



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:12 AM GMT

PDB ID : 2G18
Title : Crystal Structure of Nostoc sp. 7120 phycocyanobilin:ferredoxin oxidoreductase (PcyA) Apoprotein
Authors : Tu, S.-L.; Lagarias, J.C.; Fisher, A.J.
Deposited on : 2006-02-13
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

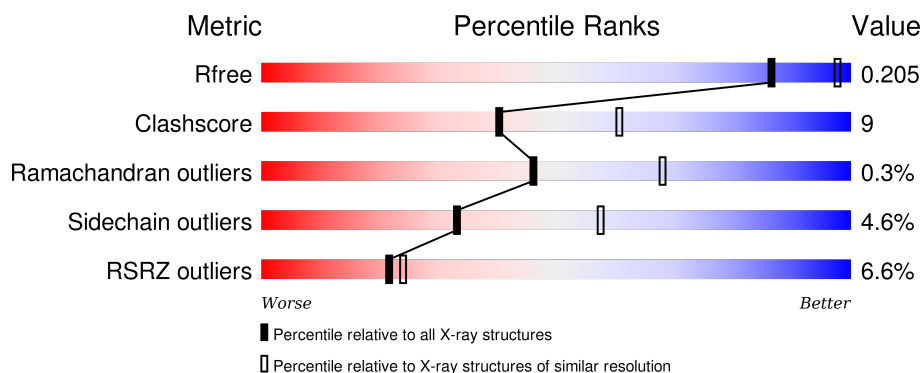
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	253	<div> <div>7%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	B	253	<div> <div>8%</div> <div>75%</div> <div>19%</div> <div>...</div> </div>
1	C	253	<div> <div>6%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	D	253	<div> <div>2%</div> <div>78%</div> <div>16%</div> <div>..</div> </div>
1	E	253	<div> <div>4%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	253	<div><div></div><div>3%</div><div>79%</div><div>17%</div><div>• •</div></div>
1	G	253	<div><div></div><div>5%</div><div>79%</div><div>18%</div><div>• •</div></div>
1	H	253	<div><div></div><div>4%</div><div>80%</div><div>16%</div><div>• •</div></div>
1	I	253	<div><div></div><div>6%</div><div>72%</div><div>21%</div><div>• 6%</div></div>
1	J	253	<div><div></div><div>6%</div><div>74%</div><div>19%</div><div>• 6%</div></div>
1	K	253	<div><div></div><div>8%</div><div>72%</div><div>21%</div><div>• 6%</div></div>
1	L	253	<div><div></div><div>16%</div><div>80%</div><div>12%</div><div>• • 6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23613 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 Phycocyanobilin:ferredoxin oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1964	1242	341	368	13			
1	B	245	Total	C	N	O	S	0	0	0
			1964	1242	341	368	13			
1	C	245	Total	C	N	O	S	0	0	0
			1964	1242	341	368	13			
1	D	248	Total	C	N	O	S	0	0	0
			1991	1261	344	373	13			
1	E	245	Total	C	N	O	S	0	0	0
			1964	1242	341	368	13			
1	F	245	Total	C	N	O	S	0	0	0
			1964	1242	341	368	13			
1	G	248	Total	C	N	O	S	0	0	0
			1991	1261	344	373	13			
1	H	245	Total	C	N	O	S	0	0	0
			1964	1242	341	368	13			
1	I	238	Total	C	N	O	S	0	0	0
			1914	1209	334	358	13			
1	J	238	Total	C	N	O	S	0	0	0
			1914	1209	334	358	13			
1	K	238	Total	C	N	O	S	0	0	0
			1914	1209	334	358	13			
1	L	238	Total	C	N	O	S	0	0	0
			1914	1209	334	358	13			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
A	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
A	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
A	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
A	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
A	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
A	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
A	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
B	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
B	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
B	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
B	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
B	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
B	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
B	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
B	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
B	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
C	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
C	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
C	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
C	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
C	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
C	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
C	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
C	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
C	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
D	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
D	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
D	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
D	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
D	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
D	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
D	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
D	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
D	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
E	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
E	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
E	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
E	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
E	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
E	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
E	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
E	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
E	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
F	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
F	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
F	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
F	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
F	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
F	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
F	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
F	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
G	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
G	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
G	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
G	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
G	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
G	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
G	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
G	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
G	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
H	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
H	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
H	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
H	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
H	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
H	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
H	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
H	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
H	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
I	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
I	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
I	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
I	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
I	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
I	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
I	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
I	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
I	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
J	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
J	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
J	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
J	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
J	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
J	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
J	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
J	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
K	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
K	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
K	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
K	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
K	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
K	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
K	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
K	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
K	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0
L	-7	GLY	-	CLONING ARTIFACT	UNP Q93TN0
L	-6	PRO	-	CLONING ARTIFACT	UNP Q93TN0
L	-5	LEU	-	CLONING ARTIFACT	UNP Q93TN0
L	-4	GLY	-	CLONING ARTIFACT	UNP Q93TN0
L	-3	SER	-	CLONING ARTIFACT	UNP Q93TN0
L	-2	PRO	-	CLONING ARTIFACT	UNP Q93TN0
L	-1	GLU	-	CLONING ARTIFACT	UNP Q93TN0
L	0	PHE	-	CLONING ARTIFACT	UNP Q93TN0
L	1	ILE	-	CLONING ARTIFACT	UNP Q93TN0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	7	Total O 7 7	0	0
3	C	16	Total O 16 16	0	0
3	D	31	Total O 31 31	0	0
3	E	18	Total O 18 18	0	0
3	F	17	Total O 17 17	0	0
3	G	18	Total O 18 18	0	0

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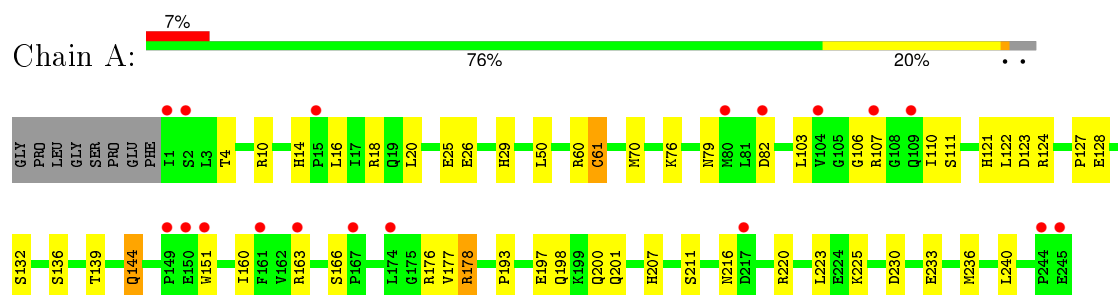
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	25	Total 25	O 25	0	0
3	I	14	Total 14	O 14	0	0
3	J	11	Total 11	O 11	0	0
3	K	13	Total 13	O 13	0	0
3	L	1	Total 1	O 1	0	0

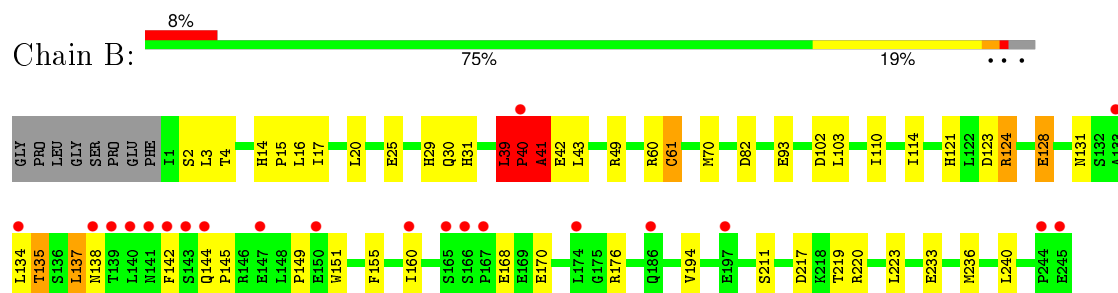
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

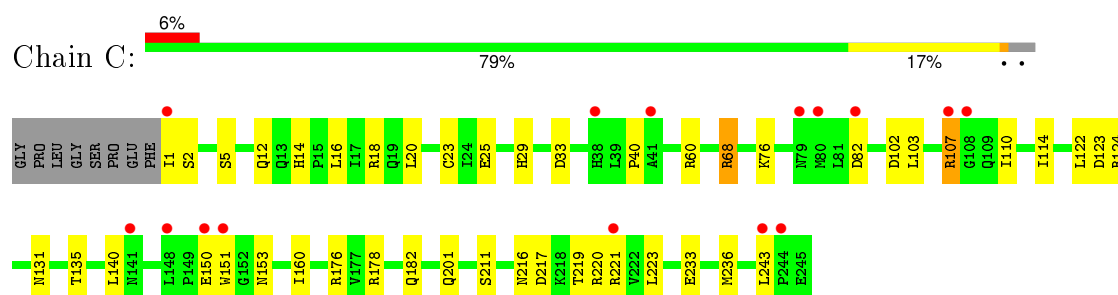
• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase



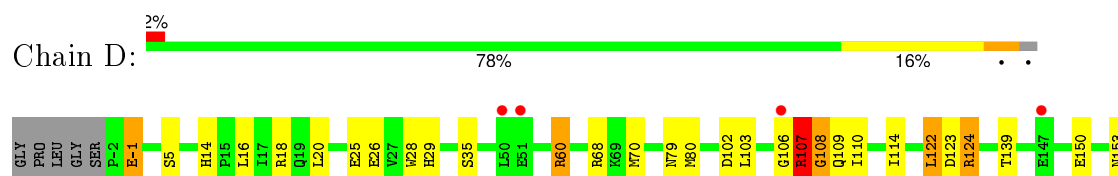
• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

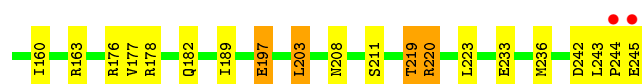


• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

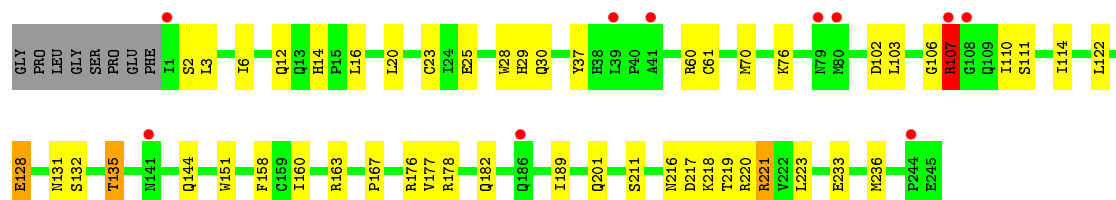
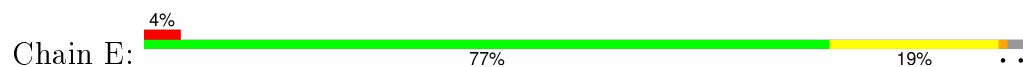


• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

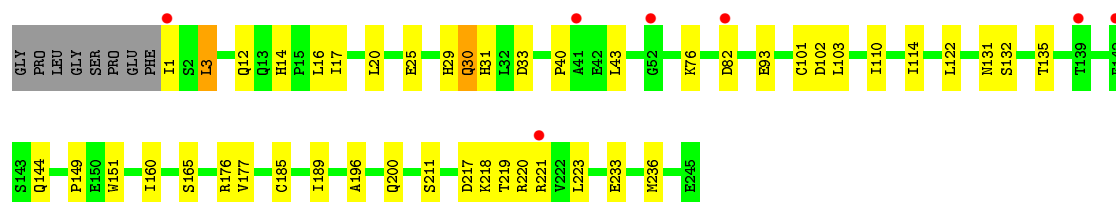
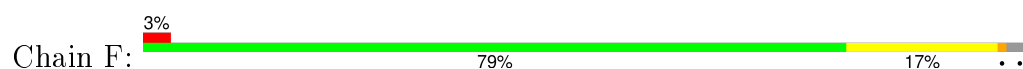




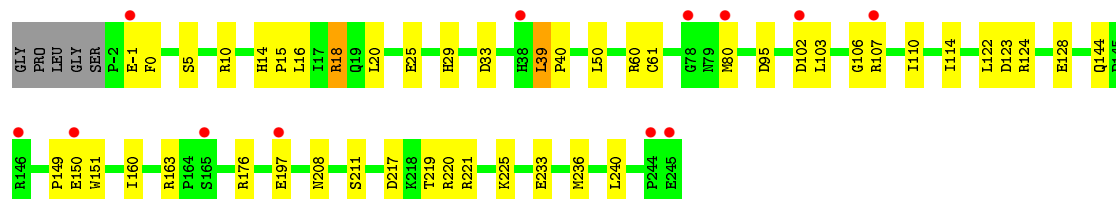
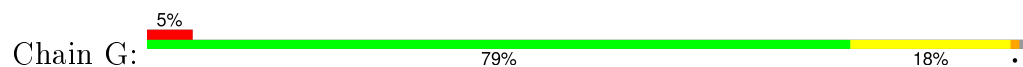
• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase



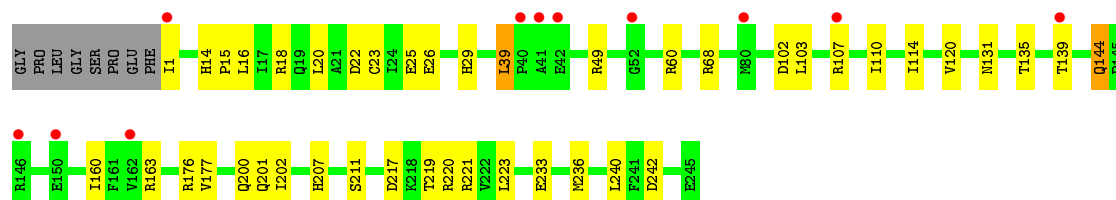
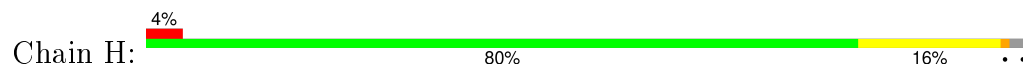
• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase



• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

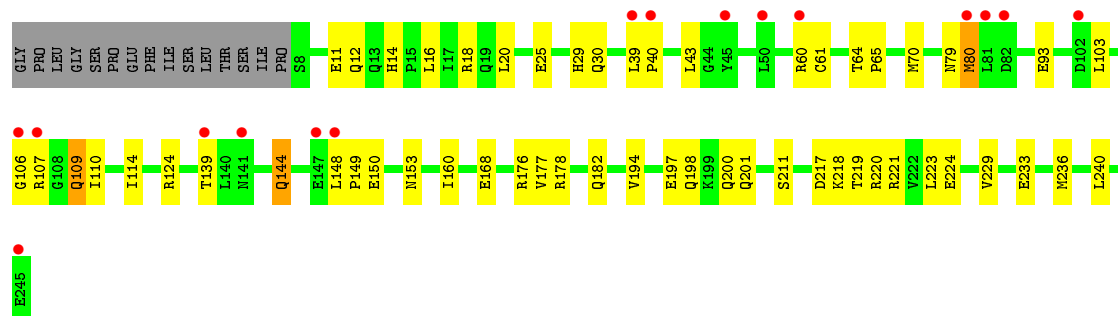


• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase



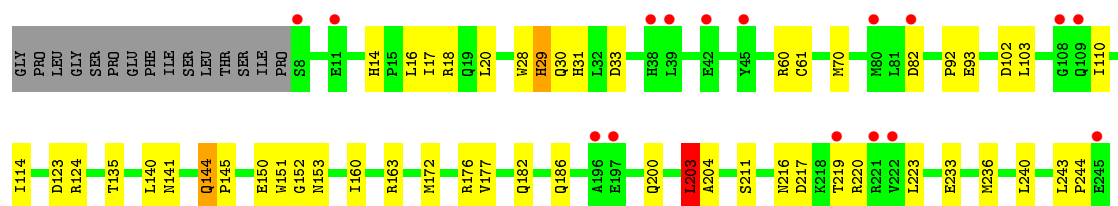
• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase





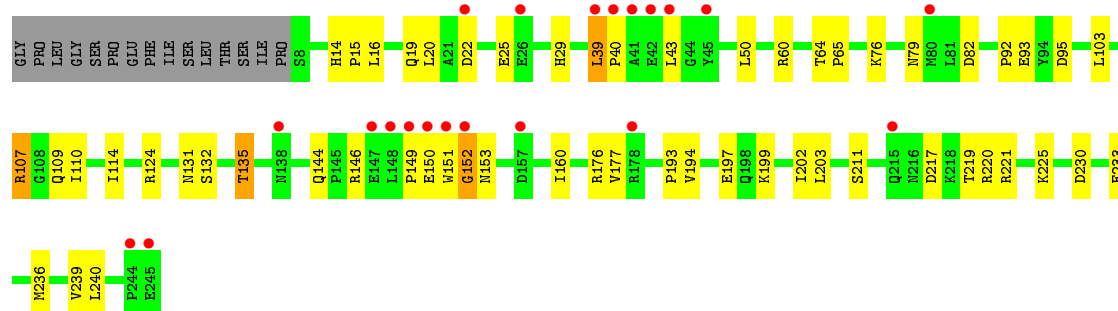
- Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

Chain J: 6% 74% 19% 6%



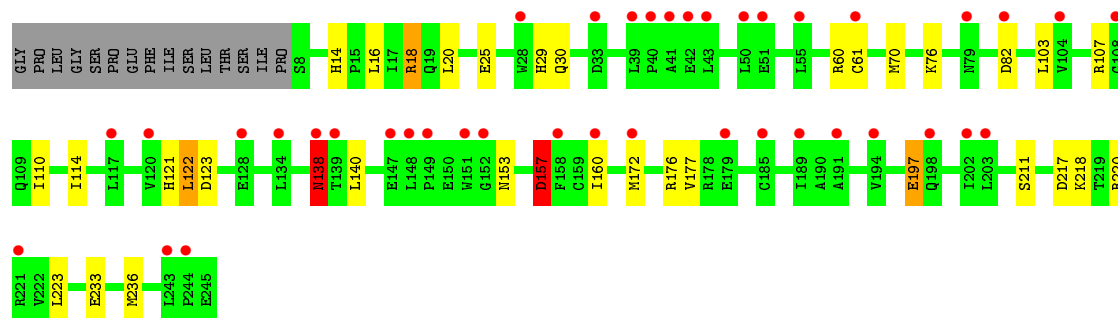
- Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

Chain K: 8% 72% 21% 6%



- Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase

Chain L: 16% 80% 12% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 141.33Å 121.84Å 90.00° 91.29° 90.00°	Depositor
Resolution (Å)	43.94 – 2.50 43.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.94-2.50) 99.6 (43.94-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.257 0.206 , 0.205	Depositor DCC
R_{free} test set	4576 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.5	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 91600 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23613	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2431e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.92	6/2012 (0.3%)	1.00	3/2729 (0.1%)
1	B	0.68	1/2012 (0.0%)	0.71	0/2729
1	C	0.77	1/2012 (0.0%)	0.94	5/2729 (0.2%)
1	D	0.84	1/2041 (0.0%)	0.84	4/2768 (0.1%)
1	E	0.82	0/2012	0.76	1/2729 (0.0%)
1	F	0.79	1/2012 (0.0%)	0.75	1/2729 (0.0%)
1	G	0.72	1/2041 (0.0%)	0.72	0/2768
1	H	0.81	0/2012	0.78	0/2729
1	I	0.73	0/1961	0.74	0/2658
1	J	0.80	2/1961 (0.1%)	0.79	3/2658 (0.1%)
1	K	0.74	0/1961	0.75	0/2658
1	L	1.24	4/1961 (0.2%)	0.70	3/2658 (0.1%)
All	All	0.83	17/23998 (0.1%)	0.79	20/32542 (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
1	B	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	197	GLU	CD-OE1	36.97	1.66	1.25
1	L	197	GLU	CD-OE2	23.40	1.51	1.25
1	L	157	ASP	CB-CG	17.69	1.89	1.51
1	A	178	ARG	NE-CZ	15.40	1.53	1.33
1	A	178	ARG	CZ-NH1	-13.96	1.15	1.33
1	A	166	SER	CB-OG	10.28	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	ARG	CZ-NH2	9.96	1.46	1.33
1	L	197	GLU	CG-CD	8.49	1.64	1.51
1	J	93	GLU	CD-OE2	7.26	1.33	1.25
1	A	111	SER	CB-OG	6.96	1.51	1.42
1	A	61	CYS	CB-SG	-6.20	1.71	1.82
1	B	61	CYS	CB-SG	-5.85	1.72	1.81
1	D	219	THR	CB-CG2	-5.77	1.33	1.52
1	F	101	CYS	CB-SG	-5.51	1.72	1.81
1	A	178	ARG	CZ-NH2	5.48	1.40	1.33
1	G	61	CYS	CB-SG	-5.14	1.73	1.81
1	J	93	GLU	CD-OE1	5.05	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH2	31.77	136.18	120.30
1	C	178	ARG	NE-CZ-NH2	-26.81	106.89	120.30
1	A	178	ARG	NE-CZ-NH1	-13.51	113.54	120.30
1	J	93	GLU	OE1-CD-OE2	-10.95	110.16	123.30
1	L	197	GLU	OE1-CD-OE2	10.62	136.04	123.30
1	L	197	GLU	CG-CD-OE1	-10.37	97.57	118.30
1	D	219	THR	OG1-CB-CG2	-9.07	89.13	110.00
1	A	178	ARG	NH1-CZ-NH2	-8.39	110.17	119.40
1	C	178	ARG	NH1-CZ-NH2	8.37	128.61	119.40
1	C	178	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	J	203	LEU	CA-CB-CG	7.33	132.17	115.30
1	C	68	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	220	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	68	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	F	122	LEU	CA-CB-CG	-5.92	101.68	115.30
1	D	122	LEU	CA-CB-CG	-5.78	102.01	115.30
1	D	163	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	J	93	GLU	CG-CD-OE2	5.29	128.88	118.30
1	L	157	ASP	CB-CG-OD1	5.17	122.96	118.30
1	E	37	TYR	N-CA-C	-5.15	97.10	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	39	LEU	Peptide
1	B	40	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	41	ALA	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	1964	0	1916	31	0
1	B	1964	0	1916	38	1
1	C	1964	0	1916	33	0
1	D	1991	0	1938	50	0
1	E	1964	0	1916	39	0
1	F	1964	0	1916	27	2
1	G	1991	0	1938	29	0
1	H	1964	0	1916	26	0
1	I	1914	0	1856	39	1
1	J	1914	0	1856	54	0
1	K	1914	0	1856	48	0
1	L	1914	0	1856	28	0
2	E	1	0	0	0	0
3	A	19	0	0	2	0
3	B	7	0	0	1	0
3	C	16	0	0	4	0
3	D	31	0	0	6	0
3	E	18	0	0	0	0
3	F	17	0	0	0	0
3	G	18	0	0	1	0
3	H	25	0	0	3	0
3	I	14	0	0	2	0
3	J	11	0	0	0	0
3	K	13	0	0	0	0
3	L	1	0	0	0	0
All	All	23613	0	22796	400	2

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 9.

All (400) 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:L:157:ASP:CB	1:L:157:ASP:CG	1.88	1.39
1:L:197:GLU:CD	1:L:197:GLU:OE1	1.66	1.31
1:K:124:ARG:NH2	1:K:153:ASN:HB2	1.66	1.08
1:D:35:SER:CB	1:J:186:GLN:NE2	2.21	1.04
1:D:35:SER:CB	1:J:186:GLN:HE22	1.69	1.04
1:E:128:GLU:H	1:E:128:GLU:CD	1.68	0.94
1:D:35:SER:HB2	1:J:186:GLN:NE2	1.83	0.92
1:I:12:GLN:OE1	3:I:259:HOH:O	1.88	0.90
1:C:68:ARG:HD3	3:C:253:HOH:O	1.70	0.90
1:D:107:ARG:O	1:D:109:GLN:N	2.05	0.89
1:D:35:SER:HB3	1:J:186:GLN:HE22	1.36	0.88
1:D:220:ARG:HD2	3:D:260:HOH:O	1.73	0.87
1:J:141:ASN:N	1:J:172:MET:HE3	1.91	0.85
1:C:221:ARG:NE	1:D:197:GLU:HG2	1.92	0.84
1:A:144:GLN:HG2	1:A:163:ARG:HB3	1.58	0.84
1:F:144:GLN:HE21	1:F:165:SER:HB3	1.41	0.84
1:C:150:GLU:HB3	1:J:33:ASP:OD2	1.78	0.83
1:K:124:ARG:HH21	1:K:153:ASN:HB2	1.42	0.82
1:B:40:PRO:O	1:B:43:LEU:HB2	1.81	0.80
1:K:149:PRO:HG2	1:K:151:TRP:CE2	2.16	0.79
1:I:106:GLY:HA3	1:I:109:GLN:O	1.83	0.79
1:B:39:LEU:CB	1:B:40:PRO:HD2	2.12	0.79
1:K:124:ARG:NH2	1:K:153:ASN:CB	2.45	0.78
1:B:14:HIS:HE1	3:B:246:HOH:O	1.65	0.78
1:E:131:ASN:O	1:E:135:THR:HG23	1.82	0.78
1:D:153:ASN:HB3	3:D:276:HOH:O	1.84	0.77
1:H:131:ASN:O	1:H:135:THR:HG23	1.86	0.76
1:J:29:HIS:CE1	1:J:30:GLN:OE1	2.39	0.76
1:K:40:PRO:HG2	1:K:43:LEU:HD12	1.66	0.76
1:F:144:GLN:NE2	1:F:165:SER:HB3	2.01	0.76
1:J:141:ASN:H	1:J:172:MET:HE3	1.52	0.75
1:K:220:ARG:NH2	1:K:233:GLU:OE2	2.20	0.74
1:D:60:ARG:NH2	1:E:3:LEU:O	2.21	0.74
1:H:120:VAL:HG23	1:H:202:ILE:HD12	1.69	0.74
1:B:220:ARG:NH2	1:B:233:GLU:OE2	2.20	0.74
1:G:10:ARG:O	1:G:18:ARG:HG3	1.88	0.74
1:D:182:GLN:NE2	1:F:33:ASP:OD2	2.20	0.73
1:K:151:TRP:C	1:K:153:ASN:H	1.92	0.73
1:H:14:HIS:HD2	1:H:16:LEU:H	1.36	0.73
1:C:220:ARG:NH2	1:C:233:GLU:OE2	2.21	0.73
1:K:151:TRP:HA	1:K:153:ASN:ND2	2.03	0.73
1:E:220:ARG:NH2	1:E:233:GLU:OE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:ARG:NH2	1:J:233:GLU:OE2	2.22	0.72
1:K:15:PRO:O	1:K:19:GLN:HG3	1.88	0.72
1:H:220:ARG:NH2	1:H:233:GLU:OE2	2.22	0.72
1:F:14:HIS:HD2	1:F:16:LEU:H	1.38	0.72
1:D:220:ARG:NH2	1:D:233:GLU:OE2	2.22	0.72
1:A:220:ARG:NH2	1:A:233:GLU:OE2	2.23	0.72
1:J:140:LEU:HB3	1:J:172:MET:CE	2.20	0.71
1:I:220:ARG:NH2	1:I:233:GLU:OE2	2.24	0.70
1:E:167:PRO:HG2	1:K:22:ASP:CB	2.21	0.70
1:H:22:ASP:O	1:H:26:GLU:HG3	1.92	0.69
1:J:140:LEU:HB3	1:J:172:MET:HE2	1.73	0.69
1:I:16:LEU:HD23	1:I:110:ILE:HD13	1.74	0.69
1:L:220:ARG:NH2	1:L:233:GLU:OE2	2.26	0.69
1:D:14:HIS:HD2	1:D:16:LEU:H	1.41	0.69
1:I:11:GLU:OE1	1:I:11:GLU:HA	1.91	0.68
1:G:220:ARG:NH2	1:G:233:GLU:OE2	2.26	0.68
1:C:151:TRP:CE2	1:C:216:ASN:HB3	2.27	0.68
1:K:131:ASN:O	1:K:135:THR:HG23	1.92	0.68
1:I:18:ARG:HH11	1:I:18:ARG:HG2	1.57	0.68
1:I:14:HIS:HD2	1:I:16:LEU:H	1.42	0.68
1:H:14:HIS:CD2	1:H:16:LEU:H	2.12	0.68
1:C:131:ASN:O	1:C:135:THR:HG23	1.94	0.67
1:F:220:ARG:NH2	1:F:233:GLU:OE2	2.26	0.67
1:A:122:LEU:H	1:J:200:GLN:NE2	1.93	0.67
1:L:121:HIS:HB3	1:L:123:ASP:OD1	1.96	0.66
1:G:208:ASN:ND2	1:I:200:GLN:OE1	2.28	0.66
1:G:25:GLU:O	1:G:29:HIS:HD2	1.79	0.66
1:C:221:ARG:HE	1:D:197:GLU:HG2	1.60	0.65
1:G:18:ARG:HG3	1:G:18:ARG:HH11	1.60	0.65
1:C:182:GLN:OE1	3:C:259:HOH:O	2.14	0.65
3:D:262:HOH:O	1:J:31:HIS:HE1	1.80	0.65
1:F:14:HIS:CD2	1:F:16:LEU:H	2.15	0.65
1:L:18:ARG:HH11	1:L:18:ARG:HG2	1.62	0.65
1:D:60:ARG:CG	3:D:258:HOH:O	2.44	0.64
1:A:121:HIS:HB2	1:A:123:ASP:OD1	1.97	0.64
1:G:14:HIS:HD2	1:G:16:LEU:H	1.46	0.64
1:D:106:GLY:C	1:D:107:ARG:HG2	2.18	0.64
1:F:16:LEU:HD23	1:F:110:ILE:HD13	1.78	0.64
1:C:14:HIS:HD2	1:C:16:LEU:H	1.46	0.64
1:K:151:TRP:C	1:K:153:ASN:N	2.49	0.64
1:B:39:LEU:CB	1:B:40:PRO:CD	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:PRO:HG2	1:K:22:ASP:HB2	1.79	0.64
1:A:128:GLU:CD	1:A:128:GLU:H	2.01	0.64
1:D:14:HIS:CD2	1:D:16:LEU:H	2.15	0.64
1:E:14:HIS:HD2	1:E:16:LEU:H	1.44	0.64
1:G:149:PRO:HG2	1:G:151:TRP:NE1	2.13	0.63
1:E:25:GLU:O	1:E:29:HIS:HD2	1.82	0.63
1:D:-1:GLU:HB3	1:K:109:GLN:HE21	1.64	0.63
1:K:16:LEU:HD23	1:K:110:ILE:HD13	1.80	0.62
1:A:25:GLU:O	1:A:29:HIS:HD2	1.82	0.62
1:H:16:LEU:HD23	1:H:110:ILE:HD13	1.82	0.61
1:L:14:HIS:HD2	1:L:16:LEU:H	1.48	0.61
1:I:14:HIS:CD2	1:I:16:LEU:H	2.17	0.61
1:A:128:GLU:OE1	1:A:128:GLU:N	2.21	0.61
1:B:39:LEU:O	1:B:41:ALA:N	2.33	0.61
1:C:25:GLU:O	1:C:29:HIS:HD2	1.83	0.61
1:C:1:ILE:N	1:C:1:ILE:HD12	2.16	0.60
1:B:128:GLU:CD	1:B:128:GLU:N	2.55	0.60
1:C:221:ARG:CZ	1:D:197:GLU:HG2	2.30	0.60
1:L:197:GLU:CG	1:L:197:GLU:OE1	2.48	0.60
1:E:14:HIS:CD2	1:E:16:LEU:H	2.19	0.60
1:G:16:LEU:HD23	1:G:110:ILE:HD13	1.83	0.60
1:B:39:LEU:HB2	1:B:40:PRO:HD2	1.82	0.59
1:B:41:ALA:O	1:B:42:GLU:HB2	2.02	0.59
1:B:16:LEU:HD23	1:B:110:ILE:HD13	1.84	0.59
1:E:128:GLU:OE2	1:E:128:GLU:N	2.35	0.59
1:J:14:HIS:CD2	1:J:16:LEU:H	2.21	0.59
1:C:16:LEU:HD23	1:C:110:ILE:HD13	1.84	0.59
1:I:18:ARG:HG2	1:I:18:ARG:NH1	2.15	0.59
1:L:14:HIS:CD2	1:L:16:LEU:H	2.21	0.59
1:I:25:GLU:O	1:I:29:HIS:HD2	1.86	0.59
1:D:189:ILE:HG22	1:F:93:GLU:HG2	1.84	0.59
1:J:123:ASP:O	1:J:124:ARG:HB2	2.03	0.58
1:E:160:ILE:CD1	1:E:176:ARG:HG2	2.33	0.58
1:J:14:HIS:HD2	1:J:16:LEU:H	1.51	0.58
1:I:20:LEU:HD23	1:I:103:LEU:HD22	1.85	0.58
1:B:124:ARG:NH1	1:B:155:PHE:O	2.36	0.58
1:D:122:LEU:HD12	1:D:122:LEU:N	2.18	0.58
1:F:25:GLU:O	1:F:29:HIS:HD2	1.87	0.58
1:J:124:ARG:HD2	1:J:153:ASN:O	2.04	0.58
1:C:14:HIS:CD2	1:C:16:LEU:H	2.21	0.58
1:J:243:LEU:HB3	1:J:244:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:PRO:HA	1:K:202:ILE:HG21	1.86	0.58
1:K:160:ILE:CD1	1:K:176:ARG:HG2	2.35	0.57
1:K:93:GLU:O	1:K:194:VAL:N	2.36	0.57
1:E:167:PRO:HG2	1:K:22:ASP:OD2	2.05	0.57
1:L:16:LEU:HD23	1:L:110:ILE:HD13	1.86	0.57
1:D:160:ILE:CD1	1:D:176:ARG:HG2	2.33	0.57
1:A:14:HIS:HD2	1:A:16:LEU:H	1.50	0.57
1:B:160:ILE:CD1	1:B:176:ARG:HG2	2.34	0.57
1:A:16:LEU:HD23	1:A:110:ILE:HD13	1.86	0.57
1:G:160:ILE:CD1	1:G:176:ARG:HG2	2.34	0.57
1:B:14:HIS:HD2	1:B:16:LEU:H	1.53	0.57
1:A:121:HIS:HA	1:J:200:GLN:HE22	1.69	0.57
1:D:16:LEU:HD23	1:D:110:ILE:HD13	1.86	0.57
1:E:167:PRO:CG	1:K:22:ASP:OD2	2.53	0.56
1:H:160:ILE:CD1	1:H:176:ARG:HG2	2.35	0.56
1:J:217:ASP:OD1	1:J:219:THR:HG23	2.05	0.56
1:E:189:ILE:HG22	1:I:144:GLN:HE22	1.70	0.56
1:G:14:HIS:CD2	1:G:16:LEU:H	2.24	0.56
1:L:138:ASN:HD22	1:L:138:ASN:N	2.04	0.56
1:C:150:GLU:CB	1:J:33:ASP:OD2	2.50	0.56
1:F:131:ASN:O	1:F:135:THR:HG23	2.05	0.56
1:A:14:HIS:CD2	1:A:16:LEU:H	2.24	0.56
1:I:80:MET:CE	1:I:80:MET:HA	2.36	0.56
1:B:128:GLU:CD	1:B:128:GLU:H	2.09	0.55
1:E:20:LEU:HD11	1:E:177:VAL:HG11	1.89	0.55
1:J:16:LEU:HD23	1:J:110:ILE:HD13	1.88	0.55
1:I:160:ILE:CD1	1:I:176:ARG:HG2	2.36	0.55
1:I:124:ARG:HD2	1:I:153:ASN:O	2.07	0.55
1:E:20:LEU:HD23	1:E:103:LEU:HD22	1.90	0.54
1:B:14:HIS:CD2	1:B:16:LEU:H	2.24	0.54
1:D:223:LEU:HD12	1:D:236:MET:CE	2.38	0.54
1:H:223:LEU:HD12	1:H:236:MET:CE	2.37	0.54
1:D:208:ASN:ND2	1:H:200:GLN:HG2	2.22	0.54
1:E:25:GLU:O	1:E:29:HIS:CD2	2.61	0.53
1:J:141:ASN:C	1:J:172:MET:HE1	2.29	0.53
1:J:29:HIS:ND1	1:J:30:GLN:OE1	2.41	0.53
1:E:106:GLY:O	1:E:107:ARG:C	2.46	0.53
1:L:25:GLU:O	1:L:29:HIS:HD2	1.92	0.53
1:D:20:LEU:HD11	1:D:177:VAL:HG11	1.91	0.53
1:I:79:ASN:HB3	1:I:107:ARG:HH12	1.73	0.53
1:K:39:LEU:HB3	1:K:40:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:ILE:CD1	1:L:176:ARG:HG2	2.39	0.53
1:H:20:LEU:HD11	1:H:177:VAL:HG11	1.91	0.53
1:G:0:PHE:CD2	1:K:95:ASP:OD2	2.62	0.53
1:H:20:LEU:HD23	1:H:103:LEU:HD22	1.90	0.52
1:A:160:ILE:CD1	1:A:176:ARG:HG2	2.39	0.52
1:C:160:ILE:CD1	1:C:176:ARG:HG2	2.39	0.52
1:J:14:HIS:CD2	1:J:110:ILE:HD11	2.44	0.52
1:A:230:ASP:OD2	1:B:49:ARG:HB3	2.10	0.52
1:D:106:GLY:O	1:D:107:ARG:HG2	2.10	0.52
1:E:135:THR:HG22	1:E:158:PHE:HZ	1.75	0.51
1:G:106:GLY:C	1:G:107:ARG:HG2	2.30	0.51
1:E:221:ARG:HG2	1:E:221:ARG:HH11	1.74	0.51
1:B:39:LEU:HB3	1:B:40:PRO:HD2	1.92	0.51
1:G:208:ASN:ND2	1:I:200:GLN:CD	2.64	0.51
1:A:122:LEU:H	1:J:200:GLN:HE22	1.57	0.51
1:K:20:LEU:HD23	1:K:103:LEU:HD22	1.91	0.51
1:E:16:LEU:HD23	1:E:110:ILE:HD13	1.93	0.51
1:F:160:ILE:CD1	1:F:176:ARG:HG2	2.41	0.51
1:A:123:ASP:OD1	1:A:124:ARG:N	2.44	0.51
1:E:122:LEU:HG	1:E:201:GLN:HG3	1.92	0.51
1:C:123:ASP:O	1:C:124:ARG:HB2	2.11	0.51
1:B:14:HIS:CD2	1:B:110:ILE:HD11	2.46	0.51
1:A:20:LEU:HD11	1:A:177:VAL:HG11	1.93	0.50
1:J:223:LEU:HD12	1:J:236:MET:CE	2.41	0.50
1:G:20:LEU:HD23	1:G:103:LEU:HD22	1.93	0.50
1:C:150:GLU:CG	1:J:33:ASP:OD2	2.60	0.50
1:D:60:ARG:HG2	3:D:258:HOH:O	2.08	0.50
1:D:20:LEU:HD23	1:D:103:LEU:HD22	1.92	0.50
1:I:217:ASP:OD1	1:I:219:THR:HG23	2.11	0.50
1:J:236:MET:HE1	1:J:240:LEU:HD12	1.92	0.50
1:K:149:PRO:HG2	1:K:151:TRP:NE1	2.26	0.50
1:D:102:ASP:HB2	1:D:114:ILE:HG22	1.94	0.50
1:I:194:VAL:HB	1:I:198:GLN:HB2	1.93	0.50
1:J:160:ILE:CD1	1:J:176:ARG:HG2	2.42	0.50
1:B:61:CYS:HA	1:B:70:MET:O	2.12	0.50
1:B:236:MET:HE1	1:B:240:LEU:HD12	1.93	0.50
1:D:223:LEU:HD12	1:D:236:MET:HE3	1.94	0.50
1:K:149:PRO:O	1:K:152:GLY:N	2.42	0.49
1:D:102:ASP:HB2	1:D:114:ILE:CG2	2.42	0.49
1:F:12:GLN:HB3	1:F:76:LYS:HE3	1.95	0.49
1:B:93:GLU:O	1:B:194:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:OD1	1:B:219:THR:HG23	2.13	0.49
1:C:223:LEU:HD12	1:C:236:MET:CE	2.43	0.49
1:J:20:LEU:HD23	1:J:103:LEU:HD22	1.95	0.49
1:F:20:LEU:HD23	1:F:103:LEU:HD22	1.95	0.49
1:H:217:ASP:OD1	1:H:219:THR:HG23	2.12	0.49
1:K:150:GLU:O	1:K:153:ASN:ND2	2.44	0.49
1:H:49:ARG:HB3	1:K:230:ASP:OD2	2.13	0.49
1:K:25:GLU:O	1:K:29:HIS:HD2	1.96	0.49
1:G:144:GLN:HB2	1:G:163:ARG:O	2.12	0.49
1:B:134:LEU:O	1:B:137:LEU:HG	2.13	0.49
1:I:144:GLN:HG3	1:I:144:GLN:O	2.11	0.49
1:D:122:LEU:HD12	1:D:122:LEU:H	1.77	0.49
1:D:35:SER:OG	1:J:186:GLN:NE2	2.46	0.48
1:E:111:SER:HA	1:E:163:ARG:HH11	1.77	0.48
1:B:30:GLN:HB3	1:B:31:HIS:CD2	2.48	0.48
1:J:144:GLN:HG2	1:J:163:ARG:HB3	1.95	0.48
1:E:30:GLN:HG2	1:J:145:PRO:HG3	1.95	0.48
1:A:151:TRP:CE2	1:A:216:ASN:HB3	2.48	0.48
1:A:121:HIS:CA	1:J:200:GLN:HE22	2.25	0.48
1:J:18:ARG:HH11	1:J:18:ARG:HG2	1.79	0.48
1:J:140:LEU:HB3	1:J:172:MET:HE3	1.93	0.48
1:I:201:GLN:OE1	3:I:258:HOH:O	2.20	0.48
1:K:199:LYS:HA	1:K:202:ILE:HD12	1.96	0.48
1:B:25:GLU:O	1:B:29:HIS:HD2	1.96	0.48
1:J:29:HIS:HE1	1:J:30:GLN:OE1	1.94	0.48
1:E:223:LEU:HD12	1:E:236:MET:CE	2.44	0.48
1:F:149:PRO:HG2	1:F:151:TRP:NE1	2.28	0.48
1:L:20:LEU:HD23	1:L:103:LEU:HD22	1.95	0.48
1:G:33:ASP:OD1	1:K:124:ARG:NH2	2.44	0.48
1:J:135:THR:HG21	1:K:107:ARG:HD2	1.96	0.48
1:F:20:LEU:HD11	1:F:177:VAL:HG11	1.97	0.47
1:C:20:LEU:HD23	1:C:103:LEU:HD22	1.96	0.47
1:J:102:ASP:HB2	1:J:114:ILE:CG2	2.44	0.47
1:A:10:ARG:HG3	1:A:18:ARG:HG3	1.95	0.47
1:L:14:HIS:CD2	1:L:110:ILE:HD11	2.49	0.47
1:D:25:GLU:O	1:D:29:HIS:HD2	1.98	0.47
1:E:14:HIS:CD2	1:E:110:ILE:HD11	2.50	0.47
1:K:217:ASP:OD1	1:K:219:THR:HG23	2.14	0.47
1:H:68:ARG:NH1	3:H:261:HOH:O	2.25	0.47
1:D:107:ARG:C	1:D:109:GLN:H	2.18	0.47
1:B:121:HIS:HB2	1:B:123:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:MET:HG2	1:G:107:ARG:NH2	2.30	0.47
1:L:20:LEU:HD11	1:L:177:VAL:HG11	1.97	0.47
1:J:61:CYS:HA	1:J:70:MET:O	2.14	0.47
1:C:122:LEU:HD12	1:C:201:GLN:HG2	1.95	0.47
1:G:102:ASP:HB2	1:G:114:ILE:CG2	2.45	0.47
1:H:220:ARG:HD2	3:H:253:HOH:O	2.15	0.47
1:A:106:GLY:O	1:A:107:ARG:HB2	2.14	0.47
1:D:26:GLU:OE1	1:D:178:ARG:NH2	2.48	0.47
1:L:140:LEU:HD22	1:L:172:MET:HG2	1.97	0.47
1:G:236:MET:HE1	1:G:240:LEU:HD12	1.97	0.47
1:D:68:ARG:NH2	1:D:242:ASP:CG	2.68	0.47
1:H:144:GLN:HB2	1:H:163:ARG:O	2.15	0.46
1:B:131:ASN:O	1:B:135:THR:OG1	2.28	0.46
1:I:14:HIS:HB2	1:I:106:GLY:O	2.15	0.46
1:A:193:PRO:HB2	1:K:150:GLU:HG2	1.98	0.46
1:D:124:ARG:HD2	1:D:153:ASN:O	2.15	0.46
1:K:14:HIS:CE1	1:K:110:ILE:HD12	2.51	0.46
1:L:114:ILE:HA	1:L:160:ILE:O	2.15	0.46
1:A:20:LEU:HD23	1:A:103:LEU:HD22	1.97	0.46
1:G:123:ASP:O	1:G:124:ARG:HB2	2.15	0.46
1:C:25:GLU:O	1:C:29:HIS:CD2	2.67	0.46
1:I:20:LEU:HD11	1:I:177:VAL:HG11	1.97	0.46
1:G:217:ASP:OD1	1:G:219:THR:HG23	2.16	0.46
1:A:127:PRO:HG3	3:A:247:HOH:O	2.16	0.46
1:D:124:ARG:HE	1:D:124:ARG:HB3	1.25	0.46
1:C:1:ILE:H1	1:C:1:ILE:HD12	1.80	0.46
1:I:93:GLU:O	1:I:194:VAL:HG22	2.15	0.45
1:D:68:ARG:NH2	1:D:242:ASP:OD2	2.49	0.45
1:C:114:ILE:HA	1:C:160:ILE:O	2.16	0.45
1:G:102:ASP:HB2	1:G:114:ILE:HG22	1.99	0.45
1:D:123:ASP:O	1:D:124:ARG:HB2	2.14	0.45
1:B:142:PHE:O	1:B:145:PRO:HD3	2.17	0.45
1:L:138:ASN:N	1:L:138:ASN:ND2	2.64	0.45
1:F:223:LEU:HD12	1:F:236:MET:CE	2.47	0.45
1:D:107:ARG:O	1:D:108:GLY:C	2.53	0.45
1:F:40:PRO:HG2	1:F:43:LEU:HD12	1.99	0.45
1:L:61:CYS:HA	1:L:70:MET:O	2.17	0.45
1:K:236:MET:HE1	1:K:240:LEU:HD12	1.99	0.45
1:F:185:CYS:O	1:F:189:ILE:HD12	2.16	0.45
1:B:102:ASP:HB2	1:B:114:ILE:CG2	2.47	0.45
1:B:223:LEU:HD12	1:B:236:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLN:NE2	1:A:201:GLN:NE2	2.65	0.45
1:J:102:ASP:HB2	1:J:114:ILE:HG22	1.99	0.45
1:L:18:ARG:NH1	1:L:18:ARG:HG2	2.31	0.44
1:B:123:ASP:O	1:B:124:ARG:HB2	2.17	0.44
1:H:39:LEU:HD12	1:H:39:LEU:H	1.82	0.44
1:A:236:MET:HE1	1:A:240:LEU:HD12	2.00	0.44
1:K:92:PRO:O	1:K:202:ILE:HD13	2.17	0.44
1:C:140:LEU:HD11	1:C:176:ARG:HB2	1.97	0.44
1:J:151:TRP:CE2	1:J:216:ASN:HB3	2.52	0.44
1:G:95:ASP:HB3	3:G:260:HOH:O	2.17	0.44
1:E:178:ARG:O	1:E:182:GLN:HG3	2.17	0.44
1:G:149:PRO:HG2	1:G:151:TRP:CE2	2.52	0.44
1:F:25:GLU:O	1:F:29:HIS:CD2	2.70	0.44
1:J:150:GLU:C	1:J:152:GLY:H	2.20	0.44
1:B:170:GLU:OE1	1:L:18:ARG:NH2	2.50	0.44
1:E:221:ARG:NH1	1:E:221:ARG:HG2	2.32	0.44
1:J:135:THR:HG21	1:K:107:ARG:CD	2.48	0.44
1:C:217:ASP:OD1	1:C:219:THR:HG23	2.17	0.44
1:C:102:ASP:HB2	1:C:114:ILE:CG2	2.48	0.44
1:D:79:ASN:ND2	3:D:251:HOH:O	2.50	0.44
1:C:243:LEU:HG	3:C:255:HOH:O	2.18	0.44
1:E:12:GLN:HB3	1:E:76:LYS:HE3	2.00	0.44
1:E:102:ASP:HB2	1:E:114:ILE:CG2	2.48	0.44
1:F:14:HIS:CD2	1:F:110:ILE:HD11	2.53	0.43
1:K:14:HIS:CE1	1:K:110:ILE:CD1	3.01	0.43
1:I:106:GLY:CA	1:I:109:GLN:O	2.61	0.43
1:F:102:ASP:HB2	1:F:114:ILE:CG2	2.49	0.43
1:J:223:LEU:HD12	1:J:236:MET:HE2	1.98	0.43
1:A:127:PRO:HD3	3:A:247:HOH:O	2.17	0.43
1:A:61:CYS:HA	1:A:70:MET:O	2.18	0.43
1:E:151:TRP:CE2	1:E:216:ASN:HB3	2.54	0.43
1:E:135:THR:HG22	1:E:158:PHE:CZ	2.53	0.43
1:E:167:PRO:HG3	1:K:22:ASP:OD2	2.17	0.43
1:E:61:CYS:HA	1:E:70:MET:O	2.18	0.43
1:D:203:LEU:HD12	1:D:244:PRO:HB2	1.99	0.43
1:B:30:GLN:HB3	1:B:31:HIS:HD2	1.83	0.43
1:F:196:ALA:O	1:F:200:GLN:HG3	2.19	0.43
1:K:114:ILE:HA	1:K:160:ILE:O	2.18	0.43
1:H:25:GLU:O	1:H:29:HIS:HD2	2.02	0.43
1:F:76:LYS:HG3	1:F:82:ASP:OD1	2.18	0.43
1:L:157:ASP:H	1:L:157:ASP:CG	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:SER:OG	1:J:182:GLN:HB3	2.18	0.43
1:A:223:LEU:HD12	1:A:236:MET:CE	2.49	0.43
1:G:25:GLU:O	1:G:29:HIS:CD2	2.65	0.43
1:L:217:ASP:OD1	1:L:218:LYS:N	2.52	0.43
1:L:122:LEU:HG	1:L:122:LEU:H	1.66	0.43
1:F:114:ILE:HA	1:F:160:ILE:O	2.18	0.42
1:J:20:LEU:HD11	1:J:177:VAL:HG11	2.01	0.42
1:G:14:HIS:HA	1:G:15:PRO:HD3	1.94	0.42
1:E:111:SER:HA	1:E:163:ARG:NH1	2.34	0.42
1:A:50:LEU:HD11	1:A:225:LYS:HB3	2.02	0.42
1:I:64:THR:HB	1:I:65:PRO:HD2	2.02	0.42
1:F:30:GLN:HG2	1:F:31:HIS:CD2	2.53	0.42
1:E:217:ASP:OD1	1:E:219:THR:HG23	2.20	0.42
1:K:149:PRO:HB2	1:K:151:TRP:CD1	2.55	0.42
1:K:39:LEU:HD22	1:K:239:VAL:HG22	2.02	0.42
1:K:76:LYS:HG3	1:K:82:ASP:OD1	2.18	0.42
1:I:178:ARG:O	1:I:182:GLN:HG3	2.20	0.42
1:J:17:ILE:CD1	1:J:82:ASP:HB3	2.48	0.42
1:D:243:LEU:HD13	1:H:207:HIS:NE2	2.34	0.42
1:G:124:ARG:HB3	1:G:124:ARG:HE	1.46	0.42
1:I:236:MET:HE1	1:I:240:LEU:HD12	2.01	0.42
1:G:50:LEU:HD11	1:G:225:LYS:HB3	2.01	0.42
1:C:12:GLN:HB3	1:C:76:LYS:HE3	2.01	0.42
1:C:150:GLU:HG2	1:J:33:ASP:OD2	2.19	0.42
1:I:114:ILE:HA	1:I:160:ILE:O	2.19	0.42
1:B:20:LEU:HD23	1:B:103:LEU:HD22	2.01	0.42
1:B:40:PRO:O	1:B:43:LEU:N	2.53	0.42
1:L:76:LYS:HG3	1:L:82:ASP:OD1	2.20	0.42
1:E:28:TRP:CE2	1:E:70:MET:HE3	2.54	0.41
1:A:200:GLN:HB3	1:J:204:ALA:HB1	2.01	0.41
1:K:20:LEU:HD11	1:K:177:VAL:HG11	2.01	0.41
1:E:28:TRP:CD2	1:E:70:MET:HE3	2.56	0.41
1:I:224:GLU:HG2	1:I:229:VAL:HA	2.02	0.41
1:H:236:MET:HE1	1:H:240:LEU:HD12	2.02	0.41
1:H:68:ARG:NH2	1:H:242:ASP:OD2	2.53	0.41
1:K:50:LEU:HD11	1:K:225:LYS:HB3	2.02	0.41
1:D:14:HIS:CD2	1:D:110:ILE:HD11	2.55	0.41
1:C:76:LYS:HG3	1:C:82:ASP:OD1	2.20	0.41
1:F:217:ASP:OD1	1:F:219:THR:HG23	2.20	0.41
1:I:223:LEU:HD12	1:I:236:MET:CE	2.50	0.41
1:B:17:ILE:CD1	1:B:82:ASP:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:LEU:HB2	1:G:40:PRO:HD2	2.01	0.41
1:I:61:CYS:HA	1:I:70:MET:O	2.20	0.41
1:I:14:HIS:CD2	1:I:110:ILE:HD11	2.55	0.41
1:K:93:GLU:HB3	1:K:193:PRO:HB3	2.03	0.41
1:I:25:GLU:O	1:I:29:HIS:CD2	2.69	0.41
1:C:124:ARG:NH1	1:C:153:ASN:O	2.53	0.41
1:E:217:ASP:OD1	1:E:218:LYS:N	2.54	0.41
1:A:76:LYS:HG3	1:A:82:ASP:OD1	2.21	0.41
1:L:157:ASP:N	1:L:157:ASP:OD1	2.50	0.41
1:J:28:TRP:CD2	1:J:70:MET:HE2	2.56	0.41
1:H:107:ARG:NH2	3:H:267:HOH:O	2.54	0.41
1:H:102:ASP:HB2	1:H:114:ILE:CG2	2.51	0.41
1:J:92:PRO:CB	1:J:203:LEU:HD13	2.51	0.40
1:B:149:PRO:HG2	1:B:151:TRP:NE1	2.36	0.40
1:B:14:HIS:HA	1:B:15:PRO:HD3	1.94	0.40
1:I:217:ASP:OD1	1:I:218:LYS:N	2.54	0.40
1:F:17:ILE:CD1	1:F:82:ASP:HB3	2.51	0.40
1:C:107:ARG:NH2	3:C:252:HOH:O	2.54	0.40
1:K:150:GLU:OE2	1:K:150:GLU:HA	2.21	0.40
1:H:14:HIS:HA	1:H:15:PRO:HD3	1.98	0.40
1:L:138:ASN:HD22	1:L:138:ASN:H	1.68	0.40
1:I:223:LEU:HD12	1:I:236:MET:HE3	2.03	0.40
1:K:64:THR:HB	1:K:65:PRO:CD	2.52	0.40
1:I:148:LEU:HA	1:I:149:PRO:HD3	1.92	0.40
1:L:223:LEU:HD12	1:L:236:MET:CE	2.50	0.40
1:I:40:PRO:O	1:I:43:LEU:N	2.46	0.40
1:H:114:ILE:HA	1:H:160:ILE:O	2.21	0.40
1:D:35:SER:HB2	1:J:186:GLN:HE22	1.51	0.40
1:D:114:ILE:HA	1:D:160:ILE:O	2.22	0.40
1:D:28:TRP:CD2	1:D:70:MET:CE	3.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:NH2	1:F:3:LEU:O[2_456]	2.16	0.04
1:F:218:LYS:NZ	1:I:197:GLU:OE1[2_446]	2.19	0.01

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	243/253 (96%)	235 (97%)	8 (3%)	0	100	100
1	B	243/253 (96%)	236 (97%)	4 (2%)	3 (1%)	16	29
1	C	243/253 (96%)	238 (98%)	4 (2%)	1 (0%)	39	61
1	D	246/253 (97%)	238 (97%)	6 (2%)	2 (1%)	24	41
1	E	243/253 (96%)	237 (98%)	5 (2%)	1 (0%)	39	61
1	F	243/253 (96%)	238 (98%)	5 (2%)	0	100	100
1	G	246/253 (97%)	240 (98%)	6 (2%)	0	100	100
1	H	243/253 (96%)	236 (97%)	7 (3%)	0	100	100
1	I	236/253 (93%)	231 (98%)	5 (2%)	0	100	100
1	J	236/253 (93%)	231 (98%)	5 (2%)	0	100	100
1	K	236/253 (93%)	228 (97%)	7 (3%)	1 (0%)	39	61
1	L	236/253 (93%)	228 (97%)	7 (3%)	1 (0%)	39	61
All	All	2894/3036 (95%)	2816 (97%)	69 (2%)	9 (0%)	46	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	PRO
1	D	108	GLY
1	D	107	ARG
1	K	152	GLY
1	B	41	ALA
1	E	107	ARG
1	L	138	ASN
1	B	138	ASN
1	C	40	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/223 (97%)	205 (94%)	12 (6%)	27	48
1	B	217/223 (97%)	206 (95%)	11 (5%)	29	52
1	C	217/223 (97%)	209 (96%)	8 (4%)	41	68
1	D	220/223 (99%)	206 (94%)	14 (6%)	22	39
1	E	217/223 (97%)	206 (95%)	11 (5%)	29	52
1	F	217/223 (97%)	211 (97%)	6 (3%)	51	78
1	G	220/223 (99%)	209 (95%)	11 (5%)	30	53
1	H	217/223 (97%)	207 (95%)	10 (5%)	33	57
1	I	210/223 (94%)	199 (95%)	11 (5%)	29	51
1	J	210/223 (94%)	205 (98%)	5 (2%)	57	82
1	K	210/223 (94%)	198 (94%)	12 (6%)	25	46
1	L	210/223 (94%)	201 (96%)	9 (4%)	35	61
All	All	2582/2676 (96%)	2462 (95%)	120 (5%)	33	57

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	26	GLU
1	A	60	ARG
1	A	79	ASN
1	A	132	SER
1	A	136	SER
1	A	139	THR
1	A	144	GLN
1	A	178	ARG
1	A	197	GLU
1	A	207	HIS
1	A	211	SER
1	B	2	SER
1	B	3	LEU

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Mol	Chain	Res	Type
1	B	4	THR
1	B	39	LEU
1	B	124	ARG
1	B	128	GLU
1	B	135	THR
1	B	137	LEU
1	B	144	GLN
1	B	168	GLU
1	B	211	SER
1	C	2	SER
1	C	5	SER
1	C	18	ARG
1	C	23	CYS
1	C	33	ASP
1	C	60	ARG
1	C	107	ARG
1	C	211	SER
1	D	-1	GLU
1	D	5	SER
1	D	18	ARG
1	D	60	ARG
1	D	80	MET
1	D	107	ARG
1	D	124	ARG
1	D	139	THR
1	D	150	GLU
1	D	197	GLU
1	D	203	LEU
1	D	211	SER
1	D	219	THR
1	D	245	GLU
1	E	2	SER
1	E	6	ILE
1	E	23	CYS
1	E	60	ARG
1	E	107	ARG
1	E	128	GLU
1	E	132	SER
1	E	135	THR
1	E	144	GLN
1	E	211	SER
1	E	221	ARG

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Mol	Chain	Res	Type
1	F	1	ILE
1	F	3	LEU
1	F	30	GLN
1	F	132	SER
1	F	211	SER
1	F	221	ARG
1	G	-1	GLU
1	G	5	SER
1	G	18	ARG
1	G	39	LEU
1	G	60	ARG
1	G	122	LEU
1	G	128	GLU
1	G	150	GLU
1	G	197	GLU
1	G	211	SER
1	G	221	ARG
1	H	1	ILE
1	H	18	ARG
1	H	23	CYS
1	H	39	LEU
1	H	60	ARG
1	H	139	THR
1	H	144	GLN
1	H	201	GLN
1	H	211	SER
1	H	221	ARG
1	I	30	GLN
1	I	39	LEU
1	I	60	ARG
1	I	80	MET
1	I	109	GLN
1	I	139	THR
1	I	144	GLN
1	I	150	GLU
1	I	168	GLU
1	I	211	SER
1	I	221	ARG
1	J	29	HIS
1	J	60	ARG
1	J	144	GLN
1	J	203	LEU

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Mol	Chain	Res	Type
1	J	211	SER
1	K	39	LEU
1	K	60	ARG
1	K	79	ASN
1	K	107	ARG
1	K	132	SER
1	K	135	THR
1	K	144	GLN
1	K	146	ARG
1	K	197	GLU
1	K	203	LEU
1	K	211	SER
1	K	221	ARG
1	L	18	ARG
1	L	30	GLN
1	L	60	ARG
1	L	107	ARG
1	L	122	LEU
1	L	138	ASN
1	L	153	ASN
1	L	157	ASP
1	L	211	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	29	HIS
1	A	31	HIS
1	A	198	GLN
1	B	14	HIS
1	B	29	HIS
1	B	31	HIS
1	C	14	HIS
1	C	29	HIS
1	C	208	ASN
1	D	14	HIS
1	D	29	HIS
1	D	31	HIS
1	D	208	ASN
1	E	14	HIS
1	E	29	HIS

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Mol	Chain	Res	Type
1	E	144	GLN
1	F	14	HIS
1	F	29	HIS
1	F	30	GLN
1	F	31	HIS
1	F	144	GLN
1	G	14	HIS
1	G	29	HIS
1	G	30	GLN
1	G	186	GLN
1	G	207	HIS
1	G	208	ASN
1	H	14	HIS
1	H	29	HIS
1	H	31	HIS
1	I	12	GLN
1	I	14	HIS
1	I	29	HIS
1	I	31	HIS
1	I	144	GLN
1	J	14	HIS
1	J	31	HIS
1	J	186	GLN
1	J	200	GLN
1	K	19	GLN
1	K	29	HIS
1	K	31	HIS
1	K	109	GLN
1	L	14	HIS
1	L	138	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	245/253 (96%)	0.65	18 (7%)	18 20	39, 51, 68, 83	0
1	B	245/253 (96%)	0.64	21 (8%)	13 14	40, 52, 73, 78	0
1	C	245/253 (96%)	0.48	15 (6%)	25 27	40, 52, 69, 79	0
1	D	248/253 (98%)	0.35	6 (2%)	62 66	40, 51, 68, 76	0
1	E	245/253 (96%)	0.44	10 (4%)	41 46	38, 52, 69, 82	0
1	F	245/253 (96%)	0.49	7 (2%)	55 60	40, 52, 66, 73	0
1	G	248/253 (98%)	0.53	12 (4%)	34 39	38, 52, 70, 77	0
1	H	245/253 (96%)	0.50	11 (4%)	37 42	39, 53, 66, 76	0
1	I	238/253 (94%)	0.57	16 (6%)	21 23	39, 52, 68, 77	0
1	J	238/253 (94%)	0.57	16 (6%)	21 23	40, 51, 66, 84	0
1	K	238/253 (94%)	0.73	21 (8%)	12 13	39, 52, 72, 90	0
1	L	238/253 (94%)	1.13	40 (16%)	2 2	39, 53, 67, 74	0
All	All	2918/3036 (96%)	0.59	193 (6%)	22 24	38, 52, 69, 90	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	51	GLU	7.7
1	F	1	ILE	6.8
1	K	151	TRP	6.7
1	B	144	GLN	5.5
1	L	42	GLU	5.4
1	F	41	ALA	5.3
1	A	80	MET	5.2
1	I	245	GLU	5.1
1	A	244	PRO	5.0
1	K	215	GLN	4.9
1	C	244	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	H	150	GLU	4.7
1	I	80	MET	4.6
1	L	151	TRP	4.5
1	K	149	PRO	4.5
1	A	150	GLU	4.3
1	J	8	SER	4.3
1	G	107	ARG	4.2
1	K	150	GLU	4.2
1	L	108	GLY	4.2
1	F	139	THR	4.1
1	J	39	LEU	4.1
1	K	152	GLY	4.0
1	B	166	SER	4.0
1	C	108	GLY	4.0
1	H	40	PRO	3.9
1	K	147	GLU	3.9
1	L	40	PRO	3.9
1	K	244	PRO	3.9
1	C	80	MET	3.9
1	L	243	LEU	3.9
1	I	50	LEU	3.8
1	B	245	GLU	3.8
1	L	41	ALA	3.8
1	J	245	GLU	3.7
1	C	150	GLU	3.7
1	A	149	PRO	3.7
1	H	139	THR	3.6
1	E	41	ALA	3.6
1	L	152	GLY	3.6
1	C	1	ILE	3.5
1	L	50	LEU	3.5
1	A	1	ILE	3.5
1	G	245	GLU	3.5
1	I	81	LEU	3.5
1	E	1	ILE	3.5
1	B	141	ASN	3.4
1	A	82	ASP	3.4
1	G	150	GLU	3.4
1	K	245	GLU	3.4
1	J	222	VAL	3.4
1	H	1	ILE	3.4
1	K	178	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	148	LEU	3.3
1	K	41	ALA	3.3
1	A	217	ASP	3.3
1	A	163	ARG	3.2
1	B	244	PRO	3.2
1	L	185	CYS	3.2
1	C	41	ALA	3.2
1	L	128	GLU	3.2
1	B	139	THR	3.2
1	E	141	ASN	3.2
1	F	142	PHE	3.2
1	K	148	LEU	3.1
1	L	149	PRO	3.1
1	D	245	GLU	3.1
1	K	39	LEU	3.1
1	H	80	MET	3.1
1	I	39	LEU	3.1
1	L	33	ASP	3.0
1	C	151	TRP	3.0
1	A	174	LEU	3.0
1	L	39	LEU	3.0
1	E	107	ARG	3.0
1	G	165	SER	3.0
1	A	104	VAL	3.0
1	L	160	ILE	3.0
1	I	40	PRO	3.0
1	H	52	GLY	2.9
1	H	41	ALA	2.9
1	D	147	GLU	2.9
1	L	43	LEU	2.9
1	C	82	ASP	2.9
1	K	26	GLU	2.9
1	E	244	PRO	2.9
1	L	82	ASP	2.9
1	L	79	ASN	2.8
1	I	141	ASN	2.8
1	E	39	LEU	2.8
1	E	80	MET	2.8
1	L	194	VAL	2.8
1	B	150	GLU	2.8
1	J	42	GLU	2.8
1	L	104	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	158	PHE	2.8
1	L	203	LEU	2.8
1	K	80	MET	2.8
1	A	109	GLN	2.7
1	G	-1	GLU	2.7
1	J	11	GLU	2.7
1	I	82	ASP	2.7
1	G	146	ARG	2.7
1	E	108	GLY	2.7
1	J	45	TYR	2.7
1	L	191	ALA	2.7
1	D	106	GLY	2.7
1	J	38	HIS	2.7
1	B	40	PRO	2.6
1	A	245	GLU	2.6
1	B	174	LEU	2.6
1	L	202	ILE	2.6
1	J	108	GLY	2.6
1	A	161	PHE	2.6
1	B	142	PHE	2.6
1	C	107	ARG	2.6
1	I	147	GLU	2.5
1	K	22	ASP	2.5
1	L	244	PRO	2.5
1	H	42	GLU	2.5
1	L	120	VAL	2.5
1	L	134	LEU	2.5
1	G	80	MET	2.5
1	I	139	THR	2.5
1	B	165	SER	2.5
1	K	45	TYR	2.5
1	A	167	PRO	2.4
1	B	147	GLU	2.4
1	E	186	GLN	2.4
1	B	160	ILE	2.4
1	K	138	ASN	2.4
1	L	147	GLU	2.4
1	J	196	ALA	2.4
1	B	134	LEU	2.4
1	C	148	LEU	2.4
1	I	45	TYR	2.4
1	G	38	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	197	GLU	2.4
1	J	80	MET	2.4
1	K	40	PRO	2.3
1	L	198	GLN	2.3
1	L	138	ASN	2.3
1	I	106	GLY	2.3
1	K	157	ASP	2.3
1	H	107	ARG	2.3
1	I	107	ARG	2.3
1	G	244	PRO	2.3
1	J	197	GLU	2.3
1	J	109	GLN	2.3
1	K	42	GLU	2.3
1	F	82	ASP	2.3
1	D	244	PRO	2.3
1	L	61	CYS	2.2
1	E	79	ASN	2.2
1	G	78	GLY	2.2
1	L	55	LEU	2.2
1	B	186	GLN	2.2
1	C	221	ARG	2.2
1	J	221	ARG	2.2
1	C	38	HIS	2.2
1	B	140	LEU	2.2
1	L	172	MET	2.2
1	C	141	ASN	2.2
1	F	52	GLY	2.1
1	B	197	GLU	2.1
1	A	15	PRO	2.1
1	B	138	ASN	2.1
1	A	2	SER	2.1
1	B	143	SER	2.1
1	L	189	ILE	2.1
1	K	43	LEU	2.1
1	J	219	THR	2.1
1	L	28	TRP	2.1
1	F	221	ARG	2.1
1	I	102	ASP	2.1
1	B	167	PRO	2.1
1	L	139	THR	2.1
1	H	146	ARG	2.1
1	A	151	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	221	ARG	2.1
1	D	50	LEU	2.1
1	L	148	LEU	2.1
1	I	60	ARG	2.0
1	C	243	LEU	2.0
1	L	117	LEU	2.0
1	C	79	ASN	2.0
1	D	51	GLU	2.0
1	B	133	ALA	2.0
1	G	102	ASP	2.0
1	J	82	ASP	2.0
1	L	179	GLU	2.0
1	H	162	VAL	2.0
1	A	107	ARG	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
2	CA	E	246	1/1	0.69	0.25	1.85	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.