



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 11:33 am BST

PDB ID : 3GKF
Title : Crystal Structure of E. coli LsrF
Authors : Miller, S.T.; Diaz, Z.C.
Deposited on : 2009-03-10
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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	:	2.11
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)	:	2.11

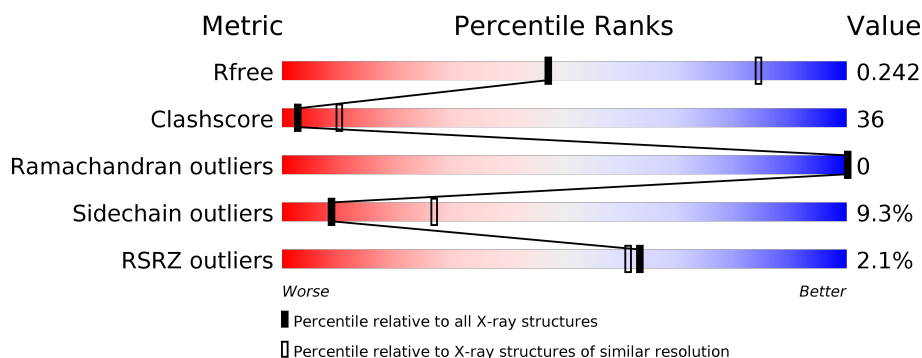
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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 $\leq 5\%$. 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	293	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>38%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	293	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>43%</div> <div>5%</div> <div>6%</div> </div> </div>
1	C	293	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>6%</div> <div>6%</div> </div> </div>
1	D	293	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>41%</div> <div>5%</div> <div>6%</div> </div> </div>
1	E	293	<div> <div>4%</div> <div> <div></div> <div>48%</div> <div>41%</div> <div>5%</div> <div>6%</div> </div> </div>
1	F	293	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>5%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	293	
1	H	293	
1	I	293	
1	J	293	
1	K	293	
1	L	293	
1	M	293	
1	N	293	
1	O	293	
1	P	293	
1	Q	293	
1	R	293	
1	S	293	
1	T	293	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 42541 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 Aldolase lsrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	L	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	M	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	N	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	K	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	F	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	I	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	H	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	G	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	J	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	S	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	P	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	Q	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	R	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	T	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			
1	E	276	Total	C	N	O	S	0	0	0
			2115	1332	374	392	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	276	Total 2115	C 1332	N 374	O 392	S 17	0	0	0
1	C	276	Total 2115	C 1332	N 374	O 392	S 17	0	0	0
1	D	276	Total 2115	C 1332	N 374	O 392	S 17	0	0	0
1	A	276	Total 2115	C 1332	N 374	O 392	S 17	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	GLY	-	EXPRESSION TAG	UNP P76143
O	0	SER	-	EXPRESSION TAG	UNP P76143
L	-1	GLY	-	EXPRESSION TAG	UNP P76143
L	0	SER	-	EXPRESSION TAG	UNP P76143
M	-1	GLY	-	EXPRESSION TAG	UNP P76143
M	0	SER	-	EXPRESSION TAG	UNP P76143
N	-1	GLY	-	EXPRESSION TAG	UNP P76143
N	0	SER	-	EXPRESSION TAG	UNP P76143
K	-1	GLY	-	EXPRESSION TAG	UNP P76143
K	0	SER	-	EXPRESSION TAG	UNP P76143
F	-1	GLY	-	EXPRESSION TAG	UNP P76143
F	0	SER	-	EXPRESSION TAG	UNP P76143
I	-1	GLY	-	EXPRESSION TAG	UNP P76143
I	0	SER	-	EXPRESSION TAG	UNP P76143
H	-1	GLY	-	EXPRESSION TAG	UNP P76143
H	0	SER	-	EXPRESSION TAG	UNP P76143
G	-1	GLY	-	EXPRESSION TAG	UNP P76143
G	0	SER	-	EXPRESSION TAG	UNP P76143
J	-1	GLY	-	EXPRESSION TAG	UNP P76143
J	0	SER	-	EXPRESSION TAG	UNP P76143
S	-1	GLY	-	EXPRESSION TAG	UNP P76143
S	0	SER	-	EXPRESSION TAG	UNP P76143
P	-1	GLY	-	EXPRESSION TAG	UNP P76143
P	0	SER	-	EXPRESSION TAG	UNP P76143
Q	-1	GLY	-	EXPRESSION TAG	UNP P76143
Q	0	SER	-	EXPRESSION TAG	UNP P76143
R	-1	GLY	-	EXPRESSION TAG	UNP P76143
R	0	SER	-	EXPRESSION TAG	UNP P76143
T	-1	GLY	-	EXPRESSION TAG	UNP P76143
T	0	SER	-	EXPRESSION TAG	UNP P76143
E	-1	GLY	-	EXPRESSION TAG	UNP P76143

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	EXPRESSION TAG	UNP P76143
B	-1	GLY	-	EXPRESSION TAG	UNP P76143
B	0	SER	-	EXPRESSION TAG	UNP P76143
C	-1	GLY	-	EXPRESSION TAG	UNP P76143
C	0	SER	-	EXPRESSION TAG	UNP P76143
D	-1	GLY	-	EXPRESSION TAG	UNP P76143
D	0	SER	-	EXPRESSION TAG	UNP P76143
A	-1	GLY	-	EXPRESSION TAG	UNP P76143
A	0	SER	-	EXPRESSION TAG	UNP P76143

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	O	13	Total O 13 13	0	0
2	L	11	Total O 11 11	0	0
2	M	13	Total O 13 13	0	0
2	N	16	Total O 16 16	0	0
2	K	6	Total O 6 6	0	0
2	F	9	Total O 9 9	0	0
2	I	9	Total O 9 9	0	0
2	H	20	Total O 20 20	0	0
2	G	16	Total O 16 16	0	0
2	J	10	Total O 10 10	0	0
2	S	10	Total O 10 10	0	0
2	P	5	Total O 5 5	0	0
2	Q	10	Total O 10 10	0	0
2	R	6	Total O 6 6	0	0
2	T	7	Total O 7 7	0	0

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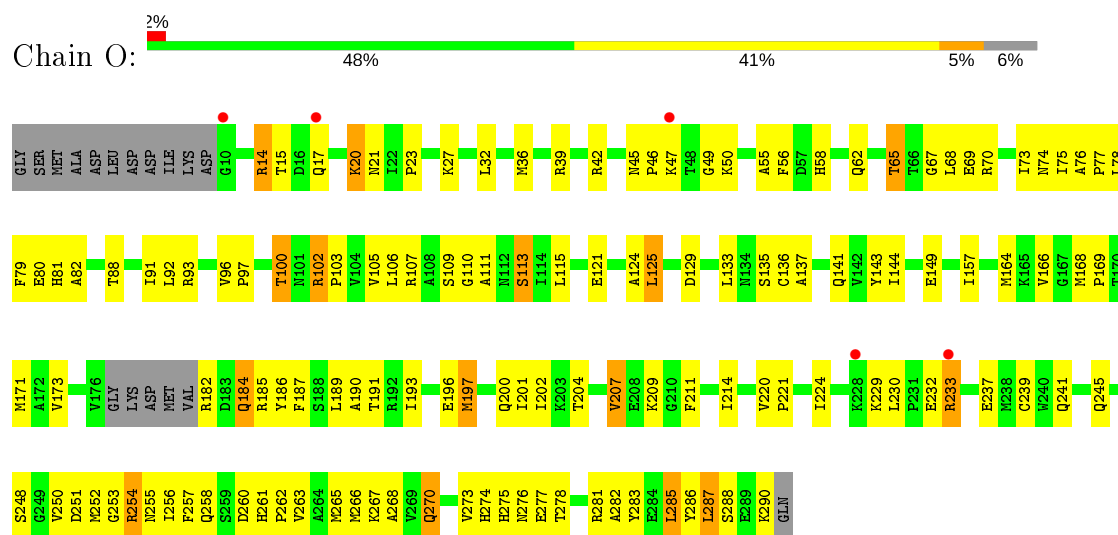
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	6	Total 6	O 6	0	0
2	B	10	Total 10	O 10	0	0
2	C	35	Total 35	O 35	0	0
2	D	18	Total 18	O 18	0	0
2	A	11	Total 11	O 11	0	0

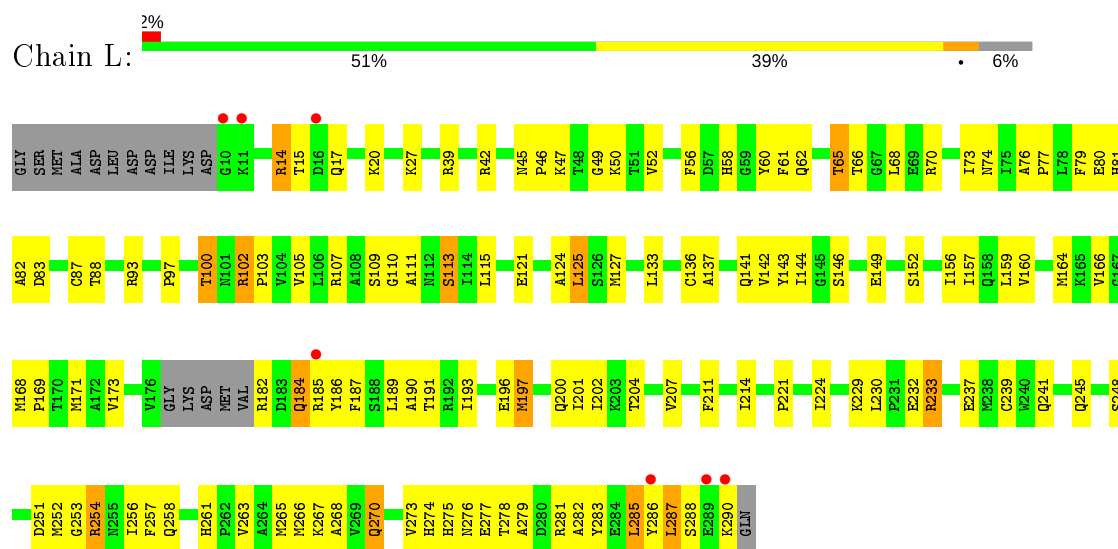
3 Residue-property plots [i](#)

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

• Molecule 1: Aldolase lsrF

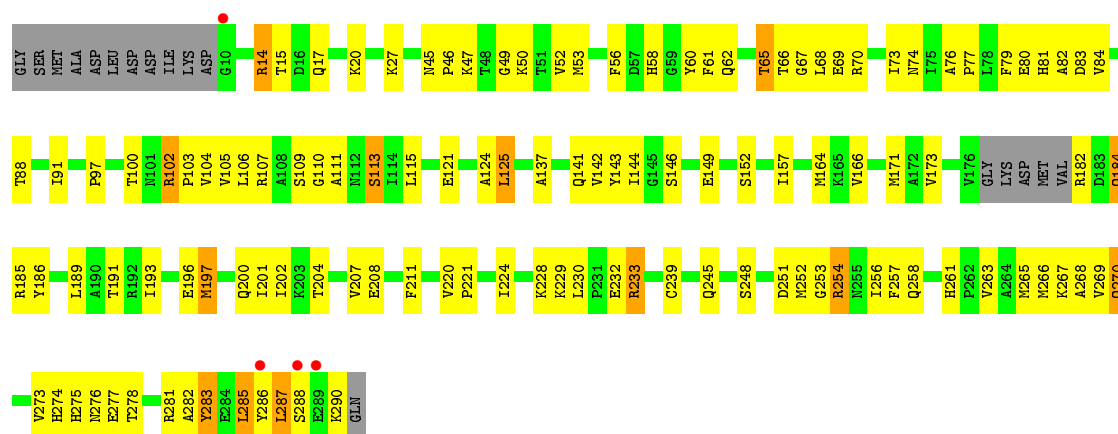


• Molecule 1: Aldolase lsrF

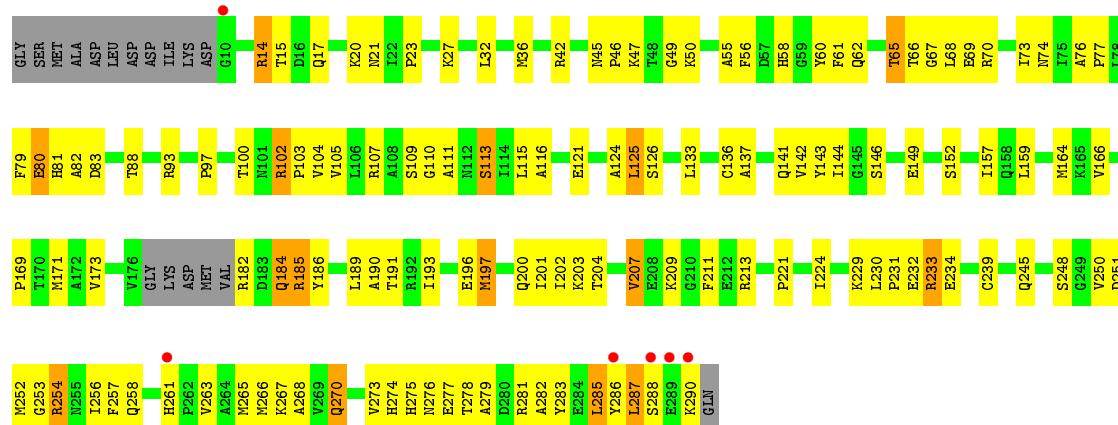


• Molecule 1: Aldolase lsrF

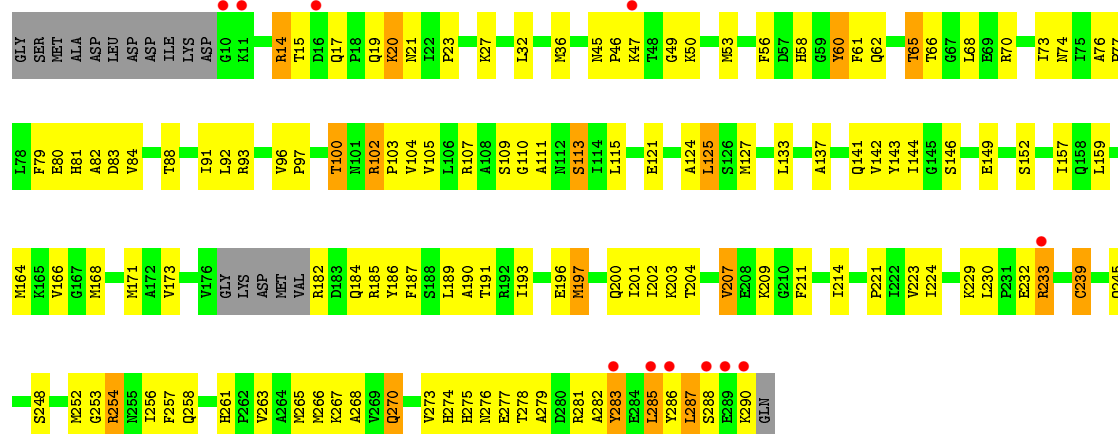




• Molecule 1: Aldolase lsrF

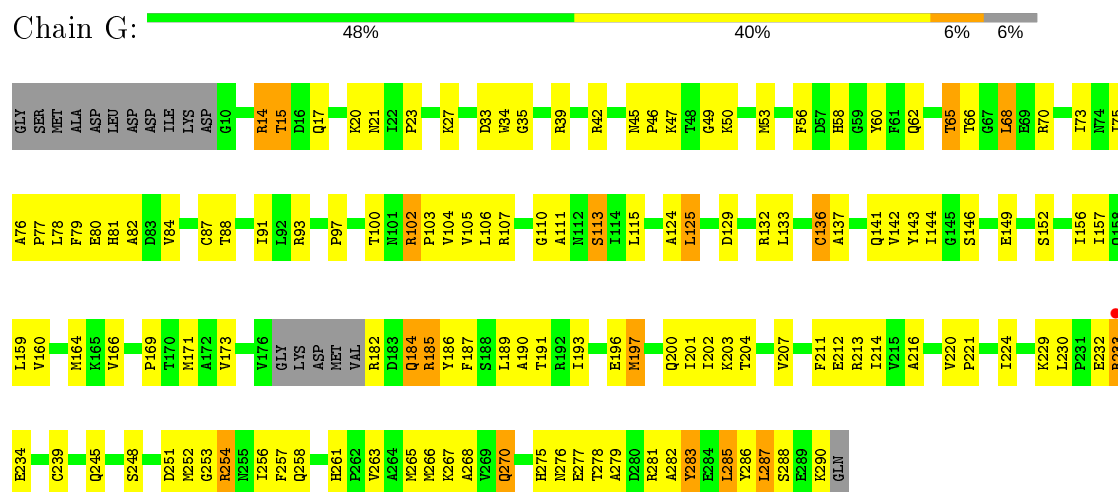


• Molecule 1: Aldolase lsrF

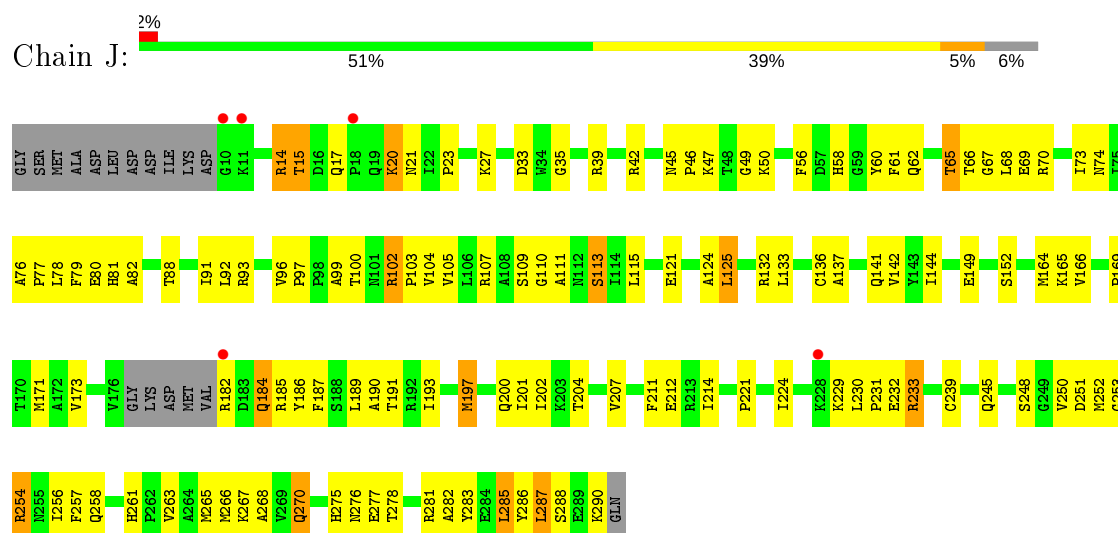


• Molecule 1: Aldolase lsrF

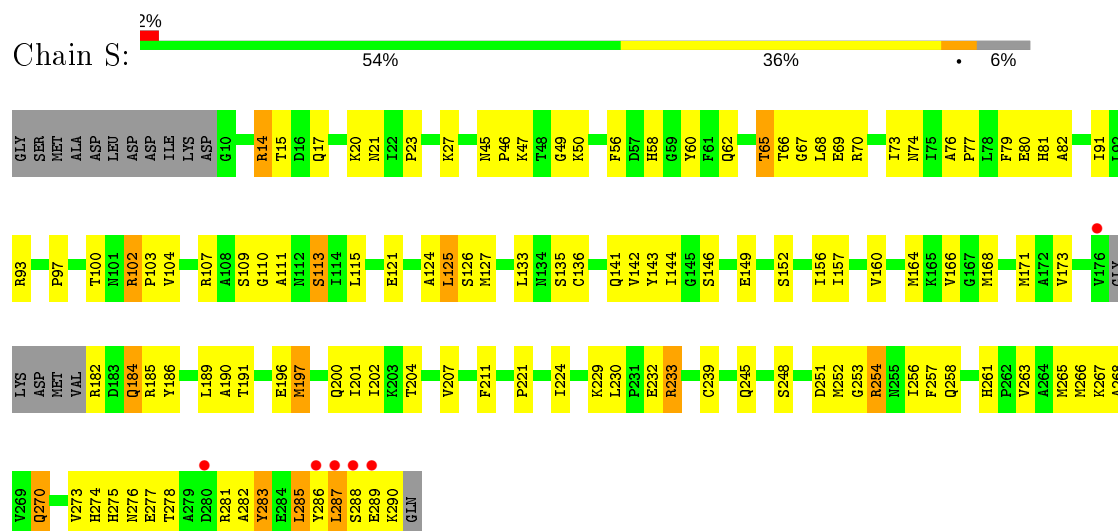
- Molecule 1: Aldolase lsrF



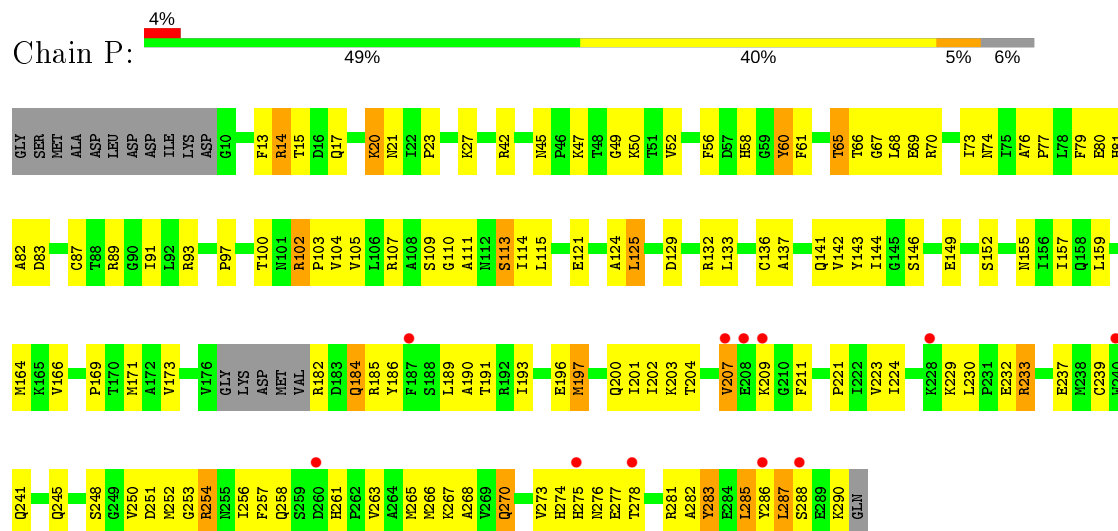
- Molecule 1: Aldolase lsrF



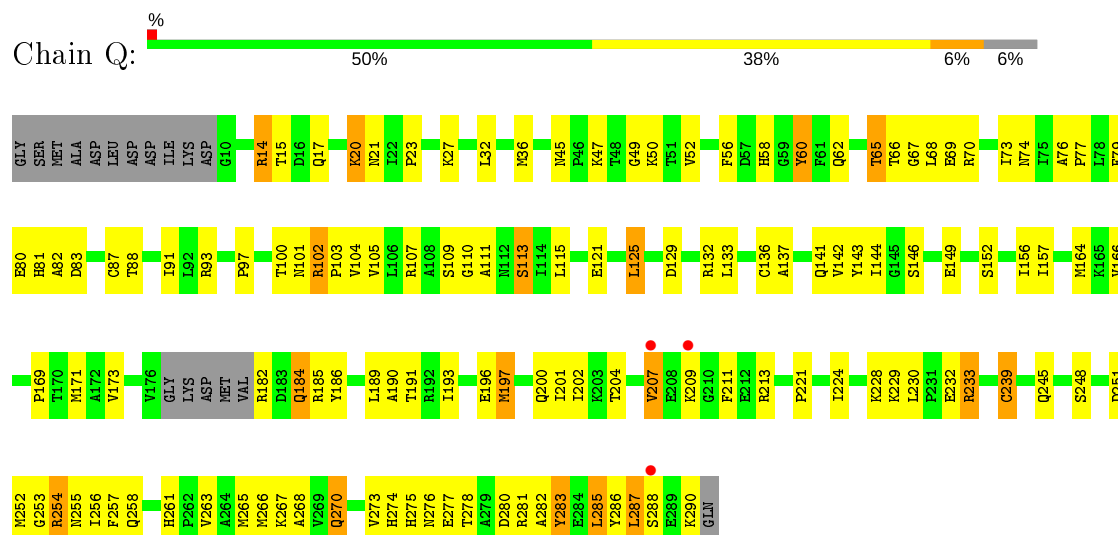
- Molecule 1: Aldolase lsrF



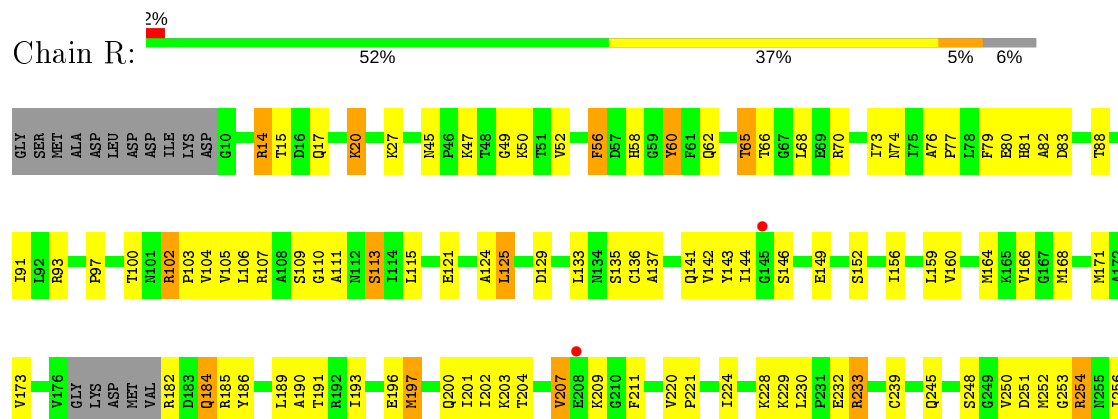
- Molecule 1: Aldolase lsrF



- Molecule 1: Aldolase lsrF

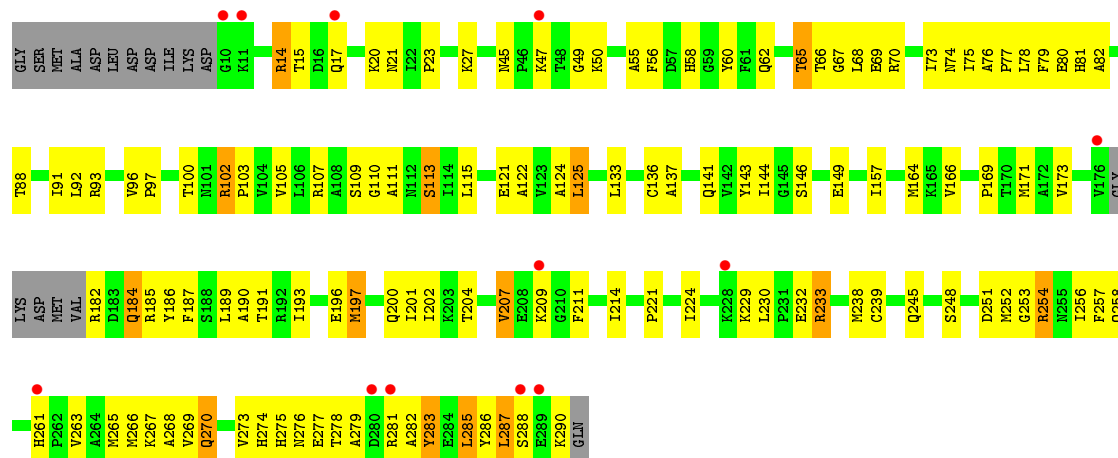


- Molecule 1: Aldolase lsrF

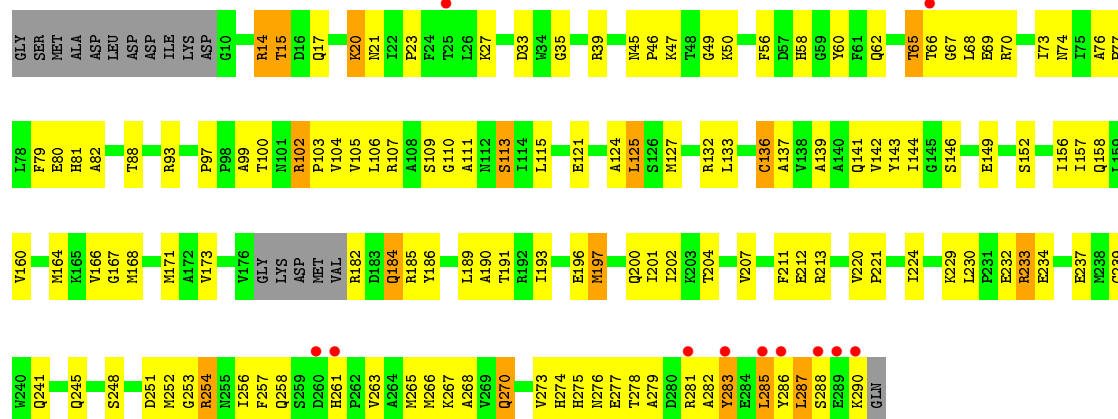




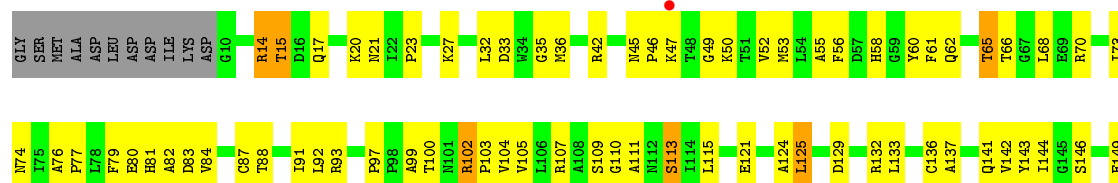
• Molecule 1: Aldolase lsrF

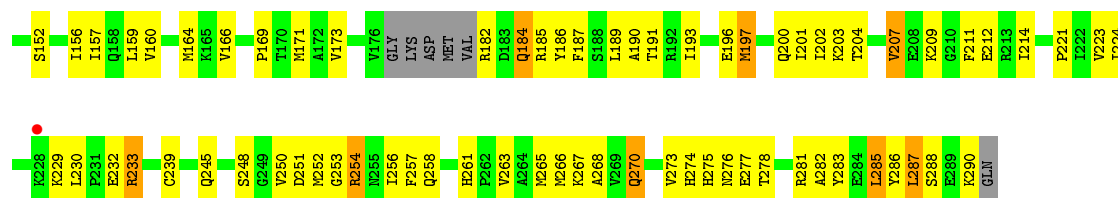


• Molecule 1: Aldolase lsrF

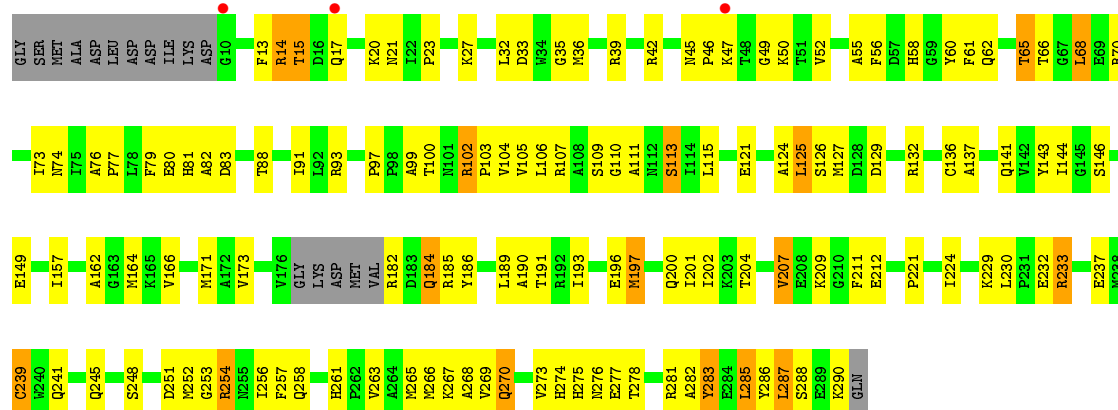


• Molecule 1: Aldolase lsrF

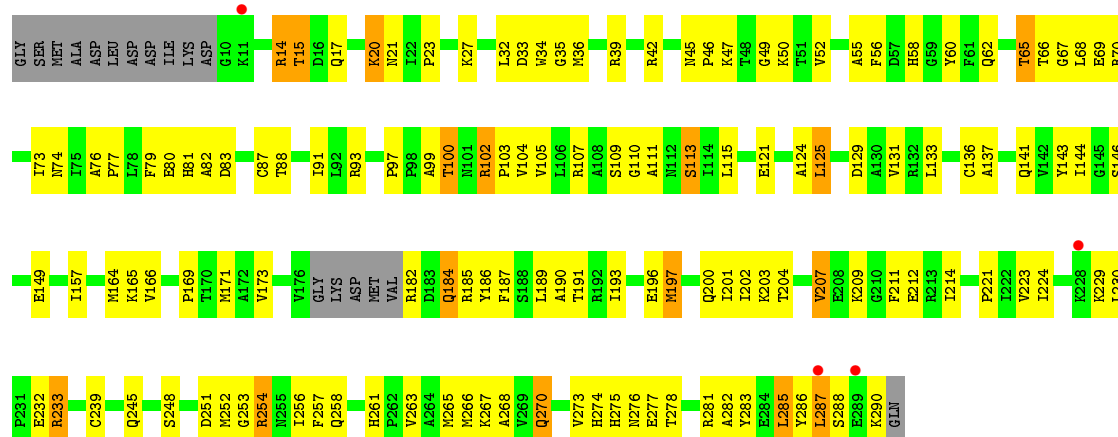




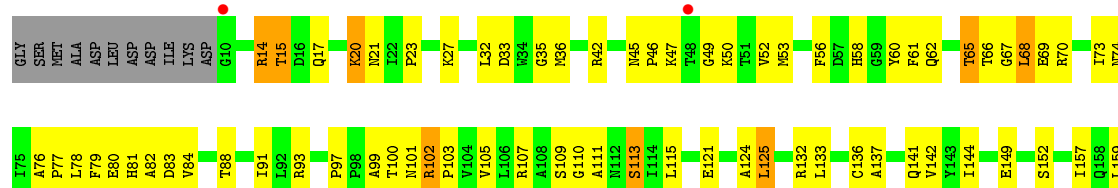
• Molecule 1: Aldolase lsrF

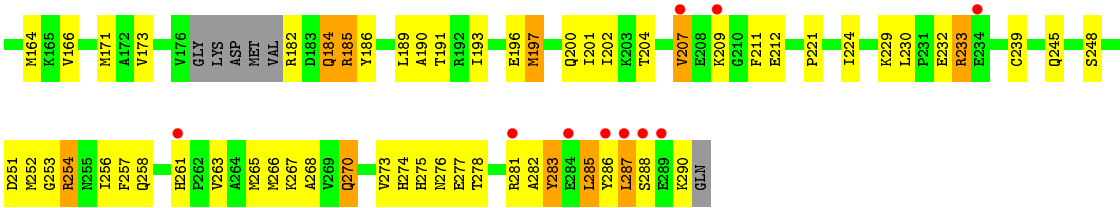


• Molecule 1: Aldolase lsrF



• Molecule 1: Aldolase lsrF





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 104.61Å 171.67Å 89.88° 79.31° 89.61°	Depositor
Resolution (Å)	29.64 – 2.90 29.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.64-2.90) 95.4 (29.65-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.209 , 0.229 0.227 , 0.242	Depositor DCC
R_{free} test set	5685 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,h-l 0.036 for -h,k,-l 0.013 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	42541	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.63	0/2153	0.70	0/2911
1	B	0.65	0/2153	0.69	0/2911
1	C	0.75	1/2153 (0.0%)	0.73	0/2911
1	D	0.65	0/2153	0.70	0/2911
1	E	0.62	1/2153 (0.0%)	0.68	0/2911
1	F	0.63	0/2153	0.68	0/2911
1	G	0.69	1/2153 (0.0%)	0.71	0/2911
1	H	0.72	1/2153 (0.0%)	0.72	0/2911
1	I	0.65	0/2153	0.71	0/2911
1	J	0.62	0/2153	0.70	0/2911
1	K	0.64	1/2153 (0.0%)	0.70	0/2911
1	L	0.69	0/2153	0.72	0/2911
1	M	0.71	0/2153	0.71	0/2911
1	N	0.71	0/2153	0.70	0/2911
1	O	0.62	0/2153	0.68	0/2911
1	P	0.60	0/2153	0.68	0/2911
1	Q	0.66	1/2153 (0.0%)	0.69	0/2911
1	R	0.70	0/2153	0.70	0/2911
1	S	0.64	0/2153	0.69	0/2911
1	T	0.61	0/2153	0.69	0/2911
All	All	0.66	6/43060 (0.0%)	0.70	0/58220

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	239	CYS	CB-SG	-6.83	1.70	1.82
1	E	136	CYS	CB-SG	-6.11	1.71	1.82
1	C	239	CYS	CB-SG	-5.75	1.72	1.81
1	H	239	CYS	CB-SG	-5.74	1.72	1.81
1	K	239	CYS	CB-SG	-5.70	1.72	1.81

There are no bond angle outliers.

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	2115	0	2126	170	0
1	B	2115	0	2126	177	1
1	C	2115	0	2126	179	0
1	D	2115	0	2126	178	2
1	E	2115	0	2126	173	1
1	F	2115	0	2125	158	0
1	G	2115	0	2126	190	0
1	H	2115	0	2126	171	0
1	I	2115	0	2126	173	0
1	J	2115	0	2126	157	2
1	K	2115	0	2126	154	0
1	L	2115	0	2126	151	3
1	M	2115	0	2126	145	3
1	N	2115	0	2126	177	1
1	O	2115	0	2126	170	3
1	P	2115	0	2126	160	0
1	Q	2115	0	2126	160	0
1	R	2115	0	2126	156	0
1	S	2115	0	2126	150	0
1	T	2115	0	2126	159	0
2	A	11	0	0	0	0
2	B	10	0	0	2	0
2	C	35	0	0	4	0
2	D	18	0	0	2	0
2	E	6	0	0	0	0
2	F	9	0	0	1	0
2	G	16	0	0	0	0
2	H	20	0	0	4	0
2	I	9	0	0	0	0
2	J	10	0	0	1	0
2	K	6	0	0	1	0
2	L	11	0	0	0	0
2	M	13	0	0	0	0
2	N	16	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	13	0	0	0	0
2	P	5	0	0	1	0
2	Q	10	0	0	5	0
2	R	6	0	0	0	0
2	S	10	0	0	1	0
2	T	7	0	0	4	0
All	All	42541	0	42519	3016	8

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 36.

The worst 5 of 3016 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:N:287:LEU:HD21	1:G:275:HIS:CE1	1.20	1.70
1:B:283:TYR:HE2	1:B:287:LEU:CD1	1.19	1.55
1:O:283:TYR:HE2	1:O:287:LEU:CD1	1.19	1.54
1:J:283:TYR:HE2	1:J:287:LEU:CD1	1.15	1.53
1:N:283:TYR:HE2	1:N:287:LEU:CD1	1.22	1.52

The worst 5 of 8 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:O:287:LEU:CD2	1:M:275:HIS:CE1[1_565]	1.57	0.63
1:O:287:LEU:CD2	1:M:275:HIS:ND1[1_565]	1.83	0.37
1:L:233:ARG:NH2	1:E:234:GLU:OE2[1_546]	1.89	0.31
1:N:281:ARG:NH2	1:D:276:ASN:ND2[1_545]	1.91	0.29
1:O:287:LEU:CD2	1:M:275:HIS:NE2[1_565]	2.00	0.20

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	272/293 (93%)	264 (97%)	8 (3%)	0	100	100
1	B	272/293 (93%)	265 (97%)	7 (3%)	0	100	100
1	C	272/293 (93%)	265 (97%)	7 (3%)	0	100	100
1	D	272/293 (93%)	262 (96%)	10 (4%)	0	100	100
1	E	272/293 (93%)	265 (97%)	7 (3%)	0	100	100
1	F	272/293 (93%)	262 (96%)	10 (4%)	0	100	100
1	G	272/293 (93%)	262 (96%)	10 (4%)	0	100	100
1	H	272/293 (93%)	263 (97%)	9 (3%)	0	100	100
1	I	272/293 (93%)	263 (97%)	9 (3%)	0	100	100
1	J	272/293 (93%)	264 (97%)	8 (3%)	0	100	100
1	K	272/293 (93%)	263 (97%)	9 (3%)	0	100	100
1	L	272/293 (93%)	264 (97%)	8 (3%)	0	100	100
1	M	272/293 (93%)	263 (97%)	9 (3%)	0	100	100
1	N	272/293 (93%)	261 (96%)	11 (4%)	0	100	100
1	O	272/293 (93%)	263 (97%)	9 (3%)	0	100	100
1	P	272/293 (93%)	262 (96%)	10 (4%)	0	100	100
1	Q	272/293 (93%)	261 (96%)	11 (4%)	0	100	100
1	R	272/293 (93%)	260 (96%)	12 (4%)	0	100	100
1	S	272/293 (93%)	262 (96%)	10 (4%)	0	100	100
1	T	272/293 (93%)	263 (97%)	9 (3%)	0	100	100
All	All	5440/5860 (93%)	5257 (97%)	183 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/238 (94%)	202 (90%)	22 (10%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	224/238 (94%)	204 (91%)	20 (9%)	9	29
1	C	224/238 (94%)	202 (90%)	22 (10%)	8	24
1	D	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	E	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	F	224/238 (94%)	204 (91%)	20 (9%)	9	29
1	G	224/238 (94%)	201 (90%)	23 (10%)	7	22
1	H	224/238 (94%)	204 (91%)	20 (9%)	9	29
1	I	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	J	224/238 (94%)	204 (91%)	20 (9%)	9	29
1	K	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	L	224/238 (94%)	204 (91%)	20 (9%)	9	29
1	M	224/238 (94%)	202 (90%)	22 (10%)	8	24
1	N	224/238 (94%)	204 (91%)	20 (9%)	9	29
1	O	224/238 (94%)	205 (92%)	19 (8%)	10	31
1	P	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	Q	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	R	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	S	224/238 (94%)	203 (91%)	21 (9%)	8	26
1	T	224/238 (94%)	204 (91%)	20 (9%)	9	29
All	All	4480/4760 (94%)	4064 (91%)	416 (9%)	9	27

5 of 416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	20	LYS
1	P	80	GLU
1	D	166	VAL
1	J	104	VAL
1	S	80	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	58	HIS

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Mol	Chain	Res	Type
1	P	241	GLN
1	D	200	GLN
1	J	200	GLN
1	S	274	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	276/293 (94%)	0.07	12 (4%) 35 31	19, 32, 60, 81	0
1	B	276/293 (94%)	-0.11	2 (0%) 87 87	19, 32, 60, 81	0
1	C	276/293 (94%)	-0.01	3 (1%) 80 80	19, 32, 60, 81	0
1	D	276/293 (94%)	0.01	4 (1%) 75 75	19, 32, 60, 81	0
1	E	276/293 (94%)	0.10	11 (3%) 38 33	19, 32, 60, 81	0
1	F	276/293 (94%)	-0.06	4 (1%) 75 75	19, 32, 60, 81	0
1	G	276/293 (94%)	-0.15	1 (0%) 92 93	19, 32, 60, 81	0
1	H	276/293 (94%)	0.06	3 (1%) 80 80	19, 32, 60, 81	0
1	I	276/293 (94%)	-0.03	3 (1%) 80 80	19, 32, 60, 81	0
1	J	276/293 (94%)	-0.09	5 (1%) 68 67	19, 32, 60, 81	0
1	K	276/293 (94%)	-0.03	11 (3%) 38 33	19, 32, 60, 81	0
1	L	276/293 (94%)	-0.07	7 (2%) 57 55	19, 32, 60, 81	0
1	M	276/293 (94%)	-0.07	4 (1%) 75 75	19, 32, 60, 81	0
1	N	276/293 (94%)	-0.02	6 (2%) 62 59	19, 32, 60, 81	0
1	O	276/293 (94%)	-0.08	5 (1%) 68 67	19, 32, 60, 81	0
1	P	276/293 (94%)	0.03	11 (3%) 38 33	19, 32, 60, 81	0
1	Q	276/293 (94%)	-0.04	3 (1%) 80 80	19, 32, 60, 81	0
1	R	276/293 (94%)	0.05	5 (1%) 68 67	19, 32, 60, 81	0
1	S	276/293 (94%)	-0.06	6 (2%) 62 59	19, 32, 60, 81	0
1	T	276/293 (94%)	0.01	12 (4%) 35 31	19, 32, 60, 81	0
All	All	5520/5860 (94%)	-0.02	118 (2%) 63 61	19, 32, 61, 81	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	GLY	7.0
1	E	289	GLU	6.6
1	E	288	SER	6.0
1	N	288	SER	5.4
1	E	286	TYR	5.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.