Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:18 PM GMT

PDB ID	:	3TIK
Title	:	Sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei in complex with the tipifarnib derivative 6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-4-(2,6-difluorophenyl)-1-methylquinolin-2(1H)-one
Authors	:	Hargrove, T.Y.; Wawrzak, Z.; Kraus, J.M.; Gelb, M.H.; Buckner, F.S.; Waterman, M.R.; Lepesheva, G.I.
Deposited on	:	2011-08-20
Resolution	:	2.05 Å(reported)

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

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

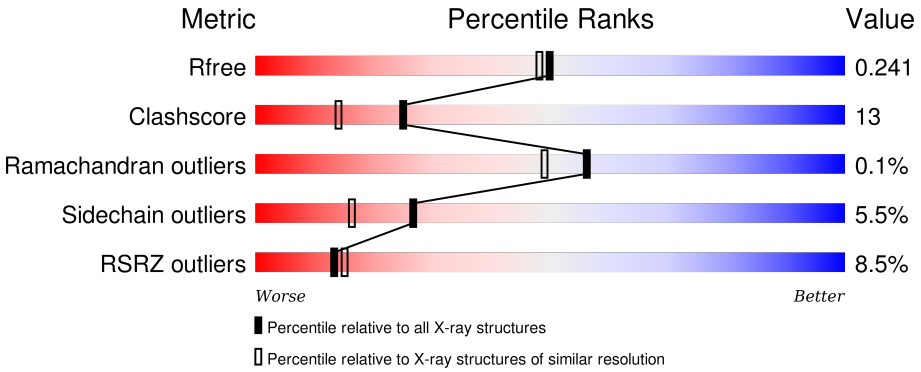
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	454	12% 77% 21%
1	B	454	8% 78% 18%
1	C	454	9% 81% 17%
1	D	454	5% 81% 15%

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	JKF	A	490	-	-	X	-
3	JKF	B	490	-	-	X	-
3	JKF	C	490	-	-	X	-
3	JKF	D	490	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14911 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.

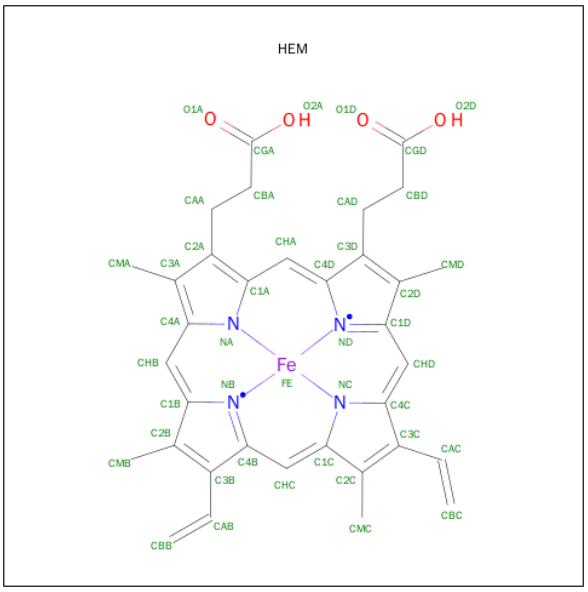
- Molecule 1 is a protein called sterol 14-alpha demethylase (CYP51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	B	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	C	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	D	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			

There are 16 discrepancies between the modelled and reference sequences:

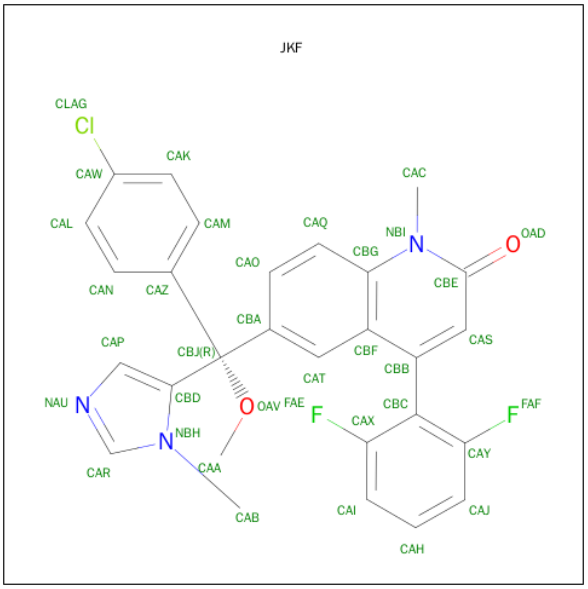
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LYS	-	EXPRESSION TAG	UNP Q385E8
A	29	GLY	-	EXPRESSION TAG	UNP Q385E8
A	30	LYS	-	EXPRESSION TAG	UNP Q385E8
A	31	LEU	-	EXPRESSION TAG	UNP Q385E8
B	28	LYS	-	EXPRESSION TAG	UNP Q385E8
B	29	GLY	-	EXPRESSION TAG	UNP Q385E8
B	30	LYS	-	EXPRESSION TAG	UNP Q385E8
B	31	LEU	-	EXPRESSION TAG	UNP Q385E8
C	28	LYS	-	EXPRESSION TAG	UNP Q385E8
C	29	GLY	-	EXPRESSION TAG	UNP Q385E8
C	30	LYS	-	EXPRESSION TAG	UNP Q385E8
C	31	LEU	-	EXPRESSION TAG	UNP Q385E8
D	28	LYS	-	EXPRESSION TAG	UNP Q385E8
D	29	GLY	-	EXPRESSION TAG	UNP Q385E8
D	30	LYS	-	EXPRESSION TAG	UNP Q385E8
D	31	LEU	-	EXPRESSION TAG	UNP Q385E8

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



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

- Molecule 3 is 6-[(R)-(4-CHLOROPHENYL)(METHOXY)(1-METHYL-1H-IMIDAZOL-5-YL)METHYL]-4-(2,6-DIFLUOROPHENYL)-1-METHYLQUINOLIN-2(1H)-ONE (three-letter code: JKF) (formula: $C_{28}H_{22}ClF_2N_3O_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		
3	B	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		
3	C	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		
3	D	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		

- Molecule 4 is water.

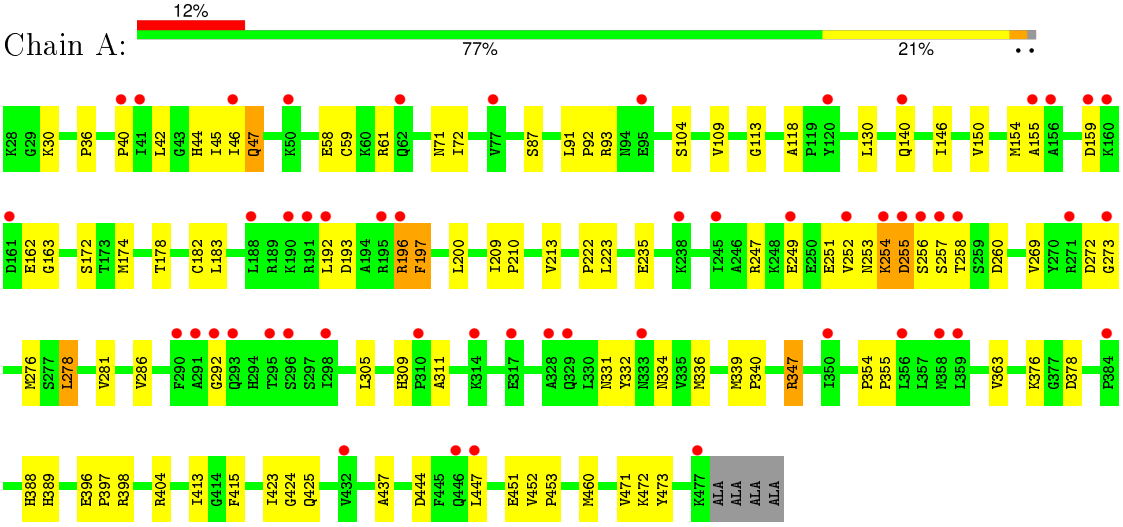
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	76	Total	O	0	0
			76	76		
4	C	59	Total	O	0	0
			59	59		
4	D	113	Total	O	0	0
			113	113		

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.

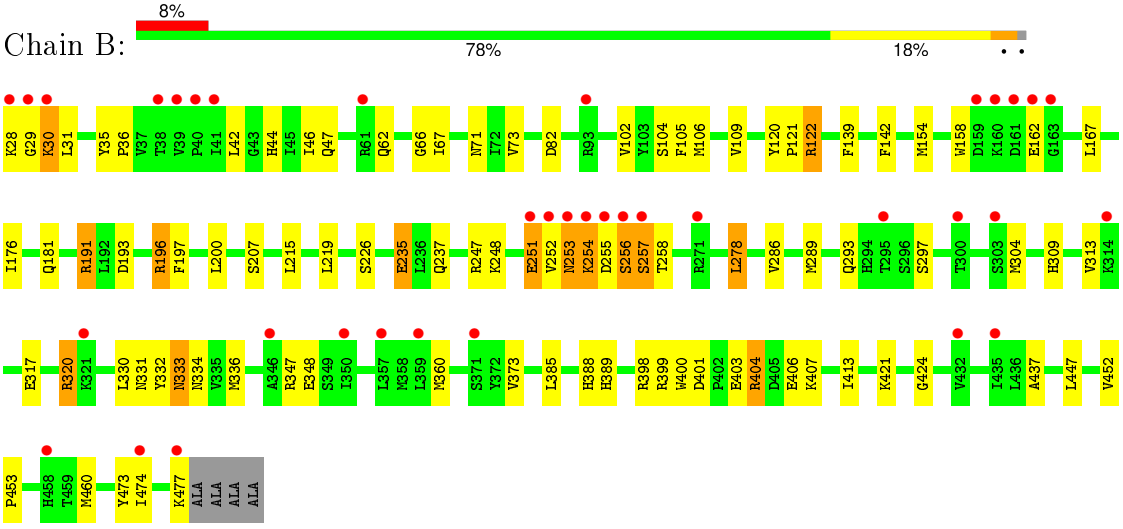
- Molecule 1: sterol 14-alpha demethylase (CYP51)

Chain A:



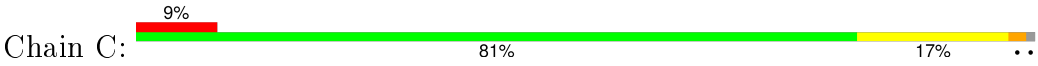
- Molecule 1: sterol 14-alpha demethylase (CYP51)

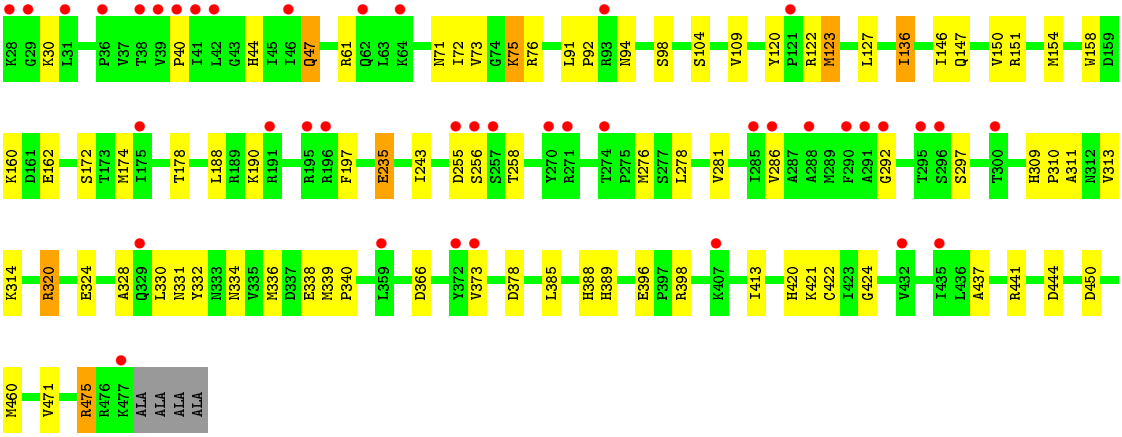
Chain B:



- Molecule 1: sterol 14-alpha demethylase (CYP51)

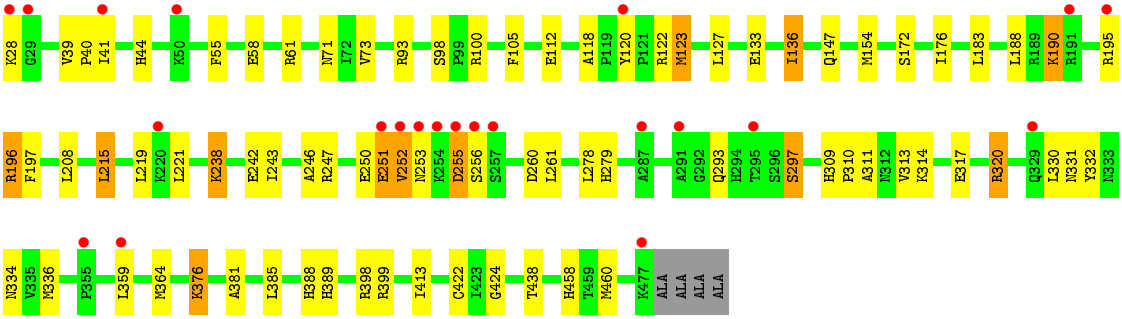
Chain C:





- Molecule 1: sterol 14-alpha demethylase (CYP51)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.72Å 79.72Å 117.52Å 74.47° 81.58° 68.05°	Depositor
Resolution (Å)	30.00 – 2.05 29.69 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.05) 91.5 (29.69-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.243 0.185 , 0.241	Depositor DCC
R_{free} test set	6066 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 121303 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14911	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, JKF

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	0.43	1/3657 (0.0%)	0.52	0/4944
1	B	0.45	0/3657	0.56	0/4944
1	C	0.43	0/3657	0.51	0/4944
1	D	0.52	0/3657	0.59	0/4944
All	All	0.46	1/14628 (0.0%)	0.55	0/19776

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	CYS	CB-SG	-5.01	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	GLU	Peptide

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	3575	0	3620	78	0
1	B	3575	0	3620	102	0
1	C	3575	0	3620	79	0
1	D	3575	0	3620	77	0
2	A	43	0	30	6	0
2	B	43	0	30	5	0
2	C	43	0	30	9	0
2	D	43	0	30	5	0
3	A	36	0	22	9	0
3	B	36	0	22	9	0
3	C	36	0	22	17	0
3	D	36	0	22	11	0
4	A	47	0	0	1	0
4	B	76	0	0	0	0
4	C	59	0	0	1	0
4	D	113	0	0	0	0
All	All	14911	0	14688	373	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 13.

All (373) 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:191:ARG:CG	1:B:191:ARG:HH11	1.61	1.14
1:A:196:ARG:CB	1:A:196:ARG:HH11	1.59	1.12
1:D:320:ARG:HH21	1:D:320:ARG:HG2	1.08	1.10
1:B:28:LYS:HD2	1:B:30:LYS:HB3	1.34	1.08
1:A:196:ARG:NH1	1:A:196:ARG:HB3	1.67	1.08
1:B:320:ARG:HG2	1:B:320:ARG:HH21	1.08	1.07
1:A:196:ARG:HB3	1:A:196:ARG:HH11	1.04	1.07
1:D:250:GLU:HB2	1:D:256:SER:HB2	1.12	1.06
1:D:250:GLU:CB	1:D:256:SER:HB2	1.86	1.05
1:B:191:ARG:HG2	1:B:191:ARG:NH1	1.50	1.04
1:B:254:LYS:HE2	1:B:254:LYS:HA	1.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HG2	1:C:320:ARG:HH21	1.24	0.98
1:C:75:LYS:HB2	1:C:75:LYS:NZ	1.80	0.96
1:C:75:LYS:HZ2	1:C:75:LYS:HB2	1.33	0.93
1:B:73:VAL:O	1:B:73:VAL:HG12	1.68	0.93
1:D:251:GLU:HA	1:D:256:SER:HB3	1.51	0.93
1:D:250:GLU:HB2	1:D:256:SER:CB	1.98	0.92
1:C:44:HIS:HD2	1:C:71:ASN:H	1.07	0.92
1:D:320:ARG:HH21	1:D:320:ARG:CG	1.84	0.91
1:A:47:GLN:HE21	1:A:47:GLN:H	1.15	0.90
1:D:44:HIS:HD2	1:D:71:ASN:H	1.13	0.90
1:B:320:ARG:HH21	1:B:320:ARG:CG	1.85	0.90
1:C:460:MET:HE2	3:C:490:JKF:CAJ	2.02	0.89
1:C:389:HIS:HE1	1:C:398:ARG:HH11	1.20	0.89
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.36	0.89
1:D:388:HIS:HE1	1:D:413:ILE:H	1.19	0.89
1:D:196:ARG:HH11	1:D:196:ARG:HB3	1.37	0.89
1:C:475:ARG:CG	1:C:475:ARG:HH11	1.86	0.88
1:B:388:HIS:HE1	1:B:413:ILE:H	1.17	0.87
1:A:196:ARG:CG	1:A:196:ARG:HH11	1.88	0.87
1:C:388:HIS:HE1	1:C:413:ILE:H	1.20	0.86
1:C:276:MET:HE2	1:C:281:VAL:HG22	1.57	0.86
1:B:193:ASP:OD1	1:B:196:ARG:HG3	1.75	0.85
1:B:251:GLU:HA	1:B:256:SER:HB2	1.59	0.85
1:B:320:ARG:HG2	1:B:320:ARG:NH2	1.90	0.84
1:B:122:ARG:CG	1:B:122:ARG:HH11	1.89	0.84
1:B:109:VAL:HG13	1:B:286:VAL:HG11	1.59	0.83
1:A:388:HIS:HE1	1:A:413:ILE:H	1.23	0.83
1:C:389:HIS:CE1	1:C:398:ARG:HH11	1.98	0.82
1:D:309:HIS:HD2	1:D:311:ALA:H	1.25	0.81
1:B:191:ARG:HG2	1:B:191:ARG:HH11	0.69	0.81
1:D:320:ARG:NH2	1:D:320:ARG:HG2	1.90	0.81
1:B:122:ARG:NH1	1:B:122:ARG:HG2	1.94	0.81
1:B:253:ASN:HB2	1:B:255:ASP:H	1.45	0.81
1:C:460:MET:CE	3:C:490:JKF:CAJ	2.59	0.81
1:C:320:ARG:CG	1:C:320:ARG:HH21	1.94	0.80
1:C:47:GLN:HE21	1:C:47:GLN:H	1.30	0.80
1:C:460:MET:HE2	3:C:490:JKF:CAY	2.12	0.80
1:A:309:HIS:CD2	1:A:311:ALA:H	2.00	0.80
1:B:28:LYS:HB3	1:B:30:LYS:H	1.47	0.79
1:B:102:VAL:HG11	1:B:360:MET:HB2	1.65	0.79
1:A:260:ASP:HA	4:A:517:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD21	1:B:235:GLU:HG2	1.64	0.78
1:B:247:ARG:O	1:B:251:GLU:HB2	1.82	0.78
1:D:389:HIS:HE1	1:D:398:ARG:HH11	1.27	0.78
1:D:247:ARG:O	1:D:251:GLU:HB2	1.83	0.78
1:A:44:HIS:HD2	1:A:71:ASN:H	1.31	0.77
1:C:332:TYR:CE1	1:C:336:MET:HG3	2.20	0.77
1:C:320:ARG:O	1:C:324:GLU:HG3	1.85	0.77
1:C:460:MET:CE	3:C:490:JKF:CAY	2.64	0.76
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.49	0.76
1:B:28:LYS:HD2	1:B:30:LYS:CB	2.14	0.76
1:B:44:HIS:HD2	1:B:71:ASN:H	1.32	0.75
1:C:475:ARG:HG2	1:C:475:ARG:HH11	1.52	0.74
1:B:196:ARG:NH1	1:B:196:ARG:HB3	2.03	0.74
1:B:42:LEU:HD13	1:B:46:ILE:HD11	1.70	0.74
1:D:331:ASN:H	1:D:334:ASN:HD22	1.36	0.74
3:B:490:JKF:HAAB	3:B:490:JKF:CAM	2.18	0.73
3:B:490:JKF:HAN	3:B:490:JKF:CAO	2.17	0.73
1:C:44:HIS:CD2	1:C:71:ASN:H	1.99	0.73
1:D:399:ARG:HG3	1:D:399:ARG:HH11	1.52	0.73
1:D:44:HIS:CD2	1:D:71:ASN:H	2.02	0.72
2:B:482:HEM:HBC2	2:B:482:HEM:HMC2	1.71	0.72
1:B:401:ASP:O	1:B:404:ARG:HG2	1.88	0.71
1:A:309:HIS:HD2	1:A:311:ALA:H	1.35	0.71
1:D:251:GLU:CA	1:D:256:SER:HB3	2.21	0.70
1:B:251:GLU:O	1:B:251:GLU:CD	2.30	0.70
1:A:47:GLN:NE2	1:A:47:GLN:H	1.89	0.70
1:A:251:GLU:O	1:A:254:LYS:HD3	1.92	0.70
1:B:333:ASN:HD22	1:B:333:ASN:H	1.41	0.69
1:D:196:ARG:CB	1:D:196:ARG:HH11	2.05	0.69
1:A:30:LYS:HG2	1:B:181:GLN:HE22	1.57	0.69
1:A:155:ALA:O	1:A:159:ASP:HB3	1.94	0.68
1:B:197:PHE:CZ	1:B:289:MET:HG3	2.28	0.68
1:B:389:HIS:HE1	1:B:398:ARG:HH11	1.42	0.68
1:A:200:LEU:HD21	1:A:235:GLU:OE1	1.93	0.68
1:D:389:HIS:CE1	1:D:398:ARG:HH11	2.10	0.68
1:C:75:LYS:CB	1:C:75:LYS:NZ	2.54	0.68
1:D:188:LEU:HD13	1:D:243:ILE:HG13	1.76	0.68
1:A:253:ASN:C	1:A:254:LYS:HG2	2.12	0.67
1:D:320:ARG:NH2	1:D:320:ARG:CG	2.49	0.67
1:B:196:ARG:HH11	1:B:196:ARG:CB	2.07	0.67
3:A:490:JKF:CAO	3:A:490:JKF:HAN	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:HIS:CD2	1:C:311:ALA:H	2.13	0.67
1:B:73:VAL:O	1:B:73:VAL:CG1	2.41	0.66
1:A:388:HIS:CE1	1:A:413:ILE:H	2.10	0.66
1:A:210:PRO:O	1:A:213:VAL:HG23	1.96	0.66
1:D:388:HIS:CE1	1:D:413:ILE:H	2.10	0.66
1:D:309:HIS:CD2	1:D:311:ALA:H	2.11	0.66
1:B:196:ARG:HH11	1:B:196:ARG:HB3	1.60	0.66
1:A:58:GLU:OE1	1:A:61:ARG:NH1	2.29	0.66
1:C:320:ARG:HG2	1:C:320:ARG:NH2	2.04	0.65
1:B:388:HIS:CE1	1:B:413:ILE:H	2.06	0.65
2:D:482:HEM:HBC2	2:D:482:HEM:HMC2	1.79	0.65
1:C:424:GLY:HA3	2:C:482:HEM:C3C	2.32	0.65
1:B:248:LYS:HA	1:B:251:GLU:HB2	1.78	0.65
1:C:331:ASN:H	1:C:334:ASN:HD22	1.46	0.64
1:D:196:ARG:NH1	1:D:196:ARG:HB3	2.11	0.64
1:B:331:ASN:H	1:B:334:ASN:HD22	1.46	0.64
1:D:247:ARG:O	1:D:251:GLU:N	2.31	0.64
1:C:276:MET:CE	1:C:281:VAL:HG22	2.26	0.64
1:A:93:ARG:HG2	1:A:93:ARG:NH1	2.10	0.64
1:B:385:LEU:O	1:B:389:HIS:HD2	1.80	0.64
1:B:139:PHE:HA	1:B:142:PHE:HB2	1.80	0.64
1:D:399:ARG:HG3	1:D:399:ARG:NH1	2.12	0.63
1:B:36:PRO:O	1:B:44:HIS:HE1	1.81	0.63
1:C:320:ARG:CG	1:C:320:ARG:NH2	2.57	0.62
1:A:309:HIS:HD2	1:A:311:ALA:N	1.97	0.62
1:D:253:ASN:HB3	1:D:255:ASP:OD1	1.99	0.62
1:B:460:MET:HE2	3:B:490:JKF:CAY	2.29	0.62
3:C:490:JKF:HAB	3:C:490:JKF:CAT	2.30	0.62
2:B:482:HEM:HMB2	2:B:482:HEM:HBB2	1.81	0.62
2:C:482:HEM:CMB	2:C:482:HEM:HBB2	2.30	0.62
1:B:197:PHE:CE2	1:B:289:MET:HG3	2.35	0.61
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.56	0.61
2:C:482:HEM:HMB2	2:C:482:HEM:HBB2	1.81	0.61
1:C:388:HIS:CE1	1:C:413:ILE:H	2.10	0.61
1:C:75:LYS:HZ3	1:C:75:LYS:HB2	1.66	0.60
1:C:460:MET:CE	3:C:490:JKF:HAJ	2.32	0.60
1:D:58:GLU:HA	1:D:61:ARG:NH1	2.16	0.60
1:B:251:GLU:C	1:B:251:GLU:CD	2.61	0.60
1:B:254:LYS:CE	1:B:254:LYS:HA	2.11	0.60
3:C:490:JKF:HAAB	3:C:490:JKF:CAM	2.30	0.60
1:D:332:TYR:CE1	1:D:336:MET:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:CB	1:C:75:LYS:HZ2	2.10	0.59
1:C:460:MET:HE1	3:C:490:JKF:HAJ	1.83	0.59
1:B:389:HIS:CE1	1:B:398:ARG:HH11	2.20	0.59
1:A:113:GLY:O	1:A:118:ALA:HB2	2.03	0.59
1:D:252:VAL:HG13	1:D:252:VAL:O	2.01	0.59
3:A:490:JKF:HAT	3:A:490:JKF:CAA	2.31	0.59
1:B:253:ASN:N	1:B:253:ASN:OD1	2.28	0.59
1:D:460:MET:HE2	3:D:490:JKF:CAY	2.33	0.59
1:C:136:ILE:C	1:C:136:ILE:HD12	2.23	0.59
2:D:482:HEM:HBC2	2:D:482:HEM:CMC	2.33	0.59
1:B:320:ARG:CG	1:B:320:ARG:NH2	2.50	0.59
1:D:98:SER:OG	1:D:120:TYR:OH	2.21	0.58
1:C:475:ARG:HG3	1:C:475:ARG:HH11	1.66	0.58
1:C:460:MET:CE	3:C:490:JKF:FAF	2.42	0.58
1:A:255:ASP:OD2	1:A:255:ASP:N	2.36	0.58
3:A:490:JKF:CAO	3:A:490:JKF:CAN	2.81	0.58
1:B:406:GLU:O	1:C:136:ILE:HD11	2.04	0.58
1:B:105:PHE:HA	1:B:219:LEU:HD21	1.85	0.58
1:B:30:LYS:HG2	1:B:31:LEU:H	1.68	0.57
1:C:190:LYS:NZ	1:C:190:LYS:HB3	2.18	0.57
1:C:76:ARG:NH2	1:C:378:ASP:OD2	2.37	0.57
1:A:45:ILE:HG23	1:A:46:ILE:HD12	1.85	0.57
3:B:490:JKF:CAN	3:B:490:JKF:CAO	2.81	0.57
1:C:309:HIS:HD2	1:C:311:ALA:H	1.51	0.57
3:A:490:JKF:HAAA	3:A:490:JKF:HAT	1.85	0.57
1:A:42:LEU:HD13	1:A:46:ILE:CD1	2.34	0.57
1:C:328:ALA:HA	1:C:441:ARG:HH21	1.70	0.57
1:D:246:ALA:O	1:D:250:GLU:HG3	2.03	0.57
1:A:309:HIS:CD2	1:A:311:ALA:HB3	2.40	0.57
1:B:333:ASN:ND2	1:B:333:ASN:H	2.02	0.57
1:D:331:ASN:H	1:D:334:ASN:ND2	2.03	0.57
1:D:251:GLU:N	1:D:256:SER:HB3	2.21	0.56
1:D:460:MET:CE	3:D:490:JKF:CAY	2.84	0.56
1:C:310:PRO:O	1:C:313:VAL:HG13	2.05	0.56
3:D:490:JKF:CAO	3:D:490:JKF:HAN	2.35	0.56
1:A:305:LEU:HD13	1:A:453:PRO:HG2	1.87	0.56
3:C:490:JKF:CAO	3:C:490:JKF:HAN	2.35	0.56
2:B:482:HEM:HBB2	2:B:482:HEM:CMB	2.35	0.56
2:A:482:HEM:CMB	2:A:482:HEM:HBB2	2.36	0.56
1:A:252:VAL:O	1:A:252:VAL:HG13	2.06	0.56
2:A:482:HEM:HMB2	2:A:482:HEM:HBB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LYS:CG	1:B:31:LEU:H	2.19	0.56
1:B:109:VAL:CG1	1:B:286:VAL:HG11	2.33	0.56
1:C:437:ALA:O	1:C:441:ARG:HB2	2.07	0.55
1:A:109:VAL:CG1	1:A:286:VAL:HG11	2.37	0.55
2:C:482:HEM:HBC2	2:C:482:HEM:CMC	2.37	0.55
1:C:94:ASN:OD1	1:C:420:HIS:NE2	2.39	0.55
1:C:47:GLN:HE21	1:C:47:GLN:N	2.01	0.54
1:B:331:ASN:H	1:B:334:ASN:ND2	2.05	0.54
1:C:314:LYS:HB2	4:C:522:HOH:O	2.06	0.54
1:D:123:MET:HE3	1:D:127:LEU:HD12	1.89	0.54
1:D:253:ASN:C	1:D:255:ASP:H	2.10	0.54
1:D:253:ASN:O	1:D:255:ASP:OD2	2.25	0.54
1:A:278:LEU:HD22	1:A:278:LEU:O	2.07	0.54
1:D:123:MET:CE	1:D:127:LEU:HD12	2.37	0.54
3:B:490:JKF:CAA	3:B:490:JKF:CAM	2.85	0.54
1:D:154:MET:HE1	1:D:438:THR:HG22	1.90	0.54
1:D:105:PHE:HA	1:D:219:LEU:HD21	1.89	0.54
1:C:98:SER:OG	1:C:120:TYR:OH	2.22	0.54
1:C:475:ARG:CG	1:C:475:ARG:NH1	2.56	0.53
1:A:109:VAL:HG13	1:A:286:VAL:HG11	1.90	0.53
1:D:208:LEU:CD1	3:D:490:JKF:HAJ	2.38	0.53
1:B:29:GLY:HA2	1:B:373:VAL:HG23	1.90	0.53
1:B:251:GLU:HA	1:B:256:SER:CB	2.36	0.53
1:D:252:VAL:O	1:D:252:VAL:CG1	2.57	0.53
3:A:490:JKF:HAAA	3:A:490:JKF:CAT	2.38	0.53
1:B:200:LEU:CD2	1:B:235:GLU:HG2	2.37	0.53
3:B:490:JKF:CAT	3:B:490:JKF:HAB	2.38	0.53
1:C:30:LYS:O	1:C:373:VAL:HG12	2.09	0.52
1:A:460:MET:HE2	3:A:490:JKF:HAS	1.91	0.52
1:C:460:MET:HE1	3:C:490:JKF:CAJ	2.35	0.52
1:B:46:ILE:H	1:B:46:ILE:HD12	1.74	0.52
1:D:385:LEU:O	1:D:389:HIS:HD2	1.92	0.52
1:A:252:VAL:O	1:A:252:VAL:CG1	2.58	0.52
1:B:399:ARG:HG3	1:B:399:ARG:HH11	1.74	0.52
1:D:253:ASN:HB3	1:D:255:ASP:CG	2.31	0.51
1:C:475:ARG:HG3	1:C:475:ARG:NH1	2.25	0.51
1:D:172:SER:HA	1:D:297:SER:HB2	1.93	0.51
1:B:460:MET:CE	3:B:490:JKF:CAY	2.88	0.50
2:A:482:HEM:CMC	2:A:482:HEM:HBC2	2.41	0.50
1:B:399:ARG:NH1	1:B:399:ARG:HG3	2.26	0.50
1:B:237:GLN:CG	1:B:278:LEU:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:CYS:HB2	2:C:482:HEM:NA	2.26	0.50
1:B:424:GLY:HA3	2:B:482:HEM:C3C	2.47	0.50
1:A:45:ILE:HD13	1:D:221:LEU:HD22	1.94	0.50
3:C:490:JKF:CAO	3:C:490:JKF:CAN	2.90	0.49
1:A:36:PRO:O	1:A:44:HIS:HE1	1.95	0.49
1:B:309:HIS:HD2	1:B:452:VAL:HG23	1.77	0.49
1:C:320:ARG:NH1	1:C:444:ASP:OD2	2.44	0.49
1:B:67:ILE:HD13	1:B:67:ILE:N	2.26	0.49
1:D:133:GLU:HG3	1:D:261:LEU:HD12	1.94	0.49
1:C:292:GLY:HA3	2:C:482:HEM:HMC3	1.94	0.49
1:A:389:HIS:HE1	1:A:398:ARG:HH11	1.60	0.49
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.74	0.49
1:B:347:ARG:HH11	1:B:347:ARG:HB3	1.78	0.49
1:C:109:VAL:CG1	1:C:286:VAL:HG11	2.43	0.49
1:A:247:ARG:NH2	1:A:258:THR:HG21	2.27	0.49
1:C:276:MET:CE	1:C:281:VAL:HA	2.43	0.49
1:A:256:SER:OG	1:A:257:SER:N	2.46	0.49
1:D:183:LEU:O	1:D:260:ASP:HB2	2.13	0.49
1:D:255:ASP:OD2	1:D:255:ASP:N	2.45	0.49
1:A:42:LEU:HD13	1:A:46:ILE:HD13	1.95	0.49
1:B:35:TYR:HD2	1:B:44:HIS:CE1	2.31	0.48
1:B:251:GLU:O	1:B:251:GLU:OE2	2.30	0.48
3:D:490:JKF:HAAB	3:D:490:JKF:CAM	2.43	0.48
1:A:162:GLU:HA	1:A:473:TYR:O	2.13	0.48
1:C:47:GLN:NE2	1:C:47:GLN:H	2.04	0.48
3:A:490:JKF:CAT	3:A:490:JKF:CAA	2.90	0.48
1:C:44:HIS:HD2	1:C:71:ASN:N	1.92	0.48
3:C:490:JKF:CAM	3:C:490:JKF:CAP	2.88	0.48
1:C:276:MET:CE	1:C:281:VAL:CG2	2.92	0.48
1:B:347:ARG:HB3	1:B:347:ARG:NH1	2.29	0.48
1:C:172:SER:HB2	1:C:297:SER:OG	2.13	0.48
1:D:147:GLN:HE22	1:D:330:LEU:HG	1.78	0.48
1:A:42:LEU:HD13	1:A:46:ILE:HD11	1.96	0.48
1:A:272:ASP:C	1:A:272:ASP:OD1	2.52	0.48
1:D:136:ILE:HG22	1:D:336:MET:CE	2.44	0.48
1:B:255:ASP:O	1:B:257:SER:N	2.44	0.47
1:B:407:LYS:HA	1:C:136:ILE:HD11	1.96	0.47
1:A:222:PRO:O	1:A:223:LEU:HD23	2.14	0.47
1:A:424:GLY:HA3	2:A:482:HEM:C3C	2.48	0.47
1:A:347:ARG:HB3	1:A:347:ARG:HH11	1.80	0.47
1:A:209:ILE:HA	1:A:210:PRO:HD2	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HD13	3:D:490:JKF:HAJ	1.95	0.47
1:D:188:LEU:CD1	1:D:243:ILE:HG13	2.42	0.47
1:C:123:MET:HE3	1:C:127:LEU:HD12	1.97	0.47
1:B:154:MET:HG2	1:B:158:TRP:CE3	2.50	0.47
3:D:490:JKF:HAB	3:D:490:JKF:CAT	2.45	0.47
1:C:174:MET:O	1:C:178:THR:HG23	2.14	0.47
1:B:196:ARG:NH1	1:B:196:ARG:CB	2.72	0.47
1:C:154:MET:HG2	1:C:158:TRP:CE3	2.48	0.47
1:A:309:HIS:CD2	1:A:311:ALA:CB	2.98	0.47
2:A:482:HEM:HMC1	2:A:482:HEM:HBC2	1.97	0.46
3:A:490:JKF:HAC	3:A:490:JKF:HAQ	1.70	0.46
1:B:237:GLN:HG3	1:B:278:LEU:HD13	1.96	0.46
1:C:339:MET:N	1:C:340:PRO:HD3	2.31	0.46
1:A:276:MET:CE	1:A:281:VAL:HA	2.46	0.46
1:C:146:ILE:O	1:C:150:VAL:HG23	2.15	0.46
1:C:314:LYS:HE3	1:C:314:LYS:HB3	1.63	0.46
1:B:154:MET:HB2	1:B:154:MET:HE3	1.61	0.46
1:B:251:GLU:OE1	1:B:252:VAL:HA	2.16	0.46
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.51	0.46
1:B:257:SER:O	1:B:258:THR:C	2.50	0.46
1:B:46:ILE:N	1:B:46:ILE:HD12	2.31	0.46
1:B:66:GLY:C	1:B:67:ILE:HD13	2.37	0.46
1:B:313:VAL:O	1:B:317:GLU:HB2	2.15	0.46
3:D:490:JKF:CAN	3:D:490:JKF:CAO	2.93	0.45
1:A:150:VAL:O	1:A:154:MET:HG3	2.16	0.45
1:B:36:PRO:O	1:B:44:HIS:CE1	2.66	0.45
1:B:109:VAL:HG13	1:B:286:VAL:CG1	2.40	0.45
1:D:100:ARG:NH2	1:D:118:ALA:O	2.50	0.45
1:B:167:LEU:HD21	1:B:304:MET:HB2	1.99	0.45
3:C:490:JKF:HAT	3:C:490:JKF:CAX	2.45	0.45
1:B:385:LEU:O	1:B:389:HIS:CD2	2.66	0.45
1:A:130:LEU:HD23	1:A:423:ILE:HD11	1.98	0.45
3:C:490:JKF:CAM	3:C:490:JKF:HAP	2.47	0.45
2:C:482:HEM:HMB2	2:C:482:HEM:CBB	2.46	0.45
1:B:406:GLU:O	1:C:136:ILE:CD1	2.65	0.45
1:A:331:ASN:H	1:A:334:ASN:HD22	1.64	0.45
1:B:460:MET:HE2	3:B:490:JKF:CAJ	2.47	0.45
1:B:330:LEU:HD11	1:B:437:ALA:HB3	1.98	0.45
1:C:424:GLY:HA3	2:C:482:HEM:C2C	2.52	0.45
1:A:363:VAL:HG12	1:A:376:LYS:HA	1.99	0.45
1:B:333:ASN:ND2	1:B:333:ASN:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:HG13	1:B:453:PRO:HD2	2.00	0.44
1:D:364:MET:O	1:D:376:LYS:HE2	2.16	0.44
1:B:348:GLU:HG3	1:B:400:TRP:CD1	2.53	0.44
1:C:147:GLN:NE2	1:C:151:ARG:HH12	2.14	0.44
3:D:490:JKF:HAC	3:D:490:JKF:HAQ	1.67	0.44
1:B:30:LYS:HD3	1:B:31:LEU:N	2.33	0.44
1:C:276:MET:HE1	1:C:281:VAL:HA	2.00	0.44
1:A:87:SER:HB2	1:A:91:LEU:HD12	1.99	0.44
1:B:473:TYR:C	1:B:474:ILE:HG13	2.38	0.44
1:D:310:PRO:O	1:D:313:VAL:HG13	2.17	0.44
1:A:183:LEU:O	1:A:260:ASP:HB2	2.18	0.43
2:D:482:HEM:HBB2	2:D:482:HEM:CMB	2.47	0.43
1:A:415:PHE:CD2	1:A:425:GLN:HB2	2.53	0.43
1:D:112:GLU:O	1:D:279:HIS:HE1	2.01	0.43
1:A:249:GLU:O	1:A:253:ASN:ND2	2.51	0.43
1:A:196:ARG:NH1	1:A:196:ARG:HG2	2.29	0.43
1:A:396:GLU:N	1:A:397:PRO:CD	2.81	0.43
1:A:174:MET:O	1:A:178:THR:HG23	2.19	0.43
1:C:385:LEU:O	1:C:389:HIS:HD2	2.01	0.43
1:C:109:VAL:HG13	1:C:286:VAL:HG11	2.01	0.43
1:C:235:GLU:O	1:C:235:GLU:HG3	2.18	0.43
1:A:192:LEU:HD11	1:A:197:PHE:HA	2.01	0.43
1:D:424:GLY:HA3	2:D:482:HEM:C3C	2.54	0.43
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.53	0.43
1:A:163:GLY:O	1:A:472:LYS:HG3	2.19	0.43
3:A:490:JKF:HAB	3:A:490:JKF:CAT	2.48	0.42
1:D:460:MET:CE	3:D:490:JKF:CAJ	2.96	0.42
1:A:451:GLU:OE2	1:A:451:GLU:HA	2.19	0.42
1:D:176:ILE:HB	1:D:293:GLN:OE1	2.18	0.42
1:C:91:LEU:N	1:C:92:PRO:CD	2.82	0.42
3:B:490:JKF:HAQ	3:B:490:JKF:HAC	1.70	0.42
1:A:91:LEU:N	1:A:92:PRO:CD	2.82	0.42
1:C:72:ILE:O	1:C:73:VAL:HG22	2.19	0.42
3:C:490:JKF:FAE	3:C:490:JKF:HAB	2.09	0.42
1:B:398:ARG:HA	1:B:398:ARG:HD2	1.84	0.42
1:B:30:LYS:CG	1:B:31:LEU:N	2.82	0.42
1:D:44:HIS:HB3	1:D:55:PHE:CZ	2.54	0.42
1:D:136:ILE:HG22	1:D:336:MET:HE1	2.01	0.42
1:D:250:GLU:HB3	1:D:256:SER:HB2	1.92	0.42
1:B:120:TYR:N	1:B:121:PRO:CD	2.83	0.42
1:D:250:GLU:C	1:D:256:SER:HB3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:CG1	1:B:286:VAL:CG1	2.98	0.42
2:C:482:HEM:CMC	2:C:482:HEM:CBC	2.97	0.42
1:C:338:GLU:C	1:C:340:PRO:HD3	2.40	0.42
1:D:460:MET:HE2	3:D:490:JKF:CAJ	2.49	0.42
1:A:292:GLY:HA3	2:A:482:HEM:HMC3	2.02	0.42
1:D:422:CYS:HA	2:D:482:HEM:C4D	2.55	0.42
1:C:123:MET:CE	1:C:127:LEU:HD12	2.50	0.41
1:D:190:LYS:HB3	1:D:190:LYS:HE2	1.68	0.41
1:D:39:VAL:HA	1:D:40:PRO:HD3	1.75	0.41
1:D:58:GLU:HA	1:D:61:ARG:HH12	1.83	0.41
1:A:45:ILE:HB	1:A:72:ILE:HG23	2.01	0.41
1:C:460:MET:HE1	3:C:490:JKF:CAY	2.50	0.41
1:B:424:GLY:HA3	2:B:482:HEM:C2C	2.55	0.41
1:D:136:ILE:CG2	1:D:336:MET:CE	2.98	0.41
1:A:339:MET:HE3	1:A:437:ALA:HB2	2.02	0.41
1:A:389:HIS:CE1	1:A:398:ARG:HH11	2.38	0.41
1:B:28:LYS:CD	1:B:30:LYS:HB3	2.26	0.41
1:B:253:ASN:HB2	1:B:255:ASP:HB3	2.03	0.41
1:A:309:HIS:HD2	1:A:311:ALA:CB	2.33	0.41
1:B:67:ILE:HD11	1:B:82:ASP:HB3	2.03	0.41
1:D:359:LEU:O	1:D:381:ALA:HA	2.21	0.41
1:D:253:ASN:CB	1:D:255:ASP:CG	2.89	0.41
1:A:276:MET:HE1	1:A:281:VAL:HA	2.02	0.41
1:A:354:PRO:HA	1:A:355:PRO:HD3	1.96	0.41
1:D:238:LYS:HD3	1:D:242:GLU:OE2	2.21	0.41
1:A:339:MET:N	1:A:340:PRO:CD	2.84	0.41
1:D:73:VAL:HG11	1:D:215:LEU:HD21	2.03	0.41
1:A:146:ILE:HG13	1:A:182:CYS:SG	2.62	0.40
1:D:332:TYR:C	1:D:332:TYR:CD2	2.94	0.40
1:C:147:GLN:NE2	1:C:330:LEU:HG	2.36	0.40
1:B:176:ILE:HB	1:B:293:GLN:OE1	2.21	0.40
1:A:309:HIS:HD2	1:A:311:ALA:HB3	1.82	0.40
1:A:269:VAL:HG13	1:A:273:GLY:O	2.21	0.40
1:C:188:LEU:HD13	1:C:243:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	448/454 (99%)	432 (96%)	15 (3%)	1 (0%)	52	43
1	B	448/454 (99%)	434 (97%)	14 (3%)	0	100	100
1	C	448/454 (99%)	429 (96%)	18 (4%)	1 (0%)	52	43
1	D	448/454 (99%)	436 (97%)	12 (3%)	0	100	100
All	All	1792/1816 (99%)	1731 (97%)	59 (3%)	2 (0%)	56	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	PRO
1	A	40	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	392/392 (100%)	375 (96%)	17 (4%)	35	27
1	B	392/392 (100%)	366 (93%)	26 (7%)	21	11
1	C	392/392 (100%)	370 (94%)	22 (6%)	26	16
1	D	392/392 (100%)	370 (94%)	22 (6%)	26	16
All	All	1568/1568 (100%)	1481 (94%)	87 (6%)	27	16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	104	SER
1	A	140	GLN
1	A	172	SER
1	A	193	ASP
1	A	196	ARG
1	A	197	PHE
1	A	254	LYS
1	A	255	ASP
1	A	278	LEU
1	A	347	ARG
1	A	378	ASP
1	A	404	ARG
1	A	444	ASP
1	A	447	LEU
1	A	452	VAL
1	A	471	VAL
1	B	30	LYS
1	B	47	GLN
1	B	62	GLN
1	B	104	SER
1	B	106	MET
1	B	122	ARG
1	B	162	GLU
1	B	191	ARG
1	B	196	ARG
1	B	207	SER
1	B	215	LEU
1	B	226	SER
1	B	235	GLU
1	B	253	ASN
1	B	254	LYS
1	B	256	SER
1	B	257	SER
1	B	278	LEU
1	B	297	SER
1	B	320	ARG
1	B	333	ASN
1	B	403	GLU
1	B	404	ARG
1	B	421	LYS
1	B	447	LEU
1	B	477	LYS

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Mol	Chain	Res	Type
1	C	47	GLN
1	C	61	ARG
1	C	75	LYS
1	C	104	SER
1	C	122	ARG
1	C	123	MET
1	C	136	ILE
1	C	160	LYS
1	C	162	GLU
1	C	197	PHE
1	C	235	GLU
1	C	255	ASP
1	C	256	SER
1	C	258	THR
1	C	278	LEU
1	C	320	ARG
1	C	366	ASP
1	C	396	GLU
1	C	421	LYS
1	C	450	ASP
1	C	471	VAL
1	C	475	ARG
1	D	28	LYS
1	D	41	ILE
1	D	93	ARG
1	D	122	ARG
1	D	123	MET
1	D	136	ILE
1	D	190	LYS
1	D	195	ARG
1	D	196	ARG
1	D	197	PHE
1	D	215	LEU
1	D	238	LYS
1	D	251	GLU
1	D	252	VAL
1	D	255	ASP
1	D	278	LEU
1	D	297	SER
1	D	314	LYS
1	D	317	GLU
1	D	320	ARG

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Mol	Chain	Res	Type
1	D	376	LYS
1	D	458	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	47	GLN
1	A	140	GLN
1	A	279	HIS
1	A	309	HIS
1	A	334	ASN
1	A	388	HIS
1	A	389	HIS
1	A	446	GLN
1	B	44	HIS
1	B	181	GLN
1	B	279	HIS
1	B	306	HIS
1	B	333	ASN
1	B	334	ASN
1	B	388	HIS
1	B	389	HIS
1	B	446	GLN
1	C	44	HIS
1	C	47	GLN
1	C	279	HIS
1	C	309	HIS
1	C	334	ASN
1	C	388	HIS
1	C	389	HIS
1	C	446	GLN
1	D	44	HIS
1	D	279	HIS
1	D	309	HIS
1	D	334	ASN
1	D	388	HIS
1	D	389	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	482	1,3	30,50,50	2.16	7 (23%)	24,82,82	2.28	10 (41%)
3	JKF	A	490	2	36,40,40	3.08	6 (16%)	52,60,60	1.73	12 (23%)
2	HEM	B	482	1,3	30,50,50	2.37	7 (23%)	24,82,82	2.40	11 (45%)
3	JKF	B	490	2	36,40,40	3.16	7 (19%)	52,60,60	1.50	6 (11%)
2	HEM	C	482	1,3	30,50,50	2.26	4 (13%)	24,82,82	2.49	10 (41%)
3	JKF	C	490	2	36,40,40	2.92	6 (16%)	52,60,60	1.65	12 (23%)
2	HEM	D	482	1,3	30,50,50	2.34	6 (20%)	24,82,82	2.44	10 (41%)
3	JKF	D	490	2	36,40,40	2.67	6 (16%)	52,60,60	1.60	6 (11%)

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	482	1,3	-	0/10/54/54	0/0/8/8
3	JKF	A	490	2	-	0/19/25/25	0/5/5/5
2	HEM	B	482	1,3	-	0/10/54/54	0/0/8/8
3	JKF	B	490	2	-	0/19/25/25	0/5/5/5
2	HEM	C	482	1,3	-	0/10/54/54	0/0/8/8
3	JKF	C	490	2	-	0/19/25/25	0/5/5/5
2	HEM	D	482	1,3	-	0/10/54/54	0/0/8/8
3	JKF	D	490	2	-	0/19/25/25	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	490	JKF	CBJ-CBA	-10.42	1.38	1.54
3	C	490	JKF	CBB-CBC	-10.05	1.39	1.50
3	C	490	JKF	CBJ-CBA	-9.90	1.38	1.54
3	A	490	JKF	CBB-CBC	-9.44	1.39	1.50
3	B	490	JKF	CBB-CBC	-9.30	1.40	1.50
3	A	490	JKF	CBJ-CAZ	-9.13	1.39	1.54
2	D	482	HEM	C3B-C4B	-8.93	1.43	1.51
2	C	482	HEM	C3B-C4B	-8.79	1.44	1.51
2	B	482	HEM	C3B-C4B	-8.55	1.44	1.51
3	B	490	JKF	CBJ-CBA	-8.40	1.41	1.54
3	B	490	JKF	CBJ-CAZ	-8.38	1.41	1.54
3	D	490	JKF	CBJ-CBA	-8.17	1.41	1.54
3	D	490	JKF	CBJ-CAZ	-8.01	1.41	1.54
3	C	490	JKF	CBJ-CAZ	-7.94	1.41	1.54
3	D	490	JKF	CBB-CBC	-7.83	1.41	1.50
2	A	482	HEM	C3B-C4B	-7.57	1.45	1.51
3	B	490	JKF	FAF-CAY	-6.53	1.19	1.35
3	B	490	JKF	FAE-CAX	-6.35	1.20	1.35
2	B	482	HEM	C3D-C4D	-5.78	1.44	1.51
2	A	482	HEM	C3D-C4D	-5.17	1.44	1.51
2	D	482	HEM	C3D-C4D	-5.06	1.45	1.51
2	C	482	HEM	C3D-C4D	-4.81	1.45	1.51
3	B	490	JKF	CBG-NBI	-4.72	1.35	1.40
3	D	490	JKF	CBG-NBI	-4.47	1.35	1.40
3	A	490	JKF	CBG-NBI	-4.41	1.35	1.40
3	A	490	JKF	FAF-CAY	-4.32	1.25	1.35
2	C	482	HEM	C2C-C1C	-4.10	1.44	1.52
3	D	490	JKF	FAF-CAY	-3.89	1.26	1.35
2	D	482	HEM	C2C-C1C	-3.88	1.45	1.52
2	B	482	HEM	C2C-C1C	-3.66	1.45	1.52
3	C	490	JKF	CBG-NBI	-3.65	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	482	HEM	C2C-C1C	-3.39	1.46	1.52
3	D	490	JKF	CBE-NBI	-2.35	1.34	1.38
2	B	482	HEM	C2D-C1D	-2.34	1.44	1.51
3	B	490	JKF	CBE-NBI	-2.29	1.34	1.38
2	A	482	HEM	C2D-C1D	-2.20	1.44	1.51
3	C	490	JKF	FAF-CAY	-2.18	1.30	1.35
2	D	482	HEM	C2D-C1D	-2.17	1.44	1.51
3	A	490	JKF	CBE-NBI	-2.15	1.35	1.38
2	C	482	HEM	C2D-C1D	-2.03	1.45	1.51
2	B	482	HEM	C3B-CAB	2.03	1.55	1.51
2	A	482	HEM	C3C-CAC	2.06	1.55	1.51
2	D	482	HEM	C4C-NC	2.11	1.38	1.36
2	A	482	HEM	C1C-NC	2.15	1.38	1.36
2	A	482	HEM	CAA-C2A	2.24	1.55	1.52
2	D	482	HEM	C3B-CAB	2.37	1.55	1.51
2	B	482	HEM	C4C-NC	2.50	1.39	1.36
2	B	482	HEM	C3C-CAC	2.60	1.56	1.51
3	C	490	JKF	CAW-CLAG	2.82	1.80	1.74

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	490	JKF	CBB-CBC-CAX	-5.25	118.72	122.90
3	B	490	JKF	CBB-CBC-CAX	-5.25	118.72	122.90
2	C	482	HEM	C3C-CAC-CBC	-4.62	117.37	124.46
2	D	482	HEM	C3C-CAC-CBC	-3.86	118.54	124.46
3	C	490	JKF	CBB-CBC-CAX	-3.74	119.93	122.90
3	D	490	JKF	NAU-CAR-NBH	-3.47	107.59	112.28
3	C	490	JKF	CAJ-CAY-CBC	-3.44	120.19	124.03
3	B	490	JKF	NAU-CAR-NBH	-3.30	107.82	112.28
3	C	490	JKF	NAU-CAR-NBH	-3.29	107.83	112.28
2	C	482	HEM	C3B-CAB-CBB	-3.28	119.42	124.46
3	D	490	JKF	CAQ-CBG-NBI	-3.26	119.28	121.78
2	D	482	HEM	C3B-CAB-CBB	-3.23	119.50	124.46
3	A	490	JKF	NAU-CAR-NBH	-3.18	107.98	112.28
3	A	490	JKF	CAJ-CAY-CBC	-3.16	120.50	124.03
3	D	490	JKF	CBB-CBC-CAX	-3.07	120.45	122.90
3	B	490	JKF	CAJ-CAY-CBC	-3.00	120.69	124.03
3	A	490	JKF	CAI-CAX-CBC	-2.94	120.76	124.03
3	D	490	JKF	CAJ-CAY-CBC	-2.90	120.80	124.03
2	C	482	HEM	CMA-C3A-C4A	-2.90	123.57	128.36
2	B	482	HEM	CBD-CAD-C3D	-2.85	105.26	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	482	HEM	CBD-CAD-C3D	-2.75	105.54	113.55
2	B	482	HEM	C3B-CAB-CBB	-2.72	120.29	124.46
2	A	482	HEM	CAA-C2A-C1A	-2.70	124.07	127.01
3	C	490	JKF	CAQ-CBG-NBI	-2.62	119.77	121.78
3	A	490	JKF	CAQ-CAO-CBA	-2.61	118.20	121.78
2	B	482	HEM	CBA-CAA-C2A	-2.50	108.05	112.53
2	B	482	HEM	CAA-CBA-CGA	-2.47	108.22	112.75
3	C	490	JKF	CAI-CAX-CBC	-2.44	121.31	124.03
2	A	482	HEM	C3B-CAB-CBB	-2.41	120.77	124.46
3	C	490	JKF	CAQ-CAO-CBA	-2.34	118.57	121.78
3	C	490	JKF	CBB-CBC-CAY	-2.31	121.06	122.90
3	C	490	JKF	CBA-CAT-CBF	-2.20	120.16	122.24
2	A	482	HEM	C3C-CAC-CBC	-2.19	121.10	124.46
2	A	482	HEM	CMA-C3A-C4A	-2.14	124.83	128.36
3	A	490	JKF	CAQ-CBG-NBI	-2.09	120.18	121.78
2	D	482	HEM	CBD-CAD-C3D	-2.06	107.55	113.55
2	D	482	HEM	CBA-CAA-C2A	-2.05	108.86	112.53
3	A	490	JKF	CAR-NBH-CBD	-2.02	106.95	110.05
3	A	490	JKF	CAO-CBA-CAT	2.02	120.83	117.75
3	B	490	JKF	CBB-CBF-CBG	2.06	120.18	117.94
3	A	490	JKF	CAP-NAU-CAR	2.13	109.06	105.71
3	C	490	JKF	CAP-NAU-CAR	2.16	109.12	105.71
3	A	490	JKF	CBB-CBF-CBG	2.20	120.33	117.94
2	B	482	HEM	C2D-C3D-C4D	2.26	105.33	101.50
2	B	482	HEM	C2C-C1C-CHC	2.28	127.15	123.68
2	A	482	HEM	C2D-C3D-C4D	2.29	105.37	101.50
3	C	490	JKF	CAN-CAL-CAW	2.31	121.80	119.23
2	D	482	HEM	C2D-C3D-C4D	2.45	105.65	101.50
2	C	482	HEM	C2D-C3D-C4D	2.46	105.68	101.50
3	D	490	JKF	CAY-CBC-CAX	2.53	117.23	114.44
3	B	490	JKF	CAB-NBH-CBD	2.63	127.54	124.35
2	A	482	HEM	CMD-C2D-C3D	2.73	126.44	114.35
3	C	490	JKF	CAB-NBH-CBD	2.86	127.83	124.35
2	D	482	HEM	CMD-C2D-C3D	2.87	127.05	114.35
2	C	482	HEM	CMD-C2D-C3D	3.02	127.72	114.35
3	B	490	JKF	CAY-CBC-CAX	3.22	117.99	114.44
2	B	482	HEM	CMD-C2D-C3D	3.23	128.64	114.35
2	D	482	HEM	CMB-C2B-C3B	3.87	126.19	116.53
2	C	482	HEM	CMB-C2B-C3B	3.92	126.32	116.53
2	A	482	HEM	CMC-C2C-C3C	3.95	126.39	116.53
2	B	482	HEM	CMC-C2C-C3C	4.02	126.56	116.53
3	A	490	JKF	CAY-CBC-CAX	4.04	118.90	114.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	490	JKF	CAY-CBC-CAX	4.09	118.95	114.44
2	B	482	HEM	CAD-C3D-C4D	4.13	127.03	112.47
2	A	482	HEM	CMB-C2B-C3B	4.13	126.85	116.53
2	C	482	HEM	CMC-C2C-C3C	4.34	127.35	116.53
2	D	482	HEM	CAD-C3D-C4D	4.38	127.92	112.47
2	C	482	HEM	CAD-C3D-C4D	4.40	127.98	112.47
2	B	482	HEM	CMB-C2B-C3B	4.40	127.52	116.53
2	A	482	HEM	CAD-C3D-C4D	4.44	128.14	112.47
3	D	490	JKF	CAB-NBH-CBD	4.51	129.83	124.35
2	C	482	HEM	CAD-C3D-C2D	4.56	126.32	113.22
2	D	482	HEM	CAD-C3D-C2D	4.59	126.41	113.22
2	A	482	HEM	CAD-C3D-C2D	4.61	126.48	113.22
2	D	482	HEM	CMC-C2C-C3C	4.80	128.51	116.53
3	A	490	JKF	CAB-NBH-CBD	4.93	130.34	124.35
2	B	482	HEM	CAD-C3D-C2D	5.02	127.64	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	482	HEM	6	0
3	A	490	JKF	9	0
2	B	482	HEM	5	0
3	B	490	JKF	9	0
2	C	482	HEM	9	0
3	C	490	JKF	17	0
2	D	482	HEM	5	0
3	D	490	JKF	11	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	450/454 (99%)	0.61	53 (11%) 6 6	33, 53, 75, 88	0
1	B	450/454 (99%)	0.56	37 (8%) 14 16	27, 47, 70, 95	0
1	C	450/454 (99%)	0.52	41 (9%) 11 12	33, 52, 73, 93	0
1	D	450/454 (99%)	0.31	22 (4%) 33 38	25, 41, 62, 85	0
All	All	1800/1816 (99%)	0.50	153 (8%) 13 15	25, 48, 72, 95	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	VAL	12.7
1	C	29	GLY	11.3
1	B	252	VAL	10.3
1	B	28	LYS	10.0
1	B	256	SER	9.5
1	C	28	LYS	8.4
1	D	28	LYS	7.7
1	C	256	SER	7.2
1	C	255	ASP	6.6
1	A	256	SER	6.3
1	B	255	ASP	6.1
1	B	251	GLU	6.1
1	B	257	SER	6.0
1	D	29	GLY	5.9
1	C	477	LYS	5.8
1	D	41	ILE	5.8
1	D	256	SER	5.4
1	B	253	ASN	5.1
1	C	257	SER	4.7
1	B	474	ILE	4.6
1	C	39	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	477	LYS	4.5
1	A	329	GLN	4.4
1	A	328	ALA	4.4
1	B	40	PRO	4.3
1	D	254	LYS	4.3
1	A	271	ARG	4.1
1	D	477	LYS	4.0
1	C	271	ARG	4.0
1	A	159	ASP	4.0
1	A	190	LYS	3.9
1	A	257	SER	3.9
1	D	253	ASN	3.9
1	B	161	ASP	3.8
1	C	36	PRO	3.8
1	C	291	ALA	3.7
1	A	120	TYR	3.6
1	C	38	THR	3.6
1	C	288	ALA	3.6
1	A	258	THR	3.6
1	D	251	GLU	3.6
1	C	373	VAL	3.5
1	D	257	SER	3.5
1	B	29	GLY	3.5
1	A	195	ARG	3.5
1	A	192	LEU	3.5
1	C	41	ILE	3.4
1	A	155	ALA	3.3
1	A	447	LEU	3.3
1	C	121	PRO	3.3
1	B	359	LEU	3.3
1	B	41	ILE	3.2
1	A	310	PRO	3.1
1	C	93	ARG	3.1
1	C	295	THR	3.1
1	D	255	ASP	3.1
1	B	432	VAL	3.1
1	A	249	GLU	3.1
1	A	317	GLU	3.1
1	D	120	TYR	3.0
1	A	140	GLN	3.0
1	C	285	ILE	3.0
1	A	293	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	252	VAL	3.0
1	B	300	THR	3.0
1	C	31	LEU	3.0
1	A	291	ALA	2.9
1	A	446	GLN	2.9
1	C	64	LYS	2.9
1	A	46	ILE	2.8
1	C	196	ARG	2.8
1	A	296	SER	2.8
1	A	188	LEU	2.8
1	C	407	LYS	2.7
1	B	321	LYS	2.7
1	B	162	GLU	2.7
1	A	156	ALA	2.7
1	C	46	ILE	2.7
1	C	359	LEU	2.6
1	C	435	ILE	2.6
1	B	61	ARG	2.6
1	B	159	ASP	2.6
1	C	432	VAL	2.6
1	D	359	LEU	2.6
1	A	238	LYS	2.6
1	B	30	LYS	2.6
1	A	77	VAL	2.6
1	A	295	THR	2.6
1	B	435	ILE	2.6
1	B	93	ARG	2.6
1	B	160	LYS	2.5
1	C	42	LEU	2.5
1	A	333	ASN	2.5
1	A	359	LEU	2.5
1	C	40	PRO	2.5
1	D	287	ALA	2.5
1	B	458	HIS	2.5
1	B	39	VAL	2.5
1	A	254	LYS	2.4
1	B	38	THR	2.4
1	B	350	ILE	2.4
1	A	40	PRO	2.4
1	A	477	LYS	2.4
1	C	372	TYR	2.4
1	B	371	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	220	LYS	2.4
1	A	95	GLU	2.4
1	C	175	ILE	2.4
1	A	196	ARG	2.4
1	C	195	ARG	2.4
1	C	296	SER	2.3
1	A	384	PRO	2.3
1	B	314	LYS	2.3
1	A	290	PHE	2.3
1	A	292	GLY	2.2
1	D	291	ALA	2.2
1	A	62	GLN	2.2
1	A	358	MET	2.2
1	B	295	THR	2.2
1	A	432	VAL	2.2
1	D	50	LYS	2.2
1	B	254	LYS	2.2
1	C	270	TYR	2.2
1	B	163	GLY	2.2
1	D	191	ARG	2.2
1	A	41	ILE	2.2
1	A	298	ILE	2.2
1	B	303	SER	2.2
1	C	290	PHE	2.1
1	D	195	ARG	2.1
1	A	356	LEU	2.1
1	C	274	THR	2.1
1	C	329	GLN	2.1
1	D	329	GLN	2.1
1	A	314	LYS	2.1
1	C	300	THR	2.1
1	B	357	LEU	2.1
1	D	355	PRO	2.1
1	C	62	GLN	2.1
1	C	191	ARG	2.1
1	A	161	ASP	2.1
1	B	346	ALA	2.1
1	A	191	ARG	2.1
1	C	286	VAL	2.1
1	D	295	THR	2.1
1	A	350	ILE	2.0
1	A	255	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	160	LYS	2.0
1	A	245	ILE	2.0
1	A	273	GLY	2.0
1	B	271	ARG	2.0
1	C	292	GLY	2.0
1	A	50	LYS	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	JKF	D	490	36/36	0.96	0.24	1.54	21,39,56,66	0
2	HEM	A	482	43/43	0.97	0.20	0.80	29,32,39,45	0
3	JKF	C	490	36/36	0.92	0.21	0.66	38,49,58,64	0
2	HEM	D	482	43/43	0.98	0.19	0.64	23,27,38,43	0
2	HEM	C	482	43/43	0.97	0.20	0.37	35,40,48,55	0
3	JKF	B	490	36/36	0.96	0.18	0.35	31,42,57,65	0
2	HEM	B	482	43/43	0.98	0.18	0.34	23,31,37,41	0
3	JKF	A	490	36/36	0.96	0.17	0.18	33,41,60,66	0

6.5 Other polymers (i)

There are no such residues in this entry.