



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 08:30 PM EST

PDB ID : 3VR9
Title : Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode *Ascaris suum* with the specific inhibitor flutolanil
Authors : Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.
Deposited on : unknown
Resolution : 3.01 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

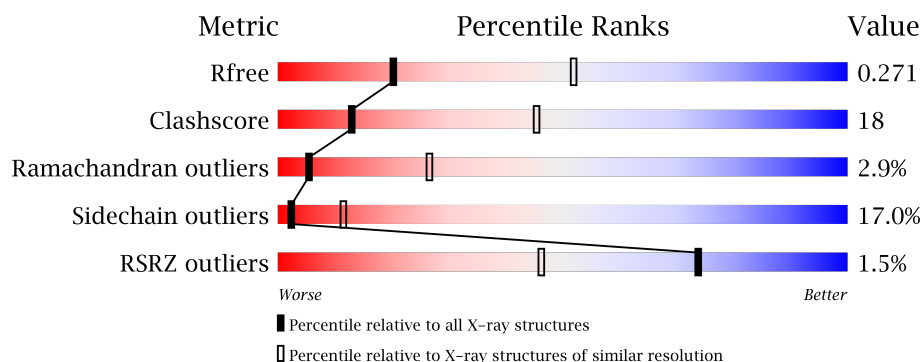
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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>0.5%</div> <div>51% 37% 7% 5%</div> </div>
1	E	645	<div> <div>0.5%</div> <div>53% 37% 5% 5%</div> </div>
2	B	282	<div> <div>0.5%</div> <div>50% 33% 5% 12%</div> </div>
2	F	282	<div> <div>0.5%</div> <div>50% 30% 7% 12%</div> </div>
3	C	188	<div> <div>4%</div> <div>46% 28% 7% 19%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	188	 2% 41% 33% 6% 19%
4	D	156	 1% 48% 28% 5% 17%
4	H	156	 3% 45% 31% 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	FTN	C	202	-	-	-	X
12	EPH	D	201	-	-	-	X
12	EPH	H	201	-	-	-	X
5	MLI	A	701	-	-	X	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			

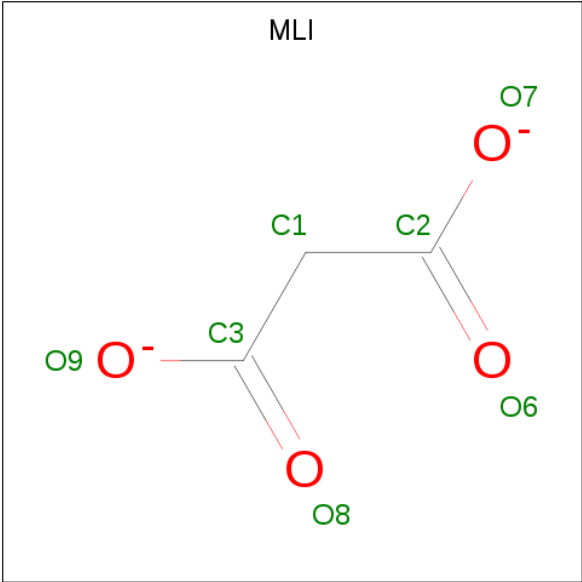
- Molecule 3 is a protein called Cytochrome b-large subunit.

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: C₃H₂O₄).



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: C₂₇H₃₃N₉O₁₅P₂).



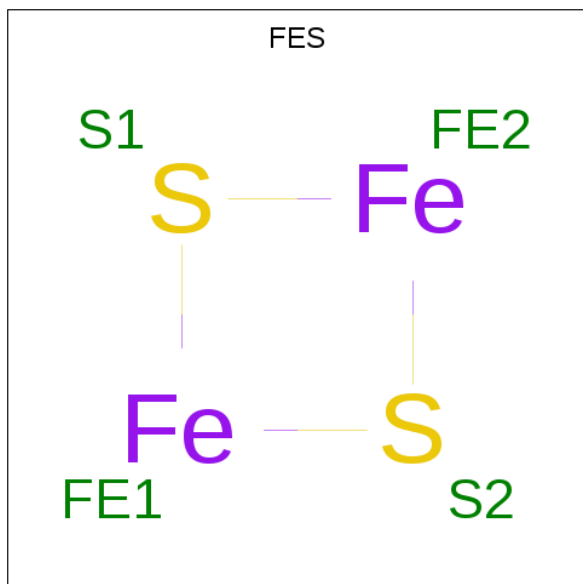
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

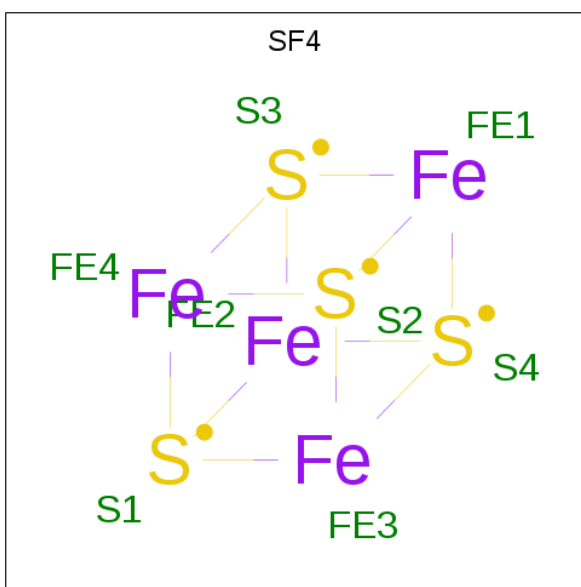
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



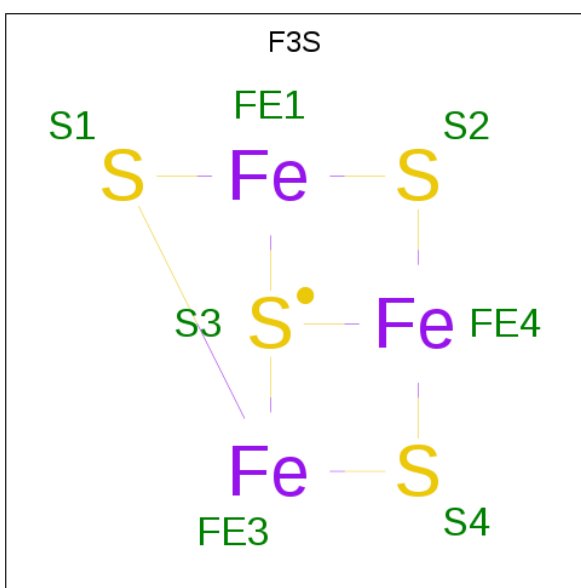
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

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



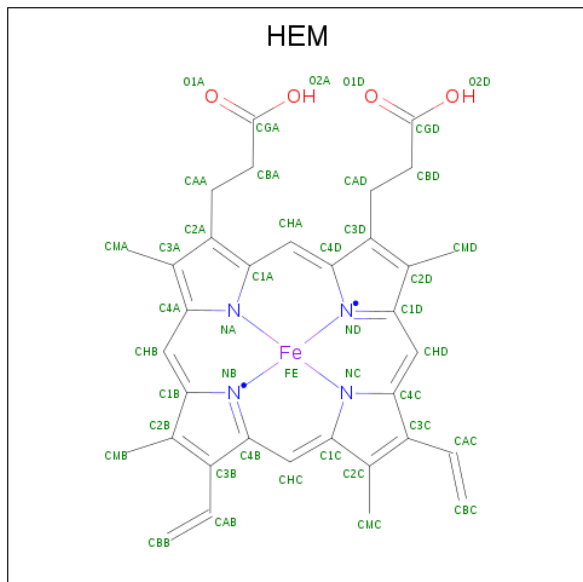
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



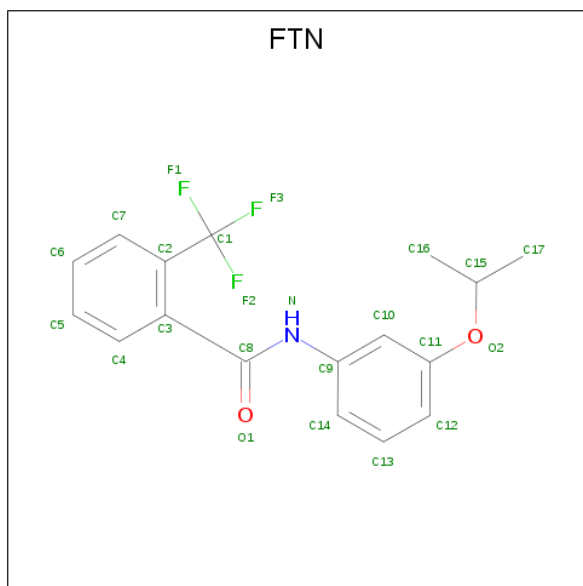
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

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



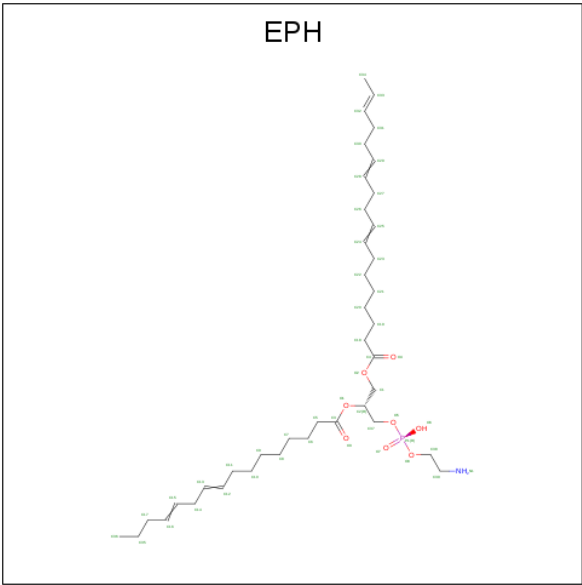
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is N-[3-(1-methylethoxy)phenyl]-2-(trifluoromethyl)benzamide (three-letter code: FTN) (formula: $C_{17}H_{16}F_3NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	F	N	O	0	0
			23	17	3	1	2		
11	F	1	Total	C	F	N	O	0	0
			23	17	3	1	2		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: C₃₉H₆₈NO₈P).

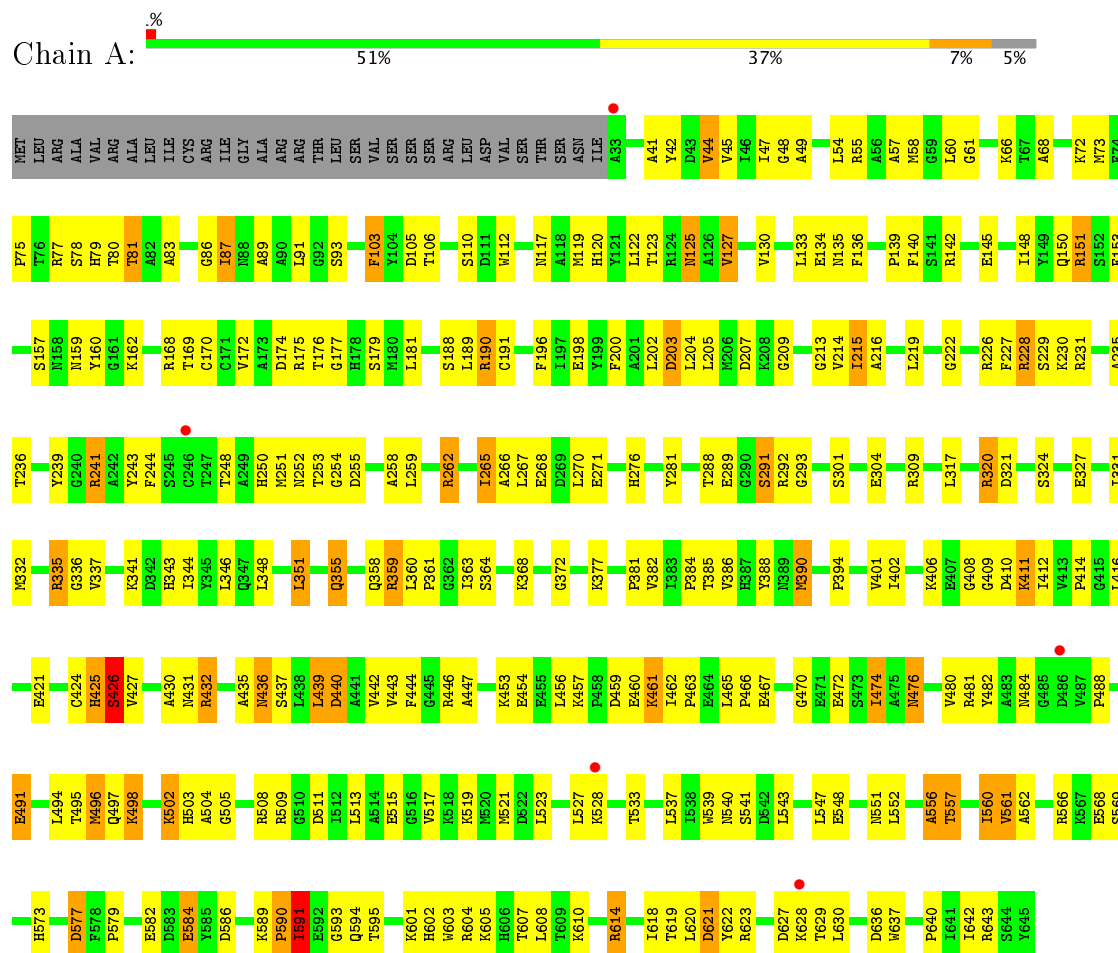


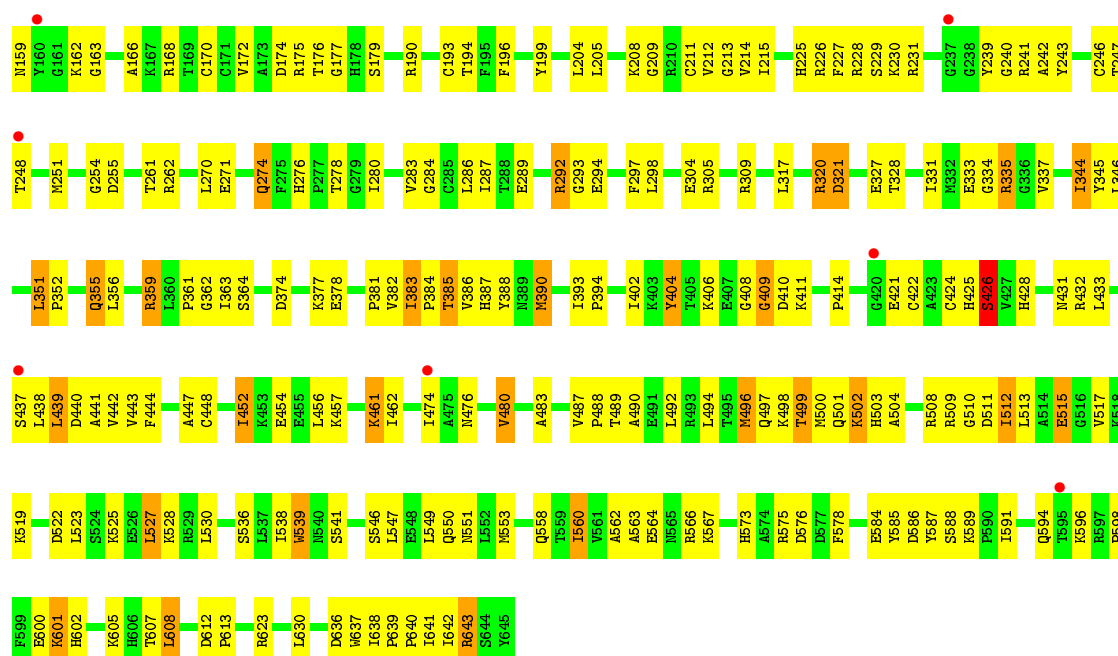
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

3 Residue-property plots

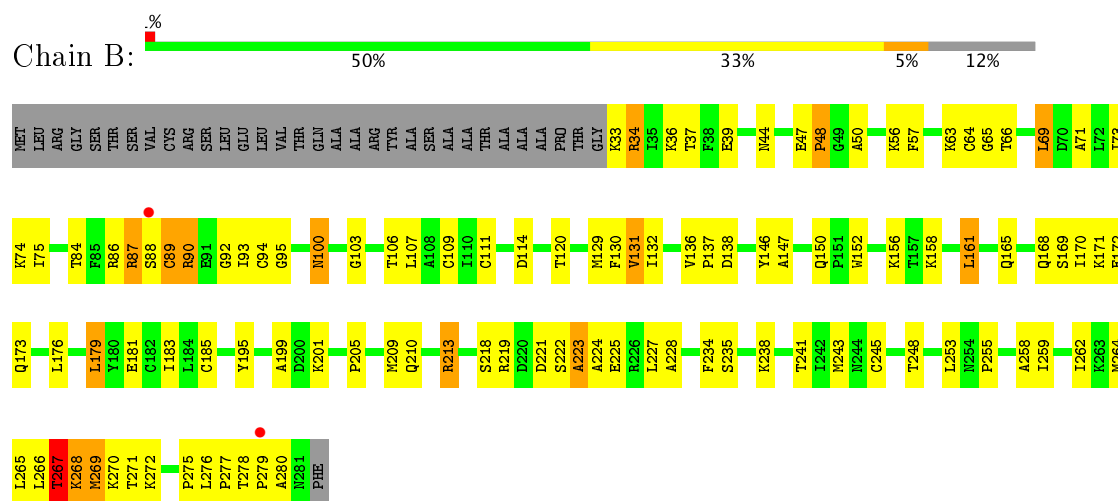
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

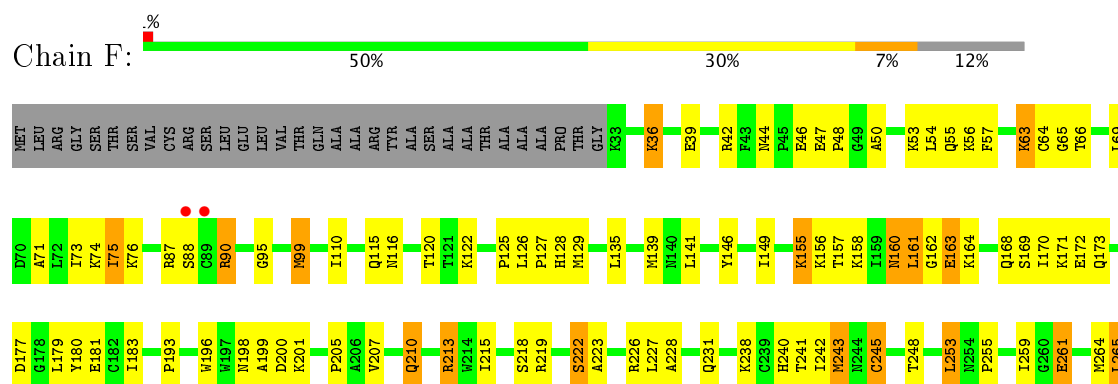




• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

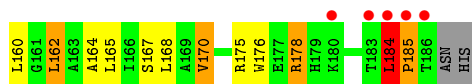
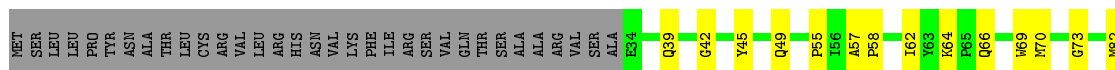


• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

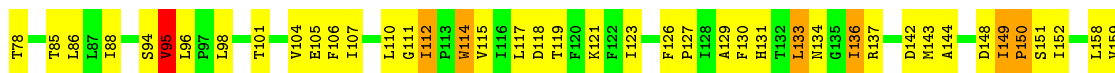
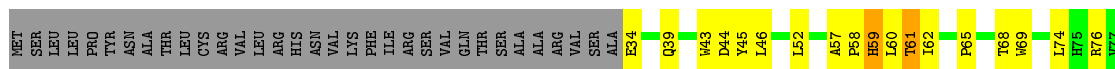




• Molecule 3: Cytochrome b-large subunit



• 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	124.01Å 135.33Å 220.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.39 – 3.01 47.39 – 3.01	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.39-3.01) 92.2 (47.39-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.277 0.214 , 0.271	Depositor DCC
R_{free} test set	3245 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18262	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, FAD, FTN

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	0.61	0/4859	0.74	0/6564
1	E	0.59	0/4859	0.72	0/6564
2	B	0.67	0/2016	0.78	1/2723 (0.0%)
2	F	0.64	0/2016	0.78	0/2723
3	C	0.61	0/1255	0.73	0/1709
3	G	0.65	0/1255	0.78	1/1709 (0.1%)
4	D	0.65	0/1026	0.77	1/1402 (0.1%)
4	H	0.65	0/1026	0.72	0/1402
All	All	0.62	0/18312	0.75	3/24796 (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
1	E	0	1
2	B	0	1
2	F	0	1
4	H	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	156	LEU	CA-CB-CG	5.83	128.70	115.30
3	G	165	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	269	MET	N-CA-C	-5.49	96.18	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	425	HIS	Peptide
2	B	267	THR	Peptide
1	E	425	HIS	Peptide
2	F	267	THR	Peptide
4	H	48	GLY	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	184	0
1	E	4758	0	4692	185	0
2	B	1973	0	1992	74	0
2	F	1973	0	1992	82	0
3	C	1217	0	1265	48	0
3	G	1217	0	1265	53	0
4	D	994	0	977	34	0
4	H	994	0	977	40	0
5	A	7	0	2	2	0
5	E	7	0	2	1	0
6	A	53	0	29	5	0
6	E	53	0	31	9	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	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	13	0
10	G	43	0	30	12	0
11	C	23	0	16	3	0
11	F	23	0	16	2	0
12	D	44	0	53	5	0
12	H	44	0	53	3	0
All	All	18262	0	18114	668	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 18.

All (668) 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:NE2	6:E:702:FAD:HM82	0.96	1.26
1:E:79:HIS:CD2	6:E:702:FAD:HM82	1.88	1.08
4:D:50:LYS:H	4:D:51:PRO:HD2	1.19	1.05
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.36	1.05
10:C:201:HEM:HHA	10:C:201:HEM:HBD1	1.39	1.02
4:D:50:LYS:H	4:D:51:PRO:CD	1.75	0.99
1:A:103:PHE:HA	1:A:123:THR:HG21	1.49	0.91
2:B:86:ARG:HH12	2:B:137:PRO:HD2	1.32	0.91
4:D:50:LYS:N	4:D:51:PRO:HD2	1.85	0.91
10:G:201:HEM:HBA2	10:G:201:HEM:HHA	1.53	0.90
1:A:432:ARG:HH21	1:A:435:ALA:H	1.19	0.89
2:B:262:ILE:HG22	2:B:266:LEU:CD2	2.03	0.88
2:B:267:THR:HB	2:B:268:LYS:HG3	1.56	0.88
1:E:320:ARG:HH12	5:E:701:MLI:C2	1.86	0.87
3:G:112:ILE:HB	3:G:117:LEU:HD11	1.55	0.87
3:C:149:ILE:HD13	3:C:149:ILE:H	1.38	0.86
2:B:223:ALA:O	2:B:227:LEU:HD12	1.75	0.86
3:G:148:ASP:OD2	3:G:150:PRO:HG2	1.75	0.86
2:B:267:THR:HG21	4:D:60:LYS:HB2	1.56	0.85
2:B:213:ARG:O	2:B:213:ARG:HD3	1.77	0.85
2:F:160:ASN:HB3	2:F:163:GLU:HB2	1.60	0.82
4:D:108:GLY:O	4:D:122:ARG:NH2	2.13	0.82
1:A:614:ARG:HH11	1:A:614:ARG:HB2	1.45	0.81
3:G:58:PRO:HB2	3:G:62:ILE:HG12	1.62	0.81
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.62	0.81
2:B:71:ALA:O	2:B:75:ILE:HG23	1.81	0.81
1:E:93:SER:H	1:E:150:GLN:HE22	1.29	0.80
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.63	0.80
2:F:181:GLU:HB2	2:F:253:LEU:HD21	1.63	0.80
1:E:502:LYS:HD3	1:E:503:HIS:CE1	2.16	0.80
2:F:71:ALA:O	2:F:75:ILE:HG23	1.83	0.79
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.64	0.79
1:A:614:ARG:HB2	1:A:614:ARG:NH1	1.99	0.78
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.66	0.78
3:C:175:ARG:O	3:C:175:ARG:HG3	1.84	0.78
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.58	0.77
2:B:262:ILE:HG22	2:B:266:LEU:HD21	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLU:HA	2:B:228:ALA:HB3	1.67	0.76
1:E:122:LEU:HD11	1:E:439:LEU:HB3	1.65	0.76
1:A:557:THR:O	1:A:560:ILE:HG22	1.86	0.76
1:A:388:TYR:CE1	1:A:421:GLU:HG3	2.21	0.76
4:D:67:ALA:O	4:D:70:VAL:HG23	1.85	0.76
3:G:123:ILE:O	3:G:127:PRO:HD2	1.84	0.76
1:A:432:ARG:NH2	1:A:435:ALA:H	1.85	0.75
2:F:278:THR:HB	2:F:279:PRO:CD	2.16	0.75
1:E:205:LEU:HB3	1:E:212:VAL:HG23	1.69	0.74
1:E:209:GLY:O	1:E:414:PRO:HD2	1.86	0.74
2:B:86:ARG:NH1	2:B:137:PRO:HD2	2.02	0.74
2:F:278:THR:HB	2:F:279:PRO:HD3	1.69	0.74
2:F:276:LEU:HD23	2:F:277:PRO:HD2	1.68	0.73
4:H:101:TRP:O	4:H:105:ASN:HB2	1.89	0.73
2:B:172:GLU:OE2	2:B:275:PRO:HD2	1.90	0.72
2:B:64:CYS:HB2	2:B:74:LYS:HE2	1.72	0.71
1:E:321:ASP:HB3	1:E:431:ASN:ND2	2.04	0.71
1:A:508:ARG:NH1	1:A:573:HIS:HD2	1.89	0.71
2:F:99:MET:CE	2:F:135:LEU:HD13	2.21	0.71
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.21	0.71
1:A:81:THR:HB	1:A:181:LEU:HD23	1.73	0.70
2:F:223:ALA:O	2:F:227:LEU:HD12	1.91	0.70
2:B:213:ARG:C	2:B:213:ARG:HD3	2.11	0.70
1:A:268:GLU:HB2	1:A:394:PRO:HG3	1.74	0.70
1:A:239:TYR:HB3	1:A:254:GLY:HA3	1.73	0.70
2:B:146:TYR:HE1	2:B:210:GLN:HG2	1.57	0.70
1:E:93:SER:H	1:E:150:GLN:NE2	1.89	0.70
1:A:91:LEU:HD23	1:A:127:VAL:CG1	2.22	0.70
4:H:104:VAL:HG21	4:H:121:VAL:O	1.91	0.70
4:D:77:TYR:HA	12:D:201:EPH:H11	1.74	0.69
1:E:120:HIS:HD2	1:E:630:LEU:HB2	1.57	0.69
1:A:327:GLU:OE2	1:A:384:PRO:HD3	1.91	0.69
2:B:47:GLU:HB3	2:B:50:ALA:HB2	1.74	0.69
4:H:69:MET:HE1	4:H:95:HIS:HB2	1.74	0.69
1:A:174:ASP:CB	1:A:361:PRO:HD2	2.22	0.69
1:E:476:ASN:O	1:E:480:VAL:HG23	1.93	0.69
3:C:158:LEU:O	3:C:162:LEU:HB2	1.92	0.69
1:E:280:ILE:HD11	1:E:287:ILE:HD11	1.75	0.69
2:F:99:MET:HE1	2:F:135:LEU:HD13	1.75	0.68
2:F:215:ILE:HG22	2:F:226:ARG:HD2	1.76	0.68
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:LEU:O	1:A:621:ASP:HB2	1.94	0.68
3:C:82:MET:HB2	10:C:201:HEM:HAC	1.74	0.68
2:F:172:GLU:OE2	2:F:275:PRO:HD2	1.92	0.68
1:A:267:LEU:HD12	1:A:270:LEU:HD11	1.76	0.67
1:A:265:ILE:HG22	1:A:266:ALA:O	1.94	0.67
1:A:590:PRO:O	1:A:591:ILE:HG22	1.94	0.67
1:E:174:ASP:OD2	1:E:362:GLY:N	2.27	0.67
3:G:133:LEU:HB3	3:G:159:VAL:HG13	1.75	0.67
1:E:280:ILE:CD1	1:E:287:ILE:HD11	2.25	0.67
1:A:133:LEU:HA	1:A:136:PHE:CD2	2.29	0.67
3:C:126:PHE:HB3	3:C:127:PRO:HD3	1.77	0.67
1:A:561:VAL:HG11	1:A:618:ILE:HD12	1.75	0.66
1:E:142:ARG:HG2	2:F:168:GLN:O	1.96	0.66
3:C:149:ILE:CD1	3:C:149:ILE:H	2.07	0.66
1:A:120:HIS:HD2	1:A:630:LEU:H	1.42	0.66
3:C:66:GLN:O	3:C:70:MET:HG3	1.95	0.65
10:G:201:HEM:HBB2	4:H:69:MET:HB3	1.79	0.65
1:A:508:ARG:NH1	1:A:573:HIS:CD2	2.64	0.65
2:B:234:PHE:CD1	2:B:238:LYS:HG3	2.32	0.65
1:E:428:HIS:HB3	1:E:432:ARG:HA	1.78	0.65
1:E:156:GLN:HB3	1:E:166:ALA:HB3	1.78	0.64
2:B:205:PRO:HA	2:B:259:ILE:HD11	1.80	0.64
4:D:107:TYR:O	4:D:109:ARG:HG2	1.96	0.64
3:C:134:ASN:O	3:C:137:ARG:HB3	1.97	0.63
2:B:267:THR:HB	2:B:268:LYS:CG	2.26	0.63
1:A:276:HIS:O	1:A:384:PRO:HA	1.97	0.63
2:B:213:ARG:C	2:B:213:ARG:CD	2.67	0.63
3:C:133:LEU:HB3	3:C:159:VAL:HG22	1.81	0.63
1:E:510:GLY:HA2	1:E:575:ARG:NH1	2.12	0.63
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.80	0.63
1:E:584:GLU:HG3	1:E:602:HIS:CE1	2.34	0.63
1:E:586:ASP:OD1	1:E:588:SER:HB3	1.99	0.63
2:B:262:ILE:O	2:B:266:LEU:HD22	1.98	0.63
2:F:146:TYR:HE1	2:F:210:GLN:HG2	1.63	0.63
1:E:174:ASP:HB2	1:E:361:PRO:CD	2.23	0.62
1:A:91:LEU:HD12	1:A:170:CYS:SG	2.39	0.62
1:A:401:VAL:HG21	1:A:416:LEU:HG	1.80	0.62
1:E:321:ASP:HB3	1:E:431:ASN:HD22	1.63	0.62
1:E:41:ALA:HB1	1:E:462:ILE:HG21	1.82	0.62
1:E:117:ASN:HD22	1:E:118:ALA:H	1.48	0.62
1:A:133:LEU:HA	1:A:136:PHE:HD2	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ASP:OD2	3:C:150:PRO:HG2	2.00	0.62
3:G:118:ASP:O	3:G:171:VAL:HG11	2.00	0.62
2:F:170:ILE:HG13	2:F:171:LYS:N	2.15	0.62
1:A:258:ALA:HB1	1:A:262:ARG:NH1	2.15	0.61
10:C:201:HEM:HBB2	10:C:201:HEM:CMB	2.30	0.61
1:A:125:ASN:HD22	1:A:125:ASN:N	1.97	0.61
1:A:412:ILE:O	1:A:414:PRO:HD3	2.00	0.61
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.14	0.61
3:C:175:ARG:HH21	3:C:178:ARG:HH12	1.47	0.61
1:E:541:SER:HB3	2:F:76:LYS:NZ	2.14	0.61
1:E:612:ASP:OD2	1:E:613:PRO:HD2	2.00	0.61
2:F:39:GLU:HG2	2:F:56:LYS:HG3	1.83	0.61
4:H:104:VAL:HG11	4:H:125:ALA:HB2	1.83	0.61
3:G:104:VAL:O	3:G:107:ILE:HG13	2.01	0.61
1:A:228:ARG:NH1	1:A:463:PRO:O	2.34	0.60
2:B:92:GLY:HA2	2:B:109:CYS:SG	2.41	0.60
1:E:527:LEU:HD13	1:E:553:MET:HG2	1.83	0.60
4:H:43:ILE:O	4:H:46:GLU:HB2	2.01	0.60
1:A:541:SER:HB2	2:B:84:THR:HG23	1.82	0.60
4:H:80:HIS:CE1	12:H:201:EPH:H371	2.37	0.60
3:C:69:TRP:CD2	11:C:202:FTN:H15	2.36	0.60
1:A:424:CYS:C	1:A:426:SER:H	2.04	0.60
3:C:86:LEU:HD21	12:D:201:EPH:H231	1.84	0.60
1:E:143:THR:O	1:E:146:GLY:N	2.35	0.60
3:G:76:ARG:HA	10:G:201:HEM:O2D	2.01	0.60
1:E:566:ARG:O	1:E:575:ARG:NH2	2.35	0.60
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.83	0.60
1:E:602:HIS:O	1:E:605:LYS:HE2	2.02	0.59
1:A:189:LEU:CD1	2:B:147:ALA:HB2	2.31	0.59
4:D:118:ALA:HB1	4:D:122:ARG:HH21	1.68	0.59
1:E:133:LEU:HA	1:E:136:PHE:HD2	1.67	0.59
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.37	0.59
1:A:91:LEU:HD23	1:A:127:VAL:HG13	1.83	0.59
1:A:93:SER:H	1:A:150:GLN:NE2	2.00	0.59
2:F:146:TYR:O	2:F:149:ILE:HG12	2.03	0.59
4:D:107:TYR:O	4:D:109:ARG:N	2.35	0.58
1:A:481:ARG:HD3	1:A:482:TYR:CE1	2.38	0.58
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.37	0.58
1:E:286:LEU:HD13	1:E:387:HIS:CE1	2.39	0.58
4:H:118:ALA:HA	4:H:121:VAL:HG22	1.85	0.58
1:A:174:ASP:HB2	1:A:361:PRO:CD	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:SER:HB2	6:E:702:FAD:H1'2	1.86	0.58
2:F:146:TYR:HA	2:F:207:VAL:HG13	1.85	0.58
2:F:267:THR:HG21	4:H:60:LYS:HB2	1.85	0.58
2:B:225:GLU:HA	2:B:228:ALA:CB	2.34	0.58
1:A:584:GLU:OE1	1:A:604:ARG:NH1	2.37	0.58
3:C:86:LEU:HD11	4:D:92:LEU:HD23	1.85	0.58
2:F:245:CYS:HB2	2:F:255:PRO:HG2	1.86	0.58
1:A:432:ARG:HH21	1:A:435:ALA:N	1.96	0.57
1:A:244:PHE:HA	1:A:497:GLN:HE21	1.69	0.57
1:A:189:LEU:HD13	2:B:147:ALA:HB2	1.86	0.57
1:E:510:GLY:CA	1:E:575:ARG:HH11	2.17	0.57
1:E:111:ASP:OD2	1:E:643:ARG:HD2	2.04	0.57
1:E:503:HIS:HE1	1:E:519:LYS:NZ	2.03	0.57
2:B:227:LEU:CD2	2:B:265:LEU:HB3	2.34	0.57
3:C:137:ARG:NH2	3:C:152:ILE:O	2.37	0.57
1:E:111:ASP:CG	1:E:643:ARG:HD2	2.25	0.57
1:E:438:LEU:HG	6:E:702:FAD:C2	2.34	0.57
3:G:149:ILE:H	3:G:149:ILE:HD13	1.68	0.57
3:C:82:MET:HG2	12:D:201:EPH:H271	1.85	0.57
3:G:143:MET:O	3:G:144:ALA:HB3	2.04	0.57
1:E:492:LEU:HB3	1:E:549:LEU:HD21	1.86	0.57
1:A:231:ARG:HE	1:A:456:LEU:HD23	1.70	0.57
2:B:245:CYS:HB2	2:B:255:PRO:HG2	1.87	0.57
1:E:262:ARG:HH12	1:E:551:ASN:ND2	2.02	0.57
1:E:44:VAL:HG21	1:E:60:LEU:CD1	2.35	0.57
4:H:71:PRO:O	4:H:74:PRO:HG2	2.04	0.57
2:B:90:ARG:O	2:B:90:ARG:HG2	2.05	0.57
1:E:591:ILE:O	1:E:594:GLN:HB2	2.05	0.57
1:A:586:ASP:H	1:A:594:GLN:NE2	2.02	0.56
10:C:201:HEM:HMB2	10:C:201:HEM:HBB2	1.86	0.56
2:B:267:THR:CG2	4:D:60:LYS:HB2	2.30	0.56
1:E:352:PRO:HG2	1:E:355:GLN:HE21	1.70	0.56
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.87	0.56
1:E:158:ASN:O	1:E:159:ASN:HB2	2.04	0.56
1:A:304:GLU:OE2	1:A:309:ARG:HD3	2.04	0.56
2:B:64:CYS:SG	2:B:65:GLY:N	2.78	0.56
3:C:45:TYR:CE2	3:C:49:GLN:HG3	2.40	0.56
1:E:243:TYR:OH	1:E:504:ALA:HB3	2.05	0.56
1:A:91:LEU:HD23	1:A:127:VAL:HG12	1.88	0.56
2:F:42:ARG:HG3	2:F:55:GLN:HE21	1.70	0.56
10:G:201:HEM:HBD1	10:G:201:HEM:HBA2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:GLY:O	2:F:219:ARG:NH2	2.38	0.56
1:A:174:ASP:HB3	1:A:361:PRO:HD2	1.86	0.56
11:F:304:FTN:H15	3:G:69:TRP:CD2	2.41	0.56
1:A:135:ASN:ND2	2:B:161:LEU:O	2.38	0.56
2:B:262:ILE:CG2	2:B:266:LEU:HD21	2.34	0.56
10:G:201:HEM:HHA	10:G:201:HEM:CBA	2.32	0.56
1:E:205:LEU:O	1:E:212:VAL:HG22	2.06	0.55
1:A:435:ALA:HA	6:A:702:FAD:O2	2.06	0.55
1:A:582:GLU:HB2	1:A:603:TRP:HB2	1.87	0.55
1:E:461:LYS:HE2	1:E:461:LYS:H	1.71	0.55
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.88	0.55
3:G:149:ILE:N	3:G:150:PRO:HD2	2.21	0.55
1:E:304:GLU:OE2	1:E:309:ARG:HD3	2.05	0.55
1:E:78:SER:O	1:E:81:THR:HG22	2.06	0.55
2:B:44:ASN:HB3	2:B:47:GLU:HB2	1.89	0.55
3:G:126:PHE:HB3	3:G:127:PRO:CD	2.37	0.55
2:B:227:LEU:HD22	2:B:265:LEU:HB3	1.89	0.55
3:C:82:MET:CB	10:C:201:HEM:HAC	2.37	0.55
1:E:278:THR:HG21	1:E:346:LEU:HD22	1.89	0.55
2:F:196:TRP:CZ3	3:G:59:HIS:HB2	2.42	0.55
3:C:105:GLU:C	3:C:107:ILE:H	2.09	0.54
1:E:72:LYS:HE2	1:E:255:ASP:OD2	2.07	0.54
1:E:270:LEU:HD12	1:E:558:GLN:HB3	1.88	0.54
2:B:131:VAL:HG23	3:C:55:PRO:HD2	1.90	0.54
1:E:117:ASN:ND2	1:E:118:ALA:H	2.04	0.54
1:E:42:TYR:O	1:E:229:SER:HA	2.07	0.54
1:E:567:LYS:HG2	1:E:578:PHE:CZ	2.43	0.54
2:F:64:CYS:HB2	2:F:74:LYS:HE2	1.88	0.54
2:B:57:PHE:CG	2:B:75:ILE:HD12	2.42	0.54
3:C:128:ILE:O	3:C:132:THR:OG1	2.26	0.54
1:E:503:HIS:HD2	1:E:512:ILE:O	1.90	0.54
3:G:60:LEU:HD12	3:G:61:THR:N	2.23	0.54
1:E:128:GLU:HG3	2:F:162:GLY:HA3	1.90	0.54
4:H:148:ARG:O	4:H:152:MET:HG3	2.07	0.54
4:D:70:VAL:O	4:D:74:PRO:HD2	2.08	0.53
3:G:142:ASP:OD2	4:H:63:ARG:NH1	2.40	0.53
4:D:108:GLY:HA2	4:D:113:LEU:HD11	1.90	0.53
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.42	0.53
1:E:109:GLY:O	1:E:431:ASN:HB3	2.07	0.53
3:G:105:GLU:C	3:G:107:ILE:H	2.11	0.53
1:A:78:SER:OG	6:A:702:FAD:H51A	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:HA3	1:A:235:ALA:O	2.09	0.53
2:F:47:GLU:O	2:F:50:ALA:HB2	2.08	0.53
1:A:103:PHE:HD1	1:A:123:THR:HG1	1.56	0.53
1:A:72:LYS:HE2	1:A:255:ASP:OD2	2.09	0.53
2:B:195:TYR:O	2:B:199:ALA:HB2	2.09	0.53
4:D:50:LYS:N	4:D:51:PRO:CD	2.49	0.53
1:E:159:ASN:HB2	1:E:163:GLY:H	1.73	0.53
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.90	0.53
1:E:509:ARG:NH1	1:E:511:ASP:OD2	2.41	0.53
4:H:70:VAL:O	4:H:74:PRO:HD2	2.09	0.53
3:G:86:LEU:HD11	4:H:92:LEU:HD23	1.91	0.53
1:A:548:GLU:O	1:A:552:LEU:HD12	2.09	0.53
1:E:50:GLY:HA3	6:E:702:FAD:O1P	2.09	0.53
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.44	0.52
2:F:168:GLN:HG3	2:F:172:GLU:HG3	1.91	0.52
2:F:238:LYS:HE3	4:H:106:ASP:OD2	2.09	0.52
4:H:84:MET:O	4:H:86:LEU:N	2.42	0.52
2:F:42:ARG:HG3	2:F:55:GLN:NE2	2.24	0.52
1:A:336:GLY:HA3	1:A:341:LYS:O	2.09	0.52
2:F:128:HIS:CD2	3:G:59:HIS:CD2	2.98	0.52
1:A:262:ARG:HH12	1:A:551:ASN:ND2	2.08	0.52
3:C:139:ILE:O	3:C:143:MET:HG2	2.08	0.52
3:G:114:TRP:HB2	3:G:175:ARG:HH22	1.75	0.52
1:A:569:SER:HB2	1:A:579:PRO:O	2.10	0.52
1:E:135:ASN:ND2	2:F:161:LEU:O	2.40	0.52
1:A:255:ASP:O	1:A:258:ALA:HB3	2.10	0.52
1:E:298:LEU:HD12	1:E:344:ILE:HD11	1.92	0.52
1:E:73:MET:HB2	1:E:77:ARG:HB2	1.91	0.52
4:D:69:MET:CE	4:D:95:HIS:HB2	2.40	0.52
1:E:293:GLY:N	1:E:317:LEU:HD21	2.25	0.52
1:A:584:GLU:HG3	1:A:602:HIS:CE1	2.45	0.52
3:C:113:PRO:HG2	3:C:116:ILE:HD12	1.92	0.52
1:E:86:GLY:HA2	1:E:176:THR:HG21	1.90	0.52
1:E:241:ARG:HD3	1:E:246:CYS:SG	2.50	0.52
3:C:121:LYS:HA	3:C:124:ILE:HD12	1.93	0.51
1:E:344:ILE:HG12	1:E:345:TYR:N	2.24	0.51
1:E:327:GLU:OE2	1:E:384:PRO:HD3	2.10	0.51
3:G:158:LEU:O	3:G:162:LEU:HB2	2.11	0.51
4:H:61:ILE:HG13	4:H:62:GLU:N	2.24	0.51
1:A:566:ARG:NH2	1:A:607:THR:OG1	2.33	0.51
1:A:44:VAL:HG21	1:A:60:LEU:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ALA:O	1:A:557:THR:C	2.48	0.51
1:E:383:ILE:HG13	1:E:384:PRO:CD	2.40	0.51
1:E:99:TRP:HH2	1:E:120:HIS:CE1	2.28	0.51
4:H:99:GLY:O	4:H:103:VAL:HG23	2.10	0.51
1:A:568:GLU:OE2	1:A:603:TRP:HB3	2.10	0.51
2:B:36:LYS:HE2	2:B:114:ASP:O	2.10	0.51
2:B:222:SER:O	2:B:224:ALA:N	2.44	0.51
2:B:265:LEU:C	2:B:267:THR:H	2.14	0.51
1:E:517:VAL:HG22	1:E:560:ILE:HG23	1.91	0.51
2:F:205:PRO:HA	2:F:259:ILE:HD11	1.93	0.51
1:A:439:LEU:HD23	1:A:443:VAL:HG23	1.93	0.51
1:E:122:LEU:HA	1:E:443:VAL:HG11	1.92	0.51
1:E:128:GLU:O	1:E:132:GLU:HB2	2.11	0.51
1:E:509:ARG:HG2	1:E:576:ASP:HB2	1.92	0.51
2:F:160:ASN:HB3	2:F:163:GLU:CB	2.36	0.51
1:A:243:TYR:CG	1:A:386:VAL:HG21	2.45	0.51
1:A:45:VAL:HG22	1:A:68:ALA:HB3	1.92	0.51
1:A:481:ARG:HA	1:A:543:LEU:HD13	1.93	0.51
1:E:215:ILE:HD12	1:E:226:ARG:HG2	1.93	0.51
1:A:390:MET:HE1	1:A:431:ASN:HA	1.93	0.51
1:A:496:MET:HG3	1:A:497:GLN:N	2.25	0.51
2:F:240:HIS:C	2:F:241:THR:HG22	2.31	0.51
1:A:517:VAL:O	1:A:521:MET:HG2	2.10	0.51
2:F:228:ALA:HA	2:F:231:GLN:NE2	2.25	0.51
3:G:126:PHE:HB3	3:G:127:PRO:HD3	1.93	0.51
1:E:215:ILE:HA	1:E:225:HIS:O	2.11	0.50
1:E:293:GLY:HA2	1:E:317:LEU:HD11	1.92	0.50
2:F:99:MET:HE1	2:F:135:LEU:CD1	2.41	0.50
3:G:65:PRO:HA	3:G:69:TRP:CZ2	2.46	0.50
1:A:360:LEU:HB3	1:A:363:ILE:HD11	1.91	0.50
1:A:557:THR:O	1:A:560:ILE:CG2	2.59	0.50
1:E:448:CYS:O	1:E:452:ILE:HB	2.11	0.50
1:A:207:ASP:OD2	1:A:466:PRO:HG3	2.12	0.50
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.94	0.50
4:H:118:ALA:HA	4:H:121:VAL:CG2	2.40	0.50
1:A:41:ALA:HB1	1:A:462:ILE:HG21	1.94	0.50
1:E:404:TYR:CD2	1:E:623:ARG:HG3	2.45	0.50
2:F:278:THR:CB	2:F:279:PRO:HD3	2.39	0.50
1:E:383:ILE:HG13	1:E:384:PRO:HD2	1.93	0.50
1:E:585:TYR:CE1	1:E:596:LYS:HB2	2.47	0.50
10:C:201:HEM:NC	4:D:95:HIS:HD2	2.03	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:O	1:A:80:THR:C	2.50	0.50
1:A:230:LYS:HD3	1:A:456:LEU:HD21	1.93	0.50
1:E:196:PHE:HB3	1:E:199:TYR:CD1	2.47	0.50
1:A:321:ASP:HB3	1:A:431:ASN:ND2	2.27	0.50
1:A:436:ASN:O	1:A:440:ASP:HB3	2.12	0.49
1:A:566:ARG:HB3	1:A:573:HIS:CE1	2.46	0.49
2:F:242:ILE:HG22	2:F:243:MET:N	2.27	0.49
1:A:49:ALA:HB1	1:A:75:PRO:HB3	1.94	0.49
4:D:101:TRP:O	4:D:105:ASN:HB2	2.12	0.49
1:A:151:ARG:O	1:A:169:THR:HB	2.13	0.49
1:A:293:GLY:HA2	1:A:317:LEU:HD11	1.94	0.49
1:A:78:SER:O	1:A:81:THR:HG22	2.12	0.49
4:D:93:THR:HG21	4:D:133:LEU:HD13	1.93	0.49
1:E:510:GLY:CA	1:E:575:ARG:NH1	2.76	0.49
1:E:289:GLU:OE1	1:E:320:ARG:HD3	2.12	0.49
1:A:390:MET:CE	1:A:431:ASN:HA	2.43	0.49
2:B:106:THR:OG1	2:B:107:LEU:N	2.45	0.49
3:C:133:LEU:O	3:C:136:ILE:HG12	2.13	0.49
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.45	0.49
1:A:509:ARG:NH1	1:A:511:ASP:OD2	2.46	0.49
1:E:149:TYR:CE1	1:E:359:ARG:NH2	2.80	0.49
1:E:510:GLY:N	1:E:575:ARG:HH11	2.09	0.49
3:C:112:ILE:HB	3:C:117:LEU:HD11	1.95	0.49
2:F:99:MET:HE2	2:F:135:LEU:HD13	1.93	0.49
1:E:276:HIS:HB2	1:E:387:HIS:CG	2.48	0.49
1:A:213:GLY:HA3	1:A:227:PHE:O	2.13	0.48
1:A:134:GLU:OE2	2:B:219:ARG:NH1	2.43	0.48
1:A:439:LEU:CD2	1:A:443:VAL:HG21	2.43	0.48
1:A:605:LYS:HD2	1:A:622:TYR:HB3	1.94	0.48
1:E:551:ASN:HD22	1:E:551:ASN:N	2.11	0.48
1:A:72:LYS:HG2	6:A:702:FAD:C4A	2.43	0.48
1:A:73:MET:HA	1:A:198:GLU:HG3	1.96	0.48
2:B:92:GLY:CA	2:B:109:CYS:SG	3.02	0.48
3:C:178:ARG:HH11	3:C:178:ARG:HB3	1.77	0.48
1:E:404:TYR:C	1:E:404:TYR:CD1	2.87	0.48
10:G:201:HEM:HBB1	4:H:70:VAL:HA	1.95	0.48
1:A:589:LYS:O	1:A:591:ILE:N	2.47	0.48
2:B:132:ILE:HB	2:B:136:VAL:HG12	1.96	0.48
2:B:47:GLU:HB3	2:B:50:ALA:CB	2.42	0.48
4:H:73:ILE:N	4:H:74:PRO:HD2	2.28	0.48
1:E:117:ASN:N	1:E:117:ASN:HD22	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:LYS:CE	1:E:461:LYS:H	2.27	0.48
1:E:522:ASP:O	1:E:525:LYS:HB2	2.14	0.48
1:A:55:ARG:HG2	1:A:442:VAL:O	2.13	0.48
2:B:95:GLY:HA2	2:B:183:ILE:HD12	1.96	0.48
2:F:44:ASN:ND2	2:F:47:GLU:HB3	2.28	0.48
1:E:42:TYR:CD2	1:E:68:ALA:HB2	2.49	0.47
2:F:57:PHE:CG	2:F:75:ILE:HD12	2.49	0.47
1:A:48:GLY:HA2	6:A:702:FAD:H1B	1.95	0.47
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.95	0.47
3:G:163:ALA:O	3:G:167:SER:HB3	2.14	0.47
1:A:488:PRO:HG2	1:A:491:GLU:HB2	1.97	0.47
2:B:156:LYS:HB2	2:B:221:ASP:HB3	1.95	0.47
1:E:547:LEU:O	1:E:550:GLN:HB2	2.15	0.47
1:A:502:LYS:HD2	1:A:503:HIS:CE1	2.49	0.47
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.50	0.47
1:A:54:LEU:HA	1:A:57:ALA:HB3	1.96	0.47
1:E:289:GLU:HA	1:E:292:ARG:NH1	2.30	0.47
1:A:189:LEU:HD13	2:B:147:ALA:CB	2.44	0.47
2:B:150:GLN:HA	2:B:152:TRP:CZ3	2.50	0.47
3:C:104:VAL:HG12	3:C:108:ARG:HH12	1.79	0.47
3:C:88:ILE:O	3:C:88:ILE:HD12	2.15	0.47
1:E:388:TYR:CD2	1:E:432:ARG:HD2	2.50	0.47
1:E:38:ILE:HG23	4:H:34:GLY:HA3	1.95	0.47
2:F:169:SER:HB3	2:F:172:GLU:HG2	1.97	0.47
1:E:536:SER:HB2	2:F:46:GLU:OE2	2.14	0.47
1:E:504:ALA:HB2	1:E:560:ILE:HD12	1.96	0.47
1:A:439:LEU:CD2	1:A:443:VAL:CG2	2.92	0.47
10:C:201:HEM:HMB2	10:C:201:HEM:CBB	2.44	0.47
10:G:201:HEM:HAB	4:H:73:ILE:HD12	1.95	0.47
1:A:271:GLU:OE2	1:A:566:ARG:NE	2.46	0.47
2:B:168:GLN:HG3	2:B:172:GLU:HG3	1.97	0.47
2:B:222:SER:O	2:B:223:ALA:C	2.54	0.47
1:E:204:LEU:HD22	1:E:211:CYS:SG	2.55	0.47
1:E:55:ARG:HG2	1:E:442:VAL:HG13	1.96	0.47
4:H:127:ILE:O	4:H:131:CYS:HB2	2.15	0.47
1:A:288:THR:HG23	1:A:291:SER:H	1.79	0.46
4:D:69:MET:HE1	4:D:95:HIS:HB2	1.97	0.46
1:E:503:HIS:CE1	1:E:519:LYS:NZ	2.82	0.46
4:H:69:MET:HB2	4:H:69:MET:HE2	1.70	0.46
2:B:179:LEU:HD12	2:B:209:MET:HG2	1.97	0.46
1:E:608:LEU:CD2	1:E:623:ARG:HB2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ASN:O	1:A:480:VAL:HG23	2.15	0.46
1:A:87:ILE:HD13	1:A:130:VAL:HG22	1.97	0.46
2:B:103:GLY:HA3	3:C:64:LYS:HB2	1.96	0.46
1:E:102:HIS:ND1	1:E:123:THR:HG22	2.30	0.46
1:E:333:GLU:OE2	1:E:335:ARG:NH2	2.49	0.46
2:B:181:GLU:HB2	2:B:253:LEU:HD21	1.96	0.46
1:A:231:ARG:HH11	1:A:456:LEU:HD23	1.79	0.46
3:G:65:PRO:HA	3:G:69:TRP:HZ2	1.81	0.46
1:A:200:PHE:O	1:A:216:ALA:HA	2.15	0.46
10:C:201:HEM:CBD	10:C:201:HEM:HHA	2.29	0.46
1:E:538:ILE:HD12	2:F:46:GLU:HG3	1.98	0.46
3:G:133:LEU:O	3:G:136:ILE:HG13	2.16	0.46
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.53	0.46
2:B:279:PRO:O	2:B:280:ALA:HB3	2.15	0.46
2:F:168:GLN:CG	2:F:172:GLU:HG3	2.46	0.46
1:A:148:ILE:H	2:B:165:GLN:HE22	1.64	0.46
1:A:289:GLU:OE2	1:A:292:ARG:NH2	2.49	0.46
1:A:504:ALA:HB2	1:A:560:ILE:HD12	1.97	0.46
1:E:510:GLY:HA2	1:E:575:ARG:HH11	1.78	0.46
2:F:268:LYS:HE3	2:F:268:LYS:HB2	1.68	0.46
2:F:47:GLU:HA	2:F:48:PRO:HD3	1.83	0.46
3:C:132:THR:HG23	10:C:201:HEM:HAB	1.95	0.45
4:D:56:GLY:O	4:D:58:LEU:N	2.49	0.45
4:H:80:HIS:HE1	12:H:201:EPH:H371	1.79	0.45
1:A:513:LEU:O	1:A:517:VAL:HG23	2.16	0.45
1:E:437:SER:O	1:E:441:ALA:HB2	2.15	0.45
1:A:105:ASP:OD2	1:A:157:SER:N	2.42	0.45
1:A:368:LYS:O	1:A:372:GLY:HA2	2.16	0.45
1:A:470:GLY:O	1:A:474:ILE:HG22	2.16	0.45
1:A:73:MET:HE3	1:A:78:SER:HA	1.98	0.45
1:E:508:ARG:O	1:E:575:ARG:HA	2.17	0.45
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.72	0.45
1:E:45:VAL:HG23	1:E:229:SER:HB3	1.97	0.45
2:F:177:ASP:OD1	2:F:180:TYR:HE2	2.00	0.45
1:A:289:GLU:OE1	1:A:320:ARG:HD3	2.17	0.45
2:F:240:HIS:C	2:F:241:THR:CG2	2.84	0.45
2:F:265:LEU:C	2:F:267:THR:H	2.19	0.45
1:A:459:ASP:OD1	1:A:460:GLU:N	2.50	0.45
1:A:55:ARG:NH2	1:A:58:MET:HB2	2.32	0.45
2:F:129:MET:H	3:G:57:ALA:HB3	1.82	0.45
4:H:77:TYR:HD2	4:H:78:PHE:CE2	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.99	0.45
1:A:61:GLY:HA3	1:A:191:CYS:O	2.17	0.45
1:E:487:VAL:HA	1:E:488:PRO:HD2	1.70	0.45
1:E:522:ASP:HA	1:E:525:LYS:HD2	1.98	0.45
2:F:155:LYS:HA	2:F:155:LYS:HD2	1.69	0.45
2:F:267:THR:HB	2:F:268:LYS:HG2	1.97	0.45
3:G:131:HIS:CD2	10:G:201:HEM:C1C	3.04	0.45
1:A:291:SER:HB2	1:A:348:LEU:HD21	1.99	0.45
1:A:498:LYS:HE3	1:A:498:LYS:HB2	1.63	0.45
1:A:89:ALA:HB2	1:A:130:VAL:HG21	1.99	0.45
3:C:184:LEU:HA	3:C:185:PRO:HD3	1.75	0.45
1:E:642:ILE:H	1:E:642:ILE:HG13	1.55	0.45
1:A:355:GLN:O	1:A:359:ARG:HB2	2.16	0.45
1:A:42:TYR:CE2	1:A:66:LYS:HE2	2.51	0.45
2:B:69:LEU:O	2:B:73:ILE:HG12	2.16	0.45
1:E:297:PHE:CD2	1:E:305:ARG:HD2	2.53	0.44
3:G:95:VAL:HG13	3:G:95:VAL:O	2.17	0.44
3:C:108:ARG:HB2	3:C:108:ARG:HH11	1.83	0.44
4:D:153:VAL:C	4:D:155:GLU:H	2.20	0.44
2:F:39:GLU:OE1	2:F:54:LEU:HD22	2.17	0.44
2:B:183:ILE:HG13	2:B:185:CYS:HB3	1.99	0.44
1:E:214:VAL:HG12	1:E:215:ILE:N	2.31	0.44
3:G:117:LEU:O	3:G:121:LYS:HE3	2.16	0.44
3:G:74:LEU:O	3:G:78:THR:HG23	2.17	0.44
4:H:51:PRO:O	4:H:53:HIS:N	2.50	0.44
1:A:262:ARG:NH1	1:A:551:ASN:ND2	2.65	0.44
1:A:586:ASP:H	1:A:594:GLN:HE22	1.64	0.44
1:A:568:GLU:CD	1:A:603:TRP:HB3	2.38	0.44
4:D:92:LEU:HD12	4:D:92:LEU:HA	1.73	0.44
1:E:242:ALA:HA	1:E:496:MET:CE	2.48	0.44
1:E:374:ASP:C	1:E:374:ASP:OD2	2.56	0.44
1:E:404:TYR:HB2	1:E:410:ASP:HB3	1.99	0.44
1:A:204:LEU:HG	1:A:259:LEU:HB3	1.98	0.44
3:C:57:ALA:HA	3:C:58:PRO:HD2	1.76	0.44
1:E:97:ASP:OD2	1:E:168:ARG:NH1	2.51	0.44
1:E:246:CYS:HA	1:E:385:THR:HG22	2.00	0.44
1:E:374:ASP:OD1	1:E:377:LYS:HD3	2.17	0.44
1:E:496:MET:CG	1:E:497:GLN:N	2.80	0.44
1:A:55:ARG:HH22	1:A:58:MET:HB2	1.82	0.44
1:E:248:THR:O	2:F:90:ARG:NH2	2.44	0.44
1:E:278:THR:HG22	1:E:382:VAL:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:143:MET:O	3:G:144:ALA:CB	2.66	0.44
3:G:149:ILE:H	3:G:149:ILE:CD1	2.28	0.44
1:E:271:GLU:HB2	1:E:563:ALA:HB2	1.99	0.44
3:G:134:ASN:O	3:G:137:ARG:HB3	2.18	0.44
3:G:114:TRP:HB2	3:G:175:ARG:NH2	2.32	0.44
1:A:202:LEU:HB2	1:A:215:ILE:HG23	1.99	0.44
1:A:190:ARG:HB3	2:B:152:TRP:CZ2	2.53	0.44
2:F:193:PRO:HD2	2:F:242:ILE:HD13	2.00	0.44
1:A:508:ARG:HH11	1:A:573:HIS:CD2	2.35	0.43
4:D:137:LEU:HA	4:D:137:LEU:HD23	1.88	0.43
2:F:126:LEU:HA	2:F:127:PRO:HD3	1.88	0.43
3:G:76:ARG:HE	10:G:201:HEM:CGD	2.31	0.43
1:A:42:TYR:O	1:A:229:SER:HA	2.18	0.43
3:C:105:GLU:C	3:C:107:ILE:N	2.71	0.43
6:E:702:FAD:H1'1	6:E:702:FAD:H9	1.69	0.43
3:C:42:GLY:O	3:C:45:TYR:HB3	2.18	0.43
1:E:383:ILE:HG13	1:E:384:PRO:N	2.33	0.43
1:E:584:GLU:OE2	1:E:587:TYR:HE1	2.01	0.43
1:A:250:HIS:HB3	2:B:87:ARG:NH1	2.32	0.43
1:A:425:HIS:HB2	1:A:427:VAL:HG13	2.01	0.43
3:C:92:GLY:O	3:C:96:LEU:HB2	2.19	0.43
1:E:424:CYS:C	1:E:426:SER:H	2.20	0.43
1:E:600:GLU:OE2	1:E:600:GLU:N	2.51	0.43
4:H:146:LEU:O	4:H:149:ALA:HB3	2.18	0.43
1:A:215:ILE:HG13	1:A:226:ARG:HG2	2.00	0.43
1:A:540:ASN:HB3	1:A:543:LEU:HB3	2.01	0.43
2:B:130:PHE:O	2:B:138:ASP:N	2.46	0.43
4:D:80:HIS:ND1	4:D:147:THR:HB	2.33	0.43
1:E:38:ILE:CG2	4:H:34:GLY:HA3	2.49	0.43
2:F:222:SER:O	2:F:223:ALA:C	2.56	0.43
1:A:258:ALA:HB1	1:A:262:ARG:HH11	1.81	0.43
1:A:608:LEU:HD22	1:A:623:ARG:HB2	2.00	0.43
1:E:138:MET:HE2	1:E:172:VAL:HG23	2.01	0.43
3:G:74:LEU:HD23	3:G:130:PHE:CZ	2.54	0.43
10:C:201:HEM:CBB	10:C:201:HEM:CMB	2.96	0.43
1:E:44:VAL:HA	1:E:231:ARG:O	2.18	0.43
1:E:331:ILE:HD11	1:E:344:ILE:HG22	2.00	0.43
1:A:203:ASP:HA	1:A:259:LEU:HG	1.99	0.43
1:A:346:LEU:HB2	1:A:382:VAL:HG21	2.00	0.43
1:A:511:ASP:O	1:A:515:GLU:HB2	2.19	0.43
1:A:432:ARG:HH22	5:A:701:MLI:C2	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:202:FTN:O1	11:C:202:FTN:H14	2.19	0.43
1:E:276:HIS:CD2	1:E:286:LEU:HD11	2.53	0.43
2:F:261:GLU:O	2:F:264:MET:HB2	2.19	0.43
2:F:127:PRO:HB3	3:G:59:HIS:HA	2.01	0.43
1:A:91:LEU:CD1	1:A:170:CYS:SG	3.07	0.43
1:A:189:LEU:CD1	2:B:147:ALA:CB	2.96	0.43
4:D:150:PHE:CE1	12:D:201:EPH:H182	2.53	0.43
1:E:109:GLY:HA3	1:E:433:LEU:HD13	2.00	0.43
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.46	0.43
2:F:95:GLY:CA	2:F:183:ILE:HD12	2.49	0.43
2:F:267:THR:HB	2:F:268:LYS:CG	2.48	0.43
3:G:110:LEU:O	3:G:112:ILE:N	2.52	0.43
4:H:150:PHE:O	4:H:151:GLU:C	2.57	0.43
4:H:82:ARG:HA	4:H:85:ASP:HB2	2.01	0.43
1:A:106:THR:HG22	1:A:119:MET:SD	2.59	0.43
1:A:253:THR:O	1:A:552:LEU:HG	2.19	0.43
2:B:234:PHE:O	2:B:235:SER:C	2.57	0.43
1:E:294:GLU:O	1:E:351:LEU:HD21	2.18	0.43
1:E:74:PHE:CD1	1:E:75:PRO:HD2	2.54	0.43
1:A:331:ILE:HD11	1:A:343:HIS:C	2.40	0.42
3:C:132:THR:HG23	10:C:201:HEM:CBB	2.49	0.42
1:E:489:THR:HG23	1:E:490:ALA:N	2.34	0.42
3:G:173:TYR:O	3:G:176:TRP:HB3	2.19	0.42
4:H:112:VAL:O	4:H:112:VAL:HG12	2.18	0.42
4:H:137:LEU:HD23	4:H:137:LEU:HA	1.71	0.42
1:A:73:MET:CE	1:A:78:SER:HA	2.48	0.42
2:B:258:ALA:O	2:B:262:ILE:HG13	2.19	0.42
2:B:34:ARG:HG2	2:B:34:ARG:HH21	1.82	0.42
1:E:511:ASP:O	1:E:515:GLU:HB2	2.20	0.42
3:C:58:PRO:HB2	3:C:62:ILE:HG12	2.01	0.42
1:E:274:GLN:HB2	1:E:390:MET:HE1	2.01	0.42
1:E:72:LYS:HG2	6:E:702:FAD:C4A	2.49	0.42
2:F:276:LEU:HA	2:F:277:PRO:HD2	1.73	0.42
3:G:137:ARG:NH2	3:G:152:ILE:O	2.51	0.42
2:B:100:ASN:ND2	2:B:100:ASN:C	2.73	0.42
3:C:105:GLU:O	3:C:107:ILE:N	2.52	0.42
1:E:94:MET:HG2	1:E:150:GLN:HB2	2.00	0.42
1:E:213:GLY:HA3	1:E:227:PHE:O	2.19	0.42
1:E:79:HIS:CD2	6:E:702:FAD:HM81	2.52	0.42
2:F:128:HIS:HD2	3:G:59:HIS:CD2	2.38	0.42
1:A:620:LEU:O	1:A:621:ASP:CB	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.02	0.42
1:E:541:SER:HB3	2:F:76:LYS:HZ1	1.81	0.42
2:F:243:MET:O	3:G:68:THR:HG21	2.19	0.42
3:G:105:GLU:O	3:G:107:ILE:N	2.53	0.42
1:A:86:GLY:HA2	1:A:176:THR:HG21	2.00	0.42
1:A:466:PRO:O	1:A:467:GLU:C	2.55	0.42
1:A:582:GLU:CB	1:A:603:TRP:HD1	2.32	0.42
10:C:201:HEM:HBB1	4:D:70:VAL:HA	2.02	0.42
1:E:231:ARG:HD3	1:E:231:ARG:HA	1.78	0.42
1:E:393:ILE:HA	1:E:394:PRO:HD3	1.94	0.42
1:E:591:ILE:HA	1:E:594:GLN:OE1	2.18	0.42
1:A:321:ASP:OD1	1:A:643:ARG:NH2	2.51	0.42
2:B:75:ILE:O	2:B:75:ILE:HG13	2.19	0.42
1:E:406:LYS:HB2	1:E:406:LYS:NZ	2.34	0.42
1:A:241:ARG:HA	1:A:241:ARG:HD3	1.66	0.42
1:A:388:TYR:CD1	1:A:421:GLU:HG3	2.54	0.42
2:B:39:GLU:HG2	2:B:56:LYS:HG2	2.02	0.42
1:E:508:ARG:HH11	1:E:573:HIS:HD2	1.68	0.42
1:E:55:ARG:HD2	1:E:55:ARG:HA	1.76	0.42
2:F:163:GLU:O	2:F:164:LYS:HB3	2.19	0.42
1:A:351:LEU:HG	1:A:355:GLN:HE22	1.85	0.42
1:A:68:ALA:HB1	1:A:196:PHE:CE1	2.55	0.42
3:C:178:ARG:NH1	3:C:178:ARG:HB3	2.35	0.42
2:F:125:PRO:O	2:F:126:LEU:C	2.58	0.42
3:G:129:ALA:HA	12:H:201:EPH:H13	2.02	0.42
10:G:201:HEM:CBB	4:H:69:MET:HB3	2.48	0.42
1:A:394:PRO:HB2	1:A:402:ILE:HG13	2.01	0.42
1:E:87:ILE:HD11	1:E:439:LEU:HA	2.01	0.42
1:E:638:ILE:HA	1:E:639:PRO:HD3	1.89	0.42
1:E:408:GLY:O	1:E:409:GLY:C	2.58	0.41
2:F:63:LYS:O	2:F:74:LYS:HE2	2.20	0.41
3:G:131:HIS:HD2	10:G:201:HEM:C1C	2.38	0.41
1:A:159:ASN:O	1:A:160:TYR:C	2.58	0.41
4:D:41:ASP:OD2	4:D:44:ALA:HB3	2.19	0.41
4:D:82:ARG:HB2	4:D:82:ARG:CZ	2.50	0.41
1:E:243:TYR:OH	1:E:504:ALA:CB	2.68	0.41
1:E:586:ASP:H	1:E:594:GLN:NE2	2.18	0.41
1:A:236:THR:O	6:A:702:FAD:H8A	2.20	0.41
1:A:265:ILE:HD12	1:A:401:VAL:HG11	2.02	0.41
1:A:461:LYS:HG3	1:A:461:LYS:H	1.70	0.41
3:C:107:ILE:CD1	4:D:156:LEU:HD13	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:TRP:CE3	11:C:202:FTN:H15	2.55	0.41
1:E:41:ALA:HA	1:E:228:ARG:HB2	2.02	0.41
1:E:247:THR:HG22	1:E:284:GLY:O	2.20	0.41
1:A:509:ARG:HA	1:A:577:ASP:OD2	2.20	0.41
2:F:198:ASN:O	2:F:200:ASP:N	2.54	0.41
3:G:107:ILE:HA	3:G:110:LEU:HD12	2.02	0.41
1:A:125:ASN:N	1:A:125:ASN:ND2	2.68	0.41
1:A:390:MET:HE3	1:A:430:ALA:O	2.20	0.41
1:A:83:ALA:HB3	1:A:177:GLY:CA	2.45	0.41
4:D:86:LEU:HA	4:D:86:LEU:HD22	1.95	0.41
1:E:502:LYS:CD	1:E:503:HIS:CE1	2.97	0.41
1:E:598:PRO:HG2	1:E:601:LYS:HB2	2.03	0.41
2:F:128:HIS:CD2	3:G:59:HIS:HD2	2.39	0.41
3:G:74:LEU:HG	3:G:130:PHE:CE1	2.56	0.41
4:H:80:HIS:HB3	4:H:81:GLY:H	1.70	0.41
2:B:172:GLU:OE2	2:B:275:PRO:CD	2.64	0.41
3:C:133:LEU:HD12	3:C:133:LEU:HA	1.83	0.41
2:F:36:LYS:HD3	2:F:36:LYS:HA	1.85	0.41
3:C:164:ALA:O	3:C:168:LEU:HB2	2.21	0.41
1:A:55:ARG:HA	1:A:58:MET:HG3	2.02	0.41
1:A:139:PRO:HB3	2:B:176:LEU:HD13	2.03	0.41
3:C:167:SER:O	3:C:170:VAL:HG12	2.21	0.41
4:D:151:GLU:HG2	12:D:201:EPH:O6	2.21	0.41
4:D:77:TYR:HD2	4:D:78:PHE:CE2	2.39	0.41
2:F:141:LEU:HD12	2:F:141:LEU:O	2.20	0.41
2:F:242:ILE:O	2:F:243:MET:HB2	2.20	0.41
2:F:273:PRO:O	2:F:275:PRO:HD3	2.20	0.41
4:H:70:VAL:N	4:H:71:PRO:HD2	2.36	0.41
2:B:47:GLU:HA	2:B:48:PRO:HD3	1.90	0.41
1:E:492:LEU:HD12	1:E:492:LEU:HA	1.92	0.41
1:E:91:LEU:HD12	1:E:170:CYS:SG	2.61	0.41
2:F:99:MET:HB3	2:F:99:MET:HE3	1.89	0.41
3:G:43:TRP:O	3:G:44:ASP:C	2.58	0.41
1:E:390:MET:HB3	1:E:428:HIS:HB2	2.02	0.41
4:H:100:VAL:HG23	4:H:101:TRP:N	2.36	0.41
1:E:174:ASP:OD2	1:E:363:ILE:N	2.43	0.40
1:E:499:THR:O	1:E:500:MET:C	2.59	0.40
1:E:530:LEU:HD12	1:E:530:LEU:HA	1.89	0.40
1:E:128:GLU:CG	2:F:162:GLY:HA3	2.51	0.40
2:F:240:HIS:CG	11:F:304:FTN:H7	2.56	0.40
4:H:41:ASP:OD1	4:H:43:ILE:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:NH1	2:B:94:CYS:O	2.43	0.40
3:G:149:ILE:HD13	3:G:149:ILE:N	2.35	0.40
1:A:209:GLY:O	1:A:414:PRO:HD2	2.21	0.40
1:A:503:HIS:CE1	1:A:519:LYS:HE3	2.57	0.40
1:A:582:GLU:HB2	1:A:603:TRP:CD1	2.56	0.40
4:D:84:MET:HG2	4:D:147:THR:HG21	2.03	0.40
4:H:84:MET:C	4:H:86:LEU:N	2.74	0.40
2:B:89:CYS:HB3	2:B:94:CYS:HB3	2.03	0.40
1:A:222:GLY:O	1:A:537:LEU:HD13	2.22	0.40
1:A:281:TYR:HB3	1:A:381:PRO:HB2	2.04	0.40
1:A:408:GLY:O	1:A:411:LYS:HD3	2.22	0.40
1:E:243:TYR:HB3	1:E:501:GLN:OE1	2.22	0.40
1:E:363:ILE:O	1:E:364:SER:C	2.60	0.40
1:E:508:ARG:HH11	1:E:573:HIS:CD2	2.39	0.40
1:E:541:SER:HB3	2:F:76:LYS:HZ3	1.84	0.40
3:G:45:TYR:O	3:G:46:LEU:C	2.59	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%)	522 (85%)	76 (12%)	13 (2%)	8	36
1	E	611/645 (95%)	537 (88%)	64 (10%)	10 (2%)	11	44
2	B	247/282 (88%)	208 (84%)	31 (13%)	8 (3%)	5	24
2	F	247/282 (88%)	202 (82%)	36 (15%)	9 (4%)	4	21
3	C	151/188 (80%)	120 (80%)	23 (15%)	8 (5%)	2	13
3	G	151/188 (80%)	114 (76%)	29 (19%)	8 (5%)	2	13
4	D	127/156 (81%)	92 (72%)	28 (22%)	7 (6%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	127/156 (81%)	105 (83%)	18 (14%)	4 (3%)	5	25
All	All	2272/2542 (89%)	1900 (84%)	305 (13%)	67 (3%)	5	26

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	PRO
1	A	591	ILE
1	A	621	ASP
3	C	184	LEU
3	C	185	PRO
4	D	50	LYS
4	D	57	THR
1	E	409	GLY
1	E	426	SER
2	F	243	MET
4	H	52	LEU
4	H	85	ASP
1	A	409	GLY
1	A	426	SER
1	A	556	ALA
2	B	243	MET
2	B	264	MET
2	B	269	MET
3	C	99	ASP
3	C	106	PHE
4	D	108	GLY
1	E	483	ALA
2	F	199	ALA
2	F	245	CYS
2	F	267	THR
2	F	269	MET
3	G	106	PHE
3	G	111	GLY
3	G	170	VAL
4	H	48	GLY
3	C	170	VAL
4	D	45	ALA
4	D	51	PRO
4	D	56	GLY
1	E	144	PRO
1	E	240	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	169	ALA
3	G	179	HIS
3	G	185	PRO
1	A	476	ASN
1	A	557	THR
1	A	629	THR
2	B	88	SER
2	B	161	LEU
4	D	86	LEU
2	F	218	SER
2	F	280	ALA
1	E	95	ASN
1	E	539	TRP
2	F	277	PRO
3	G	95	VAL
4	H	151	GLU
1	A	103	PHE
1	A	335	ARG
2	B	223	ALA
1	E	334	GLY
1	A	505	GLY
3	C	95	VAL
3	C	123	ILE
2	F	65	GLY
3	G	150	PRO
2	B	48	PRO
1	E	96	PRO
1	A	593	GLY
2	B	277	PRO
3	C	73	GLY
1	E	381	PRO

5.3.2 Protein sidechains ⓘ

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	498/526 (95%)	408 (82%)	90 (18%)	2 10
1	E	498/526 (95%)	427 (86%)	71 (14%)	4 17
2	B	219/242 (90%)	187 (85%)	32 (15%)	3 16
2	F	219/242 (90%)	182 (83%)	37 (17%)	2 11
3	C	127/158 (80%)	106 (84%)	21 (16%)	2 12
3	G	127/158 (80%)	101 (80%)	26 (20%)	1 6
4	D	96/119 (81%)	72 (75%)	24 (25%)	1 3
4	H	96/119 (81%)	77 (80%)	19 (20%)	1 7
All	All	1880/2090 (90%)	1560 (83%)	320 (17%)	2 11

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	47	ILE
1	A	81	THR
1	A	87	ILE
1	A	110	SER
1	A	117	ASN
1	A	122	LEU
1	A	125	ASN
1	A	127	VAL
1	A	142	ARG
1	A	145	GLU
1	A	151	ARG
1	A	153	PHE
1	A	162	LYS
1	A	175	ARG
1	A	179	SER
1	A	188	SER
1	A	190	ARG
1	A	203	ASP
1	A	205	LEU
1	A	214	VAL
1	A	215	ILE
1	A	228	ARG
1	A	241	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	248	THR
1	A	251	MET
1	A	252	ASN
1	A	262	ARG
1	A	265	ILE
1	A	291	SER
1	A	301	SER
1	A	320	ARG
1	A	324	SER
1	A	332	MET
1	A	335	ARG
1	A	337	VAL
1	A	344	ILE
1	A	351	LEU
1	A	355	GLN
1	A	358	GLN
1	A	359	ARG
1	A	364	SER
1	A	377	LYS
1	A	385	THR
1	A	390	MET
1	A	406	LYS
1	A	410	ASP
1	A	411	LYS
1	A	426	SER
1	A	432	ARG
1	A	436	ASN
1	A	437	SER
1	A	439	LEU
1	A	440	ASP
1	A	446	ARG
1	A	453	LYS
1	A	454	GLU
1	A	457	LYS
1	A	461	LYS
1	A	465	LEU
1	A	472	GLU
1	A	474	ILE
1	A	484	ASN
1	A	491	GLU
1	A	494	LEU
1	A	495	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	496	MET
1	A	498	LYS
1	A	502	LYS
1	A	523	LEU
1	A	527	LEU
1	A	528	LYS
1	A	533	THR
1	A	539	TRP
1	A	547	LEU
1	A	560	ILE
1	A	561	VAL
1	A	577	ASP
1	A	584	GLU
1	A	591	ILE
1	A	595	THR
1	A	601	LYS
1	A	610	LYS
1	A	614	ARG
1	A	619	THR
1	A	627	ASP
1	A	628	LYS
1	A	636	ASP
1	A	637	TRP
1	A	642	ILE
2	B	33	LYS
2	B	34	ARG
2	B	37	THR
2	B	63	LYS
2	B	66	THR
2	B	69	LEU
2	B	87	ARG
2	B	89	CYS
2	B	90	ARG
2	B	93	ILE
2	B	100	ASN
2	B	111	CYS
2	B	120	THR
2	B	129	MET
2	B	131	VAL
2	B	158	LYS
2	B	169	SER
2	B	170	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	171	LYS
2	B	173	GLN
2	B	179	LEU
2	B	213	ARG
2	B	218	SER
2	B	241	THR
2	B	248	THR
2	B	267	THR
2	B	268	LYS
2	B	270	LYS
2	B	271	THR
2	B	272	LYS
2	B	276	LEU
2	B	278	THR
3	C	85	THR
3	C	86	LEU
3	C	88	ILE
3	C	99	ASP
3	C	106	PHE
3	C	110	LEU
3	C	112	ILE
3	C	114	TRP
3	C	118	ASP
3	C	120	PHE
3	C	132	THR
3	C	133	LEU
3	C	136	ILE
3	C	145	LYS
3	C	149	ILE
3	C	160	LEU
3	C	162	LEU
3	C	165	LEU
3	C	176	TRP
3	C	178	ARG
3	C	184	LEU
4	D	46	GLU
4	D	47	LYS
4	D	50	LYS
4	D	53	HIS
4	D	57	THR
4	D	61	ILE
4	D	63	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	64	TYR
4	D	72	LEU
4	D	79	ILE
4	D	82	ARG
4	D	83	GLU
4	D	86	LEU
4	D	88	LEU
4	D	90	LEU
4	D	92	LEU
4	D	113	LEU
4	D	117	LEU
4	D	122	ARG
4	D	136	LEU
4	D	143	ASP
4	D	152	MET
4	D	154	TRP
4	D	156	LEU
1	E	44	VAL
1	E	62	GLU
1	E	117	ASN
1	E	124	ARG
1	E	142	ARG
1	E	143	THR
1	E	145	GLU
1	E	151	ARG
1	E	152	SER
1	E	153	PHE
1	E	162	LYS
1	E	175	ARG
1	E	179	SER
1	E	190	ARG
1	E	193	CYS
1	E	194	THR
1	E	208	LYS
1	E	230	LYS
1	E	251	MET
1	E	261	THR
1	E	274	GLN
1	E	283	VAL
1	E	292	ARG
1	E	320	ARG
1	E	321	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	328	THR
1	E	335	ARG
1	E	337	VAL
1	E	344	ILE
1	E	351	LEU
1	E	355	GLN
1	E	356	LEU
1	E	359	ARG
1	E	378	GLU
1	E	383	ILE
1	E	385	THR
1	E	390	MET
1	E	402	ILE
1	E	404	TYR
1	E	411	LYS
1	E	422	CYS
1	E	426	SER
1	E	439	LEU
1	E	440	ASP
1	E	452	ILE
1	E	454	GLU
1	E	456	LEU
1	E	457	LYS
1	E	461	LYS
1	E	474	ILE
1	E	480	VAL
1	E	494	LEU
1	E	496	MET
1	E	498	LYS
1	E	499	THR
1	E	502	LYS
1	E	512	ILE
1	E	515	GLU
1	E	523	LEU
1	E	527	LEU
1	E	528	LYS
1	E	539	TRP
1	E	546	SER
1	E	560	ILE
1	E	589	LYS
1	E	601	LYS
1	E	608	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	636	ASP
1	E	637	TRP
1	E	641	ILE
1	E	643	ARG
2	F	36	LYS
2	F	53	LYS
2	F	63	LYS
2	F	66	THR
2	F	69	LEU
2	F	73	ILE
2	F	75	ILE
2	F	87	ARG
2	F	88	SER
2	F	90	ARG
2	F	99	MET
2	F	110	ILE
2	F	115	GLN
2	F	116	ASN
2	F	120	THR
2	F	122	LYS
2	F	139	MET
2	F	155	LYS
2	F	156	LYS
2	F	157	THR
2	F	158	LYS
2	F	160	ASN
2	F	161	LEU
2	F	163	GLU
2	F	173	GLN
2	F	210	GLN
2	F	213	ARG
2	F	222	SER
2	F	248	THR
2	F	253	LEU
2	F	261	GLU
2	F	265	LEU
2	F	266	LEU
2	F	267	THR
2	F	268	LYS
2	F	270	LYS
2	F	276	LEU
3	G	34	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	52	LEU
3	G	59	HIS
3	G	61	THR
3	G	85	THR
3	G	88	ILE
3	G	94	SER
3	G	95	VAL
3	G	96	LEU
3	G	98	LEU
3	G	101	THR
3	G	112	ILE
3	G	114	TRP
3	G	115	VAL
3	G	119	THR
3	G	133	LEU
3	G	136	ILE
3	G	149	ILE
3	G	151	SER
3	G	160	LEU
3	G	162	LEU
3	G	165	LEU
3	G	170	VAL
3	G	172	VAL
3	G	175	ARG
3	G	177	GLU
4	H	46	GLU
4	H	49	PHE
4	H	50	LYS
4	H	53	HIS
4	H	58	LEU
4	H	61	ILE
4	H	64	TYR
4	H	79	ILE
4	H	83	GLU
4	H	86	LEU
4	H	88	LEU
4	H	90	LEU
4	H	92	LEU
4	H	121	VAL
4	H	131	CYS
4	H	136	LEU
4	H	142	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	154	TRP
4	H	155	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	95	ASN
1	A	117	ASN
1	A	120	HIS
1	A	150	GLN
1	A	187	ASN
1	A	349	HIS
1	A	355	GLN
1	A	357	HIS
1	A	431	ASN
1	A	436	ASN
1	A	451	ASN
1	A	484	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
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	112	ASN
2	B	145	GLN
2	B	165	GLN
2	B	210	GLN
2	B	244	ASN
3	C	75	HIS
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	349	HIS
1	E	355	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	431	ASN
1	E	436	ASN
1	E	451	ASN
1	E	476	ASN
1	E	484	ASN
1	E	503	HIS
1	E	550	GLN
1	E	551	ASN
1	E	565	ASN
1	E	573	HIS
1	E	602	HIS
2	F	44	ASN
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	128	HIS
2	F	145	GLN
2	F	160	ASN
2	F	165	GLN
2	F	244	ASN
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	51,58,58	1.35	6 (11%)	54,89,89	2.14	11 (20%)
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	28,50,50	2.36	10 (35%)	17,82,82	2.27	7 (41%)
11	FTN	C	202	-	24,24,24	3.37	9 (37%)	34,34,34	2.29	9 (26%)
12	EPH	D	201	-	43,43,48	1.99	10 (23%)	45,48,53	2.73	8 (17%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	1	51,58,58	1.48	8 (15%)	54,89,89	2.36	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	-
11	FTN	F	304	-	24,24,24	3.27	9 (37%)	34,34,34	2.73	9 (26%)
10	HEM	G	201	3,4	28,50,50	2.32	8 (28%)	17,82,82	1.83	5 (29%)
12	EPH	H	201	-	43,43,48	1.93	9 (20%)	45,48,53	2.68	8 (17%)

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	-	0/28/50/50	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	-	2/6/54/54	0/0/8/8
11	FTN	C	202	-	-	0/18/18/18	0/2/2/2
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	-	0/28/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

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
11	FTN	F	304	-	-	0/18/18/18	0/2/2/2
10	HEM	G	201	3,4	-	0/6/54/54	0/0/8/8
12	EPH	H	201	-	-	0/47/47/52	0/0/0/0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	C3B-C2B	-5.12	1.33	1.40
10	C	201	HEM	C3C-C2C	-4.97	1.33	1.40
11	F	304	FTN	C9-N	-4.79	1.32	1.41
10	C	201	HEM	C3B-C2B	-4.41	1.34	1.40
10	G	201	HEM	C3C-C2C	-4.13	1.34	1.40
12	D	201	EPH	C18-C4	-3.82	1.39	1.50
12	H	201	EPH	C18-C4	-3.64	1.40	1.50
11	C	202	FTN	C9-N	-3.60	1.34	1.41
11	C	202	FTN	C13-C12	-3.23	1.32	1.38
12	D	201	EPH	C27-C28	-3.12	1.33	1.50
11	F	304	FTN	C10-C9	-3.11	1.34	1.39
12	H	201	EPH	C27-C28	-3.09	1.33	1.50
11	C	202	FTN	C10-C9	-2.45	1.35	1.39
12	D	201	EPH	C10-C11	-2.33	1.43	1.52
12	H	201	EPH	C10-C11	-2.28	1.43	1.52
11	F	304	FTN	C13-C12	-2.26	1.34	1.38
10	C	201	HEM	CAA-C2A	2.02	1.55	1.52
6	A	702	FAD	C2A-N1A	2.04	1.37	1.33
6	E	702	FAD	C6-C7	2.05	1.43	1.37
11	F	304	FTN	O2-C11	2.05	1.42	1.38
10	C	201	HEM	CMB-C2B	2.09	1.56	1.51
10	G	201	HEM	CAD-C3D	2.10	1.56	1.52
12	D	201	EPH	O2-C4	2.16	1.39	1.33
10	G	201	HEM	C4C-NC	2.24	1.39	1.36
6	E	702	FAD	C2A-N1A	2.24	1.38	1.33
11	C	202	FTN	O2-C11	2.47	1.43	1.38
6	E	702	FAD	C1'-N10	2.55	1.51	1.48
10	C	201	HEM	C1C-NC	2.57	1.39	1.36
10	C	201	HEM	C4D-ND	2.58	1.39	1.36
10	C	201	HEM	C1B-NB	2.64	1.39	1.36
6	E	702	FAD	C10-N1	2.71	1.37	1.33
6	E	702	FAD	C5X-N5	2.72	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	FAD	C10-N1	2.75	1.37	1.33
12	D	201	EPH	C26-C25	2.90	1.66	1.50
12	H	201	EPH	C26-C25	2.95	1.66	1.50
6	A	702	FAD	C1'-N10	3.00	1.51	1.48
12	D	201	EPH	P1-O7	3.02	1.62	1.50
10	G	201	HEM	C4D-ND	3.08	1.40	1.36
12	H	201	EPH	P1-O7	3.09	1.62	1.50
6	A	702	FAD	C4X-N5	3.13	1.37	1.33
12	H	201	EPH	C15-C16	3.18	1.53	1.29
12	D	201	EPH	C15-C16	3.25	1.54	1.29
10	G	201	HEM	C3C-CAC	3.46	1.54	1.47
10	C	201	HEM	C3C-CAC	3.51	1.54	1.47
6	E	702	FAD	C4-N3	3.81	1.39	1.33
6	A	702	FAD	C4-N3	3.84	1.40	1.33
10	C	201	HEM	C3B-CAB	3.90	1.55	1.47
12	H	201	EPH	C13-C12	3.91	1.53	1.31
10	G	201	HEM	C3B-CAB	3.92	1.55	1.47
12	D	201	EPH	C25-C24	3.95	1.53	1.31
12	D	201	EPH	C13-C12	3.95	1.53	1.31
6	A	702	FAD	C2A-N3A	3.98	1.38	1.32
12	H	201	EPH	C25-C24	4.00	1.54	1.31
6	E	702	FAD	C2A-N3A	4.05	1.38	1.32
10	C	201	HEM	C3D-C2D	5.42	1.53	1.37
10	G	201	HEM	C3D-C2D	5.51	1.54	1.37
11	F	304	FTN	C3-C2	5.52	1.49	1.40
6	E	702	FAD	C4X-N5	5.61	1.41	1.33
11	C	202	FTN	C3-C2	6.14	1.50	1.40
11	F	304	FTN	C10-C11	6.14	1.49	1.38
11	C	202	FTN	C12-C11	6.24	1.51	1.38
11	F	304	FTN	C13-C14	6.39	1.51	1.38
11	F	304	FTN	C12-C11	6.48	1.52	1.38
11	C	202	FTN	C13-C14	6.53	1.51	1.38
12	H	201	EPH	C29-C28	7.05	1.71	1.31
12	D	201	EPH	C29-C28	7.13	1.71	1.31
11	C	202	FTN	C14-C9	7.40	1.51	1.39
11	C	202	FTN	C10-C11	7.54	1.52	1.38
11	F	304	FTN	C14-C9	7.66	1.52	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	N3A-C2A-N1A	-9.55	120.54	128.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	304	FTN	C13-C14-C9	-9.55	108.18	119.72
6	E	702	FAD	N3A-C2A-N1A	-9.53	120.56	128.86
11	F	304	FTN	C12-C11-C10	-8.72	108.70	120.53
11	C	202	FTN	C13-C14-C9	-7.45	110.71	119.72
11	C	202	FTN	C12-C11-C10	-7.04	110.98	120.53
10	C	201	HEM	CAA-CBA-CGA	-5.67	102.98	112.66
11	F	304	FTN	C11-O2-C15	-4.26	113.71	119.39
6	A	702	FAD	C4X-C4-N3	-4.07	117.69	123.48
6	E	702	FAD	C4-C4X-C10	-4.03	116.70	119.96
11	F	304	FTN	F1-C1-C2	-3.80	105.86	112.69
12	H	201	EPH	C30-C29-C28	-3.47	112.13	127.03
11	C	202	FTN	C11-O2-C15	-3.43	114.82	119.39
11	C	202	FTN	F2-C1-C2	-3.19	106.95	112.69
6	A	702	FAD	C4A-C5A-N7A	-3.12	106.39	109.41
6	A	702	FAD	O2'-C2'-C3'	-3.00	101.64	109.09
10	C	201	HEM	CMA-C3A-C4A	-2.98	123.89	128.46
10	G	201	HEM	CAA-CBA-CGA	-2.68	108.08	112.66
12	D	201	EPH	C30-C29-C28	-2.65	115.65	127.03
11	C	202	FTN	C4-C3-C2	-2.50	116.47	119.54
11	C	202	FTN	F1-C1-C2	-2.49	108.20	112.69
10	G	201	HEM	CAA-C2A-C3A	-2.49	121.90	129.00
11	C	202	FTN	O2-C11-C12	-2.39	108.22	119.92
6	A	702	FAD	C1B-N9A-C4A	-2.38	122.53	126.64
6	E	702	FAD	C4A-C5A-N7A	-2.32	107.17	109.41
6	E	702	FAD	C4X-C4-N3	-2.32	120.19	123.48
6	A	702	FAD	C4'-C3'-C2'	-2.29	108.49	113.41
12	D	201	EPH	O5-P1-O7	-2.25	100.18	109.25
6	E	702	FAD	C9A-C5X-N5	-2.18	118.99	122.24
10	C	201	HEM	C3C-C4C-NC	-2.17	106.85	110.94
11	F	304	FTN	C9-N-C8	-2.08	121.25	126.61
11	F	304	FTN	O2-C11-C12	-2.05	109.86	119.92
11	F	304	FTN	O2-C11-C10	-2.03	108.64	119.47
12	H	201	EPH	C26-C25-C24	-2.00	110.19	124.81
11	C	202	FTN	C2-C3-C8	2.05	125.66	122.76
10	G	201	HEM	C4A-C3A-C2A	2.06	108.43	107.00
6	A	702	FAD	C5X-C9A-N10	2.09	119.21	117.66
11	C	202	FTN	C9-C10-C11	2.12	122.77	119.18
6	A	702	FAD	C1'-C2'-C3'	2.12	115.89	109.82
10	C	201	HEM	CMA-C3A-C2A	2.13	128.97	124.94
11	F	304	FTN	C13-C12-C11	2.32	122.76	118.95
10	C	201	HEM	CBD-CAD-C3D	2.38	117.01	112.47
6	E	702	FAD	C1'-N10-C10	2.40	120.96	118.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	C4X-N5-C5X	2.60	119.51	116.76
6	A	702	FAD	C4X-N5-C5X	2.62	119.53	116.76
10	G	201	HEM	C4C-C3C-C2C	2.64	108.74	106.90
12	H	201	EPH	C19-C18-C4	2.69	123.42	113.58
12	D	201	EPH	C19-C18-C4	2.84	123.96	113.58
10	C	201	HEM	CBA-CAA-C2A	3.10	118.41	112.48
12	H	201	EPH	C1-O2-C4	3.34	127.19	117.13
6	A	702	FAD	C1'-N10-C9A	3.35	121.42	118.35
6	E	702	FAD	C6-C5X-N5	3.37	122.92	118.97
12	H	201	EPH	C2-O1-C3	3.46	126.04	117.88
6	E	702	FAD	C1'-C2'-C3'	3.53	119.90	109.82
11	F	304	FTN	C14-C9-C10	3.67	123.98	119.66
10	G	201	HEM	CBD-CAD-C3D	3.88	119.86	112.47
12	D	201	EPH	C14-C15-C16	4.01	148.60	124.90
10	C	201	HEM	C4C-C3C-C2C	4.05	109.72	106.90
12	H	201	EPH	C14-C15-C16	4.13	149.33	124.90
12	D	201	EPH	C1-O2-C4	4.18	129.71	117.13
12	D	201	EPH	C2-O1-C3	4.88	129.41	117.88
6	E	702	FAD	C4-C4X-N5	5.03	124.19	118.68
6	E	702	FAD	C5X-C9A-N10	5.35	121.63	117.66
6	E	702	FAD	C4-N3-C2	6.14	120.53	115.16
6	A	702	FAD	C4-N3-C2	7.37	121.61	115.16
12	H	201	EPH	C15-C14-C13	8.40	140.40	111.84
12	D	201	EPH	C15-C14-C13	8.83	141.87	111.84
12	D	201	EPH	C27-C26-C25	12.31	145.62	112.93
12	H	201	EPH	C27-C26-C25	12.47	146.05	112.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	201	HEM	C2D-C3D-CAD-CBD
10	C	201	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

10 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	MLI	2	0
6	A	702	FAD	5	0
10	C	201	HEM	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	202	FTN	3	0
12	D	201	EPH	5	0
5	E	701	MLI	1	0
6	E	702	FAD	9	0
11	F	304	FTN	2	0
10	G	201	HEM	12	0
12	H	201	EPH	3	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, 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%)	-0.33	5 (0%)	86 63	53, 79, 102, 114	0
1	E	613/645 (95%)	-0.14	8 (1%)	77 50	59, 86, 110, 119	0
2	B	249/282 (88%)	-0.32	2 (0%)	86 63	54, 71, 94, 100	0
2	F	249/282 (88%)	-0.42	2 (0%)	86 63	60, 76, 100, 117	0
3	C	153/188 (81%)	-0.13	7 (4%)	33 13	64, 83, 159, 176	0
3	G	153/188 (81%)	-0.38	3 (1%)	65 35	66, 82, 126, 149	0
4	D	129/156 (82%)	-0.36	2 (1%)	72 43	69, 88, 123, 134	0
4	H	129/156 (82%)	-0.41	5 (3%)	40 16	69, 85, 112, 121	0
All	All	2288/2542 (90%)	-0.29	34 (1%)	74 46	53, 82, 111, 176	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	186	THR	10.7
3	C	185	PRO	7.1
3	C	184	LEU	5.1
4	D	45	ALA	5.0
4	D	49	PHE	4.7
3	C	180	LYS	3.3
4	H	52	LEU	3.1
1	A	33	ALA	2.9
1	E	420	GLY	2.9
3	C	183	THR	2.9
1	E	437	SER	2.8
1	E	474	ILE	2.8
1	E	34	GLN	2.7
1	A	628	LYS	2.5
3	G	186	THR	2.5
1	E	160	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	115	ASP	2.5
1	A	528	LYS	2.5
1	E	248	THR	2.4
2	B	279	PRO	2.4
1	A	246	CYS	2.3
3	G	185	PRO	2.2
3	G	180	LYS	2.2
4	H	51	PRO	2.2
2	B	88	SER	2.2
3	C	111	GLY	2.2
1	E	237	GLY	2.2
4	H	53	HIS	2.1
4	H	49	PHE	2.1
1	E	595	THR	2.1
1	A	486	ASP	2.0
2	F	88	SER	2.0
3	C	110	LEU	2.0
2	F	89	CYS	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
12	EPH	H	201	44/49	0.80	0.42	7.34	95,106,130,131	0
12	EPH	D	201	44/49	0.79	0.53	6.22	93,119,145,146	0
5	MLI	A	701	7/7	0.95	0.33	2.97	82,83,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	FTN	C	202	23/23	0.96	0.22	2.10	73,74,77,78	0
5	MLI	E	701	7/7	0.97	0.33	1.57	82,83,85,86	0
11	FTN	F	304	23/23	0.96	0.17	1.23	65,68,72,73	0
10	HEM	C	201	43/43	0.97	0.21	0.93	74,82,89,92	0
6	FAD	E	702	53/53	0.96	0.34	0.50	61,67,70,72	0
6	FAD	A	702	53/53	0.97	0.27	0.39	52,66,72,74	0
9	F3S	B	303	7/7	1.00	0.15	0.23	55,56,60,62	0
10	HEM	G	201	43/43	0.98	0.17	0.18	63,72,75,78	0
8	SF4	F	302	8/8	1.00	0.19	-0.22	49,52,53,54	0
8	SF4	B	302	8/8	0.99	0.20	-0.31	48,49,51,55	0
9	F3S	F	303	7/7	0.99	0.12	-0.87	66,67,69,69	0
7	FES	F	301	4/4	0.99	0.21	-1.03	59,63,65,66	0
7	FES	B	301	4/4	1.00	0.20	-1.30	52,54,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.