Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:00 PM GMT

PDB ID	:	3VRA
Title	:	Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode Ascaris suum with the specific inhibitor Atpenin A5
Authors	:	Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.
Deposited on	:	2012-04-07
Resolution	:	3.44 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:

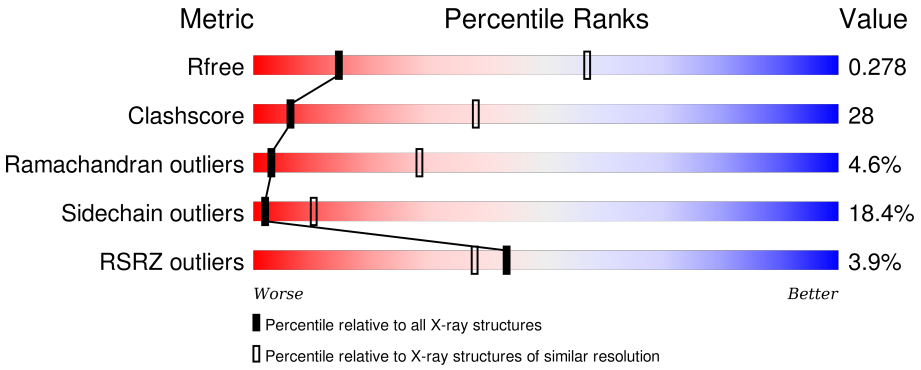
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.44 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	1007 (3.54-3.34)
Clashscore	102246	1044 (3.52-3.36)
Ramachandran outliers	100387	1013 (3.52-3.36)
Sidechain outliers	100360	1014 (3.52-3.36)
RSRZ outliers	91569	1012 (3.54-3.34)

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	645	6% 45% 41% 9% 5%
1	E	645	2% 42% 46% 7% 5%
2	B	282	% 36% 42% 11% 12%
2	F	282	2% 40% 34% 14% • 12%
3	C	188	4% 32% 39% 10% 19%

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Mol	Chain	Length	Quality of chain
3	G	188	6% 32% 42% 6% 19%
4	D	156	3% 47% 29% 5% 17%
4	H	156	3% 36% 40% 6% 17%

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
11	AT5	C	202	-	-	X	X
11	AT5	G	202	-	-	X	X
12	EPH	D	201	-	-	-	X
12	EPH	H	201	-	-	-	X
5	MLI	A	701	-	-	X	-
5	MLI	E	701	-	-	X	-
8	SF4	B	302	-	-	X	-
9	F3S	F	303	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18262 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 Flavoprotein subunit of complex II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			
1	E	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			

- Molecule 2 is a protein called Iron-sulfur subunit of succinate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			
2	F	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			

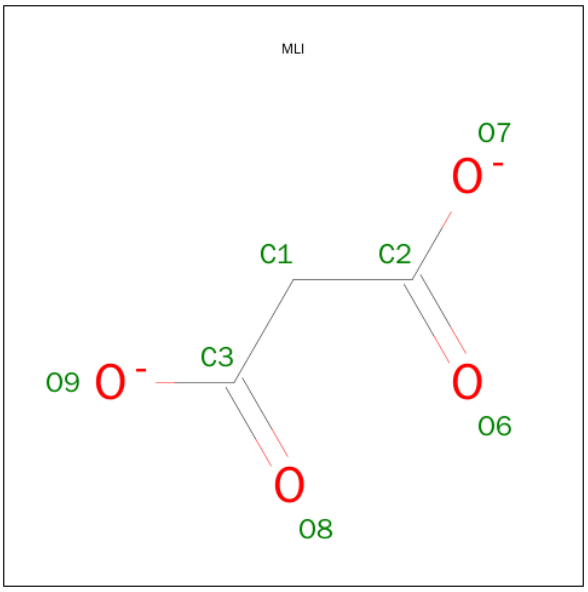
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

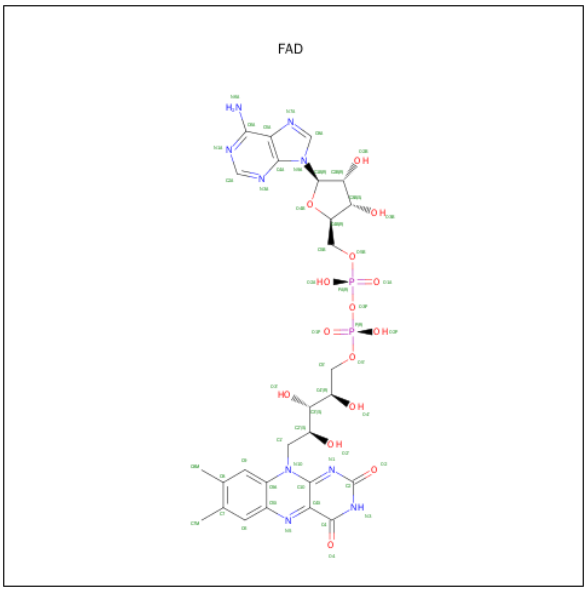
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			
4	H	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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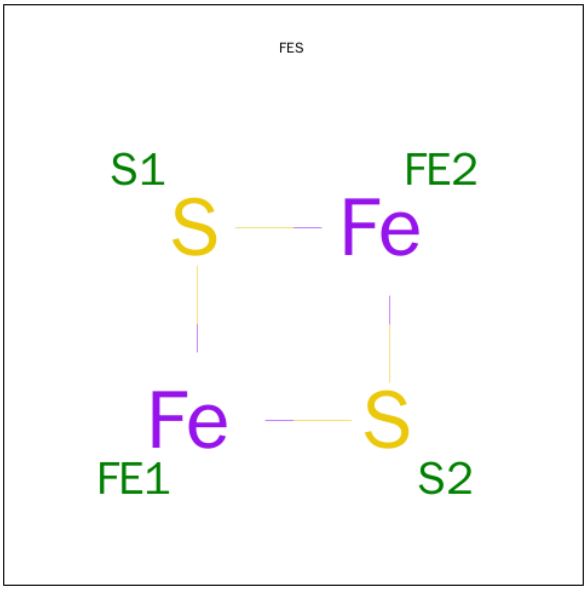
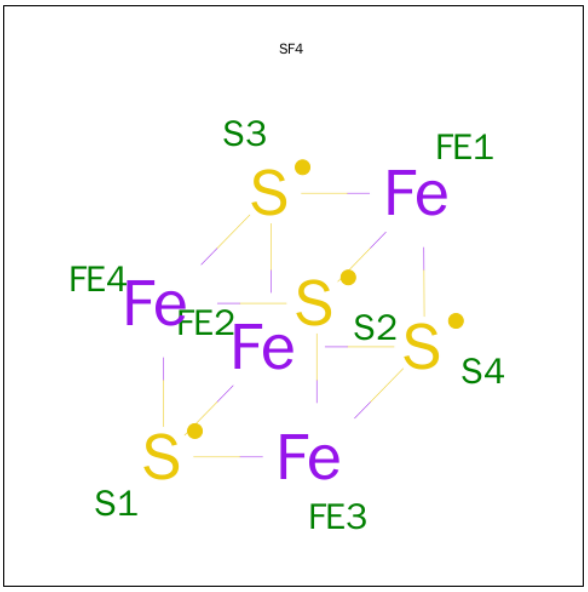
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



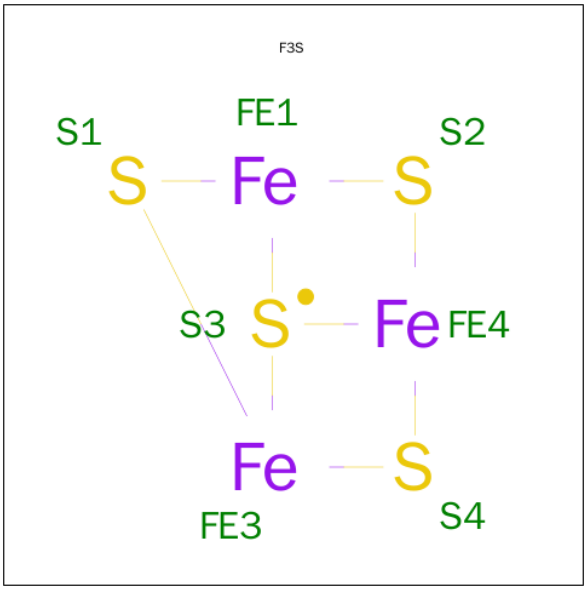
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Fe	S		0	0
			4	2	2			
7	F	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



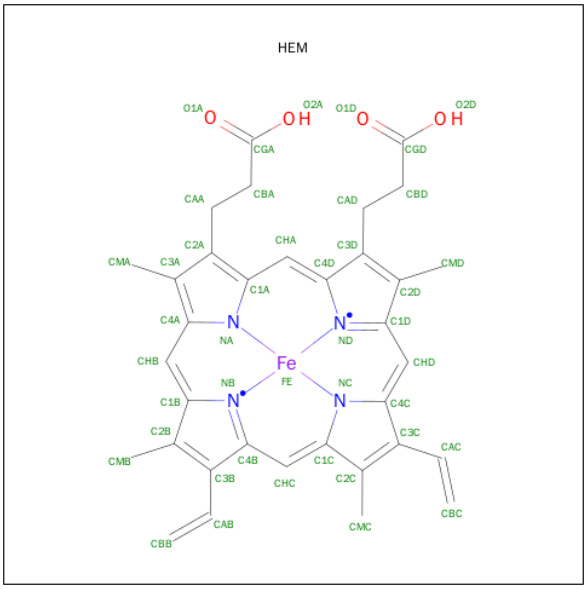
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 8 4 4	0	0
8	F	1	Total Fe S 8 4 4	0	0

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



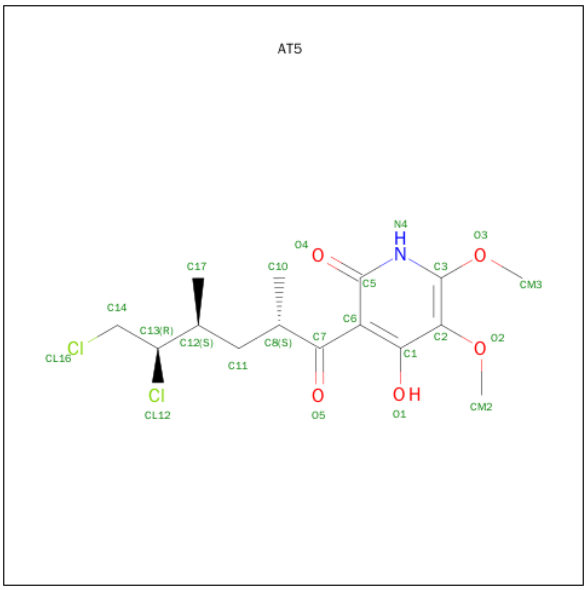
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 7 3 4	0	0
9	F	1	Total Fe S 7 3 4	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



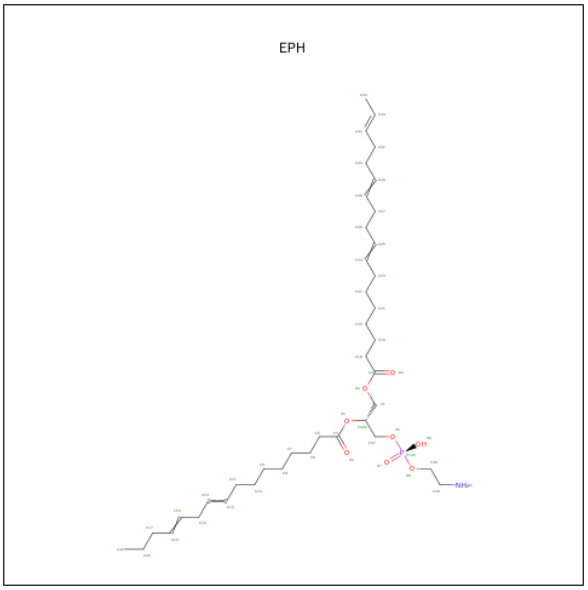
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 3-[(2S,4S,5R)-5,6-DICHLORO-2,4-DIMETHYL-1-OXOHEXYL]-4-HYDROXY-5,6-DIMETHOXY-2(1H)-PYRIDINONE (three-letter code: AT5) (formula: $C_{15}H_{21}Cl_2NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Cl	N	O	0	0
			23	15	2	1	5		
11	G	1	Total	C	Cl	N	O	0	0
			23	15	2	1	5		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



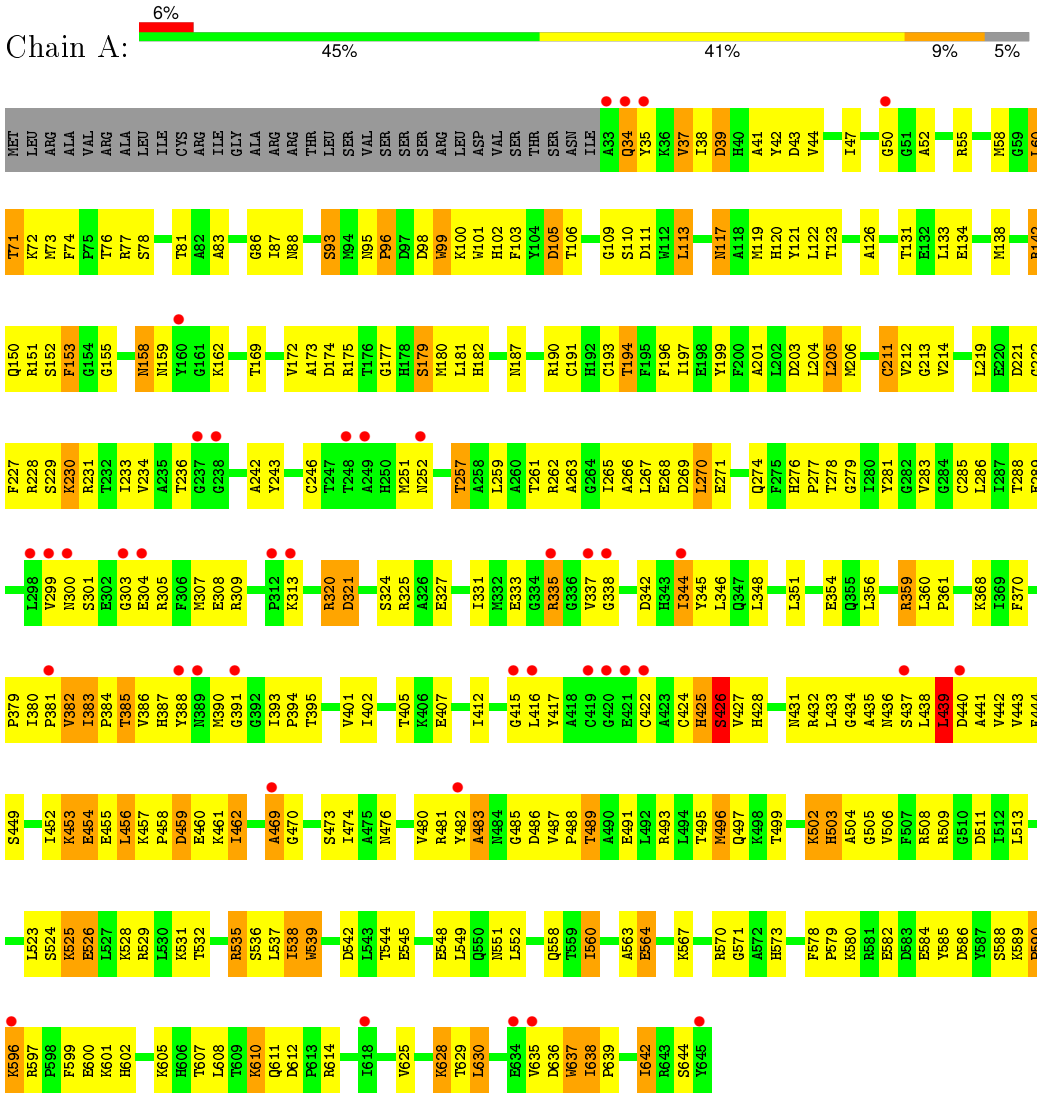
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

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.

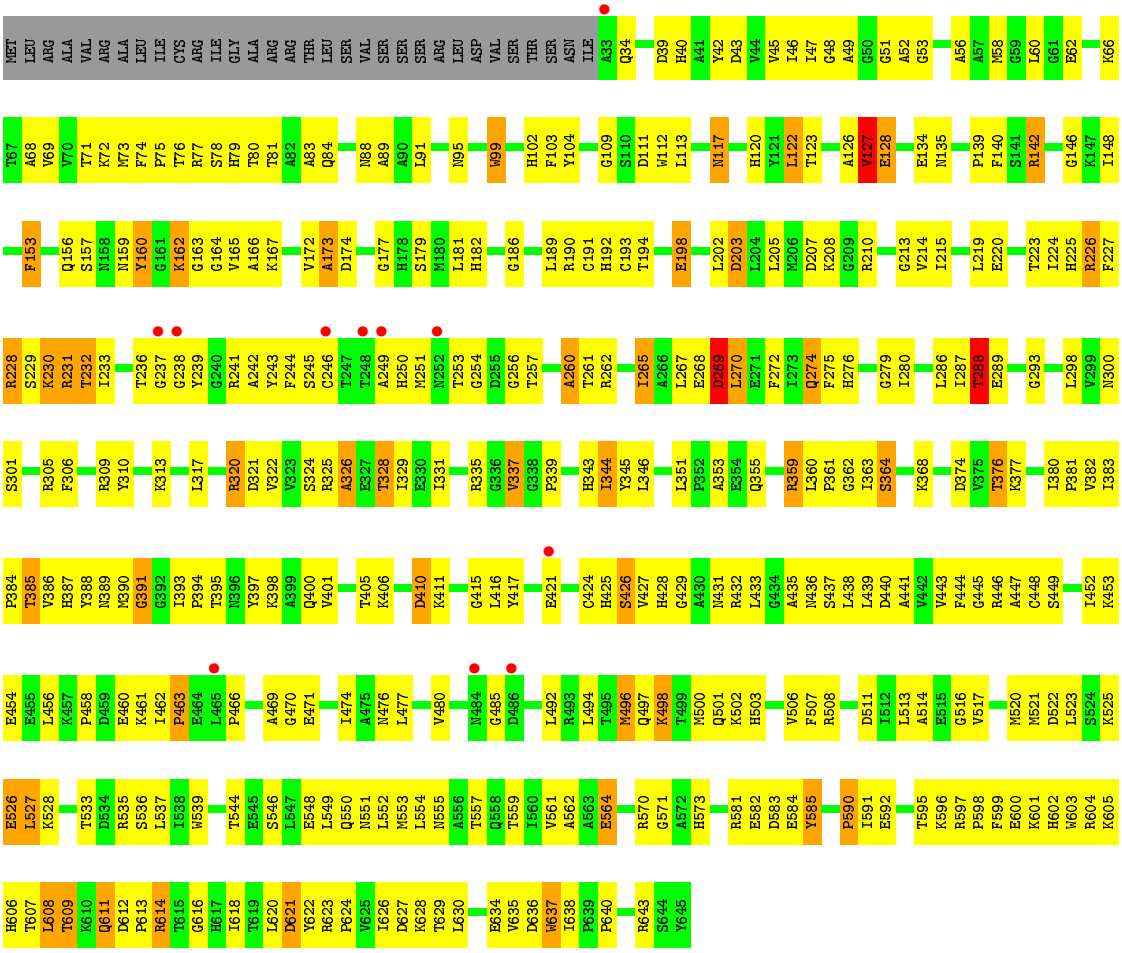
- Molecule 1: Flavoprotein subunit of complex II

Chain A:



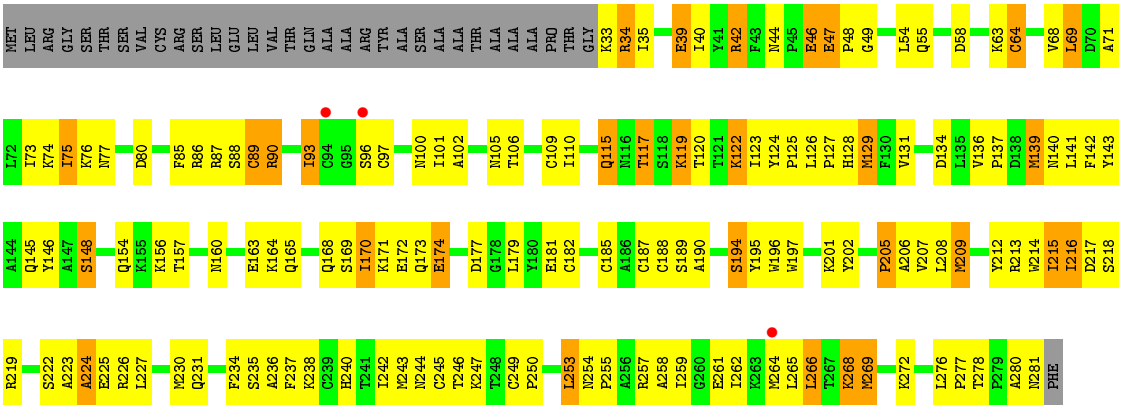
- Molecule 1: Flavoprotein subunit of complex II

Chain E:



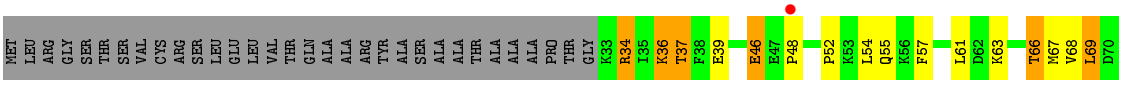
• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

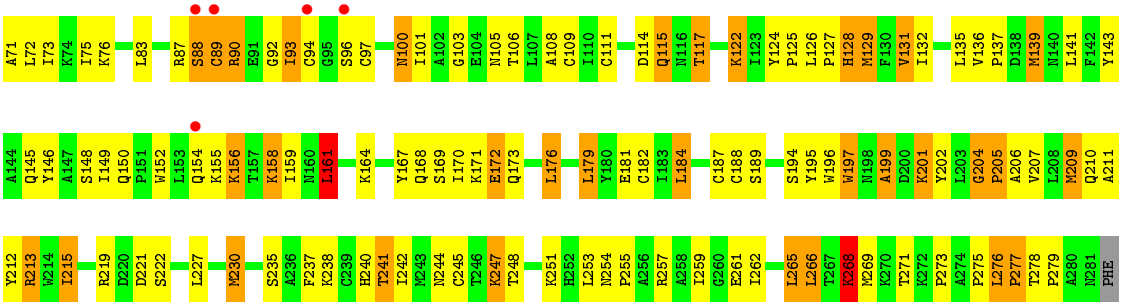
Chain B:



• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

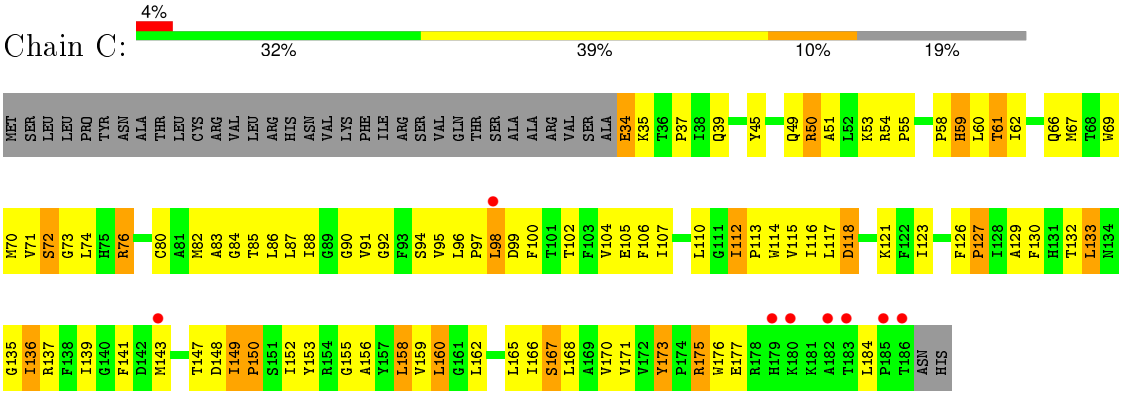
Chain F:





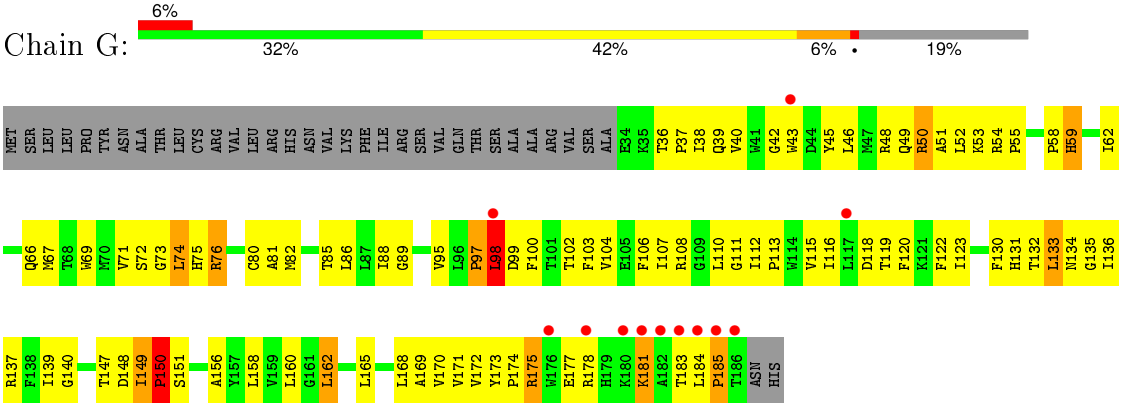
• Molecule 3: Cytochrome b-large subunit

Chain C:



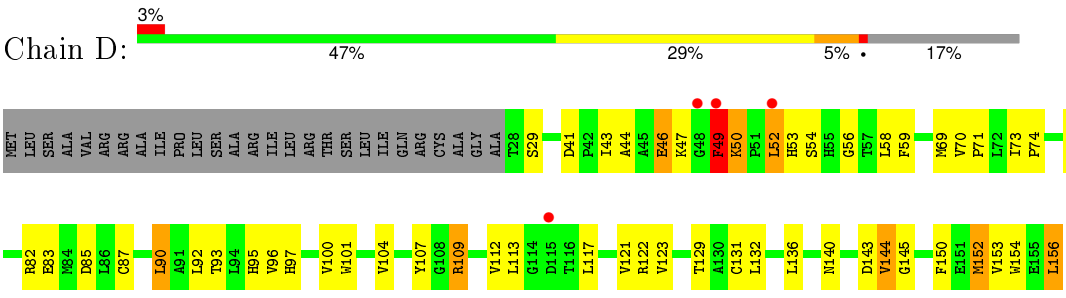
• Molecule 3: Cytochrome b-large subunit

Chain G:



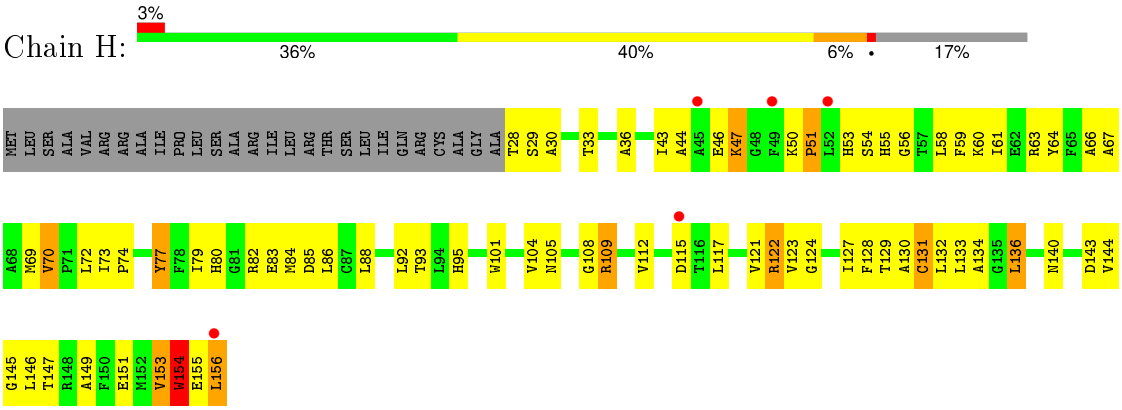
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:



• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain H:


3%
36%
40%
6%
17%
MET LEU SER ALA VAL ARG ARG ALA ILE PRO LEU SER ALA ARG ILE LEU ARG THR SER LEU ILE GLN ARG CYS ALA GLY ALA T28 S29 A30 T33 A36 I43 A44 A45 F46 K47 G48 F49 K50 P51 L52 H53 S54 H55 G56 T57 L58 F59 K60 I61 E62 R63 Y64 F65 A66 A67
A68 M69 V70 P71 L72 I73 P74 Y77 F78 I79 H80 G81 R82 E83 M84 D85 L86 C87 L88 L92 T93 L94 H95 W101 V104 N105 G108 R109 V112 D115 T116 L117 V121 R122 V123 G124 I127 F128 T129 A130 C131 L132 L133 A134 G135 L136 N140 D143 V144
G145 L146 T147 R148 A149 F150 E151 M152 V153 W154 E155 L156

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.82Å 132.25Å 220.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.44 49.72 – 3.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.72-3.44) 89.5 (49.72-3.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.205 , 0.281 0.203 , 0.278	Depositor DCC
R_{free} test set	2217 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	103.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 43349 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18262	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: SF4, MLI, F3S, FES, EPH, HEM, AT5, FAD

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	0.65	0/4859	0.77	2/6564 (0.0%)
1	E	0.68	0/4859	0.81	0/6564
2	B	0.72	1/2016 (0.0%)	0.83	0/2723
2	F	0.77	1/2016 (0.0%)	0.89	1/2723 (0.0%)
3	C	0.72	0/1255	0.83	2/1709 (0.1%)
3	G	0.71	0/1255	0.84	2/1709 (0.1%)
4	D	0.74	0/1026	0.83	1/1402 (0.1%)
4	H	0.75	0/1026	0.80	0/1402
All	All	0.70	2/18312 (0.0%)	0.81	8/24796 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	187	CYS	CB-SG	-5.08	1.73	1.81
2	B	97	CYS	CB-SG	-5.04	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	LEU	CA-CB-CG	6.64	130.58	115.30
4	D	52	LEU	CA-CB-CG	6.52	130.30	115.30
2	F	179	LEU	CA-CB-CG	6.16	129.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	184	LEU	CA-CB-CG	5.49	127.92	115.30
3	G	165	LEU	CA-CB-CG	5.24	127.35	115.30
3	G	98	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	637	TRP	CA-CB-CG	5.03	123.25	113.70
3	C	158	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	425	HIS	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	4758	0	4692	260	0
1	E	4758	0	4692	284	0
2	B	1973	0	1994	135	0
2	F	1973	0	1994	133	0
3	C	1217	0	1265	86	0
3	G	1217	0	1265	67	0
4	D	994	0	977	48	0
4	H	994	0	977	59	0
5	A	7	0	2	3	0
5	E	7	0	2	4	0
6	A	53	0	30	12	0
6	E	53	0	31	16	0
7	B	4	0	0	0	0
7	F	4	0	0	1	0
8	B	8	0	0	5	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	2	0
10	C	43	0	30	14	0
10	G	43	0	30	13	0
11	C	23	0	20	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	23	0	21	11	0
12	D	44	0	53	4	0
12	H	44	0	53	2	0
All	All	18262	0	18128	1009	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 28.

All (1009) 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:E:79:HIS:CD2	6:E:702:FAD:HM82	1.71	1.26
1:E:79:HIS:NE2	6:E:702:FAD:HM82	0.92	1.24
3:C:114:TRP:HB2	3:C:175:ARG:HH11	1.09	1.14
2:F:115:GLN:HA	2:F:115:GLN:HE21	1.14	1.08
3:C:107:ILE:HD11	4:D:156:LEU:HD22	1.35	1.07
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.33	1.07
3:G:149:ILE:H	3:G:149:ILE:HD13	1.14	1.06
10:G:201:HEM:HMB1	10:G:201:HEM:HBB2	1.39	1.04
4:D:109:ARG:HG2	4:D:109:ARG:HH21	1.15	1.04
1:A:44:VAL:HG11	1:A:60:LEU:HD22	1.37	1.03
2:F:131:VAL:HG23	3:G:55:PRO:HG2	1.39	1.02
1:A:321:ASP:HB3	1:A:431:ASN:ND2	1.75	1.01
1:A:190:ARG:HA	4:D:43:ILE:HD11	1.42	1.00
3:C:123:ILE:O	3:C:127:PRO:HD2	1.60	0.99
2:F:268:LYS:CG	2:F:269:MET:H	1.75	0.98
2:F:240:HIS:HB2	11:G:202:AT5:HM31	1.45	0.98
3:C:149:ILE:HD13	3:C:149:ILE:H	1.27	0.96
1:E:570:ARG:NH1	1:E:581:ARG:HD2	1.81	0.95
2:F:115:GLN:HA	2:F:115:GLN:NE2	1.82	0.94
2:F:240:HIS:CB	11:G:202:AT5:HM31	1.97	0.93
2:F:105:ASN:HD21	2:F:127:PRO:HD2	1.33	0.92
1:A:503:HIS:HD2	1:A:516:GLY:HA2	1.32	0.92
3:G:133:LEU:O	3:G:136:ILE:HG13	1.68	0.92
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.50	0.91
2:F:57:PHE:CD2	2:F:75:ILE:HD12	2.05	0.91
4:H:50:LYS:N	4:H:51:PRO:HD2	1.86	0.90
2:F:89:CYS:HG	7:F:301:FES:FE2	0.67	0.90
1:A:213:GLY:HA3	1:A:227:PHE:O	1.71	0.90
1:E:583:ASP:O	1:E:602:HIS:HB2	1.71	0.89
1:E:582:GLU:HB2	1:E:603:TRP:HD1	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:202:AT5:HM32	11:G:202:AT5:HM23	1.54	0.87
1:E:583:ASP:O	1:E:602:HIS:CB	2.23	0.87
1:E:43:ASP:OD2	1:E:230:LYS:HE2	1.75	0.87
2:F:268:LYS:HG3	2:F:269:MET:H	1.37	0.87
2:B:240:HIS:HB2	11:C:202:AT5:HM31	1.57	0.87
3:G:112:ILE:HB	3:G:113:PRO:CD	2.05	0.86
1:E:611:GLN:HG3	1:E:618:ILE:HG13	1.57	0.86
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.46	0.86
1:A:321:ASP:HB3	1:A:431:ASN:HD22	1.41	0.86
2:B:71:ALA:O	2:B:75:ILE:HG12	1.76	0.85
10:G:201:HEM:NC	4:H:95:HIS:CD2	2.44	0.84
1:A:503:HIS:HD2	1:A:516:GLY:CA	1.89	0.84
10:G:201:HEM:HHA	10:G:201:HEM:HBD1	1.57	0.84
2:F:34:ARG:HB2	2:F:117:THR:HG21	1.59	0.84
1:E:527:LEU:HD11	1:E:553:MET:HG3	1.58	0.84
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.13	0.84
4:H:70:VAL:O	4:H:74:PRO:HD2	1.77	0.83
3:G:149:ILE:H	3:G:149:ILE:CD1	1.88	0.83
1:A:488:PRO:HG2	1:A:491:GLU:HB2	1.61	0.82
1:E:428:HIS:HB3	1:E:432:ARG:HA	1.60	0.82
1:E:135:ASN:ND2	2:F:161:LEU:O	2.11	0.82
4:H:109:ARG:HH21	4:H:109:ARG:HG2	1.45	0.82
3:C:149:ILE:CD1	3:C:149:ILE:H	1.92	0.81
3:G:112:ILE:HB	3:G:113:PRO:HD3	1.60	0.81
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.63	0.81
2:F:150:GLN:HG2	2:F:152:TRP:CH2	2.16	0.80
1:A:205:LEU:HB3	1:A:212:VAL:HG23	1.61	0.80
1:E:584:GLU:O	1:E:597:ARG:HG3	1.82	0.80
2:F:105:ASN:HD21	2:F:127:PRO:CD	1.94	0.80
1:E:267:LEU:HD12	1:E:270:LEU:HD11	1.62	0.79
1:E:424:CYS:C	1:E:426:SER:H	1.86	0.79
1:E:492:LEU:HB3	1:E:549:LEU:HD21	1.64	0.79
2:F:240:HIS:HB2	11:G:202:AT5:CM3	2.14	0.78
2:B:242:ILE:HD11	11:C:202:AT5:HM33	1.63	0.78
1:E:320:ARG:HH12	5:E:701:MLI:C2	1.96	0.78
1:E:72:LYS:O	1:E:198:GLU:HA	1.83	0.78
2:F:128:HIS:HD2	2:F:196:TRP:HB3	1.48	0.78
4:H:151:GLU:O	4:H:155:GLU:HG3	1.83	0.78
3:G:184:LEU:HB2	3:G:185:PRO:HD2	1.66	0.78
1:E:383:ILE:HG12	1:E:384:PRO:HD2	1.65	0.78
1:E:522:ASP:O	1:E:525:LYS:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:CD2	6:A:702:FAD:H6	2.13	0.77
1:A:142:ARG:HG2	2:B:168:GLN:O	1.83	0.77
3:C:112:ILE:HD13	3:C:117:LEU:HD21	1.65	0.77
1:E:470:GLY:O	1:E:474:ILE:HG22	1.85	0.77
2:B:240:HIS:CB	11:C:202:AT5:HM31	2.15	0.76
2:B:88:SER:O	2:B:90:ARG:N	2.19	0.76
1:A:278:THR:HG21	1:A:346:LEU:HD22	1.65	0.76
3:G:115:VAL:HG23	3:G:116:ILE:HD12	1.68	0.76
3:C:114:TRP:HB2	3:C:175:ARG:NH1	1.94	0.76
2:F:268:LYS:CG	2:F:269:MET:N	2.46	0.76
1:A:103:PHE:HA	1:A:123:THR:HG21	1.67	0.76
1:E:582:GLU:HB2	1:E:603:TRP:CD1	2.20	0.76
2:F:196:TRP:CZ3	3:G:59:HIS:HB2	2.20	0.76
2:F:76:LYS:NZ	2:F:83:LEU:O	2.17	0.76
2:B:40:ILE:HG23	2:B:123:ILE:HB	1.68	0.75
1:E:182:HIS:CE1	2:F:184:LEU:HD22	2.21	0.75
1:E:561:VAL:CG2	1:E:618:ILE:HG21	2.16	0.75
11:C:202:AT5:HM32	11:C:202:AT5:HM23	1.66	0.75
1:A:231:ARG:HD3	1:A:415:GLY:HA2	1.69	0.75
4:H:67:ALA:O	4:H:70:VAL:HG23	1.87	0.74
3:C:82:MET:HB2	10:C:201:HEM:HAC	1.67	0.74
3:C:49:GLN:OE1	3:C:54:ARG:NH1	2.20	0.74
1:E:72:LYS:O	1:E:198:GLU:HG3	1.86	0.74
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.01	0.73
1:A:523:LEU:HA	1:A:526:GLU:HG3	1.70	0.73
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.71	0.73
1:E:570:ARG:HH11	1:E:581:ARG:HD2	1.52	0.73
1:E:432:ARG:HH21	1:E:435:ALA:H	1.35	0.73
3:G:177:GLU:HG3	3:G:181:LYS:HE2	1.70	0.73
2:F:271:THR:HG23	2:F:271:THR:O	1.87	0.73
1:E:561:VAL:HG21	1:E:618:ILE:CG2	2.18	0.73
1:E:159:ASN:HD22	1:E:163:GLY:HA3	1.53	0.73
1:A:443:VAL:HG12	1:A:444:PHE:CD1	2.24	0.73
1:A:504:ALA:HB2	1:A:560:ILE:HD12	1.71	0.73
3:G:149:ILE:HD13	3:G:149:ILE:N	1.99	0.72
2:B:119:LYS:HE2	2:B:119:LYS:HA	1.70	0.72
2:F:237:PHE:HE2	4:H:59:PHE:CD1	2.07	0.72
1:E:88:ASN:O	1:E:439:LEU:HD23	1.89	0.72
10:C:201:HEM:HBB2	10:C:201:HEM:HMB2	1.72	0.72
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.71	0.72
1:A:327:GLU:OE2	1:A:384:PRO:HD3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.71	0.72
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.25	0.71
1:A:503:HIS:CD2	1:A:516:GLY:HA2	2.20	0.71
1:A:159:ASN:O	1:A:162:LYS:HG2	1.91	0.71
2:B:230:MET:HE2	2:B:262:ILE:HG21	1.70	0.71
2:F:105:ASN:ND2	2:F:127:PRO:HD2	2.04	0.71
1:E:269:ASP:HB3	1:E:272:PHE:HD1	1.56	0.70
1:A:50:GLY:HA3	6:A:702:FAD:O1P	1.91	0.70
3:G:173:TYR:HD2	3:G:174:PRO:HD3	1.54	0.70
1:A:268:GLU:HB3	1:A:608:LEU:HD23	1.73	0.70
2:B:128:HIS:HD2	3:C:59:HIS:CD2	2.10	0.70
2:F:69:LEU:HA	2:F:72:LEU:HD12	1.72	0.70
4:D:71:PRO:O	4:D:74:PRO:HD2	1.91	0.70
1:A:77:ARG:HD2	2:B:96:SER:OG	1.92	0.70
4:H:50:LYS:H	4:H:51:PRO:HD2	1.55	0.69
1:A:58:MET:HA	1:A:191:CYS:SG	2.32	0.69
1:A:52:ALA:N	1:A:441:ALA:HB1	2.08	0.69
1:A:88:ASN:ND2	1:A:435:ALA:HB3	2.08	0.69
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.74	0.69
2:F:149:ILE:HD12	2:F:211:ALA:HA	1.74	0.69
2:B:128:HIS:HD2	3:C:59:HIS:HD2	1.41	0.69
2:B:246:THR:OG1	2:B:255:PRO:HD2	1.92	0.69
1:E:496:MET:HG3	1:E:497:GLN:N	2.08	0.69
3:C:112:ILE:HD12	3:C:112:ILE:H	1.57	0.69
3:C:149:ILE:N	3:C:149:ILE:HD13	2.04	0.69
2:B:268:LYS:HG2	2:B:269:MET:H	1.58	0.69
2:B:115:GLN:HA	2:B:115:GLN:HE21	1.58	0.68
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.75	0.68
4:D:109:ARG:HB2	4:D:112:VAL:HG12	1.76	0.68
4:H:50:LYS:N	4:H:51:PRO:CD	2.56	0.68
1:A:401:VAL:HG21	1:A:416:LEU:HG	1.75	0.68
1:A:286:LEU:HD23	6:A:702:FAD:H6	1.76	0.68
3:G:76:ARG:HE	10:G:201:HEM:CGD	2.07	0.68
2:B:208:LEU:HD13	2:B:259:ILE:HD11	1.75	0.68
10:C:201:HEM:HBD1	10:C:201:HEM:HHA	1.76	0.68
1:E:557:THR:O	1:E:561:VAL:HG13	1.94	0.68
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.76	0.68
1:E:280:ILE:HG13	1:E:287:ILE:HD11	1.76	0.67
1:E:45:VAL:HG22	1:E:68:ALA:HB3	1.75	0.67
2:B:64:CYS:HB2	2:B:74:LYS:HD2	1.76	0.67
3:G:69:TRP:O	3:G:73:GLY:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:GLN:HE22	2:B:195:TYR:HE1	1.43	0.67
1:E:113:LEU:HD21	1:E:269:ASP:OD1	1.95	0.67
1:E:360:LEU:HB3	1:E:363:ILE:HD11	1.76	0.67
1:A:476:ASN:O	1:A:480:VAL:HG23	1.94	0.67
1:E:269:ASP:HB3	1:E:272:PHE:CD1	2.31	0.66
1:E:508:ARG:HB3	1:E:513:LEU:HD11	1.76	0.66
1:A:43:ASP:HA	1:A:230:LYS:HE3	1.76	0.66
1:E:40:HIS:O	1:E:228:ARG:HG3	1.96	0.66
1:E:117:ASN:H	1:E:117:ASN:HD22	1.41	0.66
3:C:76:ARG:HE	10:C:201:HEM:CGD	2.07	0.66
2:B:101:ILE:HG12	2:B:123:ILE:HD12	1.76	0.66
1:A:299:VAL:HG13	1:A:303:GLY:HA2	1.78	0.66
3:C:76:ARG:HA	10:C:201:HEM:O2D	1.96	0.66
2:B:240:HIS:HB2	11:C:202:AT5:CM3	2.26	0.66
1:A:81:THR:HB	1:A:181:LEU:HD23	1.77	0.66
2:B:185:CYS:SG	8:B:302:SF4:FE1	1.87	0.66
3:C:74:LEU:HG	3:C:130:PHE:CE1	2.31	0.66
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.25	0.66
4:D:109:ARG:NH2	4:D:109:ARG:HG2	1.95	0.66
11:C:202:AT5:CM2	11:C:202:AT5:HM32	2.26	0.66
1:E:286:LEU:HD23	6:E:702:FAD:H6	1.78	0.65
1:E:78:SER:HG	6:E:702:FAD:HO3A	1.40	0.65
2:F:202:TYR:CE2	2:F:204:GLY:HA2	2.31	0.65
1:E:502:LYS:HD3	1:E:503:HIS:CE1	2.31	0.65
1:E:140:PHE:HA	1:E:172:VAL:HG22	1.79	0.65
3:G:135:GLY:HA3	10:G:201:HEM:HMB3	1.78	0.65
10:C:201:HEM:HHA	10:C:201:HEM:HBA2	1.77	0.65
1:E:215:ILE:HA	1:E:225:HIS:O	1.97	0.65
2:B:127:PRO:HB2	2:B:190:ALA:O	1.96	0.65
4:D:41:ASP:OD1	4:D:44:ALA:HB3	1.96	0.65
2:B:215:ILE:CG2	2:B:226:ARG:HD2	2.26	0.65
1:A:294:GLU:OE2	1:A:359:ARG:HG2	1.96	0.65
1:A:503:HIS:HE2	1:A:519:LYS:HE2	1.62	0.65
2:F:100:ASN:HD21	2:F:103:GLY:HA2	1.62	0.65
10:G:201:HEM:HBB2	10:G:201:HEM:CMB	2.20	0.65
1:E:228:ARG:NH1	1:E:463:PRO:O	2.30	0.65
1:E:395:THR:HA	1:E:400:GLN:O	1.97	0.65
1:E:52:ALA:H	1:E:441:ALA:HB1	1.61	0.64
1:E:583:ASP:O	1:E:602:HIS:HB3	1.97	0.64
1:A:589:LYS:O	1:A:591:ILE:N	2.26	0.64
2:F:131:VAL:CG2	3:G:55:PRO:HG2	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:197:TRP:O	4:H:109:ARG:NH2	2.31	0.64
1:E:605:LYS:HD2	1:E:622:TYR:HB3	1.79	0.64
2:F:230:MET:CE	2:F:262:ILE:HG21	2.28	0.64
1:A:337:VAL:HG22	1:A:338:GLY:H	1.62	0.64
4:D:77:TYR:CD1	12:D:201:EPH:H372	2.32	0.64
1:E:383:ILE:HG12	1:E:384:PRO:CD	2.28	0.63
2:F:268:LYS:HG3	2:F:269:MET:N	2.09	0.63
1:E:536:SER:HB2	2:F:46:GLU:CD	2.19	0.63
1:A:205:LEU:HB3	1:A:212:VAL:CG2	2.28	0.63
1:A:288:THR:HG23	1:A:291:SER:H	1.61	0.63
1:E:190:ARG:O	4:H:43:ILE:HD11	1.99	0.63
1:E:230:LYS:HE3	1:E:456:LEU:HD11	1.80	0.63
2:B:196:TRP:CZ3	3:C:59:HIS:HB2	2.33	0.63
1:E:174:ASP:CB	1:E:361:PRO:HD2	2.28	0.63
1:E:582:GLU:CB	1:E:603:TRP:HD1	2.11	0.63
1:A:41:ALA:HA	1:A:228:ARG:O	1.98	0.63
2:F:88:SER:O	2:F:90:ARG:N	2.31	0.62
2:F:237:PHE:CE2	4:H:59:PHE:CD1	2.87	0.62
3:G:36:THR:HB	3:G:37:PRO:HD2	1.81	0.62
1:A:578:PHE:N	1:A:579:PRO:HD3	2.12	0.62
1:A:38:ILE:HD12	1:A:225:HIS:CE1	2.34	0.62
1:E:242:ALA:HB2	1:E:552:LEU:HD22	1.81	0.62
1:E:620:LEU:O	1:E:621:ASP:HB2	1.99	0.62
1:E:286:LEU:HD23	6:E:702:FAD:C6	2.29	0.62
1:A:331:ILE:HG23	1:A:342:ASP:HA	1.80	0.62
3:C:133:LEU:O	3:C:136:ILE:HD12	1.99	0.62
4:H:109:ARG:NH2	4:H:109:ARG:HG2	2.12	0.62
3:C:61:THR:HB	3:C:62:ILE:HG23	1.81	0.62
1:E:286:LEU:HD12	1:E:287:ILE:N	2.15	0.62
1:A:243:TYR:CG	1:A:386:VAL:HG21	2.35	0.62
1:A:88:ASN:HD21	1:A:435:ALA:HB3	1.61	0.61
1:E:570:ARG:NH1	1:E:581:ARG:CD	2.58	0.61
2:F:89:CYS:HB2	2:F:93:ILE:HG22	1.82	0.61
1:E:424:CYS:C	1:E:426:SER:N	2.53	0.61
1:A:230:LYS:HD2	1:A:462:ILE:HA	1.82	0.61
1:E:39:ASP:OD2	1:E:226:ARG:NH1	2.33	0.61
1:E:437:SER:HB3	6:E:702:FAD:N1	2.15	0.61
4:D:109:ARG:CG	4:D:109:ARG:HH21	2.02	0.61
4:H:44:ALA:HA	4:H:47:LYS:HE2	1.83	0.61
3:C:123:ILE:O	3:C:127:PRO:CD	2.42	0.61
4:D:70:VAL:O	4:D:74:PRO:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HE3	1:A:251:MET:HG3	1.83	0.61
3:C:121:LYS:HB3	3:C:171:VAL:HG22	1.83	0.61
3:C:80:CYS:O	3:C:84:GLY:N	2.32	0.61
1:E:174:ASP:OD2	1:E:362:GLY:N	2.34	0.61
1:A:307:MET:C	1:A:309:ARG:H	2.04	0.61
3:G:120:PHE:HA	3:G:123:ILE:HD12	1.83	0.61
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.01	0.61
1:E:39:ASP:HB2	4:H:33:THR:HG22	1.83	0.61
1:E:380:ILE:HG22	1:E:382:VAL:HG13	1.82	0.61
1:A:150:GLN:HA	1:A:169:THR:O	2.01	0.60
2:F:254:ASN:CG	2:F:257:ARG:HB2	2.22	0.60
3:C:104:VAL:O	3:C:107:ILE:HG13	2.01	0.60
1:A:424:CYS:C	1:A:426:SER:H	2.02	0.60
1:A:388:TYR:HE1	1:A:437:SER:HG	1.50	0.60
2:F:188:CYS:SG	2:F:206:ALA:HB2	2.42	0.60
10:C:201:HEM:HBB2	10:C:201:HEM:CMB	2.31	0.60
1:E:432:ARG:NH2	1:E:435:ALA:H	2.00	0.60
1:A:117:ASN:H	1:A:117:ASN:HD22	1.48	0.60
2:B:242:ILE:HG23	3:C:69:TRP:HA	1.83	0.60
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.82	0.60
4:H:58:LEU:O	4:H:61:ILE:HG12	2.02	0.60
1:A:83:ALA:HB3	1:A:177:GLY:CA	2.20	0.60
3:G:112:ILE:CB	3:G:113:PRO:HD3	2.31	0.60
1:E:289:GLU:HB2	1:E:320:ARG:NH2	2.16	0.60
3:G:132:THR:HG23	10:G:201:HEM:CBB	2.32	0.60
1:A:233:ILE:HG12	1:A:417:TYR:HB2	1.83	0.59
1:A:325:ARG:NH1	1:A:571:GLY:O	2.35	0.59
1:A:276:HIS:HB2	1:A:387:HIS:CB	2.31	0.59
1:A:278:THR:CG2	1:A:346:LEU:HD22	2.32	0.59
3:G:175:ARG:HG3	3:G:175:ARG:O	2.02	0.59
2:B:129:MET:HA	2:B:129:MET:CE	2.32	0.59
1:E:71:THR:HG1	6:E:702:FAD:HO2A	1.46	0.59
2:B:268:LYS:CG	2:B:269:MET:N	2.64	0.59
1:A:39:ASP:OD1	1:A:226:ARG:NH1	2.35	0.59
2:B:128:HIS:CD2	3:C:59:HIS:HD2	2.20	0.59
1:A:628:LYS:HD3	1:A:628:LYS:H	1.66	0.59
1:E:231:ARG:HD2	1:E:415:GLY:HA2	1.84	0.59
1:E:562:ALA:HB2	1:E:609:THR:CG2	2.33	0.59
2:F:212:TYR:HB2	2:F:262:ILE:HD11	1.85	0.59
3:G:48:ARG:O	3:G:52:LEU:HG	2.03	0.59
3:G:82:MET:HB2	10:G:201:HEM:HAC	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:ARG:NH1	5:E:701:MLI:C2	2.66	0.58
2:B:276:LEU:O	2:B:278:THR:N	2.36	0.58
1:A:205:LEU:HB2	1:A:213:GLY:O	2.02	0.58
3:C:45:TYR:CE2	3:C:49:GLN:HG3	2.38	0.58
2:B:254:ASN:ND2	3:C:147:THR:O	2.27	0.58
1:A:100:LYS:HD3	1:A:635:VAL:HG21	1.85	0.58
1:E:562:ALA:HB2	1:E:609:THR:HG22	1.84	0.58
1:E:268:GLU:HG2	1:E:394:PRO:HG3	1.85	0.58
2:B:212:TYR:HB2	2:B:262:ILE:HD11	1.84	0.58
1:E:329:ILE:HD11	1:E:507:PHE:HZ	1.68	0.58
3:C:82:MET:HG2	12:D:201:EPH:H262	1.85	0.58
2:B:179:LEU:HD12	2:B:209:MET:HE2	1.85	0.58
1:A:221:ASP:HA	1:A:538:ILE:HG12	1.86	0.58
2:B:250:PRO:HD2	8:B:302:SF4:S3	2.44	0.58
2:F:247:LYS:O	2:F:247:LYS:HG3	2.02	0.58
1:E:274:GLN:HB2	1:E:390:MET:CE	2.33	0.58
1:E:279:GLY:O	1:E:382:VAL:HA	2.04	0.58
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.85	0.58
1:E:91:LEU:HD23	1:E:127:VAL:HG12	1.86	0.58
2:B:64:CYS:HB2	2:B:74:LYS:CD	2.34	0.58
3:G:158:LEU:O	3:G:162:LEU:HB2	2.03	0.58
1:A:286:LEU:CD2	6:A:702:FAD:C6	2.82	0.58
1:E:230:LYS:HB3	1:E:456:LEU:HD21	1.86	0.58
1:A:337:VAL:HG11	1:A:345:TYR:CD1	2.38	0.58
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.85	0.57
3:C:126:PHE:HA	3:C:167:SER:OG	2.03	0.57
1:A:503:HIS:NE2	1:A:519:LYS:HE2	2.20	0.57
1:A:333:GLU:HB3	1:A:335:ARG:HH12	1.69	0.57
2:F:93:ILE:O	2:F:93:ILE:HD13	2.03	0.57
1:E:128:GLU:HG2	1:E:446:ARG:HH22	1.69	0.57
1:A:276:HIS:HB2	1:A:387:HIS:HB2	1.86	0.57
2:F:254:ASN:OD1	2:F:257:ARG:HB2	2.04	0.57
3:C:156:ALA:O	3:C:160:LEU:HB2	2.04	0.57
1:A:231:ARG:CD	1:A:415:GLY:HA2	2.33	0.57
1:E:203:ASP:O	1:E:215:ILE:HG22	2.05	0.57
1:E:262:ARG:HH22	1:E:551:ASN:HD21	1.52	0.57
4:D:77:TYR:HD1	12:D:201:EPH:H372	1.68	0.57
1:E:213:GLY:HA3	1:E:227:PHE:O	2.05	0.57
1:A:432:ARG:NH2	1:A:435:ALA:H	2.02	0.57
3:G:173:TYR:CD2	3:G:174:PRO:HD3	2.38	0.57
1:A:71:THR:OG1	1:A:73:MET:O	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ALA:HA	1:E:126:ALA:HB1	1.86	0.57
2:F:268:LYS:HG2	2:F:269:MET:H	1.67	0.56
2:F:262:ILE:HG22	2:F:266:LEU:CD2	2.34	0.56
2:B:237:PHE:HE2	4:D:59:PHE:CD1	2.23	0.56
2:B:47:GLU:HG2	2:B:48:PRO:HD2	1.87	0.56
1:A:281:TYR:HA	1:A:383:ILE:HG22	1.86	0.56
1:E:71:THR:OG1	6:E:702:FAD:O2B	2.21	0.56
5:A:701:MLI:H12	6:A:702:FAD:N5	2.20	0.56
2:F:242:ILE:HG12	3:G:72:SER:OG	2.05	0.56
10:C:201:HEM:HBA2	10:C:201:HEM:CHA	2.35	0.56
1:A:42:TYR:O	1:A:229:SER:HA	2.05	0.56
1:E:139:PRO:HA	2:F:219:ARG:HH22	1.69	0.56
2:B:243:MET:HE2	3:C:141:PHE:HB3	1.87	0.56
1:E:432:ARG:HH21	1:E:435:ALA:N	2.03	0.56
1:E:517:VAL:O	1:E:521:MET:HG2	2.06	0.56
1:A:434:GLY:O	1:A:435:ALA:HB3	2.06	0.56
1:E:249:ALA:HB1	2:F:88:SER:OG	2.05	0.56
4:H:69:MET:O	4:H:73:ILE:HD12	2.06	0.56
1:A:65:PHE:HE2	1:A:456:LEU:HD12	1.69	0.56
1:E:526:GLU:C	1:E:528:LYS:H	2.09	0.56
3:G:134:ASN:O	3:G:137:ARG:HB3	2.05	0.56
2:B:35:ILE:HG22	2:B:58:ASP:HB3	1.86	0.56
3:C:133:LEU:HA	3:C:136:ILE:HD11	1.86	0.56
2:B:242:ILE:CD1	11:C:202:AT5:HM33	2.35	0.56
1:E:157:SER:HA	1:E:166:ALA:HB2	1.87	0.56
3:G:73:GLY:HA2	11:G:202:AT5:O4	2.06	0.56
1:E:43:ASP:O	1:E:230:LYS:HB2	2.05	0.56
1:E:42:TYR:O	1:E:229:SER:HA	2.06	0.56
2:F:92:GLY:HA2	2:F:109:CYS:SG	2.45	0.56
1:A:83:ALA:HA	6:A:702:FAD:N5	2.21	0.56
1:E:243:TYR:HB3	1:E:501:GLN:OE1	2.06	0.56
1:A:172:VAL:HG21	1:A:179:SER:HB3	1.88	0.56
3:G:50:ARG:HG3	3:G:51:ALA:N	2.21	0.56
2:B:230:MET:CE	2:B:262:ILE:HG21	2.35	0.56
2:F:195:TYR:O	2:F:199:ALA:HB2	2.05	0.56
4:D:97:HIS:HB2	4:D:129:THR:HG23	1.87	0.56
2:F:55:GLN:HB3	2:F:57:PHE:HE1	1.70	0.55
2:B:230:MET:HB2	2:B:236:ALA:HB2	1.88	0.55
1:A:83:ALA:CB	1:A:438:LEU:HD21	2.37	0.55
1:A:289:GLU:HB3	5:A:701:MLI:O9	2.05	0.55
1:A:151:ARG:HG3	1:A:169:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:OD1	1:A:174:ASP:O	2.24	0.55
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.41	0.55
2:B:231:GLN:HB3	4:D:54:SER:HA	1.88	0.55
1:A:489:THR:HG21	1:A:542:ASP:OD1	2.06	0.55
1:A:204:LEU:HD22	1:A:211:CYS:SG	2.47	0.55
2:F:146:TYR:O	2:F:149:ILE:HG12	2.06	0.55
3:G:184:LEU:HB2	3:G:185:PRO:CD	2.36	0.55
2:B:105:ASN:HD21	2:B:127:PRO:CD	2.20	0.55
1:A:138:MET:CE	1:A:180:MET:HB2	2.36	0.55
1:E:153:PHE:CZ	1:E:289:GLU:HB3	2.42	0.55
2:F:245:CYS:HB2	2:F:255:PRO:HG2	1.89	0.55
2:B:160:ASN:HB3	2:B:163:GLU:HB2	1.89	0.55
1:E:146:GLY:HA3	2:F:167:TYR:CE1	2.42	0.55
2:B:217:ASP:C	2:B:219:ARG:H	2.10	0.54
2:B:264:MET:SD	3:C:143:MET:HG2	2.47	0.54
4:D:97:HIS:HB2	4:D:129:THR:CG2	2.38	0.54
3:G:100:PHE:O	3:G:103:PHE:HB3	2.06	0.54
2:F:240:HIS:O	2:F:241:THR:HG23	2.07	0.54
1:E:346:LEU:HB2	1:E:382:VAL:HG21	1.90	0.54
1:E:570:ARG:HG3	1:E:581:ARG:HD2	1.89	0.54
1:A:268:GLU:HA	1:A:607:THR:O	2.08	0.54
1:A:206:MET:HG3	1:A:263:ALA:HB1	1.89	0.54
1:A:370:PHE:CZ	2:B:110:ILE:HG22	2.42	0.54
1:A:147:LYS:HA	2:B:165:GLN:NE2	2.22	0.54
1:E:286:LEU:HD22	1:E:387:HIS:CE1	2.42	0.54
1:E:102:HIS:CE1	1:E:123:THR:HG22	2.42	0.54
1:E:602:HIS:O	1:E:605:LYS:HE2	2.08	0.54
1:E:471:GLU:HA	1:E:474:ILE:CG2	2.38	0.54
3:G:42:GLY:O	3:G:45:TYR:HB3	2.07	0.54
1:A:586:ASP:OD1	1:A:588:SER:OG	2.24	0.54
2:F:241:THR:OG1	2:F:241:THR:O	2.25	0.54
4:H:66:ALA:HA	4:H:69:MET:HG3	1.90	0.54
1:A:393:ILE:HG22	1:A:401:VAL:HG13	1.90	0.54
2:B:215:ILE:HG22	2:B:226:ARG:HD2	1.89	0.54
1:A:394:PRO:O	1:A:401:VAL:HA	2.07	0.54
3:C:82:MET:CB	10:C:201:HEM:HAC	2.36	0.53
3:G:148:ASP:OD2	3:G:150:PRO:HD2	2.08	0.53
4:H:133:LEU:O	4:H:134:ALA:C	2.45	0.53
1:A:142:ARG:HB3	2:B:170:ILE:HG22	1.90	0.53
1:E:394:PRO:O	1:E:401:VAL:HA	2.08	0.53
1:A:41:ALA:HB1	1:A:462:ILE:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:VAL:O	1:E:173:ALA:HB3	2.08	0.53
1:A:226:ARG:HH21	1:A:469:ALA:HB3	1.74	0.53
1:E:220:GLU:OE2	3:G:54:ARG:NH2	2.41	0.53
1:A:605:LYS:HA	1:A:625:VAL:HG23	1.89	0.53
1:E:561:VAL:HG23	1:E:620:LEU:HD11	1.90	0.53
4:H:50:LYS:H	4:H:51:PRO:CD	2.19	0.53
2:B:237:PHE:CE2	4:D:59:PHE:CD1	2.97	0.53
4:D:71:PRO:C	4:D:74:PRO:HD2	2.29	0.53
1:A:394:PRO:HB2	1:A:402:ILE:HG13	1.90	0.53
4:H:85:ASP:OD1	4:H:145:GLY:HA3	2.09	0.53
2:F:242:ILE:HD11	11:G:202:AT5:HM33	1.90	0.52
2:B:100:ASN:N	2:B:124:TYR:O	2.36	0.52
1:A:98:ASP:OD2	1:A:100:LYS:HG3	2.09	0.52
1:E:585:TYR:HD1	1:E:585:TYR:N	2.07	0.52
2:B:88:SER:O	2:B:89:CYS:C	2.46	0.52
2:B:245:CYS:SG	2:B:255:PRO:HG2	2.49	0.52
1:E:80:THR:HG22	1:E:181:LEU:HB2	1.90	0.52
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.92	0.52
3:C:112:ILE:N	3:C:112:ILE:HD12	2.24	0.52
3:C:50:ARG:HG3	3:C:51:ALA:N	2.23	0.52
1:E:391:GLY:HA2	1:E:424:CYS:SG	2.49	0.52
1:A:119:MET:O	1:A:123:THR:HG23	2.09	0.52
4:H:28:THR:O	4:H:30:ALA:N	2.41	0.52
1:E:427:VAL:HG11	1:E:444:PHE:CE1	2.44	0.52
2:B:188:CYS:SG	2:B:206:ALA:HB2	2.50	0.52
1:E:606:HIS:HD2	1:E:623:ARG:NH1	2.08	0.52
1:A:172:VAL:HG21	1:A:179:SER:CB	2.40	0.52
3:G:58:PRO:HB2	3:G:62:ILE:HG12	1.92	0.52
1:E:363:ILE:HG13	1:E:364:SER:H	1.73	0.52
2:F:148:SER:HB3	3:G:38:ILE:HD13	1.92	0.52
1:E:598:PRO:HD2	1:E:601:LYS:HB2	1.91	0.52
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.92	0.52
1:E:355:GLN:O	1:E:359:ARG:HB2	2.10	0.52
1:A:76:THR:O	1:A:76:THR:CG2	2.58	0.52
4:D:43:ILE:O	4:D:46:GLU:HB3	2.09	0.52
1:E:428:HIS:HB3	1:E:432:ARG:CA	2.38	0.52
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.40	0.51
2:B:254:ASN:OD1	2:B:257:ARG:HB2	2.10	0.51
1:E:476:ASN:O	1:E:480:VAL:HG23	2.09	0.51
1:E:590:PRO:C	1:E:592:GLU:H	2.13	0.51
1:E:260:ALA:O	1:E:261:THR:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:ARG:O	4:D:113:LEU:HB2	2.10	0.51
2:F:271:THR:CG2	2:F:271:THR:O	2.58	0.51
3:G:173:TYR:C	3:G:175:ARG:H	2.13	0.51
1:E:268:GLU:OE1	1:E:394:PRO:HB3	2.10	0.51
1:E:74:PHE:O	1:E:76:THR:N	2.43	0.51
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.41	0.51
11:C:202:AT5:H12	4:D:107:TYR:OH	2.10	0.51
1:E:274:GLN:HB2	1:E:390:MET:HE1	1.91	0.51
4:H:131:CYS:O	4:H:132:LEU:C	2.49	0.51
2:F:261:GLU:O	2:F:265:LEU:HD12	2.10	0.51
2:B:34:ARG:HB2	2:B:117:THR:HG21	1.92	0.51
1:E:265:ILE:HD12	1:E:401:VAL:HG11	1.93	0.51
1:E:262:ARG:HH22	1:E:551:ASN:ND2	2.08	0.51
1:E:233:ILE:HA	1:E:417:TYR:O	2.09	0.51
1:E:95:ASN:HD21	1:E:167:LYS:HB2	1.75	0.51
1:A:87:ILE:HD11	1:A:439:LEU:HA	1.92	0.51
3:C:121:LYS:HE2	4:D:154:TRP:HA	1.93	0.51
1:A:257:THR:HG22	1:A:267:LEU:HD22	1.92	0.51
1:E:102:HIS:ND1	1:E:123:THR:HG22	2.25	0.51
1:E:104:TYR:CD2	1:E:160:TYR:HA	2.45	0.51
4:H:43:ILE:O	4:H:46:GLU:HB3	2.11	0.51
2:F:240:HIS:CG	11:G:202:AT5:HM31	2.45	0.51
1:A:193:CYS:O	1:A:194:THR:C	2.48	0.51
2:F:57:PHE:HD2	2:F:75:ILE:HD12	1.73	0.51
3:C:112:ILE:CD1	3:C:117:LEU:HD21	2.38	0.51
1:A:517:VAL:HG22	1:A:560:ILE:HG23	1.93	0.51
4:H:146:LEU:O	4:H:149:ALA:HB3	2.09	0.51
1:E:134:GLU:HG3	1:E:148:ILE:HD11	1.93	0.51
3:C:133:LEU:HB3	3:C:159:VAL:HG13	1.92	0.51
3:C:173:TYR:O	3:C:176:TRP:HB3	2.11	0.51
1:A:86:GLY:O	1:A:438:LEU:HD12	2.11	0.50
1:A:58:MET:HE3	1:A:187:ASN:HB3	1.92	0.50
1:E:321:ASP:OD2	1:E:571:GLY:HA2	2.12	0.50
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.92	0.50
1:A:113:LEU:HD21	1:A:269:ASP:OD1	2.12	0.50
1:E:331:ILE:HD11	1:E:344:ILE:HG23	1.92	0.50
1:E:428:HIS:ND1	1:E:432:ARG:HG3	2.26	0.50
3:C:112:ILE:HG22	3:C:113:PRO:HD2	1.93	0.50
1:A:345:TYR:CD2	1:A:379:PRO:HG2	2.46	0.50
1:E:157:SER:HB2	1:E:164:GLY:O	2.11	0.50
2:B:85:PHE:N	2:B:85:PHE:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:C	1:A:454:GLU:H	2.14	0.50
1:E:214:VAL:HG12	1:E:215:ILE:N	2.27	0.50
2:B:126:LEU:HD22	2:B:190:ALA:HB3	1.92	0.50
2:F:36:LYS:HD2	2:F:37:THR:H	1.77	0.50
1:E:45:VAL:CG2	1:E:68:ALA:HB3	2.41	0.50
4:D:58:LEU:O	4:D:58:LEU:HD23	2.12	0.50
1:E:585:TYR:CD1	1:E:585:TYR:N	2.79	0.50
1:A:126:ALA:CB	1:A:439:LEU:HD21	2.42	0.50
1:A:439:LEU:O	1:A:443:VAL:HB	2.12	0.50
2:F:179:LEU:HD12	2:F:209:MET:HE1	1.92	0.50
2:B:181:GLU:HB2	2:B:253:LEU:HD21	1.94	0.50
1:A:383:ILE:HG12	1:A:384:PRO:O	2.12	0.50
4:H:67:ALA:O	4:H:69:MET:N	2.45	0.50
3:G:169:ALA:O	3:G:173:TYR:HB3	2.12	0.50
2:B:139:MET:HB3	2:B:143:TYR:CE2	2.47	0.50
1:E:186:GLY:O	1:E:189:LEU:HB2	2.11	0.50
2:F:242:ILE:HD11	11:G:202:AT5:CM3	2.42	0.49
2:B:89:CYS:SG	2:B:90:ARG:N	2.84	0.49
1:A:73:MET:CE	1:A:78:SER:HA	2.42	0.49
1:A:37:VAL:HG21	4:D:29:SER:HA	1.92	0.49
1:E:390:MET:O	1:E:391:GLY:O	2.30	0.49
1:A:432:ARG:HH21	1:A:435:ALA:H	1.61	0.49
1:A:443:VAL:HG12	1:A:444:PHE:HD1	1.75	0.49
3:C:59:HIS:O	3:C:62:ILE:HG13	2.12	0.49
2:F:212:TYR:HA	2:F:215:ILE:HG12	1.93	0.49
3:G:86:LEU:HB2	4:H:132:LEU:HD11	1.94	0.49
3:C:148:ASP:OD2	3:C:150:PRO:HD2	2.13	0.49
2:B:181:GLU:O	2:B:182:CYS:C	2.50	0.49
4:D:101:TRP:CH2	4:D:122:ARG:HG2	2.48	0.49
3:C:149:ILE:HG12	3:C:150:PRO:HD3	1.94	0.49
10:C:201:HEM:NC	4:D:95:HIS:CD2	2.80	0.49
1:A:274:GLN:HB2	1:A:390:MET:HE1	1.95	0.49
4:H:77:TYR:HA	12:H:201:EPH:H11	1.93	0.49
1:E:43:ASP:HA	1:E:230:LYS:HD3	1.95	0.49
1:A:148:ILE:H	2:B:165:GLN:NE2	2.10	0.49
4:H:140:ASN:HA	4:H:145:GLY:HA2	1.94	0.49
2:F:124:TYR:HB3	2:F:125:PRO:CD	2.43	0.49
1:A:43:ASP:H	1:A:66:LYS:HB3	1.77	0.49
1:A:331:ILE:HD11	1:A:344:ILE:HG22	1.95	0.49
1:A:93:SER:HB3	1:A:147:LYS:CB	2.43	0.49
1:A:74:PHE:HA	1:A:197:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:HIS:O	1:A:384:PRO:HA	2.13	0.49
11:G:202:AT5:O1	11:G:202:AT5:H111	2.12	0.49
1:E:49:ALA:HB1	1:E:75:PRO:HB3	1.95	0.49
1:A:470:GLY:O	1:A:473:SER:HB2	2.12	0.49
2:F:197:TRP:HA	4:H:109:ARG:NH2	2.28	0.48
1:E:113:LEU:O	1:E:606:HIS:HE1	1.96	0.48
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.48	0.48
1:A:567:LYS:HB3	1:A:578:PHE:CE1	2.47	0.48
2:B:35:ILE:CG2	2:B:58:ASP:HB3	2.43	0.48
2:F:66:THR:HG23	2:F:67:MET:HG2	1.94	0.48
2:B:39:GLU:HA	2:B:55:GLN:O	2.13	0.48
3:C:136:ILE:HA	3:C:139:ILE:HD12	1.95	0.48
1:E:241:ARG:HA	1:E:241:ARG:HD3	1.58	0.48
1:E:268:GLU:HB3	1:E:608:LEU:HD22	1.96	0.48
3:G:71:VAL:HG11	3:G:137:ARG:NH1	2.28	0.48
3:C:91:VAL:O	3:C:92:GLY:C	2.50	0.48
3:C:88:ILE:O	3:C:92:GLY:HA3	2.13	0.48
2:F:168:GLN:NE2	2:F:173:GLN:HA	2.27	0.48
1:E:77:ARG:HD2	2:F:96:SER:OG	2.13	0.48
1:A:142:ARG:CG	2:B:168:GLN:O	2.59	0.48
1:E:508:ARG:HH11	1:E:573:HIS:HA	1.78	0.48
1:E:109:GLY:O	1:E:431:ASN:HB3	2.14	0.48
3:C:107:ILE:HD11	4:D:156:LEU:CD2	2.25	0.48
2:B:242:ILE:O	2:B:243:MET:HB2	2.13	0.48
3:G:175:ARG:HH22	3:G:178:ARG:NH2	2.11	0.48
1:E:496:MET:HE2	1:E:552:LEU:HB3	1.95	0.48
1:A:38:ILE:N	1:A:224:ILE:O	2.45	0.48
1:A:320:ARG:HG2	1:A:320:ARG:H	1.33	0.48
1:E:618:ILE:HG22	1:E:620:LEU:HD12	1.96	0.48
3:C:76:ARG:NH1	4:D:107:TYR:HE1	2.11	0.48
3:G:116:ILE:HA	3:G:119:THR:HB	1.96	0.48
1:E:139:PRO:HA	2:F:219:ARG:NH2	2.28	0.48
1:A:55:ARG:HG2	1:A:442:VAL:O	2.14	0.48
2:F:240:HIS:C	2:F:241:THR:CG2	2.82	0.48
3:C:60:LEU:HD22	11:C:202:AT5:C10	2.42	0.48
1:E:523:LEU:C	1:E:525:LYS:N	2.65	0.48
1:A:58:MET:CE	1:A:187:ASN:HB3	2.43	0.48
1:E:438:LEU:O	1:E:441:ALA:N	2.47	0.48
2:F:230:MET:HE3	2:F:262:ILE:HG21	1.95	0.48
1:A:424:CYS:C	1:A:426:SER:N	2.67	0.48
1:A:76:THR:HG23	1:A:182:HIS:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:THR:HG21	1:E:548:GLU:HB3	1.95	0.48
3:C:132:THR:HG21	4:D:73:ILE:HG21	1.96	0.48
3:G:107:ILE:HG13	3:G:108:ARG:N	2.28	0.48
5:E:701:MLI:H12	6:E:702:FAD:N5	2.29	0.48
1:A:537:LEU:O	1:A:538:ILE:C	2.51	0.48
1:E:555:ASN:O	1:E:559:THR:OG1	2.26	0.48
2:B:268:LYS:HE2	2:B:268:LYS:HB3	1.37	0.48
2:B:231:GLN:OE1	4:D:52:LEU:HG	2.13	0.48
2:F:149:ILE:O	2:F:150:GLN:HB2	2.12	0.48
1:E:103:PHE:HA	1:E:123:THR:HG21	1.96	0.48
1:A:274:GLN:N	1:A:390:MET:HE2	2.28	0.48
1:E:427:VAL:HG23	1:E:428:HIS:CD2	2.48	0.48
2:B:128:HIS:CD2	3:C:59:HIS:CD2	2.97	0.48
2:B:268:LYS:HG2	2:B:269:MET:N	2.24	0.48
2:B:142:PHE:HE1	2:B:206:ALA:HB3	1.78	0.48
2:B:205:PRO:O	2:B:206:ALA:C	2.51	0.48
1:A:558:GLN:NE2	1:A:611:GLN:HB3	2.29	0.48
1:A:549:LEU:HD12	1:A:549:LEU:O	2.14	0.48
2:F:129:MET:CE	2:F:129:MET:HA	2.44	0.48
3:C:86:LEU:HB2	4:D:132:LEU:HD11	1.96	0.47
1:E:275:PHE:CE2	1:E:386:VAL:HG23	2.49	0.47
2:B:44:ASN:HD22	2:B:47:GLU:HB2	1.79	0.47
4:D:100:VAL:O	4:D:104:VAL:HB	2.14	0.47
1:A:496:MET:CG	1:A:497:GLN:N	2.77	0.47
1:E:496:MET:CE	1:E:552:LEU:HB3	2.44	0.47
1:E:363:ILE:O	1:E:364:SER:C	2.52	0.47
1:A:325:ARG:HG2	1:A:506:VAL:HG12	1.96	0.47
1:A:508:ARG:NH1	1:A:573:HIS:HA	2.29	0.47
1:A:545:GLU:HA	1:A:548:GLU:HB2	1.97	0.47
2:F:101:ILE:HG21	2:F:111:CYS:SG	2.54	0.47
3:C:34:GLU:OE2	3:C:34:GLU:HA	2.13	0.47
3:C:129:ALA:O	3:C:133:LEU:HD22	2.13	0.47
1:E:554:LEU:HD22	1:E:611:GLN:OE1	2.14	0.47
1:E:73:MET:HB3	1:E:251:MET:HE3	1.96	0.47
2:B:86:ARG:HD2	2:B:136:VAL:HG13	1.95	0.47
1:E:99:TRP:HE3	1:E:99:TRP:O	1.96	0.47
3:G:135:GLY:HA3	10:G:201:HEM:CMB	2.44	0.47
1:A:294:GLU:CD	1:A:359:ARG:HG2	2.35	0.47
2:F:172:GLU:OE2	2:F:275:PRO:HD2	2.14	0.47
1:A:47:ILE:CG2	1:A:201:ALA:HB2	2.45	0.47
1:E:214:VAL:CG2	1:E:232:THR:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ASN:N	1:E:117:ASN:HD22	2.09	0.47
2:B:179:LEU:HD12	2:B:209:MET:CE	2.45	0.47
2:B:201:LYS:O	2:B:235:SER:HA	2.14	0.47
2:B:146:TYR:HA	2:B:207:VAL:HG13	1.97	0.47
1:E:603:TRP:O	1:E:605:LYS:N	2.44	0.47
3:C:66:GLN:HB2	3:C:69:TRP:CD1	2.49	0.47
2:F:235:SER:HB3	3:G:39:GLN:NE2	2.30	0.47
2:B:234:PHE:O	2:B:238:LYS:HB2	2.15	0.47
1:A:503:HIS:CD2	1:A:516:GLY:CA	2.81	0.47
10:G:201:HEM:HMB1	10:G:201:HEM:CBB	2.27	0.47
4:H:67:ALA:C	4:H:69:MET:N	2.68	0.47
2:B:69:LEU:HD12	2:B:109:CYS:CB	2.45	0.47
3:G:97:PRO:HG2	3:G:98:LEU:H	1.79	0.47
3:C:60:LEU:HD22	11:C:202:AT5:H101	1.97	0.47
1:E:585:TYR:HE1	1:E:596:LYS:HD3	1.80	0.47
1:A:523:LEU:C	1:A:525:LYS:H	2.19	0.47
4:H:59:PHE:O	4:H:60:LYS:C	2.53	0.47
2:B:185:CYS:SG	8:B:302:SF4:S3	3.12	0.47
4:H:93:THR:HA	4:H:132:LEU:HD23	1.96	0.47
4:H:105:ASN:HA	4:H:122:ARG:HH12	1.79	0.47
2:B:141:LEU:HB2	3:C:45:TYR:CE1	2.51	0.46
3:C:133:LEU:HD12	3:C:133:LEU:HA	1.75	0.46
1:A:331:ILE:HD11	1:A:344:ILE:CG2	2.46	0.46
1:E:103:PHE:CE2	1:E:638:ILE:HD11	2.50	0.46
2:F:36:LYS:HB2	2:F:61:LEU:CD1	2.46	0.46
1:A:493:ARG:HB2	1:A:549:LEU:HD22	1.97	0.46
1:E:58:MET:HA	1:E:191:CYS:SG	2.56	0.46
1:A:102:HIS:O	1:A:106:THR:OG1	2.27	0.46
2:F:156:LYS:HE2	2:F:156:LYS:HB3	1.67	0.46
1:E:60:LEU:HD21	1:E:449:SER:HA	1.97	0.46
4:H:133:LEU:O	4:H:136:LEU:N	2.48	0.46
1:E:613:PRO:HG2	1:E:614:ARG:HH11	1.81	0.46
1:A:457:LYS:O	1:A:459:ASP:N	2.48	0.46
4:H:54:SER:C	4:H:56:GLY:H	2.18	0.46
11:G:202:AT5:C1	11:G:202:AT5:H111	2.45	0.46
2:B:129:MET:HA	2:B:129:MET:HE2	1.97	0.46
1:A:333:GLU:O	1:A:335:ARG:NH1	2.48	0.46
1:E:142:ARG:HB2	2:F:173:GLN:HG2	1.97	0.46
1:A:111:ASP:O	1:A:570:ARG:HD3	2.16	0.46
1:E:182:HIS:ND1	2:F:184:LEU:HD22	2.30	0.46
3:C:118:ASP:O	3:C:171:VAL:HG11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:HB2	1:A:169:THR:OG1	2.15	0.46
4:H:108:GLY:O	4:H:122:ARG:NH2	2.48	0.46
1:E:202:LEU:HD11	1:E:477:LEU:HD13	1.97	0.46
1:E:245:SER:OG	1:E:385:THR:HG21	2.15	0.46
1:E:34:GLN:HA	1:E:34:GLN:OE1	2.16	0.46
1:E:52:ALA:N	1:E:441:ALA:HB1	2.30	0.46
1:A:307:MET:C	1:A:309:ARG:N	2.69	0.46
1:E:139:PRO:HB3	2:F:176:LEU:HD23	1.97	0.46
2:B:86:ARG:HH12	2:B:139:MET:HB2	1.81	0.46
1:E:77:ARG:HA	2:F:94:CYS:HB2	1.97	0.46
1:E:298:LEU:HB3	1:E:306:PHE:CE2	2.51	0.46
1:E:544:THR:C	1:E:546:SER:N	2.68	0.46
1:A:276:HIS:CE1	1:A:286:LEU:CD1	2.99	0.46
2:F:238:LYS:O	2:F:240:HIS:CD2	2.69	0.46
2:F:242:ILE:HB	9:F:303:F3S:S4	2.55	0.46
2:B:258:ALA:O	2:B:259:ILE:C	2.53	0.46
3:G:122:PHE:HA	3:G:171:VAL:HG21	1.97	0.46
1:E:231:ARG:HD3	1:E:231:ARG:HA	1.55	0.46
1:A:538:ILE:O	1:A:539:TRP:C	2.55	0.46
1:E:363:ILE:HG13	1:E:364:SER:N	2.31	0.46
1:A:274:GLN:HB2	1:A:390:MET:CE	2.46	0.46
2:B:89:CYS:HB2	2:B:93:ILE:HG22	1.98	0.46
1:E:496:MET:O	1:E:500:MET:HB2	2.15	0.46
2:B:126:LEU:HB3	2:B:190:ALA:CB	2.45	0.46
1:A:390:MET:SD	1:A:432:ARG:HB2	2.56	0.45
1:E:249:ALA:C	1:E:251:MET:H	2.19	0.45
1:E:361:PRO:HG2	1:E:362:GLY:H	1.80	0.45
2:B:215:ILE:HG23	2:B:226:ARG:HD2	1.97	0.45
1:A:120:HIS:HD2	1:A:630:LEU:H	1.64	0.45
1:A:268:GLU:HB3	1:A:608:LEU:CD2	2.43	0.45
2:F:36:LYS:HB2	2:F:61:LEU:HD12	1.98	0.45
1:E:241:ARG:HH22	2:F:90:ARG:HH12	1.64	0.45
2:B:214:TRP:HB3	2:B:226:ARG:CZ	2.45	0.45
1:E:526:GLU:C	1:E:528:LYS:N	2.70	0.45
2:F:213:ARG:HD3	2:F:213:ARG:C	2.37	0.45
1:E:46:ILE:HG12	1:E:233:ILE:HD12	1.99	0.45
4:D:101:TRP:CZ3	4:D:122:ARG:HG2	2.51	0.45
1:A:74:PHE:HA	1:A:197:ILE:CG2	2.46	0.45
1:E:246:CYS:HA	1:E:386:VAL:O	2.16	0.45
1:A:47:ILE:HG21	1:A:201:ALA:CB	2.46	0.45
3:G:171:VAL:HA	4:H:154:TRP:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:514:ALA:HA	1:E:517:VAL:HG23	1.97	0.45
1:A:360:LEU:N	1:A:361:PRO:CD	2.79	0.45
2:B:217:ASP:C	2:B:219:ARG:N	2.70	0.45
1:E:612:ASP:HB3	1:E:616:GLY:H	1.82	0.45
1:A:276:HIS:HB2	1:A:387:HIS:CG	2.51	0.45
10:C:201:HEM:HBB1	4:D:70:VAL:HA	1.98	0.45
1:A:121:TYR:CE1	1:A:447:ALA:HB2	2.51	0.45
1:A:337:VAL:CG1	1:A:345:TYR:CD1	2.99	0.45
2:F:257:ARG:HG2	3:G:147:THR:OG1	2.16	0.45
1:E:280:ILE:CG1	1:E:287:ILE:HD11	2.46	0.45
4:H:93:THR:HG21	4:H:133:LEU:HB2	1.98	0.45
1:E:122:LEU:HA	1:E:443:VAL:HG11	1.98	0.45
2:B:47:GLU:OE2	2:B:48:PRO:O	2.35	0.45
2:B:76:LYS:HA	2:B:80:ASP:O	2.16	0.45
1:A:481:ARG:NH2	1:A:537:LEU:HG	2.32	0.45
1:A:246:CYS:O	2:B:90:ARG:NH2	2.50	0.45
1:E:514:ALA:HB2	1:E:564:GLU:HG3	1.99	0.45
3:G:52:LEU:HD12	3:G:54:ARG:NH1	2.31	0.45
1:E:437:SER:OG	6:E:702:FAD:H2'	2.17	0.45
1:A:277:PRO:HA	1:A:324:SER:OG	2.17	0.45
2:F:89:CYS:SG	2:F:90:ARG:N	2.90	0.45
2:B:242:ILE:HD11	11:C:202:AT5:CM3	2.43	0.45
1:E:99:TRP:CE3	1:E:99:TRP:C	2.90	0.45
1:A:638:ILE:HA	1:A:639:PRO:HD3	1.85	0.45
2:F:136:VAL:HA	2:F:137:PRO:HD3	1.64	0.45
1:E:353:ALA:HB2	1:E:376:THR:HG21	1.97	0.45
1:E:635:VAL:HG22	1:E:636:ASP:H	1.80	0.45
1:E:388:TYR:CD2	1:E:432:ARG:HD2	2.52	0.45
2:B:249:CYS:HA	8:B:302:SF4:S3	2.57	0.45
2:B:125:PRO:O	2:B:126:LEU:C	2.55	0.45
1:A:628:LYS:H	1:A:628:LYS:CD	2.29	0.45
1:E:275:PHE:CE1	1:E:506:VAL:HA	2.52	0.45
1:A:196:PHE:O	1:A:199:TYR:CD1	2.70	0.45
4:D:140:ASN:ND2	4:D:140:ASN:N	2.62	0.45
1:E:584:GLU:C	1:E:585:TYR:HD1	2.21	0.44
1:A:78:SER:O	1:A:81:THR:HG22	2.17	0.44
3:C:152:ILE:HG22	3:C:153:TYR:N	2.31	0.44
2:F:268:LYS:HE2	2:F:268:LYS:HB3	1.65	0.44
2:B:131:VAL:O	3:C:54:ARG:HD3	2.18	0.44
4:D:144:VAL:HG21	4:D:152:MET:HE1	1.99	0.44
1:A:642:ILE:HG13	1:A:642:ILE:H	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:129:THR:O	4:H:130:ALA:C	2.55	0.44
2:F:115:GLN:CA	2:F:115:GLN:HE21	2.05	0.44
2:F:240:HIS:C	2:F:241:THR:HG23	2.37	0.44
2:F:100:ASN:HD21	2:F:103:GLY:CA	2.28	0.44
1:A:495:THR:O	1:A:499:THR:HG23	2.18	0.44
2:B:194:SER:HB3	2:B:202:TYR:CD2	2.52	0.44
2:F:205:PRO:HD3	9:F:303:F3S:S3	2.58	0.44
1:E:605:LYS:HD2	1:E:622:TYR:CB	2.47	0.44
2:B:71:ALA:O	2:B:75:ILE:CG1	2.58	0.44
4:H:104:VAL:CG1	4:H:121:VAL:HG12	2.46	0.44
1:A:325:ARG:HG2	1:A:506:VAL:CG1	2.48	0.44
1:A:635:VAL:HG22	1:A:636:ASP:H	1.81	0.44
1:E:608:LEU:N	1:E:608:LEU:HD23	2.32	0.44
1:E:74:PHE:CD1	1:E:75:PRO:HD2	2.53	0.44
4:D:140:ASN:HD22	4:D:140:ASN:N	2.16	0.44
1:A:600:GLU:N	1:A:600:GLU:OE2	2.51	0.44
2:F:196:TRP:CH2	3:G:59:HIS:HB2	2.53	0.44
4:H:47:LYS:HB2	4:H:47:LYS:HE3	1.72	0.44
2:B:217:ASP:O	2:B:219:ARG:N	2.50	0.44
1:A:599:PHE:HA	1:A:602:HIS:CD2	2.52	0.44
2:F:154:GLN:HE21	2:F:222:SER:HB2	1.83	0.44
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.52	0.44
2:F:251:LYS:HB2	2:F:253:LEU:HG	2.00	0.44
3:C:132:THR:HG23	10:C:201:HEM:CBB	2.48	0.44
1:E:388:TYR:HE1	1:E:421:GLU:HG3	1.75	0.44
1:A:538:ILE:O	1:A:539:TRP:O	2.35	0.44
1:A:76:THR:CG2	1:A:182:HIS:NE2	2.81	0.44
1:A:101:TRP:CE3	1:A:158:ASN:HB3	2.52	0.44
1:E:325:ARG:O	1:E:326:ALA:C	2.56	0.44
1:A:486:ASP:OD2	1:A:529:ARG:HG2	2.17	0.44
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.00	0.44
1:E:570:ARG:HG3	1:E:581:ARG:CD	2.48	0.44
1:E:603:TRP:HZ3	1:E:622:TYR:CE2	2.36	0.44
11:C:202:AT5:H142	4:D:107:TYR:CE2	2.52	0.44
1:E:214:VAL:HG23	1:E:232:THR:HG21	1.99	0.44
1:A:148:ILE:H	2:B:165:GLN:HE22	1.64	0.44
1:E:598:PRO:O	1:E:600:GLU:N	2.51	0.44
1:E:46:ILE:HB	1:E:69:VAL:HG22	2.00	0.44
2:B:141:LEU:HB2	3:C:45:TYR:CZ	2.53	0.44
1:E:437:SER:O	1:E:440:ASP:HB3	2.17	0.44
1:E:83:ALA:HB3	1:E:177:GLY:CA	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LEU:HG	6:A:702:FAD:C2	2.48	0.44
1:A:109:GLY:O	1:A:431:ASN:HB3	2.18	0.44
1:E:274:GLN:HB2	1:E:390:MET:HE2	2.00	0.44
2:F:36:LYS:NZ	2:F:114:ASP:O	2.46	0.44
1:A:432:ARG:NH2	6:A:702:FAD:C2	2.81	0.43
3:C:45:TYR:O	3:C:49:GLN:HG2	2.18	0.43
3:C:100:PHE:O	3:C:104:VAL:HG23	2.18	0.43
10:G:201:HEM:CMB	10:G:201:HEM:CBB	2.93	0.43
2:F:34:ARG:HD3	2:F:34:ARG:O	2.18	0.43
1:E:270:LEU:O	1:E:559:THR:HG23	2.18	0.43
1:A:126:ALA:HB2	1:A:439:LEU:HD11	2.01	0.43
1:A:416:LEU:C	1:A:417:TYR:HD1	2.21	0.43
1:A:138:MET:HE1	1:A:180:MET:HB2	2.00	0.43
4:D:131:CYS:O	4:D:132:LEU:C	2.56	0.43
2:B:102:ALA:HA	2:B:122:LYS:NZ	2.33	0.43
3:G:168:LEU:O	3:G:172:VAL:HG12	2.18	0.43
3:C:35:LYS:O	4:D:49:PHE:HE1	2.01	0.43
1:E:287:ILE:O	1:E:288:THR:O	2.37	0.43
2:B:145:GLN:O	2:B:148:SER:HB3	2.18	0.43
2:F:154:GLN:HE21	2:F:222:SER:CB	2.30	0.43
2:F:205:PRO:HA	2:F:259:ILE:HD11	2.01	0.43
3:C:71:VAL:HG12	3:C:72:SER:N	2.32	0.43
2:F:146:TYR:CE1	2:F:210:GLN:HG2	2.53	0.43
1:E:224:ILE:HG13	1:E:474:ILE:HD13	1.99	0.43
3:C:105:GLU:C	3:C:107:ILE:H	2.21	0.43
1:A:155:GLY:HA3	1:A:433:LEU:HD11	1.99	0.43
4:H:67:ALA:C	4:H:69:MET:H	2.22	0.43
1:A:508:ARG:HB3	1:A:513:LEU:HD11	2.01	0.43
1:A:242:ALA:HB2	1:A:552:LEU:HD22	2.00	0.43
4:H:101:TRP:CH2	4:H:122:ARG:HG2	2.54	0.43
3:G:74:LEU:HD23	3:G:130:PHE:CE1	2.53	0.43
10:G:201:HEM:C1C	4:H:95:HIS:CD2	3.07	0.43
1:E:241:ARG:C	1:E:243:TYR:H	2.22	0.43
4:D:73:ILE:N	4:D:74:PRO:CD	2.81	0.43
2:F:230:MET:HE1	2:F:262:ILE:HG21	2.00	0.43
1:A:578:PHE:N	1:A:579:PRO:CD	2.82	0.43
1:A:267:LEU:HB3	1:A:270:LEU:HD21	1.99	0.43
1:E:111:ASP:OD2	1:E:643:ARG:HD2	2.19	0.43
1:A:433:LEU:HD12	1:A:434:GLY:H	1.84	0.43
1:A:122:LEU:HG	1:A:439:LEU:CD1	2.48	0.43
1:E:117:ASN:OD1	1:E:397:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD12	1:A:558:GLN:OE1	2.18	0.43
4:H:77:TYR:HA	12:H:201:EPH:C1	2.48	0.43
1:A:428:HIS:HE1	1:A:436:ASN:HB3	1.83	0.43
1:E:337:VAL:HG12	1:E:343:HIS:O	2.19	0.43
1:E:84:GLN:HB2	1:E:288:THR:HB	2.01	0.43
3:C:136:ILE:HG13	3:C:136:ILE:H	1.59	0.43
3:C:58:PRO:HB2	3:C:62:ILE:HG12	2.00	0.43
4:H:92:LEU:O	4:H:93:THR:C	2.57	0.43
1:E:623:ARG:HG3	1:E:624:PRO:HD2	2.01	0.43
1:A:76:THR:HG22	1:A:76:THR:O	2.18	0.43
1:A:105:ASP:N	1:A:105:ASP:OD1	2.50	0.43
2:B:73:ILE:HG22	2:B:77:ASN:HD21	1.84	0.43
1:E:320:ARG:NH1	5:E:701:MLI:O6	2.52	0.43
4:H:59:PHE:HE2	4:H:63:ARG:NH2	2.17	0.43
1:A:291:SER:HB2	1:A:348:LEU:HD21	2.01	0.43
1:E:191:CYS:O	1:E:193:CYS:N	2.52	0.43
2:F:276:LEU:HA	2:F:277:PRO:HD2	1.87	0.43
4:D:156:LEU:H	4:D:156:LEU:HG	1.67	0.42
3:C:71:VAL:HG11	3:C:137:ARG:NH1	2.34	0.42
2:B:68:VAL:HG21	2:B:101:ILE:HD13	2.01	0.42
2:B:86:ARG:CD	2:B:136:VAL:HG13	2.49	0.42
1:E:300:ASN:HB3	1:E:306:PHE:CD2	2.54	0.42
3:G:80:CYS:O	3:G:81:ALA:C	2.57	0.42
1:A:509:ARG:HB3	1:A:511:ASP:OD2	2.20	0.42
1:A:88:ASN:ND2	1:A:435:ALA:CB	2.80	0.42
3:C:126:PHE:HB3	3:C:127:PRO:HD3	2.01	0.42
1:A:78:SER:HB2	1:A:181:LEU:HD21	2.02	0.42
4:D:54:SER:C	4:D:56:GLY:H	2.21	0.42
1:A:72:LYS:HE2	6:A:702:FAD:C8A	2.49	0.42
1:A:205:LEU:HD22	1:A:214:VAL:O	2.19	0.42
1:E:444:PHE:O	1:E:447:ALA:HB3	2.19	0.42
2:B:262:ILE:HG22	2:B:266:LEU:HD22	2.01	0.42
1:A:134:GLU:OE2	2:B:219:ARG:NH1	2.45	0.42
2:B:86:ARG:HH11	2:B:137:PRO:HD2	1.83	0.42
3:G:156:ALA:O	3:G:160:LEU:HB2	2.19	0.42
4:D:87:CYS:HA	4:D:90:LEU:HB2	2.01	0.42
1:A:453:LYS:O	1:A:453:LYS:HG3	2.18	0.42
3:C:126:PHE:HA	3:C:129:ALA:HB3	2.02	0.42
10:C:201:HEM:CBB	10:C:201:HEM:HMB2	2.45	0.42
2:F:146:TYR:HE1	2:F:210:GLN:HG2	1.85	0.42
2:B:208:LEU:HD13	2:B:259:ILE:CD1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:TYR:CD2	1:E:66:LYS:HG2	2.54	0.42
1:A:370:PHE:HZ	2:B:110:ILE:HG22	1.84	0.42
3:G:85:THR:O	3:G:89:GLY:N	2.52	0.42
1:E:289:GLU:CD	1:E:320:ARG:HH21	2.23	0.42
3:C:66:GLN:O	3:C:70:MET:HB2	2.19	0.42
1:E:388:TYR:CE2	1:E:432:ARG:HD2	2.55	0.42
3:C:112:ILE:HG22	3:C:116:ILE:HD13	2.01	0.42
1:E:331:ILE:CD1	1:E:344:ILE:HG23	2.49	0.42
3:G:85:THR:HA	3:G:88:ILE:HG13	2.00	0.42
1:E:182:HIS:HE1	2:F:184:LEU:HD22	1.77	0.42
2:B:212:TYR:CZ	2:B:216:ILE:HG12	2.55	0.42
3:G:104:VAL:HG13	4:H:156:LEU:HD23	2.02	0.42
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.79	0.42
2:F:141:LEU:O	2:F:145:GLN:HG3	2.19	0.42
1:A:590:PRO:O	1:A:592:GLU:N	2.35	0.42
6:E:702:FAD:H1'1	6:E:702:FAD:H9	1.76	0.42
2:F:57:PHE:CG	2:F:75:ILE:HD12	2.52	0.42
2:F:146:TYR:HA	2:F:207:VAL:HG13	2.01	0.42
3:G:170:VAL:O	3:G:174:PRO:HD2	2.18	0.42
1:E:45:VAL:O	1:E:232:THR:HA	2.20	0.42
2:B:187:CYS:HB2	8:B:302:SF4:S3	2.60	0.42
1:A:147:LYS:HA	2:B:165:GLN:HE22	1.83	0.42
1:A:93:SER:HB3	1:A:147:LYS:HB2	2.01	0.42
1:A:34:GLN:NE2	1:A:35:TYR:H	2.18	0.42
3:G:43:TRP:O	3:G:46:LEU:N	2.52	0.42
1:A:482:TYR:O	1:A:483:ALA:C	2.58	0.42
1:A:585:TYR:CE1	1:A:596:LYS:HA	2.55	0.42
1:E:410:ASP:N	1:E:410:ASP:OD2	2.52	0.42
1:E:56:ALA:HA	1:E:445:GLY:O	2.20	0.42
2:B:261:GLU:O	2:B:265:LEU:HD12	2.20	0.42
1:E:146:GLY:HA3	2:F:167:TYR:HE1	1.84	0.42
1:A:452:ILE:C	1:A:454:GLU:N	2.73	0.42
1:A:110:SER:HA	1:A:428:HIS:O	2.19	0.42
10:G:201:HEM:NC	4:H:95:HIS:HD2	1.99	0.42
4:D:109:ARG:NH2	4:D:109:ARG:CG	2.72	0.42
1:A:580:LYS:HB3	1:A:582:GLU:OE1	2.20	0.42
1:A:234:VAL:HG12	1:A:236:THR:HG23	2.02	0.42
1:A:73:MET:HE3	1:A:78:SER:HA	2.01	0.42
1:A:385:THR:O	1:A:386:VAL:C	2.58	0.42
1:A:219:LEU:HD21	1:A:544:THR:HG21	2.01	0.42
1:E:309:ARG:NH2	1:E:310:TYR:CE2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:LEU:HA	2:F:135:LEU:HD23	1.80	0.42
1:E:72:LYS:HE2	6:E:702:FAD:N7A	2.34	0.41
3:C:73:GLY:O	3:C:76:ARG:HB2	2.19	0.41
3:G:173:TYR:C	3:G:175:ARG:N	2.74	0.41
1:E:401:VAL:HG21	1:E:416:LEU:HG	2.01	0.41
2:B:224:ALA:HB3	2:B:225:GLU:OE2	2.19	0.41
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.20	0.41
1:E:83:ALA:HA	6:E:702:FAD:C5X	2.50	0.41
1:E:79:HIS:NE2	6:E:702:FAD:C8	2.75	0.41
2:F:71:ALA:O	2:F:75:ILE:HG12	2.20	0.41
2:B:222:SER:O	2:B:223:ALA:C	2.58	0.41
4:H:80:HIS:HA	4:H:147:THR:HG21	2.01	0.41
1:E:207:ASP:OD1	1:E:208:LYS:HG3	2.20	0.41
1:A:536:SER:HB2	2:B:46:GLU:OE1	2.20	0.41
1:A:72:LYS:HE2	6:A:702:FAD:N7A	2.35	0.41
2:B:242:ILE:HG12	3:C:72:SER:OG	2.20	0.41
1:E:237:GLY:HA2	1:E:421:GLU:HB3	2.02	0.41
1:A:231:ARG:HH11	1:A:456:LEU:HD23	1.85	0.41
2:B:131:VAL:CG2	3:C:55:PRO:HG2	2.50	0.41
1:E:88:ASN:ND2	1:E:156:GLN:HE22	2.17	0.41
2:F:125:PRO:O	2:F:126:LEU:C	2.58	0.41
1:E:466:PRO:O	1:E:469:ALA:HB2	2.20	0.41
2:F:97:CYS:HB2	2:F:108:ALA:HB3	2.03	0.41
2:F:39:GLU:HB2	2:F:122:LYS:HB2	2.01	0.41
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.89	0.41
2:B:42:ARG:HD2	2:B:42:ARG:HA	1.85	0.41
1:E:448:CYS:O	1:E:452:ILE:HG13	2.19	0.41
4:H:153:VAL:C	4:H:155:GLU:H	2.24	0.41
1:A:346:LEU:HB2	1:A:382:VAL:HG21	2.02	0.41
1:A:268:GLU:CB	1:A:608:LEU:HD23	2.46	0.41
4:D:140:ASN:HD22	4:D:145:GLY:HA2	1.86	0.41
1:E:325:ARG:O	1:E:328:THR:N	2.52	0.41
1:A:375:VAL:HG12	1:A:380:ILE:HD11	2.02	0.41
1:E:238:GLY:HA3	1:E:389:ASN:ND2	2.34	0.41
1:E:276:HIS:NE2	1:E:286:LEU:HD11	2.35	0.41
1:E:231:ARG:HH11	1:E:456:LEU:HD23	1.85	0.41
1:A:99:TRP:CZ2	1:A:100:LYS:HE3	2.56	0.41
2:B:33:LYS:HZ3	2:B:35:ILE:HD11	1.85	0.41
1:A:277:PRO:HD3	1:A:320:ARG:HB3	2.01	0.41
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.82	0.41
2:B:181:GLU:CD	2:B:181:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HH12	1:A:551:ASN:ND2	2.18	0.41
2:F:158:LYS:HB2	2:F:158:LYS:HE3	1.42	0.41
2:F:242:ILE:CG1	11:G:202:AT5:HM33	2.51	0.41
2:F:68:VAL:O	2:F:69:LEU:C	2.57	0.41
4:H:117:LEU:O	4:H:121:VAL:HG23	2.21	0.41
2:B:142:PHE:CE1	2:B:206:ALA:HB3	2.56	0.41
2:B:69:LEU:HD12	2:B:109:CYS:HB3	2.02	0.41
1:A:509:ARG:HD2	1:A:511:ASP:OD2	2.21	0.41
3:C:135:GLY:O	3:C:136:ILE:C	2.59	0.41
4:H:50:LYS:O	4:H:51:PRO:C	2.59	0.41
3:C:137:ARG:NH2	3:C:141:PHE:HZ	2.19	0.41
2:B:196:TRP:CE3	3:C:59:HIS:HB2	2.55	0.41
1:A:393:ILE:O	1:A:395:THR:HG23	2.20	0.41
1:A:43:ASP:HB2	1:A:66:LYS:O	2.21	0.41
2:B:100:ASN:OD1	2:B:105:ASN:ND2	2.53	0.41
3:G:137:ARG:O	3:G:140:GLY:N	2.53	0.41
1:E:480:VAL:HG21	1:E:550:GLN:NE2	2.35	0.41
1:E:142:ARG:HG2	2:F:168:GLN:O	2.20	0.41
1:A:300:ASN:HB2	1:A:301:SER:H	1.72	0.41
3:C:166:ILE:O	3:C:170:VAL:HB	2.21	0.41
1:E:244:PHE:CD1	1:E:498:LYS:HE3	2.56	0.41
1:E:122:LEU:CD1	1:E:440:ASP:HA	2.51	0.41
2:F:242:ILE:HG23	3:G:69:TRP:HA	2.03	0.41
1:E:159:ASN:O	1:E:162:LYS:HG2	2.20	0.41
1:E:159:ASN:O	1:E:160:TYR:C	2.60	0.41
1:E:214:VAL:HG12	1:E:215:ILE:H	1.85	0.41
1:E:117:ASN:O	1:E:120:HIS:HB3	2.20	0.41
3:G:49:GLN:OE1	3:G:54:ARG:NH1	2.54	0.41
1:A:172:VAL:O	1:A:174:ASP:N	2.54	0.41
1:A:499:THR:O	1:A:502:LYS:N	2.53	0.41
1:A:585:TYR:CZ	1:A:596:LYS:HD3	2.56	0.41
2:F:181:GLU:O	2:F:182:CYS:C	2.60	0.41
2:F:155:LYS:HA	2:F:221:ASP:HB2	2.02	0.41
1:E:433:LEU:HA	1:E:433:LEU:HD12	1.92	0.41
1:E:492:LEU:HD21	1:E:527:LEU:HD12	2.02	0.41
1:E:513:LEU:O	1:E:517:VAL:HG23	2.21	0.41
1:A:98:ASP:O	1:A:100:LYS:N	2.54	0.41
1:A:99:TRP:HH2	1:A:120:HIS:HE1	1.69	0.41
1:A:93:SER:HB3	1:A:147:LYS:HB3	2.02	0.41
2:B:189:SER:HA	2:B:205:PRO:HG2	2.03	0.41
2:B:174:GLU:O	2:B:177:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:627:ASP:O	1:E:637:TRP:HB2	2.21	0.41
2:B:197:TRP:O	4:D:109:ARG:NH2	2.54	0.40
1:A:230:LYS:CD	1:A:462:ILE:HA	2.49	0.40
1:E:562:ALA:HB1	1:E:607:THR:HG21	2.02	0.40
1:A:496:MET:HE2	1:A:552:LEU:HD13	2.02	0.40
2:B:69:LEU:HB2	2:B:109:CYS:HA	2.03	0.40
4:H:127:ILE:HA	4:H:127:ILE:HD13	1.80	0.40
1:E:219:LEU:HD23	1:E:219:LEU:HA	1.78	0.40
4:H:124:GLY:O	4:H:128:PHE:N	2.55	0.40
1:E:48:GLY:HA2	6:E:702:FAD:H1B	2.02	0.40
1:E:516:GLY:O	1:E:517:VAL:C	2.59	0.40
1:A:98:ASP:C	1:A:100:LYS:H	2.24	0.40
4:H:85:ASP:CG	4:H:146:LEU:H	2.24	0.40
1:E:77:ARG:NH1	2:F:94:CYS:O	2.54	0.40
3:C:83:ALA:HB1	4:D:96:VAL:HG11	2.04	0.40
1:E:374:ASP:OD1	1:E:374:ASP:C	2.60	0.40
1:A:434:GLY:O	1:A:435:ALA:CB	2.70	0.40
1:E:561:VAL:CG2	1:E:620:LEU:HD11	2.51	0.40
2:F:197:TRP:HA	4:H:109:ARG:HH22	1.85	0.40
1:A:121:TYR:HE1	1:A:447:ALA:HB2	1.87	0.40
1:E:361:PRO:HG2	1:E:362:GLY:N	2.35	0.40
2:F:188:CYS:SG	2:F:189:SER:N	2.94	0.40
3:G:71:VAL:HG11	3:G:137:ARG:HH12	1.86	0.40
1:E:612:ASP:HA	1:E:613:PRO:HD2	1.76	0.40
1:E:337:VAL:HG11	1:E:345:TYR:CD1	2.56	0.40
2:F:39:GLU:HB3	2:F:54:LEU:HD22	2.03	0.40
1:A:532:THR:OG1	1:A:535:ARG:NH2	2.51	0.40
1:A:271:GLU:HB2	1:A:563:ALA:HB2	2.03	0.40
1:E:623:ARG:NH2	1:E:626:ILE:HD11	2.36	0.40
1:E:397:TYR:CE1	1:E:398:LYS:HG3	2.56	0.40
1:E:393:ILE:HA	1:E:394:PRO:HD3	1.97	0.40
1:A:266:ALA:HB2	1:A:610:LYS:CG	2.52	0.40
2:F:105:ASN:O	2:F:106:THR:HB	2.22	0.40
1:A:279:GLY:HA3	1:A:385:THR:OG1	2.21	0.40
3:G:75:HIS:CE1	3:G:131:HIS:CE1	3.09	0.40
1:A:95:ASN:HA	1:A:96:PRO:HD2	1.90	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	611/645 (95%)	493 (81%)	92 (15%)	26 (4%)	3	30
1	E	611/645 (95%)	499 (82%)	82 (13%)	30 (5%)	3	26
2	B	247/282 (88%)	204 (83%)	34 (14%)	9 (4%)	4	36
2	F	247/282 (88%)	192 (78%)	42 (17%)	13 (5%)	2	23
3	C	151/188 (80%)	110 (73%)	34 (22%)	7 (5%)	3	28
3	G	151/188 (80%)	118 (78%)	25 (17%)	8 (5%)	2	23
4	D	127/156 (81%)	96 (76%)	27 (21%)	4 (3%)	5	40
4	H	127/156 (81%)	87 (68%)	32 (25%)	8 (6%)	2	19
All	All	2272/2542 (89%)	1799 (79%)	368 (16%)	105 (5%)	3	28

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	THR
1	A	614	ARG
2	B	89	CYS
3	C	97	PRO
4	D	49	PHE
1	E	127	VAL
1	E	269	ASP
1	E	288	THR
1	E	339	PRO
1	E	485	GLY
1	E	590	PRO
1	E	591	ILE
1	E	599	PHE
2	F	89	CYS
3	G	98	LEU
3	G	111	GLY
4	H	29	SER

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Mol	Chain	Res	Type
4	H	115	ASP
1	A	305	ARG
1	A	391	GLY
1	A	407	GLU
1	A	426	SER
1	A	458	PRO
1	A	460	GLU
1	A	469	ALA
1	A	485	GLY
1	A	539	TRP
2	B	49	GLY
2	B	134	ASP
2	B	224	ALA
2	B	277	PRO
3	C	155	GLY
1	E	51	GLY
1	E	326	ALA
1	E	391	GLY
1	E	460	GLU
1	E	621	ASP
2	F	132	ILE
2	F	161	LEU
2	F	199	ALA
3	G	185	PRO
4	H	51	PRO
1	A	259	LEU
1	A	483	ALA
1	A	524	SER
1	A	538	ILE
1	A	592	GLU
2	B	205	PRO
2	B	218	SER
3	C	37	PRO
3	C	90	GLY
3	C	106	PHE
4	D	47	LYS
4	D	85	ASP
1	E	173	ALA
1	E	260	ALA
1	E	527	LEU
2	F	204	GLY
2	F	205	PRO

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Mol	Chain	Res	Type
2	F	268	LYS
2	F	279	PRO
3	G	74	LEU
3	G	183	THR
1	A	99	TRP
1	A	173	ALA
1	A	590	PRO
2	B	280	ALA
3	C	98	LEU
1	E	53	GLY
1	E	128	GLU
1	E	179	SER
1	E	192	HIS
1	E	364	SER
1	E	463	PRO
1	E	604	ARG
1	E	629	THR
2	F	277	PRO
4	H	55	HIS
1	A	96	PRO
1	A	194	THR
1	A	252	ASN
1	A	308	GLU
1	A	591	ILE
2	B	140	ASN
3	C	150	PRO
1	E	250	HIS
1	E	305	ARG
2	F	48	PRO
2	F	52	PRO
3	G	59	HIS
3	G	97	PRO
4	H	77	TYR
1	A	381	PRO
1	E	429	GLY
1	E	458	PRO
2	F	88	SER
4	H	154	TRP
4	D	50	LYS
1	E	462	ILE
2	F	273	PRO
3	G	150	PRO

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Mol	Chain	Res	Type
1	A	505	GLY
1	E	381	PRO
4	H	36	ALA
4	H	144	VAL

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	498/526 (95%)	415 (83%)	83 (17%)	3 15
1	E	498/526 (95%)	424 (85%)	74 (15%)	4 20
2	B	219/242 (90%)	173 (79%)	46 (21%)	1 6
2	F	219/242 (90%)	172 (78%)	47 (22%)	1 6
3	C	127/158 (80%)	94 (74%)	33 (26%)	0 3
3	G	127/158 (80%)	106 (84%)	21 (16%)	3 15
4	D	96/119 (81%)	75 (78%)	21 (22%)	1 5
4	H	96/119 (81%)	75 (78%)	21 (22%)	1 5
All	All	1880/2090 (90%)	1534 (82%)	346 (18%)	2 10

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	37	VAL
1	A	39	ASP
1	A	60	LEU
1	A	71	THR
1	A	93	SER
1	A	105	ASP
1	A	113	LEU
1	A	117	ASN
1	A	131	THR
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	152	SER
1	A	153	PHE
1	A	158	ASN
1	A	175	ARG
1	A	179	SER
1	A	203	ASP
1	A	205	LEU
1	A	211	CYS
1	A	230	LYS
1	A	257	THR
1	A	261	THR
1	A	265	ILE
1	A	270	LEU
1	A	283	VAL
1	A	285	CYS
1	A	304	GLU
1	A	313	LYS
1	A	320	ARG
1	A	321	ASP
1	A	335	ARG
1	A	344	ILE
1	A	351	LEU
1	A	354	GLU
1	A	356	LEU
1	A	359	ARG
1	A	368	LYS
1	A	377	LYS
1	A	382	VAL
1	A	383	ILE
1	A	385	THR
1	A	405	THR
1	A	412	ILE
1	A	422	CYS
1	A	425	HIS
1	A	426	SER
1	A	427	VAL
1	A	439	LEU
1	A	440	ASP
1	A	446	ARG
1	A	449	SER
1	A	453	LYS
1	A	454	GLU

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Mol	Chain	Res	Type
1	A	455	GLU
1	A	456	LEU
1	A	459	ASP
1	A	461	LYS
1	A	462	ILE
1	A	474	ILE
1	A	487	VAL
1	A	496	MET
1	A	502	LYS
1	A	503	HIS
1	A	525	LYS
1	A	526	GLU
1	A	528	LYS
1	A	531	LYS
1	A	535	ARG
1	A	560	ILE
1	A	564	GLU
1	A	584	GLU
1	A	596	LYS
1	A	597	ARG
1	A	601	LYS
1	A	610	LYS
1	A	612	ASP
1	A	628	LYS
1	A	629	THR
1	A	630	LEU
1	A	637	TRP
1	A	638	ILE
1	A	642	ILE
1	A	644	SER
2	B	34	ARG
2	B	39	GLU
2	B	42	ARG
2	B	46	GLU
2	B	47	GLU
2	B	54	LEU
2	B	63	LYS
2	B	64	CYS
2	B	69	LEU
2	B	75	ILE
2	B	87	ARG
2	B	90	ARG

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Mol	Chain	Res	Type
2	B	93	ILE
2	B	106	THR
2	B	115	GLN
2	B	117	THR
2	B	119	LYS
2	B	120	THR
2	B	122	LYS
2	B	129	MET
2	B	139	MET
2	B	148	SER
2	B	154	GLN
2	B	156	LYS
2	B	157	THR
2	B	164	LYS
2	B	169	SER
2	B	170	ILE
2	B	171	LYS
2	B	172	GLU
2	B	173	GLN
2	B	174	GLU
2	B	194	SER
2	B	209	MET
2	B	213	ARG
2	B	215	ILE
2	B	216	ILE
2	B	227	LEU
2	B	244	ASN
2	B	247	LYS
2	B	253	LEU
2	B	266	LEU
2	B	268	LYS
2	B	269	MET
2	B	272	LYS
2	B	281	ASN
3	C	34	GLU
3	C	50	ARG
3	C	53	LYS
3	C	59	HIS
3	C	61	THR
3	C	67	MET
3	C	72	SER
3	C	76	ARG

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Mol	Chain	Res	Type
3	C	85	THR
3	C	87	LEU
3	C	94	SER
3	C	95	VAL
3	C	96	LEU
3	C	98	LEU
3	C	99	ASP
3	C	102	THR
3	C	110	LEU
3	C	112	ILE
3	C	115	VAL
3	C	118	ASP
3	C	127	PRO
3	C	133	LEU
3	C	136	ILE
3	C	149	ILE
3	C	158	LEU
3	C	160	LEU
3	C	162	LEU
3	C	165	LEU
3	C	167	SER
3	C	168	LEU
3	C	173	TYR
3	C	175	ARG
3	C	177	GLU
4	D	46	GLU
4	D	49	PHE
4	D	50	LYS
4	D	53	HIS
4	D	69	MET
4	D	79	ILE
4	D	82	ARG
4	D	83	GLU
4	D	90	LEU
4	D	92	LEU
4	D	93	THR
4	D	109	ARG
4	D	117	LEU
4	D	121	VAL
4	D	123	VAL
4	D	136	LEU
4	D	143	ASP

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Mol	Chain	Res	Type
4	D	144	VAL
4	D	152	MET
4	D	153	VAL
4	D	156	LEU
1	E	47	ILE
1	E	62	GLU
1	E	81	THR
1	E	99	TRP
1	E	117	ASN
1	E	122	LEU
1	E	127	VAL
1	E	142	ARG
1	E	153	PHE
1	E	160	TYR
1	E	162	LYS
1	E	165	VAL
1	E	194	THR
1	E	198	GLU
1	E	203	ASP
1	E	205	LEU
1	E	210	ARG
1	E	223	THR
1	E	226	ARG
1	E	228	ARG
1	E	230	LYS
1	E	231	ARG
1	E	232	THR
1	E	257	THR
1	E	265	ILE
1	E	269	ASP
1	E	270	LEU
1	E	274	GLN
1	E	288	THR
1	E	301	SER
1	E	313	LYS
1	E	320	ARG
1	E	322	VAL
1	E	324	SER
1	E	328	THR
1	E	335	ARG
1	E	337	VAL
1	E	344	ILE

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Mol	Chain	Res	Type
1	E	351	LEU
1	E	359	ARG
1	E	368	LYS
1	E	376	THR
1	E	377	LYS
1	E	385	THR
1	E	405	THR
1	E	406	LYS
1	E	410	ASP
1	E	411	LYS
1	E	425	HIS
1	E	426	SER
1	E	436	ASN
1	E	453	LYS
1	E	454	GLU
1	E	461	LYS
1	E	494	LEU
1	E	496	MET
1	E	498	LYS
1	E	511	ASP
1	E	520	MET
1	E	526	GLU
1	E	533	THR
1	E	535	ARG
1	E	537	LEU
1	E	539	TRP
1	E	564	GLU
1	E	585	TYR
1	E	595	THR
1	E	608	LEU
1	E	609	THR
1	E	611	GLN
1	E	614	ARG
1	E	628	LYS
1	E	634	GLU
1	E	637	TRP
2	F	34	ARG
2	F	36	LYS
2	F	37	THR
2	F	46	GLU
2	F	63	LYS
2	F	66	THR

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Mol	Chain	Res	Type
2	F	69	LEU
2	F	73	ILE
2	F	87	ARG
2	F	90	ARG
2	F	93	ILE
2	F	100	ASN
2	F	115	GLN
2	F	117	THR
2	F	122	LYS
2	F	128	HIS
2	F	129	MET
2	F	131	VAL
2	F	139	MET
2	F	156	LYS
2	F	158	LYS
2	F	159	ILE
2	F	161	LEU
2	F	164	LYS
2	F	169	SER
2	F	170	ILE
2	F	171	LYS
2	F	172	GLU
2	F	176	LEU
2	F	184	LEU
2	F	194	SER
2	F	197	TRP
2	F	201	LYS
2	F	209	MET
2	F	213	ARG
2	F	215	ILE
2	F	227	LEU
2	F	230	MET
2	F	241	THR
2	F	244	ASN
2	F	247	LYS
2	F	248	THR
2	F	265	LEU
2	F	266	LEU
2	F	268	LYS
2	F	276	LEU
2	F	278	THR
3	G	40	VAL

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Mol	Chain	Res	Type
3	G	50	ARG
3	G	53	LYS
3	G	66	GLN
3	G	67	MET
3	G	76	ARG
3	G	95	VAL
3	G	98	LEU
3	G	99	ASP
3	G	102	THR
3	G	106	PHE
3	G	110	LEU
3	G	118	ASP
3	G	133	LEU
3	G	139	ILE
3	G	149	ILE
3	G	150	PRO
3	G	151	SER
3	G	162	LEU
3	G	175	ARG
3	G	181	LYS
4	H	47	LYS
4	H	53	HIS
4	H	64	TYR
4	H	70	VAL
4	H	72	LEU
4	H	79	ILE
4	H	82	ARG
4	H	83	GLU
4	H	84	MET
4	H	86	LEU
4	H	88	LEU
4	H	109	ARG
4	H	112	VAL
4	H	122	ARG
4	H	123	VAL
4	H	131	CYS
4	H	136	LEU
4	H	143	ASP
4	H	153	VAL
4	H	154	TRP
4	H	156	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	95	ASN
1	A	117	ASN
1	A	120	HIS
1	A	150	GLN
1	A	252	ASN
1	A	349	HIS
1	A	428	HIS
1	A	431	ASN
1	A	436	ASN
1	A	451	ASN
1	A	476	ASN
1	A	484	ASN
1	A	503	HIS
1	A	551	ASN
1	A	565	ASN
2	B	44	ASN
2	B	55	GLN
2	B	77	ASN
2	B	100	ASN
2	B	105	ASN
2	B	115	GLN
2	B	128	HIS
2	B	145	GLN
2	B	160	ASN
2	B	165	GLN
3	C	59	HIS
3	C	66	GLN
4	D	140	ASN
1	E	88	ASN
1	E	95	ASN
1	E	117	ASN
1	E	120	HIS
1	E	125	ASN
1	E	156	GLN
1	E	159	ASN
1	E	178	HIS
1	E	182	HIS
1	E	347	GLN
1	E	349	HIS
1	E	355	GLN

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Mol	Chain	Res	Type
1	E	389	ASN
1	E	436	ASN
1	E	451	ASN
1	E	484	ASN
1	E	503	HIS
1	E	550	GLN
1	E	551	ASN
1	E	558	GLN
1	E	606	HIS
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	112	ASN
2	F	115	GLN
2	F	116	ASN
2	F	128	HIS
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
2	F	168	GLN
2	F	210	GLN
2	F	244	ASN
3	G	75	HIS
4	H	140	ASN

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

16 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	$\#\|Z\| > 2$
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	A	702	1	48,58,58	1.34	7 (14%)	54,89,89	2.44	16 (29%)
7	FES	B	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	C	201	3,4	30,50,50	2.11	9 (30%)	24,82,82	2.51	10 (41%)
11	AT5	C	202	-	19,23,23	1.57	3 (15%)	16,32,32	2.44	5 (31%)
12	EPH	D	201	-	42,43,48	1.98	8 (19%)	43,48,53	2.65	9 (20%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	1	48,58,58	1.37	6 (12%)	54,89,89	2.60	13 (24%)
7	FES	F	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	F	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	F	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	G	201	3,4	30,50,50	1.97	7 (23%)	24,82,82	2.29	8 (33%)
11	AT5	G	202	-	19,23,23	1.47	3 (15%)	16,32,32	2.60	5 (31%)
12	EPH	H	201	-	42,43,48	2.12	12 (28%)	43,48,53	2.95	10 (23%)

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	MLI	A	701	-	-	0/0/4/4	0/0/0/0
6	FAD	A	702	1	-	0/30/50/50	0/6/6/6
7	FES	B	301	2	-	0/0/4/4	0/1/1/1
8	SF4	B	302	2	-	0/0/48/48	0/6/5/5
9	F3S	B	303	2	-	0/0/24/24	0/0/3/3
10	HEM	C	201	3,4	-	0/10/54/54	0/0/8/8
11	AT5	C	202	-	-	2/22/22/22	0/1/1/1
12	EPH	D	201	-	-	0/47/47/52	0/0/0/0
5	MLI	E	701	-	-	0/0/4/4	0/0/0/0
6	FAD	E	702	1	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	F	301	2	-	0/0/4/4	0/1/1/1
8	SF4	F	302	2	-	0/0/48/48	0/6/5/5
9	F3S	F	303	2	-	0/0/24/24	0/0/3/3
10	HEM	G	201	3,4	-	0/10/54/54	0/0/8/8
11	AT5	G	202	-	-	0/22/22/22	0/1/1/1
12	EPH	H	201	-	-	0/47/47/52	0/0/0/0

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	201	HEM	C3B-C4B	-6.31	1.46	1.51
10	G	201	HEM	C3B-C4B	-6.12	1.46	1.51
10	C	201	HEM	C2C-C1C	-4.40	1.44	1.52
10	G	201	HEM	C2C-C1C	-4.10	1.44	1.52
10	C	201	HEM	C3D-C4D	-3.81	1.46	1.51
12	D	201	EPH	C27-C28	-3.81	1.33	1.50
12	D	201	EPH	C18-C4	-3.62	1.39	1.50
12	H	201	EPH	C27-C28	-3.51	1.34	1.50
12	H	201	EPH	C18-C4	-3.45	1.40	1.50
10	G	201	HEM	C3D-C4D	-3.39	1.47	1.51
11	C	202	AT5	C11-C12	-2.55	1.49	1.54
11	G	202	AT5	C11-C12	-2.54	1.49	1.54
6	A	702	FAD	C10-N10	-2.50	1.36	1.39
10	C	201	HEM	C2B-C1B	-2.33	1.44	1.51
6	A	702	FAD	C9A-N10	-2.19	1.35	1.38
11	C	202	AT5	C5-C6	-2.18	1.39	1.44
12	H	201	EPH	C10-C11	-2.11	1.44	1.52
10	C	201	HEM	C2D-C1D	-2.00	1.45	1.51
10	C	201	HEM	FE-ND	2.02	2.08	1.97
6	E	702	FAD	C10-N1	2.07	1.39	1.35
10	G	201	HEM	CAA-C2A	2.09	1.55	1.52
10	G	201	HEM	C1C-NC	2.21	1.38	1.36
6	A	702	FAD	C5X-N5	2.25	1.38	1.35
12	H	201	EPH	O2-C4	2.32	1.40	1.33
12	H	201	EPH	C37-C2	2.33	1.57	1.50
6	A	702	FAD	C4-N3	2.38	1.37	1.33
6	E	702	FAD	C2A-N1A	2.41	1.38	1.33
10	G	201	HEM	C3B-CAB	2.41	1.55	1.51
6	E	702	FAD	C1'-N10	2.45	1.51	1.48
10	C	201	HEM	C4C-NC	2.50	1.39	1.36
10	C	201	HEM	C3B-CAB	2.51	1.56	1.51
12	H	201	EPH	P1-O7	2.52	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	FE-ND	2.53	2.10	1.97
12	H	201	EPH	C5-C3	2.66	1.58	1.50
6	A	702	FAD	C2A-N1A	2.70	1.39	1.33
11	G	202	AT5	C6-C7	2.70	1.56	1.49
12	D	201	EPH	P1-O7	2.77	1.61	1.51
12	D	201	EPH	C15-C16	3.35	1.54	1.29
12	H	201	EPH	C15-C16	3.39	1.54	1.29
10	C	201	HEM	FE-NC	3.39	2.09	1.95
12	D	201	EPH	C26-C25	3.63	1.66	1.50
6	A	702	FAD	C2A-N3A	3.64	1.38	1.32
6	E	702	FAD	C2A-N3A	3.65	1.38	1.32
12	H	201	EPH	C26-C25	3.72	1.66	1.50
6	E	702	FAD	C4X-N5	3.75	1.39	1.33
12	D	201	EPH	C25-C24	3.80	1.53	1.31
12	H	201	EPH	C25-C24	3.87	1.54	1.31
12	H	201	EPH	C13-C12	3.87	1.54	1.31
12	D	201	EPH	C13-C12	3.94	1.54	1.31
6	E	702	FAD	C4-N3	3.98	1.40	1.33
11	G	202	AT5	O4-C5	4.27	1.34	1.24
6	A	702	FAD	C4X-N5	4.52	1.40	1.33
11	C	202	AT5	O4-C5	4.91	1.36	1.24
12	D	201	EPH	C29-C28	6.93	1.71	1.31
12	H	201	EPH	C29-C28	7.06	1.72	1.31

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	702	FAD	N3A-C2A-N1A	-12.58	119.26	128.89
6	A	702	FAD	N3A-C2A-N1A	-11.06	120.43	128.89
11	G	202	AT5	CM3-O3-C3	-7.78	109.58	117.31
11	C	202	AT5	C6-C5-N4	-5.99	119.65	124.19
11	C	202	AT5	C11-C12-C13	-4.77	101.92	110.28
6	E	702	FAD	P-O3P-PA	-4.65	119.68	132.73
6	A	702	FAD	C4-C4X-C10	-4.40	117.12	119.94
11	G	202	AT5	C6-C5-N4	-4.28	120.95	124.19
6	E	702	FAD	C1B-N9A-C4A	-4.03	120.86	126.94
10	G	201	HEM	C3C-CAC-CBC	-3.76	118.69	124.46
10	C	201	HEM	C3C-CAC-CBC	-3.75	118.70	124.46
6	A	702	FAD	P-O3P-PA	-3.67	122.43	132.73
6	E	702	FAD	C8M-C8-C9	-3.35	111.17	120.28
11	G	202	AT5	C11-C12-C13	-3.33	104.44	110.28
11	C	202	AT5	CM3-O3-C3	-3.26	114.07	117.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	201	HEM	CAA-CBA-CGA	-3.21	106.86	112.75
6	E	702	FAD	C4-C4X-C10	-3.17	117.91	119.94
12	D	201	EPH	C30-C29-C28	-2.92	113.69	127.06
6	A	702	FAD	C4A-C5A-N7A	-2.77	106.93	109.48
10	C	201	HEM	CAA-C2A-C3A	-2.67	121.39	129.00
6	E	702	FAD	O2'-C2'-C3'	-2.35	103.11	109.02
12	D	201	EPH	C37-C2-C1	-2.35	106.58	112.07
12	H	201	EPH	O5-P1-O7	-2.34	100.54	109.62
6	A	702	FAD	C4X-C4-N3	-2.34	120.39	123.59
6	E	702	FAD	C4A-C5A-N7A	-2.27	107.39	109.48
10	G	201	HEM	C3B-CAB-CBB	-2.18	121.11	124.46
6	E	702	FAD	C2B-C1B-N9A	-2.16	110.99	114.29
12	H	201	EPH	C30-C29-C28	-2.14	117.27	127.06
11	C	202	AT5	O3-C3-N4	-2.12	115.97	118.99
11	G	202	AT5	C17-C12-C11	-2.04	107.59	110.76
6	A	702	FAD	C2B-C1B-N9A	-2.03	111.20	114.29
6	A	702	FAD	C9A-C5X-N5	-2.02	119.37	122.36
6	A	702	FAD	C8M-C8-C9	-2.00	114.83	120.28
6	A	702	FAD	C8M-C8-C7	2.00	125.13	120.73
6	E	702	FAD	C1'-C2'-C3'	2.07	115.75	109.82
10	C	201	HEM	C3B-C4B-CHC	2.11	126.14	123.16
12	D	201	EPH	C10-C11-C12	2.12	123.58	112.45
12	H	201	EPH	O2-C4-C18	2.19	118.58	111.90
12	H	201	EPH	O1-C2-C37	2.23	116.20	108.36
12	D	201	EPH	C19-C18-C4	2.24	122.41	113.59
12	D	201	EPH	C1-O2-C4	2.39	123.54	116.85
6	A	702	FAD	O3P-PA-O5B	2.40	109.29	102.94
6	A	702	FAD	C6-C5X-N5	2.41	122.06	118.96
6	E	702	FAD	O4B-C1B-N9A	2.42	113.17	108.10
6	A	702	FAD	O4B-C1B-N9A	2.49	113.30	108.10
10	C	201	HEM	CMD-C2D-C3D	2.58	125.75	114.35
10	G	201	HEM	CMD-C2D-C3D	2.62	125.93	114.35
11	G	202	AT5	C5-N4-C3	2.63	121.13	117.79
6	A	702	FAD	C4B-O4B-C1B	2.66	112.64	109.72
10	G	201	HEM	C3B-C4B-CHC	2.71	126.98	123.16
12	H	201	EPH	O2-C1-C2	2.91	116.53	108.69
12	H	201	EPH	C1-O2-C4	3.05	125.37	116.85
6	E	702	FAD	C8M-C8-C7	3.40	128.19	120.73
6	A	702	FAD	C4-C4X-N5	3.49	122.96	118.72
11	C	202	AT5	C5-N4-C3	3.53	122.27	117.79
10	G	201	HEM	CMB-C2B-C3B	3.71	125.79	116.53
10	C	201	HEM	CAA-C2A-C1A	3.80	131.13	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	201	HEM	CMC-C2C-C3C	3.91	126.30	116.53
12	H	201	EPH	C14-C15-C16	3.96	149.48	125.00
10	C	201	HEM	CMC-C2C-C3C	3.99	126.49	116.53
6	A	702	FAD	C5X-C9A-N10	4.07	120.72	117.62
12	D	201	EPH	C14-C15-C16	4.14	150.58	125.00
10	C	201	HEM	CAD-C3D-C2D	4.40	125.88	113.22
12	D	201	EPH	C2-O1-C3	4.44	128.53	117.89
10	C	201	HEM	CMB-C2B-C3B	4.44	127.62	116.53
10	G	201	HEM	CAD-C3D-C2D	4.48	126.10	113.22
10	C	201	HEM	CAD-C3D-C4D	4.97	129.99	112.47
10	G	201	HEM	CAD-C3D-C4D	5.01	130.13	112.47
6	E	702	FAD	C4-N3-C2	5.57	120.06	115.25
6	E	702	FAD	C5X-C9A-N10	5.71	121.96	117.62
6	A	702	FAD	C4-N3-C2	6.92	121.23	115.25
12	H	201	EPH	C2-O1-C3	7.20	135.17	117.89
12	D	201	EPH	C15-C14-C13	8.64	140.76	112.00
12	H	201	EPH	C15-C14-C13	8.82	141.35	112.00
12	D	201	EPH	C27-C26-C25	11.58	144.08	112.86
12	H	201	EPH	C27-C26-C25	12.46	146.45	112.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	202	AT5	CM3-O3-C3-C2
11	C	202	AT5	CM3-O3-C3-N4

There are no ring outliers.

13 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	MLI	3	0
6	A	702	FAD	12	0
8	B	302	SF4	5	0
10	C	201	HEM	14	0
11	C	202	AT5	12	0
12	D	201	EPH	4	0
5	E	701	MLI	4	0
6	E	702	FAD	16	0
7	F	301	FES	1	0
9	F	303	F3S	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	201	HEM	13	0
11	G	202	AT5	11	0
12	H	201	EPH	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	613/645 (95%)	0.29	41 (6%)	21	19	84, 111, 132, 145	0
1	E	613/645 (95%)	-0.06	11 (1%)	71	65	78, 105, 126, 141	0
2	B	249/282 (88%)	-0.15	3 (1%)	81	75	78, 99, 125, 146	0
2	F	249/282 (88%)	0.04	6 (2%)	62	56	71, 92, 114, 130	0
3	C	153/188 (81%)	-0.05	8 (5%)	31	27	89, 107, 148, 165	0
3	G	153/188 (81%)	0.16	12 (7%)	16	15	88, 101, 172, 199	0
4	D	129/156 (82%)	-0.19	4 (3%)	52	47	92, 107, 131, 142	0
4	H	129/156 (82%)	-0.03	5 (3%)	43	38	90, 109, 145, 151	0
All	All	2288/2542 (90%)	0.05	90 (3%)	43	38	71, 106, 134, 199	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	185	PRO	12.1
3	G	184	LEU	9.0
4	H	49	PHE	7.0
3	G	186	THR	6.4
3	G	181	LYS	5.4
4	D	49	PHE	5.1
1	A	415	GLY	5.1
3	C	185	PRO	4.6
3	C	186	THR	4.4
1	A	299	VAL	4.2
1	A	237	GLY	4.0
1	A	437	SER	3.9
4	H	45	ALA	3.8
3	G	183	THR	3.7
1	A	596	LYS	3.6
3	C	180	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	595	THR	3.3
1	E	33	ALA	3.2
1	E	237	GLY	3.1
1	A	313	LYS	3.1
1	A	440	ASP	3.1
3	G	180	LYS	3.0
1	A	381	PRO	3.0
1	A	416	LEU	2.9
1	A	300	ASN	2.9
1	E	246	CYS	2.9
3	C	183	THR	2.9
1	A	335	ARG	2.9
1	A	420	GLY	2.8
1	A	50	GLY	2.8
1	A	422	CYS	2.8
1	E	252	ASN	2.7
4	D	115	ASP	2.7
1	A	35	TYR	2.7
2	F	48	PRO	2.7
1	A	249	ALA	2.6
1	E	421	GLU	2.6
1	A	312	PRO	2.6
2	B	264	MET	2.6
2	F	88	SER	2.6
4	H	156	LEU	2.5
3	G	43	TRP	2.5
3	C	179	HIS	2.5
1	A	344	ILE	2.5
1	A	469	ALA	2.5
1	A	248	THR	2.4
3	C	143	MET	2.4
1	A	160	TYR	2.4
2	B	94	CYS	2.4
1	A	635	VAL	2.4
4	D	48	GLY	2.4
3	G	117	LEU	2.4
1	E	249	ALA	2.4
4	H	115	ASP	2.3
1	A	298	LEU	2.3
1	A	419	CYS	2.3
2	F	89	CYS	2.3
3	G	98	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	52	LEU	2.3
1	E	465	LEU	2.3
1	A	421	GLU	2.3
1	A	238	GLY	2.3
2	F	94	CYS	2.3
1	E	238	GLY	2.3
3	G	178	ARG	2.2
2	B	96	SER	2.2
1	A	389	ASN	2.2
1	A	634	GLU	2.2
1	E	486	ASP	2.2
3	C	182	ALA	2.2
2	F	96	SER	2.2
3	G	176	TRP	2.2
1	A	34	GLN	2.2
4	H	52	LEU	2.2
1	E	248	THR	2.1
1	A	645	TYR	2.1
3	C	98	LEU	2.1
1	A	482	TYR	2.1
1	A	337	VAL	2.1
1	A	618	ILE	2.1
1	A	252	ASN	2.1
1	E	484	ASN	2.1
1	A	303	GLY	2.1
1	A	388	TYR	2.1
1	A	338	GLY	2.1
3	G	182	ALA	2.1
1	A	304	GLU	2.1
1	A	391	GLY	2.0
2	F	154	GLN	2.0
1	A	33	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

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
12	EPH	D	201	44/49	0.88	0.45	8.17	114,133,158,158	0
12	EPH	H	201	44/49	0.85	0.72	7.53	101,138,160,161	0
11	AT5	C	202	23/23	0.92	0.25	2.84	110,115,144,151	0
11	AT5	G	202	23/23	0.90	0.30	2.22	115,121,134,148	0
10	HEM	G	201	43/43	0.94	0.28	1.55	111,117,126,129	0
5	MLI	A	701	7/7	0.92	0.37	1.00	99,101,101,102	0
10	HEM	C	201	43/43	0.97	0.21	0.69	105,108,121,127	0
6	FAD	A	702	53/53	0.95	0.36	0.13	69,90,95,96	0
5	MLI	E	701	7/7	0.97	0.24	0.07	95,96,96,96	0
8	SF4	B	302	8/8	1.00	0.20	-0.10	67,72,75,75	0
8	SF4	F	302	8/8	1.00	0.21	-0.30	57,65,68,68	0
6	FAD	E	702	53/53	0.98	0.26	-0.34	63,76,88,90	0
9	F3S	F	303	7/7	1.00	0.17	-0.38	79,82,83,83	0
7	FES	B	301	4/4	1.00	0.25	-0.80	78,78,80,82	0
7	FES	F	301	4/4	1.00	0.24	-0.90	82,85,88,89	0
9	F3S	B	303	7/7	0.99	0.15	-0.97	89,90,92,93	0

6.5 Other polymers

There are no such residues in this entry.