143:GLY:O	1:C:146:LYS:HB2	1.95	0.67
1:D:414:ARG:HG3	1:D:414:ARG:HH11	1.59	0.66
1:A:59:ASP:HA	1:A:62:ARG:NH1	2.10	0.66
1:D:328:GLN:O	1:D:332:GLN:HG3	1.95	0.66
1:B:451:MET:HG3	1:B:452:GLU:N	2.09	0.65
1:A:55:PRO:HD3	1:A:481:PHE:CE1	2.30	0.65
1:B:303:PHE:CE1	1:B:307:MET:HE1	2.31	0.65
1:B:54:THR:N	1:B:55:PRO:HD2	2.12	0.65
1:D:38:LEU:HB2	1:D:39:PRO:HD3	1.79	0.65
1:B:143:GLY:HA2	1:B:146:LYS:HE3	1.80	0.64
1:C:55:PRO:HD3	1:C:481:PHE:CZ	2.32	0.64
1:D:276:LEU:HD23	1:D:279:MET:HE1	1.79	0.64
1:C:55:PRO:CD	1:C:481:PHE:CE1	2.80	0.64
1:B:104:VAL:HG12	1:B:107:THR:HG23	1.79	0.64
1:B:85:ALA:HB3	5:B:522:HOH:O	1.98	0.64
1:B:309:THR:HB	2:B:800:HEM:HAB	1.80	0.63
1:A:206:LEU:HD23	1:A:307:MET:SD	2.39	0.63
1:A:232:HIS:O	1:A:234:PRO:HD3	1.99	0.63
1:B:474:ARG:HH11	1:B:474:ARG:HG2	1.63	0.63
1:B:227:VAL:HG12	1:B:229:VAL:HG12	1.80	0.62
1:D:149:LEU:O	1:D:153:VAL:HG23	2.00	0.62
1:A:303:PHE:CD1	1:A:307:MET:CE	2.83	0.62
1:A:59:ASP:HA	1:A:62:ARG:HH12	1.65	0.62
1:C:224:LEU:HD23	1:C:231:LEU:HD23	1.81	0.61
1:C:368:ASP:HB3	5:C:530:HOH:O	2.00	0.61
1:D:63:ARG:HH11	1:D:63:ARG:HG2	1.64	0.61
1:B:440:ARG:NH2	1:B:440:ARG:HG3	2.15	0.61
1:A:446:GLU:HB3	1:A:447:PRO:HD3	1.82	0.61
1:D:414:ARG:HH11	1:D:414:ARG:CG	2.14	0.60
1:C:206:LEU:HD23	1:C:307:MET:HE2	1.83	0.60
1:D:303:PHE:HE2	1:D:307:MET:HE2	1.67	0.60
1:C:216:GLU:HA	1:C:221:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:PHE:CD2	1:D:295:LEU:HD13	2.37	0.59
1:B:220:LEU:HD13	1:B:224:LEU:HD13	1.83	0.59
1:B:233:ILE:HB	1:B:236:LEU:HD23	1.85	0.59
1:A:91:LEU:HD11	1:A:397:THR:HG21	1.84	0.59
1:D:359:VAL:O	1:D:363:VAL:HG23	2.01	0.59
1:B:303:PHE:CD1	1:B:307:MET:HE1	2.36	0.59
1:B:226:ALA:O	1:B:228:PRO:HD3	2.02	0.58
1:B:279:MET:HE1	1:B:295:LEU:HD22	1.85	0.58
1:B:105:PRO:O	1:B:108:GLN:HG3	2.02	0.58
1:D:63:ARG:NH1	1:D:63:ARG:HG2	2.17	0.58
1:A:221:ARG:O	1:A:225:ASN:HB2	2.04	0.58
1:D:104:VAL:HA	1:D:225:ASN:HD21	1.69	0.58
1:C:328:GLN:O	1:C:332:GLN:HG3	2.03	0.58
1:C:233:ILE:HD12	1:C:233:ILE:N	2.19	0.58
1:D:335:ILE:HG12	1:D:353:MET:HE1	1.84	0.58
1:D:205:LEU:HD13	1:D:250:GLN:HG3	1.86	0.57
1:D:279:MET:HE1	1:D:295:LEU:HD22	1.85	0.57
1:D:221:ARG:O	1:D:225:ASN:HB2	2.04	0.57
1:A:50:ASP:OD1	1:A:52:GLN:HG2	2.04	0.57
1:A:276:LEU:HA	1:A:279:MET:HE3	1.87	0.57
1:D:213:LEU:HD22	1:D:308:VAL:HG21	1.86	0.57
1:C:309:THR:HB	2:C:800:HEM:HAB	1.87	0.57
1:A:335:ILE:HG12	1:A:353:MET:HE1	1.85	0.57
1:A:276:LEU:HD23	1:A:279:MET:CE	2.34	0.57
1:A:109:ILE:CG2	1:A:245:LYS:HD2	2.35	0.57
1:C:276:LEU:HD23	1:C:279:MET:CE	2.36	0.56
1:D:227:VAL:HG12	1:D:229:VAL:HG12	1.87	0.56
1:D:219:PHE:O	1:D:223:VAL:HG23	2.05	0.56
1:B:303:PHE:HD1	1:B:307:MET:CE	2.18	0.56
1:A:339:ILE:HG23	1:A:343:ARG:NH1	2.20	0.56
1:C:233:ILE:H	1:C:233:ILE:HD12	1.71	0.56
1:B:303:PHE:CD1	1:B:307:MET:HE3	2.41	0.56
1:D:331:VAL:HG13	1:D:356:THR:OG1	2.06	0.56
1:D:95:GLY:HA3	1:D:440:ARG:NH2	2.21	0.55
1:A:75:TRP:CZ3	1:A:226:ALA:HB2	2.41	0.55
1:D:33:LEU:N	1:D:33:LEU:HD12	2.21	0.55
1:B:105:PRO:HD2	1:B:225:ASN:OD1	2.06	0.55
1:D:152:TRP:HH2	1:D:194:ARG:HB3	1.71	0.55
1:D:183:SER:OG	1:D:307:MET:HB2	2.07	0.55
1:C:110:LEU:HD22	1:C:248:LEU:HD12	1.88	0.54
1:B:139:LEU:HB3	1:B:144:LEU:HD12	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:HIS:CE1	1:D:426:HIS:HE2	2.25	0.54
1:B:224:LEU:HD21	1:B:236:LEU:HB3	1.90	0.54
1:B:91:LEU:HD11	1:B:397:THR:HG21	1.89	0.54
1:D:382:ILE:HG13	1:D:389:ILE:HB	1.89	0.54
1:D:208:LEU:HD22	1:D:246:ALA:HB3	1.88	0.54
1:D:35:PRO:HB2	1:D:65:PHE:HB3	1.90	0.54
1:B:334:GLU:OE1	1:B:353:MET:HA	2.07	0.54
1:A:308:VAL:HG22	1:A:308:VAL:O	2.08	0.53
1:A:84:LEU:O	1:A:88:ARG:HB2	2.07	0.53
1:D:279:MET:CE	1:D:295:LEU:HD22	2.38	0.53
1:D:339:ILE:HG12	1:D:349:ASP:OD1	2.07	0.53
1:B:474:ARG:NH1	1:B:474:ARG:HG2	2.21	0.53
1:C:245:LYS:HB3	1:C:245:LYS:NZ	2.23	0.53
1:B:89:GLU:O	1:B:93:THR:HB	2.08	0.53
1:A:303:PHE:CE1	1:A:307:MET:HE2	2.44	0.53
1:A:104:VAL:HG12	1:A:106:ILE:HG22	1.91	0.53
1:D:196:GLU:HA	1:D:196:GLU:OE1	2.08	0.53
1:C:40:LEU:HD23	1:C:43:LEU:HD12	1.90	0.53
1:D:303:PHE:CE2	1:D:307:MET:HE2	2.44	0.53
1:B:174:PRO:HD3	1:B:492:LEU:HD22	1.91	0.53
1:D:215:GLU:O	1:D:221:ARG:HG2	2.09	0.52
1:D:109:ILE:HG22	1:D:245:LYS:HE2	1.91	0.52
1:D:84:LEU:HD11	1:D:88:ARG:HD2	1.91	0.52
1:D:170:ARG:HH11	1:D:170:ARG:HG3	1.75	0.52
1:A:97:ASP:OD2	1:A:380:ARG:HD2	2.09	0.52
1:B:355:TYR:O	1:B:359:VAL:HG23	2.09	0.52
1:D:352:HIS:C	1:D:354:PRO:HD3	2.29	0.52
1:B:303:PHE:CE1	1:B:307:MET:CE	2.92	0.52
1:B:104:VAL:CG1	1:B:107:THR:HG23	2.40	0.52
1:D:91:LEU:HD11	1:D:397:THR:HG21	1.91	0.52
1:C:215:GLU:OE1	1:C:244:GLN:HG3	2.10	0.52
1:D:232:HIS:O	1:D:234:PRO:HD3	2.09	0.52
1:A:151:GLN:O	1:A:155:GLU:HG3	2.10	0.52
1:B:331:VAL:HG13	1:B:356:THR:OG1	2.10	0.51
1:B:104:VAL:HA	1:B:225:ASN:HD21	1.75	0.51
1:C:183:SER:OG	1:C:307:MET:HG3	2.10	0.51
1:D:71:LEU:HD12	1:D:71:LEU:O	2.10	0.51
1:D:38:LEU:N	1:D:38:LEU:HD12	2.25	0.51
1:B:60:GLN:O	1:B:64:ARG:HG3	2.11	0.51
2:A:800:HEM:C1D	3:A:503:PN0:H14	2.45	0.51
1:A:441:ARG:HB2	5:A:530:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HG12	1:C:353:MET:HE1	1.92	0.50
1:B:59:ASP:O	1:B:63:ARG:HD3	2.11	0.50
1:D:71:LEU:CD1	1:D:73:LEU:HG	2.41	0.50
1:A:450:ARG:HD2	5:A:550:HOH:O	2.12	0.50
1:D:215:GLU:OE1	1:D:244:GLN:HG3	2.12	0.50
1:B:319:LEU:HB2	1:B:490:TYR:CE2	2.47	0.50
1:A:369:ILE:HD12	1:A:484:LEU:HD11	1.94	0.50
1:D:428:VAL:O	1:D:430:PRO:HD3	2.12	0.50
1:C:469:PRO:HB2	1:C:472:GLN:NE2	2.27	0.50
1:D:334:GLU:OE1	1:D:353:MET:HA	2.12	0.50
1:B:424:GLN:HB2	1:B:426:HIS:CE1	2.47	0.49
1:B:377:MET:HA	1:B:393:THR:O	2.12	0.49
1:C:104:VAL:HG12	1:C:106:ILE:HG22	1.94	0.49
1:C:152:TRP:HH2	1:C:194:ARG:HB3	1.76	0.49
1:B:445:GLY:HA3	2:B:800:HEM:C3C	2.47	0.49
1:A:104:VAL:HA	1:A:225:ASN:HD21	1.78	0.49
1:A:215:GLU:OE1	1:A:243:PHE:HB2	2.13	0.49
1:D:369:ILE:HG13	1:D:370:VAL:CG2	2.41	0.49
1:C:350:GLN:HG3	1:C:454:PHE:CD2	2.48	0.49
1:D:106:ILE:HD11	1:D:240:VAL:HG21	1.95	0.49
1:C:221:ARG:CG	1:C:221:ARG:HH11	2.22	0.49
1:C:262:TRP:CD1	1:C:273:GLU:HG2	2.48	0.49
2:D:800:HEM:C1D	3:D:503:PN0:H14	2.48	0.49
1:C:326:ASP:OD2	1:C:326:ASP:N	2.46	0.49
1:B:422:ASP:OD1	1:B:424:GLN:HG3	2.13	0.48
1:B:132:ARG:HD2	1:B:444:LEU:HD12	1.94	0.48
1:D:339:ILE:HA	1:D:343:ARG:HH12	1.79	0.48
1:D:421:LEU:HA	1:D:426:HIS:O	2.13	0.48
1:A:88:ARG:CZ	5:A:512:HOH:O	2.61	0.48
1:A:409:TRP:O	1:D:411:LYS:NZ	2.45	0.48
1:B:420:PHE:O	1:B:427:PHE:HA	2.14	0.48
1:D:38:LEU:H	1:D:38:LEU:HD12	1.77	0.48
1:B:129:ARG:NH1	5:B:512:HOH:O	2.47	0.48
1:D:309:THR:HB	2:D:800:HEM:CAB	2.43	0.48
1:C:140:ARG:HA	1:C:144:LEU:HB2	1.96	0.48
1:C:101:ARG:HG2	1:C:441:ARG:NH2	2.29	0.48
1:A:40:LEU:HB3	1:A:41:PRO:CD	2.39	0.47
1:D:106:ILE:HG13	1:D:241:LEU:HD11	1.96	0.47
1:B:336:ASP:OD2	1:B:497:ARG:NH2	2.47	0.47
1:C:440:ARG:HH21	1:C:440:ARG:HG3	1.79	0.47
1:A:224:LEU:HD12	1:A:240:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:HD13	1:C:47:LEU:HD11	1.97	0.47
1:D:451:MET:HG3	1:D:452:GLU:N	2.30	0.47
2:A:800:HEM:ND	3:A:503:PN0:H14	2.29	0.47
1:B:266:GLN:HG3	1:B:267:PRO:HD2	1.96	0.47
1:C:91:LEU:HD11	1:C:397:THR:HG21	1.95	0.47
1:C:205:LEU:HD13	1:C:250:GLN:HG3	1.95	0.47
1:C:476:SER:C	1:C:478:HIS:H	2.17	0.47
1:A:40:LEU:CB	1:A:41:PRO:HD2	2.37	0.47
1:C:152:TRP:O	1:C:152:TRP:CE3	2.67	0.47
1:D:414:ARG:NH1	1:D:414:ARG:CG	2.74	0.47
1:B:54:THR:HG21	1:B:372:LEU:HD11	1.97	0.47
1:C:205:LEU:HD13	1:C:250:GLN:CG	2.45	0.47
1:A:205:LEU:HD13	1:A:250:GLN:CG	2.45	0.47
1:D:308:VAL:HG22	1:D:308:VAL:O	2.15	0.47
1:C:280:GLU:OE2	1:C:283:LYS:HE2	2.15	0.47
1:D:293:GLU:OE1	1:D:293:GLU:N	2.45	0.47
1:C:180:LYS:HE2	1:C:203:LEU:CD2	2.45	0.46
1:D:187:ALA:HB2	1:D:303:PHE:HE1	1.80	0.46
1:D:339:ILE:HD13	1:D:345:PRO:HB3	1.97	0.46
1:B:105:PRO:HD2	1:B:225:ASN:CG	2.35	0.46
1:B:220:LEU:O	1:B:224:LEU:HD13	2.15	0.46
1:C:435:PRO:HG2	1:C:436:PHE:CD1	2.50	0.46
1:A:170:ARG:HA	1:A:171:PRO:HD3	1.84	0.46
1:D:382:ILE:CG1	1:D:389:ILE:HB	2.45	0.46
1:C:443:CYS:HB2	2:C:800:HEM:NA	2.29	0.46
1:B:176:GLY:O	1:B:180:LYS:HG3	2.16	0.46
1:C:473:PRO:O	1:C:474:ARG:C	2.53	0.46
1:C:152:TRP:CH2	1:C:194:ARG:HB3	2.50	0.46
1:C:446:GLU:HB3	1:C:447:PRO:HD3	1.97	0.46
1:D:383:GLU:HA	1:D:387:PHE:O	2.16	0.46
1:D:440:ARG:NH2	1:D:440:ARG:CG	2.72	0.46
1:D:316:TRP:O	1:D:320:LEU:HG	2.16	0.46
1:C:176:GLY:O	1:C:180:LYS:HG3	2.15	0.46
1:A:64:ARG:HD2	1:A:65:PHE:CZ	2.51	0.46
1:A:330:ARG:HB2	1:A:355:TYR:CE2	2.51	0.45
1:C:216:GLU:HA	1:C:221:ARG:HH12	1.81	0.45
1:D:205:LEU:HD13	1:D:250:GLN:CG	2.47	0.45
1:D:436:PHE:CE1	1:D:446:GLU:HG3	2.51	0.45
1:A:437:SER:HB3	2:A:800:HEM:HBA1	1.99	0.45
1:A:35:PRO:HD3	1:A:387:PHE:CE2	2.52	0.45
1:D:174:PRO:HD3	1:D:492:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.81	0.45
1:C:449:ALA:O	1:C:453:LEU:HG	2.16	0.45
1:A:227:VAL:HG12	1:A:229:VAL:HG22	1.99	0.45
1:B:144:LEU:HD21	1:B:448:LEU:HA	1.98	0.45
1:D:110:LEU:HD22	1:D:248:LEU:CD1	2.44	0.45
1:C:151:GLN:O	1:C:155:GLU:HG3	2.17	0.45
1:B:380:ARG:HG2	1:B:381:ASP:N	2.32	0.45
1:D:480:VAL:O	1:D:480:VAL:HG13	2.16	0.45
1:A:416:HIS:HB3	1:A:419:HIS:CE1	2.51	0.45
1:B:183:SER:OG	1:B:307:MET:HG3	2.17	0.45
1:B:220:LEU:HD13	1:B:220:LEU:C	2.37	0.45
1:A:327:VAL:O	1:A:331:VAL:HG23	2.17	0.45
1:A:284:GLY:O	1:A:286:PRO:HD3	2.16	0.45
1:C:323:LEU:HA	1:C:323:LEU:HD12	1.87	0.45
1:C:331:VAL:HG11	1:C:461:LEU:HD12	1.99	0.45
1:B:54:THR:N	1:B:55:PRO:CD	2.80	0.44
1:D:184:ASN:ND2	1:D:194:ARG:HB2	2.32	0.44
1:C:151:GLN:HA	1:C:154:THR:OG1	2.18	0.44
1:A:79:VAL:HG23	1:A:393:THR:HG21	1.99	0.44
1:A:176:GLY:O	1:A:180:LYS:HG3	2.16	0.44
1:C:55:PRO:HG2	1:C:481:PHE:CE1	2.53	0.44
1:A:244:GLN:HG2	3:A:503:PN0:H4	1.98	0.44
1:D:303:PHE:HE2	1:D:307:MET:CE	2.29	0.44
1:A:416:HIS:NE2	1:A:418:GLU:HB2	2.31	0.44
1:C:180:LYS:HG2	1:C:206:LEU:CD1	2.46	0.44
1:C:451:MET:HG3	1:C:452:GLU:N	2.33	0.44
1:A:303:PHE:CE1	1:A:307:MET:CE	3.01	0.44
1:C:149:LEU:O	1:C:153:VAL:HG23	2.18	0.44
1:C:180:LYS:HG2	1:C:206:LEU:HD11	2.00	0.44
1:C:233:ILE:CD1	1:C:233:ILE:H	2.30	0.44
1:D:362:GLU:HG3	1:D:415:PHE:CD1	2.53	0.44
1:D:133:ARG:HD3	1:D:133:ARG:HA	1.88	0.44
1:B:199:ASP:O	1:B:203:LEU:HG	2.17	0.44
1:C:43:LEU:CD1	1:C:47:LEU:HD11	2.48	0.44
1:C:37:PRO:HG2	1:C:45:ASN:ND2	2.32	0.44
1:A:150:GLU:HG2	1:A:347:MET:HG2	2.00	0.43
1:C:54:THR:N	1:C:55:PRO:CD	2.81	0.43
1:B:336:ASP:CG	1:B:497:ARG:HH22	2.21	0.43
1:A:369:ILE:HG13	1:A:370:VAL:CG2	2.43	0.43
1:C:320:LEU:HD12	1:C:363:VAL:HG22	2.01	0.43
1:A:221:ARG:HG3	1:A:222:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HG22	1:A:109:ILE:O	2.17	0.43
1:A:421:LEU:HA	1:A:426:HIS:O	2.19	0.43
1:D:276:LEU:HD23	1:D:279:MET:CE	2.49	0.43
1:D:153:VAL:HG21	1:D:451:MET:SD	2.59	0.43
1:B:220:LEU:HD13	1:B:220:LEU:O	2.18	0.43
1:A:88:ARG:NE	5:A:512:HOH:O	2.51	0.43
1:D:433:PHE:CZ	1:D:435:PRO:HG3	2.53	0.43
1:C:309:THR:HB	2:C:800:HEM:CAB	2.47	0.43
1:A:73:LEU:O	1:A:74:ALA:HB3	2.19	0.43
1:B:219:PHE:O	1:B:223:VAL:HG23	2.19	0.43
1:B:328:GLN:O	1:B:332:GLN:HG3	2.18	0.43
1:A:39:PRO:HA	1:A:45:ASN:ND2	2.34	0.43
1:C:441:ARG:HD2	2:C:800:HEM:O2D	2.18	0.43
1:B:144:LEU:HA	1:B:149:LEU:HD12	2.01	0.43
1:A:323:LEU:CD1	1:A:475:PRO:HD2	2.49	0.43
1:C:141:ASN:O	1:C:146:LYS:HE2	2.19	0.42
1:C:104:VAL:CG1	1:C:106:ILE:HG22	2.49	0.42
1:D:323:LEU:HD12	1:D:323:LEU:HA	1.89	0.42
1:B:70:SER:O	1:B:71:LEU:HD23	2.19	0.42
1:C:40:LEU:HG	1:C:41:PRO:CD	2.47	0.42
1:A:326:ASP:OD2	1:A:326:ASP:N	2.51	0.42
1:A:139:LEU:HB3	1:A:144:LEU:HD12	2.00	0.42
1:C:221:ARG:CG	1:C:221:ARG:NH1	2.83	0.42
1:D:104:VAL:HG12	1:D:225:ASN:HD21	1.85	0.42
1:C:322:ILE:HG22	1:C:466:PHE:C	2.40	0.42
1:A:237:ALA:HA	1:A:240:VAL:CG2	2.50	0.42
1:B:323:LEU:HD13	1:B:475:PRO:HG2	2.01	0.42
1:C:276:LEU:HA	1:C:279:MET:HE3	2.00	0.42
1:C:40:LEU:HD22	1:C:47:LEU:HD12	2.01	0.42
1:D:170:ARG:NH1	1:D:170:ARG:HG3	2.33	0.42
1:D:437:SER:OG	1:D:438:ALA:N	2.49	0.42
1:C:55:PRO:HG2	1:C:481:PHE:CD1	2.54	0.42
1:B:205:LEU:HD13	1:B:250:GLN:HB3	2.01	0.42
1:C:167:HIS:O	1:C:170:ARG:HB2	2.20	0.42
1:B:227:VAL:CG1	1:B:229:VAL:HG12	2.48	0.42
1:A:205:LEU:HD13	1:A:250:GLN:HG3	2.02	0.42
1:C:331:VAL:HG13	1:C:356:THR:OG1	2.20	0.42
1:A:341:GLN:HE22	1:A:497:ARG:C	2.23	0.42
1:D:33:LEU:N	1:D:33:LEU:CD1	2.83	0.42
1:A:331:VAL:HG11	1:A:461:LEU:HD12	2.02	0.42
1:C:170:ARG:HA	1:C:171:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:HB3	1:C:65:PHE:CD1	2.55	0.42
1:D:279:MET:HE2	1:D:295:LEU:HB2	2.00	0.41
1:C:437:SER:HB3	2:C:800:HEM:HBA1	2.02	0.41
1:B:192:GLY:O	1:B:269:ARG:NH2	2.53	0.41
1:D:224:LEU:HD12	1:D:240:VAL:HG11	2.02	0.41
1:D:52:GLN:O	1:D:55:PRO:HD2	2.19	0.41
1:B:339:ILE:HG12	1:B:349:ASP:OD1	2.21	0.41
1:D:355:TYR:O	1:D:359:VAL:HG23	2.20	0.41
2:C:800:HEM:C1D	3:C:503:PN0:H14	2.54	0.41
1:D:204:ARG:O	1:D:208:LEU:HG	2.20	0.41
1:D:428:VAL:HG23	1:D:428:VAL:O	2.20	0.41
1:D:321:MET:CE	1:D:321:MET:HA	2.50	0.41
1:B:117:GLN:HB3	1:B:122:ALA:HA	2.03	0.41
1:B:320:LEU:HD13	1:B:415:PHE:CD1	2.55	0.41
1:A:495:VAL:O	1:A:495:VAL:HG23	2.19	0.41
1:C:58:PHE:HA	1:C:61:LEU:HD12	2.02	0.41
1:C:107:THR:HB	1:C:112:PHE:CD2	2.54	0.41
1:B:334:GLU:OE1	1:B:354:PRO:HD2	2.21	0.41
1:C:224:LEU:N	1:C:224:LEU:HD12	2.35	0.41
1:A:309:THR:HB	2:A:800:HEM:CAB	2.50	0.41
1:C:462:GLN:HG2	1:C:462:GLN:O	2.20	0.41
1:C:428:VAL:O	1:C:428:VAL:HG23	2.19	0.41
1:C:303:PHE:CE1	1:C:307:MET:HE1	2.55	0.41
1:B:428:VAL:O	1:B:428:VAL:HG23	2.20	0.41
1:C:316:TRP:CD1	1:C:487:PRO:HD3	2.56	0.41
1:C:221:ARG:NH1	1:C:221:ARG:HG2	2.28	0.41
1:A:220:LEU:CD2	1:A:224:LEU:HG	2.51	0.41
1:A:55:PRO:CD	1:A:481:PHE:CE1	3.01	0.41
1:D:303:PHE:CE2	1:D:307:MET:CE	3.04	0.41
1:B:331:VAL:O	1:B:335:ILE:HG13	2.20	0.41
1:A:303:PHE:CD1	1:A:307:MET:HE2	2.56	0.41
1:C:424:GLN:O	1:C:424:GLN:HG3	2.21	0.41
1:B:308:VAL:O	1:B:484:LEU:HD21	2.20	0.41
1:C:95:GLY:HA3	5:C:511:HOH:O	2.20	0.41
1:A:416:HIS:HB3	1:A:419:HIS:ND1	2.36	0.40
1:B:369:ILE:HG13	1:B:370:VAL:HG23	2.03	0.40
1:D:444:LEU:C	1:D:444:LEU:HD12	2.41	0.40
1:A:365:ARG:HH22	1:A:404:LYS:HD3	1.86	0.40
1:C:206:LEU:HD23	1:C:307:MET:CE	2.48	0.40
1:D:367:GLY:O	1:D:368:ASP:C	2.59	0.40
1:C:40:LEU:CD2	1:C:47:LEU:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ILE:HG13	1:B:370:VAL:CG2	2.51	0.40
1:D:297:ILE:O	1:D:301:ASP:HB2	2.21	0.40
1:A:34:PRO:HA	1:A:387:PHE:CD2	2.56	0.40
1:A:316:TRP:CD1	1:A:487:PRO:HD3	2.56	0.40
1:D:495:VAL:HG23	1:D:495:VAL:O	2.21	0.40
1:B:84:LEU:HD11	1:B:88:ARG:HD2	2.03	0.40
1:D:368:ASP:OD1	1:D:403:LEU:HD12	2.21	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	465/479 (97%)	438 (94%)	26 (6%)	1 (0%)	52	79
1	B	452/479 (94%)	427 (94%)	24 (5%)	1 (0%)	52	79
1	C	465/479 (97%)	439 (94%)	24 (5%)	2 (0%)	39	67
1	D	452/479 (94%)	432 (96%)	19 (4%)	1 (0%)	52	79
All	All	1834/1916 (96%)	1736 (95%)	93 (5%)	5 (0%)	46	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	GLY
1	D	143	GLY
1	C	143	GLY
1	C	41	PRO
1	A	143	GLY

### 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	398/409 (97%)	379 (95%)	19 (5%)	31	59
1	B	390/409 (95%)	371 (95%)	19 (5%)	31	58
1	C	398/409 (97%)	381 (96%)	17 (4%)	35	64
1	D	390/409 (95%)	376 (96%)	14 (4%)	42	71
All	All	1576/1636 (96%)	1507 (96%)	69 (4%)	35	63

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	75	TRP
1	A	115	ARG
1	A	133	ARG
1	A	147	LYS
1	A	149	LEU
1	A	189	LEU
1	A	220	LEU
1	A	221	ARG
1	A	240	VAL
1	A	259	ARG
1	A	270	ASP
1	A	303	PHE
1	A	323	LEU
1	A	414	ARG
1	A	463	HIS
1	A	480	VAL
1	A	484	LEU
1	A	492	LEU
1	B	32	LYS
1	B	52	GLN
1	B	75	TRP
1	B	149	LEU
1	B	154	THR

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	210	GLN
1	B	216	GLU
1	B	221	ARG
1	B	222	GLU
1	B	303	PHE
1	B	350	GLN
1	B	370	VAL
1	B	434	LEU
1	B	451	MET
1	B	465	SER
1	B	468	VAL
1	B	477	HIS
1	B	492	LEU
1	C	59	ASP
1	C	115	ARG
1	C	133	ARG
1	C	149	LEU
1	C	173	ARG
1	C	189	LEU
1	C	204	ARG
1	C	221	ARG
1	C	303	PHE
1	C	310	THR
1	C	395	LEU
1	C	431	GLU
1	C	451	MET
1	C	463	HIS
1	C	480	VAL
1	C	484	LEU
1	C	492	LEU
1	D	115	ARG
1	D	149	LEU
1	D	151	GLN
1	D	152	TRP
1	D	189	LEU
1	D	221	ARG
1	D	255	LEU
1	D	414	ARG
1	D	451	MET
1	D	465	SER
1	D	470	THR

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Mol	Chain	Res	Type
1	D	477	HIS
1	D	484	LEU
1	D	492	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	GLN
1	C	108	GLN
1	C	472	GLN
1	D	151	GLN
1	D	266	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 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z  > 2$
3	PN0	A	503	2	28,30,30	1.78	7 (25%)	36,44,44	1.76	7 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	800	1,3	30,50,50	3.58	12 (40%)	24,82,82	2.62	10 (41%)
3	PN0	B	503	2	28,30,30	1.72	7 (25%)	36,44,44	1.77	7 (19%)
2	HEM	B	800	1,3	30,50,50	3.79	14 (46%)	24,82,82	2.63	10 (41%)
3	PN0	C	503	2	28,30,30	1.85	8 (28%)	36,44,44	1.71	6 (16%)
2	HEM	C	800	1,3	30,50,50	3.78	13 (43%)	24,82,82	2.75	9 (37%)
3	PN0	D	503	2	28,30,30	1.67	7 (25%)	36,44,44	1.77	8 (22%)
2	HEM	D	800	1,3	30,50,50	3.59	14 (46%)	24,82,82	2.69	10 (41%)

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	PN0	A	503	2	-	0/21/39/39	0/2/3/3
2	HEM	A	800	1,3	-	0/10/54/54	0/0/8/8
3	PN0	B	503	2	-	0/21/39/39	0/2/3/3
2	HEM	B	800	1,3	-	0/10/54/54	0/0/8/8
3	PN0	C	503	2	-	0/21/39/39	0/2/3/3
2	HEM	C	800	1,3	-	0/10/54/54	0/0/8/8
3	PN0	D	503	2	-	0/21/39/39	0/2/3/3
2	HEM	D	800	1,3	-	0/10/54/54	0/0/8/8

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	HEM	C3B-C4B	-11.55	1.41	1.51
2	B	800	HEM	C3B-C4B	-11.15	1.41	1.51
2	A	800	HEM	C3B-C4B	-9.93	1.43	1.51
2	D	800	HEM	C3B-C4B	-9.03	1.43	1.51
2	D	800	HEM	C3D-C4D	-8.95	1.40	1.51
2	C	800	HEM	C3D-C4D	-8.90	1.40	1.51
2	B	800	HEM	C3D-C4D	-8.53	1.40	1.51
2	A	800	HEM	C3D-C4D	-8.09	1.41	1.51
2	B	800	HEM	C2C-C1C	-7.26	1.38	1.52
2	D	800	HEM	C2C-C1C	-7.23	1.38	1.52
2	D	800	HEM	C3C-CAC	-6.81	1.38	1.51
2	B	800	HEM	C3C-CAC	-6.67	1.38	1.51
2	A	800	HEM	C3C-CAC	-6.67	1.38	1.51
2	C	800	HEM	C2C-C1C	-6.47	1.40	1.52
2	B	800	HEM	C2D-C3D	-6.34	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C2C-C1C	-6.27	1.40	1.52
2	C	800	HEM	C3C-CAC	-6.13	1.39	1.51
2	C	800	HEM	C2D-C3D	-6.03	1.36	1.54
2	A	800	HEM	C2D-C3D	-5.99	1.36	1.54
2	D	800	HEM	C2D-C3D	-5.75	1.37	1.54
2	A	800	HEM	C3B-CAB	-5.27	1.41	1.51
3	C	503	PN0	C1-S1	-5.23	1.79	1.84
3	A	503	PN0	C1-S1	-4.96	1.79	1.84
2	C	800	HEM	C3B-CAB	-4.57	1.42	1.51
2	B	800	HEM	C3B-CAB	-4.51	1.42	1.51
2	D	800	HEM	C3B-CAB	-4.21	1.43	1.51
3	B	503	PN0	C1-S1	-3.79	1.81	1.84
2	D	800	HEM	C2D-C1D	-3.78	1.39	1.51
2	B	800	HEM	C2D-C1D	-3.58	1.40	1.51
2	A	800	HEM	C2D-C1D	-3.51	1.40	1.51
2	C	800	HEM	C2D-C1D	-3.42	1.40	1.51
3	B	503	PN0	C5-S2	-3.33	1.71	1.76
3	D	503	PN0	C5-S2	-3.16	1.71	1.76
2	B	800	HEM	C2B-C1B	-2.97	1.42	1.51
2	C	800	HEM	C2B-C1B	-2.91	1.42	1.51
3	A	503	PN0	C5-S2	-2.82	1.72	1.76
2	A	800	HEM	C2B-C1B	-2.64	1.43	1.51
3	D	503	PN0	C1-S1	-2.54	1.82	1.84
2	D	800	HEM	C2B-C1B	-2.50	1.43	1.51
2	B	800	HEM	C1C-NC	-2.46	1.32	1.36
3	A	503	PN0	O1-C11	-2.30	1.34	1.39
3	C	503	PN0	O1-C11	-2.26	1.34	1.39
2	D	800	HEM	C1C-NC	-2.25	1.33	1.36
2	C	800	HEM	C1C-NC	-2.24	1.33	1.36
3	B	503	PN0	O1-C11	-2.22	1.34	1.39
3	C	503	PN0	C5-S2	-2.16	1.73	1.76
3	B	503	PN0	C15-C14	2.04	1.42	1.38
2	D	800	HEM	CBC-CAC	2.05	1.41	1.29
2	D	800	HEM	CAA-C2A	2.05	1.55	1.52
2	B	800	HEM	CBC-CAC	2.05	1.41	1.29
2	B	800	HEM	FE-ND	2.05	2.08	1.97
3	C	503	PN0	C9-C8	2.12	1.42	1.38
3	D	503	PN0	C7-C8	2.13	1.42	1.38
2	C	800	HEM	CBC-CAC	2.14	1.41	1.29
2	A	800	HEM	FE-ND	2.19	2.09	1.97
3	A	503	PN0	C7-C8	2.19	1.43	1.38
3	D	503	PN0	C10-C5	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	PN0	C3-N1	2.25	1.51	1.48
3	B	503	PN0	C7-C8	2.26	1.43	1.38
2	B	800	HEM	FE-NC	2.31	2.04	1.95
3	B	503	PN0	C6-C5	2.50	1.42	1.38
2	A	800	HEM	FE-NC	2.53	2.05	1.95
3	C	503	PN0	C7-C8	2.55	1.43	1.38
2	D	800	HEM	FE-NC	2.56	2.05	1.95
2	C	800	HEM	FE-NC	2.57	2.06	1.95
3	A	503	PN0	C10-C5	2.61	1.43	1.38
3	C	503	PN0	C6-C5	2.63	1.43	1.38
3	A	503	PN0	C6-C5	2.70	1.43	1.38
3	C	503	PN0	C10-C5	2.80	1.43	1.38
3	A	503	PN0	C15-C11	2.85	1.44	1.38
2	C	800	HEM	CBB-CAB	2.88	1.46	1.29
3	B	503	PN0	C15-C11	2.97	1.44	1.38
2	D	800	HEM	CBB-CAB	3.02	1.46	1.29
2	D	800	HEM	CMA-C3A	3.08	1.58	1.51
3	D	503	PN0	C15-C11	3.09	1.44	1.38
2	B	800	HEM	CBB-CAB	3.10	1.47	1.29
3	D	503	PN0	C6-C5	3.10	1.43	1.38
2	A	800	HEM	CBB-CAB	3.10	1.47	1.29
2	A	800	HEM	CMA-C3A	3.17	1.58	1.51
2	B	800	HEM	CMA-C3A	3.26	1.58	1.51
3	C	503	PN0	C15-C11	3.46	1.45	1.38
2	C	800	HEM	CMA-C3A	3.67	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	PN0	C18-C1-C17	-5.39	103.26	109.63
3	A	503	PN0	C18-C1-C17	-4.85	103.90	109.63
3	C	503	PN0	C18-C1-C17	-4.75	104.02	109.63
3	D	503	PN0	C18-C1-C17	-4.74	104.03	109.63
3	C	503	PN0	O2-S2-C5	-4.51	102.14	108.00
3	D	503	PN0	O2-S2-C5	-4.41	102.28	108.00
3	A	503	PN0	O2-S2-C5	-4.26	102.48	108.00
3	B	503	PN0	O2-S2-C5	-4.15	102.62	108.00
3	D	503	PN0	O1-C11-C12	-2.54	110.31	119.42
3	C	503	PN0	O1-C11-C12	-2.51	110.42	119.42
3	B	503	PN0	O1-C11-C12	-2.43	110.70	119.42
3	A	503	PN0	O1-C11-C12	-2.41	110.77	119.42
3	D	503	PN0	C2-N1-S2	-2.15	115.54	119.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	PN0	C6-C5-S2	-2.01	117.57	119.79
3	A	503	PN0	O4-N3-C16	2.15	122.91	119.86
2	D	800	HEM	CBA-CAA-C2A	2.16	116.40	112.53
2	B	800	HEM	CBA-CAA-C2A	2.18	116.44	112.53
3	D	503	PN0	O4-N3-C16	2.26	123.06	119.86
3	B	503	PN0	O4-N3-C16	2.32	123.15	119.86
2	D	800	HEM	C1D-CHD-C4C	2.36	129.76	125.82
2	B	800	HEM	CMD-C2D-C3D	2.45	125.17	114.35
2	A	800	HEM	CMD-C2D-C3D	2.45	125.18	114.35
2	C	800	HEM	CMD-C2D-C3D	2.47	125.28	114.35
2	B	800	HEM	C1D-CHD-C4C	2.50	130.00	125.82
2	C	800	HEM	C1D-CHD-C4C	2.51	130.01	125.82
2	A	800	HEM	CBA-CAA-C2A	2.56	117.12	112.53
3	A	503	PN0	O1-C11-C15	2.59	128.71	119.42
2	A	800	HEM	C1D-CHD-C4C	2.60	130.17	125.82
2	D	800	HEM	CMD-C2D-C3D	2.61	125.91	114.35
3	B	503	PN0	O1-C11-C15	2.63	128.85	119.42
3	C	503	PN0	O1-C11-C15	2.70	129.09	119.42
3	D	503	PN0	O1-C11-C15	2.73	129.19	119.42
2	D	800	HEM	C4B-CHC-C1C	2.78	130.46	125.82
3	C	503	PN0	C5-S2-N1	3.06	112.38	107.38
3	B	503	PN0	C5-S2-N1	3.21	112.63	107.38
2	B	800	HEM	C4B-CHC-C1C	3.34	131.41	125.82
2	C	800	HEM	C4B-CHC-C1C	3.38	131.47	125.82
2	D	800	HEM	C3C-CAC-CBC	3.51	129.84	124.46
2	A	800	HEM	C4B-CHC-C1C	3.64	131.91	125.82
3	A	503	PN0	C11-O1-C8	3.80	128.27	118.81
2	D	800	HEM	CAD-C3D-C4D	3.93	126.32	112.47
3	B	503	PN0	C11-O1-C8	3.96	128.68	118.81
2	A	800	HEM	CMC-C2C-C3C	3.97	126.43	116.53
2	B	800	HEM	C3C-CAC-CBC	3.97	130.54	124.46
2	C	800	HEM	CMC-C2C-C3C	3.98	126.47	116.53
3	C	503	PN0	C11-O1-C8	4.03	128.84	118.81
2	C	800	HEM	CAD-C3D-C4D	4.11	126.97	112.47
2	D	800	HEM	CMC-C2C-C3C	4.14	126.87	116.53
2	B	800	HEM	CAD-C3D-C4D	4.15	127.11	112.47
3	A	503	PN0	C5-S2-N1	4.19	114.23	107.38
2	B	800	HEM	CMC-C2C-C3C	4.19	127.00	116.53
2	A	800	HEM	C3C-CAC-CBC	4.21	130.91	124.46
2	A	800	HEM	C3B-CAB-CBB	4.21	130.92	124.46
2	A	800	HEM	CAD-C3D-C4D	4.36	127.86	112.47
3	D	503	PN0	C11-O1-C8	4.51	130.04	118.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C3B-CAB-CBB	4.53	131.41	124.46
2	A	800	HEM	CAD-C3D-C2D	5.00	127.59	113.22
2	C	800	HEM	C3C-CAC-CBC	5.03	132.18	124.46
2	A	800	HEM	CMB-C2B-C3B	5.18	129.46	116.53
2	C	800	HEM	C3B-CAB-CBB	5.20	132.43	124.46
2	B	800	HEM	CAD-C3D-C2D	5.24	128.28	113.22
2	C	800	HEM	CAD-C3D-C2D	5.28	128.41	113.22
2	D	800	HEM	CMB-C2B-C3B	5.33	129.82	116.53
2	D	800	HEM	CAD-C3D-C2D	5.46	128.92	113.22
2	B	800	HEM	CMB-C2B-C3B	5.52	130.30	116.53
2	C	800	HEM	CMB-C2B-C3B	5.54	130.36	116.53
2	D	800	HEM	C3B-CAB-CBB	5.64	133.10	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	PN0	3	0
2	A	800	HEM	4	0
2	B	800	HEM	2	0
3	C	503	PN0	1	0
2	C	800	HEM	6	0
3	D	503	PN0	1	0
2	D	800	HEM	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<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	467/479 (97%)	0.15	26 (5%)	28	25	20, 36, 79, 91	1 (0%)
1	B	456/479 (95%)	0.36	39 (8%)	13	10	25, 42, 87, 100	0
1	C	467/479 (97%)	0.18	29 (6%)	24	22	20, 37, 87, 107	1 (0%)
1	D	456/479 (95%)	0.26	34 (7%)	17	14	25, 44, 83, 96	0
All	All	1846/1916 (96%)	0.24	128 (6%)	20	18	20, 40, 84, 107	2 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	GLY	8.1
1	A	38	LEU	7.6
1	C	38	LEU	7.4
1	B	145	GLY	7.1
1	B	230	LEU	7.1
1	A	145	GLY	6.7
1	C	145	GLY	6.6
1	B	75	TRP	6.5
1	C	40	LEU	6.2
1	C	41	PRO	6.1
1	C	47	LEU	6.0
1	A	342	VAL	5.7
1	B	38	LEU	5.5
1	C	46	LEU	5.3
1	A	47	LEU	5.1
1	D	75	TRP	5.1
1	B	63	ARG	4.9
1	A	217	SER	4.9
1	C	48	HIS	4.9
1	A	40	LEU	4.8
1	C	43	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	75	TRP	4.4
1	B	232	HIS	4.4
1	B	60	GLN	4.3
1	C	39	PRO	4.3
1	D	238	GLY	4.2
1	A	43	LEU	4.2
1	B	342	VAL	4.2
1	B	231	LEU	4.1
1	B	229	VAL	4.0
1	A	48	HIS	3.9
1	D	39	PRO	3.9
1	B	236	LEU	3.8
1	B	234	PRO	3.8
1	B	219	PHE	3.8
1	A	75	TRP	3.8
1	A	41	PRO	3.7
1	D	144	LEU	3.7
1	D	76	THR	3.7
1	A	39	PRO	3.7
1	C	44	GLY	3.7
1	B	144	LEU	3.6
1	D	240	VAL	3.6
1	B	65	PHE	3.5
1	C	45	ASN	3.5
1	D	237	ALA	3.5
1	C	340	GLY	3.5
1	B	217	SER	3.5
1	D	38	LEU	3.5
1	A	219	PHE	3.4
1	D	229	VAL	3.4
1	B	39	PRO	3.4
1	D	151	GLN	3.4
1	C	342	VAL	3.4
1	C	219	PHE	3.4
1	B	147	LYS	3.3
1	B	37	PRO	3.3
1	A	144	LEU	3.2
1	B	227	VAL	3.2
1	C	37	PRO	3.2
1	D	342	VAL	3.2
1	C	234	PRO	3.2
1	D	50	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	3.1
1	C	151	GLN	3.1
1	B	341	GLN	3.0
1	B	233	ILE	3.0
1	C	42	GLY	3.0
1	D	146	LYS	3.0
1	C	147	LYS	3.0
1	D	147	LYS	3.0
1	B	216	GLU	3.0
1	B	50	ASP	2.9
1	D	65	PHE	2.9
1	C	51	PHE	2.9
1	B	64	ARG	2.9
1	D	236	LEU	2.9
1	B	72	GLN	2.8
1	C	233	ILE	2.8
1	B	168	SER	2.8
1	B	235	ALA	2.8
1	D	235	ALA	2.8
1	C	144	LEU	2.8
1	A	477	HIS	2.8
1	A	146	LYS	2.8
1	B	240	VAL	2.7
1	B	463	HIS	2.7
1	D	73	LEU	2.7
1	A	216	GLU	2.7
1	D	228	PRO	2.7
1	D	64	ARG	2.7
1	A	231	LEU	2.6
1	B	56	TYR	2.6
1	B	33	LEU	2.6
1	B	61	LEU	2.6
1	D	33	LEU	2.6
1	C	341	GLN	2.6
1	A	147	LYS	2.6
1	B	151	GLN	2.5
1	B	214	LYS	2.5
1	D	37	PRO	2.5
1	A	341	GLN	2.4
1	C	50	ASP	2.4
1	C	229	VAL	2.4
1	D	74	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	234	PRO	2.4
1	D	232	HIS	2.4
1	A	234	PRO	2.3
1	A	236	LEU	2.3
1	D	51	PHE	2.3
1	C	477	HIS	2.3
1	D	168	SER	2.3
1	D	233	ILE	2.3
1	A	214	LYS	2.3
1	D	63	ARG	2.3
1	C	231	LEU	2.2
1	A	229	VAL	2.2
1	B	464	PHE	2.2
1	B	218	GLY	2.2
1	B	215	GLU	2.2
1	D	166	ASN	2.2
1	C	49	VAL	2.1
1	A	233	ILE	2.1
1	A	237	ALA	2.1
1	D	72	GLN	2.0
1	A	343	ARG	2.0
1	B	77	PRO	2.0
1	D	219	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<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( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	800	43/43	0.98	0.20	0.63	16,21,25,26	0
3	PN0	C	503	28/28	0.95	0.21	0.29	36,45,51,55	0
2	HEM	B	800	43/43	0.98	0.19	0.13	23,27,30,34	0
2	HEM	C	800	43/43	0.98	0.18	0.08	14,19,23,25	0
3	PN0	A	503	28/28	0.94	0.21	0.05	35,48,53,55	0
3	PN0	B	503	28/28	0.95	0.20	0.02	40,48,51,54	0
3	PN0	D	503	28/28	0.96	0.19	-0.10	40,50,52,54	0
2	HEM	D	800	43/43	0.98	0.17	-0.30	23,25,28,32	0
4	ZN	A	601	1/1	0.99	0.10	-1.15	34,34,34,34	0
4	ZN	A	600	1/1	1.00	0.08	-2.19	29,29,29,29	0
4	ZN	C	600	1/1	1.00	0.07	-2.53	35,35,35,35	0
4	ZN	B	600	1/1	1.00	0.07	-2.84	29,29,29,29	0
4	ZN	D	600	1/1	1.00	0.06	-3.83	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.