



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 AM GMT

PDB ID : 2BS2
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-
GENES
Authors : Lancaster, C.R.D.
Deposited on : 2005-05-14
Resolution : 1.78 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

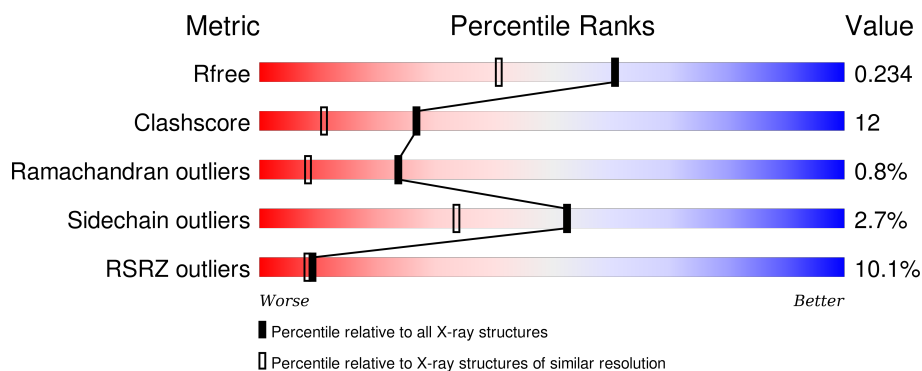
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	660	<div> <div>8%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	D	660	<div> <div>10%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	B	241	<div> <div>6%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
2	E	241	<div> <div>5%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
3	C	256	<div> <div>18%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	256	

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	LMT	C	1257	-	-	-	X
11	LMT	F	1257	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19666 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 QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	27	5	1
			5145	3219	927	967	32			
1	D	656	Total	C	N	O	S	32	3	1
			5125	3207	921	965	32			

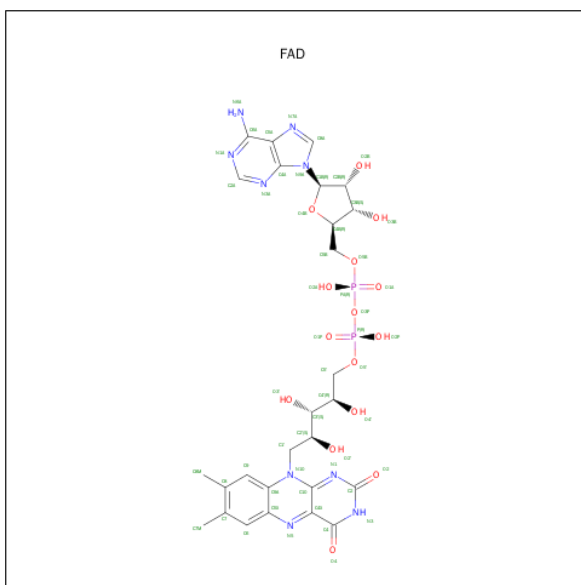
- Molecule 2 is a protein called QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			
2	E	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			

- Molecule 3 is a protein called QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C.

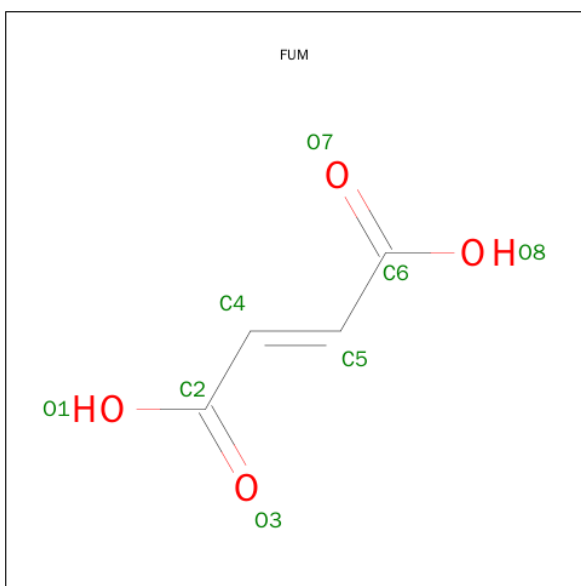
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	255	Total	C	N	O	S	16	2	1
			2099	1398	336	351	14			
3	F	255	Total	C	N	O	S	12	2	1
			2099	1398	336	351	14			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).

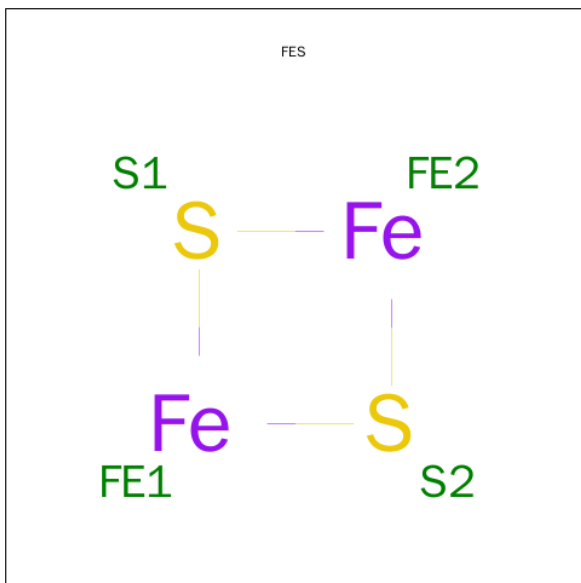


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

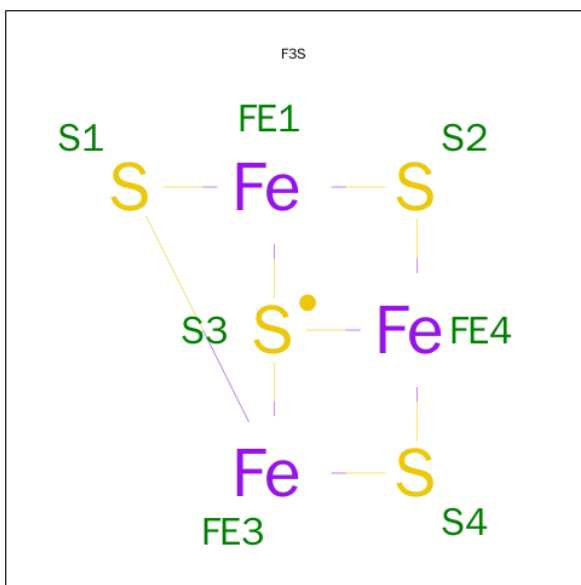
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



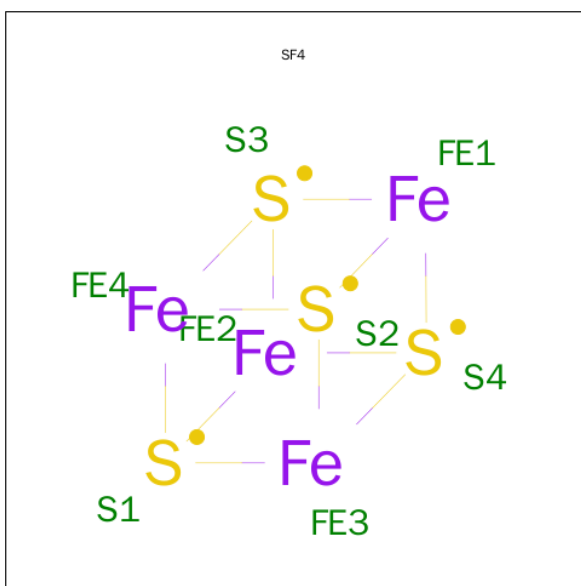
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



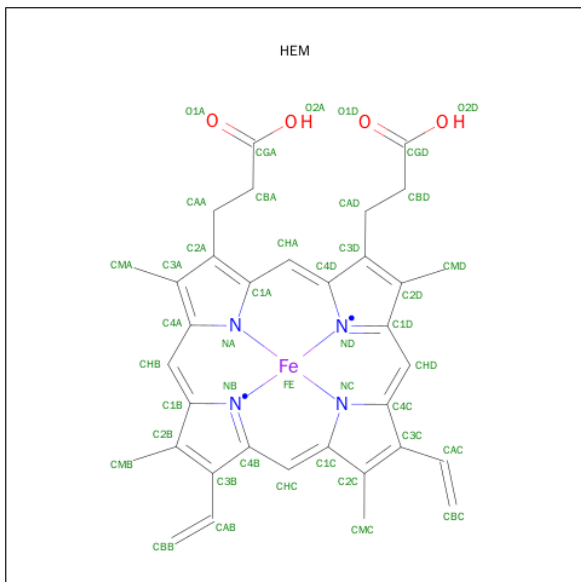
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



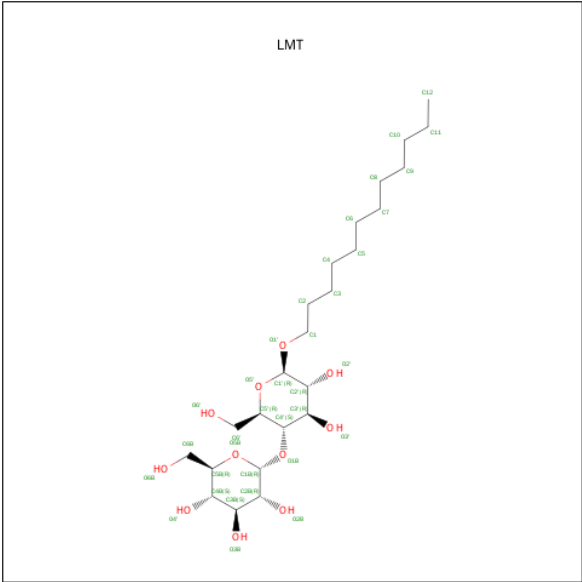
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		

- 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	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	16	0
			35	24	11		
11	F	1	Total	C	O	16	0
			35	24	11		

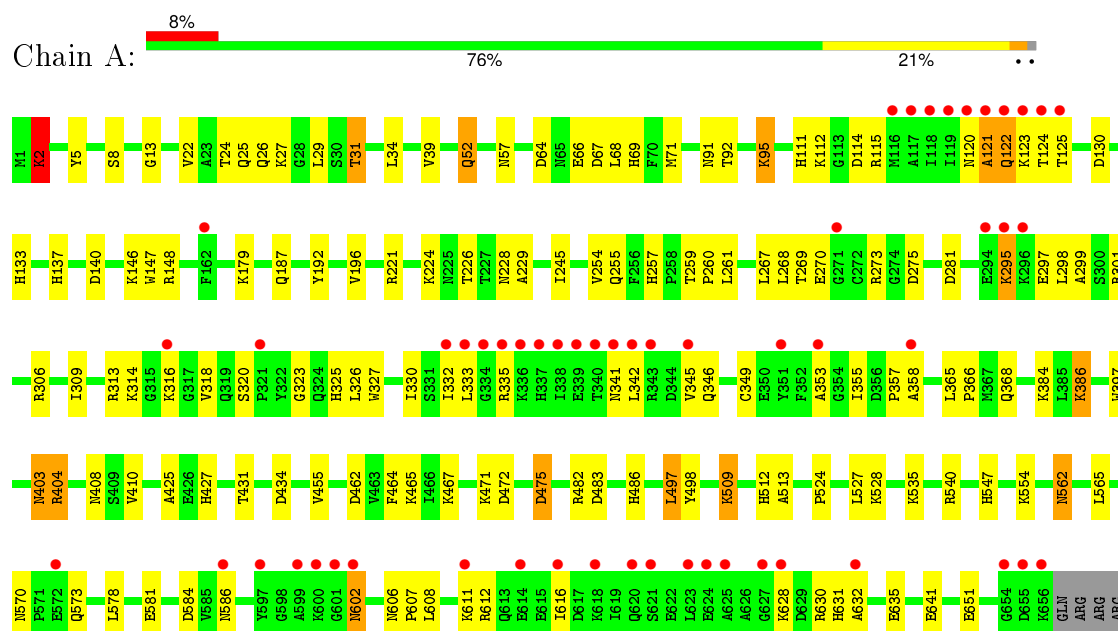
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	273	Total	O	1	0
			273	273		
12	B	155	Total	O	0	0
			155	155		
12	C	55	Total	O	0	0
			55	55		
12	D	287	Total	O	4	0
			287	287		
12	E	164	Total	O	0	0
			164	164		
12	F	56	Total	O	0	0
			56	56		

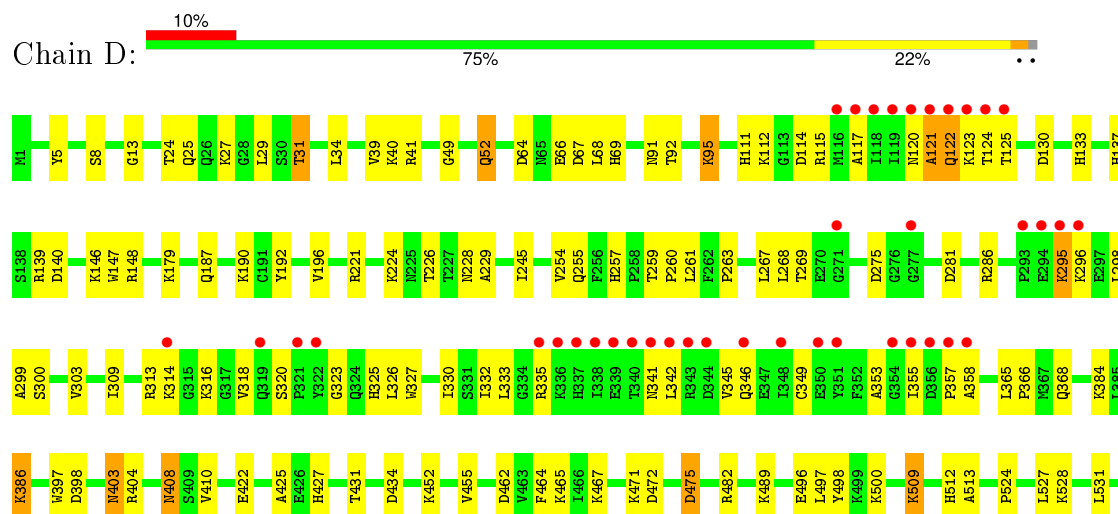
3 Residue-property plots

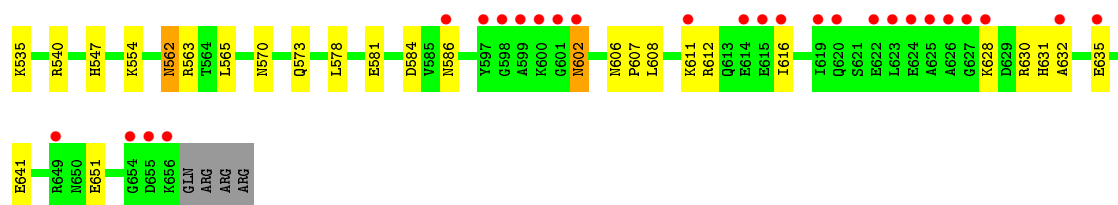
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

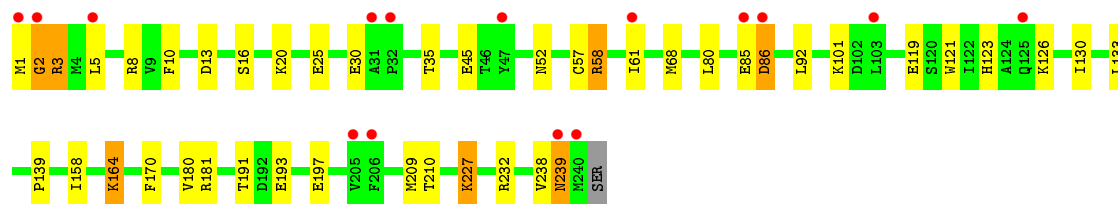
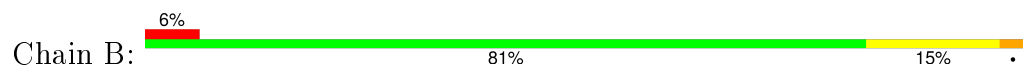


• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

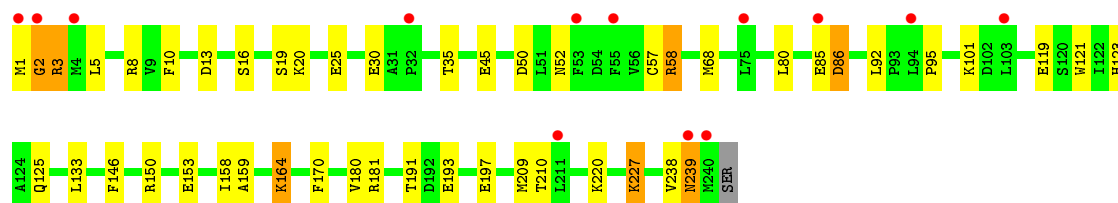
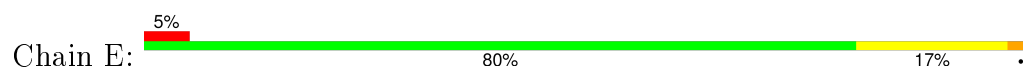




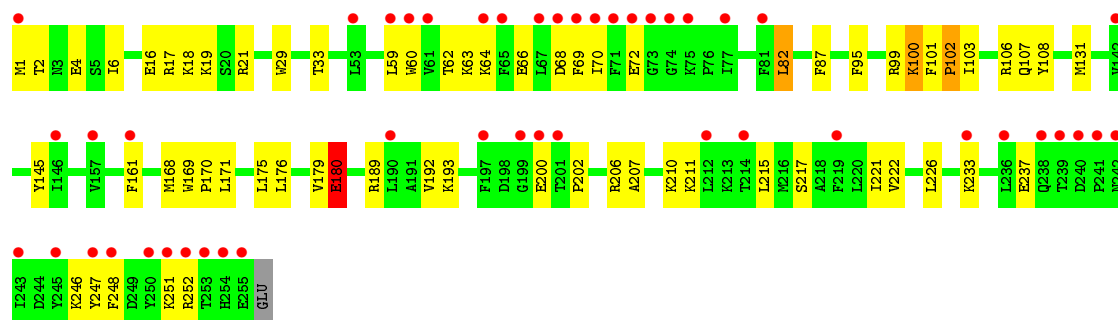
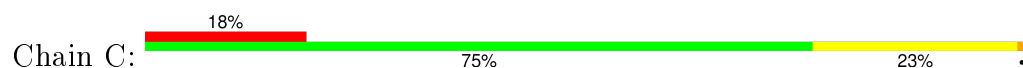
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B



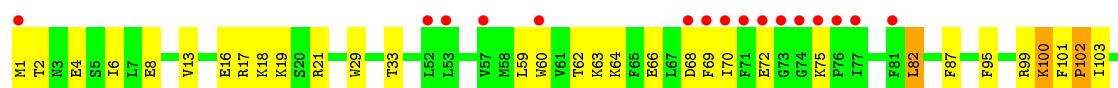
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

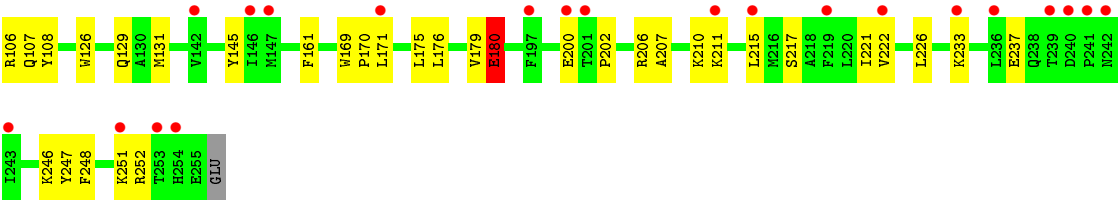


• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C



• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.10Å 188.77Å 117.82Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	28.70 – 1.78 28.70 – 1.78	Depositor EDS
% Data completeness (in resolution range)	92.5 (28.70-1.78) 92.3 (28.70-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.237 0.226 , 0.234	Depositor DCC
R_{free} test set	4488 reflections (1.44%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 317966 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19666	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SF4, LMT, F3S, FES, HEM, FUM, 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	2.00	2/5241 (0.0%)	0.61	3/7063 (0.0%)
1	D	0.32	0/5221	0.59	1/7038 (0.0%)
2	B	0.34	0/1939	0.59	0/2616
2	E	0.35	0/1939	0.59	0/2616
3	C	2.35	2/2165 (0.1%)	2.34	3/2930 (0.1%)
3	F	7.27	6/2165 (0.3%)	2.64	9/2930 (0.3%)
All	All	2.82	10/18670 (0.1%)	1.31	16/25193 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	180[A]	GLU	CD-OE2	220.23	3.67	1.25
3	F	180[B]	GLU	CD-OE2	220.23	3.67	1.25
1	A	2[A]	LYS	CE-NZ	101.15	4.01	1.49
1	A	2[B]	LYS	CE-NZ	101.15	4.01	1.49
3	F	180[A]	GLU	CG-CD	83.46	2.77	1.51
3	F	180[B]	GLU	CG-CD	83.46	2.77	1.51
3	C	180[A]	GLU	CD-OE2	76.70	2.10	1.25
3	C	180[B]	GLU	CD-OE2	76.70	2.10	1.25
3	F	180[A]	GLU	CD-OE1	40.43	1.70	1.25
3	F	180[B]	GLU	CD-OE1	40.43	1.70	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	180[A]	GLU	OE1-CD-OE2	-87.28	18.56	123.30
3	C	180[B]	GLU	OE1-CD-OE2	-87.28	18.56	123.30
3	F	180[A]	GLU	OE1-CD-OE2	-84.43	21.99	123.30
3	F	180[B]	GLU	OE1-CD-OE2	-84.43	21.99	123.30
3	F	180[A]	GLU	CG-CD-OE2	-38.95	40.40	118.30
3	F	180[B]	GLU	CG-CD-OE2	-38.95	40.40	118.30
3	F	180[A]	GLU	CG-CD-OE1	-29.66	58.98	118.30
3	F	180[B]	GLU	CG-CD-OE1	-29.66	58.98	118.30
3	F	180[A]	GLU	CB-CG-CD	-18.86	63.28	114.20
3	F	180[B]	GLU	CB-CG-CD	-18.86	63.28	114.20
1	A	2[A]	LYS	CD-CE-NZ	-10.05	88.58	111.70
1	A	2[B]	LYS	CD-CE-NZ	-10.05	88.58	111.70
3	F	102	PRO	N-CA-C	-5.60	97.55	112.10
3	C	102	PRO	N-CA-C	-5.58	97.60	112.10
1	D	397	TRP	N-CA-C	-5.19	96.98	111.00
1	A	397	TRP	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	180[A]	GLU	Sidechain
3	F	180[A]	GLU	Sidechain

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	5145	0	5124	126	0
1	D	5125	0	5100	128	0
2	B	1902	0	1869	44	0
2	E	1902	0	1869	49	0
3	C	2099	0	2111	56	0
3	F	2099	0	2111	67	0
4	A	53	0	29	3	0
4	D	53	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	2	0	0
5	D	8	0	2	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
8	B	7	0	0	0	0
8	E	7	0	0	0	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
10	C	86	0	60	1	0
10	F	86	0	60	1	0
11	C	35	0	46	8	0
11	F	35	0	46	9	0
12	A	273	0	0	9	0
12	B	155	0	0	3	0
12	C	55	0	0	1	0
12	D	287	0	0	5	0
12	E	164	0	0	2	0
12	F	56	0	0	1	0
All	All	19666	0	18458	444	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 12.

All (444) 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)
3:F:180[B]:GLU:CG	3:F:180[B]:GLU:CD	1.80	1.47
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:OE1	1.70	1.31
3:F:180[B]:GLU:HG2	3:F:180[B]:GLU:OE1	1.47	1.11
2:B:1:MET:HG2	2:B:2:GLY:H	1.24	1.01
2:E:1:MET:HG2	2:E:2:GLY:H	1.24	0.98
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:HB2	1.84	0.97
1:D:64:ASP:HB2	1:D:146:LYS:HG2	1.47	0.96
1:A:64:ASP:HB2	1:A:146:LYS:HG2	1.47	0.95
3:F:180[A]:GLU:OE2	3:F:180[A]:GLU:HG3	1.68	0.93
2:B:8:ARG:HG2	2:B:25:GLU:HG2	1.52	0.90
2:E:8:ARG:HG2	2:E:25:GLU:HG2	1.53	0.89
1:D:27:LYS:HD2	1:D:425:ALA:HB1	1.56	0.86
1:A:27:LYS:HD2	1:A:425:ALA:HB1	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:MET:SD	3:F:100:LYS:HG3	2.17	0.85
1:A:52:GLN:HG2	1:A:69:HIS:NE2	1.92	0.85
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:HG2	1.76	0.84
2:B:209:MET:SD	3:C:100:LYS:HG3	2.17	0.84
1:D:52:GLN:HG2	1:D:69:HIS:NE2	1.92	0.83
1:A:535:LYS:HG3	1:A:578:LEU:HD11	1.60	0.83
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:CB	2.49	0.81
1:D:535:LYS:HG3	1:D:578:LEU:HD11	1.61	0.81
3:F:131:MET:HG2	11:F:1257:LMT:H123	1.63	0.80
1:A:330:ILE:HD11	1:A:357:PRO:HB2	1.63	0.80
3:F:103:ILE:H	3:F:107:GLN:NE2	1.80	0.80
3:C:131:MET:HG2	11:C:1257:LMT:H123	1.63	0.79
1:D:330:ILE:HD11	1:D:357:PRO:HB2	1.63	0.79
1:D:112:LYS:H	1:D:133:HIS:HD2	1.31	0.79
2:E:180:VAL:HG11	2:E:227:LYS:HG3	1.65	0.78
3:C:103:ILE:H	3:C:107:GLN:NE2	1.82	0.78
1:A:611:LYS:NZ	1:A:611:LYS:HB3	2.00	0.76
1:D:611:LYS:NZ	1:D:611:LYS:HB3	2.00	0.76
1:D:628:LYS:HG3	1:D:632:ALA:HB3	1.68	0.76
1:A:628:LYS:HG3	1:A:632:ALA:HB3	1.67	0.76
2:E:238:VAL:O	2:E:239:ASN:HB2	1.85	0.75
1:A:112:LYS:H	1:A:133:HIS:HD2	1.32	0.75
2:B:180:VAL:HG11	2:B:227:LYS:HG3	1.67	0.75
3:C:180[B]:GLU:HG3	3:C:180[B]:GLU:OE2	1.87	0.74
1:D:268:LEU:HD22	1:D:345:VAL:HG23	1.70	0.74
2:E:1:MET:HG2	2:E:2:GLY:N	2.02	0.74
1:A:346:GLN:HA	1:A:357:PRO:HG3	1.70	0.74
2:B:238:VAL:O	2:B:239:ASN:HB2	1.86	0.74
1:D:179:LYS:HG3	1:D:196:VAL:HG11	1.70	0.73
1:D:112:LYS:HG3	1:D:130:ASP:HA	1.70	0.73
1:D:482:ARG:HH11	1:D:547:HIS:HD2	1.36	0.73
1:D:346:GLN:HA	1:D:357:PRO:HG3	1.69	0.73
1:A:179:LYS:HG3	1:A:196:VAL:HG11	1.70	0.72
1:A:268:LEU:HD22	1:A:345:VAL:HG23	1.70	0.72
1:A:112:LYS:HG3	1:A:130:ASP:HA	1.70	0.72
1:A:482:ARG:HH11	1:A:547:HIS:HD2	1.36	0.72
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:CG	2.38	0.72
1:A:179:LYS:HG3	1:A:196:VAL:CG1	2.20	0.71
1:D:179:LYS:HG3	1:D:196:VAL:CG1	2.20	0.71
3:C:4:GLU:H	3:C:4:GLU:CD	1.94	0.71
2:B:1:MET:HG2	2:B:2:GLY:N	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:GLU:CD	3:F:4:GLU:H	1.94	0.70
3:F:180[A]:GLU:CG	3:F:180[A]:GLU:OE1	2.39	0.70
3:F:180[A]:GLU:CG	3:F:180[A]:GLU:OE2	2.38	0.70
3:C:95:PHE:HE1	11:F:1257:LMT:H101	1.58	0.69
3:F:131:MET:HG2	11:F:1257:LMT:C12	2.23	0.68
3:C:131:MET:HG2	11:C:1257:LMT:C12	2.23	0.67
1:D:320:SER:HB3	1:D:323:GLY:O	1.94	0.67
1:A:386:LYS:HG3	12:A:2164:HOH:O	1.95	0.66
1:D:386:LYS:HG3	12:D:2164:HOH:O	1.95	0.66
1:A:320:SER:HB3	1:A:323:GLY:O	1.94	0.66
1:D:121:ALA:O	1:D:122:GLN:HG3	1.96	0.66
1:A:64:ASP:CB	1:A:146:LYS:HG2	2.25	0.66
2:E:191:THR:OG1	2:E:193:GLU:HG2	1.96	0.65
1:D:64:ASP:CB	1:D:146:LYS:HG2	2.25	0.65
1:D:540:ARG:HH22	1:D:562:ASN:ND2	1.95	0.65
1:A:540:ARG:HH22	1:A:562:ASN:ND2	1.93	0.65
2:B:126:LYS:HG2	12:B:2083:HOH:O	1.96	0.65
1:A:342:LEU:HB3	1:A:345:VAL:HG12	1.79	0.64
3:C:69:PHE:CD1	3:C:70:ILE:HG13	2.32	0.64
3:F:69:PHE:HD1	3:F:70:ILE:HG13	1.62	0.64
2:E:68:MET:HB2	2:E:92:LEU:HB2	1.79	0.64
1:A:121:ALA:O	1:A:122:GLN:HG3	1.97	0.64
2:B:191:THR:OG1	2:B:193:GLU:HG2	1.97	0.64
2:B:68:MET:HB2	2:B:92:LEU:HB2	1.80	0.64
2:E:119:GLU:OE1	2:E:123:HIS:HE1	1.81	0.64
2:B:119:GLU:OE1	2:B:123:HIS:HE1	1.80	0.64
1:A:342:LEU:HB3	1:A:345:VAL:CG1	2.29	0.63
3:F:69:PHE:CD1	3:F:70:ILE:HG13	2.32	0.63
1:D:342:LEU:HB3	1:D:345:VAL:CG1	2.28	0.63
1:D:342:LEU:HB3	1:D:345:VAL:HG12	1.79	0.63
1:D:64:ASP:HB2	1:D:146:LYS:CG	2.27	0.63
1:D:115[A]:ARG:HD2	1:D:117:ALA:HB2	1.81	0.63
3:C:69:PHE:HD1	3:C:70:ILE:HG13	1.62	0.63
1:A:540:ARG:HH22	1:A:562:ASN:HD22	1.45	0.63
1:D:221:ARG:HD2	1:D:226:THR:HG21	1.81	0.63
1:D:540:ARG:HH22	1:D:562:ASN:HD22	1.46	0.62
3:C:1:MET:HE3	3:C:6:ILE:HD11	1.82	0.62
1:A:342:LEU:O	1:A:345:VAL:HG12	2.00	0.62
1:A:27:LYS:HD2	1:A:425:ALA:CB	2.29	0.61
1:D:224:LYS:HB3	1:D:475:ASP:OD2	2.00	0.61
1:A:651:GLU:OE2	2:B:133:LEU:HD23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HG2	2:B:3:ARG:H	1.66	0.61
3:C:103:ILE:H	3:C:107:GLN:HE21	1.48	0.61
2:B:2:GLY:O	2:B:30:GLU:HB3	2.01	0.61
3:F:103:ILE:H	3:F:107:GLN:HE21	1.48	0.61
1:D:342:LEU:O	1:D:345:VAL:HG12	2.00	0.61
2:E:2:GLY:O	2:E:30:GLU:HB3	2.01	0.61
3:F:180[B]:GLU:CB	3:F:180[B]:GLU:CD	2.63	0.61
1:A:64:ASP:HB2	1:A:146:LYS:CG	2.26	0.61
3:F:180[B]:GLU:CG	3:F:180[B]:GLU:OE1	2.38	0.60
1:D:295:LYS:HG2	1:D:299:ALA:HA	1.83	0.60
2:E:1:MET:HG2	2:E:3:ARG:H	1.66	0.60
1:D:651:GLU:OE2	2:E:133:LEU:HD23	2.00	0.60
1:D:27:LYS:HD2	1:D:425:ALA:CB	2.30	0.60
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:OE1	2.19	0.59
2:E:180:VAL:HG11	2:E:227:LYS:CG	2.32	0.59
3:F:180[A]:GLU:OE1	3:F:180[A]:GLU:OE2	2.20	0.59
1:A:221:ARG:HD2	1:A:226:THR:HG21	1.84	0.59
2:E:13:ASP:HA	2:E:101:LYS:HG3	1.84	0.59
3:F:233:LYS:O	3:F:237:GLU:HG3	2.03	0.59
3:C:17:ARG:NH1	2:E:16:SER:O	2.35	0.59
1:A:295:LYS:HG2	1:A:299:ALA:HA	1.83	0.59
2:B:13:ASP:HA	2:B:101:LYS:HG3	1.84	0.59
1:D:257:HIS:HD2	1:D:259:THR:H	1.51	0.59
11:C:1257:LMT:H101	3:F:95:PHE:HE1	1.68	0.59
2:B:180:VAL:HG11	2:B:227:LYS:CG	2.33	0.58
1:D:92:THR:O	1:D:95:LYS:HG3	2.03	0.58
3:C:233:LYS:O	3:C:237:GLU:HG3	2.03	0.58
2:E:2:GLY:O	2:E:3:ARG:HG2	2.04	0.58
2:B:2:GLY:O	2:B:3:ARG:HG2	2.03	0.58
1:A:332:ILE:HD12	1:A:333:LEU:N	2.19	0.58
1:A:562:ASN:HD22	1:A:562:ASN:C	2.07	0.58
1:A:224:LYS:HB3	1:A:475:ASP:OD2	2.03	0.58
1:A:92:THR:O	1:A:95:LYS:HG3	2.04	0.58
1:D:562:ASN:C	1:D:562:ASN:HD22	2.06	0.57
1:A:257:HIS:HD2	1:A:259:THR:H	1.51	0.57
1:D:257:HIS:CE1	1:D:267:LEU:HD11	2.39	0.57
1:A:257:HIS:CE1	1:A:267:LEU:HD11	2.39	0.57
3:F:207:ALA:O	3:F:211:LYS:HG3	2.04	0.57
1:D:464:PHE:CD1	2:E:45:GLU:HG2	2.40	0.57
3:C:206:ARG:O	3:C:210:LYS:HG3	2.04	0.57
1:D:570:ASN:O	1:D:573:GLN:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:TYR:HA	1:A:527:LEU:HD13	1.87	0.57
1:A:455:VAL:O	1:A:509:LYS:HD2	2.04	0.57
3:F:206:ARG:O	3:F:210:LYS:HG3	2.04	0.57
3:C:207:ALA:O	3:C:211:LYS:HG3	2.05	0.57
1:D:455:VAL:O	1:D:509:LYS:HD2	2.05	0.57
1:D:332:ILE:HD12	1:D:333:LEU:N	2.19	0.56
1:A:8:SER:HB2	1:A:31:THR:HB	1.87	0.56
3:F:102:PRO:O	11:F:1257:LMT:H62	2.05	0.56
3:C:102:PRO:O	11:C:1257:LMT:H62	2.06	0.56
3:C:95:PHE:CE1	11:F:1257:LMT:H51	2.42	0.55
2:E:121:TRP:O	2:E:123:HIS:HD2	1.89	0.55
1:D:498:TYR:HA	1:D:527:LEU:HD13	1.87	0.55
1:A:306:ARG:HD2	12:A:2241:HOH:O	2.07	0.55
1:A:611:LYS:HZ3	1:A:611:LYS:HB3	1.72	0.54
2:B:85:GLU:O	2:B:86:ASP:HB2	2.07	0.54
2:E:85:GLU:O	2:E:86:ASP:HB2	2.07	0.54
3:F:248:PHE:HE2	3:F:252:ARG:HH21	1.55	0.54
3:C:211:LYS:O	3:C:215:LEU:HD23	2.07	0.54
3:C:217:SER:O	3:C:221:ILE:HG12	2.08	0.54
2:E:10:PHE:HB2	2:E:92:LEU:HD23	1.90	0.54
1:A:570:ASN:O	1:A:573:GLN:HG2	2.06	0.54
3:F:217:SER:O	3:F:221:ILE:HG12	2.07	0.54
1:A:464:PHE:CD1	2:B:45:GLU:HG2	2.42	0.54
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:CD	2.46	0.54
1:A:114:ASP:HB3	1:A:125:THR:HG21	1.89	0.54
2:B:121:TRP:O	2:B:123:HIS:HD2	1.91	0.53
2:B:197:GLU:OE1	3:C:19:LYS:HG3	2.08	0.53
2:E:197:GLU:O	3:F:19:LYS:HD2	2.09	0.53
1:D:114:ASP:HB3	1:D:125:THR:HG21	1.89	0.53
1:A:260:PRO:HD2	1:A:365:LEU:O	2.07	0.53
3:F:211:LYS:O	3:F:215:LEU:HD23	2.09	0.53
3:C:169:TRP:N	3:C:170:PRO:HD2	2.24	0.53
2:B:10:PHE:HB2	2:B:92:LEU:HD23	1.90	0.53
3:C:248:PHE:HE2	3:C:252:ARG:HH21	1.56	0.53
3:C:145:TYR:OH	3:F:170:PRO:HG2	2.09	0.53
2:B:197:GLU:O	3:C:19:LYS:HD2	2.09	0.53
2:B:158:ILE:HG23	2:B:164:LYS:HD3	1.91	0.53
1:D:8:SER:HB2	1:D:31:THR:HB	1.91	0.53
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:CG	2.77	0.52
1:A:112:LYS:HG3	1:A:130:ASP:CA	2.40	0.52
1:D:260:PRO:HD2	1:D:365:LEU:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ASP:HB2	1:D:147:TRP:CE2	2.45	0.52
3:F:169:TRP:N	3:F:170:PRO:HD2	2.24	0.52
1:A:140:ASP:HB2	1:A:147:TRP:CE2	2.45	0.52
1:D:482:ARG:NH1	1:D:547:HIS:HD2	2.06	0.52
1:D:257:HIS:CD2	1:D:259:THR:H	2.28	0.52
3:C:170:PRO:HG2	3:F:145:TYR:OH	2.09	0.52
1:D:24:THR:OG1	1:D:31:THR:HG21	2.10	0.51
2:E:158:ILE:HG23	2:E:164:LYS:HD3	1.91	0.51
1:A:434:ASP:OD1	1:D:434:ASP:OD1	2.28	0.51
1:A:24:THR:OG1	1:A:31:THR:HG21	2.11	0.51
3:F:1:MET:CE	3:F:6:ILE:HD11	2.41	0.51
2:E:197:GLU:OE1	3:F:19:LYS:HG3	2.10	0.51
1:D:255:GLN:HE21	1:D:403:ASN:ND2	2.08	0.51
1:D:122:GLN:O	1:D:124:THR:N	2.36	0.51
1:A:467:LYS:O	1:A:471:LYS:HG3	2.11	0.51
1:A:245:ILE:O	1:A:384:LYS:HE2	2.10	0.51
1:D:524:PRO:O	1:D:528:LYS:HG3	2.10	0.51
1:A:295:LYS:CG	1:A:299:ALA:HA	2.41	0.51
1:A:52:GLN:HG3	1:A:148:ARG:HD2	1.94	0.51
1:D:295:LYS:CG	1:D:299:ALA:HA	2.41	0.51
3:C:168:MET:HE2	12:C:2043:HOH:O	2.10	0.51
2:B:61:ILE:HG23	12:B:2038:HOH:O	2.10	0.51
1:A:64:ASP:HA	1:A:68:LEU:HD12	1.94	0.50
1:A:257:HIS:CD2	1:A:259:THR:H	2.28	0.50
3:C:1:MET:CE	3:C:6:ILE:HD11	2.40	0.50
3:C:17:ARG:HD2	2:E:19:SER:O	2.11	0.50
1:A:325:HIS:HD2	1:A:326:LEU:O	1.94	0.50
3:F:101:PHE:HB3	11:F:1257:LMT:H71	1.93	0.50
1:D:482:ARG:HH11	1:D:547:HIS:CD2	2.23	0.50
1:A:482:ARG:HH11	1:A:547:HIS:CD2	2.23	0.50
2:E:1:MET:CG	2:E:2:GLY:H	2.09	0.50
1:A:611:LYS:HZ2	1:A:611:LYS:HB3	1.75	0.50
2:E:52:ASN:OD1	2:E:101:LYS:HE3	2.11	0.50
1:A:270:GLU:HG3	1:A:273[A]:ARG:HH22	1.76	0.50
3:C:175:LEU:O	3:C:179:VAL:HG12	2.12	0.50
3:C:16[B]:GLU:HA	2:E:20:LYS:CE	2.42	0.50
3:C:16[B]:GLU:HA	2:E:20:LYS:HE3	1.92	0.50
1:A:482:ARG:NH1	1:A:547:HIS:HD2	2.06	0.50
1:A:255:GLN:HE21	1:A:403:ASN:ND2	2.10	0.50
2:E:239:ASN:CG	3:F:21:ARG:HE	2.15	0.50
1:A:257:HIS:O	1:A:366:PRO:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ILE:O	1:D:384:LYS:HE2	2.12	0.50
3:F:1:MET:HE1	3:F:6:ILE:HD11	1.93	0.50
3:C:62:THR:O	3:C:66:GLU:HG3	2.12	0.50
1:D:452:LYS:NZ	12:D:2200:HOH:O	2.45	0.49
1:D:64:ASP:HA	1:D:68:LEU:HD12	1.93	0.49
2:E:52:ASN:CG	2:E:101:LYS:HE3	2.33	0.49
1:D:281:ASP:HB2	1:D:316:LYS:HG3	1.93	0.49
2:B:1:MET:CG	2:B:2:GLY:H	2.09	0.49
3:F:62:THR:O	3:F:66:GLU:HG3	2.12	0.49
1:D:467:LYS:O	1:D:471:LYS:HG3	2.11	0.49
1:D:112:LYS:HG3	1:D:130:ASP:CA	2.40	0.49
1:A:111:HIS:HA	1:A:133:HIS:CD2	2.48	0.49
1:A:631:HIS:O	1:A:635:GLU:HG3	2.12	0.49
1:D:341:ASN:C	1:D:342:LEU:HD12	2.33	0.49
1:D:325:HIS:HD2	1:D:326:LEU:O	1.95	0.49
1:A:228:ASN:HD22	1:A:228:ASN:N	2.10	0.49
1:A:427:HIS:O	1:A:431:THR:HG22	2.13	0.49
1:A:281:ASP:HB2	1:A:316:LYS:HG3	1.93	0.49
1:D:651:GLU:HG2	2:E:133:LEU:CD2	2.43	0.49
1:D:111:HIS:HA	1:D:133:HIS:CD2	2.48	0.49
2:B:239:ASN:CG	3:C:21:ARG:HE	2.15	0.49
1:A:651:GLU:HG2	2:B:133:LEU:CD2	2.43	0.49
1:A:524:PRO:O	1:A:528:LYS:HG3	2.12	0.49
1:D:52:GLN:HG3	1:D:148:ARG:HD2	1.94	0.48
3:C:99:ARG:HG2	11:F:1257:LMT:H32	1.95	0.48
3:C:101:PHE:HB3	11:C:1257:LMT:H71	1.94	0.48
3:F:175:LEU:O	3:F:179:VAL:HG12	2.13	0.48
2:B:52:ASN:CG	2:B:101:LYS:HE3	2.33	0.48
1:D:259:THR:N	1:D:260:PRO:HD3	2.29	0.48
1:A:462:ASP:HB3	1:A:465:LYS:HD3	1.94	0.48
1:D:611:LYS:HZ2	1:D:611:LYS:HB3	1.74	0.48
1:A:341:ASN:C	1:A:342:LEU:HD12	2.33	0.48
1:A:384:LYS:NZ	12:A:2166:HOH:O	2.44	0.48
1:D:427:HIS:O	1:D:431:THR:HG22	2.13	0.48
1:D:631:HIS:O	1:D:635:GLU:HG3	2.12	0.48
1:D:462:ASP:HB3	1:D:465:LYS:HD3	1.95	0.48
1:D:257:HIS:O	1:D:366:PRO:HA	2.13	0.48
1:D:228:ASN:N	1:D:228:ASN:HD22	2.12	0.48
1:D:342:LEU:HD12	1:D:342:LEU:N	2.29	0.48
1:D:190:LYS:HE3	12:D:2069:HOH:O	2.14	0.48
1:D:179:LYS:CG	1:D:196:VAL:HG11	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:CG	1:A:196:VAL:HG11	2.42	0.47
3:F:2:THR:OG1	3:F:4:GLU:HG2	2.15	0.47
1:D:384:LYS:NZ	12:D:2165:HOH:O	2.43	0.47
1:A:410:VAL:HG13	4:A:1656:FAD:C2	2.44	0.47
1:D:309:ILE:O	1:D:313:ARG:HG3	2.14	0.47
11:C:1257:LMT:H32	3:F:99:ARG:HG2	1.97	0.47
1:A:342:LEU:HD12	1:A:342:LEU:N	2.30	0.47
1:D:67:ASP:OD2	1:D:630:ARG:HD2	2.14	0.47
1:A:25:GLN:OE1	1:A:31:THR:HG23	2.14	0.47
1:A:120:ASN:HB3	1:A:298:LEU:CD1	2.45	0.47
2:B:130:ILE:HG12	12:B:2087:HOH:O	2.14	0.47
3:C:16[A]:GLU:HA	2:E:20:LYS:HE3	1.95	0.47
3:C:16[A]:GLU:HA	2:E:20:LYS:CE	2.45	0.47
1:D:410:VAL:HG13	4:D:1656:FAD:C2	2.45	0.47
1:D:120:ASN:HB3	1:D:298:LEU:CD1	2.45	0.47
1:A:259:THR:N	1:A:260:PRO:HD3	2.30	0.47
1:D:120:ASN:HB3	1:D:298:LEU:HD13	1.97	0.47
1:D:66:GLU:HG2	1:D:91:ASN:HD22	1.79	0.47
2:B:2:GLY:O	2:B:3:ARG:CG	2.64	0.47
3:F:108:TYR:CD2	11:F:1257:LMT:H52	2.50	0.47
1:A:120:ASN:HB3	1:A:298:LEU:HD13	1.97	0.47
3:C:108:TYR:CD2	11:C:1257:LMT:H52	2.50	0.46
3:C:176:LEU:O	3:C:180[B]:GLU:HB2	2.15	0.46
1:A:270:GLU:HG3	1:A:273[A]:ARG:NH2	2.30	0.46
1:D:607:PRO:HG2	1:D:608:LEU:HD12	1.96	0.46
1:A:607:PRO:HG2	1:A:608:LEU:HD12	1.97	0.46
2:E:57:CYS:O	2:E:58:ARG:HG3	2.14	0.46
1:A:115[B]:ARG:HB2	12:A:2055:HOH:O	2.15	0.46
1:A:554:LYS:HG2	1:A:602:ASN:ND2	2.31	0.46
1:D:611:LYS:HB3	1:D:611:LYS:HZ3	1.75	0.46
1:A:273[A]:ARG:NH1	1:A:273[A]:ARG:HB2	2.30	0.46
1:A:67:ASP:OD2	1:A:630:ARG:HD2	2.15	0.46
1:D:261:LEU:HD21	1:D:353:ALA:HB2	1.97	0.46
3:C:2:THR:OG1	3:C:4:GLU:HG2	2.15	0.46
2:B:52:ASN:OD1	2:B:101:LYS:HE3	2.15	0.46
1:A:410:VAL:HG13	4:A:1656:FAD:N1	2.31	0.46
1:A:122:GLN:O	1:A:124:THR:N	2.37	0.46
1:D:187:GLN:HB3	1:D:192:TYR:HE2	1.81	0.46
2:B:57:CYS:O	2:B:58:ARG:HG3	2.16	0.46
1:A:540:ARG:NH2	1:A:562:ASN:ND2	2.63	0.45
1:A:13:GLY:HA3	1:A:39:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:GLY:O	2:E:3:ARG:CG	2.64	0.45
3:F:171:LEU:HD23	3:F:171:LEU:C	2.37	0.45
1:A:261:LEU:HD21	1:A:353:ALA:HB2	1.98	0.45
1:A:309:ILE:O	1:A:313:ARG:HG3	2.16	0.45
1:A:187:GLN:HB3	1:A:192:TYR:HE2	1.81	0.45
1:A:297:GLU:CD	1:A:297:GLU:H	2.19	0.45
3:C:59:LEU:HD22	3:C:252:ARG:NH1	2.32	0.45
4:D:1656:FAD:H1'1	4:D:1656:FAD:H9	1.61	0.45
1:A:5:TYR:CD1	1:A:5:TYR:C	2.89	0.45
1:A:66:GLU:HG2	1:A:91:ASN:HD22	1.80	0.45
3:F:59:LEU:HD22	3:F:252:ARG:NH1	2.32	0.45
3:C:171:LEU:HD23	3:C:171:LEU:C	2.36	0.45
1:D:410:VAL:HG13	4:D:1656:FAD:N1	2.32	0.45
2:E:125:GLN:HG2	12:E:2094:HOH:O	2.16	0.45
1:D:13:GLY:HA3	1:D:39:VAL:HG12	1.98	0.45
1:D:5:TYR:CD1	1:D:5:TYR:C	2.89	0.45
2:E:52:ASN:OD1	2:E:101:LYS:CE	2.64	0.45
1:D:554:LYS:HG2	1:D:602:ASN:ND2	2.31	0.45
3:F:176:LEU:O	3:F:180[B]:GLU:HB2	2.17	0.45
11:C:1257:LMT:H51	3:F:95:PHE:CE1	2.52	0.44
1:D:540:ARG:NH2	1:D:562:ASN:ND2	2.64	0.44
2:B:193:GLU:H	2:B:193:GLU:CD	2.21	0.44
1:D:221:ARG:HD3	1:D:229:ALA:O	2.17	0.44
2:B:35:THR:HG22	2:B:80:LEU:HD23	1.98	0.44
1:A:455:VAL:CG1	1:A:509:LYS:HG3	2.48	0.44
1:A:554:LYS:HG2	1:A:602:ASN:HD22	1.83	0.44
2:E:193:GLU:CD	2:E:193:GLU:H	2.20	0.44
2:E:35:THR:HG22	2:E:80:LEU:HD23	2.00	0.44
1:D:25:GLN:OE1	1:D:31:THR:HG23	2.18	0.44
1:A:608:LEU:HD12	1:A:608:LEU:N	2.33	0.44
1:D:422:GLU:HG2	12:D:2177:HOH:O	2.18	0.44
1:D:49:GLY:HA2	1:D:139[A]:ARG:HH21	1.82	0.44
1:A:34:LEU:HD22	1:A:179:LYS:HG2	2.00	0.44
1:A:2[A]:LYS:HE3	12:A:2108:HOH:O	2.18	0.44
2:B:85:GLU:HA	2:B:85:GLU:OE2	2.18	0.43
3:F:8:GLU:HA	3:F:13:VAL:O	2.18	0.43
3:F:247:TYR:O	3:F:251:LYS:HG3	2.18	0.43
2:E:210:THR:HG22	2:E:210:THR:O	2.18	0.43
3:F:82:LEU:HD12	10:F:1256:HEM:CBB	2.49	0.43
1:A:52:GLN:HB2	1:A:52:GLN:HE21	1.51	0.43
3:C:2:THR:HB	3:C:4:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:THR:HB	3:F:4:GLU:OE2	2.19	0.43
1:D:554:LYS:HG2	1:D:602:ASN:HD22	1.83	0.43
1:A:497:LEU:HA	1:A:497:LEU:HD12	1.86	0.43
2:B:164:LYS:HG2	2:B:170:PHE:HD2	1.84	0.43
2:E:5:LEU:HD11	2:E:30:GLU:HB2	2.01	0.43
2:E:164:LYS:HG2	2:E:170:PHE:HD2	1.83	0.43
1:D:314:LYS:NZ	1:D:314:LYS:HB3	2.34	0.43
1:A:318:VAL:HG21	1:A:327:TRP:NE1	2.33	0.43
1:D:124:THR:OG1	1:D:125:THR:N	2.52	0.42
2:B:16:SER:O	3:F:17:ARG:NH1	2.45	0.42
1:A:584:ASP:OD1	1:A:586:ASN:HB2	2.19	0.42
3:F:29:TRP:O	3:F:33:THR:HG23	2.19	0.42
1:D:455:VAL:HG13	1:D:509:LYS:HG3	2.02	0.42
2:E:95:PRO:HD2	2:E:159:ALA:HB1	2.01	0.42
3:F:126:TRP:O	3:F:129:GLN:HB2	2.19	0.42
1:A:254:VAL:CG1	1:A:368:GLN:HG2	2.49	0.42
2:E:85:GLU:OE2	2:E:85:GLU:HA	2.19	0.42
1:A:335:ARG:NH1	1:A:358:ALA:HB3	2.35	0.42
3:C:200:GLU:C	3:C:202:PRO:HD3	2.40	0.42
3:C:59:LEU:O	3:C:63:LYS:HG3	2.20	0.42
1:A:608:LEU:HD12	1:A:608:LEU:H	1.84	0.42
1:A:115[A]:ARG:HB2	12:A:2055:HOH:O	2.20	0.42
2:B:52:ASN:OD1	2:B:101:LYS:CE	2.67	0.42
1:D:286:ARG:NH2	1:D:296:LYS:HE2	2.35	0.42
1:D:254:VAL:CG1	1:D:368:GLN:HG2	2.50	0.42
2:E:121:TRP:O	2:E:123:HIS:CD2	2.72	0.42
3:C:63:LYS:HE2	3:C:68:ASP:OD2	2.20	0.42
1:D:584:ASP:OD1	1:D:586:ASN:HB2	2.19	0.42
3:C:247:TYR:O	3:C:251:LYS:HG3	2.19	0.42
1:D:34:LEU:HD22	1:D:179:LYS:HG2	2.01	0.42
1:D:224:LYS:HD3	1:D:472:ASP:OD1	2.20	0.42
1:A:95:LYS:HE3	1:A:95:LYS:HB3	1.91	0.42
1:D:455:VAL:CG1	1:D:509:LYS:HG3	2.49	0.42
3:F:59:LEU:O	3:F:63:LYS:HG3	2.20	0.42
1:D:565:LEU:HD11	1:D:581:GLU:HB2	2.01	0.42
1:A:349:CYS:HB3	1:A:355:ILE:HG13	2.00	0.42
3:C:161:PHE:CD2	3:C:246:LYS:HE3	2.55	0.42
3:F:200:GLU:C	3:F:202:PRO:HD3	2.40	0.42
3:C:29:TRP:O	3:C:33:THR:HG23	2.20	0.42
1:D:612:ARG:O	1:D:616:ILE:HG13	2.19	0.42
2:B:232:ARG:CZ	3:C:193:LYS:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:ASP:HA	12:E:2035:HOH:O	2.20	0.41
1:D:512:HIS:O	1:D:513:ALA:C	2.58	0.41
2:B:210:THR:HG22	2:B:210:THR:O	2.19	0.41
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.85	0.41
3:F:161:PHE:CD2	3:F:246:LYS:HE3	2.55	0.41
1:A:612:ARG:O	1:A:616:ILE:HG13	2.20	0.41
1:D:455:VAL:HG13	1:D:509:LYS:CD	2.50	0.41
1:D:608:LEU:N	1:D:608:LEU:HD12	2.34	0.41
1:D:606:ASN:OD1	1:D:608:LEU:HD13	2.20	0.41
1:D:349:CYS:HB3	1:D:355:ILE:HG13	2.01	0.41
1:A:512:HIS:O	1:A:513:ALA:C	2.58	0.41
3:C:82:LEU:HD13	3:C:82:LEU:O	2.20	0.41
2:B:5:LEU:HD11	2:B:30:GLU:HB2	2.01	0.41
1:A:111:HIS:HB3	2:B:139:PRO:HG3	2.03	0.41
1:A:224:LYS:HD3	1:A:472:ASP:OD1	2.21	0.41
1:A:455:VAL:HG13	1:A:509:LYS:HG3	2.01	0.41
3:C:82:LEU:HD12	10:C:1256:HEM:CBB	2.49	0.41
3:F:60:TRP:CZ2	3:F:64:LYS:HD2	2.55	0.41
1:D:268:LEU:HD22	1:D:345:VAL:CG2	2.47	0.41
1:A:455:VAL:HG13	1:A:509:LYS:CD	2.50	0.41
1:A:565:LEU:HD11	1:A:581:GLU:HB2	2.02	0.41
1:A:71:MET:HE2	12:A:2027:HOH:O	2.21	0.41
1:D:300:SER:HB3	1:D:303:VAL:HG23	2.03	0.41
1:D:27:LYS:HB3	1:D:27:LYS:HE3	1.89	0.41
1:A:29:LEU:O	1:A:31:THR:HG22	2.19	0.41
1:D:608:LEU:HD12	1:D:608:LEU:H	1.85	0.41
1:D:335:ARG:NH1	1:D:358:ALA:HB3	2.35	0.41
1:A:314:LYS:HB3	1:A:314:LYS:NZ	2.35	0.41
1:A:221:ARG:HD3	1:A:229:ALA:O	2.21	0.41
1:A:606:ASN:OD1	1:A:608:LEU:HD13	2.20	0.41
1:D:318:VAL:HG21	1:D:327:TRP:NE1	2.35	0.41
3:F:75:LYS:HE2	12:F:2021:HOH:O	2.21	0.41
1:A:224:LYS:NZ	12:A:2207:HOH:O	2.54	0.41
1:A:301:ARG:HH12	1:A:404:ARG:NH1	2.19	0.41
1:D:52:GLN:HG2	1:D:69:HIS:CE1	2.54	0.41
2:B:227:LYS:HD3	2:B:227:LYS:HA	1.95	0.41
4:A:1656:FAD:H1'1	4:A:1656:FAD:H9	1.62	0.41
1:D:49:GLY:HA2	1:D:139[A]:ARG:NH2	2.35	0.41
3:F:17:ARG:O	3:F:17:ARG:HG2	2.21	0.41
3:C:222:VAL:O	3:C:226:LEU:HG	2.21	0.41
2:E:146:PHE:O	2:E:150:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LYS:HE2	2:E:153:GLU:CD	2.41	0.41
1:A:57:ASN:HB2	12:A:2023:HOH:O	2.20	0.41
3:F:222:VAL:O	3:F:226:LEU:HG	2.21	0.41
1:D:455:VAL:HG13	1:D:509:LYS:HD3	2.03	0.41
3:F:63:LYS:HE2	3:F:68:ASP:OD2	2.20	0.41
1:A:483:ASP:CG	1:A:486:HIS:HD1	2.25	0.41
3:C:60:TRP:CZ2	3:C:64:LYS:HD2	2.55	0.41
1:D:52:GLN:HB3	1:D:408:ASN:HD22	1.87	0.40
1:D:496:GLU:O	1:D:500:LYS:HG3	2.21	0.40
1:D:531:LEU:O	1:D:535:LYS:HB3	2.21	0.40
3:C:169:TRP:N	3:C:170:PRO:CD	2.84	0.40
3:C:189:ARG:HA	3:C:192:VAL:HG22	2.02	0.40
2:E:220:LYS:HE2	2:E:220:LYS:HA	2.03	0.40
2:B:20:LYS:HE3	3:F:16[B]:GLU:HA	2.03	0.40
1:A:22:VAL:O	1:A:26:GLN:HG2	2.21	0.40
1:D:489:LYS:HB3	1:D:489:LYS:HE2	1.95	0.40
1:A:52:GLN:HG2	1:A:69:HIS:CE1	2.56	0.40
3:F:108:TYR:HD2	11:F:1257:LMT:H52	1.87	0.40
1:D:341:ASN:HB2	1:D:342:LEU:HD12	2.04	0.40
1:D:29:LEU:O	1:D:31:THR:HG22	2.21	0.40
1:D:398:ASP:OD2	1:D:563:ARG:NE	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	659/660 (100%)	634 (96%)	21 (3%)	4 (1%)	30	13
1	D	657/660 (100%)	631 (96%)	22 (3%)	4 (1%)	30	13
2	B	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	11	2
2	E	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	11	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	39	22
3	F	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	39	22
All	All	2304/2314 (100%)	2213 (96%)	73 (3%)	18 (1%)	24	8

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
2	B	86	ASP
3	C	72	GLU
1	D	121	ALA
2	E	86	ASP
3	F	72	GLU
1	A	123	LYS
2	B	3	ARG
1	D	123	LYS
2	E	3	ARG
1	A	269	THR
2	B	239	ASN
1	D	269	THR
2	E	2	GLY
2	E	239	ASN
1	A	122	GLN
2	B	2	GLY
1	D	122	GLN

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	537/537 (100%)	519 (97%)	18 (3%)	44	24
1	D	535/537 (100%)	518 (97%)	17 (3%)	46	26
2	B	212/213 (100%)	208 (98%)	4 (2%)	65	49
2	E	212/213 (100%)	208 (98%)	4 (2%)	65	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	223/223 (100%)	218 (98%)	5 (2%)	60	42
3	F	223/223 (100%)	218 (98%)	5 (2%)	60	42
All	All	1942/1946 (100%)	1889 (97%)	53 (3%)	52	34

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2[A]	LYS
1	A	2[B]	LYS
1	A	31	THR
1	A	52	GLN
1	A	95	LYS
1	A	137	HIS
1	A	275	ASP
1	A	295	LYS
1	A	386	LYS
1	A	403	ASN
1	A	404	ARG
1	A	408	ASN
1	A	475	ASP
1	A	497	LEU
1	A	509	LYS
1	A	562	ASN
1	A	602	ASN
1	A	641	GLU
2	B	58	ARG
2	B	164	LYS
2	B	181	ARG
2	B	227	LYS
3	C	18	LYS
3	C	82	LEU
3	C	87	PHE
3	C	100	LYS
3	C	106	ARG
1	D	31	THR
1	D	52	GLN
1	D	95	LYS
1	D	137	HIS
1	D	263	PRO
1	D	275	ASP
1	D	295	LYS

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Mol	Chain	Res	Type
1	D	386	LYS
1	D	403	ASN
1	D	404	ARG
1	D	408	ASN
1	D	475	ASP
1	D	497	LEU
1	D	509	LYS
1	D	562	ASN
1	D	602	ASN
1	D	641	GLU
2	E	58	ARG
2	E	164	LYS
2	E	181	ARG
2	E	227	LYS
3	F	18	LYS
3	F	82	LEU
3	F	87	PHE
3	F	100	LYS
3	F	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	48	GLN
1	A	57	ASN
1	A	91	ASN
1	A	133	HIS
1	A	225	ASN
1	A	228	ASN
1	A	257	HIS
1	A	325	HIS
1	A	403	ASN
1	A	408	ASN
1	A	430	ASN
1	A	468	ASN
1	A	547	HIS
1	A	562	ASN
1	A	586	ASN
1	A	602	ASN
2	B	116	GLN
2	B	123	HIS

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Mol	Chain	Res	Type
2	B	177	ASN
3	C	107	GLN
1	D	26	GLN
1	D	48	GLN
1	D	57	ASN
1	D	91	ASN
1	D	133	HIS
1	D	225	ASN
1	D	228	ASN
1	D	257	HIS
1	D	325	HIS
1	D	403	ASN
1	D	408	ASN
1	D	430	ASN
1	D	468	ASN
1	D	547	HIS
1	D	562	ASN
1	D	586	ASN
1	D	602	ASN
2	E	116	GLN
2	E	123	HIS
2	E	177	ASN
3	F	107	GLN

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 ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	FAD	A	1656	1	48,58,58	1.91	12 (25%)	54,89,89	2.05	11 (20%)
5	FUM	A	1657	-	1,7,7	1.50	0	0,8,8	0.00	-
7	FES	B	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	B	1241	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF4	B	1242	2	0,12,12	0.00	-	0,24,24	0.00	-
10	HEM	C	1255	3	30,50,50	2.91	12 (40%)	24,82,82	2.13	7 (29%)
10	HEM	C	1256	3	30,50,50	2.98	11 (36%)	24,82,82	2.15	7 (29%)
11	LMT	C	1257	-	36,36,36	1.08	2 (5%)	47,47,47	1.28	4 (8%)
4	FAD	D	1656	1	48,58,58	1.75	11 (22%)	54,89,89	2.07	12 (22%)
5	FUM	D	1657	-	1,7,7	1.48	0	0,8,8	0.00	-
7	FES	E	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	E	1241	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF4	E	1242	2	0,12,12	0.00	-	0,24,24	0.00	-
10	HEM	F	1255	3	30,50,50	2.82	11 (36%)	24,82,82	2.14	7 (29%)
10	HEM	F	1256	3	30,50,50	2.94	10 (33%)	24,82,82	2.15	7 (29%)
11	LMT	F	1257	-	36,36,36	1.08	2 (5%)	47,47,47	1.28	4 (8%)

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
4	FAD	A	1656	1	-	0/30/50/50	0/6/6/6
5	FUM	A	1657	-	-	0/0/5/5	0/0/0/0
7	FES	B	1240	2	-	0/0/4/4	0/1/1/1
8	F3S	B	1241	2	-	0/0/24/24	0/0/3/3
9	SF4	B	1242	2	-	0/0/48/48	0/6/5/5
10	HEM	C	1255	3	-	0/10/54/54	0/0/8/8
10	HEM	C	1256	3	-	0/10/54/54	0/0/8/8
11	LMT	C	1257	-	-	0/21/61/61	0/2/2/2
4	FAD	D	1656	1	-	0/30/50/50	0/6/6/6
5	FUM	D	1657	-	-	0/0/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	E	1240	2	-	0/0/4/4	0/1/1/1
8	F3S	E	1241	2	-	0/0/24/24	0/0/3/3
9	SF4	E	1242	2	-	0/0/48/48	0/6/5/5
10	HEM	F	1255	3	-	0/10/54/54	0/0/8/8
10	HEM	F	1256	3	-	0/10/54/54	0/0/8/8
11	LMT	F	1257	-	-	0/21/61/61	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1256	HEM	C3B-C4B	-8.01	1.44	1.51
10	F	1256	HEM	C3B-C4B	-7.87	1.44	1.51
10	C	1255	HEM	C3B-C4B	-7.55	1.45	1.51
10	F	1255	HEM	C3B-C4B	-7.11	1.45	1.51
10	C	1256	HEM	C2D-C3D	-6.37	1.35	1.54
10	F	1256	HEM	C2D-C3D	-6.35	1.35	1.54
10	F	1256	HEM	C3B-CAB	-6.26	1.39	1.51
10	C	1255	HEM	C2D-C3D	-6.22	1.35	1.54
10	F	1255	HEM	C2D-C3D	-6.22	1.35	1.54
10	C	1256	HEM	C3B-CAB	-6.13	1.39	1.51
10	C	1256	HEM	C3C-CAC	-5.83	1.40	1.51
10	F	1256	HEM	C3C-CAC	-5.78	1.40	1.51
10	C	1255	HEM	C3C-CAC	-5.75	1.40	1.51
10	F	1255	HEM	C3C-CAC	-5.74	1.40	1.51
10	C	1255	HEM	C3B-CAB	-5.70	1.40	1.51
10	C	1256	HEM	C3D-C4D	-5.42	1.44	1.51
10	F	1255	HEM	C3B-CAB	-5.25	1.41	1.51
10	F	1256	HEM	C3D-C4D	-5.15	1.45	1.51
10	F	1255	HEM	C3D-C4D	-5.08	1.45	1.51
10	C	1255	HEM	C3D-C4D	-4.95	1.45	1.51
10	C	1255	HEM	C2C-C1C	-4.15	1.44	1.52
4	A	1656	FAD	PA-O2A	-4.13	1.37	1.54
10	F	1255	HEM	C2C-C1C	-4.09	1.44	1.52
10	F	1256	HEM	C2C-C1C	-4.09	1.44	1.52
4	D	1656	FAD	PA-O2A	-4.08	1.37	1.54
10	C	1256	HEM	C2C-C1C	-3.90	1.45	1.52
4	A	1656	FAD	P-O2P	-3.60	1.39	1.54
4	D	1656	FAD	P-O2P	-3.20	1.41	1.54
4	A	1656	FAD	C10-N10	-3.05	1.35	1.39
4	D	1656	FAD	C10-N10	-2.37	1.36	1.39
10	C	1256	HEM	C2D-C1D	-2.26	1.44	1.51
10	F	1256	HEM	C2D-C1D	-2.22	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	1256	HEM	C2B-C1B	-2.18	1.44	1.51
10	F	1255	HEM	C2D-C1D	-2.14	1.44	1.51
10	C	1256	HEM	C2B-C1B	-2.11	1.44	1.51
10	C	1255	HEM	C2B-C1B	-2.06	1.45	1.51
10	F	1255	HEM	C2B-C1B	-2.04	1.45	1.51
10	C	1255	HEM	C2D-C1D	-2.02	1.45	1.51
4	D	1656	FAD	C5X-N5	2.00	1.38	1.35
4	A	1656	FAD	C8-C7	2.00	1.46	1.41
4	D	1656	FAD	C4X-N5	2.03	1.36	1.33
10	F	1255	HEM	C1C-NC	2.03	1.38	1.36
4	A	1656	FAD	C2A-N1A	2.07	1.37	1.33
4	A	1656	FAD	C5X-N5	2.09	1.38	1.35
10	C	1255	HEM	C4C-NC	2.11	1.38	1.36
4	D	1656	FAD	C4A-N3A	2.13	1.38	1.35
4	A	1656	FAD	C4A-N3A	2.34	1.39	1.35
10	C	1256	HEM	FE-NC	2.50	2.05	1.95
10	C	1255	HEM	FE-NC	2.66	2.06	1.95
10	C	1255	HEM	CBB-CAB	2.71	1.44	1.29
11	C	1257	LMT	C3'-C4'	2.73	1.60	1.52
4	D	1656	FAD	C4-N3	2.74	1.38	1.33
10	C	1256	HEM	CBB-CAB	2.74	1.45	1.29
10	F	1256	HEM	CBC-CAC	2.77	1.45	1.29
11	F	1257	LMT	C3'-C4'	2.77	1.60	1.52
10	F	1255	HEM	CBB-CAB	2.77	1.45	1.29
10	F	1256	HEM	CBB-CAB	2.80	1.45	1.29
10	C	1255	HEM	CBC-CAC	2.82	1.45	1.29
10	C	1256	HEM	CBC-CAC	2.88	1.46	1.29
10	F	1255	HEM	CBC-CAC	2.88	1.46	1.29
4	A	1656	FAD	C4-N3	2.93	1.38	1.33
11	C	1257	LMT	O5B-C1B	3.29	1.50	1.41
11	F	1257	LMT	O5B-C1B	3.33	1.50	1.41
4	D	1656	FAD	O5'-C5'	3.38	1.58	1.44
4	D	1656	FAD	C4X-C10	3.43	1.47	1.41
4	A	1656	FAD	O5'-C5'	3.46	1.59	1.44
4	D	1656	FAD	C9A-N10	3.54	1.43	1.38
4	A	1656	FAD	C4X-C10	3.71	1.48	1.41
4	A	1656	FAD	C9A-N10	4.51	1.45	1.38
4	D	1656	FAD	O4B-C1B	4.73	1.47	1.41
4	A	1656	FAD	O4B-C1B	4.93	1.47	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1656	FAD	C1'-N10-C9A	-5.91	112.23	118.86
4	A	1656	FAD	C1'-N10-C9A	-5.87	112.27	118.86
4	D	1656	FAD	C4X-C4-N3	-4.75	117.10	123.59
4	A	1656	FAD	C4X-C4-N3	-4.73	117.12	123.59
4	A	1656	FAD	C4X-C10-N10	-4.71	117.75	120.52
4	D	1656	FAD	C4X-C10-N10	-4.53	117.85	120.52
4	D	1656	FAD	N3A-C2A-N1A	-3.78	126.00	128.89
4	A	1656	FAD	N3A-C2A-N1A	-3.50	126.21	128.89
11	C	1257	LMT	C3'-C4'-C5'	-3.28	103.41	110.84
11	F	1257	LMT	C3'-C4'-C5'	-3.28	103.43	110.84
11	C	1257	LMT	O1'-C1'-C2'	-3.03	104.21	108.04
11	F	1257	LMT	O1'-C1'-C2'	-3.01	104.23	108.04
4	D	1656	FAD	O4B-C1B-N9A	-2.99	101.83	108.10
4	A	1656	FAD	O4B-C1B-N9A	-2.97	101.87	108.10
4	A	1656	FAD	C4-C4X-C10	-2.97	118.04	119.94
4	D	1656	FAD	C4-C4X-C10	-2.77	118.17	119.94
4	A	1656	FAD	C4B-O4B-C1B	-2.17	107.34	109.72
4	D	1656	FAD	C4B-O4B-C1B	-2.07	107.44	109.72
10	F	1255	HEM	C3C-CAC-CBC	2.03	127.56	124.46
4	D	1656	FAD	C4A-C5A-N7A	2.03	111.35	109.48
11	F	1257	LMT	O1B-C4'-C3'	2.14	112.69	107.17
11	C	1257	LMT	O1B-C4'-C3'	2.15	112.72	107.17
10	C	1255	HEM	C3C-CAC-CBC	2.25	127.90	124.46
4	A	1656	FAD	C2B-C1B-N9A	2.25	117.74	114.29
4	A	1656	FAD	C2A-N1A-C6A	2.29	122.86	118.77
4	D	1656	FAD	C2B-C1B-N9A	2.32	117.83	114.29
10	F	1256	HEM	CMD-C2D-C3D	2.35	124.73	114.35
4	D	1656	FAD	C2A-N1A-C6A	2.35	122.96	118.77
10	C	1256	HEM	CMD-C2D-C3D	2.38	124.89	114.35
4	A	1656	FAD	O3P-P-O5'	2.66	109.99	102.94
10	C	1255	HEM	CMD-C2D-C3D	2.83	126.87	114.35
10	F	1256	HEM	CAD-C3D-C2D	2.93	121.64	113.22
10	C	1256	HEM	CAD-C3D-C2D	2.96	121.72	113.22
10	F	1255	HEM	CMD-C2D-C3D	2.99	127.57	114.35
4	D	1656	FAD	O3P-P-O5'	2.99	110.88	102.94
10	F	1255	HEM	C2D-C3D-C4D	3.25	107.00	101.50
10	C	1255	HEM	C2D-C3D-C4D	3.25	107.01	101.50
10	F	1255	HEM	CMC-C2C-C3C	3.33	124.85	116.53
10	F	1256	HEM	CBA-CAA-C2A	3.33	118.51	112.53
10	F	1256	HEM	C2D-C3D-C4D	3.35	107.17	101.50
10	C	1256	HEM	C2D-C3D-C4D	3.43	107.32	101.50
10	C	1255	HEM	CMC-C2C-C3C	3.53	125.35	116.53
10	C	1256	HEM	CBA-CAA-C2A	3.62	119.01	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1255	HEM	CAD-C3D-C4D	3.82	125.96	112.47
10	F	1255	HEM	CAD-C3D-C4D	3.84	126.00	112.47
10	F	1256	HEM	CMB-C2B-C3B	3.95	126.39	116.53
10	C	1256	HEM	CMB-C2B-C3B	4.02	126.55	116.53
10	F	1256	HEM	CMC-C2C-C3C	4.28	127.20	116.53
10	C	1256	HEM	CMC-C2C-C3C	4.33	127.35	116.53
11	C	1257	LMT	C1-O1'-C1'	4.62	122.02	113.94
11	F	1257	LMT	C1-O1'-C1'	4.67	122.11	113.94
10	C	1255	HEM	CMB-C2B-C3B	4.71	128.30	116.53
10	F	1255	HEM	CAD-C3D-C2D	4.79	126.99	113.22
10	C	1255	HEM	CAD-C3D-C2D	4.80	127.03	113.22
10	F	1255	HEM	CMB-C2B-C3B	4.89	128.74	116.53
10	C	1256	HEM	CAD-C3D-C4D	5.23	130.93	112.47
10	F	1256	HEM	CAD-C3D-C4D	5.30	131.16	112.47
4	A	1656	FAD	C4-N3-C2	7.58	121.80	115.25
4	D	1656	FAD	C4-N3-C2	7.71	121.91	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1656	FAD	3	0
10	C	1256	HEM	1	0
11	C	1257	LMT	8	0
4	D	1656	FAD	3	0
10	F	1256	HEM	1	0
11	F	1257	LMT	9	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	656/660 (99%)	0.51	55 (8%)	14 13	19, 33, 69, 80	14 (2%)
1	D	656/660 (99%)	0.59	65 (9%)	9 8	19, 33, 69, 80	16 (2%)
2	B	240/241 (99%)	0.35	15 (6%)	23 22	21, 29, 50, 74	2 (0%)
2	E	240/241 (99%)	0.40	13 (5%)	29 27	20, 28, 51, 74	2 (0%)
3	C	255/256 (99%)	1.05	47 (18%)	2 1	26, 44, 77, 91	11 (4%)
3	F	255/256 (99%)	0.88	37 (14%)	3 3	25, 43, 76, 90	10 (3%)
All	All	2302/2314 (99%)	0.61	232 (10%)	9 8	19, 34, 70, 91	55 (2%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	121	ALA	13.9
2	B	1	MET	11.8
3	C	254	HIS	11.3
1	A	121	ALA	10.5
1	A	122	GLN	10.2
1	D	122	GLN	10.1
1	A	124	THR	9.3
2	E	1	MET	9.1
1	D	599	ALA	8.8
1	D	338	ILE	8.4
2	B	240	MET	8.2
3	F	243	ILE	8.2
1	D	342	LEU	8.1
1	A	123	LYS	8.0
3	C	255	GLU	7.9
3	C	243	ILE	7.9
3	C	253	THR	7.9
3	C	69	PHE	7.5
1	D	124	THR	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	625	ALA	7.3
3	F	253	THR	7.2
3	C	71	PHE	7.1
1	D	623	LEU	7.0
1	A	597	TYR	7.0
1	D	116	MET	7.0
1	D	341	ASN	6.9
3	C	60	TRP	6.8
3	F	74	GLY	6.8
1	A	627	GLY	6.5
1	A	118	ILE	6.4
3	C	239	THR	6.4
3	F	69	PHE	6.4
3	C	248	PHE	6.3
1	A	120	ASN	6.3
3	C	242	ASN	6.1
1	D	337	HIS	6.1
3	C	72	GLU	5.9
3	F	72	GLU	5.9
1	D	600	LYS	5.8
1	A	117	ALA	5.8
2	E	240	MET	5.7
3	C	236	LEU	5.7
3	F	60	TRP	5.7
1	D	123	LYS	5.6
1	A	116	MET	5.5
3	C	67	LEU	5.4
1	D	119	ILE	5.4
2	B	85	GLU	5.3
3	F	215	LEU	5.3
2	E	4	MET	5.3
3	F	254	HIS	5.2
1	A	624	GLU	5.2
1	A	334	GLY	5.2
2	B	2	GLY	5.2
1	A	623	LEU	5.2
1	D	117	ALA	5.1
1	D	626	ALA	5.1
3	C	74	GLY	5.1
1	D	340	THR	5.0
1	A	337	HIS	4.9
1	D	627	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
3	F	1	MET	4.9
3	C	250	TYR	4.9
1	A	336	LYS	4.8
1	A	340	THR	4.8
1	A	341	ASN	4.8
1	A	600	LYS	4.8
3	F	81	PHE	4.7
1	D	597	TYR	4.6
1	A	351	TYR	4.6
1	D	335	ARG	4.5
3	C	200	GLU	4.5
1	D	358	ALA	4.5
3	F	71	PHE	4.4
3	C	77	ILE	4.4
1	A	125	THR	4.4
1	D	656	LYS	4.3
3	C	70	ILE	4.3
3	C	73	GLY	4.3
1	D	625	ALA	4.3
1	A	339	GLU	4.2
3	F	241	PRO	4.2
3	C	64	LYS	4.1
1	D	339	GLU	4.1
1	D	336	LYS	4.0
1	D	343	ARG	3.9
1	A	654	GLY	3.9
3	F	77	ILE	3.9
1	A	621	SER	3.9
3	C	146	ILE	3.8
2	B	31	ALA	3.8
1	A	353	ALA	3.8
3	C	1	MET	3.8
1	A	656	LYS	3.7
1	D	598	GLY	3.7
3	C	68	ASP	3.7
3	C	65	PHE	3.7
3	C	245	TYR	3.6
1	A	338	ILE	3.6
1	D	624	GLU	3.6
1	A	601	GLY	3.5
3	C	81	PHE	3.5
1	A	333	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	3.5
3	F	200	GLU	3.5
3	C	53	LEU	3.5
1	D	601	GLY	3.5
3	F	73	GLY	3.5
2	B	47	TYR	3.5
1	D	611	LYS	3.4
1	A	599	ALA	3.4
3	F	242	ASN	3.4
3	F	53	LEU	3.3
1	A	628	LYS	3.3
1	D	628	LYS	3.3
1	D	354	GLY	3.3
3	C	247	TYR	3.3
1	A	632	ALA	3.3
3	F	233	LYS	3.3
1	D	118	ILE	3.3
1	D	322	TYR	3.2
2	E	85	GLU	3.2
1	D	294	GLU	3.2
3	F	68	ASP	3.1
2	E	2	GLY	3.1
1	A	295	LYS	3.1
3	C	233	LYS	3.1
1	A	620	GLN	3.1
3	C	251	LYS	3.1
1	A	611	LYS	3.1
1	D	125	THR	3.1
1	D	619	ILE	3.1
1	A	602	ASN	3.1
2	B	205	VAL	3.0
1	A	294	GLU	3.0
3	C	201	THR	3.0
3	F	76	PRO	3.0
1	D	293	PRO	3.0
3	F	52	LEU	3.0
3	C	240	ASP	2.9
3	F	240	ASP	2.9
3	F	146	ILE	2.9
3	C	75	LYS	2.9
3	F	75	LYS	2.9
1	A	119	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	654	GLY	2.9
1	D	346	GLN	2.9
1	D	655	ASP	2.9
3	F	70	ILE	2.9
1	D	614	GLU	2.8
3	C	199	GLY	2.8
1	D	620	GLN	2.8
2	B	125	GLN	2.8
3	F	211	LYS	2.8
3	F	201	THR	2.7
1	A	614	GLU	2.7
3	F	251	LYS	2.7
3	C	241	PRO	2.7
3	C	157	VAL	2.7
1	A	358	ALA	2.7
3	C	197	PHE	2.6
1	D	356	ASP	2.6
1	D	602	ASN	2.6
1	A	586	ASN	2.6
3	C	61	VAL	2.6
3	C	161	PHE	2.6
3	F	239	THR	2.5
1	D	319	GLN	2.5
3	F	197	PHE	2.5
3	C	59	LEU	2.5
3	C	238	GLN	2.5
1	A	343	ARG	2.5
3	C	252	ARG	2.5
1	D	622	GLU	2.5
3	F	57	VAL	2.5
1	D	344	ASP	2.5
1	D	348	ILE	2.5
3	F	236	LEU	2.5
1	A	655	ASP	2.4
3	C	214	THR	2.4
2	E	32	PRO	2.4
1	A	345	VAL	2.4
2	E	211	LEU	2.4
1	A	271	GLY	2.4
2	B	239	ASN	2.4
2	E	103	LEU	2.4
1	D	355	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	219	PHE	2.4
1	A	296	LYS	2.3
1	A	335	ARG	2.3
1	D	632	ALA	2.3
1	A	572	GLU	2.3
1	D	350	GLU	2.3
1	A	618	LYS	2.3
1	A	332	ILE	2.3
1	D	635	GLU	2.3
3	C	219	PHE	2.3
3	C	212	LEU	2.3
1	D	295	LYS	2.3
1	D	616	ILE	2.3
2	B	206	PHE	2.3
3	C	142	VAL	2.2
3	F	142	VAL	2.2
3	F	222	VAL	2.2
1	D	120	ASN	2.2
2	B	32	PRO	2.2
1	A	616	ILE	2.2
1	D	351	TYR	2.2
2	B	86	ASP	2.2
2	B	5	LEU	2.2
2	B	103	LEU	2.2
3	F	171	LEU	2.2
2	E	239	ASN	2.2
1	A	162	PHE	2.1
2	E	53	PHE	2.1
1	D	314	LYS	2.1
2	E	94	LEU	2.1
1	D	321	PRO	2.1
1	D	586	ASN	2.1
3	C	190	LEU	2.1
1	D	277	GLY	2.1
1	D	615	GLU	2.1
2	B	61	ILE	2.1
1	D	271	GLY	2.0
1	A	316	LYS	2.0
1	D	296	LYS	2.0
1	A	321	PRO	2.0
1	D	357	PRO	2.0
1	D	649	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	55	PHE	2.0
2	E	75	LEU	2.0
3	F	147	MET	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	LMT	C	1257	35/35	0.55	0.34	8.64	59,63,68,69	16
11	LMT	F	1257	35/35	0.73	0.25	7.51	59,63,69,69	16
5	FUM	D	1657	8/8	0.79	0.18	1.28	43,46,47,48	0
5	FUM	A	1657	8/8	0.76	0.17	1.22	42,46,48,50	0
10	HEM	C	1256	43/43	0.96	0.13	0.37	38,40,43,45	0
10	HEM	F	1256	43/43	0.96	0.13	-0.00	36,40,43,45	0
10	HEM	C	1255	43/43	0.96	0.10	-0.21	26,31,34,38	0
10	HEM	F	1255	43/43	0.97	0.10	-0.24	26,32,35,38	0
6	NA	D	1658	1/1	0.96	0.08	-0.47	26,26,26,26	0
4	FAD	D	1656	53/53	0.97	0.09	-0.50	18,22,25,25	0
4	FAD	A	1656	53/53	0.98	0.08	-0.88	16,22,25,27	0
8	F3S	E	1241	7/7	0.99	0.09	-1.05	23,24,25,25	0
9	SF4	E	1242	8/8	0.99	0.06	-1.19	21,23,23,24	0
8	F3S	B	1241	7/7	0.99	0.07	-1.31	24,25,26,27	0
9	SF4	B	1242	8/8	0.99	0.05	-1.34	22,24,25,25	0
7	FES	E	1240	4/4	0.99	0.06	-1.48	21,21,21,23	0
7	FES	B	1240	4/4	0.99	0.06	-1.54	22,22,23,24	0
6	NA	A	1658	1/1	0.99	0.03	-3.90	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.