Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 11:20 PM EDT

PDB ID	:	3GFG
Title	:	Structure of putative oxidoreductase yvaA from Bacillus subtilis in triclinic form
Authors	:	Ramagopal, U.A.; Toro, R.; Gilmore, M.; Chang, S.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-02-26
Resolution	:	2.59 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

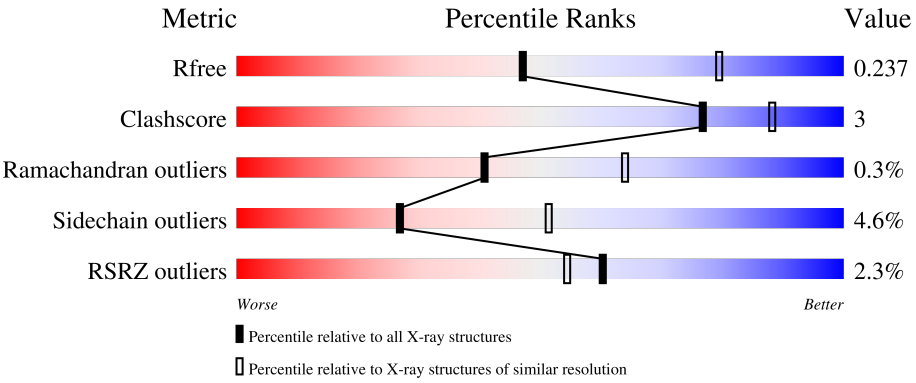
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	367	2% 84% 8% • 7%
1	B	367	% 85% 10% • 5%
1	C	367	3% 84% 10% 6%
1	D	367	2% 83% 8% 9%
1	E	367	84% 9% 7%

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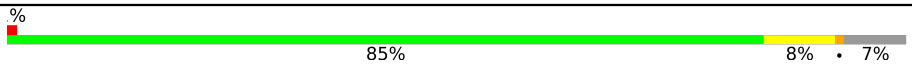
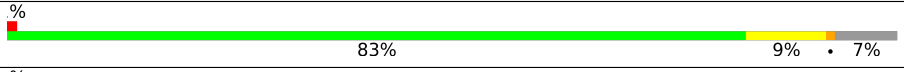
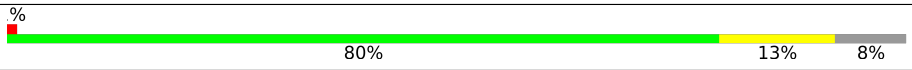
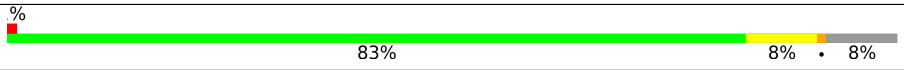
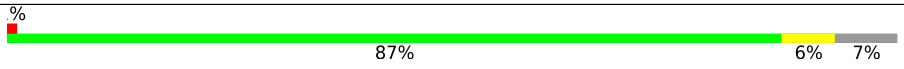
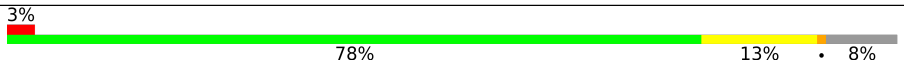
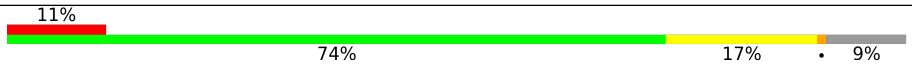
Mol	Chain	Length	Quality of chain
1	F	367	
1	G	367	
1	H	367	
1	I	367	
1	J	367	
1	K	367	
1	L	367	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32457 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 Uncharacterized oxidoreductase yvaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2655	1675	449	522	9			
1	B	350	Total	C	N	O	S	0	3	0
			2763	1742	468	544	9			
1	C	346	Total	C	N	O	S	0	1	0
			2708	1709	460	530	9			
1	D	335	Total	C	N	O	S	0	1	0
			2622	1656	440	517	9			
1	E	342	Total	C	N	O	S	0	4	0
			2696	1701	458	528	9			
1	F	342	Total	C	N	O	S	0	2	0
			2674	1688	450	527	9			
1	G	340	Total	C	N	O	S	0	2	0
			2667	1683	451	524	9			
1	H	339	Total	C	N	O	S	0	1	0
			2653	1675	448	521	9			
1	I	336	Total	C	N	O	S	0	0	0
			2634	1661	444	520	9			
1	J	340	Total	C	N	O	S	0	0	0
			2650	1675	446	520	9			
1	K	337	Total	C	N	O	S	0	0	0
			2628	1659	441	519	9			
1	L	334	Total	C	N	O	S	0	0	0
			2591	1639	435	508	9			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP O32223
A	1	SER	-	expression tag	UNP O32223
A	2	LEU	-	expression tag	UNP O32223
A	359	GLU	-	expression tag	UNP O32223
A	360	GLY	-	expression tag	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
A	361	HIS	-	expression tag	UNP O32223
A	362	HIS	-	expression tag	UNP O32223
A	363	HIS	-	expression tag	UNP O32223
A	364	HIS	-	expression tag	UNP O32223
A	365	HIS	-	expression tag	UNP O32223
A	366	HIS	-	expression tag	UNP O32223
B	0	MET	-	expression tag	UNP O32223
B	1	SER	-	expression tag	UNP O32223
B	2	LEU	-	expression tag	UNP O32223
B	359	GLU	-	expression tag	UNP O32223
B	360	GLY	-	expression tag	UNP O32223
B	361	HIS	-	expression tag	UNP O32223
B	362	HIS	-	expression tag	UNP O32223
B	363	HIS	-	expression tag	UNP O32223
B	364	HIS	-	expression tag	UNP O32223
B	365	HIS	-	expression tag	UNP O32223
B	366	HIS	-	expression tag	UNP O32223
C	0	MET	-	expression tag	UNP O32223
C	1	SER	-	expression tag	UNP O32223
C	2	LEU	-	expression tag	UNP O32223
C	359	GLU	-	expression tag	UNP O32223
C	360	GLY	-	expression tag	UNP O32223
C	361	HIS	-	expression tag	UNP O32223
C	362	HIS	-	expression tag	UNP O32223
C	363	HIS	-	expression tag	UNP O32223
C	364	HIS	-	expression tag	UNP O32223
C	365	HIS	-	expression tag	UNP O32223
C	366	HIS	-	expression tag	UNP O32223
D	0	MET	-	expression tag	UNP O32223
D	1	SER	-	expression tag	UNP O32223
D	2	LEU	-	expression tag	UNP O32223
D	359	GLU	-	expression tag	UNP O32223
D	360	GLY	-	expression tag	UNP O32223
D	361	HIS	-	expression tag	UNP O32223
D	362	HIS	-	expression tag	UNP O32223
D	363	HIS	-	expression tag	UNP O32223
D	364	HIS	-	expression tag	UNP O32223
D	365	HIS	-	expression tag	UNP O32223
D	366	HIS	-	expression tag	UNP O32223
E	0	MET	-	expression tag	UNP O32223
E	1	SER	-	expression tag	UNP O32223
E	2	LEU	-	expression tag	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
E	359	GLU	-	expression tag	UNP O32223
E	360	GLY	-	expression tag	UNP O32223
E	361	HIS	-	expression tag	UNP O32223
E	362	HIS	-	expression tag	UNP O32223
E	363	HIS	-	expression tag	UNP O32223
E	364	HIS	-	expression tag	UNP O32223
E	365	HIS	-	expression tag	UNP O32223
E	366	HIS	-	expression tag	UNP O32223
F	0	MET	-	expression tag	UNP O32223
F	1	SER	-	expression tag	UNP O32223
F	2	LEU	-	expression tag	UNP O32223
F	359	GLU	-	expression tag	UNP O32223
F	360	GLY	-	expression tag	UNP O32223
F	361	HIS	-	expression tag	UNP O32223
F	362	HIS	-	expression tag	UNP O32223
F	363	HIS	-	expression tag	UNP O32223
F	364	HIS	-	expression tag	UNP O32223
F	365	HIS	-	expression tag	UNP O32223
F	366	HIS	-	expression tag	UNP O32223
G	0	MET	-	expression tag	UNP O32223
G	1	SER	-	expression tag	UNP O32223
G	2	LEU	-	expression tag	UNP O32223
G	359	GLU	-	expression tag	UNP O32223
G	360	GLY	-	expression tag	UNP O32223
G	361	HIS	-	expression tag	UNP O32223
G	362	HIS	-	expression tag	UNP O32223
G	363	HIS	-	expression tag	UNP O32223
G	364	HIS	-	expression tag	UNP O32223
G	365	HIS	-	expression tag	UNP O32223
G	366	HIS	-	expression tag	UNP O32223
H	0	MET	-	expression tag	UNP O32223
H	1	SER	-	expression tag	UNP O32223
H	2	LEU	-	expression tag	UNP O32223
H	359	GLU	-	expression tag	UNP O32223
H	360	GLY	-	expression tag	UNP O32223
H	361	HIS	-	expression tag	UNP O32223
H	362	HIS	-	expression tag	UNP O32223
H	363	HIS	-	expression tag	UNP O32223
H	364	HIS	-	expression tag	UNP O32223
H	365	HIS	-	expression tag	UNP O32223
H	366	HIS	-	expression tag	UNP O32223
I	0	MET	-	expression tag	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1	SER	-	expression tag	UNP O32223
I	2	LEU	-	expression tag	UNP O32223
I	359	GLU	-	expression tag	UNP O32223
I	360	GLY	-	expression tag	UNP O32223
I	361	HIS	-	expression tag	UNP O32223
I	362	HIS	-	expression tag	UNP O32223
I	363	HIS	-	expression tag	UNP O32223
I	364	HIS	-	expression tag	UNP O32223
I	365	HIS	-	expression tag	UNP O32223
I	366	HIS	-	expression tag	UNP O32223
J	0	MET	-	expression tag	UNP O32223
J	1	SER	-	expression tag	UNP O32223
J	2	LEU	-	expression tag	UNP O32223
J	359	GLU	-	expression tag	UNP O32223
J	360	GLY	-	expression tag	UNP O32223
J	361	HIS	-	expression tag	UNP O32223
J	362	HIS	-	expression tag	UNP O32223
J	363	HIS	-	expression tag	UNP O32223
J	364	HIS	-	expression tag	UNP O32223
J	365	HIS	-	expression tag	UNP O32223
J	366	HIS	-	expression tag	UNP O32223
K	0	MET	-	expression tag	UNP O32223
K	1	SER	-	expression tag	UNP O32223
K	2	LEU	-	expression tag	UNP O32223
K	359	GLU	-	expression tag	UNP O32223
K	360	GLY	-	expression tag	UNP O32223
K	361	HIS	-	expression tag	UNP O32223
K	362	HIS	-	expression tag	UNP O32223
K	363	HIS	-	expression tag	UNP O32223
K	364	HIS	-	expression tag	UNP O32223
K	365	HIS	-	expression tag	UNP O32223
K	366	HIS	-	expression tag	UNP O32223
L	0	MET	-	expression tag	UNP O32223
L	1	SER	-	expression tag	UNP O32223
L	2	LEU	-	expression tag	UNP O32223
L	359	GLU	-	expression tag	UNP O32223
L	360	GLY	-	expression tag	UNP O32223
L	361	HIS	-	expression tag	UNP O32223
L	362	HIS	-	expression tag	UNP O32223
L	363	HIS	-	expression tag	UNP O32223
L	364	HIS	-	expression tag	UNP O32223
L	365	HIS	-	expression tag	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
L	366	HIS	-	expression tag	UNP O32223

- Molecule 2 is water.

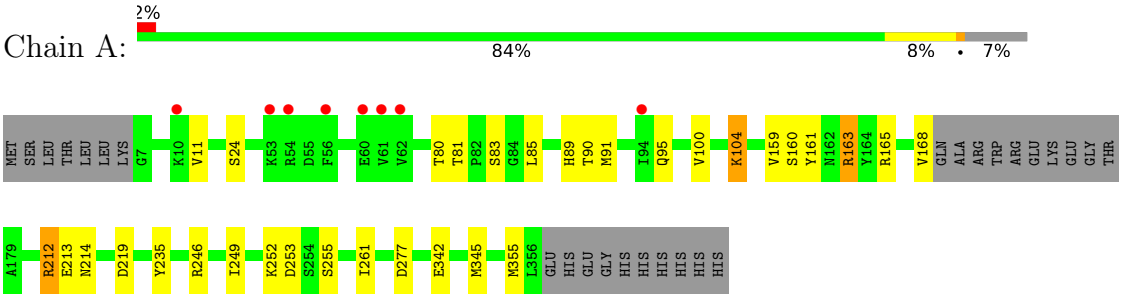
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	71	Total O 71 71	0	0
2	C	38	Total O 38 38	0	0
2	D	49	Total O 49 49	0	0
2	E	85	Total O 85 85	0	0
2	F	66	Total O 66 66	0	0
2	G	36	Total O 36 36	0	0
2	H	49	Total O 49 49	0	0
2	I	19	Total O 19 19	0	0
2	J	36	Total O 36 36	0	0
2	K	6	Total O 6 6	0	0
2	L	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

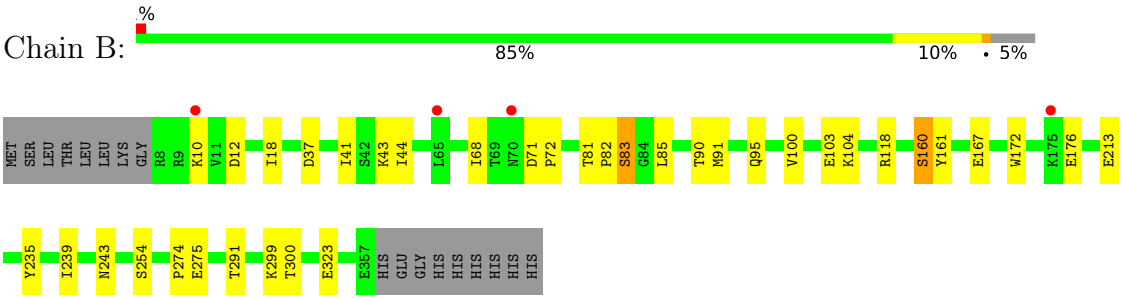
• Molecule 1: Uncharacterized oxidoreductase yvaA

Chain A:



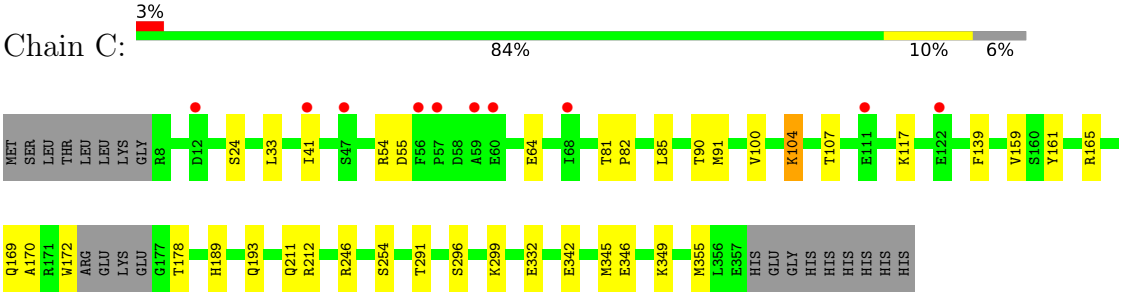
• Molecule 1: Uncharacterized oxidoreductase yvaA

Chain B:



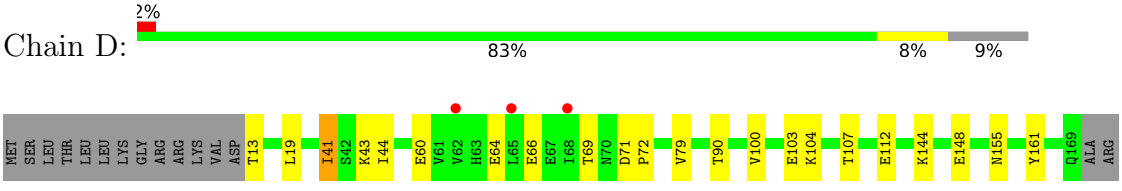
• Molecule 1: Uncharacterized oxidoreductase yvaA

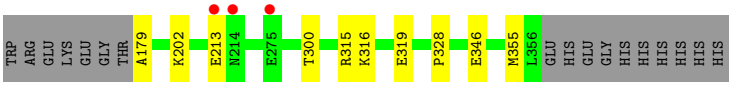
Chain C:



• Molecule 1: Uncharacterized oxidoreductase yvaA

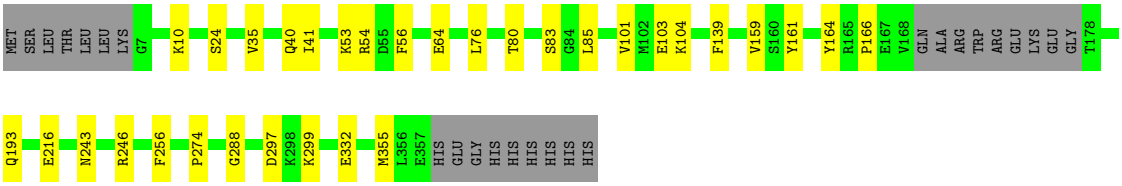
Chain D:





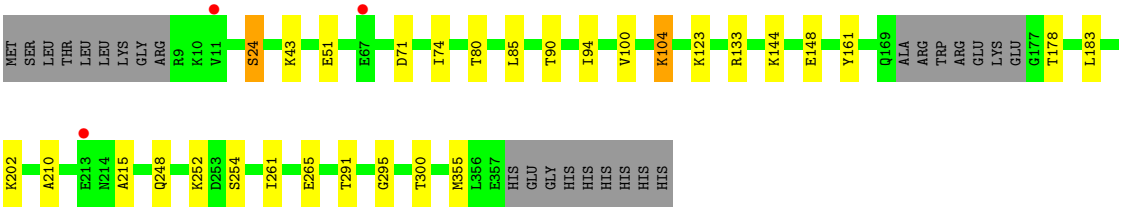
• Molecule 1: Uncharacterized oxidoreductase yvaA

Chain E:



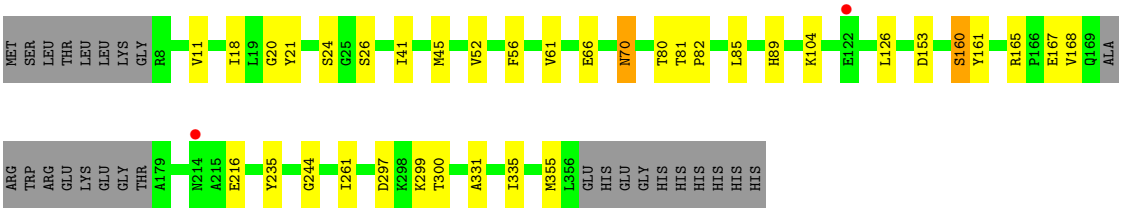
• Molecule 1: Uncharacterized oxidoreductase yvaA

Chain F:



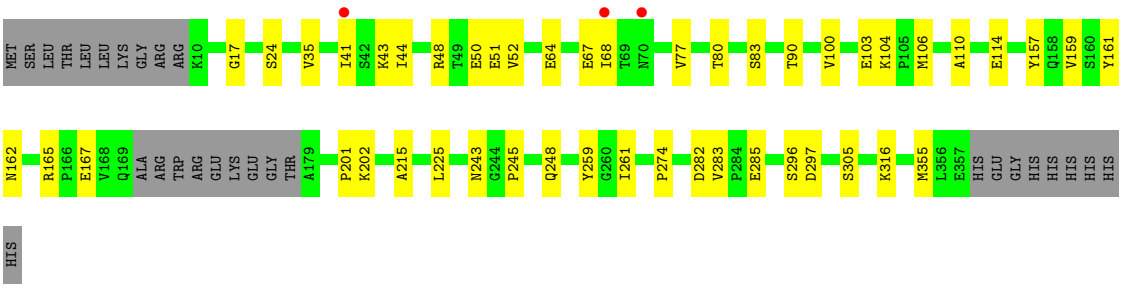
• Molecule 1: Uncharacterized oxidoreductase yvaA

Chain G:

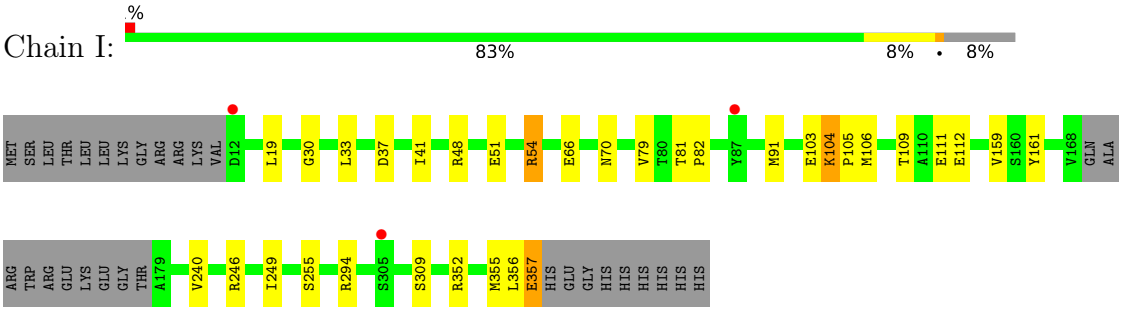


• Molecule 1: Uncharacterized oxidoreductase yvaA

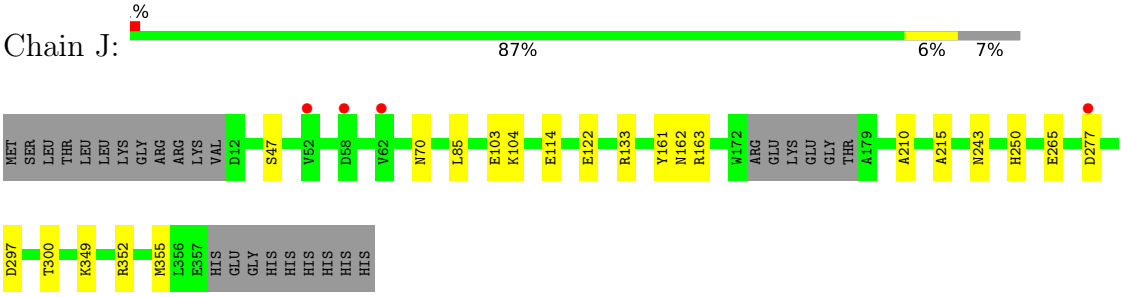
Chain H:



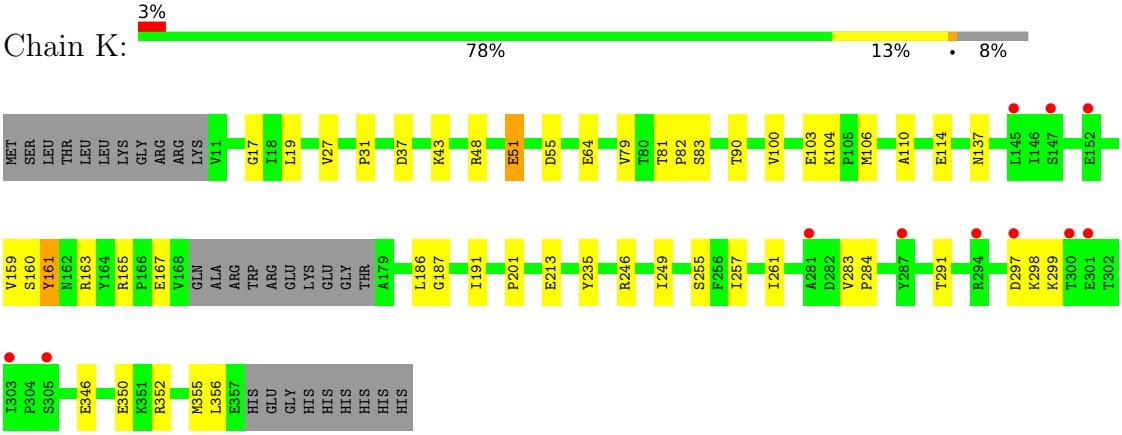
• Molecule 1: Uncharacterized oxidoreductase yvaA



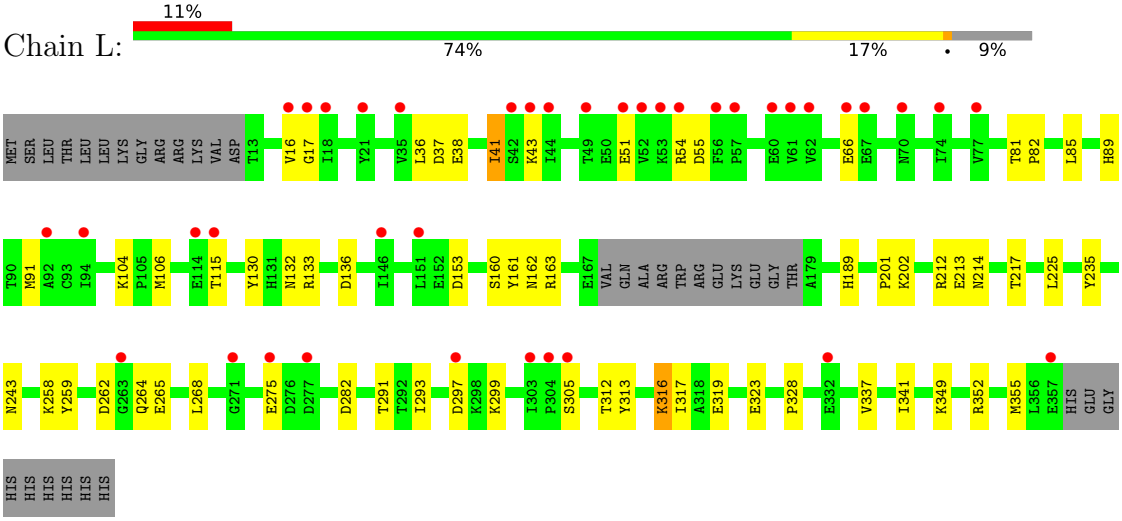
• Molecule 1: Uncharacterized oxidoreductase yvaA



• Molecule 1: Uncharacterized oxidoreductase yvaA



• Molecule 1: Uncharacterized oxidoreductase yvaA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.93Å 92.14Å 187.59Å 95.31° 94.19° 95.21°	Depositor
Resolution (Å)	45.41 – 2.59 44.55 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.41-2.59) 97.7 (44.55-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.236 0.184 , 0.237	Depositor DCC
R_{free} test set	7368 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32457	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 20.87 % 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 7.9220e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.65	0/2704	0.66	0/3660
1	B	0.62	0/2824	0.68	0/3822
1	C	0.58	0/2762	0.64	0/3740
1	D	0.61	0/2674	0.68	0/3621
1	E	0.68	1/2757 (0.0%)	0.70	0/3730
1	F	0.66	0/2729	0.70	0/3695
1	G	0.61	0/2722	0.68	1/3685 (0.0%)
1	H	0.58	0/2705	0.65	0/3662
1	I	0.57	0/2683	0.66	0/3632
1	J	0.60	1/2701 (0.0%)	0.65	0/3660
1	K	0.49	0/2677	0.60	0/3627
1	L	0.49	0/2640	0.59	0/3577
All	All	0.60	2/32578 (0.0%)	0.66	1/44111 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	114	GLU	CG-CD	5.50	1.60	1.51
1	E	332	GLU	CG-CD	5.10	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	244	GLY	N-CA-C	-5.17	100.17	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2655	0	2625	15	0
1	B	2763	0	2729	14	0
1	C	2708	0	2672	18	0
1	D	2622	0	2589	13	0
1	E	2696	0	2676	13	0
1	F	2674	0	2637	14	0
1	G	2667	0	2634	15	0
1	H	2653	0	2624	22	0
1	I	2634	0	2602	13	0
1	J	2650	0	2604	6	0
1	K	2628	0	2587	25	0
1	L	2591	0	2548	28	0
2	A	57	0	0	0	0
2	B	71	0	0	1	0
2	C	38	0	0	0	0
2	D	49	0	0	1	0
2	E	85	0	0	1	0
2	F	66	0	0	3	0
2	G	36	0	0	1	0
2	H	49	0	0	2	0
2	I	19	0	0	0	0
2	J	36	0	0	0	0
2	K	6	0	0	0	0
2	L	4	0	0	0	0
All	All	32457	0	31527	190	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 3.

All (190) 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:I:356:LEU:O	1:I:357:GLU:HB2	1.78	0.81
1:J:210:ALA:HB1	1:J:215:ALA:HB3	1.65	0.79
1:L:41:ILE:H	1:L:41:ILE:HD12	1.48	0.78
1:E:40[A]:GLN:HE21	1:E:41:ILE:H	1.35	0.74
1:G:24:SER:HB2	1:G:80:THR:HB	1.70	0.74
1:K:165:ARG:HG2	1:K:165:ARG:HH11	1.57	0.69
1:B:160:SER:HB2	1:B:235:TYR:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASN:HB3	2:B:419:HOH:O	1.93	0.67
1:K:298:LYS:HG2	1:K:299:LYS:H	1.60	0.67
1:G:52:VAL:HG11	1:G:61:VAL:HG22	1.77	0.66
1:G:85:LEU:HD23	1:G:89:HIS:CE1	2.32	0.64
1:C:82:PRO:HD2	1:C:85:LEU:HD12	1.80	0.63
1:F:90:THR:HG23	1:F:100:VAL:HG11	1.78	0.63
1:C:117:LYS:HE2	1:C:332:GLU:OE1	1.99	0.63
1:A:90:THR:HG23	1:A:100:VAL:HG11	1.80	0.62
1:L:160:SER:HB3	1:L:235:TYR:CZ	2.34	0.62
1:J:210:ALA:HB1	1:J:215:ALA:CB	2.30	0.61
1:L:133:ARG:HG2	1:L:189:HIS:ND1	2.16	0.60
1:G:85:LEU:HD23	1:G:89:HIS:HE1	1.66	0.60
1:B:160:SER:HB2	1:B:235:TYR:CZ	2.38	0.59
1:C:81:THR:HB	1:C:82:PRO:HD2	1.83	0.59
1:B:10:LYS:HE3	1:B:12:ASP:OD1	2.01	0.58
1:D:144:LYS:O	1:D:148:GLU:HG3	2.02	0.58
1:D:90:THR:HG23	1:D:100:VAL:HG11	1.85	0.58
1:C:54:ARG:NH1	1:C:55:ASP:OD1	2.38	0.57
1:D:41:ILE:HD11	1:D:44:ILE:HG13	1.86	0.57
1:K:298:LYS:HG2	1:K:299:LYS:N	2.20	0.56
1:C:90:THR:HG23	1:C:100:VAL:HG11	1.85	0.56
1:H:215:ALA:HB1	2:H:508:HOH:O	2.05	0.56
1:I:33:LEU:HB3	1:I:41:ILE:HD11	1.86	0.56
1:H:90:THR:HG23	1:H:100:VAL:HG11	1.86	0.56
1:C:81:THR:HB	1:C:82:PRO:CD	2.37	0.55
1:L:81:THR:HB	1:L:82:PRO:HD2	1.88	0.55
1:A:165:ARG:HB2	1:A:212:ARG:HH11	1.71	0.55
1:C:169:GLN:HE21	1:K:48:ARG:NH2	2.05	0.55
1:I:81:THR:HB	1:I:82:PRO:HD2	1.88	0.55
1:C:342:GLU:HA	1:C:345:MET:HE2	1.88	0.55
1:J:133:ARG:HH22	1:J:265:GLU:CD	2.10	0.55
1:D:41:ILE:HD11	1:D:44:ILE:CG1	2.37	0.54
1:G:21:TYR:CE1	1:G:26:SER:HA	2.42	0.54
1:G:41:ILE:HD12	1:G:56:PHE:CE1	2.42	0.54
1:A:342:GLU:HA	1:A:345:MET:HE2	1.88	0.54
1:H:283:VAL:HG12	1:H:285:GLU:HG2	1.88	0.54
1:A:212:ARG:HD2	1:A:219:ASP:OD2	2.06	0.54
1:A:11:VAL:HG23	1:A:11:VAL:O	2.08	0.54
1:L:319:GLU:O	1:L:323:GLU:HB2	2.08	0.54
1:F:24:SER:HB3	1:F:80:THR:HB	1.90	0.54
1:H:50:GLU:OE2	1:H:50:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:THR:HB	1:D:112:GLU:OE1	2.08	0.53
1:H:35:VAL:HG21	1:H:274:PRO:HG2	1.91	0.53
1:H:48:ARG:HB3	1:H:51:GLU:HG3	1.90	0.52
1:I:159:VAL:HA	1:I:246:ARG:O	2.09	0.52
1:G:70:ASN:HD22	1:G:70:ASN:N	2.08	0.52
1:F:51:GLU:N	1:F:51:GLU:OE1	2.43	0.52
1:D:66:GLU:HA	1:D:69:THR:OG1	2.09	0.51
1:K:246:ARG:NH1	1:K:261:ILE:HG22	2.25	0.51
1:A:91:MET:O	1:A:95:GLN:HG2	2.10	0.50
1:K:19:LEU:HD12	1:K:79:VAL:HG22	1.93	0.50
1:H:41:ILE:HD12	1:H:41:ILE:N	2.26	0.50
1:K:249:ILE:O	1:K:255:SER:HA	2.11	0.50
1:B:81:THR:HB	1:B:82:PRO:HD2	1.94	0.50
1:I:81:THR:HB	1:I:82:PRO:CD	2.42	0.50
1:G:24:SER:CB	1:G:80:THR:HB	2.40	0.50
1:F:210:ALA:HB1	1:F:215:ALA:HB3	1.93	0.49
1:E:40[A]:GLN:NE2	1:E:41:ILE:H	2.06	0.49
1:H:245:PRO:HG2	1:H:248:GLN:HE21	1.76	0.49
1:B:172:TRP:O	1:B:176:GLU:HB2	2.13	0.49
1:B:323[B]:GLU:OE1	1:B:323[B]:GLU:HA	2.13	0.49
1:G:331:ALA:O	1:G:335:ILE:HG13	2.13	0.49
1:K:187:GLY:O	1:K:191:ILE:HG13	2.13	0.49
1:A:249:ILE:O	1:A:255:SER:HA	2.13	0.48
1:B:90:THR:HG23	1:B:100:VAL:HG11	1.95	0.48
1:E:40[A]:GLN:HE21	1:E:41:ILE:N	2.07	0.48
1:I:19:LEU:HD12	1:I:79:VAL:HG22	1.95	0.48
1:I:109:THR:OG1	1:I:112:GLU:HG3	2.13	0.48
1:F:261:ILE:HG13	2:F:377:HOH:O	2.13	0.48
1:I:51:GLU:HG3	1:I:54:ARG:NH2	2.27	0.48
1:K:159:VAL:HA	1:K:246:ARG:O	2.13	0.48
1:D:179:ALA:N	2:D:454:HOH:O	2.47	0.48
1:G:126:LEU:HA	2:G:1338:HOH:O	2.13	0.47
1:H:44:ILE:HD12	1:H:52:VAL:HG13	1.96	0.47
1:L:130:TYR:CE2	1:L:132:ASN:ND2	2.82	0.47
1:K:201:PRO:O	1:K:356:LEU:HD12	2.14	0.47
1:H:245:PRO:HG2	1:H:248:GLN:NE2	2.29	0.47
1:L:85:LEU:HD23	1:L:89:HIS:CE1	2.49	0.47
1:L:312:THR:HG22	1:L:316:LYS:HE3	1.96	0.47
1:H:43:LYS:HB3	1:H:68:ILE:HD11	1.96	0.47
1:K:165:ARG:HH11	1:K:165:ARG:CG	2.26	0.47
1:C:172:TRP:CZ3	1:K:31:PRO:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:ARG:HB3	1:K:51:GLU:CG	2.45	0.47
1:L:162:ASN:HB2	1:L:243:ASN:OD1	2.15	0.47
1:C:104:LYS:HE3	1:C:189:HIS:CE1	2.50	0.47
1:L:337:VAL:O	1:L:341:ILE:HG13	2.15	0.46
1:E:164:TYR:CZ	1:E:166:PRO:HG3	2.50	0.46
1:H:282:ASP:HB2	1:H:305:SER:HB2	1.97	0.46
1:C:159:VAL:HA	1:C:246:ARG:O	2.16	0.46
1:L:282:ASP:HB2	1:L:305:SER:HB2	1.98	0.46
1:C:254:SER:HA	1:C:291:THR:O	2.16	0.46
1:K:48:ARG:HB3	1:K:51:GLU:HG3	1.98	0.46
1:L:312:THR:CG2	1:L:316:LYS:HE3	2.45	0.46
1:A:81:THR:HG21	1:A:89:HIS:CE1	2.50	0.46
1:E:35:VAL:HG21	1:E:274:PRO:HG2	1.97	0.46
1:C:139:PHE:CE1	1:C:193:GLN:HB3	2.51	0.46
1:K:346:GLU:O	1:K:350:GLU:HG2	2.16	0.46
1:H:162:ASN:HB2	1:H:243:ASN:OD1	2.15	0.46
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.81	0.46
1:E:76:LEU:HD11	1:E:101:VAL:HG23	1.97	0.46
1:B:43:LYS:HB3	1:B:68:ILE:HD11	1.98	0.45
1:E:24:SER:HB2	1:E:80:THR:HB	1.97	0.45
1:L:36:LEU:HB3	1:L:38:GLU:OE1	2.17	0.45
1:L:313:TYR:O	1:L:317:ILE:HG12	2.16	0.45
1:A:159:VAL:HA	1:A:246:ARG:O	2.17	0.44
1:F:94:ILE:O	1:F:123:LYS:HG2	2.17	0.44
1:J:162:ASN:HB2	1:J:243:ASN:OD1	2.18	0.44
1:K:81:THR:HB	1:K:82:PRO:CD	2.46	0.44
1:K:110:ALA:O	1:K:114:GLU:HG2	2.17	0.44
1:L:212:ARG:HE	1:L:212:ARG:HB2	1.66	0.44
1:C:104:LYS:O	1:C:104:LYS:HD3	2.18	0.44
1:C:41:ILE:HD12	1:C:41:ILE:N	2.32	0.44
1:L:133:ARG:HD2	1:L:136:ASP:OD2	2.18	0.44
1:I:240:VAL:HG13	1:J:250:HIS:CE1	2.52	0.44
1:G:11:VAL:O	1:G:11:VAL:HG23	2.18	0.44
1:H:243:ASN:HB3	2:H:393:HOH:O	2.18	0.44
1:K:352:ARG:HA	1:L:352:ARG:HA	2.00	0.44
1:L:316:LYS:HB3	1:L:328:PRO:HD3	2.00	0.44
1:F:104:LYS:O	1:F:104:LYS:HD3	2.19	0.43
1:F:248:GLN:HG3	2:F:565:HOH:O	2.17	0.43
1:H:157:TYR:CE2	1:H:159:VAL:CG2	3.01	0.43
1:D:43:LYS:HA	1:D:60:GLU:O	2.18	0.43
1:D:315:ARG:O	1:D:319:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:ILE:H	1:L:41:ILE:CD1	2.18	0.43
1:L:293:ILE:HA	1:L:297:ASP:O	2.18	0.43
1:A:163:ARG:HG3	1:A:165:ARG:HG3	2.01	0.43
1:L:265:GLU:HA	1:L:268:LEU:HD12	2.00	0.43
1:L:201:PRO:HG3	1:L:225:LEU:HG	2.00	0.43
1:A:24:SER:HB2	1:A:80:THR:HB	2.00	0.43
1:I:66:GLU:O	1:I:70:ASN:HB2	2.18	0.43
1:A:213:GLU:HG2	1:A:214:ASN:OD1	2.18	0.43
1:F:254:SER:HA	1:F:291:THR:O	2.19	0.43
1:B:160:SER:CB	1:B:235:TYR:CZ	3.01	0.42
1:E:159:VAL:HA	1:E:246:ARG:O	2.19	0.42
1:H:64:GLU:O	1:H:67:GLU:HG3	2.19	0.42
1:H:110:ALA:O	1:H:114:GLU:HG2	2.19	0.42
1:C:211:GLN:NE2	1:D:155:ASN:HB2	2.34	0.42
1:K:160:SER:HA	1:K:235:TYR:O	2.19	0.42
1:E:41:ILE:HD12	1:E:56:PHE:CE1	2.54	0.42
1:E:139:PHE:CE1	1:E:193:GLN:HB3	2.55	0.42
1:D:19:LEU:HD12	1:D:79:VAL:HG22	2.00	0.42
1:F:183:LEU:HB3	2:F:1317:HOH:O	2.19	0.42
1:K:17:GLY:HA2	1:K:43:LYS:O	2.20	0.42
1:D:71:ASP:HA	1:D:72:PRO:HD2	1.89	0.42
1:I:249:ILE:O	1:I:255:SER:HA	2.18	0.42
1:I:352:ARG:HA	1:J:352:ARG:HA	2.02	0.42
1:D:316:LYS:HD3	1:D:328:PRO:HB3	2.02	0.42
1:E:243:ASN:HB3	2:E:588:HOH:O	2.20	0.42
1:L:130:TYR:CE1	1:L:132:ASN:HB3	2.55	0.42
1:H:245:PRO:HD3	1:H:259:TYR:CZ	2.55	0.42
1:B:254:SER:HA	1:B:291:THR:O	2.19	0.41
1:E:54:ARG:HH21	1:E:54:ARG:CG	2.33	0.41
1:F:43:LYS:HE3	1:F:71:ASP:OD2	2.19	0.41
1:F:144:LYS:HE3	1:F:148:GLU:OE2	2.20	0.41
1:K:27:VAL:O	1:K:31:PRO:HG2	2.20	0.41
1:G:52:VAL:CG1	1:G:61:VAL:HG22	2.48	0.41
1:I:104:LYS:HA	1:I:105:PRO:C	2.39	0.41
1:B:71:ASP:HA	1:B:72:PRO:HD2	1.87	0.41
1:F:133:ARG:HH22	1:F:265:GLU:CD	2.23	0.41
1:H:24:SER:HB2	1:H:80:THR:HB	2.01	0.41
1:B:91:MET:O	1:B:95:GLN:HG2	2.20	0.41
1:G:81:THR:HB	1:G:82:PRO:HD2	2.01	0.41
1:H:17:GLY:O	1:H:77:VAL:HA	2.21	0.41
1:K:90:THR:HG23	1:K:100:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:17:GLY:HA2	1:L:43:LYS:O	2.21	0.41
1:L:291:THR:HA	1:L:299:LYS:O	2.20	0.41
1:F:71:ASP:HB3	1:F:74:ILE:HG12	2.03	0.41
1:G:18:ILE:HG22	1:G:20:GLY:O	2.21	0.41
1:H:157:TYR:CE2	1:H:159:VAL:HG21	2.55	0.41
1:K:246:ARG:HH11	1:K:261:ILE:HG22	1.85	0.41
1:L:81:THR:CB	1:L:82:PRO:HD2	2.48	0.41
1:A:104:LYS:O	1:A:104:LYS:HD3	2.21	0.41
1:A:160:SER:HA	1:A:235:TYR:O	2.21	0.41
1:L:258:LYS:HG2	1:L:259:TYR:O	2.21	0.41
1:G:160:SER:OG	1:G:235:TYR:CE1	2.73	0.41
1:K:283:VAL:HA	1:K:284:PRO:HD2	1.72	0.41
1:C:33:LEU:HB3	1:C:41:ILE:HD11	2.03	0.40
1:E:256:PHE:CZ	1:E:288:GLY:HA3	2.56	0.40
1:H:201:PRO:HG3	1:H:225:LEU:HG	2.03	0.40
1:K:161:TYR:CD1	1:K:186:LEU:HB3	2.56	0.40
1:L:262:ASP:OD2	1:L:264:GLN:HB2	2.20	0.40
1:C:165:ARG:O	1:C:212:ARG:NH1	2.47	0.40
1:B:18:ILE:O	1:B:44:ILE:HA	2.21	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	336/367 (92%)	327 (97%)	9 (3%)	0	100	100
1	B	351/367 (96%)	336 (96%)	13 (4%)	2 (1%)	25	47
1	C	343/367 (94%)	331 (96%)	11 (3%)	1 (0%)	41	64
1	D	332/367 (90%)	317 (96%)	15 (4%)	0	100	100
1	E	342/367 (93%)	333 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	340/367 (93%)	329 (97%)	10 (3%)	1 (0%)	41 64
1	G	338/367 (92%)	322 (95%)	15 (4%)	1 (0%)	41 64
1	H	336/367 (92%)	325 (97%)	10 (3%)	1 (0%)	41 64
1	I	332/367 (90%)	317 (96%)	12 (4%)	3 (1%)	17 35
1	J	336/367 (92%)	319 (95%)	17 (5%)	0	100 100
1	K	333/367 (91%)	312 (94%)	20 (6%)	1 (0%)	41 64
1	L	330/367 (90%)	311 (94%)	18 (6%)	1 (0%)	41 64
All	All	4049/4404 (92%)	3879 (96%)	159 (4%)	11 (0%)	41 64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	153	ASP
1	I	30	GLY
1	B	83	SER
1	C	170	ALA
1	L	106	MET
1	H	106	MET
1	I	48	ARG
1	K	106	MET
1	I	106	MET
1	F	295	GLY
1	B	274	PRO

5.3.2 Protein sidechains (i)

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	286/312 (92%)	274 (96%)	12 (4%)	30 55
1	B	297/312 (95%)	282 (95%)	15 (5%)	24 46
1	C	290/312 (93%)	278 (96%)	12 (4%)	30 56
1	D	283/312 (91%)	272 (96%)	11 (4%)	32 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	291/312 (93%)	279 (96%)	12 (4%)	30 56
1	F	287/312 (92%)	278 (97%)	9 (3%)	40 66
1	G	287/312 (92%)	272 (95%)	15 (5%)	23 46
1	H	286/312 (92%)	274 (96%)	12 (4%)	30 55
1	I	285/312 (91%)	274 (96%)	11 (4%)	32 58
1	J	283/312 (91%)	270 (95%)	13 (5%)	27 51
1	K	283/312 (91%)	267 (94%)	16 (6%)	20 41
1	L	276/312 (88%)	255 (92%)	21 (8%)	13 26
All	All	3434/3744 (92%)	3275 (95%)	159 (5%)	27 51

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	A	85	LEU
1	A	104	LYS
1	A	161	TYR
1	A	163	ARG
1	A	168	VAL
1	A	212	ARG
1	A	252	LYS
1	A	253	ASP
1	A	261	ILE
1	A	277	ASP
1	A	355	MET
1	B	37	ASP
1	B	41	ILE
1	B	83	SER
1	B	85	LEU
1	B	103	GLU
1	B	104	LYS
1	B	118	ARG
1	B	160	SER
1	B	161	TYR
1	B	167	GLU
1	B	213	GLU
1	B	239	ILE
1	B	275	GLU
1	B	299	LYS

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Mol	Chain	Res	Type
1	B	300	THR
1	C	24	SER
1	C	64	GLU
1	C	91	MET
1	C	104	LYS
1	C	107	THR
1	C	161	TYR
1	C	178	THR
1	C	296	SER
1	C	299	LYS
1	C	346	GLU
1	C	349	LYS
1	C	355	MET
1	D	13	THR
1	D	41	ILE
1	D	64	GLU
1	D	103	GLU
1	D	104	LYS
1	D	161	TYR
1	D	202	LYS
1	D	213	GLU
1	D	300	THR
1	D	346	GLU
1	D	355	MET
1	E	10	LYS
1	E	53	LYS
1	E	64	GLU
1	E	83	SER
1	E	85	LEU
1	E	103	GLU
1	E	104	LYS
1	E	161	TYR
1	E	216	GLU
1	E	297	ASP
1	E	299	LYS
1	E	355	MET
1	F	24	SER
1	F	85	LEU
1	F	104	LYS
1	F	161	TYR
1	F	178	THR
1	F	202	LYS

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Mol	Chain	Res	Type
1	F	252	LYS
1	F	300	THR
1	F	355	MET
1	G	45	MET
1	G	66	GLU
1	G	70	ASN
1	G	104	LYS
1	G	160	SER
1	G	161	TYR
1	G	165	ARG
1	G	167	GLU
1	G	168	VAL
1	G	216	GLU
1	G	261	ILE
1	G	297	ASP
1	G	299	LYS
1	G	300	THR
1	G	355	MET
1	H	83	SER
1	H	103	GLU
1	H	104	LYS
1	H	161	TYR
1	H	165	ARG
1	H	167	GLU
1	H	202	LYS
1	H	261	ILE
1	H	296	SER
1	H	297	ASP
1	H	316	LYS
1	H	355	MET
1	I	37	ASP
1	I	54	ARG
1	I	91	MET
1	I	103	GLU
1	I	104	LYS
1	I	111	GLU
1	I	161	TYR
1	I	294	ARG
1	I	309	SER
1	I	355	MET
1	I	357	GLU
1	J	47	SER

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Mol	Chain	Res	Type
1	J	70	ASN
1	J	85	LEU
1	J	103	GLU
1	J	104	LYS
1	J	122	GLU
1	J	161	TYR
1	J	163	ARG
1	J	277	ASP
1	J	297	ASP
1	J	300	THR
1	J	349	LYS
1	J	355	MET
1	K	37	ASP
1	K	51	GLU
1	K	55	ASP
1	K	64	GLU
1	K	83	SER
1	K	103	GLU
1	K	104	LYS
1	K	137	ASN
1	K	161	TYR
1	K	163	ARG
1	K	167	GLU
1	K	213	GLU
1	K	257	ILE
1	K	291	THR
1	K	297	ASP
1	K	355	MET
1	L	16	VAL
1	L	37	ASP
1	L	41	ILE
1	L	51	GLU
1	L	54	ARG
1	L	55	ASP
1	L	66	GLU
1	L	91	MET
1	L	104	LYS
1	L	115	THR
1	L	153	ASP
1	L	161	TYR
1	L	163	ARG
1	L	202	LYS

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Mol	Chain	Res	Type
1	L	213	GLU
1	L	214	ASN
1	L	217	THR
1	L	275	GLU
1	L	316	LYS
1	L	349	LYS
1	L	355	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	B	207	ASN
1	C	169	GLN
1	C	189	HIS
1	C	222	HIS
1	D	158	GLN
1	F	40	GLN
1	G	70	ASN
1	G	95	GLN
1	H	248	GLN
1	J	207	ASN
1	K	231	GLN
1	L	207	ASN
1	L	214	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	340/367 (92%)	0.08	8 (2%) 59 53	12, 21, 33, 54	0
1	B	350/367 (95%)	-0.01	4 (1%) 80 78	12, 19, 33, 60	0
1	C	346/367 (94%)	0.14	10 (2%) 51 45	13, 21, 36, 54	0
1	D	335/367 (91%)	0.05	6 (1%) 68 64	11, 20, 32, 40	0
1	E	342/367 (93%)	-0.06	0 100 100	9, 18, 30, 51	0
1	F	342/367 (93%)	-0.06	3 (0%) 84 82	12, 19, 31, 52	0
1	G	340/367 (92%)	0.10	2 (0%) 89 88	12, 20, 37, 52	0
1	H	339/367 (92%)	0.07	3 (0%) 84 82	11, 21, 32, 52	0
1	I	336/367 (91%)	0.12	3 (0%) 84 82	13, 22, 33, 46	0
1	J	340/367 (92%)	0.06	4 (1%) 79 76	13, 21, 33, 42	0
1	K	337/367 (91%)	0.29	11 (3%) 46 39	15, 23, 34, 52	0
1	L	334/367 (91%)	0.66	39 (11%) 4 3	15, 24, 35, 38	0
All	All	4081/4404 (92%)	0.12	93 (2%) 60 54	9, 21, 33, 60	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	53	LYS	5.2
1	L	56	PHE	4.5
1	L	43	LYS	4.4
1	L	67	GLU	4.1
1	L	115	THR	4.0
1	L	277	ASP	4.0
1	L	42	SER	3.8
1	K	147	SER	3.3
1	C	68	ILE	3.2
1	C	56	PHE	3.2
1	L	57	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	60	GLU	3.1
1	L	305	SER	3.1
1	L	151	LEU	3.1
1	C	57	PRO	3.1
1	K	287	TYR	3.0
1	L	49	THR	3.0
1	L	62	VAL	3.0
1	L	146	ILE	3.0
1	L	54	ARG	2.9
1	D	68	ILE	2.9
1	L	275	GLU	2.8
1	L	66	GLU	2.8
1	L	52	VAL	2.7
1	K	300	THR	2.7
1	L	16	VAL	2.7
1	L	44	ILE	2.7
1	L	74	ILE	2.7
1	C	60	GLU	2.7
1	D	214	ASN	2.7
1	L	92	ALA	2.6
1	A	61	VAL	2.6
1	L	70	ASN	2.6
1	K	303	ILE	2.6
1	L	303	ILE	2.6
1	L	304	PRO	2.6
1	L	51	GLU	2.6
1	L	271	GLY	2.5
1	L	21	TYR	2.5
1	A	53	LYS	2.5
1	C	59	ALA	2.5
1	C	111	GLU	2.5
1	L	18	ILE	2.5
1	G	214	ASN	2.5
1	B	65	LEU	2.5
1	K	297	ASP	2.4
1	K	294	ARG	2.4
1	C	12	ASP	2.4
1	D	275	GLU	2.4
1	A	54	ARG	2.4
1	C	47	SER	2.4
1	F	67	GLU	2.4
1	G	122	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	17	GLY	2.3
1	H	41	ILE	2.3
1	L	61	VAL	2.3
1	L	332	GLU	2.3
1	A	62	VAL	2.3
1	D	213	GLU	2.3
1	K	305	SER	2.3
1	I	12	ASP	2.3
1	B	70	ASN	2.3
1	L	357	GLU	2.3
1	F	11	VAL	2.3
1	K	281	ALA	2.3
1	L	263	GLY	2.2
1	B	175	LYS	2.2
1	J	277	ASP	2.2
1	L	94	ILE	2.2
1	A	56	PHE	2.1
1	F	213	GLU	2.1
1	A	10	LYS	2.1
1	I	305	SER	2.1
1	B	10	LYS	2.1
1	I	87	TYR	2.1
1	J	52	VAL	2.1
1	C	41	ILE	2.1
1	K	145	LEU	2.1
1	A	60	GLU	2.1
1	J	58	ASP	2.1
1	K	301	GLU	2.1
1	C	122	GLU	2.1
1	L	297	ASP	2.1
1	L	35	VAL	2.1
1	A	94	ILE	2.1
1	D	65	LEU	2.1
1	J	62	VAL	2.0
1	K	152	GLU	2.0
1	L	77	VAL	2.0
1	L	114	GLU	2.0
1	D	62	VAL	2.0
1	H	70	ASN	2.0
1	H	68	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.