Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:25 AM GMT

PDB ID	:	2QPE
Title	:	An unexpected outcome of surface-engineering an integral membrane protein: Improved crystallization of cytochrome ba3 oxidase from Thermus thermophilus
Authors	:	Liu, B.; Luna, V.M.; Chen, Y.; Stout, C.D.; Fee, J.A.
Deposited on	:	2007-07-23
Resolution	:	2.90 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 (i)) 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 2.90 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	Percentile Ranks	Value
Rfree		0.285
Clashscore		32
Ramachandran outliers		4.7%
Sidechain outliers		15.8%
RSRZ outliers		4.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
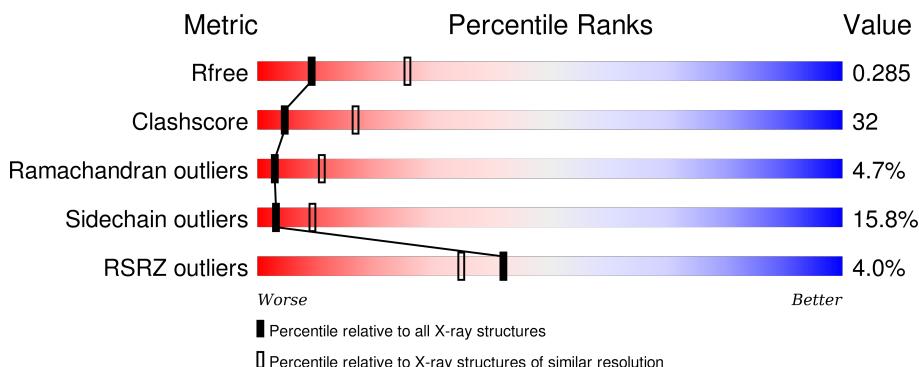
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	568	4% ■ 40% / 46% / 11% ··
2	B	168	3% ■ 51% / 42% / 6% ·
3	C	34	44% / 38% / 15% ·
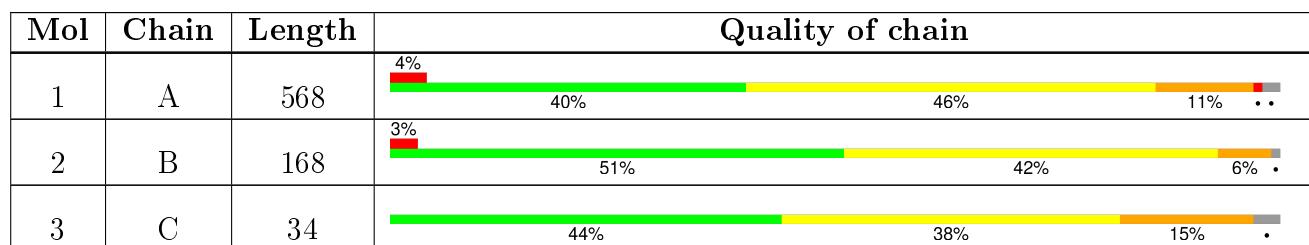
2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6077 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total 4409	C 2985	N 709	O 699	S 16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	258	ARG	LYS	ENGINEERED	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total 1298	C 844	N 217	O 233	S 4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	ENGINEERED	UNP Q5SJ80

- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total 259	C 179	N 39	O 41	0	0	0

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total　Cu 1　　　1		0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
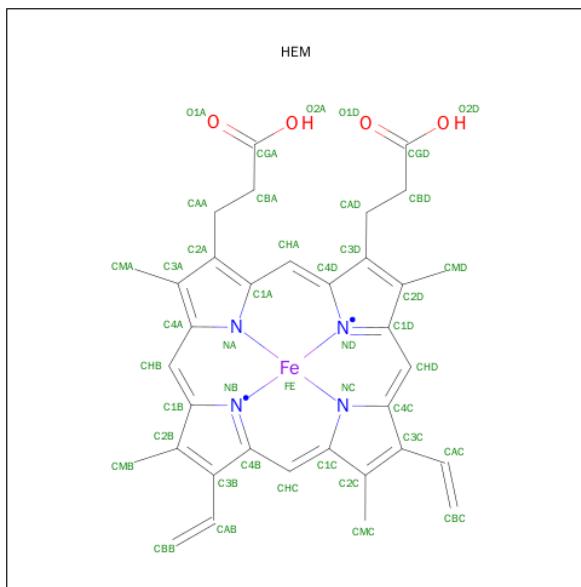
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 65	C 54	Fe 1	N 4	O 6	0	0

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).
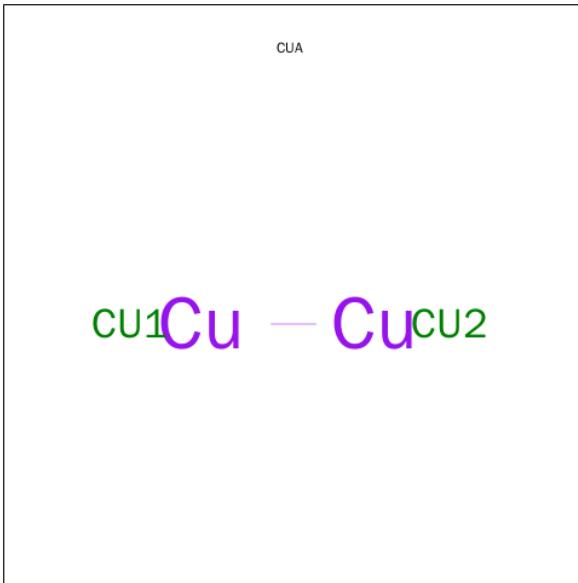
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 2	Cu 2	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Cytochrome c oxidase subunit 1
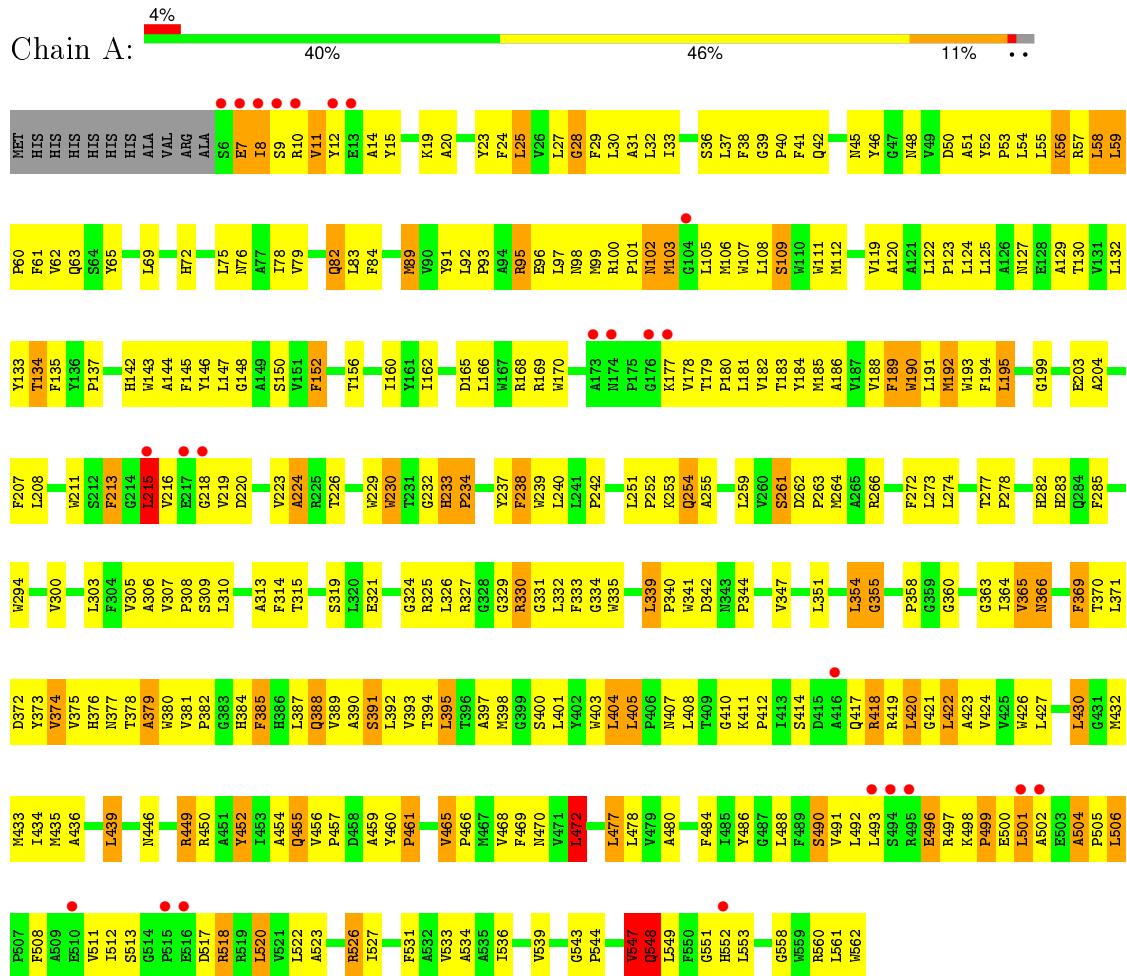
• Molecule 2: Cytochrome c oxidase subunit 2

P76 N77 Q78 Y82 V83 L84 A85 F86 A87 F88 P92 I95 E96 V97 P98 Q99 G100 A101 E102 I103 V104 F105 K106 I107 D111 V112 I113 E119 N122 V127 V132 S133 T134 V135 R136 F139 K140 R141 P142 Y145 R146 I147 I148 C149 N150 G154 L155 G156 H157

Q158 N159 M160 F161 V166 K167 E168

• Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:

44%   38%   15%   •

MET E2 K6 L9 A10 V11 I12 L13 V14 L15 T16 L20 L24 G25 V26 Y27 A28 V29 F30 F31 A32 R33 G34

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.64Å 114.64Å 148.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.99-2.90) 95.1 (19.99-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.33 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.302 0.196 , 0.285	Depositor DCC
R_{free} test set	1083 reflections (5.33%)	DCC
Wilson B-factor (Å²)	93.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 78.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\|L\|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 21408 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HAS, CUA, CU1

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	0.95	2/4566 (0.0%)	1.05	13/6266 (0.2%)
2	B	0.92	1/1335 (0.1%)	1.03	1/1822 (0.1%)
3	C	1.08	0/265	1.03	0/359
All	All	0.95	3/6166 (0.0%)	1.04	14/8447 (0.2%)

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	A	0	1
2	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	TRP	CB-CG	5.94	1.60	1.50
2	B	16	LYS	CE-NZ	5.44	1.62	1.49
1	A	203	GLU	CB-CG	5.21	1.62	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	CB-CG-CD1	-10.17	93.71	111.00
1	A	493	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	215	LEU	CA-CB-CG	6.22	129.61	115.30
2	B	37	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	520	LEU	CA-CB-CG	5.76	128.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	75	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	354	LEU	CB-CG-CD1	5.34	120.07	111.00
1	A	192	MET	CG-SD-CE	5.31	108.70	100.20
1	A	218	GLY	N-CA-C	5.21	126.12	113.10
1	A	371	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	A	472	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	A	58	LEU	CB-CG-CD1	5.15	119.76	111.00
1	A	122	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	ILE	Peptide
2	B	87	ALA	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	4409	0	4515	339	0
2	B	1298	0	1282	61	0
3	C	259	0	279	11	0
4	A	1	0	0	0	0
5	A	43	0	30	7	0
6	A	65	0	61	15	0
7	B	2	0	0	0	0
All	All	6077	0	6167	392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.71	1.53
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.79	1.27
1:A:385:PHE:CB	6:A:801:HAS:HMA2	1.73	1.18
1:A:385:PHE:CG	6:A:801:HAS:HMA2	1.81	1.16
1:A:410:GLY:CA	1:A:502:ALA:HB2	1.74	1.16
1:A:182:VAL:HG21	1:A:508:PHE:HE2	1.08	1.12
1:A:518:ARG:HH21	1:A:518:ARG:HG3	1.08	1.11
1:A:7:GLU:HB3	1:A:10:ARG:HA	1.30	1.08
1:A:182:VAL:HG21	1:A:508:PHE:CE2	1.91	1.04
1:A:410:GLY:HA2	1:A:502:ALA:CB	1.90	1.01
2:B:142:PRO:HA	2:B:166:VAL:CG2	1.90	1.00
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.48	0.95
1:A:506:LEU:HD23	1:A:506:LEU:H	1.32	0.94
1:A:385:PHE:HB2	6:A:801:HAS:CMA	1.98	0.93
1:A:410:GLY:HA2	1:A:502:ALA:HB2	0.94	0.93
1:A:430:LEU:O	1:A:434:ILE:HG13	1.70	0.91
1:A:562:TRP:HA	2:B:155:LEU:HD12	1.52	0.91
1:A:518:ARG:NH2	1:A:518:ARG:HG3	1.79	0.91
1:A:497:ARG:C	1:A:499:PRO:HD3	1.91	0.90
1:A:76:ASN:HB3	5:A:800:HEM:HBC2	1.53	0.89
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.61	0.89
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.91	0.88
1:A:385:PHE:HB2	6:A:801:HAS:HMA2	1.52	0.88
1:A:412:PRO:HB3	1:A:501:LEU:HD21	1.56	0.87
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.91	0.87
1:A:385:PHE:CB	6:A:801:HAS:CMA	2.53	0.87
1:A:12:TYR:CD1	1:A:19:LYS:HB2	2.10	0.86
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.58	0.85
1:A:45:ASN:ND2	1:A:65:TYR:CE1	2.47	0.83
1:A:385:PHE:CG	6:A:801:HAS:CMA	2.61	0.83
1:A:7:GLU:CB	1:A:10:ARG:HA	2.11	0.81
1:A:329:GLY:HA2	1:A:330:ARG:HE	1.43	0.81
1:A:374:VAL:HG12	1:A:375:VAL:HG13	1.63	0.80
1:A:454:ALA:O	1:A:457:PRO:HG3	1.80	0.80
1:A:277:THR:H	1:A:278:PRO:HD2	1.46	0.80
1:A:233:HIS:CE1	1:A:282:HIS:HE1	2.01	0.79
1:A:277:THR:N	1:A:278:PRO:HD2	1.98	0.78
1:A:385:PHE:CD2	6:A:801:HAS:HMA2	2.19	0.78
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.19	0.78
1:A:307:VAL:HA	1:A:310:LEU:HD12	1.65	0.77
1:A:162:ILE:O	1:A:165:ASP:HB3	1.84	0.77
1:A:124:LEU:HD21	1:A:145:PHE:HD1	1.46	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLY:CA	1:A:502:ALA:CB	2.60	0.74
1:A:547:VAL:HG12	1:A:548:GLN:N	2.02	0.74
2:B:92:PRO:HD2	2:B:95:ILE:HD11	1.68	0.74
1:A:124:LEU:HD21	1:A:145:PHE:CD1	2.21	0.74
1:A:108:LEU:O	1:A:112:MET:HG3	1.87	0.74
1:A:518:ARG:HH21	1:A:518:ARG:CG	1.95	0.73
1:A:549:LEU:O	1:A:553:LEU:HD23	1.88	0.73
2:B:103:ILE:HD13	2:B:139:PHE:HD1	1.54	0.73
1:A:497:ARG:O	1:A:499:PRO:HD3	1.89	0.73
1:A:63:GLN:CG	1:A:127:ASN:HD22	2.02	0.73
1:A:10:ARG:O	1:A:12:TYR:N	2.22	0.72
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.20	0.72
1:A:52:TYR:O	1:A:56:LYS:HB2	1.90	0.72
1:A:370:THR:HA	1:A:373:TYR:CE1	2.25	0.72
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.72	0.71
1:A:407:ASN:HD21	1:A:506:LEU:CD2	2.03	0.71
1:A:152:PHE:CD2	1:A:152:PHE:C	2.62	0.71
1:A:107:TRP:O	1:A:111:TRP:HD1	1.73	0.71
1:A:365:VAL:HG12	1:A:366:ASN:N	2.05	0.71
1:A:390:ALA:O	1:A:394:THR:HB	1.91	0.71
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.78	0.70
1:A:152:PHE:HD2	1:A:152:PHE:C	1.95	0.70
1:A:407:ASN:HD21	1:A:506:LEU:HD23	1.56	0.70
1:A:331:GLY:H	1:A:334:GLY:HA3	1.57	0.70
1:A:455:GLN:C	1:A:457:PRO:HD3	2.11	0.70
1:A:459:ALA:C	1:A:461:PRO:HD2	2.12	0.70
1:A:277:THR:N	1:A:278:PRO:CD	2.55	0.70
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.27	0.69
1:A:277:THR:H	1:A:278:PRO:CD	2.05	0.69
1:A:7:GLU:HB3	1:A:10:ARG:CA	2.15	0.69
1:A:220:ASP:OD2	2:B:52:ARG:NH1	2.26	0.69
1:A:76:ASN:HB3	5:A:800:HEM:CBC	2.21	0.69
1:A:27:LEU:HD23	1:A:83:LEU:CD2	2.23	0.68
1:A:233:HIS:CE1	1:A:282:HIS:CE1	2.80	0.68
1:A:329:GLY:HA2	1:A:330:ARG:NE	2.09	0.68
2:B:97:VAL:O	2:B:166:VAL:HA	1.93	0.68
1:A:27:LEU:HD23	1:A:83:LEU:HD22	1.74	0.68
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.28	0.68
1:A:321:GLU:OE1	1:A:325:ARG:NH2	2.26	0.67
2:B:55:PRO:O	2:B:58:VAL:HG12	1.94	0.67
1:A:499:PRO:HB3	1:A:502:ALA:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:HB3	6:A:801:HAS:HMC3	1.76	0.66
1:A:14:ALA:O	1:A:100:ARG:NH1	2.29	0.66
1:A:294:TRP:HZ2	1:A:544:PRO:HG2	1.60	0.65
1:A:234:PRO:HG3	1:A:277:THR:HA	1.79	0.65
1:A:152:PHE:CD2	1:A:152:PHE:O	2.50	0.65
1:A:97:LEU:HD21	1:A:180:PRO:HG2	1.78	0.65
2:B:86:PHE:O	2:B:88:PHE:N	2.28	0.65
1:A:63:GLN:HG3	1:A:127:ASN:HD22	1.60	0.65
1:A:45:ASN:ND2	1:A:65:TYR:HE1	1.96	0.64
1:A:156:THR:O	1:A:160:ILE:HG13	1.98	0.64
1:A:330:ARG:N	1:A:330:ARG:HD2	2.12	0.64
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.33	0.64
1:A:59:LEU:HB2	1:A:61:PHE:HE1	1.62	0.64
1:A:506:LEU:H	1:A:506:LEU:CD2	2.02	0.63
1:A:414:SER:OG	1:A:417:GLN:HG3	1.97	0.63
1:A:435:MET:HG2	1:A:439:LEU:HD22	1.79	0.63
1:A:330:ARG:N	1:A:330:ARG:CD	2.61	0.63
1:A:107:TRP:O	1:A:111:TRP:CD1	2.52	0.62
1:A:213:PHE:HB3	1:A:215:LEU:HD22	1.80	0.62
1:A:120:ALA:O	1:A:123:PRO:HD2	2.00	0.62
1:A:342:ASP:HB2	1:A:418:ARG:HH22	1.64	0.62
1:A:28:GLY:O	1:A:31:ALA:HB3	1.99	0.62
1:A:233:HIS:ND1	1:A:282:HIS:HE1	1.94	0.61
1:A:78:ILE:HG22	1:A:79:VAL:N	2.14	0.61
1:A:233:HIS:CD2	1:A:237:TYR:CD2	2.89	0.61
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.81	0.61
1:A:477:LEU:HA	1:A:480:ALA:HB3	1.83	0.61
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.31	0.61
1:A:385:PHE:O	1:A:389:VAL:HG12	2.01	0.61
2:B:142:PRO:HA	2:B:166:VAL:HG21	1.81	0.60
1:A:477:LEU:HD13	5:A:800:HEM:HMB1	1.83	0.60
2:B:83:VAL:HG12	2:B:84:LEU:N	2.17	0.60
1:A:233:HIS:C	1:A:233:HIS:CD2	2.74	0.60
1:A:335:TRP:O	1:A:339:LEU:HD22	2.02	0.60
1:A:370:THR:HA	1:A:373:TYR:CD1	2.36	0.60
1:A:56:LYS:O	1:A:60:PRO:HA	2.01	0.60
1:A:539:VAL:O	1:A:543:GLY:HA3	2.03	0.59
1:A:102:ASN:OD1	1:A:102:ASN:O	2.21	0.59
1:A:307:VAL:HA	1:A:310:LEU:CD1	2.32	0.59
1:A:385:PHE:HB2	6:A:801:HAS:HMA1	1.84	0.59
1:A:388:GLN:HE21	1:A:388:GLN:N	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:O	1:A:53:PRO:HD2	2.03	0.58
1:A:52:TYR:N	1:A:53:PRO:HD2	2.19	0.58
1:A:342:ASP:O	1:A:418:ARG:NH2	2.36	0.58
2:B:92:PRO:HD2	2:B:95:ILE:CD1	2.32	0.58
1:A:233:HIS:HB3	1:A:234:PRO:HD2	1.84	0.58
1:A:547:VAL:CG1	1:A:548:GLN:N	2.67	0.58
1:A:137:PRO:HG2	1:A:224:ALA:CB	2.34	0.58
1:A:137:PRO:CG	1:A:224:ALA:HB1	2.33	0.58
1:A:59:LEU:HB2	1:A:61:PHE:CE1	2.37	0.58
1:A:420:LEU:HD12	1:A:424:VAL:HG23	1.84	0.58
1:A:186:ALA:O	1:A:190:TRP:HD1	1.86	0.57
1:A:186:ALA:O	1:A:190:TRP:CD1	2.57	0.57
1:A:400:SER:O	1:A:404:LEU:HB2	2.04	0.57
1:A:523:ALA:O	1:A:526:ARG:HG3	2.03	0.57
1:A:310:LEU:O	1:A:313:ALA:HB3	2.04	0.57
1:A:137:PRO:HG2	1:A:224:ALA:HB1	1.85	0.57
1:A:562:TRP:CA	2:B:155:LEU:HD12	2.30	0.57
1:A:446:ASN:OD1	2:B:119:GLU:HG3	2.04	0.57
1:A:98:ASN:O	1:A:98:ASN:ND2	2.38	0.57
1:A:146:TYR:CD2	1:A:208:LEU:HD13	2.41	0.56
1:A:211:TRP:HZ2	1:A:558:GLY:HA3	1.70	0.56
2:B:32:LEU:O	2:B:35:TYR:HB3	2.06	0.56
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.41	0.56
1:A:261:SER:HB3	1:A:264:MET:HB2	1.87	0.56
1:A:63:GLN:CG	1:A:127:ASN:ND2	2.67	0.56
1:A:377:ASN:HB3	2:B:150:ASN:O	2.06	0.56
1:A:459:ALA:O	2:B:146:ARG:NH1	2.34	0.56
1:A:119:VAL:HG12	1:A:148:GLY:CA	2.35	0.56
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.87	0.55
1:A:91:TYR:CE1	1:A:95:ARG:HD2	2.42	0.55
1:A:410:GLY:HA3	1:A:499:PRO:HG3	1.88	0.55
1:A:191:LEU:HB3	1:A:531:PHE:CD2	2.41	0.55
1:A:20:ALA:HB3	1:A:106:MET:CE	2.38	0.54
1:A:330:ARG:H	1:A:334:GLY:HA3	1.73	0.54
2:B:70:ALA:HB1	2:B:82:TYR:O	2.07	0.54
1:A:314:PHE:CZ	2:B:14:TYR:HB3	2.43	0.54
1:A:391:SER:O	1:A:395:LEU:HD12	2.07	0.54
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.41	0.54
1:A:388:GLN:CA	1:A:388:GLN:NE2	2.70	0.54
1:A:389:VAL:HG22	5:A:800:HEM:HAC	1.88	0.54
1:A:547:VAL:HG12	1:A:548:GLN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:CD1	1:A:274:LEU:N	2.70	0.54
1:A:456:VAL:O	1:A:456:VAL:HG23	2.08	0.54
2:B:157:HIS:O	2:B:159:ASN:N	2.40	0.54
1:A:551:GLY:C	1:A:552:HIS:ND1	2.61	0.54
1:A:460:TYR:N	1:A:461:PRO:CD	2.70	0.54
2:B:96:GLU:HB3	2:B:167:LYS:NZ	2.22	0.54
1:A:152:PHE:HD2	1:A:152:PHE:O	1.90	0.53
1:A:344:PRO:HG3	1:A:422:LEU:HG	1.90	0.53
2:B:105:PHE:CZ	2:B:139:PHE:HE1	2.26	0.53
1:A:300:VAL:HG22	2:B:30:ILE:HD13	1.90	0.53
2:B:42:ALA:HB1	2:B:45:ILE:HD12	1.90	0.53
3:C:26:VAL:O	3:C:27:TYR:C	2.47	0.53
2:B:3:ASP:OD1	3:C:2:GLU:HB3	2.09	0.53
1:A:181:LEU:O	1:A:185:MET:HG3	2.09	0.53
1:A:388:GLN:HA	1:A:388:GLN:NE2	2.24	0.53
1:A:135:PHE:O	1:A:137:PRO:HD3	2.08	0.53
1:A:20:ALA:HB3	1:A:106:MET:HE1	1.90	0.52
1:A:106:MET:O	1:A:109:SER:HB3	2.08	0.52
1:A:423:ALA:O	1:A:427:LEU:HB2	2.10	0.52
1:A:391:SER:HB2	1:A:395:LEU:HD11	1.92	0.52
1:A:189:PHE:O	1:A:192:MET:N	2.41	0.52
2:B:105:PHE:HZ	2:B:139:PHE:HE1	1.58	0.52
1:A:274:LEU:N	1:A:274:LEU:HD12	2.22	0.52
1:A:426:TRP:O	1:A:430:LEU:HD22	2.11	0.51
3:C:10:ALA:O	3:C:14:VAL:HG23	2.10	0.51
1:A:36:SER:O	1:A:40:PRO:HD3	2.10	0.51
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.92	0.51
1:A:513:SER:O	2:B:5:HIS:CE1	2.63	0.51
1:A:195:LEU:CD2	1:A:534:ALA:HB1	2.40	0.51
1:A:240:LEU:HA	1:A:393:VAL:HG22	1.92	0.51
1:A:398:MET:HG2	1:A:484:PHE:CE1	2.46	0.51
1:A:52:TYR:N	1:A:53:PRO:CD	2.74	0.51
1:A:332:LEU:CD2	1:A:333:PHE:CE2	2.94	0.51
1:A:433:MET:O	1:A:436:ALA:HB3	2.11	0.51
1:A:7:GLU:O	1:A:10:ARG:HG3	2.11	0.51
1:A:56:LYS:CE	1:A:62:VAL:O	2.59	0.51
2:B:157:HIS:C	2:B:159:ASN:H	2.13	0.50
1:A:146:TYR:HD2	1:A:208:LEU:HD13	1.76	0.50
1:A:46:TYR:CE1	5:A:800:HEM:HBA2	2.46	0.50
1:A:465:VAL:O	1:A:468:VAL:HG23	2.10	0.50
1:A:384:HIS:O	1:A:388:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ARG:O	2:B:157:HIS:HD2	1.94	0.50
1:A:95:ARG:CZ	1:A:95:ARG:HA	2.41	0.50
2:B:113:ILE:HA	2:B:127:VAL:O	2.11	0.50
1:A:365:VAL:HG12	1:A:366:ASN:H	1.74	0.50
1:A:101:PRO:HA	1:A:166:LEU:HD11	1.94	0.50
1:A:379:ALA:O	1:A:382:PRO:HD2	2.12	0.50
1:A:37:LEU:O	1:A:40:PRO:HD2	2.12	0.50
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.78	0.50
1:A:124:LEU:CD2	1:A:129:ALA:HB3	2.41	0.50
2:B:86:PHE:CD1	2:B:86:PHE:C	2.86	0.50
1:A:93:PRO:HB3	1:A:183:THR:HA	1.94	0.49
1:A:233:HIS:CB	1:A:234:PRO:CD	2.87	0.49
2:B:145:TYR:CE1	2:B:166:VAL:HG13	2.47	0.49
1:A:385:PHE:HB3	6:A:801:HAS:HMA2	1.82	0.49
1:A:410:GLY:O	1:A:501:LEU:HD11	2.12	0.49
1:A:410:GLY:O	1:A:501:LEU:CD1	2.61	0.49
2:B:99:GLN:O	2:B:99:GLN:HG3	2.10	0.49
1:A:63:GLN:HB2	1:A:127:ASN:ND2	2.28	0.49
1:A:182:VAL:CG2	1:A:508:PHE:HE2	2.00	0.49
1:A:192:MET:HG3	1:A:272:PHE:O	2.12	0.49
2:B:64:TRP:CD1	2:B:83:VAL:O	2.65	0.49
1:A:27:LEU:O	1:A:28:GLY:C	2.51	0.49
1:A:240:LEU:O	1:A:240:LEU:HG	2.12	0.49
1:A:101:PRO:HB3	1:A:166:LEU:HD11	1.94	0.49
2:B:47:ALA:HB2	2:B:134:THR:HB	1.95	0.49
1:A:459:ALA:O	1:A:461:PRO:HD2	2.12	0.48
1:A:498:LYS:N	1:A:499:PRO:HD3	2.27	0.48
1:A:119:VAL:HG12	1:A:148:GLY:HA2	1.95	0.48
2:B:27:PHE:HA	2:B:30:ILE:HG13	1.95	0.48
1:A:79:VAL:HG13	1:A:152:PHE:HE1	1.79	0.48
1:A:420:LEU:O	1:A:421:GLY:C	2.52	0.48
1:A:388:GLN:CA	1:A:388:GLN:HE21	2.26	0.48
1:A:252:PRO:O	1:A:255:ALA:HB3	2.14	0.48
1:A:63:GLN:CB	1:A:127:ASN:ND2	2.77	0.48
1:A:262:ASP:N	1:A:263:PRO:HD2	2.28	0.48
1:A:330:ARG:H	1:A:330:ARG:HD2	1.79	0.47
1:A:488:LEU:CD1	1:A:492:LEU:HD12	2.44	0.47
3:C:29:VAL:O	3:C:30:PHE:C	2.51	0.47
1:A:373:TYR:OH	2:B:45:ILE:HG12	2.13	0.47
1:A:101:PRO:O	1:A:103:MET:N	2.47	0.47
1:A:41:PHE:CE1	1:A:55:LEU:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HG12	2:B:84:LEU:H	1.79	0.47
1:A:518:ARG:HA	1:A:518:ARG:HD2	1.69	0.47
2:B:142:PRO:CA	2:B:166:VAL:HG22	2.32	0.47
1:A:33:ILE:O	1:A:33:ILE:HG22	2.14	0.47
1:A:450:ARG:O	2:B:157:HIS:CD2	2.67	0.47
1:A:41:PHE:CD1	1:A:55:LEU:HD12	2.49	0.47
1:A:504:ALA:HA	1:A:505:PRO:HD3	1.84	0.47
2:B:63:PRO:HG2	2:B:82:TYR:CD2	2.50	0.47
1:A:407:ASN:ND2	1:A:506:LEU:HD22	2.30	0.46
1:A:314:PHE:CD1	2:B:15:GLU:HG2	2.50	0.46
1:A:193:TRP:HA	1:A:193:TRP:CE3	2.50	0.46
1:A:78:ILE:O	1:A:82:GLN:HB2	2.15	0.46
1:A:89:MET:HB2	1:A:190:TRP:CZ2	2.50	0.46
2:B:26:LEU:O	2:B:30:ILE:HG13	2.14	0.46
1:A:79:VAL:HG13	1:A:152:PHE:CE1	2.50	0.46
1:A:192:MET:CG	1:A:273:LEU:HA	2.44	0.46
1:A:101:PRO:O	1:A:103:MET:HG2	2.15	0.46
1:A:32:LEU:HA	1:A:76:ASN:ND2	2.30	0.46
1:A:374:VAL:HG21	3:C:30:PHE:HA	1.98	0.46
2:B:119:GLU:OE2	2:B:146:ARG:NH2	2.46	0.46
1:A:360:GLY:O	1:A:364:ILE:HG13	2.16	0.46
1:A:460:TYR:N	1:A:461:PRO:HD2	2.28	0.46
1:A:518:ARG:NH2	1:A:518:ARG:CG	2.59	0.46
1:A:42:GLN:HG2	1:A:52:TYR:OH	2.16	0.46
1:A:39:GLY:C	5:A:800:HEM:HMB3	2.36	0.46
1:A:12:TYR:CE1	1:A:19:LYS:HB2	2.50	0.46
1:A:56:LYS:NZ	1:A:62:VAL:O	2.49	0.46
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.51	0.46
1:A:96:GLU:HG2	1:A:96:GLU:O	2.16	0.46
1:A:143:TRP:CE3	1:A:213:PHE:HE2	2.33	0.45
1:A:403:TRP:CZ3	1:A:404:LEU:HD22	2.51	0.45
1:A:372:ASP:OD1	1:A:376:HIS:HB2	2.17	0.45
3:C:12:ILE:HA	3:C:15:LEU:HB3	1.98	0.45
2:B:148:ILE:HG23	2:B:161:PHE:CE2	2.52	0.45
2:B:101:ALA:O	2:B:103:ILE:HD12	2.16	0.45
2:B:154:GLY:O	2:B:157:HIS:HB2	2.16	0.45
1:A:407:ASN:ND2	1:A:506:LEU:CD2	2.77	0.45
1:A:390:ALA:HB1	1:A:432:MET:HE1	1.99	0.45
1:A:181:LEU:CD1	1:A:266:ARG:HG3	2.46	0.45
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.54	0.45
1:A:459:ALA:C	1:A:461:PRO:CD	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLY:HA3	1:A:230:TRP:HB3	1.99	0.45
1:A:363:GLY:O	1:A:366:ASN:HB2	2.17	0.45
1:A:390:ALA:HB1	1:A:432:MET:CE	2.47	0.45
3:C:31:PHE:O	3:C:34:GLY:N	2.44	0.45
1:A:207:PHE:CD1	1:A:219:VAL:HG13	2.52	0.45
2:B:157:HIS:C	2:B:159:ASN:N	2.70	0.44
1:A:548:GLN:O	1:A:551:GLY:N	2.50	0.44
1:A:439:LEU:HD13	1:A:470:ASN:OD1	2.15	0.44
1:A:404:LEU:O	1:A:408:LEU:HG	2.17	0.44
1:A:24:PHE:HZ	1:A:109:SER:OG	2.00	0.44
1:A:355:GLY:HA2	1:A:358:PRO:HD2	1.99	0.44
1:A:391:SER:C	1:A:395:LEU:HD12	2.38	0.44
1:A:381:VAL:HG12	1:A:385:PHE:CD2	2.52	0.44
1:A:119:VAL:CG1	1:A:148:GLY:HA2	2.48	0.44
1:A:264:MET:HA	1:A:264:MET:CE	2.48	0.44
1:A:499:PRO:HB3	1:A:502:ALA:CB	2.47	0.44
2:B:74:THR:HG23	2:B:78:GLN:HB3	1.99	0.44
1:A:488:LEU:HD11	1:A:492:LEU:HD12	1.99	0.44
1:A:146:TYR:CD2	1:A:208:LEU:HB3	2.53	0.44
1:A:41:PHE:HD2	1:A:51:ALA:HB3	1.82	0.44
1:A:10:ARG:O	1:A:11:VAL:C	2.56	0.44
1:A:262:ASP:O	1:A:263:PRO:C	2.56	0.44
1:A:69:LEU:HD23	1:A:132:LEU:HD22	2.00	0.43
3:C:6:LYS:HA	3:C:9:LEU:HD12	2.00	0.43
1:A:506:LEU:O	1:A:508:PHE:N	2.49	0.43
1:A:365:VAL:O	1:A:366:ASN:C	2.57	0.43
1:A:374:VAL:HG23	2:B:122:ASN:ND2	2.34	0.43
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.57	0.43
1:A:184:TYR:CD1	1:A:527:ILE:HD11	2.53	0.43
1:A:310:LEU:HB3	2:B:18:TRP:CZ2	2.54	0.43
1:A:142:HIS:ND1	1:A:144:ALA:HB3	2.33	0.43
1:A:69:LEU:HD23	1:A:132:LEU:CD2	2.49	0.43
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.80	0.43
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.83	0.43
1:A:132:LEU:C	1:A:134:THR:H	2.22	0.43
1:A:486:TYR:O	1:A:490:SER:HB3	2.19	0.43
1:A:324:GLY:HA3	1:A:335:TRP:HB2	2.01	0.42
1:A:307:VAL:CA	1:A:310:LEU:HD12	2.42	0.42
1:A:420:LEU:HD12	1:A:420:LEU:O	2.19	0.42
1:A:401:LEU:O	1:A:405:LEU:HB2	2.19	0.42
1:A:522:LEU:HA	1:A:522:LEU:HD12	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:HG21	2:B:127:VAL:HG21	2.00	0.42
2:B:51:GLU:OE2	2:B:132:VAL:HB	2.18	0.42
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.31	0.42
1:A:239:TRP:O	1:A:242:PRO:HD2	2.20	0.42
1:A:378:THR:OG1	1:A:380:TRP:HB3	2.19	0.42
3:C:16:THR:O	3:C:20:LEU:HG	2.19	0.42
1:A:347:VAL:HG12	1:A:351:LEU:HD12	2.00	0.42
1:A:204:ALA:HA	1:A:208:LEU:HB2	2.01	0.42
2:B:96:GLU:HB3	2:B:167:LYS:HZ3	1.84	0.42
1:A:325:ARG:NH1	1:A:331:GLY:O	2.53	0.42
2:B:105:PHE:HZ	2:B:139:PHE:CE1	2.36	0.42
1:A:188:VAL:O	1:A:189:PHE:O	2.37	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD23	2.00	0.42
1:A:84:PHE:CE1	1:A:397:ALA:HA	2.54	0.42
1:A:282:HIS:HA	1:A:285:PHE:CE2	2.54	0.42
1:A:511:VAL:HG12	1:A:512:ILE:C	2.39	0.42
1:A:342:ASP:HB2	1:A:418:ARG:NH2	2.34	0.42
1:A:130:THR:HG22	1:A:130:THR:O	2.19	0.42
2:B:24:ALA:O	2:B:28:VAL:HG23	2.20	0.42
1:A:351:LEU:HD21	1:A:426:TRP:CH2	2.54	0.42
1:A:273:LEU:C	1:A:274:LEU:HD12	2.40	0.42
1:A:27:LEU:HD23	1:A:83:LEU:HD21	2.01	0.42
1:A:61:PHE:HD1	1:A:61:PHE:H	1.68	0.42
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.72	0.42
1:A:229:TRP:HZ3	1:A:232:GLY:O	2.02	0.42
1:A:251:LEU:HA	1:A:254:GLN:CG	2.50	0.42
1:A:56:LYS:HD3	1:A:62:VAL:O	2.20	0.41
1:A:82:GLN:HG2	1:A:238:PHE:CZ	2.55	0.41
1:A:340:PRO:C	1:A:342:ASP:H	2.23	0.41
1:A:178:VAL:HG22	1:A:522:LEU:CD1	2.50	0.41
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.86	0.41
1:A:72:HIS:HE1	5:A:800:HEM:C4B	2.38	0.41
1:A:306:ALA:O	1:A:310:LEU:HD12	2.20	0.41
1:A:105:LEU:O	1:A:108:LEU:HB3	2.21	0.41
1:A:25:LEU:O	1:A:29:PHE:HD1	2.04	0.41
2:B:10:ALA:O	2:B:14:TYR:HD1	2.04	0.41
1:A:381:VAL:HB	1:A:382:PRO:HD3	2.03	0.41
1:A:15:TYR:CZ	1:A:95:ARG:NH1	2.89	0.41
1:A:82:GLN:NE2	1:A:156:THR:HG23	2.34	0.41
2:B:140:LYS:HE3	2:B:140:LYS:HB3	1.69	0.41
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HG11	3:C:26:VAL:HG13	2.02	0.41
1:A:259:LEU:HG	1:A:261:SER:H	1.85	0.41
1:A:411:LYS:HA	1:A:412:PRO:HD3	1.83	0.41
3:C:24:LEU:HD12	3:C:24:LEU:HA	1.97	0.41
1:A:38:PHE:HE2	1:A:62:VAL:HG21	1.86	0.41
1:A:223:VAL:O	1:A:226:THR:N	2.53	0.41
1:A:132:LEU:O	1:A:134:THR:N	2.54	0.41
2:B:40:HIS:CD2	2:B:41:THR:HG23	2.56	0.41
1:A:466:PRO:O	1:A:469:PHE:N	2.54	0.41
1:A:385:PHE:CD1	1:A:385:PHE:C	2.94	0.41
2:B:155:LEU:O	2:B:155:LEU:HD23	2.21	0.41
1:A:92:LEU:O	1:A:93:PRO:C	2.57	0.41
1:A:488:LEU:HD11	1:A:492:LEU:CD1	2.51	0.41
1:A:233:HIS:CD2	1:A:234:PRO:N	2.89	0.40
1:A:192:MET:HG2	1:A:273:LEU:HA	2.03	0.40
1:A:417:GLN:HE22	1:A:491:VAL:HA	1.86	0.40
1:A:303:LEU:HD13	2:B:30:ILE:HG12	2.03	0.40
1:A:9:SER:OG	1:A:11:VAL:HG23	2.22	0.40
1:A:369:PHE:HE2	1:A:373:TYR:HH	1.68	0.40
1:A:388:GLN:CB	6:A:801:HAS:HMC3	2.48	0.40
1:A:254:GLN:HG2	1:A:254:GLN:H	1.73	0.40
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.91	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	555/568 (98%)	427 (77%)	100 (18%)	28 (5%)	3	9
2	B	164/168 (98%)	139 (85%)	21 (13%)	4 (2%)	7	29
3	C	31/34 (91%)	19 (61%)	9 (29%)	3 (10%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	750/770 (97%)	585 (78%)	130 (17%)	35 (5%)	3	11

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	58	LEU
1	A	102	ASN
1	A	189	PHE
1	A	366	ASN
2	B	87	ALA
2	B	88	PHE
3	C	32	ALA
1	A	190	TRP
1	A	365	VAL
1	A	379	ALA
1	A	496	GLU
1	A	526	ARG
2	B	158	GLN
3	C	15	LEU
3	C	16	THR
1	A	109	SER
1	A	341	TRP
1	A	504	ALA
1	A	517	ASP
1	A	461	PRO
1	A	57	ARG
1	A	89	MET
1	A	224	ALA
1	A	392	LEU
1	A	422	LEU
1	A	452	TYR
1	A	548	GLN
2	B	4	GLN
1	A	234	PRO
1	A	233	HIS
1	A	355	GLY
1	A	499	PRO
1	A	547	VAL
1	A	28	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/462 (98%)	382 (84%)	71 (16%)	3	9
2	B	136/138 (99%)	114 (84%)	22 (16%)	3	9
3	C	26/27 (96%)	22 (85%)	4 (15%)	3	10
All	All	615/627 (98%)	518 (84%)	97 (16%)	3	9

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	ILE
1	A	23	TYR
1	A	48	ASN
1	A	54	LEU
1	A	56	LYS
1	A	59	LEU
1	A	82	GLN
1	A	95	ARG
1	A	99	MET
1	A	103	MET
1	A	125	LEU
1	A	133	TYR
1	A	134	THR
1	A	147	LEU
1	A	150	SER
1	A	152	PHE
1	A	168	ARG
1	A	169	ARG
1	A	177	LYS
1	A	179	THR
1	A	195	LEU
1	A	213	PHE
1	A	215	LEU
1	A	216	VAL
1	A	230	TRP

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Mol	Chain	Res	Type
1	A	238	PHE
1	A	253	LYS
1	A	254	GLN
1	A	261	SER
1	A	305	VAL
1	A	309	SER
1	A	315	THR
1	A	319	SER
1	A	326	LEU
1	A	327	ARG
1	A	330	ARG
1	A	339	LEU
1	A	354	LEU
1	A	369	PHE
1	A	374	VAL
1	A	385	PHE
1	A	388	GLN
1	A	391	SER
1	A	395	LEU
1	A	404	LEU
1	A	405	LEU
1	A	418	ARG
1	A	419	ARG
1	A	420	LEU
1	A	430	LEU
1	A	439	LEU
1	A	449	ARG
1	A	452	TYR
1	A	455	GLN
1	A	465	VAL
1	A	472	LEU
1	A	477	LEU
1	A	478	LEU
1	A	490	SER
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	506	LEU
1	A	518	ARG
1	A	520	LEU
1	A	533	VAL
1	A	536	ILE

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Mol	Chain	Res	Type
1	A	547	VAL
1	A	548	GLN
1	A	560	ARG
2	B	6	LYS
2	B	9	LYS
2	B	12	LEU
2	B	16	LYS
2	B	19	LEU
2	B	23	LEU
2	B	26	LEU
2	B	30	ILE
2	B	39	THR
2	B	46	PRO
2	B	52	ARG
2	B	59	ARG
2	B	72	VAL
2	B	95	ILE
2	B	99	GLN
2	B	111	ASP
2	B	136	ARG
2	B	140	LYS
2	B	141	ARG
2	B	149	CYS
2	B	166	VAL
2	B	168	GLU
3	C	2	GLU
3	C	6	LYS
3	C	13	LEU
3	C	24	LEU

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

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	ASN
1	A	127	ASN
1	A	254	GLN
1	A	388	GLN
2	B	5	HIS
2	B	122	ASN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	#$|Z| > 2$
5	HEM	A	800	1	30,50,50	1.96	6 (20%)	24,82,82	4.16	15 (62%)
6	HAS	A	801	1	45,72,72	1.85	9 (20%)	47,109,109	4.55	21 (44%)
7	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-

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
5	HEM	A	800	1	-	0/10/54/54	0/0/8/8
6	HAS	A	801	1	-	0/30/82/82	0/0/8/8
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-7.31	1.45	1.51
6	A	801	HAS	C3C-CAC	-6.36	1.34	1.47
5	A	800	HEM	C3D-C4D	-3.42	1.47	1.51
5	A	800	HEM	C2C-C1C	-3.16	1.46	1.52
5	A	800	HEM	C3B-CAB	2.05	1.55	1.51
6	A	801	HAS	C14-C15	2.08	1.37	1.33
5	A	800	HEM	CMA-C3A	2.55	1.56	1.51
5	A	800	HEM	C4C-NC	2.88	1.39	1.36
6	A	801	HAS	C1A-CHA	2.92	1.47	1.39
6	A	801	HAS	C3C-C2C	2.95	1.44	1.40
6	A	801	HAS	C2D-C3D	3.11	1.44	1.40
6	A	801	HAS	C1C-CHC	3.38	1.49	1.39
6	A	801	HAS	C4A-CHD	3.80	1.50	1.39
6	A	801	HAS	C1D-CHB	4.23	1.51	1.39
6	A	801	HAS	C2A-C3A	4.46	1.50	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	C3C-CAC-CBC	-11.11	107.42	124.46
6	A	801	HAS	CBA-CAA-C2A	-8.49	97.32	112.53
5	A	800	HEM	CAA-C2A-C1A	-8.25	118.06	127.01
5	A	800	HEM	CAA-CBA-CGA	-7.02	99.88	112.75
6	A	801	HAS	CAA-C2A-C1A	-6.80	119.63	127.01
6	A	801	HAS	CMC-C2C-C1C	-6.52	117.58	128.36
6	A	801	HAS	CMA-C3A-C2A	-5.93	112.84	125.24
6	A	801	HAS	CMC-C2C-C3C	-5.80	113.75	125.09
6	A	801	HAS	OMD-CMD-C2D	-5.67	113.65	125.11
6	A	801	HAS	C4D-C3D-C2D	-4.84	102.23	107.07
5	A	800	HEM	CMA-C3A-C4A	-3.69	122.26	128.36
6	A	801	HAS	CAA-C2A-C3A	-3.21	119.84	129.00
6	A	801	HAS	CMA-C3A-C4A	-3.00	123.41	128.36
6	A	801	HAS	C20-C19-C18	-2.87	115.62	121.05
6	A	801	HAS	C24-C23-C22	-2.54	116.22	121.05
6	A	801	HAS	C3C-C4C-NC	-2.53	106.16	110.94
6	A	801	HAS	C31-C30-C29	-2.50	114.56	122.61
5	A	800	HEM	CAD-CBD-CGD	-2.48	102.91	113.02
6	A	801	HAS	C17-C18-C19	-2.05	123.30	127.76
6	A	801	HAS	C21-C22-C23	-2.04	123.33	127.76
6	A	801	HAS	C20-C21-C22	-2.03	106.38	111.69
6	A	801	HAS	CAA-CBA-CGA	-2.03	109.03	112.75
5	A	800	HEM	C3B-CAB-CBB	-2.02	121.35	124.46
5	A	800	HEM	C2C-C1C-CHC	2.43	127.37	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	CMD-C2D-C3D	2.83	126.86	114.35
5	A	800	HEM	C2D-C3D-C4D	2.89	106.40	101.50
6	A	801	HAS	CAD-C3D-C4D	3.38	130.67	127.01
5	A	800	HEM	CMA-C3A-C2A	3.50	132.54	125.24
5	A	800	HEM	CMC-C2C-C3C	3.63	125.60	116.53
6	A	801	HAS	C25-C23-C24	4.06	121.61	115.41
5	A	800	HEM	CMB-C2B-C3B	4.24	127.11	116.53
5	A	800	HEM	CAD-C3D-C2D	4.28	125.52	113.22
5	A	800	HEM	CAD-C3D-C4D	4.43	128.08	112.47
6	A	801	HAS	C27-C19-C20	5.08	123.17	115.41
5	A	800	HEM	CBA-CAA-C2A	6.37	123.95	112.53
6	A	801	HAS	C3C-CAC-CBC	23.16	173.70	126.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	7	0
6	A	801	HAS	15	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 (i)

6.1   Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	557/568 (98%)	-0.28	25 (4%)	37	31	64, 88, 129, 216	0
2	B	166/168 (98%)	-0.40	5 (3%)	54	47	71, 88, 124, 174	0
3	C	33/34 (97%)	-0.62	0	100	100	69, 79, 133, 154	0
All	All	756/770 (98%)	-0.32	30 (3%)	42	35	64, 88, 131, 216	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	SER	8.0
1	A	515	PRO	6.0
1	A	9	SER	5.9
1	A	173	ALA	5.0
1	A	10	ARG	4.4
1	A	493	LEU	4.3
1	A	495	ARG	4.1
1	A	12	TYR	3.7
2	B	76	PRO	3.6
1	A	217	GLU	3.4
1	A	501	LEU	3.4
2	B	4	GLN	3.3
1	A	218	GLY	3.1
1	A	8	ILE	3.1
2	B	73	GLN	2.8
1	A	104	GLY	2.8
1	A	215	LEU	2.8
1	A	516	GLU	2.8
2	B	52	ARG	2.7
1	A	510	GLU	2.7
1	A	174	ASN	2.6
2	B	72	VAL	2.4
1	A	13	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	177	LYS	2.2
1	A	494	SER	2.2
1	A	502	ALA	2.2
1	A	176	GLY	2.1
1	A	7	GLU	2.0
1	A	552	HIS	2.0
1	A	416	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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
6	HAS	A	801	65/65	0.97	0.13	-0.19	53,74,87,93	0
5	HEM	A	800	43/43	0.98	0.11	-0.76	50,68,90,98	0
7	CUA	B	802	2/2	1.00	0.08	-2.03	88,88,88,90	0
4	CU1	A	803	1/1	0.99	0.11	-	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.