



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:00 AM GMT

PDB ID : 3GND
Title : Crystal Structure of E. coli LsrF in complex with Ribulose-5-phosphate
Authors : Miller, S.T.; Diaz, Z.C.
Deposited on : 2009-03-17
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
<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

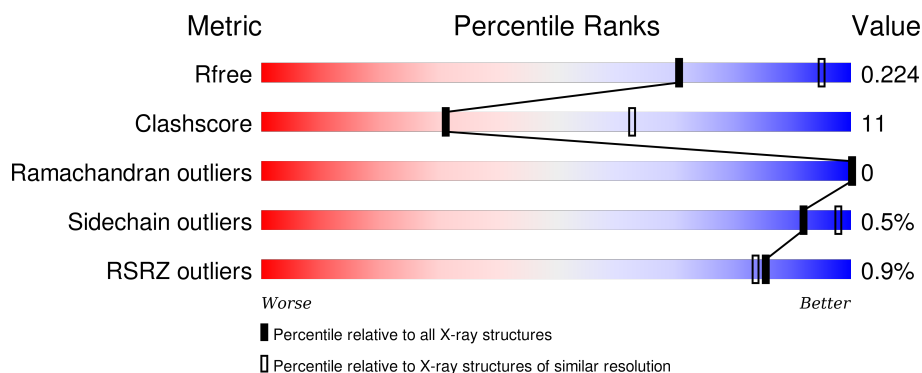
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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	295	<div> <div></div> <div>74%20%6%</div> </div>
1	B	295	<div> <div></div> <div>76%17%6%</div> </div>
1	C	295	<div> <div>%</div> <div>75%19%6%</div> </div>
1	D	295	<div> <div></div> <div>75%18%6%</div> </div>
1	E	295	<div> <div>3%</div> <div>73%21%6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	295	
1	G	295	
1	H	295	
1	I	295	
1	J	295	
1	K	295	
1	L	295	
1	M	295	
1	N	295	
1	O	295	
1	P	295	
1	Q	295	
1	R	295	
1	S	295	
1	T	295	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5RP	D	984	-	-	-	X
2	5RP	H	984	-	-	-	X
2	5RP	J	984	-	-	-	X
2	5RP	L	984	-	-	-	X
2	5RP	M	984	-	-	-	X
2	5RP	P	984	-	-	-	X
2	5RP	T	984	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42916 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	A	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	B	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	C	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	D	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	E	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	F	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	G	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	H	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	I	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	J	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	K	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	L	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	M	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	N	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	O	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	P	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	R	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	S	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	T	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P76143
A	-2	SER	-	EXPRESSION TAG	UNP P76143
A	-1	PHE	-	EXPRESSION TAG	UNP P76143
A	0	THR	-	EXPRESSION TAG	UNP P76143
B	-3	GLY	-	EXPRESSION TAG	UNP P76143
B	-2	SER	-	EXPRESSION TAG	UNP P76143
B	-1	PHE	-	EXPRESSION TAG	UNP P76143
B	0	THR	-	EXPRESSION TAG	UNP P76143
C	-3	GLY	-	EXPRESSION TAG	UNP P76143
C	-2	SER	-	EXPRESSION TAG	UNP P76143
C	-1	PHE	-	EXPRESSION TAG	UNP P76143
C	0	THR	-	EXPRESSION TAG	UNP P76143
D	-3	GLY	-	EXPRESSION TAG	UNP P76143
D	-2	SER	-	EXPRESSION TAG	UNP P76143
D	-1	PHE	-	EXPRESSION TAG	UNP P76143
D	0	THR	-	EXPRESSION TAG	UNP P76143
E	-3	GLY	-	EXPRESSION TAG	UNP P76143
E	-2	SER	-	EXPRESSION TAG	UNP P76143
E	-1	PHE	-	EXPRESSION TAG	UNP P76143
E	0	THR	-	EXPRESSION TAG	UNP P76143
F	-3	GLY	-	EXPRESSION TAG	UNP P76143
F	-2	SER	-	EXPRESSION TAG	UNP P76143
F	-1	PHE	-	EXPRESSION TAG	UNP P76143
F	0	THR	-	EXPRESSION TAG	UNP P76143
G	-3	GLY	-	EXPRESSION TAG	UNP P76143
G	-2	SER	-	EXPRESSION TAG	UNP P76143
G	-1	PHE	-	EXPRESSION TAG	UNP P76143
G	0	THR	-	EXPRESSION TAG	UNP P76143
H	-3	GLY	-	EXPRESSION TAG	UNP P76143
H	-2	SER	-	EXPRESSION TAG	UNP P76143
H	-1	PHE	-	EXPRESSION TAG	UNP P76143

Continued on next page...

Continued from previous page...

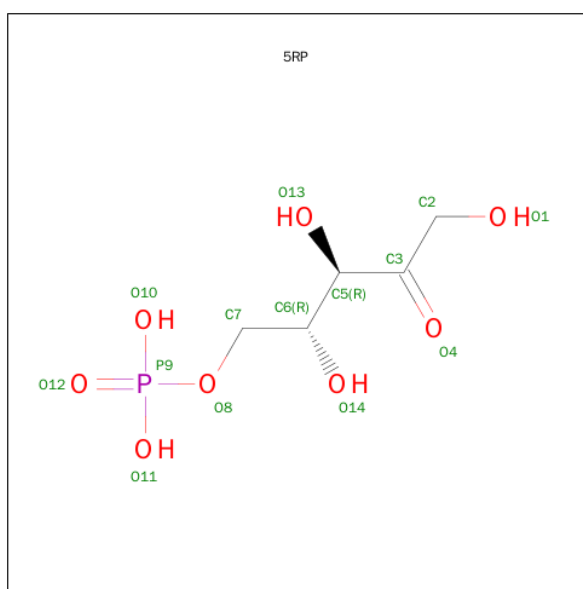
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	THR	-	EXPRESSION TAG	UNP P76143
I	-3	GLY	-	EXPRESSION TAG	UNP P76143
I	-2	SER	-	EXPRESSION TAG	UNP P76143
I	-1	PHE	-	EXPRESSION TAG	UNP P76143
I	0	THR	-	EXPRESSION TAG	UNP P76143
J	-3	GLY	-	EXPRESSION TAG	UNP P76143
J	-2	SER	-	EXPRESSION TAG	UNP P76143
J	-1	PHE	-	EXPRESSION TAG	UNP P76143
J	0	THR	-	EXPRESSION TAG	UNP P76143
K	-3	GLY	-	EXPRESSION TAG	UNP P76143
K	-2	SER	-	EXPRESSION TAG	UNP P76143
K	-1	PHE	-	EXPRESSION TAG	UNP P76143
K	0	THR	-	EXPRESSION TAG	UNP P76143
L	-3	GLY	-	EXPRESSION TAG	UNP P76143
L	-2	SER	-	EXPRESSION TAG	UNP P76143
L	-1	PHE	-	EXPRESSION TAG	UNP P76143
L	0	THR	-	EXPRESSION TAG	UNP P76143
M	-3	GLY	-	EXPRESSION TAG	UNP P76143
M	-2	SER	-	EXPRESSION TAG	UNP P76143
M	-1	PHE	-	EXPRESSION TAG	UNP P76143
M	0	THR	-	EXPRESSION TAG	UNP P76143
N	-3	GLY	-	EXPRESSION TAG	UNP P76143
N	-2	SER	-	EXPRESSION TAG	UNP P76143
N	-1	PHE	-	EXPRESSION TAG	UNP P76143
N	0	THR	-	EXPRESSION TAG	UNP P76143
O	-3	GLY	-	EXPRESSION TAG	UNP P76143
O	-2	SER	-	EXPRESSION TAG	UNP P76143
O	-1	PHE	-	EXPRESSION TAG	UNP P76143
O	0	THR	-	EXPRESSION TAG	UNP P76143
P	-3	GLY	-	EXPRESSION TAG	UNP P76143
P	-2	SER	-	EXPRESSION TAG	UNP P76143
P	-1	PHE	-	EXPRESSION TAG	UNP P76143
P	0	THR	-	EXPRESSION TAG	UNP P76143
Q	-3	GLY	-	EXPRESSION TAG	UNP P76143
Q	-2	SER	-	EXPRESSION TAG	UNP P76143
Q	-1	PHE	-	EXPRESSION TAG	UNP P76143
Q	0	THR	-	EXPRESSION TAG	UNP P76143
R	-3	GLY	-	EXPRESSION TAG	UNP P76143
R	-2	SER	-	EXPRESSION TAG	UNP P76143
R	-1	PHE	-	EXPRESSION TAG	UNP P76143
R	0	THR	-	EXPRESSION TAG	UNP P76143
S	-3	GLY	-	EXPRESSION TAG	UNP P76143

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	EXPRESSION TAG	UNP P76143
S	-1	PHE	-	EXPRESSION TAG	UNP P76143
S	0	THR	-	EXPRESSION TAG	UNP P76143
T	-3	GLY	-	EXPRESSION TAG	UNP P76143
T	-2	SER	-	EXPRESSION TAG	UNP P76143
T	-1	PHE	-	EXPRESSION TAG	UNP P76143
T	0	THR	-	EXPRESSION TAG	UNP P76143

- Molecule 2 is SUGAR (RIBULOSE-5-PHOSPHATE) (three-letter code: 5RP) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	8	1		
2	B	1	Total	C	O	P	0	0
			14	5	8	1		
2	C	1	Total	C	O	P	0	0
			14	5	8	1		
2	D	1	Total	C	O	P	0	0
			14	5	8	1		
2	E	1	Total	C	O	P	0	0
			14	5	8	1		
2	F	1	Total	C	O	P	0	0
			14	5	8	1		
2	G	1	Total	C	O	P	0	0
			14	5	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total 14	C 5	O 8	P 1	0	0
2	I	1	Total 14	C 5	O 8	P 1	0	0
2	J	1	Total 14	C 5	O 8	P 1	0	0
2	K	1	Total 14	C 5	O 8	P 1	0	0
2	L	1	Total 14	C 5	O 8	P 1	0	0
2	M	1	Total 14	C 5	O 8	P 1	0	0
2	N	1	Total 14	C 5	O 8	P 1	0	0
2	O	1	Total 14	C 5	O 8	P 1	0	0
2	P	1	Total 14	C 5	O 8	P 1	0	0
2	Q	1	Total 14	C 5	O 8	P 1	0	0
2	R	1	Total 14	C 5	O 8	P 1	0	0
2	S	1	Total 14	C 5	O 8	P 1	0	0
2	T	1	Total 14	C 5	O 8	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	L	35	Total 35	O 35	0	0
3	B	11	Total 11	O 11	0	0
3	C	17	Total 17	O 17	0	0
3	D	23	Total 23	O 23	0	0
3	E	20	Total 20	O 20	0	0

Continued on next page...

Continued from previous page...

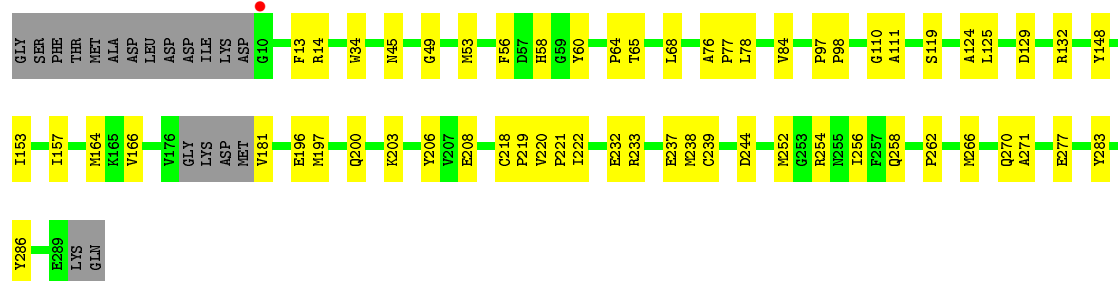
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	20	Total 20	O 20	0	0
3	G	34	Total 34	O 34	0	0
3	H	23	Total 23	O 23	0	0
3	I	18	Total 18	O 18	0	0
3	J	8	Total 8	O 8	0	0
3	K	18	Total 18	O 18	0	0
3	M	13	Total 13	O 13	0	0
3	N	12	Total 12	O 12	0	0
3	O	13	Total 13	O 13	0	0
3	P	9	Total 9	O 9	0	0
3	Q	11	Total 11	O 11	0	0
3	R	27	Total 27	O 27	0	0
3	S	22	Total 22	O 22	0	0
3	T	15	Total 15	O 15	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 ($RSRZ > 2$). 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.

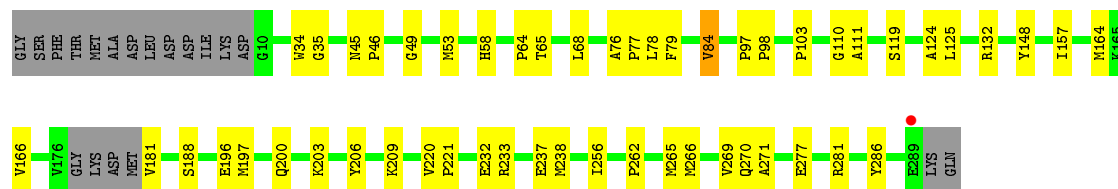
• Molecule 1: Aldolase lsrF

Chain A: 




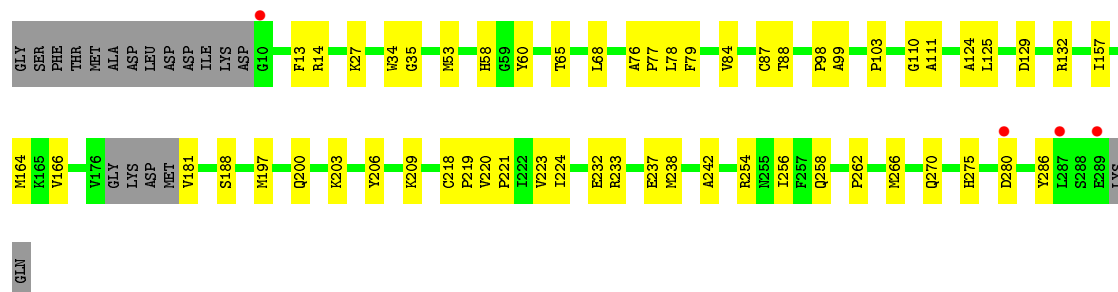
• Molecule 1: Aldolase lsrF

Chain B: 



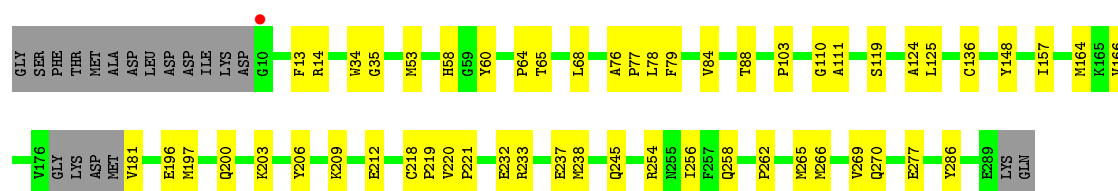
• Molecule 1: Aldolase lsrF

Chain C: 

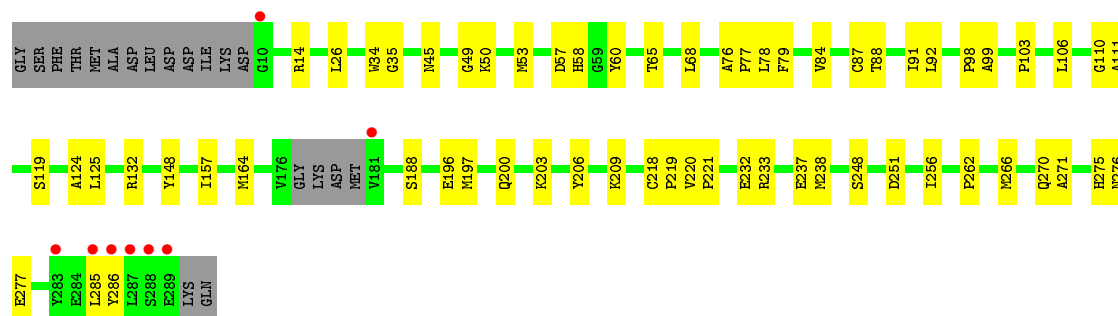
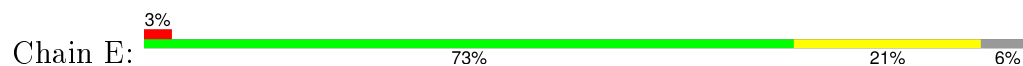


• Molecule 1: Aldolase lsrF

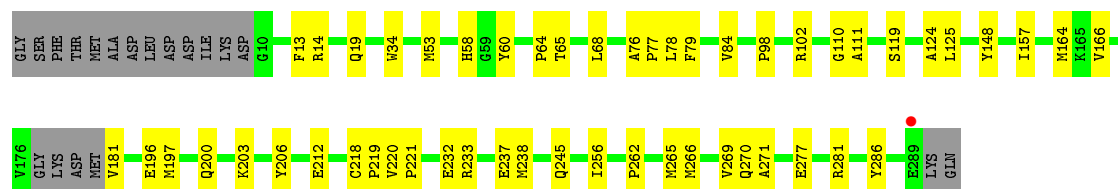
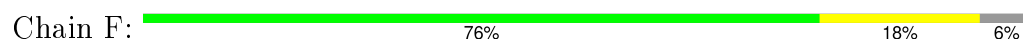
Chain D: 



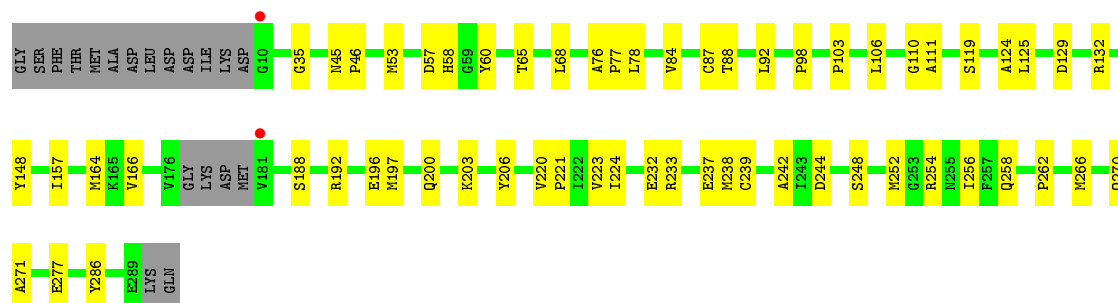
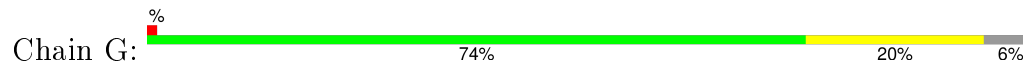
- Molecule 1: Aldolase lsrF



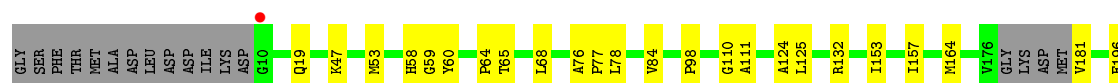
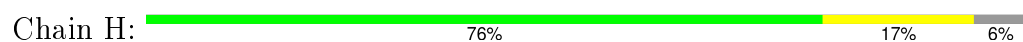
- Molecule 1: Aldolase lsrF



- Molecule 1: Aldolase lsrF

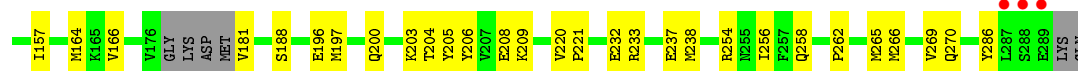
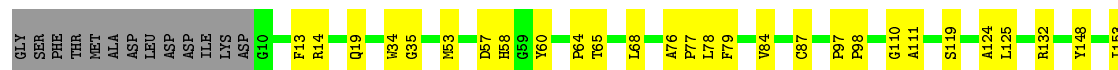
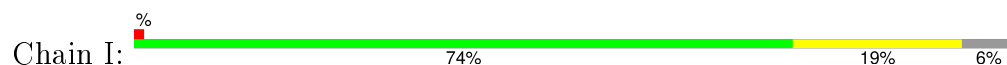


- Molecule 1: Aldolase lsrF

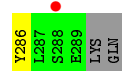
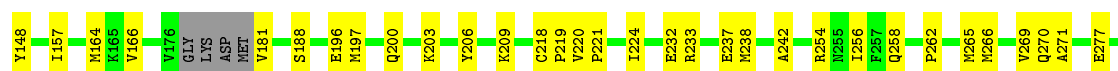
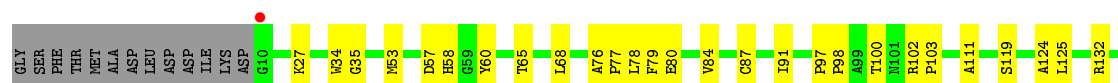
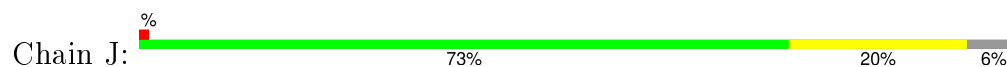




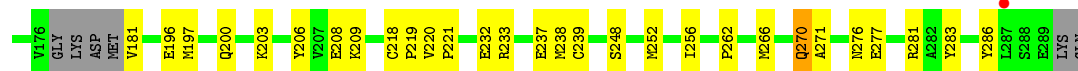
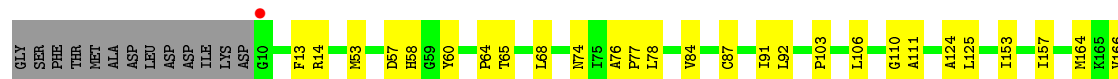
- Molecule 1: Aldolase lsrF



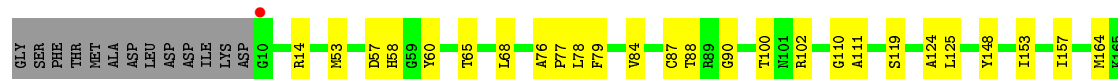
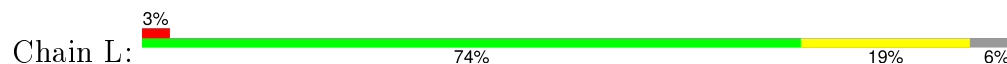
- Molecule 1: Aldolase lsrF



- Molecule 1: Aldolase lsrF



- Molecule 1: Aldolase lsrF



GLY	SER	PHE	THR	MET	ALA	ASP	LEU	ASP	TLE	LYS	ASP
G10	F13	R14	M63	H88	G99	Y60	P64	T65	L68	A76	P77
L78	F79	V84	T88	R93	T100	N101	R102	P103	G110	A111	A124
L125	L133	I157	M164	K165	V166	V176					

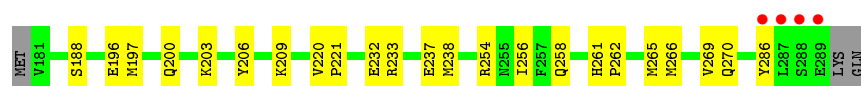
GLY	LYS	ASP	MET	V181	E196	M197	Q200	K203	Y206	K209	E212
V220	P221	E232	R233	E237	M238	Q245	R254	N255	I256	F257	Q258
P262	M266	Q270	E277	Y286	E289	LYS	GLN				

[illegible]

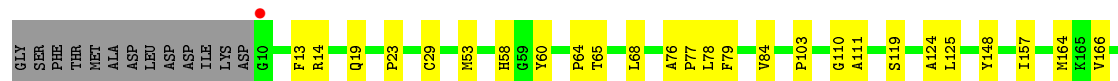
GLY	SER	THR	MET	ALA	ASP	LEU	ASP	ASP	ILE	LYS	ASP	K11	R14	R21	M53	D57	H58	G59	V60	P64	T65	L68	A76	P77	L78	F79	A82	D83	V84	C87	L92	R102	P103	L106	G110	A111	S119	A124	L125	Y148
I157	M164	V176	GLY	LYS	ASP	MET	V181	S188	E196	Q200	K203	Y206	V220	P221	P231	E232	R233	E237	M238	C239	M252	L256	P262	M265	M266	V269	Q270	A271	E277	Y283	Y286	L287	S288	E289	LYS	GLN				

M164	GLY	M165	PER	M166	THR	M167	MET	M168	ALA	M169	ASP	M170	LEU	M171	ASP	M172	ASP	M173	ILE	M174	LYS	M175	ASP	M176	GLN	M177	I22	M178	P23	M179	M45	M180	M53	M181	H58	M182	G59	M183	Y60	M184	T65	M185	P221	M186	L68	M187	A76	M188	P77	M189	L78	M190	A82	M191	B83	M192	V84	M193	T88	M194	P87	M195	P98	M196	R102	M197	P103	M198	G110	M199	A111	M200	S119	M201	A124	M202	L125	M203	L125	M204	Y148	M205	LNS	M206	I153	M207	L157
M164	GLY	M165	PER	M166	THR	M167	MET	M168	ALA	M169	ASP	M170	LEU	M171	ASP	M172	ASP	M173	ILE	M174	LYS	M175	ASP	M176	GLN	M177	I22	M178	P23	M179	M45	M180	M53	M181	H58	M182	G59	M183	Y60	M184	T65	M185	P221	M186	L68	M187	A76	M188	P77	M189	L78	M190	A82	M191	B83	M192	V84	M193	T88	M194	P87	M195	P98	M196	R102	M197	P103	M198	G110	M199	A111	M200	S119	M201	A124	M202	L125	M203	L125	M204	Y148	M205	LNS	M206	I153	M207	L157

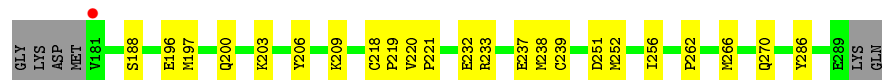
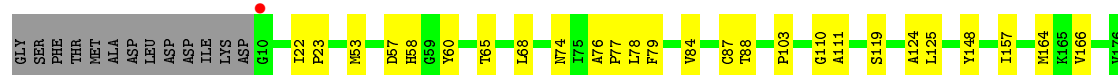
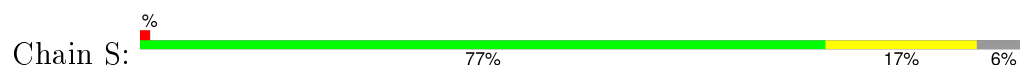
GLY	SER	PHE	THR	MET	ALA	ASP	ASP	ASP	ASP	ASP	ASP	GLU	R14	M63	D67	H68	G69	Y60	T65	L68	A76	P77	L78	F79	V84	C87	T100	M101	R102	P103	G110	A111	A124	L125	I153	I157	M164	K165	V166	V176	GLY	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----



- 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	78.74Å 107.10Å 169.52Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	49.03 – 2.90 49.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.03-2.90) 94.2 (49.02-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.195 , 0.228 0.207 , 0.224	Depositor DCC
R_{free} test set	5678 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 0.5	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l 0.317 for -h,k,-l 0.024 for -h,-k,h+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 112883 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	42916	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5RP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/2151	0.63	0/2910
1	B	0.52	0/2151	0.59	0/2910
1	C	0.53	0/2151	0.58	0/2910
1	D	0.56	0/2151	0.61	0/2910
1	E	0.63	0/2151	0.64	0/2910
1	F	0.60	0/2151	0.62	0/2910
1	G	0.62	0/2151	0.66	0/2910
1	H	0.66	0/2151	0.63	0/2910
1	I	0.54	0/2151	0.60	0/2910
1	J	0.51	0/2151	0.59	0/2910
1	K	0.64	0/2151	0.64	0/2910
1	L	0.66	0/2151	0.66	0/2910
1	M	0.59	0/2151	0.64	0/2910
1	N	0.55	0/2151	0.60	0/2910
1	O	0.54	0/2151	0.60	0/2910
1	P	0.54	0/2151	0.60	0/2910
1	Q	0.55	0/2151	0.61	0/2910
1	R	0.65	1/2151 (0.0%)	0.63	0/2910
1	S	0.61	0/2151	0.62	0/2910
1	T	0.59	1/2151 (0.0%)	0.63	0/2910
All	All	0.59	2/43020 (0.0%)	0.62	0/58200

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	29	CYS	CB-SG	-6.11	1.71	1.82
1	R	29	CYS	CB-SG	-5.43	1.73	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	2113	0	2122	53	1
1	B	2113	0	2122	49	0
1	C	2113	0	2122	50	2
1	D	2113	0	2122	48	1
1	E	2113	0	2122	61	0
1	F	2113	0	2122	46	1
1	G	2113	0	2122	55	0
1	H	2113	0	2122	71	1
1	I	2113	0	2122	50	0
1	J	2113	0	2122	52	0
1	K	2113	0	2122	56	1
1	L	2113	0	2122	79	0
1	M	2113	0	2122	46	1
1	N	2113	0	2122	49	0
1	O	2113	0	2122	47	1
1	P	2113	0	2122	47	1
1	Q	2113	0	2122	45	0
1	R	2113	0	2122	55	1
1	S	2113	0	2122	45	0
1	T	2113	0	2122	50	1
2	A	14	0	9	4	0
2	B	14	0	9	4	0
2	C	14	0	9	4	0
2	D	14	0	9	4	0
2	E	14	0	9	4	0
2	F	14	0	9	3	0
2	G	14	0	9	3	0
2	H	14	0	9	4	0
2	I	14	0	9	4	0
2	J	14	0	9	4	0
2	K	14	0	9	3	0
2	L	14	0	9	4	0
2	M	14	0	9	4	0
2	N	14	0	9	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	14	0	9	4	0
2	P	14	0	9	3	0
2	Q	14	0	9	4	0
2	R	14	0	9	4	0
2	S	14	0	9	4	0
2	T	14	0	9	3	0
3	A	27	0	0	5	0
3	B	11	0	0	0	0
3	C	17	0	0	2	0
3	D	23	0	0	1	0
3	E	20	0	0	1	0
3	F	20	0	0	1	0
3	G	34	0	0	6	0
3	H	23	0	0	2	0
3	I	18	0	0	2	0
3	J	8	0	0	1	0
3	K	18	0	0	7	0
3	L	35	0	0	3	0
3	M	13	0	0	1	0
3	N	12	0	0	1	0
3	O	13	0	0	3	0
3	P	9	0	0	3	0
3	Q	11	0	0	2	0
3	R	27	0	0	5	0
3	S	22	0	0	2	0
3	T	15	0	0	4	0
All	All	42916	0	42620	916	6

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 11.

The worst 5 of 916 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:H:275:HIS:NE2	1:L:287:LEU:CD2	2.07	1.16
1:H:275:HIS:NE2	1:L:287:LEU:HD22	1.61	1.13
1:H:281:ARG:CZ	1:L:233:ARG:HH21	1.74	0.99
1:E:285:LEU:HD21	1:K:281:ARG:NH2	1.79	0.96
1:H:275:HIS:CE1	1:L:287:LEU:CD2	2.57	0.88

The worst 5 of 6 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:R:260:ASP:OD2	1:T:281:ARG:NH1[1_565]	1.47	0.73
1:F:281:ARG:NH1	1:H:260:ASP:OD2[1_545]	1.65	0.55
1:K:283:TYR:OH	1:M:277:GLU:OE2[1_545]	1.69	0.51
1:C:275:HIS:CE1	1:P:287:LEU:CD1[1_554]	1.79	0.41
1:A:283:TYR:OH	1:D:277:GLU:OE2[1_545]	1.80	0.40

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	272/295 (92%)	259 (95%)	13 (5%)	0	100	100
1	B	272/295 (92%)	260 (96%)	12 (4%)	0	100	100
1	C	272/295 (92%)	257 (94%)	15 (6%)	0	100	100
1	D	272/295 (92%)	260 (96%)	12 (4%)	0	100	100
1	E	272/295 (92%)	257 (94%)	15 (6%)	0	100	100
1	F	272/295 (92%)	262 (96%)	10 (4%)	0	100	100
1	G	272/295 (92%)	258 (95%)	14 (5%)	0	100	100
1	H	272/295 (92%)	263 (97%)	9 (3%)	0	100	100
1	I	272/295 (92%)	258 (95%)	14 (5%)	0	100	100
1	J	272/295 (92%)	258 (95%)	14 (5%)	0	100	100
1	K	272/295 (92%)	258 (95%)	14 (5%)	0	100	100
1	L	272/295 (92%)	261 (96%)	11 (4%)	0	100	100
1	M	272/295 (92%)	258 (95%)	14 (5%)	0	100	100
1	N	272/295 (92%)	259 (95%)	13 (5%)	0	100	100
1	O	272/295 (92%)	260 (96%)	12 (4%)	0	100	100
1	P	272/295 (92%)	259 (95%)	13 (5%)	0	100	100
1	Q	272/295 (92%)	262 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	272/295 (92%)	259 (95%)	13 (5%)	0	100	100
1	S	272/295 (92%)	259 (95%)	13 (5%)	0	100	100
1	T	272/295 (92%)	260 (96%)	12 (4%)	0	100	100
All	All	5440/5900 (92%)	5187 (95%)	253 (5%)	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	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	B	224/240 (93%)	222 (99%)	2 (1%)	84	96
1	C	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	D	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	E	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	F	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	G	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	H	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	I	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	J	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	K	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	L	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	M	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	N	224/240 (93%)	221 (99%)	3 (1%)	76	94
1	O	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	P	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	Q	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	R	224/240 (93%)	223 (100%)	1 (0%)	93	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	224/240 (93%)	223 (100%)	1 (0%)	93	98
1	T	224/240 (93%)	223 (100%)	1 (0%)	93	98
All	All	4480/4800 (93%)	4457 (100%)	23 (0%)	92	98

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	270	GLN
1	L	270	GLN
1	S	270	GLN
1	K	270	GLN
1	M	270	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	58	HIS
1	K	276	ASN
1	S	58	HIS
1	J	200	GLN
1	K	184	GLN

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](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	5RP	A	984	-	13,13,13	1.57	2 (15%)	11,18,18	1.44	2 (18%)
2	5RP	B	984	-	13,13,13	1.71	3 (23%)	11,18,18	1.32	2 (18%)
2	5RP	C	984	-	13,13,13	1.79	3 (23%)	11,18,18	1.49	2 (18%)
2	5RP	D	984	-	13,13,13	1.71	3 (23%)	11,18,18	1.38	2 (18%)
2	5RP	E	984	-	13,13,13	1.88	2 (15%)	11,18,18	1.61	2 (18%)
2	5RP	F	984	-	13,13,13	1.84	3 (23%)	11,18,18	1.47	2 (18%)
2	5RP	G	984	-	13,13,13	1.79	3 (23%)	11,18,18	1.56	2 (18%)
2	5RP	H	984	-	13,13,13	1.67	3 (23%)	11,18,18	1.47	3 (27%)
2	5RP	I	984	-	13,13,13	1.74	3 (23%)	11,18,18	1.58	3 (27%)
2	5RP	J	984	-	13,13,13	1.86	2 (15%)	11,18,18	1.34	1 (9%)
2	5RP	K	984	-	13,13,13	1.62	3 (23%)	11,18,18	1.65	2 (18%)
2	5RP	L	984	-	13,13,13	1.88	3 (23%)	11,18,18	1.64	4 (36%)
2	5RP	M	984	-	13,13,13	1.65	3 (23%)	11,18,18	1.64	3 (27%)
2	5RP	N	984	-	13,13,13	1.84	3 (23%)	11,18,18	1.45	2 (18%)
2	5RP	O	984	-	13,13,13	1.89	2 (15%)	11,18,18	1.23	1 (9%)
2	5RP	P	984	-	13,13,13	1.79	3 (23%)	11,18,18	1.57	2 (18%)
2	5RP	Q	984	-	13,13,13	1.79	3 (23%)	11,18,18	1.55	3 (27%)
2	5RP	R	984	-	13,13,13	1.78	2 (15%)	11,18,18	1.44	2 (18%)
2	5RP	S	984	-	13,13,13	1.94	3 (23%)	11,18,18	1.60	4 (36%)
2	5RP	T	984	-	13,13,13	1.77	3 (23%)	11,18,18	1.47	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5RP	A	984	-	-	0/16/16/16	0/0/0/0
2	5RP	B	984	-	-	0/16/16/16	0/0/0/0
2	5RP	C	984	-	-	0/16/16/16	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5RP	D	984	-	-	0/16/16/16	0/0/0/0
2	5RP	E	984	-	-	0/16/16/16	0/0/0/0
2	5RP	F	984	-	-	0/16/16/16	0/0/0/0
2	5RP	G	984	-	-	0/16/16/16	0/0/0/0
2	5RP	H	984	-	-	0/16/16/16	0/0/0/0
2	5RP	I	984	-	-	0/16/16/16	0/0/0/0
2	5RP	J	984	-	-	0/16/16/16	0/0/0/0
2	5RP	K	984	-	-	0/16/16/16	0/0/0/0
2	5RP	L	984	-	-	0/16/16/16	0/0/0/0
2	5RP	M	984	-	-	0/16/16/16	0/0/0/0
2	5RP	N	984	-	-	0/16/16/16	0/0/0/0
2	5RP	O	984	-	-	0/16/16/16	0/0/0/0
2	5RP	P	984	-	-	0/16/16/16	0/0/0/0
2	5RP	Q	984	-	-	0/16/16/16	0/0/0/0
2	5RP	R	984	-	-	0/16/16/16	0/0/0/0
2	5RP	S	984	-	-	0/16/16/16	0/0/0/0
2	5RP	T	984	-	-	0/16/16/16	0/0/0/0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	984	5RP	P9-O10	-2.44	1.46	1.54
2	B	984	5RP	P9-O10	-2.40	1.46	1.54
2	L	984	5RP	P9-O10	-2.40	1.46	1.54
2	M	984	5RP	P9-O10	-2.37	1.46	1.54
2	Q	984	5RP	P9-O10	-2.32	1.46	1.54

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	984	5RP	O14-C6-C7	2.00	114.56	110.19
2	B	984	5RP	O1-C2-C3	2.01	118.07	112.66
2	S	984	5RP	O13-C5-C3	2.02	114.75	111.01
2	D	984	5RP	O1-C2-C3	2.03	118.13	112.66
2	S	984	5RP	O10-P9-O8	2.11	112.63	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	984	5RP	4	0
2	B	984	5RP	4	0
2	C	984	5RP	4	0
2	D	984	5RP	4	0
2	E	984	5RP	4	0
2	F	984	5RP	3	0
2	G	984	5RP	3	0
2	H	984	5RP	4	0
2	I	984	5RP	4	0
2	J	984	5RP	4	0
2	K	984	5RP	3	0
2	L	984	5RP	4	0
2	M	984	5RP	4	0
2	N	984	5RP	4	0
2	O	984	5RP	4	0
2	P	984	5RP	3	0
2	Q	984	5RP	4	0
2	R	984	5RP	4	0
2	S	984	5RP	4	0
2	T	984	5RP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/295 (93%)	-0.53	1 (0%) 93 92	6, 20, 52, 75	0
1	B	276/295 (93%)	-0.40	1 (0%) 93 92	6, 20, 52, 75	0
1	C	276/295 (93%)	-0.30	4 (1%) 78 76	6, 20, 52, 75	0
1	D	276/295 (93%)	-0.50	1 (0%) 93 92	6, 20, 52, 75	0
1	E	276/295 (93%)	-0.36	8 (2%) 55 49	6, 20, 52, 75	0
1	F	276/295 (93%)	-0.52	1 (0%) 93 92	6, 20, 52, 75	0
1	G	276/295 (93%)	-0.46	2 (0%) 89 88	6, 20, 52, 75	0
1	H	276/295 (93%)	-0.48	1 (0%) 93 92	6, 20, 52, 75	0
1	I	276/295 (93%)	-0.46	3 (1%) 82 80	6, 20, 52, 75	0
1	J	276/295 (93%)	-0.35	2 (0%) 89 88	6, 20, 52, 75	0
1	K	276/295 (93%)	-0.50	2 (0%) 89 88	6, 20, 52, 75	0
1	L	276/295 (93%)	-0.34	8 (2%) 55 49	6, 20, 52, 75	0
1	M	276/295 (93%)	-0.49	2 (0%) 89 88	6, 20, 52, 75	0
1	N	276/295 (93%)	-0.47	5 (1%) 71 68	6, 20, 52, 75	0
1	O	276/295 (93%)	-0.48	3 (1%) 82 80	6, 20, 52, 75	0
1	P	276/295 (93%)	-0.43	0 100 100	6, 20, 52, 75	0
1	Q	276/295 (93%)	-0.49	4 (1%) 78 76	6, 20, 52, 75	0
1	R	276/295 (93%)	-0.50	1 (0%) 93 92	6, 20, 52, 75	0
1	S	276/295 (93%)	-0.44	2 (0%) 89 88	6, 20, 52, 75	0
1	T	276/295 (93%)	-0.50	0 100 100	6, 20, 52, 75	0
All	All	5520/5900 (93%)	-0.45	51 (0%) 85 84	6, 20, 53, 75	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	GLU	6.1
1	E	181	VAL	4.7
1	Q	288	SER	4.5
1	S	181	VAL	4.5
1	C	10	GLY	4.4

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	5RP	M	984	14/14	0.91	0.25	3.02	36,55,65,67	0
2	5RP	J	984	14/14	0.94	0.29	2.62	36,55,65,66	0
2	5RP	T	984	14/14	0.92	0.22	2.42	36,56,65,67	0
2	5RP	P	984	14/14	0.85	0.28	2.26	36,55,65,66	0
2	5RP	H	984	14/14	0.94	0.21	2.22	36,55,65,66	0
2	5RP	L	984	14/14	0.92	0.25	2.19	36,55,65,66	0
2	5RP	D	984	14/14	0.90	0.25	2.15	36,55,65,67	0
2	5RP	K	984	14/14	0.93	0.23	1.95	36,55,65,66	0
2	5RP	R	984	14/14	0.93	0.21	1.80	36,56,65,66	0
2	5RP	G	984	14/14	0.93	0.23	1.66	36,55,65,66	0
2	5RP	O	984	14/14	0.94	0.22	1.48	36,55,65,66	0
2	5RP	N	984	14/14	0.93	0.21	1.40	36,55,65,67	0
2	5RP	I	984	14/14	0.90	0.22	1.33	36,55,64,66	0
2	5RP	Q	984	14/14	0.95	0.19	1.08	36,55,64,66	0
2	5RP	F	984	14/14	0.94	0.19	0.82	36,55,65,66	0
2	5RP	E	984	14/14	0.93	0.20	0.81	36,56,65,66	0
2	5RP	C	984	14/14	0.90	0.21	0.75	36,55,64,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	5RP	A	984	14/14	0.95	0.18	0.74	36,55,64,66	0
2	5RP	S	984	14/14	0.92	0.18	0.51	36,55,65,66	0
2	5RP	B	984	14/14	0.95	0.18	0.31	36,55,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.