



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:00 PM GMT

PDB ID : 3VR8
Title : Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode *Ascaris suum*
Authors : Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.
Deposited on : 2012-04-07
Resolution : 2.81 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

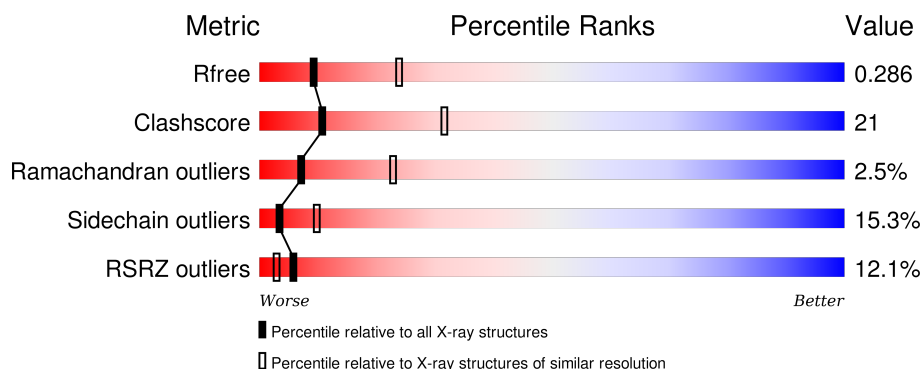
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	<div> <div>14%</div> <div>52%</div> <div>37%</div> <div>6%</div> <div>5%</div> </div>
1	E	645	<div> <div>10%</div> <div>51%</div> <div>38%</div> <div>6%</div> <div>5%</div> </div>
2	B	282	<div> <div>9%</div> <div>48%</div> <div>30%</div> <div>10%</div> <div>12%</div> </div>
2	F	282	<div> <div>13%</div> <div>45%</div> <div>35%</div> <div>7%</div> <div>12%</div> </div>
3	C	188	<div> <div>5%</div> <div>48%</div> <div>27%</div> <div>5%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	188	
4	D	156	
4	H	156	

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	RQX	C	202	-	-	-	X
11	RQX	G	202	-	-	-	X
5	MLI	A	701	-	-	X	-
6	FAD	A	702	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18232 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			

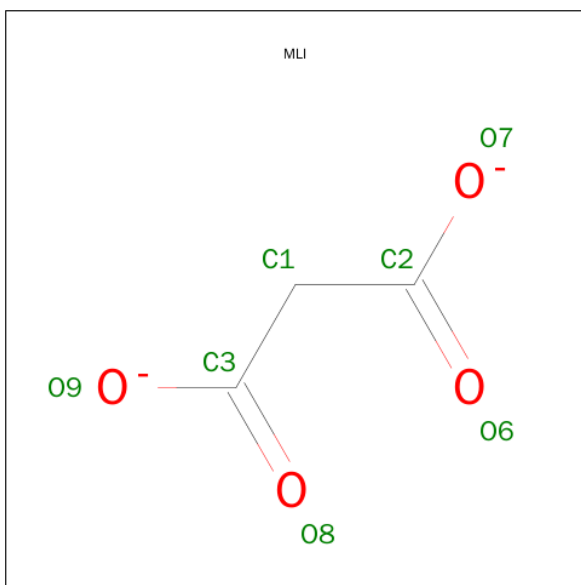
- Molecule 3 is a protein called Cytochrome b-large subunit.

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	150	Total	C	N	O	S	0	0	0
			1195	798	201	190	6			

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

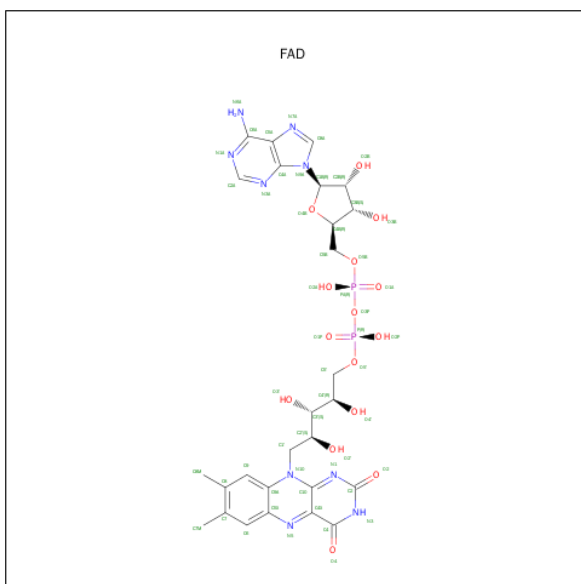
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			
4	H	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



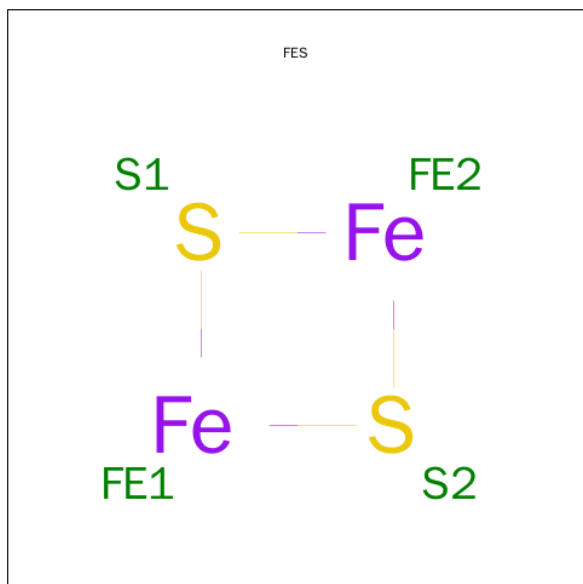
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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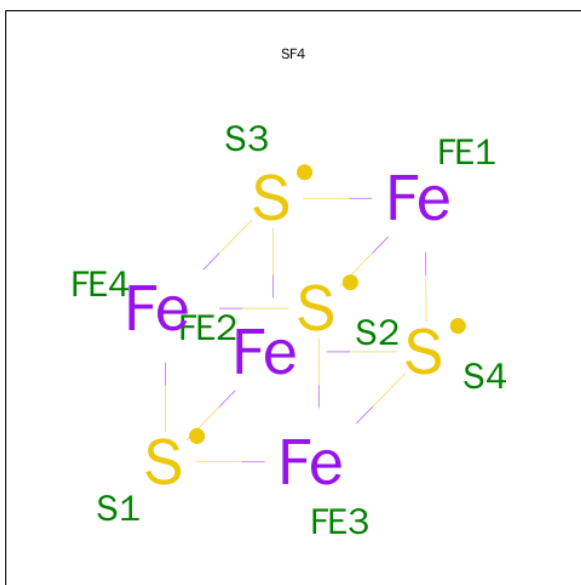
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



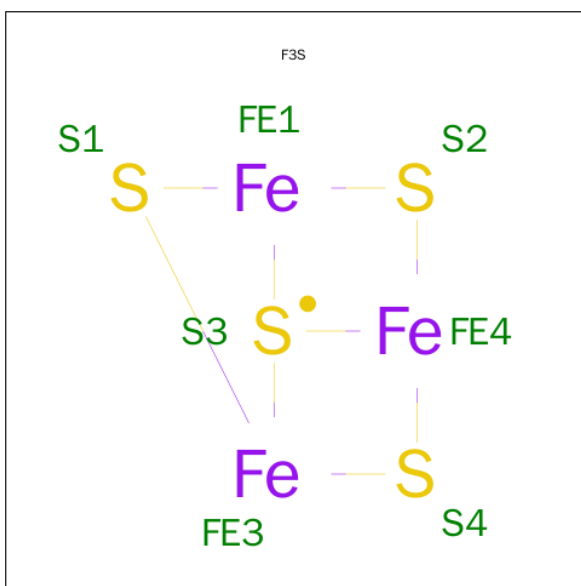
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

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



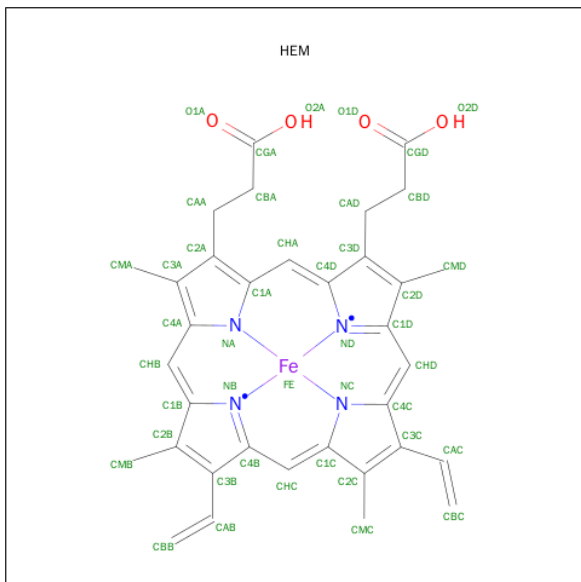
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



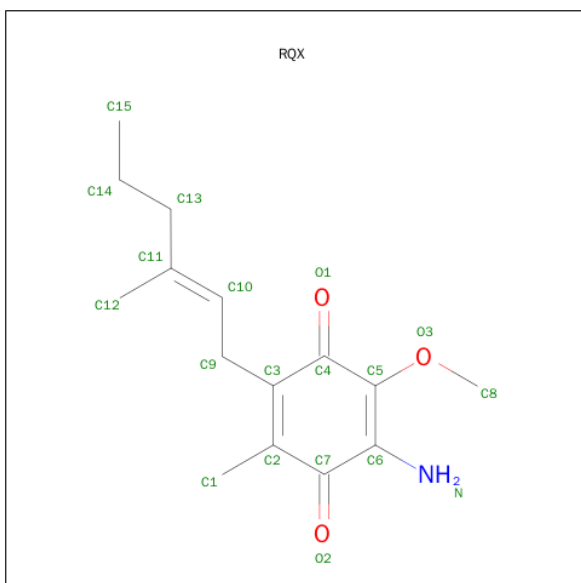
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



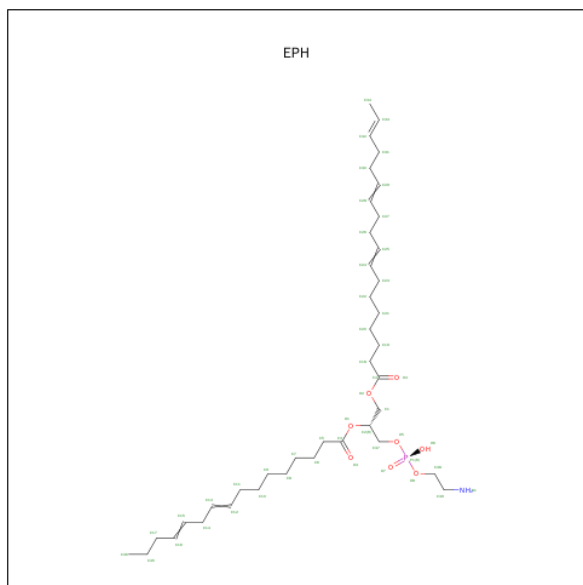
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is 2-AMINO-3-METHOXY-6-METHYL-5-[(2E)-3-METHYLHEX-2-EN-1-YL]CYCLOHEXA-2,5-DIENE-1,4-DIONE (three-letter code: RQX) (formula: C₁₅H₂₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			19	15	1	3		
11	G	1	Total	C	N	O	0	0
			19	15	1	3		

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

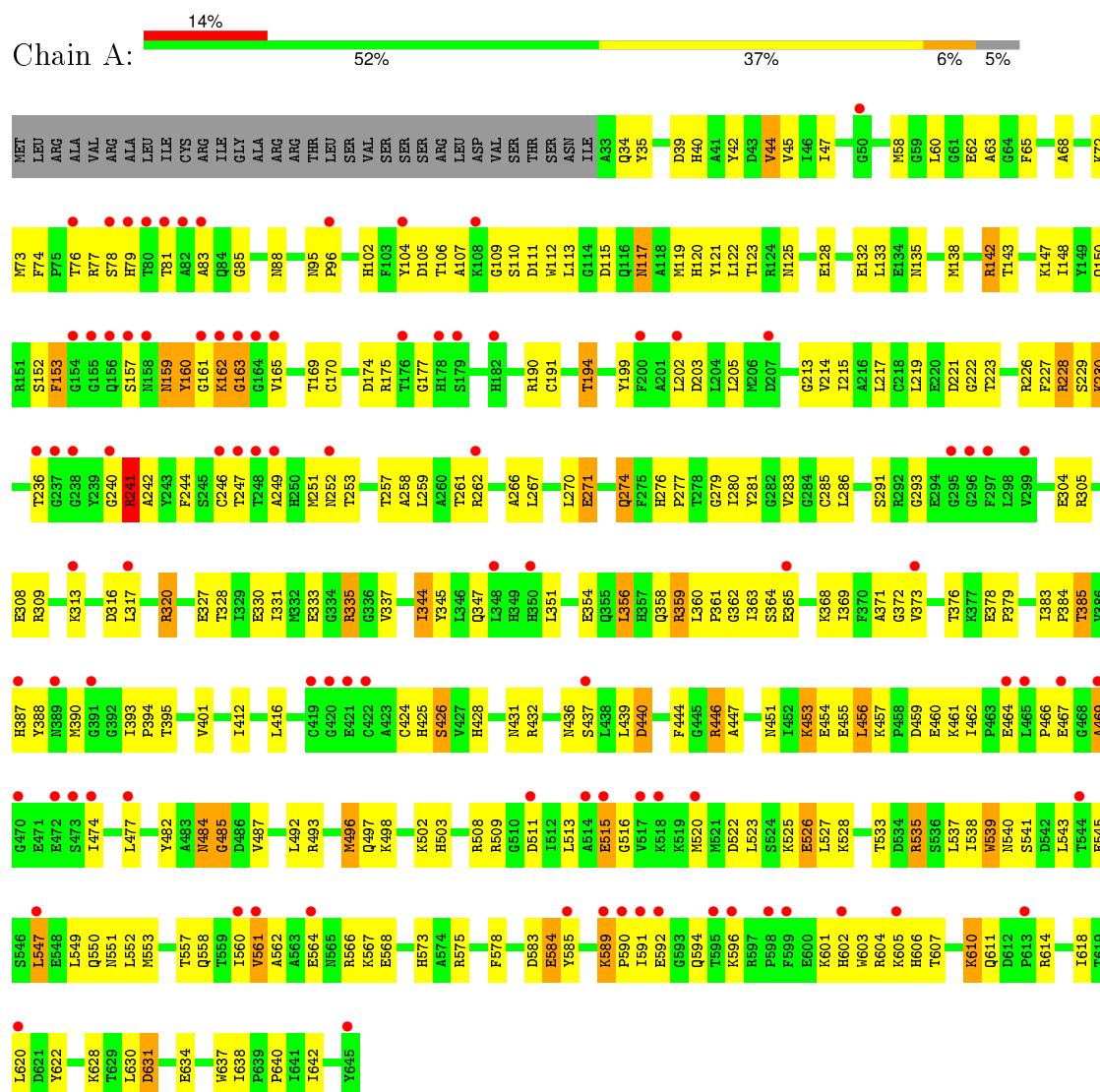


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

3 Residue-property plots

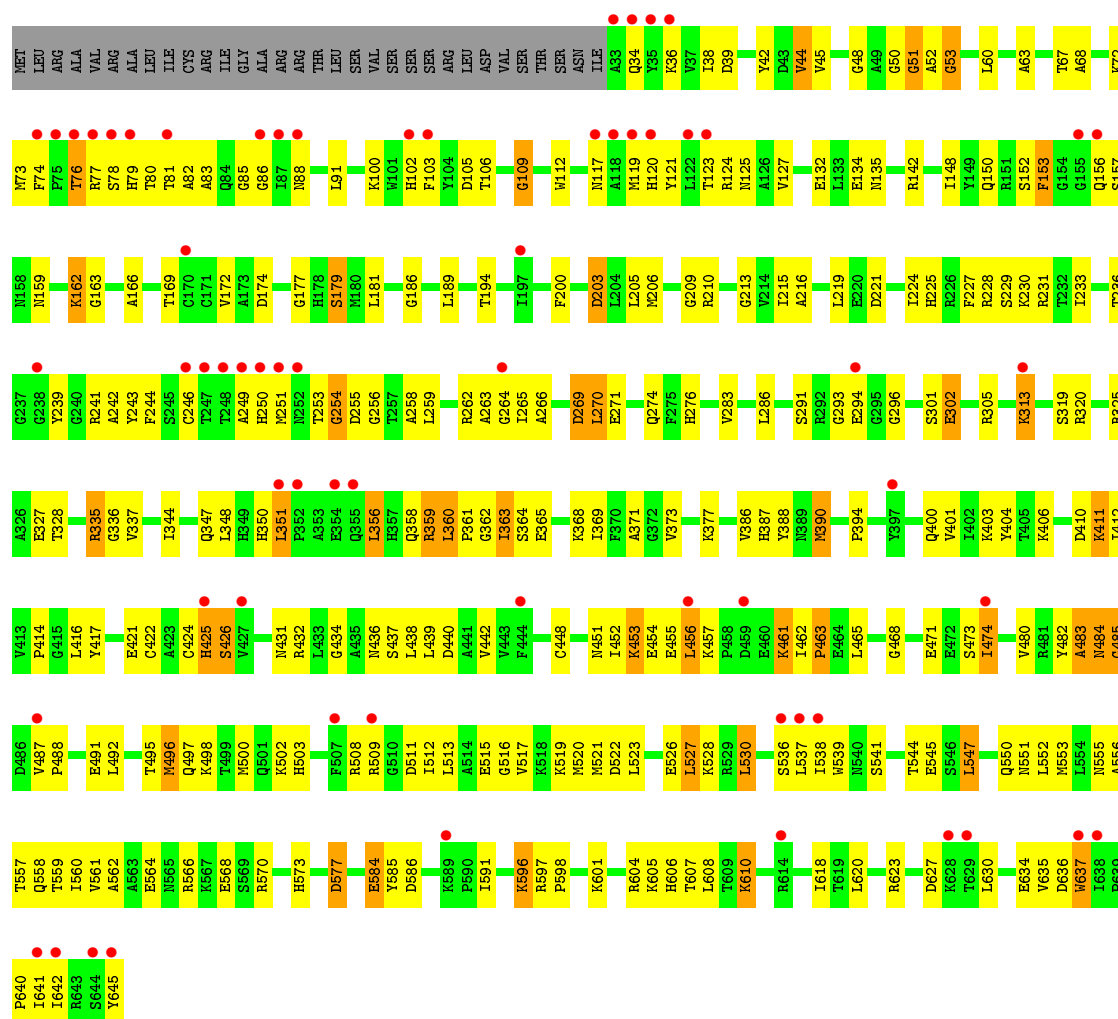
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

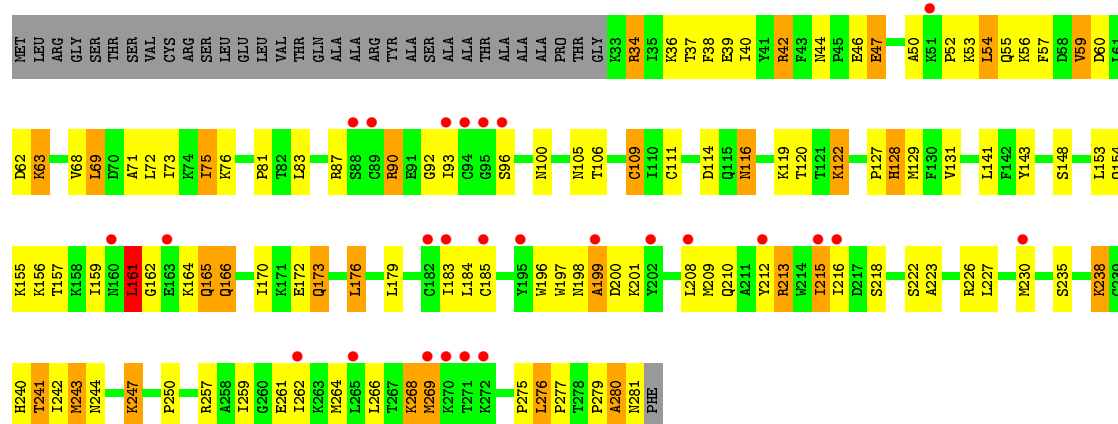


• Molecule 1: Flavoprotein subunit of complex II



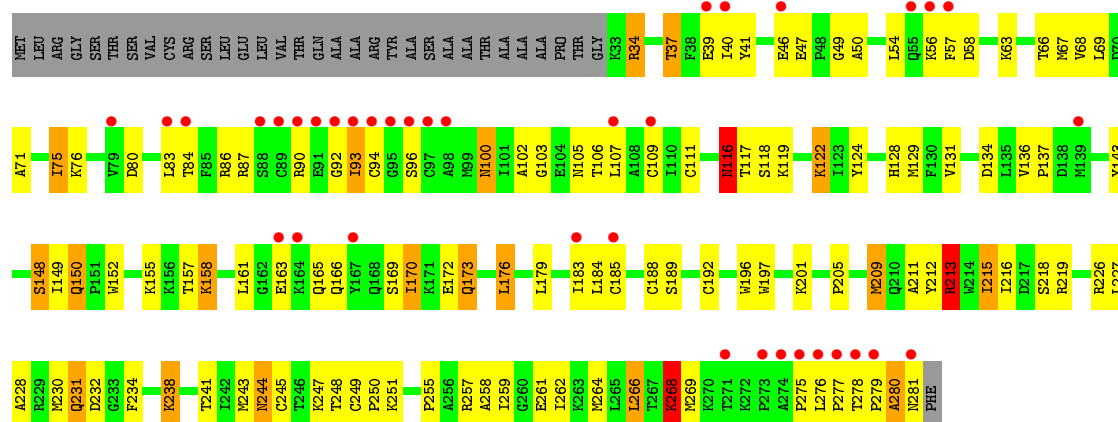


● Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

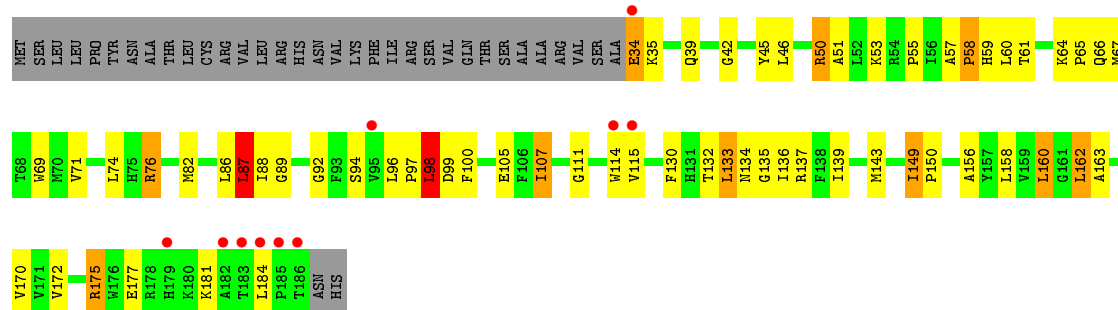


● Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

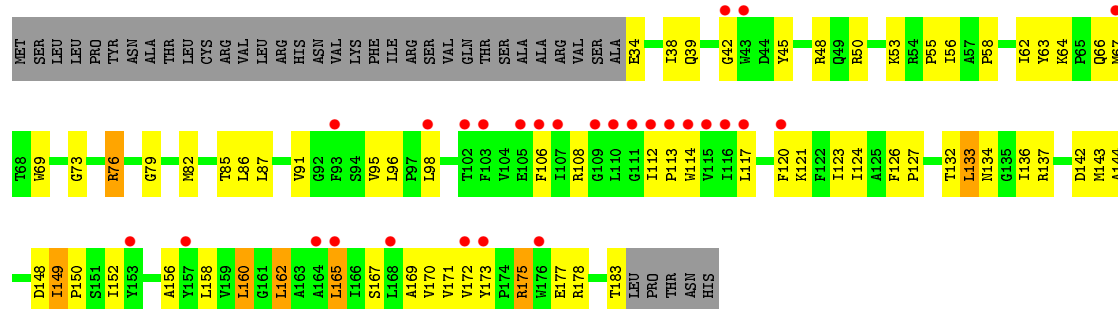
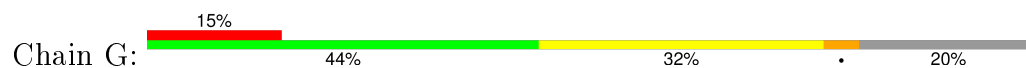




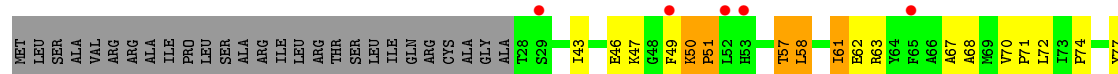
• Molecule 3: Cytochrome b-large subunit



• Molecule 3: Cytochrome b-large subunit

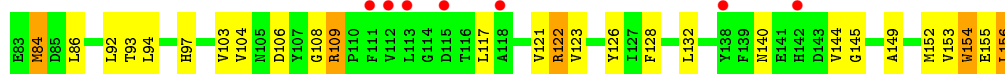


• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.71Å 129.09Å 221.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.81 48.56 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.56-2.81) 92.0 (48.56-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.231 , 0.297 0.223 , 0.286	Depositor DCC
R_{free} test set	4025 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 39.6	EDS
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 80036 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MLI, RQX, F3S, FES, EPH, HEM, 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	0.62	0/4859	0.75	1/6564 (0.0%)
1	E	0.64	0/4859	0.77	1/6564 (0.0%)
2	B	0.68	0/2016	0.81	0/2723
2	F	0.74	0/2016	0.81	0/2723
3	C	0.65	0/1255	0.78	1/1709 (0.1%)
3	G	0.63	0/1232	0.68	0/1676
4	D	0.66	0/1026	0.74	1/1402 (0.1%)
4	H	0.63	0/1026	0.74	1/1402 (0.1%)
All	All	0.65	0/18289	0.77	5/24763 (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	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	98	LEU	CA-CB-CG	7.37	132.24	115.30
1	E	351	LEU	CA-CB-CG	6.39	130.00	115.30
4	D	156	LEU	CA-CB-CG	5.49	127.92	115.30
4	H	156	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	142	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	HIS	Peptide

5.2 Too-close contacts ⓘ

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	203	0
1	E	4758	0	4692	207	0
2	B	1973	0	1993	93	0
2	F	1973	0	1992	107	0
3	C	1217	0	1265	53	0
3	G	1195	0	1240	70	0
4	D	994	0	977	43	0
4	H	994	0	977	37	0
5	A	7	0	2	2	0
5	E	7	0	2	0	0
6	A	53	0	31	7	0
6	E	53	0	31	10	0
7	B	4	0	0	1	0
7	F	4	0	0	0	0
8	B	8	0	0	1	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	15	0
10	G	43	0	30	9	0
11	C	19	0	21	8	0
11	G	19	0	21	6	0
12	D	44	0	53	6	0
12	H	44	0	53	8	0
All	All	18232	0	18102	764	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 21.

All (764) 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:79:HIS:NE2	6:A:702:FAD:HM82	1.00	1.31
1:E:79:HIS:NE2	6:E:702:FAD:HM82	0.88	1.20
1:A:446:ARG:HH11	1:A:446:ARG:HG3	1.07	1.18
2:F:34:ARG:HH21	2:F:34:ARG:HG2	1.14	1.12
1:E:79:HIS:CD2	6:E:702:FAD:HM82	1.85	1.10
3:C:149:ILE:HD13	3:C:149:ILE:H	1.05	1.09
2:F:268:LYS:HG2	2:F:269:MET:H	0.91	1.08
3:G:149:ILE:HD13	3:G:149:ILE:H	1.08	1.07
1:A:79:HIS:CE1	6:A:702:FAD:HM82	1.89	1.05
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.40	1.03
2:F:268:LYS:HG2	2:F:269:MET:N	1.72	1.03
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.40	1.03
4:H:109:ARG:HG2	4:H:109:ARG:HH21	1.24	1.02
3:C:149:ILE:CD1	3:C:149:ILE:H	1.75	1.00
2:F:268:LYS:CG	2:F:269:MET:H	1.75	0.99
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.44	0.99
1:A:117:ASN:HD22	1:A:117:ASN:H	1.03	0.94
3:C:34:GLU:OE2	3:C:34:GLU:HA	1.65	0.94
3:G:76:ARG:HG2	10:G:201:HEM:O2D	1.69	0.93
4:D:50:LYS:N	4:D:51:PRO:HD2	1.83	0.92
1:A:280:ILE:HD12	1:A:285:CYS:HB2	1.50	0.91
1:E:536:SER:HB2	2:F:46:GLU:OE1	1.70	0.90
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.07	0.89
1:A:120:HIS:HD2	1:A:630:LEU:H	1.19	0.89
3:C:133:LEU:O	3:C:136:ILE:HG13	1.73	0.89
4:D:151:GLU:HG2	12:D:201:EPH:O7	1.74	0.88
1:A:117:ASN:HD22	1:A:117:ASN:N	1.71	0.88
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.56	0.88
1:E:480:VAL:CG2	1:E:550:GLN:HE22	1.87	0.87
3:G:149:ILE:H	3:G:149:ILE:CD1	1.83	0.87
1:A:120:HIS:CD2	1:A:630:LEU:HB2	2.10	0.87
3:G:132:THR:HG23	10:G:201:HEM:CAB	2.06	0.85
3:G:132:THR:HG23	10:G:201:HEM:HAB	1.56	0.85
1:E:508:ARG:HH11	1:E:573:HIS:HD2	1.20	0.85
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.54	0.85
2:F:37:THR:HB	2:F:58:ASP:OD2	1.76	0.85
3:C:114:TRP:HB2	3:C:175:ARG:HH11	1.42	0.85
1:E:78:SER:O	1:E:81:THR:HG22	1.77	0.84
1:E:480:VAL:HG21	1:E:550:GLN:NE2	1.93	0.84
1:E:541:SER:O	1:E:545:GLU:HG3	1.76	0.84
3:C:149:ILE:N	3:C:149:ILE:HD13	1.90	0.84
10:C:201:HEM:HBA1	10:C:201:HEM:HHA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:50:LYS:H	4:H:51:PRO:HD3	1.43	0.83
1:E:480:VAL:HG21	1:E:550:GLN:HE22	1.42	0.82
1:A:509:ARG:HD2	1:A:511:ASP:OD2	1.79	0.82
2:B:36:LYS:HE3	2:B:119:LYS:O	1.79	0.82
2:B:179:LEU:HD23	2:B:213:ARG:HA	1.62	0.82
1:A:304:GLU:OE2	1:A:309:ARG:HD3	1.80	0.82
1:A:148:ILE:H	2:B:165:GLN:HE22	1.21	0.82
1:E:327:GLU:HG2	1:E:344:ILE:HD13	1.62	0.82
1:A:77:ARG:HD2	2:B:96:SER:OG	1.80	0.81
3:G:114:TRP:HB2	3:G:175:ARG:NH1	1.94	0.81
1:A:230:LYS:HD2	1:A:462:ILE:HA	1.60	0.81
1:A:117:ASN:H	1:A:117:ASN:ND2	1.78	0.81
3:C:114:TRP:HB2	3:C:175:ARG:NH1	1.96	0.80
3:G:133:LEU:O	3:G:136:ILE:HG13	1.82	0.80
3:C:76:ARG:HH12	11:C:202:RQX:C5	1.96	0.79
3:C:82:MET:HB2	10:C:201:HEM:HAC	1.63	0.79
1:E:120:HIS:HD2	1:E:630:LEU:HB2	1.46	0.79
3:G:149:ILE:HD13	3:G:149:ILE:N	1.93	0.79
10:C:201:HEM:HAA1	4:D:63:ARG:HH12	1.48	0.79
1:E:254:GLY:HA3	1:E:555:ASN:ND2	1.97	0.79
1:E:508:ARG:NH1	1:E:573:HIS:HD2	1.81	0.79
1:A:446:ARG:HG3	1:A:446:ARG:NH1	1.87	0.79
2:B:116:ASN:C	2:B:116:ASN:HD22	1.86	0.79
2:F:227:LEU:HD22	2:F:266:LEU:HD13	1.64	0.79
2:B:268:LYS:CG	2:B:269:MET:H	1.96	0.78
2:F:71:ALA:O	2:F:75:ILE:HG23	1.84	0.78
1:A:620:LEU:HD23	1:A:622:TYR:OH	1.83	0.78
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.66	0.77
1:E:79:HIS:CE1	6:E:702:FAD:HM82	2.08	0.77
1:E:480:VAL:CG2	1:E:550:GLN:NE2	2.46	0.77
3:C:135:GLY:O	3:C:139:ILE:HG13	1.84	0.77
1:A:492:LEU:HD11	1:A:526:GLU:HB2	1.65	0.77
1:A:589:LYS:HB3	1:A:590:PRO:HD2	1.67	0.77
1:A:320:ARG:HH12	5:A:701:MLI:C2	1.98	0.76
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.68	0.76
1:A:589:LYS:HB3	1:A:590:PRO:CD	2.16	0.76
1:E:508:ARG:HH11	1:E:573:HIS:CD2	2.04	0.76
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.69	0.75
1:E:503:HIS:HD2	1:E:512:ILE:O	1.70	0.74
1:A:541:SER:O	1:A:545:GLU:HG3	1.88	0.74
10:C:201:HEM:HBD1	10:C:201:HEM:HHA	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:109:ARG:NH2	4:H:109:ARG:HG2	1.98	0.73
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.70	0.73
2:F:34:ARG:HH21	2:F:34:ARG:CG	1.97	0.73
1:E:159:ASN:HD22	1:E:163:GLY:HA3	1.54	0.73
1:A:333:GLU:HB3	1:A:335:ARG:HH12	1.53	0.73
1:A:221:ASP:OD2	1:A:223:THR:OG1	2.06	0.73
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.23	0.73
1:E:42:TYR:O	1:E:229:SER:HA	1.89	0.73
1:E:291:SER:HB2	1:E:348:LEU:HD21	1.71	0.72
3:C:158:LEU:O	3:C:162:LEU:HB2	1.88	0.72
1:E:91:LEU:HD23	1:E:127:VAL:HG13	1.70	0.72
1:E:401:VAL:HG21	1:E:416:LEU:HG	1.70	0.72
1:E:584:GLU:OE2	1:E:604:ARG:NH1	2.23	0.72
2:F:34:ARG:NH2	2:F:34:ARG:HG2	1.94	0.72
3:C:76:ARG:HG3	3:C:76:ARG:HH11	1.55	0.71
2:F:86:ARG:NH1	2:F:137:PRO:HD2	2.06	0.71
1:E:557:THR:O	1:E:560:ILE:HG22	1.90	0.71
1:E:80:THR:HG22	1:E:181:LEU:HB2	1.73	0.71
4:H:50:LYS:N	4:H:51:PRO:HD3	2.04	0.71
4:D:101:TRP:CH2	4:D:122:ARG:HG2	2.25	0.71
3:C:76:ARG:HE	4:D:103:VAL:HG22	1.55	0.71
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.27	0.70
1:A:371:ALA:O	1:A:373:VAL:HG23	1.91	0.70
1:E:203:ASP:HB2	1:E:473:SER:OG	1.92	0.70
1:E:627:ASP:HB3	1:E:637:TRP:CD1	2.27	0.69
2:B:197:TRP:NE1	11:C:202:RQX:O1	2.21	0.69
1:A:39:ASP:OD1	1:A:226:ARG:NH1	2.26	0.69
3:C:149:ILE:HG12	3:C:150:PRO:HD3	1.74	0.69
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.27	0.69
1:E:262:ARG:HH12	1:E:551:ASN:HD21	1.40	0.69
1:E:135:ASN:ND2	2:F:161:LEU:O	2.25	0.69
1:A:228:ARG:HH11	1:A:464:GLU:HA	1.58	0.68
1:E:262:ARG:NH1	1:E:551:ASN:HD21	1.89	0.68
1:E:120:HIS:HD2	1:E:630:LEU:H	1.40	0.68
2:B:268:LYS:CG	2:B:269:MET:N	2.56	0.68
1:E:44:VAL:HG21	1:E:60:LEU:HD13	1.75	0.68
2:B:131:VAL:CG2	3:C:55:PRO:HG2	2.24	0.68
3:G:175:ARG:HH22	3:G:178:ARG:NH2	1.92	0.67
2:F:124:TYR:CE1	3:G:62:ILE:HG21	2.30	0.67
2:B:71:ALA:O	2:B:75:ILE:HG23	1.93	0.67
4:H:92:LEU:HD21	12:H:201:EPH:H222	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:598:PRO:HG2	1:E:601:LYS:HD3	1.76	0.67
1:A:174:ASP:OD2	1:A:362:GLY:N	2.28	0.66
2:B:172:GLU:OE2	2:B:275:PRO:HD2	1.95	0.66
2:F:155:LYS:NZ	2:F:219:ARG:O	2.29	0.66
1:A:79:HIS:NE2	6:A:702:FAD:HM81	2.07	0.66
2:F:122:LYS:N	2:F:122:LYS:HD3	2.12	0.66
1:E:527:LEU:HD11	1:E:553:MET:HG3	1.78	0.65
1:A:631:ASP:HB3	1:A:634:GLU:HB2	1.79	0.65
1:A:502:LYS:HD3	1:A:503:HIS:CE1	2.32	0.65
3:G:170:VAL:HG11	12:H:201:EPH:H61	1.78	0.65
1:A:365:GLU:O	1:A:369:ILE:HG12	1.95	0.65
1:E:103:PHE:HA	1:E:123:THR:HG21	1.78	0.65
1:E:249:ALA:C	1:E:251:MET:H	2.00	0.64
1:A:446:ARG:CG	1:A:446:ARG:HH11	1.97	0.64
1:A:277:PRO:HD3	1:A:320:ARG:HB3	1.79	0.64
1:A:65:PHE:HE2	1:A:456:LEU:HD12	1.63	0.64
1:E:100:LYS:HD3	1:E:635:VAL:HG23	1.78	0.64
2:B:155:LYS:HD2	2:B:166:GLN:NE2	2.12	0.64
1:A:63:ALA:HB1	1:A:453:LYS:HD2	1.78	0.64
2:F:268:LYS:CG	2:F:269:MET:N	2.41	0.64
4:D:50:LYS:N	4:D:51:PRO:CD	2.59	0.64
3:G:86:LEU:HD11	4:H:92:LEU:HD23	1.79	0.64
3:G:126:PHE:HA	3:G:167:SER:OG	1.97	0.64
1:E:244:PHE:HA	1:E:497:GLN:HB3	1.80	0.64
3:C:156:ALA:O	3:C:160:LEU:HB2	1.98	0.64
3:C:82:MET:CB	10:C:201:HEM:HAC	2.27	0.64
3:G:114:TRP:HD1	3:G:175:ARG:HE	1.44	0.64
2:B:268:LYS:HG3	2:B:269:MET:H	1.62	0.64
1:E:105:ASP:OD2	1:E:157:SER:N	2.30	0.63
1:A:42:TYR:O	1:A:229:SER:HA	1.98	0.63
1:E:120:HIS:CD2	1:E:630:LEU:H	2.17	0.63
3:G:126:PHE:HB3	3:G:127:PRO:HD3	1.81	0.63
4:H:156:LEU:HD12	4:H:156:LEU:O	1.99	0.63
1:E:502:LYS:HD2	1:E:503:HIS:CE1	2.34	0.63
3:C:133:LEU:HD23	3:C:163:ALA:HB2	1.80	0.63
2:F:230:MET:HE3	2:F:262:ILE:HG21	1.80	0.63
1:E:451:ASN:O	1:E:455:GLU:HG3	1.99	0.63
11:C:202:RQX:H20	4:D:107:TYR:CE2	2.33	0.62
1:E:48:GLY:HA2	6:E:702:FAD:H1B	1.81	0.62
2:F:92:GLY:O	2:F:251:LYS:NZ	2.33	0.62
1:A:105:ASP:OD2	1:A:157:SER:N	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ILE:HG22	2:B:226:ARG:HD2	1.81	0.62
4:D:72:LEU:HD21	4:D:88:LEU:HD23	1.80	0.62
1:A:244:PHE:HA	1:A:497:GLN:HB3	1.81	0.62
2:F:258:ALA:O	2:F:262:ILE:HG13	1.99	0.62
1:A:159:ASN:O	1:A:161:GLY:N	2.32	0.62
2:F:150:GLN:HB3	2:F:152:TRP:CH2	2.35	0.62
4:D:154:TRP:HB3	12:D:201:EPH:H381	1.81	0.62
2:F:197:TRP:NE1	11:G:202:RQX:O1	2.25	0.61
1:E:186:GLY:HA2	1:E:189:LEU:HD12	1.82	0.61
4:D:93:THR:HA	4:D:132:LEU:HD23	1.83	0.61
2:F:215:ILE:HG22	2:F:226:ARG:HD2	1.82	0.61
1:E:77:ARG:HA	2:F:94:CYS:HB2	1.81	0.61
1:E:327:GLU:HG2	1:E:344:ILE:CD1	2.31	0.61
1:A:79:HIS:CD2	6:A:702:FAD:C8M	2.80	0.61
1:A:262:ARG:HH22	1:A:551:ASN:HD21	1.49	0.61
1:A:358:GLN:HG3	1:A:359:ARG:HE	1.66	0.61
1:E:320:ARG:NH1	1:E:434:GLY:HA2	2.16	0.61
3:C:74:LEU:HD23	3:C:130:PHE:CE1	2.35	0.60
4:H:109:ARG:CG	4:H:109:ARG:HH21	2.07	0.60
1:A:34:GLN:HE21	1:A:35:TYR:H	1.49	0.60
1:A:228:ARG:NH1	1:A:464:GLU:HA	2.17	0.60
4:H:140:ASN:HD22	4:H:145:GLY:HA2	1.67	0.60
2:B:222:SER:O	2:B:223:ALA:C	2.40	0.60
1:E:242:ALA:O	1:E:497:GLN:HA	2.00	0.60
2:F:183:ILE:HG13	2:F:185:CYS:HB3	1.83	0.60
2:F:262:ILE:HG22	2:F:266:LEU:HD22	1.83	0.60
1:E:109:GLY:O	1:E:431:ASN:HB3	2.01	0.60
3:C:149:ILE:CD1	3:C:149:ILE:N	2.57	0.59
1:A:120:HIS:CD2	1:A:630:LEU:H	2.09	0.59
1:A:73:MET:SD	1:A:251:MET:HG2	2.42	0.59
1:E:264:GLY:O	1:E:403:LYS:NZ	2.31	0.59
2:B:39:GLU:OE1	2:B:54:LEU:HD13	2.01	0.59
1:E:44:VAL:HG22	1:E:67:THR:HG23	1.84	0.59
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.83	0.59
1:A:492:LEU:HD11	1:A:526:GLU:CB	2.32	0.59
1:E:150:GLN:HA	1:E:169:THR:O	2.03	0.59
1:A:484:ASN:O	1:A:485:GLY:O	2.19	0.59
10:C:201:HEM:HHC	10:C:201:HEM:CBB	2.24	0.59
1:E:38:ILE:HG23	4:H:34:GLY:HA3	1.84	0.59
1:A:122:LEU:HG	1:A:439:LEU:HD12	1.85	0.59
1:A:117:ASN:N	1:A:117:ASN:ND2	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HB3	1:A:549:LEU:HD21	1.84	0.59
1:A:281:TYR:HA	1:A:383:ILE:HG22	1.85	0.59
1:A:72:LYS:HE3	1:A:251:MET:HG3	1.84	0.58
1:A:85:GLY:HA3	1:A:153:PHE:CZ	2.38	0.58
1:E:557:THR:O	1:E:561:VAL:HG13	2.03	0.58
3:G:112:ILE:HB	3:G:113:PRO:CD	2.33	0.58
1:A:241:ARG:HH22	2:B:90:ARG:NH2	2.01	0.58
1:E:219:LEU:HD21	1:E:544:THR:HG21	1.84	0.58
4:D:43:ILE:O	4:D:46:GLU:HB3	2.03	0.58
1:A:247:THR:HG21	1:A:286:LEU:HD13	1.85	0.58
3:C:46:LEU:HD13	4:D:111:PHE:CD1	2.38	0.58
1:E:112:TRP:CH2	1:E:641:ILE:HG13	2.39	0.58
1:A:106:THR:HG22	1:A:119:MET:SD	2.43	0.58
1:A:148:ILE:N	2:B:165:GLN:HE22	1.99	0.58
2:B:154:GLN:HG3	2:B:222:SER:OG	2.03	0.58
3:G:156:ALA:O	3:G:160:LEU:HB2	2.04	0.58
1:E:566:ARG:NH2	1:E:605:LYS:O	2.34	0.58
2:B:116:ASN:ND2	2:B:116:ASN:C	2.58	0.58
2:F:230:MET:HE1	2:F:262:ILE:HD13	1.86	0.57
1:A:253:THR:HG22	1:A:552:LEU:CD1	2.34	0.57
1:E:159:ASN:HB2	1:E:163:GLY:CA	2.35	0.57
4:H:77:TYR:HA	12:H:201:EPH:H11	1.86	0.57
1:A:451:ASN:O	1:A:455:GLU:HG3	2.04	0.57
1:A:363:ILE:HG13	1:A:364:SER:N	2.18	0.57
3:C:76:ARG:HG3	3:C:76:ARG:NH1	2.19	0.57
2:F:212:TYR:OH	2:F:261:GLU:HG2	2.04	0.57
1:E:495:THR:OG1	1:E:523:LEU:HD21	2.04	0.57
3:C:114:TRP:CB	3:C:175:ARG:HH11	2.17	0.57
2:B:128:HIS:CD2	2:B:196:TRP:HB3	2.40	0.57
1:A:120:HIS:HD2	1:A:630:LEU:N	1.97	0.57
1:A:83:ALA:HB3	1:A:177:GLY:CA	2.33	0.57
3:C:92:GLY:O	3:C:96:LEU:HB2	2.05	0.57
1:E:262:ARG:HH12	1:E:551:ASN:ND2	2.02	0.57
1:E:400:GLN:HB3	1:E:412:ILE:HG23	1.87	0.56
1:E:148:ILE:H	2:F:165:GLN:HE22	1.52	0.56
1:E:241:ARG:NH2	1:E:246:CYS:SG	2.77	0.56
2:F:116:ASN:ND2	2:F:118:SER:OG	2.39	0.56
2:B:268:LYS:HG3	2:B:269:MET:N	2.21	0.56
1:A:135:ASN:O	2:B:153:LEU:HD23	2.05	0.56
2:F:227:LEU:CD2	2:F:266:LEU:HD13	2.35	0.56
3:C:181:LYS:HA	3:C:184:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:LYS:HE2	1:E:251:MET:HG3	1.86	0.56
1:E:86:GLY:HA3	1:E:169:THR:CG2	2.36	0.56
1:A:522:ASP:O	1:A:525:LYS:HB2	2.04	0.56
2:B:92:GLY:HA2	7:B:301:FES:S2	2.46	0.56
2:F:234:PHE:O	2:F:238:LYS:HB2	2.06	0.56
2:B:276:LEU:HD23	2:B:277:PRO:HD2	1.88	0.56
3:C:64:LYS:O	3:C:66:GLN:HG3	2.06	0.56
2:F:34:ARG:NH2	2:F:34:ARG:CG	2.64	0.56
4:H:109:ARG:CD	4:H:109:ARG:H	2.18	0.56
1:E:159:ASN:HB2	1:E:163:GLY:HA3	1.88	0.55
4:D:79:ILE:O	4:D:79:ILE:HG13	2.05	0.55
1:E:254:GLY:HA3	1:E:555:ASN:HD21	1.67	0.55
4:D:50:LYS:H	4:D:51:PRO:HD2	1.66	0.55
1:E:120:HIS:HD2	1:E:630:LEU:CB	2.16	0.55
2:B:36:LYS:NZ	2:B:114:ASP:HB3	2.22	0.55
3:C:65:PRO:HA	3:C:69:TRP:CZ2	2.41	0.55
1:E:262:ARG:NH1	1:E:551:ASN:ND2	2.53	0.55
4:H:108:GLY:O	4:H:122:ARG:NH2	2.40	0.55
1:A:327:GLU:O	1:A:331:ILE:HG12	2.07	0.55
2:F:116:ASN:HD22	2:F:116:ASN:C	2.09	0.55
1:A:132:GLU:HG2	2:B:161:LEU:HG	1.89	0.55
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.89	0.55
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.88	0.55
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.07	0.55
1:E:394:PRO:HA	1:E:424:CYS:O	2.05	0.55
2:B:172:GLU:CD	2:B:275:PRO:HD2	2.28	0.54
2:B:153:LEU:HD21	2:B:166:GLN:HE22	1.73	0.54
1:E:496:MET:HB2	1:E:520:MET:HE1	1.89	0.54
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.43	0.54
1:A:249:ALA:HB3	1:A:252:ASN:HD22	1.72	0.54
10:G:201:HEM:HBA1	10:G:201:HEM:HHA	1.89	0.54
1:E:231:ARG:NH1	1:E:456:LEU:HD23	2.21	0.54
1:E:517:VAL:HG21	1:E:564:GLU:HG3	1.89	0.54
10:C:201:HEM:NC	4:D:95:HIS:CD2	2.74	0.54
3:G:114:TRP:HD1	3:G:175:ARG:NE	2.06	0.54
2:B:59:VAL:CG2	2:B:75:ILE:HG22	2.38	0.54
1:A:213:GLY:HA3	1:A:227:PHE:O	2.08	0.54
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.90	0.54
3:G:134:ASN:O	3:G:137:ARG:HB3	2.06	0.54
3:C:86:LEU:HD11	4:D:92:LEU:HD23	1.88	0.54
3:G:79:GLY:O	10:G:201:HEM:HMD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:NZ	1:A:460:GLU:O	2.40	0.54
1:A:242:ALA:HA	1:A:496:MET:HE1	1.90	0.54
1:E:52:ALA:O	1:E:53:GLY:C	2.44	0.54
2:B:179:LEU:HD23	2:B:213:ARG:CA	2.35	0.54
2:F:150:GLN:HE22	4:H:46:GLU:CG	2.20	0.54
1:A:203:ASP:HA	1:A:259:LEU:HG	1.90	0.54
3:G:64:LYS:O	3:G:66:GLN:HG3	2.07	0.53
1:A:508:ARG:NH1	1:A:573:HIS:HD2	2.06	0.53
1:E:249:ALA:C	1:E:251:MET:N	2.61	0.53
1:E:496:MET:HB2	1:E:520:MET:CE	2.38	0.53
1:A:327:GLU:OE2	1:A:384:PRO:HD3	2.08	0.53
1:A:631:ASP:HB3	1:A:634:GLU:CB	2.37	0.53
1:A:249:ALA:C	1:A:251:MET:H	2.10	0.53
1:E:77:ARG:HD2	2:F:96:SER:OG	2.08	0.53
2:B:179:LEU:CD2	2:B:216:ILE:HD11	2.39	0.53
2:B:223:ALA:O	2:B:227:LEU:HD12	2.09	0.53
3:G:42:GLY:O	3:G:45:TYR:HB3	2.08	0.53
10:C:201:HEM:HBA1	10:C:201:HEM:HBD1	1.89	0.53
2:B:198:ASN:O	2:B:200:ASP:N	2.42	0.53
1:A:230:LYS:HD2	1:A:462:ILE:CA	2.34	0.53
1:E:50:GLY:O	1:E:51:GLY:C	2.47	0.53
4:D:71:PRO:O	4:D:74:PRO:HD2	2.10	0.52
1:A:558:GLN:HA	1:A:618:ILE:HD13	1.91	0.52
1:E:233:ILE:HA	1:E:417:TYR:O	2.09	0.52
2:B:47:GLU:HB3	2:B:50:ALA:HB2	1.91	0.52
2:F:179:LEU:HD11	2:F:257:ARG:HH22	1.74	0.52
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.92	0.52
1:E:215:ILE:HA	1:E:225:HIS:O	2.08	0.52
3:C:76:ARG:NH1	11:C:202:RQX:C5	2.69	0.52
1:E:541:SER:HB2	2:F:84:THR:HG23	1.92	0.52
3:G:169:ALA:O	3:G:173:TYR:HB3	2.08	0.52
1:A:47:ILE:HG22	1:A:236:THR:HG22	1.91	0.52
2:B:183:ILE:HG13	2:B:185:CYS:HB3	1.91	0.52
3:G:82:MET:HB2	10:G:201:HEM:HAC	1.92	0.52
1:E:432:ARG:HD2	1:E:437:SER:HB2	1.92	0.52
2:F:179:LEU:CD1	2:F:257:ARG:HH22	2.22	0.52
1:A:121:TYR:O	1:A:125:ASN:OD1	2.27	0.52
2:F:205:PRO:HA	2:F:259:ILE:HD11	1.90	0.52
1:A:174:ASP:CB	1:A:361:PRO:HD2	2.28	0.52
4:D:101:TRP:HH2	4:D:122:ARG:HG2	1.75	0.52
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:84:MET:HA	4:H:84:MET:CE	2.40	0.52
1:E:206:MET:HG3	1:E:263:ALA:HB1	1.92	0.52
3:G:76:ARG:NH2	4:H:106:ASP:OD2	2.43	0.52
2:F:124:TYR:CE1	3:G:62:ILE:CG2	2.92	0.52
2:B:34:ARG:HD2	2:B:62:ASP:OD1	2.09	0.52
1:A:73:MET:CE	1:A:78:SER:HA	2.40	0.52
10:C:201:HEM:HBC2	4:D:96:VAL:CG2	2.40	0.52
1:A:117:ASN:O	1:A:120:HIS:HB3	2.09	0.52
1:E:541:SER:HB3	2:F:76:LYS:HZ3	1.75	0.52
1:E:401:VAL:CG2	1:E:416:LEU:HG	2.39	0.52
1:E:172:VAL:HG21	1:E:179:SER:HB3	1.91	0.52
1:E:48:GLY:O	1:E:53:GLY:HA3	2.10	0.51
2:F:57:PHE:CG	2:F:75:ILE:HD12	2.45	0.51
2:B:40:ILE:CD1	2:B:75:ILE:HD11	2.41	0.51
3:G:120:PHE:O	3:G:124:ILE:HG13	2.09	0.51
1:E:153:PHE:HD1	1:E:434:GLY:HA3	1.75	0.51
2:F:172:GLU:OE2	2:F:275:PRO:HD2	2.10	0.51
3:G:76:ARG:NH1	11:G:202:RQX:O3	2.43	0.51
2:B:230:MET:CE	2:B:262:ILE:HG21	2.41	0.51
1:E:347:GLN:HG2	1:E:350:HIS:ND1	2.25	0.51
3:G:183:THR:HG23	3:G:183:THR:O	2.10	0.51
1:A:493:ARG:HB2	1:A:549:LEU:HD13	1.92	0.51
1:A:371:ALA:O	1:A:373:VAL:N	2.44	0.51
1:A:135:ASN:ND2	2:B:161:LEU:O	2.43	0.51
2:B:279:PRO:O	2:B:280:ALA:CB	2.58	0.51
1:E:301:SER:HB3	1:E:336:GLY:O	2.09	0.51
1:A:120:HIS:HD2	1:A:630:LEU:HB2	1.72	0.51
1:E:513:LEU:O	1:E:517:VAL:HG23	2.11	0.51
2:F:131:VAL:CG2	3:G:55:PRO:HG2	2.41	0.51
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.46	0.51
1:A:291:SER:HA	1:A:360:LEU:HD11	1.91	0.51
3:G:69:TRP:HE3	11:G:202:RQX:H3	1.76	0.51
2:F:54:LEU:HD11	2:F:124:TYR:OH	2.10	0.51
2:F:40:ILE:HG21	2:F:83:LEU:HD11	1.93	0.51
1:E:585:TYR:CZ	1:E:596:LYS:HD3	2.46	0.51
1:A:591:ILE:HA	1:A:594:GLN:NE2	2.26	0.51
3:C:87:LEU:O	3:C:89:GLY:N	2.44	0.50
4:D:88:LEU:O	4:D:92:LEU:HB2	2.11	0.50
4:D:153:VAL:O	4:D:156:LEU:HD12	2.11	0.50
3:C:100:PHE:CE1	4:D:149:ALA:HA	2.46	0.50
11:C:202:RQX:H20	4:D:107:TYR:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:GLY:HA2	2:F:109:CYS:SG	2.51	0.50
3:G:69:TRP:HE3	11:G:202:RQX:C1	2.24	0.50
1:E:439:LEU:HD13	1:E:439:LEU:C	2.31	0.50
1:A:221:ASP:HA	1:A:538:ILE:HG12	1.92	0.50
1:A:378:GLU:HB3	1:A:379:PRO:CD	2.42	0.50
1:E:120:HIS:HD2	1:E:630:LEU:N	2.08	0.50
1:E:586:ASP:OD1	1:E:586:ASP:C	2.50	0.50
1:E:356:LEU:HD12	1:E:360:LEU:HD12	1.93	0.50
2:B:36:LYS:NZ	2:B:114:ASP:O	2.44	0.50
1:E:88:ASN:ND2	1:E:169:THR:OG1	2.45	0.50
2:B:38:PHE:O	2:B:56:LYS:HA	2.12	0.50
1:A:78:SER:O	1:A:81:THR:HG22	2.11	0.50
2:B:39:GLU:HB2	2:B:122:LYS:HB3	1.94	0.50
4:H:144:VAL:HG11	4:H:152:MET:HE1	1.92	0.50
1:E:106:THR:HG22	1:E:119:MET:SD	2.51	0.50
1:E:253:THR:HG22	1:E:552:LEU:HD11	1.92	0.50
2:B:198:ASN:C	2:B:200:ASP:H	2.15	0.49
2:B:238:LYS:O	2:B:240:HIS:HD2	1.95	0.49
1:A:270:LEU:HD12	1:A:558:GLN:HB3	1.93	0.49
2:F:131:VAL:HG22	3:G:55:PRO:O	2.12	0.49
2:F:173:GLN:O	2:F:176:LEU:HB2	2.12	0.49
3:G:121:LYS:HB3	3:G:171:VAL:HG22	1.94	0.49
1:E:635:VAL:HG22	1:E:636:ASP:H	1.77	0.49
4:H:140:ASN:ND2	4:H:145:GLY:HA2	2.26	0.49
2:F:244:ASN:HD21	3:G:66:GLN:NE2	2.10	0.49
1:A:242:ALA:HA	1:A:496:MET:CE	2.43	0.49
1:A:222:GLY:O	1:A:537:LEU:HD13	2.12	0.49
3:G:79:GLY:C	10:G:201:HEM:HMD1	2.33	0.49
1:A:557:THR:O	1:A:560:ILE:HG22	2.11	0.49
2:F:102:ALA:HA	2:F:122:LYS:HE2	1.95	0.49
1:E:566:ARG:NH1	1:E:568:GLU:OE2	2.44	0.49
1:E:294:GLU:OE1	1:E:359:ARG:HG2	2.12	0.49
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.48	0.49
1:E:541:SER:CB	2:F:76:LYS:HZ3	2.26	0.49
1:A:246:CYS:O	2:B:90:ARG:NH2	2.46	0.49
1:A:520:MET:HG2	1:A:560:ILE:HG21	1.95	0.49
1:A:58:MET:HA	1:A:191:CYS:SG	2.53	0.49
1:E:241:ARG:HH11	1:E:250:HIS:CE1	2.31	0.49
1:A:246:CYS:HA	1:A:385:THR:HG22	1.95	0.49
1:A:508:ARG:NH1	1:A:573:HIS:CD2	2.81	0.49
2:F:47:GLU:HB3	2:F:50:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ASP:HA	1:E:538:ILE:HG12	1.94	0.48
2:F:124:TYR:CZ	3:G:62:ILE:HG21	2.48	0.48
1:E:547:LEU:HD12	1:E:547:LEU:HA	1.61	0.48
1:E:452:ILE:O	1:E:453:LYS:C	2.51	0.48
4:H:50:LYS:N	4:H:51:PRO:CD	2.75	0.48
2:F:122:LYS:N	2:F:122:LYS:CD	2.75	0.48
1:E:320:ARG:HH11	1:E:434:GLY:HA2	1.78	0.48
1:A:253:THR:HG22	1:A:552:LEU:HD11	1.95	0.48
2:F:68:VAL:HG23	2:F:111:CYS:O	2.12	0.48
1:E:606:HIS:CD2	1:E:623:ARG:NH1	2.81	0.48
3:G:62:ILE:HD12	3:G:63:TYR:N	2.29	0.48
1:A:199:TYR:HA	1:A:217:LEU:O	2.14	0.48
3:G:95:VAL:HG13	3:G:96:LEU:HD12	1.95	0.48
1:A:45:VAL:HG22	1:A:68:ALA:HB3	1.95	0.48
2:F:150:GLN:HA	2:F:152:TRP:CZ3	2.48	0.48
1:E:276:HIS:NE2	1:E:320:ARG:NH2	2.62	0.48
2:F:244:ASN:ND2	3:G:66:GLN:NE2	2.62	0.48
4:D:126:TYR:H	4:D:126:TYR:HD1	1.62	0.48
1:E:72:LYS:NZ	1:E:255:ASP:OD2	2.44	0.48
1:A:276:HIS:O	1:A:384:PRO:HA	2.13	0.48
1:E:200:PHE:O	1:E:216:ALA:HB1	2.14	0.48
1:A:527:LEU:HD11	1:A:553:MET:HG3	1.96	0.48
2:F:155:LYS:HD2	2:F:166:GLN:NE2	2.29	0.48
4:D:113:LEU:HD22	4:D:117:LEU:HD22	1.96	0.48
2:B:250:PRO:HD2	8:B:302:SF4:S3	2.54	0.48
2:F:86:ARG:HH11	2:F:137:PRO:HD2	1.77	0.48
2:F:179:LEU:CD2	2:F:216:ILE:HD11	2.44	0.48
1:E:492:LEU:HD23	1:E:530:LEU:HD12	1.95	0.48
1:A:44:VAL:HG21	1:A:60:LEU:HD13	1.96	0.48
2:B:155:LYS:HD2	2:B:166:GLN:HE21	1.77	0.47
1:A:477:LEU:HD12	1:A:543:LEU:HD11	1.96	0.47
2:B:208:LEU:HD13	2:B:259:ILE:HG12	1.96	0.47
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.97	0.47
2:B:244:ASN:ND2	3:C:66:GLN:NE2	2.61	0.47
2:F:40:ILE:HG22	2:F:41:TYR:O	2.14	0.47
1:E:258:ALA:O	1:E:259:LEU:C	2.52	0.47
10:C:201:HEM:HBA1	10:C:201:HEM:CHA	2.35	0.47
1:E:484:ASN:O	1:E:485:GLY:O	2.33	0.47
3:G:114:TRP:HB2	3:G:175:ARG:CZ	2.44	0.47
1:A:47:ILE:HD11	1:A:214:VAL:CG2	2.45	0.47
1:E:561:VAL:CG2	1:E:618:ILE:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PHE:CA	1:A:497:GLN:HB3	2.44	0.47
1:A:85:GLY:HA3	1:A:153:PHE:HZ	1.80	0.47
1:A:378:GLU:HB3	1:A:379:PRO:HD2	1.96	0.47
2:F:150:GLN:HB3	2:F:152:TRP:CZ2	2.49	0.47
1:E:519:LYS:O	1:E:522:ASP:HB2	2.14	0.47
1:E:517:VAL:O	1:E:521:MET:HG2	2.14	0.47
1:A:394:PRO:O	1:A:395:THR:HG22	2.14	0.47
3:G:148:ASP:OD2	3:G:150:PRO:HD2	2.13	0.47
3:C:76:ARG:HA	10:C:201:HEM:O2D	2.15	0.47
4:H:149:ALA:O	4:H:153:VAL:HG23	2.14	0.47
1:E:156:GLN:HB3	1:E:166:ALA:HB3	1.97	0.47
2:F:100:ASN:HD21	2:F:103:GLY:CA	2.27	0.47
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.97	0.47
2:B:179:LEU:CD1	2:B:257:ARG:HH22	2.28	0.47
4:D:108:GLY:HA2	4:D:113:LEU:HD11	1.97	0.47
1:A:107:ALA:O	1:A:110:SER:OG	2.31	0.47
1:E:121:TYR:HB2	1:E:630:LEU:HD11	1.95	0.47
2:B:179:LEU:HD22	2:B:216:ILE:HD11	1.96	0.47
1:E:80:THR:CG2	1:E:181:LEU:HB2	2.42	0.47
2:B:198:ASN:C	2:B:200:ASP:N	2.67	0.47
1:A:270:LEU:HD12	1:A:558:GLN:CB	2.45	0.47
1:A:44:VAL:HG11	1:A:60:LEU:HD22	1.96	0.47
1:E:471:GLU:HA	1:E:474:ILE:HG23	1.95	0.47
3:C:76:ARG:CG	3:C:76:ARG:NH1	2.77	0.47
2:B:268:LYS:HG2	2:B:269:MET:H	1.74	0.47
1:E:492:LEU:HD12	1:E:523:LEU:HD23	1.97	0.47
4:D:126:TYR:CD1	4:D:126:TYR:N	2.83	0.47
1:A:432:ARG:NE	1:A:437:SER:HB2	2.30	0.46
2:F:264:MET:SD	3:G:143:MET:HG2	2.55	0.46
1:A:102:HIS:CE1	1:A:123:THR:HG22	2.50	0.46
1:A:401:VAL:HG21	1:A:416:LEU:HG	1.97	0.46
2:F:245:CYS:HB2	2:F:255:PRO:HG2	1.97	0.46
2:B:238:LYS:HE3	4:D:106:ASP:OD1	2.15	0.46
1:E:159:ASN:HB2	1:E:163:GLY:N	2.29	0.46
11:C:202:RQX:H15	4:D:107:TYR:CE2	2.50	0.46
1:A:115:ASP:HB3	1:A:117:ASN:HD21	1.81	0.46
2:F:197:TRP:HZ2	11:G:202:RQX:H11	1.81	0.46
2:B:179:LEU:HD11	2:B:257:ARG:HH22	1.79	0.46
1:E:132:GLU:HG2	2:F:161:LEU:HG	1.97	0.46
1:A:159:ASN:O	1:A:162:LYS:N	2.48	0.46
2:B:230:MET:HE3	2:B:262:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:GLY:HA3	1:E:227:PHE:O	2.15	0.46
3:C:35:LYS:HB3	3:C:39:GLN:HB3	1.97	0.46
2:B:72:LEU:HA	2:B:72:LEU:HD23	1.77	0.46
1:A:78:SER:OG	6:A:702:FAD:O3B	2.19	0.46
1:A:267:LEU:HD12	1:A:270:LEU:HD11	1.98	0.46
2:B:105:ASN:HD21	2:B:127:PRO:CD	2.28	0.46
10:C:201:HEM:CAA	4:D:63:ARG:HH12	2.23	0.46
1:A:122:LEU:HD11	1:A:440:ASP:HA	1.97	0.46
1:E:552:LEU:O	1:E:556:ALA:N	2.43	0.46
1:E:74:PHE:CE2	1:E:76:THR:HB	2.51	0.46
11:G:202:RQX:H9	11:G:202:RQX:H1	1.60	0.46
1:E:390:MET:CE	1:E:431:ASN:HA	2.46	0.46
1:E:313:LYS:HB2	1:E:645:TYR:O	2.15	0.46
1:A:466:PRO:O	1:A:469:ALA:HB2	2.16	0.46
1:A:585:TYR:CE1	1:A:596:LYS:HA	2.50	0.46
1:A:511:ASP:O	1:A:515:GLU:HB2	2.15	0.46
1:E:610:LYS:O	1:E:618:ILE:HA	2.14	0.46
1:A:274:GLN:HB3	1:A:388:TYR:HB3	1.97	0.46
1:A:293:GLY:HA2	1:A:317:LEU:HD11	1.98	0.46
1:E:404:TYR:HB3	1:E:608:LEU:HD11	1.98	0.46
2:B:240:HIS:C	2:B:241:THR:HG23	2.37	0.46
1:A:276:HIS:HB2	1:A:387:HIS:CG	2.51	0.46
1:E:296:GLY:HA3	1:E:348:LEU:HD23	1.98	0.46
3:G:58:PRO:HB2	3:G:62:ILE:HG12	1.98	0.46
1:A:159:ASN:O	1:A:160:TYR:C	2.54	0.46
1:E:320:ARG:NH1	1:E:432:ARG:NH2	2.64	0.46
2:F:100:ASN:HD21	2:F:103:GLY:HA2	1.81	0.46
2:F:209:MET:HE3	2:F:258:ALA:CB	2.45	0.45
1:E:266:ALA:HB2	1:E:610:LYS:HG2	1.97	0.45
3:G:124:ILE:HG23	12:H:201:EPH:H272	1.97	0.45
1:A:42:TYR:CD2	1:A:68:ALA:HB2	2.51	0.45
2:B:39:GLU:HA	2:B:55:GLN:O	2.15	0.45
4:D:67:ALA:HA	4:D:70:VAL:HG23	1.98	0.45
1:A:482:TYR:CE2	1:A:535:ARG:HG2	2.50	0.45
2:B:68:VAL:HG23	2:B:111:CYS:O	2.16	0.45
2:B:44:ASN:HD22	2:B:47:GLU:HB2	1.81	0.45
1:A:113:LEU:O	1:A:606:HIS:HE1	1.99	0.45
3:C:86:LEU:CD1	4:D:92:LEU:HD23	2.47	0.45
1:A:279:GLY:HA3	1:A:385:THR:OG1	2.16	0.45
2:B:244:ASN:HD21	3:C:66:GLN:NE2	2.15	0.45
1:E:457:LYS:HD3	1:E:457:LYS:HA	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:LYS:O	2:B:247:LYS:HG3	2.16	0.45
4:D:143:ASP:OD2	4:D:144:VAL:HG22	2.15	0.45
1:A:541:SER:HB3	2:B:76:LYS:NZ	2.32	0.45
1:E:570:ARG:HH22	1:E:604:ARG:HG3	1.81	0.45
3:G:149:ILE:N	3:G:149:ILE:CD1	2.62	0.45
1:A:502:LYS:HD3	1:A:503:HIS:HE1	1.78	0.45
3:G:126:PHE:HB3	3:G:127:PRO:CD	2.44	0.45
1:A:540:ASN:HB3	1:A:543:LEU:HB3	1.98	0.45
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.98	0.45
1:E:243:TYR:CD2	1:E:386:VAL:HG21	2.52	0.45
1:A:503:HIS:CD2	1:A:516:GLY:CA	3.00	0.45
2:B:83:LEU:HA	2:B:83:LEU:HD12	1.76	0.45
1:E:85:GLY:N	6:E:702:FAD:O4	2.50	0.45
1:A:148:ILE:HG13	2:B:165:GLN:NE2	2.31	0.45
1:A:65:PHE:CE2	1:A:456:LEU:HD12	2.47	0.45
3:G:112:ILE:HB	3:G:113:PRO:HD3	1.98	0.45
1:E:45:VAL:HG21	1:E:227:PHE:HB3	1.98	0.45
1:E:152:SER:O	1:E:293:GLY:HA3	2.17	0.45
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.17	0.45
1:A:133:LEU:HD13	1:A:138:MET:SD	2.57	0.45
1:E:174:ASP:OD2	1:E:362:GLY:N	2.49	0.45
1:A:276:HIS:ND1	1:A:277:PRO:HD2	2.32	0.45
1:A:40:HIS:HB3	1:A:42:TYR:HE1	1.81	0.45
4:D:68:ALA:O	4:D:71:PRO:HD2	2.17	0.45
1:A:344:ILE:HG12	1:A:345:TYR:N	2.32	0.45
1:E:488:PRO:HB2	1:E:491:GLU:HG3	1.99	0.45
1:E:480:VAL:HG22	1:E:550:GLN:NE2	2.29	0.45
2:F:84:THR:HB	2:F:134:ASP:HB2	1.98	0.45
2:F:279:PRO:O	2:F:280:ALA:CB	2.65	0.45
2:B:141:LEU:HD21	2:B:199:ALA:O	2.17	0.45
1:A:230:LYS:CD	1:A:462:ILE:HA	2.39	0.44
1:E:468:GLY:O	1:E:471:GLU:HB2	2.17	0.44
1:E:509:ARG:HA	1:E:577:ASP:OD2	2.16	0.44
4:D:77:TYR:HA	12:D:201:EPH:H11	1.98	0.44
2:B:59:VAL:HG21	2:B:75:ILE:HG22	1.98	0.44
1:A:88:ASN:ND2	1:A:169:THR:OG1	2.51	0.44
3:G:76:ARG:HE	4:H:103:VAL:HG22	1.82	0.44
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.98	0.44
1:E:461:LYS:HB3	1:E:461:LYS:HE2	1.61	0.44
1:A:333:GLU:HB3	1:A:335:ARG:NH1	2.27	0.44
1:E:570:ARG:NH2	1:E:604:ARG:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:112:ILE:HD12	3:G:117:LEU:HG	1.99	0.44
2:F:100:ASN:C	2:F:100:ASN:HD22	2.21	0.44
4:H:55:HIS:CG	4:H:55:HIS:O	2.71	0.44
1:E:86:GLY:HA3	1:E:169:THR:HG22	1.99	0.44
1:A:566:ARG:HB3	1:A:573:HIS:CE1	2.53	0.44
3:G:121:LYS:HB3	3:G:171:VAL:CG2	2.47	0.44
1:A:109:GLY:O	1:A:431:ASN:HB3	2.16	0.44
1:A:190:ARG:HG2	1:A:190:ARG:O	2.16	0.44
1:A:611:GLN:HG3	1:A:618:ILE:HG12	1.99	0.44
4:H:57:THR:O	4:H:61:ILE:HG23	2.18	0.44
2:B:42:ARG:O	2:B:52:PRO:HA	2.17	0.44
3:G:76:ARG:HH21	4:H:103:VAL:HA	1.82	0.44
3:C:114:TRP:HB2	3:C:175:ARG:CZ	2.48	0.44
2:F:150:GLN:HE22	4:H:46:GLU:HG3	1.82	0.44
2:B:196:TRP:CZ3	3:C:59:HIS:HB2	2.52	0.44
4:H:84:MET:HE2	4:H:84:MET:HA	1.99	0.44
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.48	0.44
3:C:86:LEU:HD22	4:D:136:LEU:HD11	1.98	0.44
2:B:116:ASN:ND2	2:B:119:LYS:H	2.16	0.44
2:B:60:ASP:OD2	2:B:63:LYS:HE2	2.17	0.44
3:G:165:LEU:HD22	3:G:165:LEU:HA	1.92	0.44
6:A:702:FAD:H1'1	6:A:702:FAD:H9	1.77	0.44
1:A:262:ARG:HH12	1:A:551:ASN:ND2	2.15	0.44
1:A:128:GLU:HG2	2:B:162:GLY:HA3	2.00	0.44
1:A:584:GLU:HG3	1:A:602:HIS:CE1	2.53	0.44
3:C:50:ARG:HG3	3:C:51:ALA:N	2.33	0.44
3:G:114:TRP:CD1	3:G:175:ARG:NE	2.86	0.43
1:A:47:ILE:HD11	1:A:214:VAL:HG21	2.00	0.43
3:G:143:MET:O	3:G:144:ALA:HB3	2.18	0.43
2:F:228:ALA:HA	2:F:231:GLN:CG	2.48	0.43
1:A:568:GLU:O	1:A:575:ARG:HG2	2.18	0.43
1:A:104:TYR:HD1	1:A:638:ILE:HD13	1.83	0.43
1:A:202:LEU:HB2	1:A:215:ILE:HG23	1.99	0.43
1:A:562:ALA:HB1	1:A:607:THR:HG21	2.00	0.43
1:E:500:MET:HE1	1:E:560:ILE:HB	2.00	0.43
2:F:39:GLU:HB2	2:F:122:LYS:HB3	1.99	0.43
2:F:148:SER:HB3	3:G:38:ILE:HD13	2.01	0.43
1:E:124:ARG:HD2	1:E:634:GLU:OE2	2.18	0.43
1:E:363:ILE:HG13	1:E:364:SER:N	2.34	0.43
4:D:136:LEU:O	4:D:137:LEU:C	2.55	0.43
4:D:126:TYR:N	4:D:126:TYR:HD1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:209:MET:HE3	2:F:258:ALA:HB2	2.00	0.43
2:F:100:ASN:ND2	2:F:100:ASN:C	2.72	0.43
1:E:74:PHE:CD1	2:F:143:TYR:CZ	3.06	0.43
1:A:74:PHE:CD1	2:B:143:TYR:CE2	3.06	0.43
3:G:114:TRP:HB2	3:G:175:ARG:HH11	1.80	0.43
3:G:85:THR:HG21	12:H:201:EPH:H271	2.01	0.43
1:E:294:GLU:CD	1:E:359:ARG:HG2	2.39	0.43
4:D:58:LEU:O	4:D:62:GLU:HG2	2.19	0.43
2:F:188:CYS:SG	2:F:189:SER:N	2.92	0.43
1:E:286:LEU:HA	1:E:286:LEU:HD12	1.76	0.43
1:E:448:CYS:O	1:E:452:ILE:HG13	2.18	0.43
1:A:428:HIS:CE1	1:A:432:ARG:HG3	2.54	0.43
1:A:249:ALA:C	1:A:251:MET:N	2.72	0.43
1:A:73:MET:HE3	1:A:78:SER:HA	2.00	0.43
3:C:86:LEU:HA	3:C:86:LEU:HD23	1.84	0.43
2:B:92:GLY:HA2	2:B:109:CYS:SG	2.59	0.43
3:G:158:LEU:O	3:G:162:LEU:HB2	2.18	0.43
4:H:155:GLU:HB2	12:H:201:EPH:N1	2.34	0.43
2:B:264:MET:SD	3:C:143:MET:HG2	2.59	0.43
1:E:209:GLY:O	1:E:414:PRO:HD2	2.18	0.43
1:E:74:PHE:CE1	2:F:143:TYR:CD1	3.07	0.42
2:F:39:GLU:HG2	2:F:56:LYS:HG3	2.00	0.42
2:F:67:MET:HG3	2:F:109:CYS:O	2.18	0.42
2:F:107:LEU:HD11	2:F:183:ILE:HD11	2.00	0.42
1:A:320:ARG:NH1	5:A:701:MLI:C2	2.74	0.42
2:B:172:GLU:OE2	2:B:275:PRO:CD	2.67	0.42
1:A:42:TYR:HE2	1:A:194:THR:CG2	2.32	0.42
3:C:71:VAL:HG13	3:C:130:PHE:HZ	1.84	0.42
1:E:210:ARG:CZ	1:E:414:PRO:HB3	2.49	0.42
2:B:242:ILE:O	2:B:243:MET:HB2	2.18	0.42
1:A:356:LEU:HD23	1:A:376:THR:HG22	2.01	0.42
1:E:537:LEU:HA	1:E:537:LEU:HD23	1.90	0.42
2:F:243:MET:HB3	3:G:152:ILE:HD13	2.01	0.42
1:A:162:LYS:HG2	1:A:162:LYS:H	1.68	0.42
1:E:38:ILE:CG2	4:H:34:GLY:HA3	2.46	0.42
1:A:121:TYR:C	1:A:121:TYR:CD1	2.93	0.42
1:E:606:HIS:HD2	1:E:623:ARG:NH1	2.18	0.42
3:G:162:LEU:HA	3:G:162:LEU:HD22	1.75	0.42
1:A:424:CYS:C	1:A:426:SER:H	2.21	0.42
1:A:547:LEU:O	1:A:550:GLN:HB2	2.19	0.42
1:A:305:ARG:NH2	1:A:316:ASP:OD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:93:THR:HA	4:H:132:LEU:HD23	2.02	0.42
1:A:603:TRP:O	1:A:605:LYS:N	2.52	0.42
1:A:242:ALA:HB2	1:A:552:LEU:HD22	2.01	0.42
4:H:65:PHE:CZ	4:H:94:LEU:HD23	2.55	0.42
1:A:95:ASN:HB2	1:A:96:PRO:HD2	2.02	0.42
1:A:148:ILE:HG21	1:A:170:CYS:HB3	2.01	0.42
4:H:77:TYR:O	12:H:201:EPH:H371	2.19	0.42
1:E:462:ILE:O	1:E:463:PRO:C	2.57	0.42
1:A:614:ARG:CZ	1:A:614:ARG:HB3	2.49	0.42
2:B:69:LEU:O	2:B:73:ILE:HG13	2.19	0.42
2:F:249:CYS:HA	2:F:250:PRO:HD2	1.81	0.42
1:E:390:MET:SD	1:E:390:MET:N	2.93	0.42
1:E:519:LYS:O	1:E:523:LEU:HD12	2.19	0.42
1:A:567:LYS:HB3	1:A:578:PHE:CD1	2.55	0.42
6:E:702:FAD:H1'1	6:E:702:FAD:H9	1.81	0.42
3:G:112:ILE:HG13	3:G:112:ILE:H	1.73	0.42
1:A:267:LEU:HA	1:A:394:PRO:HD3	2.02	0.42
4:D:92:LEU:HD21	12:D:201:EPH:H222	2.02	0.41
1:E:73:MET:CE	1:E:78:SER:HA	2.49	0.41
1:A:333:GLU:CB	1:A:335:ARG:HH12	2.29	0.41
1:E:134:GLU:HB2	1:E:148:ILE:HD11	2.02	0.41
2:F:172:GLU:CD	2:F:275:PRO:HD2	2.39	0.41
2:F:149:ILE:HG21	2:F:211:ALA:HB2	2.01	0.41
3:C:105:GLU:C	3:C:107:ILE:H	2.23	0.41
1:E:83:ALA:HA	6:E:702:FAD:C6	2.50	0.41
3:G:69:TRP:O	3:G:73:GLY:N	2.51	0.41
1:E:77:ARG:HD3	2:F:94:CYS:O	2.19	0.41
1:A:508:ARG:HH11	1:A:573:HIS:CD2	2.37	0.41
4:D:57:THR:O	4:D:61:ILE:HG23	2.20	0.41
1:E:371:ALA:O	1:E:373:VAL:HG23	2.20	0.41
3:C:134:ASN:O	3:C:137:ARG:HB3	2.20	0.41
1:E:302:GLU:HG2	1:E:335:ARG:HG2	2.01	0.41
1:E:410:ASP:C	1:E:411:LYS:HG2	2.40	0.41
3:C:57:ALA:HA	3:C:58:PRO:HD2	1.89	0.41
1:E:72:LYS:HD3	6:E:702:FAD:C5A	2.50	0.41
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.79	0.41
2:B:244:ASN:OD1	3:C:69:TRP:HB3	2.19	0.41
2:F:105:ASN:O	2:F:106:THR:HB	2.21	0.41
2:F:169:SER:O	2:F:170:ILE:C	2.58	0.41
3:G:76:ARG:CG	10:G:201:HEM:O2D	2.55	0.41
2:F:213:ARG:O	2:F:213:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:HA	1:A:169:THR:O	2.20	0.41
1:A:271:GLU:OE2	1:A:562:ALA:HB1	2.20	0.41
1:E:482:TYR:O	1:E:483:ALA:C	2.59	0.41
2:F:93:ILE:HD13	2:F:93:ILE:O	2.20	0.41
3:C:170:VAL:HG11	12:D:201:EPH:H61	2.01	0.41
1:E:512:ILE:HG13	1:E:512:ILE:H	1.65	0.41
4:H:97:HIS:HE1	4:H:126:TYR:CE2	2.39	0.41
11:C:202:RQX:H6	4:D:106:ASP:OD2	2.20	0.41
2:F:230:MET:CE	2:F:262:ILE:HG21	2.49	0.41
2:B:40:ILE:HD12	2:B:57:PHE:CD1	2.56	0.41
1:A:240:GLY:O	1:A:242:ALA:N	2.53	0.41
1:E:215:ILE:HD11	1:E:224:ILE:HG21	2.01	0.41
1:E:228:ARG:NH1	1:E:463:PRO:O	2.53	0.41
4:H:104:VAL:HG13	4:H:121:VAL:HG12	2.02	0.41
1:E:239:TYR:OH	1:E:270:LEU:HD22	2.20	0.41
2:F:75:ILE:HG21	2:F:75:ILE:HD13	1.80	0.41
2:F:86:ARG:CZ	2:F:136:VAL:HG13	2.51	0.41
4:H:154:TRP:CE2	12:H:201:EPH:H52	2.55	0.41
1:A:258:ALA:O	1:A:262:ARG:HB2	2.20	0.41
1:A:253:THR:HG22	1:A:552:LEU:HD12	2.03	0.41
1:A:584:GLU:N	1:A:584:GLU:OE2	2.54	0.41
1:E:79:HIS:CD2	6:E:702:FAD:HM81	2.47	0.41
11:C:202:RQX:H9	11:C:202:RQX:H1	1.36	0.41
2:B:268:LYS:HB3	2:B:268:LYS:HE2	1.33	0.41
1:A:393:ILE:CG2	1:A:401:VAL:HG13	2.51	0.41
3:C:42:GLY:O	3:C:45:TYR:HB3	2.21	0.41
2:B:173:GLN:O	2:B:176:LEU:HB2	2.21	0.41
1:E:325:ARG:O	1:E:328:THR:N	2.52	0.41
1:E:162:LYS:HG2	1:E:162:LYS:H	1.69	0.41
4:H:70:VAL:O	4:H:74:PRO:HD2	2.19	0.41
10:C:201:HEM:CBA	10:C:201:HEM:HHA	2.41	0.41
3:G:133:LEU:O	3:G:136:ILE:N	2.54	0.41
1:E:363:ILE:HG13	1:E:364:SER:H	1.86	0.41
1:E:270:LEU:HD12	1:E:558:GLN:HB3	2.02	0.41
3:G:142:ASP:OD2	4:H:63:ARG:NH1	2.53	0.41
1:A:219:LEU:H	1:A:219:LEU:HD12	1.85	0.41
1:E:465:LEU:HA	1:E:465:LEU:HD23	1.91	0.41
2:B:212:TYR:O	2:B:216:ILE:HG13	2.21	0.41
1:E:390:MET:HE3	1:E:431:ASN:HA	2.03	0.41
1:E:231:ARG:HH11	1:E:456:LEU:HD23	1.86	0.41
1:E:523:LEU:HA	1:E:526:GLU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ILE:HG13	1:A:560:ILE:O	2.20	0.40
1:A:276:HIS:CG	1:A:286:LEU:HD11	2.56	0.40
2:B:90:ARG:C	2:B:90:ARG:HD2	2.41	0.40
1:A:388:TYR:CZ	1:A:432:ARG:HD2	2.57	0.40
2:F:268:LYS:HE2	2:F:268:LYS:HB3	1.38	0.40
2:B:36:LYS:HZ1	2:B:114:ASP:HB3	1.86	0.40
1:E:102:HIS:CE1	1:E:123:THR:HG22	2.56	0.40
1:E:516:GLY:O	1:E:520:MET:HB2	2.21	0.40
1:A:557:THR:O	1:A:561:VAL:HG13	2.21	0.40
1:E:45:VAL:HG22	1:E:68:ALA:HB3	2.03	0.40
1:E:270:LEU:O	1:E:559:THR:HG23	2.21	0.40
1:E:438:LEU:O	1:E:442:VAL:HG23	2.22	0.40
1:E:365:GLU:OE1	1:E:369:ILE:HD11	2.21	0.40
1:E:269:ASP:O	1:E:271:GLU:N	2.54	0.40
1:A:78:SER:OG	6:A:702:FAD:C3B	2.68	0.40
1:E:276:HIS:HD2	1:E:387:HIS:CD2	2.39	0.40
2:F:244:ASN:HD21	3:G:66:GLN:HE21	1.68	0.40
1:A:561:VAL:HG11	1:A:618:ILE:HD12	2.04	0.40
2:F:80:ASP:C	2:F:80:ASP:OD2	2.60	0.40
1:E:79:HIS:O	1:E:82:ALA:N	2.42	0.40
1:A:162:LYS:O	1:A:163:GLY:O	2.38	0.40
1:A:262:ARG:HH22	1:A:551:ASN:ND2	2.18	0.40
2:F:128:HIS:ND1	2:F:128:HIS:O	2.54	0.40
2:F:128:HIS:HA	3:G:56:ILE:HG23	2.03	0.40
1:E:461:LYS:H	1:E:461:LYS:HG2	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/645 (95%)	531 (87%)	68 (11%)	12 (2%)	9	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	611/645 (95%)	540 (88%)	56 (9%)	15 (2%)	7	23
2	B	247/282 (88%)	214 (87%)	26 (10%)	7 (3%)	6	20
2	F	247/282 (88%)	206 (83%)	33 (13%)	8 (3%)	5	16
3	C	151/188 (80%)	127 (84%)	18 (12%)	6 (4%)	4	11
3	G	148/188 (79%)	127 (86%)	18 (12%)	3 (2%)	9	29
4	D	127/156 (81%)	109 (86%)	16 (13%)	2 (2%)	12	36
4	H	127/156 (81%)	105 (83%)	18 (14%)	4 (3%)	5	17
All	All	2269/2542 (89%)	1959 (86%)	253 (11%)	57 (2%)	7	23

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	TYR
1	A	163	GLY
1	A	372	GLY
1	A	485	GLY
2	B	161	LEU
3	C	97	PRO
3	C	98	LEU
4	D	47	LYS
1	E	485	GLY
1	E	591	ILE
2	F	158	LYS
2	F	280	ALA
3	G	98	LEU
4	H	50	LYS
1	A	539	TRP
2	B	109	CYS
2	B	243	MET
2	B	280	ALA
3	C	111	GLY
1	E	51	GLY
1	E	269	ASP
1	E	305	ARG
1	E	426	SER
2	F	268	LYS
3	G	48	ARG
4	H	48	GLY
4	H	82	ARG
1	A	159	ASN

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Mol	Chain	Res	Type
1	A	241	ARG
1	A	330	GLU
1	A	469	ALA
1	A	592	GLU
3	C	58	PRO
4	D	51	PRO
1	E	63	ALA
1	E	109	GLY
1	E	254	GLY
1	E	270	LEU
1	E	463	PRO
2	F	213	ARG
1	A	604	ARG
2	B	218	SER
1	E	539	TRP
2	F	49	GLY
2	F	116	ASN
2	F	218	SER
4	H	46	GLU
2	B	199	ALA
3	C	87	LEU
1	E	125	ASN
2	F	277	PRO
1	E	483	ALA
3	G	123	ILE
2	B	81	PRO
3	C	88	ILE
1	A	589	LYS
1	E	53	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	498/526 (95%)	425 (85%)	73 (15%)	4 11
1	E	498/526 (95%)	437 (88%)	61 (12%)	6 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	219/242 (90%)	173 (79%)	46 (21%)	1	4
2	F	219/242 (90%)	179 (82%)	40 (18%)	2	6
3	C	127/158 (80%)	107 (84%)	20 (16%)	3	9
3	G	124/158 (78%)	108 (87%)	16 (13%)	5	15
4	D	96/119 (81%)	79 (82%)	17 (18%)	2	6
4	H	96/119 (81%)	82 (85%)	14 (15%)	4	11
All	All	1877/2090 (90%)	1590 (85%)	287 (15%)	3	10

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	62	GLU
1	A	76	THR
1	A	111	ASP
1	A	117	ASN
1	A	142	ARG
1	A	143	THR
1	A	147	LYS
1	A	152	SER
1	A	153	PHE
1	A	162	LYS
1	A	165	VAL
1	A	175	ARG
1	A	194	THR
1	A	205	LEU
1	A	228	ARG
1	A	230	LYS
1	A	241	ARG
1	A	257	THR
1	A	261	THR
1	A	271	GLU
1	A	274	GLN
1	A	283	VAL
1	A	308	GLU
1	A	313	LYS
1	A	320	ARG
1	A	328	THR
1	A	335	ARG
1	A	337	VAL

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Mol	Chain	Res	Type
1	A	344	ILE
1	A	347	GLN
1	A	351	LEU
1	A	354	GLU
1	A	356	LEU
1	A	359	ARG
1	A	368	LYS
1	A	385	THR
1	A	390	MET
1	A	412	ILE
1	A	425	HIS
1	A	426	SER
1	A	436	ASN
1	A	440	ASP
1	A	446	ARG
1	A	453	LYS
1	A	454	GLU
1	A	456	LEU
1	A	457	LYS
1	A	459	ASP
1	A	461	LYS
1	A	467	GLU
1	A	474	ILE
1	A	484	ASN
1	A	487	VAL
1	A	496	MET
1	A	498	LYS
1	A	515	GLU
1	A	523	LEU
1	A	526	GLU
1	A	528	LYS
1	A	533	THR
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	561	VAL
1	A	583	ASP
1	A	584	GLU
1	A	601	LYS
1	A	610	LYS
1	A	628	LYS
1	A	631	ASP

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Mol	Chain	Res	Type
1	A	637	TRP
1	A	642	ILE
2	B	34	ARG
2	B	37	THR
2	B	42	ARG
2	B	46	GLU
2	B	47	GLU
2	B	53	LYS
2	B	54	LEU
2	B	59	VAL
2	B	63	LYS
2	B	69	LEU
2	B	75	ILE
2	B	87	ARG
2	B	90	ARG
2	B	93	ILE
2	B	100	ASN
2	B	106	THR
2	B	116	ASN
2	B	120	THR
2	B	122	LYS
2	B	128	HIS
2	B	129	MET
2	B	148	SER
2	B	156	LYS
2	B	157	THR
2	B	159	ILE
2	B	161	LEU
2	B	164	LYS
2	B	165	GLN
2	B	166	GLN
2	B	170	ILE
2	B	173	GLN
2	B	176	LEU
2	B	184	LEU
2	B	209	MET
2	B	210	GLN
2	B	213	ARG
2	B	215	ILE
2	B	235	SER
2	B	238	LYS
2	B	241	THR

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Mol	Chain	Res	Type
2	B	247	LYS
2	B	266	LEU
2	B	268	LYS
2	B	269	MET
2	B	276	LEU
2	B	281	ASN
3	C	34	GLU
3	C	50	ARG
3	C	53	LYS
3	C	60	LEU
3	C	61	THR
3	C	67	MET
3	C	76	ARG
3	C	87	LEU
3	C	94	SER
3	C	98	LEU
3	C	99	ASP
3	C	107	ILE
3	C	115	VAL
3	C	133	LEU
3	C	149	ILE
3	C	160	LEU
3	C	162	LEU
3	C	172	VAL
3	C	175	ARG
3	C	177	GLU
4	D	49	PHE
4	D	50	LYS
4	D	57	THR
4	D	58	LEU
4	D	61	ILE
4	D	79	ILE
4	D	90	LEU
4	D	92	LEU
4	D	109	ARG
4	D	112	VAL
4	D	116	THR
4	D	122	ARG
4	D	123	VAL
4	D	136	LEU
4	D	144	VAL
4	D	154	TRP

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Mol	Chain	Res	Type
4	D	156	LEU
1	E	34	GLN
1	E	36	LYS
1	E	39	ASP
1	E	44	VAL
1	E	76	THR
1	E	117	ASN
1	E	142	ARG
1	E	153	PHE
1	E	162	LYS
1	E	179	SER
1	E	194	THR
1	E	203	ASP
1	E	205	LEU
1	E	230	LYS
1	E	265	ILE
1	E	274	GLN
1	E	283	VAL
1	E	302	GLU
1	E	313	LYS
1	E	319	SER
1	E	335	ARG
1	E	337	VAL
1	E	351	LEU
1	E	356	LEU
1	E	358	GLN
1	E	359	ARG
1	E	360	LEU
1	E	363	ILE
1	E	368	LYS
1	E	377	LYS
1	E	390	MET
1	E	406	LYS
1	E	411	LYS
1	E	422	CYS
1	E	425	HIS
1	E	426	SER
1	E	436	ASN
1	E	440	ASP
1	E	453	LYS
1	E	454	GLU
1	E	456	LEU

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Mol	Chain	Res	Type
1	E	461	LYS
1	E	474	ILE
1	E	484	ASN
1	E	487	VAL
1	E	496	MET
1	E	498	LYS
1	E	511	ASP
1	E	515	GLU
1	E	527	LEU
1	E	528	LYS
1	E	530	LEU
1	E	547	LEU
1	E	577	ASP
1	E	584	GLU
1	E	596	LYS
1	E	597	ARG
1	E	610	LYS
1	E	620	LEU
1	E	637	TRP
1	E	642	ILE
2	F	34	ARG
2	F	37	THR
2	F	63	LYS
2	F	66	THR
2	F	69	LEU
2	F	75	ILE
2	F	87	ARG
2	F	90	ARG
2	F	93	ILE
2	F	100	ASN
2	F	116	ASN
2	F	117	THR
2	F	119	LYS
2	F	122	LYS
2	F	129	MET
2	F	148	SER
2	F	150	GLN
2	F	157	THR
2	F	158	LYS
2	F	163	GLU
2	F	170	ILE
2	F	173	GLN

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Mol	Chain	Res	Type
2	F	176	LEU
2	F	184	LEU
2	F	192	CYS
2	F	209	MET
2	F	213	ARG
2	F	215	ILE
2	F	231	GLN
2	F	232	ASP
2	F	238	LYS
2	F	241	THR
2	F	244	ASN
2	F	247	LYS
2	F	248	THR
2	F	266	LEU
2	F	268	LYS
2	F	276	LEU
2	F	278	THR
2	F	281	ASN
3	G	34	GLU
3	G	50	ARG
3	G	53	LYS
3	G	67	MET
3	G	76	ARG
3	G	91	VAL
3	G	106	PHE
3	G	108	ARG
3	G	133	LEU
3	G	149	ILE
3	G	160	LEU
3	G	162	LEU
3	G	165	LEU
3	G	172	VAL
3	G	175	ARG
3	G	177	GLU
4	H	46	GLU
4	H	50	LYS
4	H	57	THR
4	H	58	LEU
4	H	64	TYR
4	H	73	ILE
4	H	79	ILE
4	H	84	MET

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Mol	Chain	Res	Type
4	H	86	LEU
4	H	109	ARG
4	H	117	LEU
4	H	122	ARG
4	H	123	VAL
4	H	154	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	125	ASN
1	A	150	GLN
1	A	252	ASN
1	A	349	HIS
1	A	355	GLN
1	A	389	ASN
1	A	431	ASN
1	A	436	ASN
1	A	451	ASN
1	A	497	GLN
1	A	503	HIS
1	A	550	GLN
1	A	551	ASN
1	A	573	HIS
1	A	594	GLN
1	A	606	HIS
2	B	44	ASN
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	115	GLN
2	B	116	ASN
2	B	145	GLN
2	B	165	GLN
2	B	166	GLN
2	B	173	GLN
2	B	240	HIS
2	B	244	ASN

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Mol	Chain	Res	Type
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	150	GLN
1	E	159	ASN
1	E	252	ASN
1	E	349	HIS
1	E	355	GLN
1	E	431	ASN
1	E	436	ASN
1	E	451	ASN
1	E	497	GLN
1	E	503	HIS
1	E	550	GLN
1	E	551	ASN
1	E	555	ASN
1	E	565	ASN
1	E	573	HIS
1	E	606	HIS
2	F	100	ASN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	140	ASN
2	F	145	GLN
2	F	150	GLN
2	F	165	GLN
2	F	168	GLN
2	F	244	ASN
2	F	281	ASN
3	G	66	GLN
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	1.26	4 (8%)	54,89,89	2.40	13 (24%)
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	2.12	10 (33%)	24,82,82	2.49	11 (45%)
11	RQX	C	202	-	19,19,19	2.27	3 (15%)	21,26,26	2.24	5 (23%)
12	EPH	D	201	-	42,43,48	1.95	8 (19%)	43,48,53	2.68	9 (20%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	1	48,58,58	1.46	6 (12%)	54,89,89	2.59	12 (22%)
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	2.09	6 (20%)	24,82,82	2.39	8 (33%)
11	RQX	G	202	-	19,19,19	2.47	2 (10%)	21,26,26	1.83	4 (19%)
12	EPH	H	201	-	42,43,48	1.95	9 (21%)	43,48,53	2.60	7 (16%)

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	RQX	C	202	-	-	0/10/34/34	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
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	RQX	G	202	-	-	0/10/34/34	0/1/1/1
12	EPH	H	201	-	-	0/47/47/52	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	C3B-C4B	-7.97	1.44	1.51
10	C	201	HEM	C3B-C4B	-7.29	1.45	1.51
10	C	201	HEM	C3D-C4D	-3.93	1.46	1.51
12	D	201	EPH	C18-C4	-3.92	1.38	1.50
12	D	201	EPH	C27-C28	-3.82	1.33	1.50
12	H	201	EPH	C27-C28	-3.74	1.33	1.50
12	H	201	EPH	C18-C4	-3.68	1.39	1.50
10	G	201	HEM	C3D-C4D	-3.63	1.46	1.51
10	G	201	HEM	C2C-C1C	-3.22	1.46	1.52
10	C	201	HEM	C2C-C1C	-2.87	1.47	1.52
12	H	201	EPH	C10-C11	-2.37	1.43	1.52
6	E	702	FAD	O4B-C4B	-2.22	1.39	1.45
10	C	201	HEM	C2D-C1D	-2.06	1.45	1.51
10	C	201	HEM	C2B-C1B	-2.05	1.45	1.51
10	G	201	HEM	C2D-C1D	-2.05	1.45	1.51
10	C	201	HEM	C3C-CAC	2.08	1.55	1.51
10	C	201	HEM	CAA-C2A	2.13	1.55	1.52
10	G	201	HEM	FE-ND	2.17	2.08	1.97
10	C	201	HEM	C4C-NC	2.27	1.38	1.36
11	C	202	RQX	C3-C4	2.28	1.52	1.46
6	E	702	FAD	C5X-N5	2.32	1.39	1.35
6	E	702	FAD	C1'-N10	2.41	1.50	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	201	EPH	P1-O7	2.61	1.60	1.51
6	A	702	FAD	C2A-N1A	2.81	1.39	1.33
10	C	201	HEM	FE-ND	2.83	2.12	1.97
12	H	201	EPH	P1-O7	2.89	1.61	1.51
10	G	201	HEM	C1C-NC	2.98	1.39	1.36
10	C	201	HEM	C1C-NC	3.05	1.39	1.36
6	A	702	FAD	C4-N3	3.17	1.39	1.33
12	H	201	EPH	C15-C16	3.24	1.53	1.29
12	D	201	EPH	C26-C25	3.27	1.64	1.50
12	H	201	EPH	C26-C25	3.28	1.64	1.50
12	D	201	EPH	C15-C16	3.35	1.54	1.29
12	D	201	EPH	C25-C24	3.64	1.52	1.31
6	A	702	FAD	C4X-N5	3.72	1.39	1.33
12	D	201	EPH	C13-C12	3.75	1.53	1.31
6	E	702	FAD	C2A-N3A	3.76	1.38	1.32
6	E	702	FAD	C4-N3	3.81	1.40	1.33
12	H	201	EPH	C13-C12	3.83	1.53	1.31
12	H	201	EPH	C25-C24	3.93	1.54	1.31
6	A	702	FAD	C2A-N3A	4.03	1.39	1.32
6	E	702	FAD	C4X-N5	4.63	1.40	1.33
11	C	202	RQX	C3-C2	5.10	1.47	1.35
11	G	202	RQX	C3-C2	6.15	1.49	1.35
12	H	201	EPH	C29-C28	6.80	1.71	1.31
12	D	201	EPH	C29-C28	6.97	1.72	1.31
11	C	202	RQX	C6-C5	7.40	1.50	1.39
11	G	202	RQX	C6-C5	7.58	1.50	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	N3A-C2A-N1A	-12.14	119.60	128.89
6	A	702	FAD	N3A-C2A-N1A	-11.79	119.87	128.89
6	E	702	FAD	P-O3P-PA	-5.24	118.02	132.73
10	G	201	HEM	C3C-CAC-CBC	-4.22	117.98	124.46
11	C	202	RQX	C1-C2-C3	-4.06	115.42	124.10
6	E	702	FAD	O2'-C2'-C3'	-3.91	99.19	109.02
6	E	702	FAD	C4X-C4-N3	-3.86	118.31	123.59
6	A	702	FAD	P-O3P-PA	-3.48	122.96	132.73
10	G	201	HEM	C3B-CAB-CBB	-3.22	119.51	124.46
10	C	201	HEM	C3B-CAB-CBB	-3.12	119.67	124.46
10	C	201	HEM	CAA-C2A-C1A	-3.12	123.62	127.01
12	D	201	EPH	C30-C29-C28	-3.11	112.86	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	201	HEM	C3C-CAC-CBC	-3.06	119.77	124.46
6	A	702	FAD	O3B-C3B-C4B	-2.88	102.42	111.05
6	A	702	FAD	C2B-C1B-N9A	-2.86	109.92	114.29
12	H	201	EPH	C30-C29-C28	-2.77	114.41	127.06
6	A	702	FAD	C4X-C4-N3	-2.76	119.81	123.59
10	C	201	HEM	CBA-CAA-C2A	-2.68	107.73	112.53
11	G	202	RQX	C1-C2-C3	-2.57	118.59	124.10
10	C	201	HEM	CMA-C3A-C4A	-2.57	124.11	128.36
6	E	702	FAD	C9A-C5X-N5	-2.56	118.56	122.36
11	C	202	RQX	C5-C6-N	-2.54	119.45	125.40
6	A	702	FAD	O2'-C2'-C3'	-2.47	102.80	109.02
11	G	202	RQX	C2-C3-C4	-2.09	117.74	120.12
12	D	201	EPH	C26-C25-C24	-2.08	110.84	125.34
6	A	702	FAD	C9A-C5X-N5	-2.08	119.28	122.36
6	E	702	FAD	C4A-C5A-N7A	-2.06	107.58	109.48
12	H	201	EPH	O5-P1-O7	-2.02	101.79	109.62
10	G	201	HEM	CBD-CAD-C3D	2.04	119.51	113.55
6	A	702	FAD	O3P-P-O5'	2.07	108.42	102.94
6	A	702	FAD	O2B-C2B-C3B	2.09	118.64	111.83
12	D	201	EPH	C10-C11-C12	2.11	123.50	112.45
11	G	202	RQX	C10-C9-C3	2.17	118.16	111.64
12	D	201	EPH	C1-O2-C4	2.21	123.02	116.85
6	E	702	FAD	C6-C5X-N5	2.24	121.85	118.96
11	C	202	RQX	C7-C6-N	2.28	120.79	114.74
12	D	201	EPH	O2-C4-C18	2.28	118.85	111.90
10	C	201	HEM	CBD-CAD-C3D	2.31	120.27	113.55
6	E	702	FAD	C1'-C2'-C3'	2.59	117.23	109.82
10	C	201	HEM	CMD-C2D-C3D	2.65	126.08	114.35
12	H	201	EPH	O2-C4-C18	2.74	120.24	111.90
10	G	201	HEM	CMD-C2D-C3D	2.75	126.52	114.35
6	A	702	FAD	O3'-C3'-C4'	2.87	115.98	108.75
6	E	702	FAD	C4-C4X-N5	3.00	122.36	118.72
11	C	202	RQX	C12-C11-C13	3.08	120.11	115.41
10	G	201	HEM	CAD-C3D-C2D	3.40	122.98	113.22
12	H	201	EPH	C2-O1-C3	3.51	126.31	117.89
6	E	702	FAD	C5X-C9A-N10	3.59	120.35	117.62
10	C	201	HEM	CAD-C3D-C2D	3.59	123.54	113.22
10	C	201	HEM	CMB-C2B-C3B	3.62	125.56	116.53
6	A	702	FAD	C4-C4X-N5	3.63	123.13	118.72
10	C	201	HEM	CMC-C2C-C3C	3.86	126.17	116.53
10	G	201	HEM	CMC-C2C-C3C	3.87	126.18	116.53
10	G	201	HEM	CMB-C2B-C3B	3.87	126.19	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	C14-C15-C16	4.03	149.90	125.00
6	A	702	FAD	C4X-N5-C5X	4.21	121.61	116.76
6	E	702	FAD	C4X-N5-C5X	4.28	121.68	116.76
12	D	201	EPH	C14-C15-C16	4.40	152.22	125.00
6	A	702	FAD	C4-N3-C2	5.23	119.77	115.25
11	G	202	RQX	C9-C3-C4	5.67	125.23	118.56
10	G	201	HEM	CAD-C3D-C4D	5.83	133.04	112.47
10	C	201	HEM	CAD-C3D-C4D	5.95	133.47	112.47
12	D	201	EPH	C2-O1-C3	6.22	132.81	117.89
6	E	702	FAD	C4-N3-C2	6.93	121.24	115.25
11	C	202	RQX	C9-C3-C4	6.97	126.75	118.56
12	D	201	EPH	C15-C14-C13	8.16	139.13	112.00
12	H	201	EPH	C15-C14-C13	8.16	139.16	112.00
12	D	201	EPH	C27-C26-C25	11.40	143.60	112.86
12	H	201	EPH	C27-C26-C25	11.97	145.13	112.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	MLI	2	0
6	A	702	FAD	7	0
7	B	301	FES	1	0
8	B	302	SF4	1	0
10	C	201	HEM	15	0
11	C	202	RQX	8	0
12	D	201	EPH	6	0
6	E	702	FAD	10	0
10	G	201	HEM	9	0
11	G	202	RQX	6	0
12	H	201	EPH	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	613/645 (95%)	0.44	90 (14%) 3 2	71, 96, 118, 136	0
1	E	613/645 (95%)	0.23	64 (10%) 8 4	70, 90, 113, 126	0
2	B	249/282 (88%)	0.17	26 (10%) 8 4	72, 89, 117, 137	0
2	F	249/282 (88%)	0.46	37 (14%) 3 2	67, 86, 109, 120	0
3	C	153/188 (81%)	0.21	10 (6%) 22 13	78, 97, 142, 162	0
3	G	150/188 (79%)	0.62	28 (18%) 2 1	77, 100, 151, 156	0
4	D	129/156 (82%)	0.19	11 (8%) 13 6	89, 101, 129, 142	0
4	H	129/156 (82%)	0.17	10 (7%) 16 8	86, 103, 133, 146	0
All	All	2285/2542 (89%)	0.32	276 (12%) 6 3	67, 94, 124, 162	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	PRO	9.9
4	D	49	PHE	7.4
3	G	115	VAL	6.5
3	C	183	THR	6.3
3	G	112	ILE	6.3
3	G	110	LEU	6.2
1	A	645	TYR	6.2
1	E	537	LEU	6.2
3	G	116	ILE	6.0
1	A	154	GLY	5.9
3	G	113	PRO	5.7
3	G	107	ILE	5.7
2	F	89	CYS	5.4
3	C	182	ALA	5.3
1	A	237	GLY	5.3
1	E	103	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
4	H	78	PHE	5.2
2	F	88	SER	5.1
1	E	538	ILE	5.1
3	G	168	LEU	5.0
1	A	313	LYS	5.0
2	F	94	CYS	5.0
3	C	186	THR	4.8
3	G	106	PHE	4.8
1	E	355	GLN	4.6
1	A	421	GLU	4.6
1	A	599	PHE	4.6
1	A	158	ASN	4.4
1	A	465	LEU	4.4
4	H	52	LEU	4.4
2	F	281	ASN	4.3
3	G	111	GLY	4.2
1	A	155	GLY	4.2
3	G	103	PHE	4.2
1	E	88	ASN	4.2
2	B	89	CYS	4.2
1	A	422	CYS	4.1
1	E	249	ALA	4.1
2	F	276	LEU	4.1
2	B	94	CYS	4.0
1	A	164	GLY	4.0
1	E	119	MET	4.0
1	A	474	ILE	4.0
1	A	515	GLU	3.9
1	A	472	GLU	3.9
2	B	163	GLU	3.9
1	E	33	ALA	3.9
3	G	102	THR	3.8
1	A	238	GLY	3.8
1	A	317	LEU	3.8
1	E	352	PRO	3.8
1	A	437	SER	3.7
1	A	420	GLY	3.7
1	E	459	ASP	3.7
2	F	83	LEU	3.7
1	A	179	SER	3.7
1	A	514	ALA	3.7
3	G	114	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	269	MET	3.7
1	A	247	THR	3.7
1	E	86	GLY	3.7
2	B	88	SER	3.6
2	F	96	SER	3.6
1	A	246	CYS	3.6
1	E	122	LEU	3.6
1	A	79	HIS	3.6
4	D	115	ASP	3.6
1	A	96	PRO	3.6
1	A	477	LEU	3.5
2	F	57	PHE	3.5
3	C	179	HIS	3.5
2	F	46	GLU	3.5
1	E	250	HIS	3.5
1	A	252	ASN	3.5
4	D	52	LEU	3.5
2	F	92	GLY	3.5
1	A	560	ILE	3.4
2	B	183	ILE	3.4
1	E	123	THR	3.4
2	F	97	CYS	3.3
2	B	199	ALA	3.3
4	H	46	GLU	3.3
1	A	590	PRO	3.3
1	A	596	LYS	3.3
3	G	176	TRP	3.3
2	F	271	THR	3.3
2	F	95	GLY	3.3
1	E	251	MET	3.3
1	E	117	ASN	3.2
1	A	464	GLU	3.2
1	E	81	THR	3.2
2	B	95	GLY	3.2
3	C	34	GLU	3.2
4	H	111	PHE	3.2
1	E	102	HIS	3.2
2	F	274	ALA	3.2
1	E	246	CYS	3.2
2	F	164	LYS	3.2
3	G	157	TYR	3.2
3	G	105	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLN	3.1
1	E	444	PHE	3.1
1	E	118	ALA	3.1
2	F	279	PRO	3.1
1	A	80	THR	3.1
1	E	76	THR	3.1
1	A	547	LEU	3.1
3	G	117	LEU	3.1
1	A	248	THR	3.1
4	D	116	THR	3.1
2	B	96	SER	3.1
1	E	507	PHE	3.1
1	A	249	ALA	3.1
4	H	115	ASP	3.1
3	G	172	VAL	3.1
1	A	544	THR	3.1
2	F	79	VAL	3.1
1	E	642	ILE	3.1
1	E	35	TYR	3.1
1	A	165	VAL	3.1
1	E	78	SER	3.1
1	A	162	LYS	3.1
4	H	113	LEU	3.1
1	A	591	ILE	3.0
1	A	613	PRO	3.0
1	A	592	GLU	3.0
2	F	39	GLU	3.0
1	A	207	ASP	3.0
1	A	81	THR	3.0
1	A	391	GLY	3.0
1	A	389	ASN	3.0
3	G	98	LEU	3.0
2	F	163	GLU	3.0
2	F	185	CYS	3.0
4	D	113	LEU	3.0
2	B	270	LYS	2.9
1	E	238	GLY	2.9
1	A	469	ALA	2.9
1	E	156	GLN	2.9
2	F	91	GLU	2.9
3	C	115	VAL	2.9
1	E	644	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	200	PHE	2.9
2	F	56	LYS	2.9
1	A	470	GLY	2.9
1	A	373	VAL	2.8
2	B	212	TYR	2.8
3	G	153	TYR	2.8
1	A	76	THR	2.8
1	A	595	THR	2.8
1	A	473	SER	2.8
1	E	77	ARG	2.8
1	A	82	ALA	2.8
4	H	142	HIS	2.8
1	A	176	THR	2.8
1	E	509	ARG	2.8
2	F	109	CYS	2.8
1	E	87	ILE	2.7
1	A	517	VAL	2.7
1	E	427	VAL	2.7
1	A	350	HIS	2.7
2	F	167	TYR	2.7
2	B	262	ILE	2.7
1	E	629	THR	2.7
1	A	161	GLY	2.7
2	F	84	THR	2.7
2	F	273	PRO	2.7
2	B	93	ILE	2.7
2	B	208	LEU	2.6
1	A	157	SER	2.6
1	A	518	LYS	2.6
2	F	139	MET	2.6
2	B	182	CYS	2.6
4	D	90	LEU	2.6
3	G	109	GLY	2.6
1	E	247	THR	2.6
1	E	248	THR	2.6
3	G	67	MET	2.6
1	E	354	GLU	2.6
2	F	90	ARG	2.6
2	F	55	GLN	2.6
1	A	605	LYS	2.6
1	A	236	THR	2.6
2	B	265	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	43	TRP	2.5
1	A	83	ALA	2.5
1	E	474	ILE	2.5
1	E	614	ARG	2.5
1	A	202	LEU	2.5
2	F	93	ILE	2.5
1	A	419	CYS	2.5
2	F	183	ILE	2.5
4	H	118	ALA	2.5
1	A	589	LYS	2.5
3	G	165	LEU	2.5
2	B	271	THR	2.4
1	E	252	ASN	2.4
1	E	74	PHE	2.4
1	A	348	LEU	2.4
1	E	155	GLY	2.4
3	C	114	TRP	2.4
1	E	397	TYR	2.4
2	B	51	LYS	2.4
3	C	184	LEU	2.4
2	B	215	ILE	2.4
1	A	511	ASP	2.4
1	A	50	GLY	2.3
2	F	40	ILE	2.3
1	A	620	LEU	2.3
1	E	425	HIS	2.3
4	D	117	LEU	2.3
1	A	564	GLU	2.3
1	E	34	GLN	2.3
1	A	602	HIS	2.3
1	E	637	TRP	2.3
1	A	520	MET	2.3
1	A	240	GLY	2.3
2	F	98	ALA	2.3
4	D	65	PHE	2.3
1	E	628	LYS	2.3
1	E	75	PRO	2.3
2	B	202	TYR	2.3
3	G	164	ALA	2.3
1	A	178	HIS	2.3
1	A	598	PRO	2.3
1	A	108	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	365	GLU	2.3
2	B	185	CYS	2.3
1	A	104	TYR	2.2
1	A	585	TYR	2.2
1	A	262	ARG	2.2
3	G	93	PHE	2.2
1	E	536	SER	2.2
3	G	173	TYR	2.2
1	A	163	GLY	2.2
1	A	296	GLY	2.2
4	D	148	ARG	2.2
1	E	641	ILE	2.2
3	G	120	PHE	2.2
4	H	138	TYR	2.2
1	E	294	GLU	2.2
1	E	264	GLY	2.2
2	B	160	ASN	2.2
1	E	197	ILE	2.2
1	E	351	LEU	2.2
2	B	195	TYR	2.2
2	B	272	LYS	2.1
1	E	638	ILE	2.1
1	A	387	HIS	2.1
1	A	561	VAL	2.1
1	E	120	HIS	2.1
1	A	295	GLY	2.1
2	B	216	ILE	2.1
1	A	467	GLU	2.1
1	A	299	VAL	2.1
3	C	95	VAL	2.1
1	E	79	HIS	2.1
2	F	278	THR	2.1
4	H	112	VAL	2.1
1	A	297	PHE	2.1
1	E	170	CYS	2.1
3	G	42	GLY	2.1
1	E	36	LYS	2.1
1	E	589	LYS	2.1
1	E	645	TYR	2.1
2	F	275	PRO	2.1
1	A	78	SER	2.0
1	E	487	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	53	HIS	2.0
1	E	313	LYS	2.0
4	D	29	SER	2.0
2	B	230	MET	2.0
2	F	277	PRO	2.0
1	A	182	HIS	2.0
1	E	456	LEU	2.0
2	F	107	LEU	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
11	RQX	G	202	19/19	0.80	0.35	2.94	120,125,127,127	0
11	RQX	C	202	19/19	0.79	0.29	2.16	113,116,119,119	0
12	EPH	H	201	44/49	0.80	0.34	1.53	97,113,134,135	0
12	EPH	D	201	44/49	0.88	0.24	1.12	94,102,121,122	0
5	MLI	A	701	7/7	0.90	0.32	1.06	102,103,106,106	0
6	FAD	A	702	53/53	0.92	0.40	0.75	77,83,87,89	0
10	HEM	C	201	43/43	0.97	0.20	0.22	89,93,96,98	0
10	HEM	G	201	43/43	0.98	0.19	0.22	92,97,103,106	0
9	F3S	F	303	7/7	0.99	0.18	0.20	82,83,84,87	0
8	SF4	F	302	8/8	0.99	0.22	-0.07	57,61,64,65	0
6	FAD	E	702	53/53	0.96	0.26	-0.12	63,79,88,89	0
8	SF4	B	302	8/8	0.99	0.20	-0.22	63,66,68,70	0
9	F3S	B	303	7/7	0.98	0.15	-0.39	83,85,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MLI	E	701	7/7	0.95	0.21	-0.50	92,93,93,93	0
7	FES	B	301	4/4	1.00	0.27	-0.99	70,70,72,78	0
7	FES	F	301	4/4	0.99	0.29	-2.15	60,66,68,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.