Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X2N
Title	:	X-ray structure of cyp51 from trypanosoma brucei in complex with posaconazole in two different conformations
Authors	:	Chen, C.-K.; Leung, S.S.F.; Guilbert, C.; Jacobson, M.; Mckerrow, J.H.; Podust, L.M.
Deposited on	:	2010-01-14
Resolution	:	2.60 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:

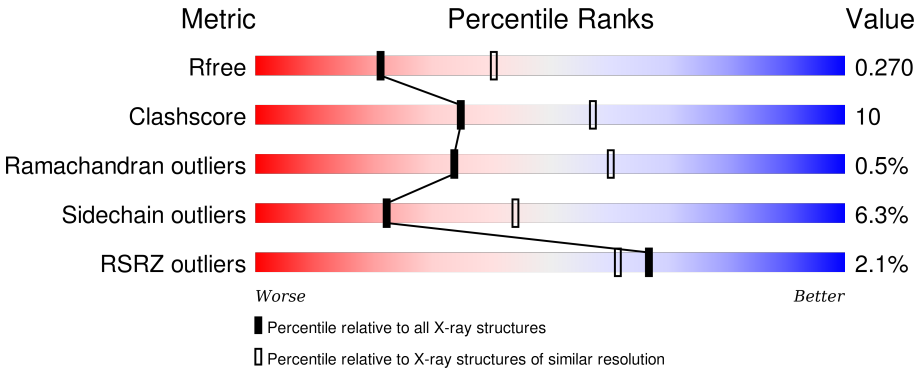
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	2% 75% 17% • 6%
1	B	475	3% 77% 14% • 7%
1	C	475	% 71% 20% • 7%
1	D	475	2% 68% 23% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14674 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.

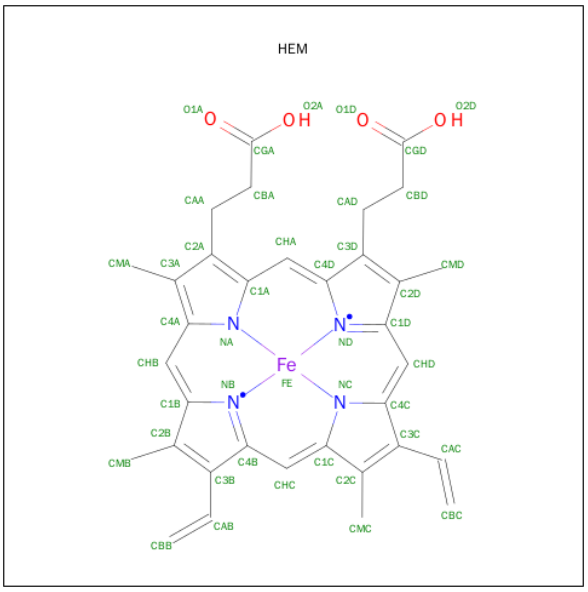
- Molecule 1 is a protein called LANOSTEROL 14-ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	1	0
			3534	2257	619	631	27			
1	B	444	Total	C	N	O	S	0	1	0
			3493	2234	609	623	27			
1	C	441	Total	C	N	O	S	0	1	0
			3488	2230	608	623	27			
1	D	447	Total	C	N	O	S	0	3	0
			3533	2255	619	632	27			

There are 12 discrepancies between the modelled and reference sequences:

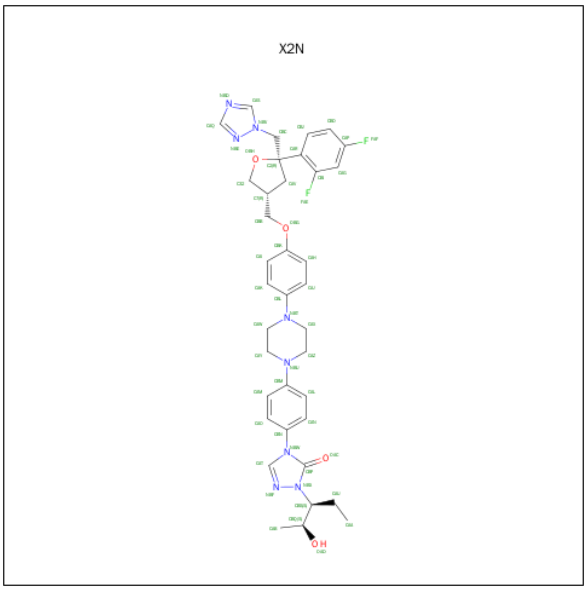
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
A	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
A	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
B	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
B	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
B	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
C	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
C	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
C	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
D	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
D	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
D	251	ALA	GLU	ENGINEERED MUTATION	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 POSACONAZOLE (three-letter code: X2N) (formula: $C_{37}H_{42}F_2N_8O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			51	37	2	8	4		
3	B	1	Total	C	F	N	O	0	0
			51	37	2	8	4		
3	C	1	Total	C	F	N	O	0	0
			51	37	2	8	4		
3	D	1	Total	C	F	N	O	0	0
			51	37	2	8	4		

- Molecule 4 is water.

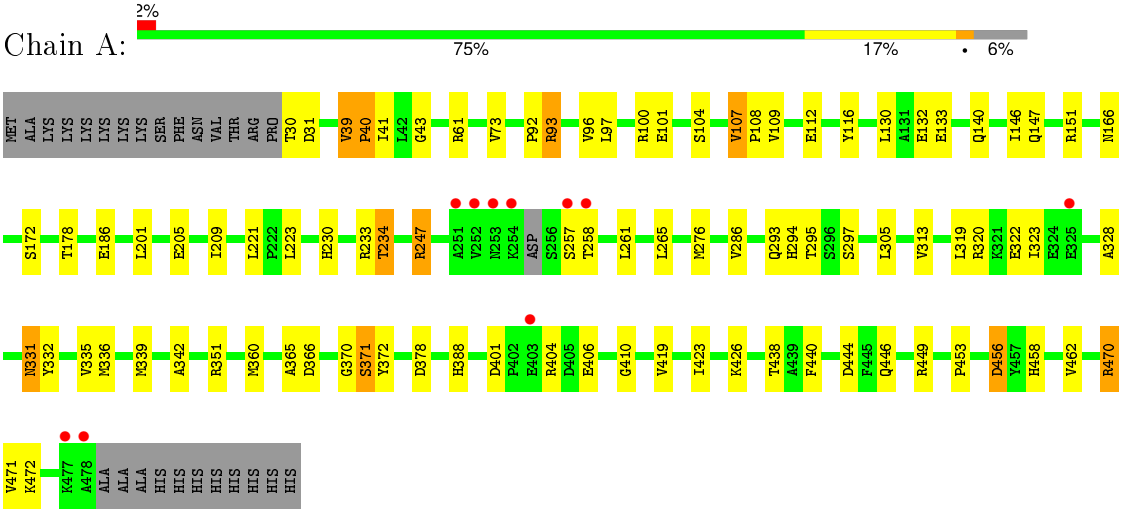
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	47	Total	O	0	0
			47	47		
4	C	69	Total	O	0	0
			69	69		
4	D	75	Total	O	0	0
			75	75		

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.

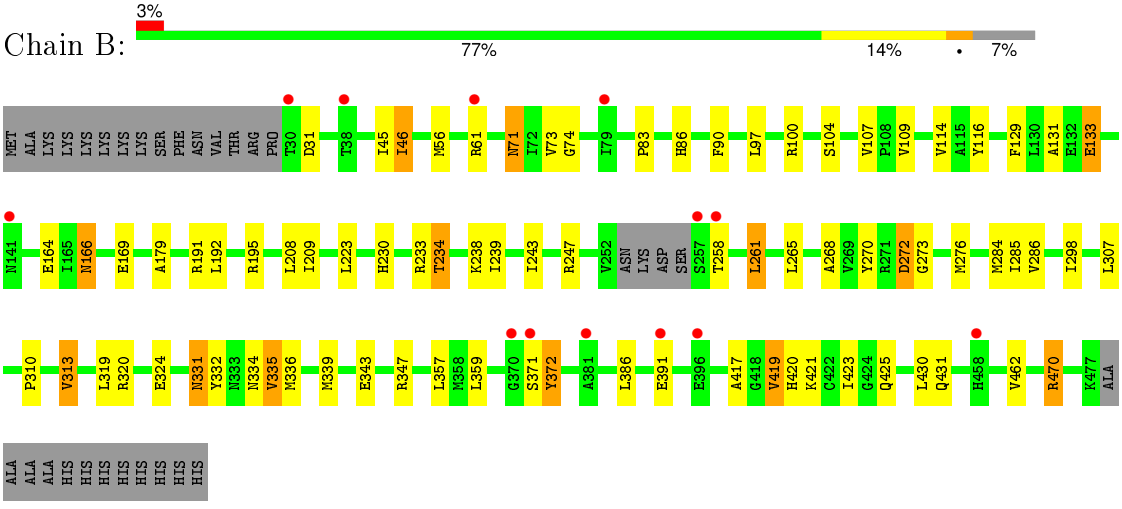
- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain A:



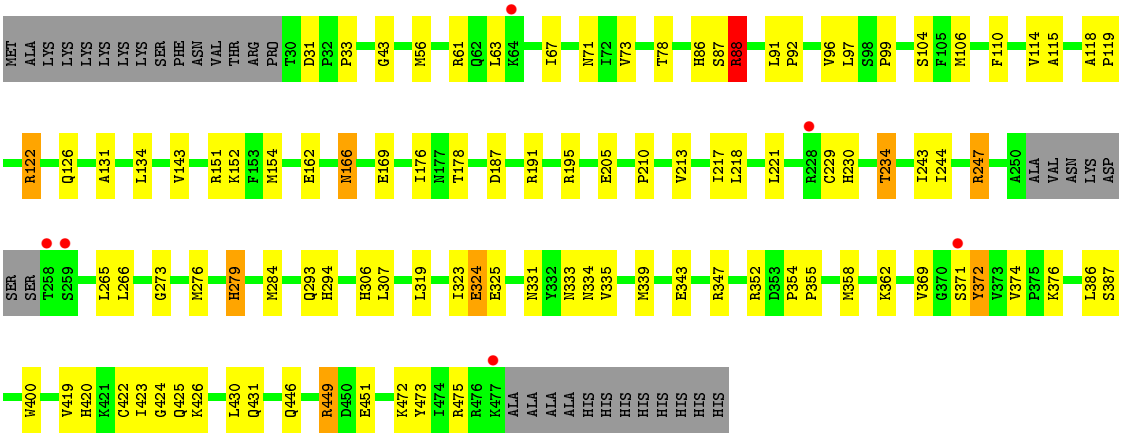
- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain B:



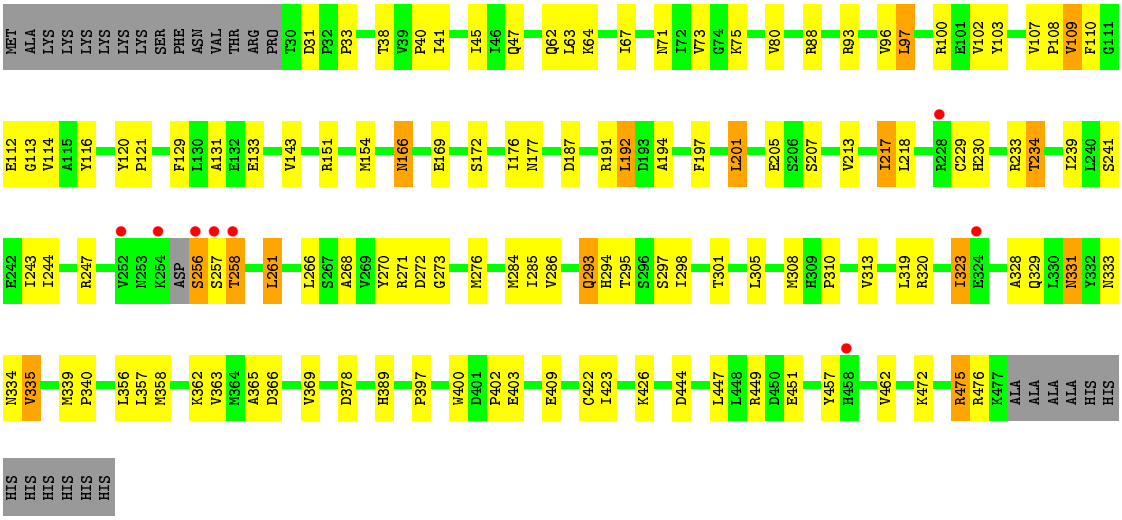
- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain C:



- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	199.89Å 114.53Å 138.09Å 90.00° 131.83° 90.00°	Depositor
Resolution (Å)	102.90 – 2.60 21.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (102.90-2.60) 99.9 (21.25-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.191 , 0.264 0.204 , 0.270	Depositor DCC
R_{free} test set	3572 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 71152 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14674	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, X2N

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	0.72	2/3616 (0.1%)	0.81	7/4898 (0.1%)
1	B	0.71	0/3575	0.78	3/4844 (0.1%)
1	C	0.74	2/3569 (0.1%)	0.79	4/4833 (0.1%)
1	D	0.85	1/3614 (0.0%)	0.83	1/4897 (0.0%)
All	All	0.76	5/14374 (0.0%)	0.80	15/19472 (0.1%)

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
1	C	0	1
1	D	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	229	CYS	CB-SG	-7.06	1.70	1.82
1	A	101	GLU	CG-CD	6.37	1.61	1.51
1	D	256	SER	CA-CB	5.69	1.61	1.52
1	A	101	GLU	CB-CG	5.55	1.62	1.52
1	C	324	GLU	CG-CD	5.16	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	ARG	NE-CZ-NH1	8.69	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	470	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	247	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	C	88	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	470	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	93	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	247	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	195	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	D	323	ILE	CB-CA-C	-5.61	100.38	111.60
1	A	456	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	93	ARG	CG-CD-NE	5.14	122.60	111.80
1	C	352	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	470	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	456	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	272	ASP	CB-CG-OD1	5.09	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	273	GLY	Peptide
1	C	273	GLY	Peptide
1	D	273	GLY	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	3534	0	3540	60	0
1	B	3493	0	3490	54	0
1	C	3488	0	3493	67	0
1	D	3533	0	3523	90	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
2	C	43	0	30	4	0
2	D	43	0	30	5	0
3	A	51	0	42	2	0
3	B	51	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	51	0	42	5	0
3	D	51	0	42	2	0
4	A	59	0	0	5	0
4	B	47	0	0	1	0
4	C	69	0	0	2	0
4	D	75	0	0	2	0
All	All	14674	0	14334	286	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 10.

All (286) 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)
2:B:1478:HEM:HBC2	2:B:1478:HEM:HMC2	1.38	1.02
2:B:1478:HEM:CMC	2:B:1478:HEM:HBC2	1.95	0.94
2:A:1479:HEM:HMC2	2:A:1479:HEM:HBC2	1.48	0.92
1:B:192:LEU:HD11	1:B:239:ILE:HD13	1.52	0.91
1:D:205:GLU:OE2	1:D:294:HIS:CE1	2.24	0.91
1:C:323:ILE:HG22	4:C:2059:HOH:O	1.75	0.86
1:A:320:ARG:NH1	1:A:444:ASP:OD2	2.09	0.85
1:D:100:ARG:HG3	1:D:116:TYR:O	1.77	0.84
1:D:192:LEU:HD12	1:D:239:ILE:HD13	1.57	0.84
1:D:187:ASP:OD2	1:D:247:ARG:HD2	1.79	0.82
1:B:331:ASN:HD22	1:B:331:ASN:C	1.83	0.82
1:D:151:ARG:NH2	1:D:328:ALA:O	2.13	0.82
1:A:230:HIS:O	1:A:234:THR:HG23	1.81	0.80
2:A:1479:HEM:HBC2	2:A:1479:HEM:CMC	2.09	0.80
1:D:177:ASN:HD22	1:D:194:ALA:CB	1.95	0.79
1:D:205:GLU:OE2	1:D:294:HIS:HE1	1.68	0.77
1:A:205:GLU:OE1	1:A:294:HIS:HE1	1.67	0.76
1:B:230:HIS:O	1:B:234:THR:HG23	1.84	0.76
1:B:192:LEU:HD13	1:B:239:ILE:HG21	1.66	0.76
1:A:335:VAL:HA	1:A:339:MET:HE3	1.69	0.75
1:C:166:ASN:HD22	1:C:169:GLU:H	1.33	0.74
1:D:151:ARG:HA	1:D:154:MET:HE2	1.69	0.74
1:B:192:LEU:CD1	1:B:239:ILE:HD13	2.17	0.73
1:D:230:HIS:O	1:D:234:THR:HG23	1.88	0.73
1:B:265:LEU:HB3	1:B:276:MET:HE3	1.71	0.73
1:A:39:VAL:HG23	4:A:2003:HOH:O	1.91	0.71
1:D:114:VAL:HG12	1:D:284:MET:HE1	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:GLU:HG2	1:D:261:LEU:HD23	1.73	0.69
1:A:146:ILE:HG23	1:A:178:THR:HG21	1.73	0.69
1:C:106:MET:HE1	3:C:1479:X2N:HAV1	1.75	0.68
1:A:209:ILE:HD11	1:A:223:LEU:HD12	1.76	0.68
1:A:335:VAL:HG23	1:A:339:MET:HE3	1.76	0.67
1:C:151:ARG:HA	1:C:154:MET:HE2	1.77	0.67
1:A:335:VAL:HA	1:A:339:MET:CE	2.25	0.66
1:C:230:HIS:O	1:C:234:THR:HG23	1.96	0.66
2:B:1478:HEM:HBB2	2:B:1478:HEM:HMB2	1.77	0.66
1:D:331:ASN:ND2	1:D:333:ASN:H	1.93	0.66
2:B:1478:HEM:HMC2	2:B:1478:HEM:CBC	2.20	0.65
2:B:1478:HEM:HBB2	2:B:1478:HEM:CMB	2.26	0.65
1:A:112:GLU:OE1	1:C:279:HIS:CD2	2.50	0.65
1:A:151:ARG:NH2	1:A:328:ALA:O	2.29	0.65
1:B:419:VAL:HG22	1:B:420:HIS:CD2	2.32	0.65
1:B:331:ASN:ND2	1:B:334:ASN:H	1.95	0.64
1:B:233:ARG:HD2	4:B:2009:HOH:O	1.96	0.64
1:C:335:VAL:HG22	1:C:339:MET:CE	2.27	0.64
1:D:335:VAL:HB	1:D:339:MET:HE3	1.79	0.63
1:D:33:PRO:HB2	1:D:63:LEU:HD22	1.81	0.63
1:D:177:ASN:ND2	1:D:194:ALA:CB	2.61	0.62
1:B:347:ARG:HH12	1:B:425:GLN:HE21	1.46	0.62
1:D:177:ASN:ND2	1:D:194:ALA:HB3	2.16	0.61
1:D:192:LEU:CD1	1:D:239:ILE:HD13	2.29	0.61
1:D:331:ASN:HD22	1:D:333:ASN:H	1.46	0.61
1:C:166:ASN:ND2	1:C:169:GLU:H	1.98	0.61
1:C:187:ASP:OD2	1:C:247:ARG:HD2	2.01	0.61
1:D:177:ASN:HD22	1:D:194:ALA:HB1	1.65	0.61
1:C:335:VAL:HG22	1:C:339:MET:HE3	1.83	0.61
1:D:331:ASN:ND2	1:D:333:ASN:N	2.49	0.60
1:C:419:VAL:HG22	1:C:420:HIS:CD2	2.36	0.60
1:D:73:VAL:O	1:D:73:VAL:HG12	2.02	0.60
1:D:310:PRO:O	1:D:313:VAL:HG13	2.02	0.60
1:D:143:VAL:HG21	1:D:335:VAL:CG1	2.32	0.60
1:B:371:SER:O	1:B:372:TYR:HB2	2.01	0.60
1:C:88:ARG:CG	1:C:88:ARG:HH11	2.15	0.60
1:A:209:ILE:CD1	1:A:223:LEU:HD12	2.31	0.59
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.36	0.59
1:B:104:SER:O	1:B:107:VAL:HG23	2.03	0.59
1:A:265:LEU:HD22	1:A:276:MET:HE1	1.85	0.59
3:C:1479:X2N:OAC	3:C:1479:X2N:HAA2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:C	4:A:2003:HOH:O	2.41	0.59
1:C:176:ILE:HB	1:C:293:GLN:NE2	2.18	0.59
1:C:118:ALA:HB1	1:C:119:PRO:HD2	1.84	0.59
1:A:370:GLY:C	1:A:371:SER:O	2.38	0.58
1:C:331:ASN:HD21	1:C:333:ASN:HB2	1.69	0.58
1:C:78:THR:HG21	1:C:374:VAL:HG22	1.84	0.58
1:C:343:GLU:OE2	1:C:347:ARG:NH2	2.37	0.58
1:A:100:ARG:HG3	1:A:116:TYR:O	2.04	0.57
1:B:371:SER:O	1:B:372:TYR:CB	2.52	0.57
1:D:102:VAL:O	1:D:213:VAL:HG22	2.04	0.57
2:A:1479:HEM:CBC	2:A:1479:HEM:HMC2	2.30	0.57
1:D:114:VAL:CG1	1:D:284:MET:HE1	2.35	0.57
1:B:71:ASN:HD22	1:B:71:ASN:C	2.08	0.57
2:D:1478:HEM:HHD	2:D:1478:HEM:HBC2	1.86	0.57
1:A:205:GLU:OE1	1:A:294:HIS:CE1	2.55	0.57
1:B:133:GLU:HG2	1:B:261:LEU:HD23	1.87	0.56
1:D:331:ASN:HD21	1:D:333:ASN:HB2	1.68	0.56
1:A:401:ASP:O	1:A:404:ARG:HG2	2.06	0.56
3:C:1479:X2N:NBF	3:C:1479:X2N:HAB2	2.20	0.56
1:D:143:VAL:CG2	1:D:335:VAL:HG11	2.35	0.55
1:C:118:ALA:HB1	1:C:119:PRO:CD	2.37	0.55
1:B:71:ASN:HD21	1:B:74:GLY:H	1.53	0.55
1:C:307:LEU:HD13	1:C:319:LEU:HD22	1.87	0.55
1:D:192:LEU:HD21	1:D:197:PHE:HD1	1.70	0.55
1:A:40:PRO:N	4:A:2003:HOH:O	2.40	0.55
1:A:320:ARG:NH2	1:A:440:PHE:O	2.40	0.55
1:B:419:VAL:CG2	1:B:420:HIS:CD2	2.89	0.54
1:C:67:ILE:HD13	1:C:369:VAL:HG12	1.90	0.54
1:D:114:VAL:CG1	1:D:284:MET:CE	2.86	0.53
1:D:363:VAL:HG23	1:D:378:ASP:O	2.07	0.53
1:B:261:LEU:HD13	1:B:285:ILE:HG12	1.89	0.53
1:D:331:ASN:H	1:D:334:ASN:HD22	1.55	0.53
1:B:73:VAL:O	1:B:73:VAL:HG12	2.09	0.53
1:D:270:TYR:O	1:D:272:ASP:O	2.27	0.53
1:C:244:ILE:HG12	1:C:266:LEU:HD11	1.89	0.53
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.43	0.53
1:C:143:VAL:HG22	1:C:430:LEU:HD11	1.89	0.53
1:C:134:LEU:HD11	2:C:1478:HEM:CBC	2.38	0.53
1:B:179:ALA:HB2	1:B:431:GLN:HE22	1.74	0.53
1:C:43:GLY:HA3	1:C:71:ASN:HD22	1.74	0.52
1:A:73:VAL:O	1:A:73:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ASN:HD22	1:D:169:GLU:H	1.56	0.52
1:A:322:GLU:HB3	1:A:323:ILE:HD12	1.91	0.52
1:D:331:ASN:H	1:D:334:ASN:ND2	2.08	0.52
1:A:323:ILE:HG22	1:A:323:ILE:O	2.10	0.52
1:A:360:MET:CE	3:A:1480:X2N:HAJ	2.40	0.52
1:D:244:ILE:CD1	1:D:266:LEU:HD11	2.40	0.52
1:D:172:SER:HA	1:D:297:SER:OG	2.09	0.52
1:D:261:LEU:HD13	1:D:285:ILE:HG12	1.91	0.51
1:C:205:GLU:OE1	1:C:294:HIS:HE1	1.93	0.51
1:C:210:PRO:O	1:C:213:VAL:HG23	2.10	0.51
1:B:331:ASN:ND2	1:B:331:ASN:C	2.55	0.51
1:C:92:PRO:HG2	1:C:97:LEU:HD22	1.92	0.51
1:C:176:ILE:CA	1:C:293:GLN:HE22	2.22	0.51
1:D:331:ASN:HD22	1:D:333:ASN:N	2.08	0.51
1:D:357:LEU:HD11	1:D:462:VAL:HG21	1.92	0.51
1:B:335:VAL:CG2	1:B:430:LEU:HD12	2.41	0.51
1:A:209:ILE:CD1	1:A:223:LEU:CD1	2.88	0.50
1:D:192:LEU:CD2	1:D:197:PHE:HD1	2.24	0.50
1:D:96:VAL:HG12	1:D:97:LEU:HD13	1.93	0.50
1:A:230:HIS:O	1:A:234:THR:CG2	2.56	0.50
1:D:365:ALA:O	1:D:366:ASP:C	2.48	0.50
1:B:230:HIS:CE1	1:D:112:GLU:HG3	2.46	0.50
2:B:1478:HEM:CBB	2:B:1478:HEM:HMB2	2.41	0.50
1:A:147:GLN:NE2	1:A:151:ARG:NH2	2.60	0.50
1:B:71:ASN:ND2	1:B:74:GLY:H	2.10	0.50
1:C:131:ALA:HA	1:C:423:ILE:HD12	1.94	0.49
1:C:265:LEU:HB3	1:C:276:MET:HE3	1.93	0.49
1:C:176:ILE:HD13	1:C:293:GLN:HE21	1.78	0.49
1:C:96:VAL:HG12	1:C:97:LEU:HD13	1.94	0.49
1:B:166:ASN:HD22	1:B:169:GLU:H	1.61	0.49
1:B:71:ASN:ND2	1:B:71:ASN:C	2.65	0.49
1:B:131:ALA:HA	1:B:423:ILE:HD12	1.93	0.49
1:D:320:ARG:NH2	1:D:444:ASP:OD1	2.46	0.48
1:C:56:MET:HB3	1:C:386:LEU:HD13	1.94	0.48
1:A:323:ILE:O	1:A:323:ILE:CG2	2.61	0.48
1:B:129:PHE:CE1	1:B:268:ALA:HB1	2.48	0.48
1:B:310:PRO:O	1:B:313:VAL:HG22	2.14	0.48
1:D:335:VAL:HA	1:D:339:MET:HE2	1.95	0.48
1:C:43:GLY:CA	1:C:71:ASN:HD22	2.26	0.48
1:C:73:VAL:HG12	1:C:73:VAL:O	2.14	0.48
1:D:67:ILE:CD1	1:D:369:VAL:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:VAL:HG22	1:D:335:VAL:HG11	1.94	0.48
1:D:298:ILE:HD13	1:D:462:VAL:O	2.12	0.48
1:B:100:ARG:HG2	1:B:116:TYR:O	2.14	0.47
1:D:400:TRP:CH2	1:D:402:PRO:HG3	2.49	0.47
1:C:335:VAL:HG13	1:C:339:MET:HE3	1.96	0.47
1:C:331:ASN:ND2	1:C:333:ASN:H	2.12	0.47
1:D:258:THR:HA	4:D:2029:HOH:O	2.13	0.47
1:B:258:THR:O	1:B:258:THR:HG22	2.15	0.47
1:C:422:CYS:HA	2:C:1478:HEM:CHA	2.44	0.47
1:B:83:PRO:HA	1:B:86:HIS:CD2	2.50	0.47
1:D:45:ILE:HD12	1:D:73:VAL:HG23	1.96	0.47
1:C:371:SER:O	1:C:372:TYR:CG	2.68	0.47
1:B:109:VAL:HG13	1:B:286:VAL:HG22	1.97	0.47
1:D:422:CYS:HA	2:D:1478:HEM:CHA	2.45	0.47
1:B:109:VAL:HG13	1:B:286:VAL:CG2	2.44	0.47
1:A:109:VAL:HG13	1:A:286:VAL:HG23	1.97	0.47
1:A:172:SER:HA	1:A:297:SER:OG	2.15	0.47
1:B:90:PHE:CG	1:B:417:ALA:HB3	2.50	0.47
1:B:335:VAL:HG21	1:B:430:LEU:HD12	1.97	0.47
1:B:114:VAL:CG1	1:B:284:MET:HE2	2.44	0.47
1:B:164:GLU:OE2	1:B:470:ARG:HD3	2.14	0.47
1:B:209:ILE:CD1	1:B:223:LEU:HD13	2.46	0.46
1:B:191:ARG:HG3	1:B:243:ILE:HD11	1.96	0.46
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.29	0.46
1:C:424:GLY:HA3	2:C:1478:HEM:C3C	2.51	0.46
1:A:331:ASN:C	1:A:331:ASN:HD22	2.19	0.46
1:A:92:PRO:HG2	1:A:97:LEU:HD22	1.98	0.46
1:C:110:PHE:CD1	1:C:115:ALA:CB	2.98	0.46
2:C:1478:HEM:HBC2	2:C:1478:HEM:HHD	1.97	0.46
1:B:166:ASN:ND2	1:B:169:GLU:H	2.14	0.46
1:D:207:SER:HB2	1:D:229:CYS:HB2	1.96	0.46
1:D:201:LEU:HD22	1:D:205:GLU:HG3	1.98	0.46
1:B:357:LEU:HD21	1:B:462:VAL:HG21	1.97	0.46
1:D:113:GLY:C	1:D:114:VAL:HG23	2.35	0.46
1:D:108:PRO:HA	1:D:233[B]:ARG:NH2	2.30	0.46
1:A:446:GLN:HB3	1:A:472:LYS:HB3	1.96	0.46
1:B:307:LEU:HD13	1:B:319:LEU:HD22	1.98	0.46
1:D:301:THR:HG22	1:D:305:LEU:HD11	1.97	0.46
1:D:191:ARG:HG3	1:D:243:ILE:HD11	1.98	0.46
1:A:146:ILE:HG23	1:A:178:THR:CG2	2.43	0.45
1:C:347:ARG:NH1	1:C:425:GLN:HE21	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:LEU:HD11	1:D:457:TYR:HD1	1.81	0.45
1:A:233:ARG:HD2	4:A:2006:HOH:O	2.17	0.45
1:A:133:GLU:HG2	1:A:261:LEU:HD12	1.97	0.45
1:D:403[B]:GLU:HG2	4:D:2053:HOH:O	2.16	0.45
1:D:102:VAL:HG23	1:D:103:TYR:CD1	2.52	0.45
1:D:166:ASN:ND2	1:D:169:GLU:H	2.14	0.45
1:A:305:LEU:HD13	1:A:453:PRO:HD2	1.98	0.45
1:B:320:ARG:O	1:B:324:GLU:HB2	2.17	0.45
1:D:295:THR:HB	2:D:1478:HEM:CAB	2.47	0.45
1:B:56:MET:HB3	1:B:386:LEU:HD13	1.99	0.45
1:B:334:ASN:O	1:B:339:MET:HG3	2.17	0.45
2:D:1478:HEM:HBB2	2:D:1478:HEM:HHC	1.99	0.45
1:C:205:GLU:OE1	1:C:294:HIS:CE1	2.70	0.45
1:C:126:GLN:HB3	1:C:284:MET:HE3	1.98	0.45
1:C:106:MET:HE1	3:C:1479:X2N:CAV	2.46	0.45
1:D:80:VAL:HG12	1:D:80:VAL:O	2.16	0.44
1:D:256:SER:O	1:D:257:SER:HB2	2.17	0.44
1:D:176:ILE:HB	1:D:293:GLN:NE2	2.32	0.44
1:D:422:CYS:HA	2:D:1478:HEM:C4D	2.53	0.44
1:C:323:ILE:O	1:C:323:ILE:HG22	2.17	0.44
1:C:78:THR:HG21	1:C:374:VAL:CG2	2.48	0.44
1:C:114:VAL:CG1	1:C:284:MET:HE1	2.47	0.44
1:C:191:ARG:HG3	1:C:243:ILE:HD11	1.99	0.44
1:A:406:GLU:OE2	1:A:410:GLY:N	2.44	0.44
1:D:319:LEU:O	1:D:323:ILE:HG13	2.17	0.44
1:D:268:ALA:HB3	1:D:276:MET:HE2	2.00	0.44
1:B:359:LEU:HD22	2:B:1478:HEM:CGA	2.46	0.44
1:A:351:ARG:HD2	1:A:388:HIS:HB3	1.99	0.44
1:A:265:LEU:HB3	1:A:276:MET:HE1	2.00	0.43
1:A:339:MET:HB3	1:A:342:ALA:HB3	2.00	0.43
1:C:449:ARG:HD3	1:C:451:GLU:O	2.17	0.43
3:D:1479:X2N:HAB1	3:D:1479:X2N:OAC	2.19	0.43
1:C:87:SER:HB2	1:C:91:LEU:HD12	2.00	0.43
1:D:335:VAL:HB	1:D:339:MET:CE	2.45	0.43
1:B:45:ILE:HG23	1:B:46:ILE:HD13	2.01	0.43
1:A:39:VAL:HG22	1:A:43:GLY:O	2.19	0.43
1:D:131:ALA:HA	1:D:423:ILE:HD12	2.01	0.43
1:A:96:VAL:HG12	1:A:97:LEU:HD13	2.00	0.43
1:D:88:ARG:HA	1:D:88:ARG:HD2	1.87	0.43
1:D:389:HIS:CD2	1:D:397:PRO:HB2	2.53	0.43
1:C:335:VAL:HA	1:C:339:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD23	1:A:423:ILE:HD11	2.00	0.43
1:B:357:LEU:HD11	1:B:462:VAL:HG21	2.01	0.43
1:C:306:HIS:CD2	1:C:400:TRP:CD1	3.07	0.43
1:A:293:GLN:HE21	1:A:293:GLN:HA	1.83	0.42
1:D:447:LEU:HD21	1:D:451:GLU:O	2.19	0.42
1:B:261:LEU:HD22	1:B:265:LEU:HD11	2.00	0.42
1:D:143:VAL:CG2	1:D:335:VAL:CG1	2.96	0.42
1:C:371:SER:O	1:C:372:TYR:CD2	2.72	0.42
1:C:335:VAL:HA	1:C:339:MET:CE	2.49	0.42
1:D:268:ALA:HB3	1:D:276:MET:CE	2.50	0.42
1:D:270:TYR:OH	1:D:276:MET:HG2	2.20	0.42
1:A:107:VAL:N	1:A:108:PRO:CD	2.82	0.42
1:D:308:MET:HB3	1:D:308:MET:HE2	1.60	0.42
1:A:295:THR:HB	2:A:1479:HEM:CAB	2.50	0.42
1:C:86:HIS:NE2	1:C:387:SER:OG	2.50	0.42
1:A:335:VAL:CA	1:A:339:MET:HE3	2.46	0.42
1:A:151:ARG:NH1	1:A:438:THR:HG23	2.34	0.42
1:D:339:MET:N	1:D:340:PRO:CD	2.83	0.42
1:C:331:ASN:H	1:C:334:ASN:HD22	1.68	0.42
1:D:129:PHE:CE1	1:D:268:ALA:HB1	2.55	0.42
1:C:178:THR:OG1	1:C:431:GLN:NE2	2.47	0.42
1:C:354:PRO:HA	1:C:355:PRO:HD3	1.89	0.41
1:D:109:VAL:HG12	1:D:110:PHE:N	2.34	0.41
1:D:114:VAL:HG13	1:D:284:MET:HE2	2.01	0.41
1:C:88:ARG:HH11	1:C:88:ARG:HG3	1.85	0.41
1:B:114:VAL:HG12	1:B:284:MET:HE2	2.02	0.41
1:A:471:VAL:CG1	1:A:472:LYS:N	2.84	0.41
1:D:217:ILE:HG22	1:D:218:LEU:CD1	2.51	0.41
1:A:319:LEU:O	1:A:323:ILE:CD1	2.68	0.41
1:C:33:PRO:HB2	1:C:63:LEU:HD22	2.03	0.41
1:A:456:ASP:O	1:A:462:VAL:HG13	2.20	0.41
1:C:176:ILE:HB	1:C:293:GLN:HE22	1.84	0.41
1:C:162:GLU:HA	1:C:473:TYR:O	2.20	0.41
1:B:270:TYR:O	1:B:272:ASP:O	2.39	0.41
1:D:331:ASN:C	1:D:331:ASN:ND2	2.74	0.41
1:D:143:VAL:HG21	1:D:335:VAL:HG11	1.98	0.41
1:C:265:LEU:HB3	1:C:276:MET:CE	2.50	0.41
1:A:335:VAL:CG2	1:A:339:MET:HE3	2.47	0.41
1:A:41:ILE:N	4:A:2003:HOH:O	2.53	0.41
1:A:265:LEU:HD22	1:A:276:MET:CE	2.50	0.41
1:D:120:TYR:N	1:D:121:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PRO:HG3	1:C:420:HIS:CE1	2.56	0.40
1:D:107:VAL:N	1:D:108:PRO:HD2	2.35	0.40
1:A:456:ASP:OD2	1:A:458[B]:HIS:HD2	2.05	0.40
1:D:177:ASN:ND2	1:D:194:ALA:HB1	2.31	0.40
3:C:1479:X2N:CAB	3:C:1479:X2N:NBF	2.83	0.40
3:A:1480:X2N:HAX2	3:A:1480:X2N:HAL	2.02	0.40
1:A:133:GLU:HG2	1:A:261:LEU:CD1	2.50	0.40
1:D:356:LEU:HD11	3:D:1479:X2N:HBC2	2.03	0.40
1:B:298:ILE:HD13	1:B:462:VAL:O	2.20	0.40
1:C:446:GLN:OE1	1:C:472:LYS:HE2	2.22	0.40
1:C:122:ARG:NE	4:C:2011:HOH:O	2.52	0.40
1:D:63:LEU:O	1:D:64:LYS:C	2.60	0.40
1:A:365:ALA:O	1:A:366:ASP:C	2.58	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	445/475 (94%)	421 (95%)	20 (4%)	4 (1%)	21	42
1	B	441/475 (93%)	422 (96%)	18 (4%)	1 (0%)	52	77
1	C	438/475 (92%)	414 (94%)	23 (5%)	1 (0%)	52	77
1	D	446/475 (94%)	406 (91%)	38 (8%)	2 (0%)	39	65
All	All	1770/1900 (93%)	1663 (94%)	99 (6%)	8 (0%)	34	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	372	TYR
1	D	40	PRO

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Mol	Chain	Res	Type
1	B	372	TYR
1	A	371	SER
1	D	475	ARG
1	A	40	PRO
1	A	104	SER
1	A	372	TYR

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	381/410 (93%)	358 (94%)	23 (6%)	24	47
1	B	375/410 (92%)	355 (95%)	20 (5%)	28	53
1	C	376/410 (92%)	356 (95%)	20 (5%)	28	53
1	D	379/410 (92%)	347 (92%)	32 (8%)	14	26
All	All	1511/1640 (92%)	1416 (94%)	95 (6%)	22	44

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	31	ASP
1	A	39	VAL
1	A	61	ARG
1	A	93	ARG
1	A	107	VAL
1	A	132	GLU
1	A	140	GLN
1	A	166	ASN
1	A	186	GLU
1	A	201	LEU
1	A	221	LEU
1	A	234	THR
1	A	247	ARG
1	A	257	SER

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Mol	Chain	Res	Type
1	A	258	THR
1	A	313	VAL
1	A	331	ASN
1	A	378	ASP
1	A	419	VAL
1	A	426	LYS
1	A	449	ARG
1	A	470	ARG
1	B	31	ASP
1	B	46	ILE
1	B	61	ARG
1	B	71	ASN
1	B	97	LEU
1	B	133	GLU
1	B	166	ASN
1	B	195	ARG
1	B	208	LEU
1	B	234	THR
1	B	238	LYS
1	B	247	ARG
1	B	261	LEU
1	B	313	VAL
1	B	331	ASN
1	B	335	VAL
1	B	343	GLU
1	B	391	GLU
1	B	419	VAL
1	B	421	LYS
1	C	31	ASP
1	C	61	ARG
1	C	88	ARG
1	C	104	SER
1	C	122	ARG
1	C	152	LYS
1	C	166	ASN
1	C	217	ILE
1	C	218	LEU
1	C	221	LEU
1	C	234	THR
1	C	279	HIS
1	C	324	GLU
1	C	325	GLU

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Mol	Chain	Res	Type
1	C	358	MET
1	C	362	LYS
1	C	376	LYS
1	C	426	LYS
1	C	449	ARG
1	C	475	ARG
1	D	31	ASP
1	D	38	THR
1	D	41	ILE
1	D	47	GLN
1	D	62	GLN
1	D	71	ASN
1	D	75	LYS
1	D	93	ARG
1	D	97	LEU
1	D	109	VAL
1	D	166	ASN
1	D	192	LEU
1	D	201	LEU
1	D	217	ILE
1	D	234	THR
1	D	241	SER
1	D	258	THR
1	D	261	LEU
1	D	271	ARG
1	D	286	VAL
1	D	293	GLN
1	D	329	GLN
1	D	331	ASN
1	D	335	VAL
1	D	358	MET
1	D	362	LYS
1	D	409	GLU
1	D	426	LYS
1	D	449	ARG
1	D	472	LYS
1	D	475	ARG
1	D	476	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	62	GLN
1	A	166	ASN
1	A	181	GLN
1	A	293	GLN
1	A	294	HIS
1	A	329	GLN
1	A	331	ASN
1	A	334	ASN
1	A	425	GLN
1	A	431	GLN
1	B	62	GLN
1	B	71	ASN
1	B	166	ASN
1	B	293	GLN
1	B	331	ASN
1	B	334	ASN
1	B	425	GLN
1	B	431	GLN
1	C	71	ASN
1	C	157	ASN
1	C	166	ASN
1	C	279	HIS
1	C	293	GLN
1	C	294	HIS
1	C	331	ASN
1	C	334	ASN
1	C	431	GLN
1	D	71	ASN
1	D	166	ASN
1	D	177	ASN
1	D	181	GLN
1	D	293	GLN
1	D	294	HIS
1	D	306	HIS
1	D	329	GLN
1	D	331	ASN
1	D	334	ASN
1	D	431	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1479	1,3	30,50,50	2.58	6 (20%)	24,82,82	2.57	12 (50%)
3	X2N	A	1480	2	46,57,57	1.71	4 (8%)	51,82,82	2.26	15 (29%)
2	HEM	B	1478	1,3	30,50,50	2.43	4 (13%)	24,82,82	2.73	9 (37%)
3	X2N	B	1479	2	46,57,57	1.76	5 (10%)	51,82,82	2.47	16 (31%)
2	HEM	C	1478	1,3	30,50,50	2.48	5 (16%)	24,82,82	2.19	8 (33%)
3	X2N	C	1479	2	46,57,57	1.91	4 (8%)	51,82,82	2.63	17 (33%)
2	HEM	D	1478	1,3	30,50,50	2.22	5 (16%)	24,82,82	2.24	8 (33%)
3	X2N	D	1479	2	46,57,57	1.81	6 (13%)	51,82,82	2.40	17 (33%)

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	1479	1,3	-	0/10/54/54	0/0/8/8
3	X2N	A	1480	2	-	1/34/59/59	1/7/7/7
2	HEM	B	1478	1,3	-	0/10/54/54	0/0/8/8
3	X2N	B	1479	2	-	1/34/59/59	1/7/7/7
2	HEM	C	1478	1,3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X2N	C	1479	2	-	1/34/59/59	1/7/7/7
2	HEM	D	1478	1,3	-	0/10/54/54	0/0/8/8
3	X2N	D	1479	2	-	0/34/59/59	0/7/7/7

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1479	HEM	C3B-C4B	-10.86	1.42	1.51
2	B	1478	HEM	C3B-C4B	-9.67	1.43	1.51
2	C	1478	HEM	C3B-C4B	-9.21	1.43	1.51
3	C	1479	X2N	CBN-NBW	-8.40	1.34	1.44
3	B	1479	X2N	CBN-NBW	-8.08	1.34	1.44
2	D	1478	HEM	C3B-C4B	-7.73	1.45	1.51
3	D	1479	X2N	CBN-NBW	-7.44	1.35	1.44
3	A	1480	X2N	CBN-NBW	-7.06	1.35	1.44
2	D	1478	HEM	C3D-C4D	-5.75	1.44	1.51
2	B	1478	HEM	C3D-C4D	-5.62	1.44	1.51
2	C	1478	HEM	C3D-C4D	-5.51	1.44	1.51
2	C	1478	HEM	C2C-C1C	-5.37	1.42	1.52
2	A	1479	HEM	C3D-C4D	-5.24	1.44	1.51
2	D	1478	HEM	C2C-C1C	-4.20	1.44	1.52
2	B	1478	HEM	C2C-C1C	-3.87	1.45	1.52
2	A	1479	HEM	C2C-C1C	-3.39	1.46	1.52
3	D	1479	X2N	C2-CAR	-2.62	1.50	1.52
2	B	1478	HEM	C2D-C1D	-2.59	1.43	1.51
2	A	1479	HEM	C2D-C1D	-2.38	1.44	1.51
3	A	1480	X2N	FAE-CBI	-2.18	1.30	1.35
3	B	1479	X2N	C2-CAR	-2.00	1.50	1.52
2	A	1479	HEM	CMA-C3A	2.03	1.55	1.51
2	C	1478	HEM	CAA-C2A	2.04	1.55	1.52
3	B	1479	X2N	NBE-NBV	2.12	1.38	1.35
3	D	1479	X2N	CAN-CBN	2.20	1.42	1.38
2	D	1478	HEM	CMA-C3A	2.26	1.56	1.51
2	D	1478	HEM	FE-NC	2.38	2.05	1.95
3	D	1479	X2N	NBE-NBV	2.55	1.39	1.35
2	A	1479	HEM	FE-NC	2.55	2.05	1.95
3	C	1479	X2N	NBE-NBV	3.01	1.39	1.35
2	C	1478	HEM	FE-NC	3.04	2.07	1.95
3	D	1479	X2N	CAT-NBF	3.93	1.36	1.30
3	B	1479	X2N	CAT-NBF	4.25	1.37	1.30
3	A	1480	X2N	CAT-NBF	4.37	1.37	1.30
3	C	1479	X2N	CAT-NBF	4.71	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1479	X2N	CAR-CBI	5.35	1.47	1.38
3	C	1479	X2N	CAR-CBI	6.03	1.48	1.38
3	A	1480	X2N	CAR-CBI	6.16	1.48	1.38
3	D	1479	X2N	CAR-CBI	6.36	1.48	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1478	HEM	C3C-CAC-CBC	-6.43	114.60	124.46
3	C	1479	X2N	CAY-NBU-CBM	-5.53	103.09	117.92
3	D	1479	X2N	CAX-CAZ-NBU	-5.34	100.05	110.63
3	B	1479	X2N	CAJ-CBL-NBT	-4.88	114.82	121.38
3	A	1480	X2N	CAY-NBU-CBM	-4.81	105.02	117.92
2	D	1478	HEM	C3C-CAC-CBC	-4.60	117.40	124.46
3	D	1479	X2N	CAG-CBI-CAR	-4.45	120.77	124.21
3	B	1479	X2N	C2-CAR-CBI	-4.12	119.56	122.90
3	C	1479	X2N	CAL-CBM-NBU	-4.07	115.92	121.38
3	A	1480	X2N	CAO-CBN-CAN	-3.96	115.06	121.21
2	A	1479	HEM	C3C-CAC-CBC	-3.96	118.38	124.46
2	A	1479	HEM	C3B-CAB-CBB	-3.76	118.69	124.46
3	B	1479	X2N	CAO-CBN-CAN	-3.72	115.43	121.21
3	C	1479	X2N	CAG-CBI-CAR	-3.65	121.39	124.21
3	C	1479	X2N	CAO-CBN-CAN	-3.54	115.71	121.21
3	B	1479	X2N	CAG-CBI-CAR	-3.49	121.52	124.21
3	D	1479	X2N	C2-CAR-CBI	-3.33	120.20	122.90
3	D	1479	X2N	CAW-CAY-NBU	-3.27	104.14	110.63
3	C	1479	X2N	CBO-CAP-CAG	-3.14	119.29	123.35
3	D	1479	X2N	CAO-CBN-CAN	-3.12	116.36	121.21
3	D	1479	X2N	CAJ-CBL-NBT	-2.88	117.51	121.38
3	D	1479	X2N	CAX-NBT-CBL	-2.84	110.32	117.92
3	D	1479	X2N	CAL-CBM-NBU	-2.82	117.59	121.38
3	A	1480	X2N	CAM-CBM-NBU	-2.77	117.66	121.38
2	B	1478	HEM	C3B-CAB-CBB	-2.66	120.38	124.46
3	D	1479	X2N	CAZ-NBU-CBM	-2.63	110.86	117.92
3	A	1480	X2N	CBO-CAP-CAG	-2.59	120.01	123.35
2	D	1478	HEM	C3B-CAB-CBB	-2.57	120.52	124.46
3	B	1479	X2N	CAY-CAW-NBT	-2.53	105.61	110.63
2	C	1478	HEM	C3C-CAC-CBC	-2.50	120.61	124.46
2	A	1479	HEM	CBD-CAD-C3D	-2.47	106.35	113.55
3	B	1479	X2N	CAZ-NBU-CBM	-2.46	111.32	117.92
2	C	1478	HEM	C1D-CHD-C4C	-2.33	121.93	125.82
2	A	1479	HEM	CAA-C2A-C1A	-2.19	124.63	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1479	X2N	C2-CAR-CBI	-2.16	121.15	122.90
2	B	1478	HEM	CAD-CBD-CGD	-2.03	104.74	113.02
3	A	1480	X2N	CAV-C7-CBB	2.01	118.06	110.86
3	A	1480	X2N	CAO-CBN-NBW	2.02	122.27	119.50
2	A	1479	HEM	CHC-C4B-NB	2.05	129.46	124.52
3	C	1479	X2N	CAB-CBQ-CBS	2.06	116.35	112.59
3	A	1480	X2N	OBG-CBB-C7	2.06	112.72	107.97
2	A	1479	HEM	C2C-C1C-CHC	2.09	126.86	123.68
2	D	1478	HEM	CMC-C2C-C3C	2.12	121.83	116.53
2	B	1478	HEM	CAD-C3D-C4D	2.12	119.96	112.47
2	C	1478	HEM	C2D-C3D-C4D	2.15	105.14	101.50
3	A	1480	X2N	CAL-CBM-NBU	2.16	124.29	121.38
3	B	1479	X2N	CBB-OBG-CBK	2.25	122.72	117.89
2	A	1479	HEM	C2D-C3D-C4D	2.28	105.37	101.50
3	B	1479	X2N	C2-CAV-C7	2.28	105.86	103.78
3	B	1479	X2N	CAX-NBT-CAW	2.29	116.39	111.59
2	D	1478	HEM	C3B-C4B-CHC	2.31	126.41	123.16
3	A	1480	X2N	CAN-CBN-NBW	2.32	122.67	119.50
3	B	1479	X2N	OBG-CBB-C7	2.32	113.31	107.97
3	D	1479	X2N	CAK-CBL-NBT	2.40	124.61	121.38
3	D	1479	X2N	CBI-CAG-CAP	2.46	119.20	116.63
2	B	1478	HEM	CAA-C2A-C1A	2.58	129.81	127.01
3	A	1480	X2N	CBB-OBG-CBK	2.64	123.56	117.89
3	B	1479	X2N	CBJ-CBO-CAP	2.64	121.20	118.35
3	D	1479	X2N	CAL-CAN-CBN	2.67	121.95	119.23
3	D	1479	X2N	CAO-CBN-NBW	2.67	123.16	119.50
3	C	1479	X2N	CAX-NBT-CAW	2.75	117.36	111.59
2	A	1479	HEM	CMD-C2D-C3D	2.75	126.52	114.35
3	D	1479	X2N	CAM-CAO-CBN	2.83	122.11	119.23
3	C	1479	X2N	CAM-CAO-CBN	2.84	122.13	119.23
2	C	1478	HEM	CMD-C2D-C3D	2.97	127.49	114.35
2	D	1478	HEM	CMD-C2D-C3D	3.02	127.72	114.35
2	C	1478	HEM	CMC-C2C-C3C	3.03	124.09	116.53
3	B	1479	X2N	CAO-CBN-NBW	3.08	123.71	119.50
3	C	1479	X2N	CAO-CBN-NBW	3.10	123.75	119.50
3	A	1480	X2N	CAL-CAN-CBN	3.12	122.41	119.23
3	C	1479	X2N	CBJ-CBO-CAP	3.14	121.74	118.35
2	C	1478	HEM	CAD-C3D-C4D	3.15	123.59	112.47
2	B	1478	HEM	CMB-C2B-C3B	3.16	124.41	116.53
3	D	1479	X2N	CBJ-CBO-CAP	3.20	121.81	118.35
3	D	1479	X2N	OBG-CBB-C7	3.27	115.50	107.97
3	B	1479	X2N	CAM-CAO-CBN	3.29	122.58	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1478	HEM	CMB-C2B-C3B	3.33	124.83	116.53
3	B	1479	X2N	CAL-CAN-CBN	3.41	122.70	119.23
3	C	1479	X2N	CBI-CAG-CAP	3.43	120.22	116.63
3	C	1479	X2N	C2-CAV-C7	3.58	107.03	103.78
2	D	1478	HEM	CAD-C3D-C4D	3.60	125.17	112.47
3	C	1479	X2N	OBG-CBB-C7	3.71	116.52	107.97
3	A	1480	X2N	CBJ-CBO-CAP	3.78	122.43	118.35
2	B	1478	HEM	CMC-C2C-C3C	3.84	126.11	116.53
3	C	1479	X2N	CAM-CBM-NBU	3.89	126.61	121.38
2	B	1478	HEM	CMD-C2D-C3D	3.91	131.64	114.35
3	C	1479	X2N	CAL-CAN-CBN	3.91	123.21	119.23
3	A	1480	X2N	CAM-CAO-CBN	4.03	123.33	119.23
2	C	1478	HEM	CMB-C2B-C3B	4.15	126.88	116.53
2	A	1479	HEM	CMC-C2C-C3C	4.19	127.00	116.53
2	A	1479	HEM	CAD-C3D-C4D	4.26	127.49	112.47
3	B	1479	X2N	CAK-CBL-NBT	4.52	127.46	121.38
2	A	1479	HEM	CMB-C2B-C3B	4.59	127.99	116.53
2	A	1479	HEM	CAD-C3D-C2D	4.84	127.13	113.22
3	A	1480	X2N	C2-CAV-C7	5.30	108.60	103.78
2	D	1478	HEM	CAD-C3D-C2D	5.82	129.94	113.22
2	C	1478	HEM	CAD-C3D-C2D	6.25	131.19	113.22
2	B	1478	HEM	CAD-C3D-C2D	7.68	135.30	113.22
3	A	1480	X2N	CAS-NBD-CAQ	9.09	108.30	102.25
3	D	1479	X2N	CAS-NBD-CAQ	9.55	108.61	102.25
3	B	1479	X2N	CAS-NBD-CAQ	10.72	109.39	102.25
3	C	1479	X2N	CAS-NBD-CAQ	11.19	109.70	102.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1479	X2N	C2-CBC-NBV-CAS
3	A	1480	X2N	C2-CBC-NBV-CAS
3	B	1479	X2N	C2-CBC-NBV-CAS

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1479	X2N	CAW-CAX-CAY-CAZ-NBT-NBU
3	A	1480	X2N	CAW-CAX-CAY-CAZ-NBT-NBU
3	B	1479	X2N	CAW-CAX-CAY-CAZ-NBT-NBU

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1479	HEM	4	0
3	A	1480	X2N	2	0
2	B	1478	HEM	7	0
2	C	1478	HEM	4	0
3	C	1479	X2N	5	0
2	D	1478	HEM	5	0
3	D	1479	X2N	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	448/475 (94%)	-0.13	10 (2%)	65	59	43, 53, 67, 74	0
1	B	444/475 (93%)	-0.15	13 (2%)	55	48	43, 54, 67, 74	0
1	C	441/475 (92%)	-0.19	6 (1%)	78	74	43, 53, 67, 74	0
1	D	447/475 (94%)	-0.19	8 (1%)	71	66	44, 54, 68, 76	0
All	All	1780/1900 (93%)	-0.16	37 (2%)	67	61	43, 54, 68, 76	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	257	SER	5.8
1	A	257	SER	3.9
1	A	478	ALA	3.7
1	D	258	THR	3.7
1	C	258	THR	3.7
1	A	251	ALA	3.5
1	A	258	THR	3.2
1	A	252	VAL	3.1
1	C	477	LYS	3.0
1	D	228	ARG	3.0
1	D	257	SER	3.0
1	B	258	THR	2.9
1	A	254	LYS	2.9
1	B	458[A]	HIS	2.9
1	A	253	ASN	2.9
1	B	371	SER	2.7
1	B	391	GLU	2.7
1	B	38	THR	2.7
1	D	252	VAL	2.6
1	B	141	ASN	2.5
1	D	324	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	228	ARG	2.5
1	D	458	HIS	2.5
1	B	30	THR	2.4
1	C	259	SER	2.4
1	B	79	ILE	2.3
1	D	254	LYS	2.3
1	A	477	LYS	2.2
1	C	371	SER	2.2
1	B	381	ALA	2.1
1	C	64	LYS	2.1
1	A	325	GLU	2.1
1	B	396	GLU	2.1
1	D	256	SER	2.1
1	B	61	ARG	2.1
1	A	403	GLU	2.1
1	B	370	GLY	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	X2N	C	1479	51/51	0.84	0.21	1.49	21,44,78,78	0
3	X2N	D	1479	51/51	0.86	0.19	0.87	28,44,75,76	0
3	X2N	A	1480	51/51	0.87	0.20	0.46	17,41,72,73	0
2	HEM	D	1478	43/43	0.97	0.16	0.19	38,45,51,56	0
2	HEM	B	1478	43/43	0.98	0.15	0.10	46,52,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	X2N	B	1479	51/51	0.90	0.15	-0.18	35,47,73,73	0
2	HEM	C	1478	43/43	0.98	0.14	-0.35	47,49,54,57	0
2	HEM	A	1479	43/43	0.98	0.14	-0.35	38,44,47,49	0

6.5 Other polymers (i)

There are no such residues in this entry.