



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:30 PM GMT

PDB ID : 4P2V  
Title : Structure of the AI-2 processing enzyme LsrF in complex with the product of the LsrG reaction P-HPD  
Authors : Miller, S.T.; Oh, I.K.; Xavier, K.B.  
Deposited on : 2014-03-05  
Resolution : 2.51 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](mailto: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.

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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

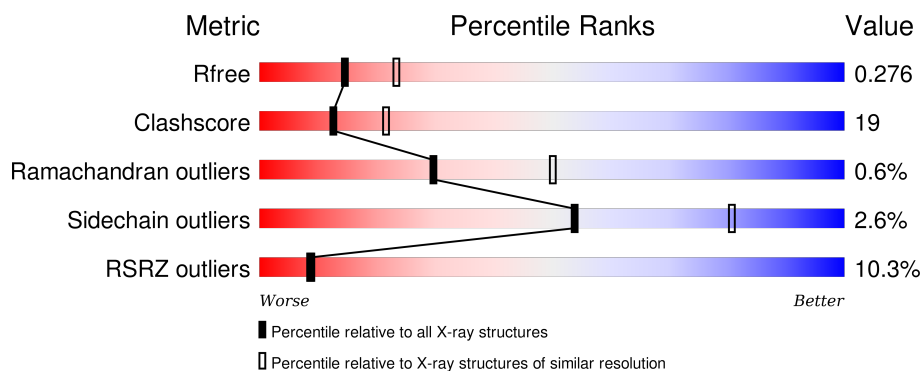
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	293	<div> <div>13%</div> <div>59%</div> <div>34%</div> <div>• •</div> </div>
1	B	293	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>•</div> </div>
1	C	293	<div> <div>10%</div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
1	D	293	<div> <div>18%</div> <div>51%</div> <div>38%</div> <div>7%</div> <div>•</div> </div>
1	E	293	<div> <div>5%</div> <div>67%</div> <div>29%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	293	<div><div>2%</div><div><div></div><div></div><div></div></div><div>72%</div><div>23%</div><div></div><div></div></div>
1	G	293	<div><div>18%</div><div><div></div><div></div><div></div></div><div>59%</div><div>33%</div><div></div><div></div></div>
1	H	293	<div><div>14%</div><div><div></div><div></div><div></div></div><div>60%</div><div>35%</div><div></div><div></div></div>
1	I	293	<div><div>6%</div><div><div></div><div></div><div></div></div><div>62%</div><div>31%</div><div></div><div></div></div>
1	K	293	<div><div>9%</div><div><div></div><div></div><div></div></div><div>61%</div><div>33%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22178 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 aldolase LsrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	B	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	C	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	D	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	E	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	F	280	Total	C	N	O	S	0	0	0
			2138	1345	377	398	18			
1	G	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	H	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	I	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	K	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			

There are 30 discrepancies between the modelled and reference sequences:

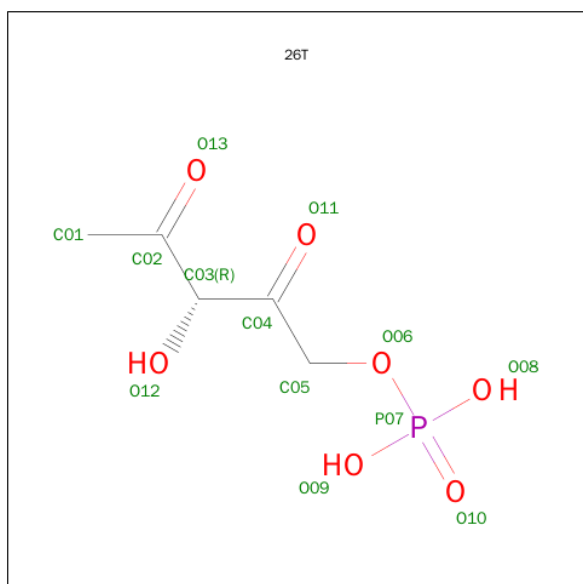
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P76143
A	0	SER	-	expression tag	UNP P76143
A	203	ALA	LYS	engineered mutation	UNP P76143
B	-1	GLY	-	expression tag	UNP P76143
B	0	SER	-	expression tag	UNP P76143
B	203	ALA	LYS	engineered mutation	UNP P76143
C	-1	GLY	-	expression tag	UNP P76143
C	0	SER	-	expression tag	UNP P76143
C	203	ALA	LYS	engineered mutation	UNP P76143

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P76143
D	0	SER	-	expression tag	UNP P76143
D	203	ALA	LYS	engineered mutation	UNP P76143
E	-1	GLY	-	expression tag	UNP P76143
E	0	SER	-	expression tag	UNP P76143
E	203	ALA	LYS	engineered mutation	UNP P76143
F	-1	GLY	-	expression tag	UNP P76143
F	0	SER	-	expression tag	UNP P76143
F	203	ALA	LYS	engineered mutation	UNP P76143
G	-1	GLY	-	expression tag	UNP P76143
G	0	SER	-	expression tag	UNP P76143
G	203	ALA	LYS	engineered mutation	UNP P76143
H	-1	GLY	-	expression tag	UNP P76143
H	0	SER	-	expression tag	UNP P76143
H	203	ALA	LYS	engineered mutation	UNP P76143
I	-1	GLY	-	expression tag	UNP P76143
I	0	SER	-	expression tag	UNP P76143
I	203	ALA	LYS	engineered mutation	UNP P76143
K	-1	GLY	-	expression tag	UNP P76143
K	0	SER	-	expression tag	UNP P76143
K	203	ALA	LYS	engineered mutation	UNP P76143

- Molecule 2 is (3R)-3-hydroxy-2,4-dioxopentyl dihydrogen phosphate (three-letter code: 26T) (formula: C<sub>5</sub>H<sub>9</sub>O<sub>7</sub>P).

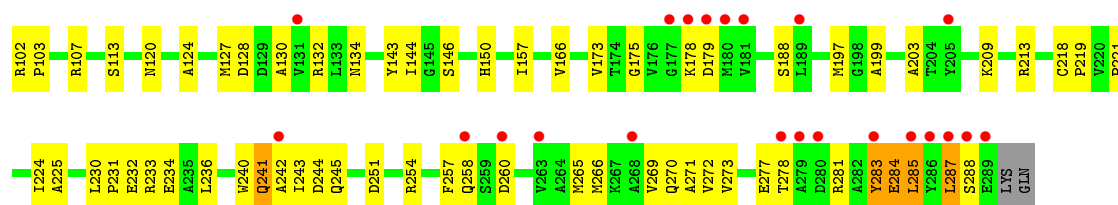


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 13 5 7 1	0	0
2	B	1	Total C O P 13 5 7 1	0	0
2	C	1	Total C O P 13 5 7 1	0	0
2	D	1	Total C O P 13 5 7 1	0	0
2	E	1	Total C O P 13 5 7 1	0	0
2	F	1	Total C O P 13 5 7 1	0	0
2	G	1	Total C O P 13 5 7 1	0	0
2	H	1	Total C O P 13 5 7 1	0	0
2	I	1	Total C O P 13 5 7 1	0	0
2	K	1	Total C O P 13 5 7 1	0	0

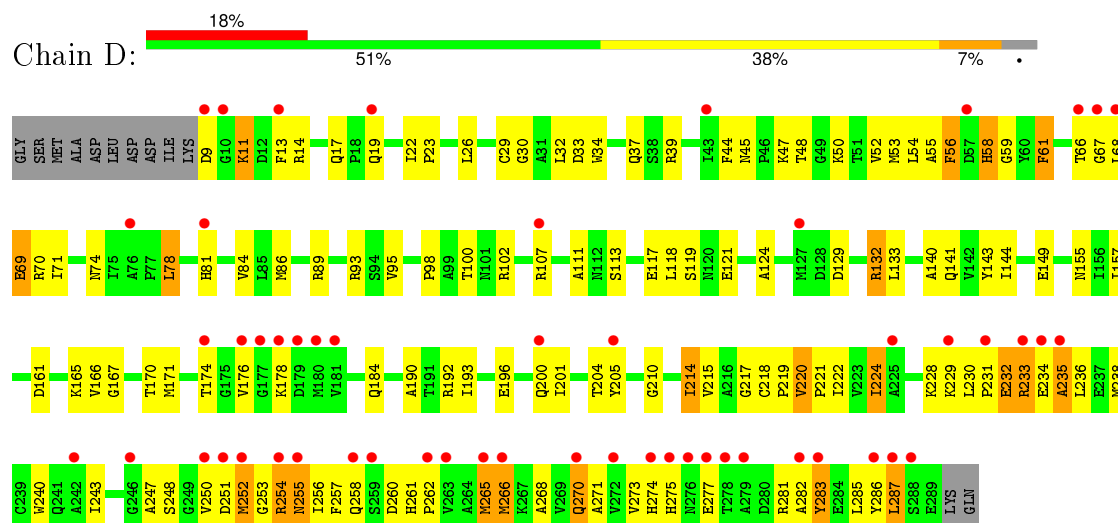
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total O 47 47	0	0
3	B	73	Total O 73 73	0	0
3	C	66	Total O 66 66	0	0
3	D	38	Total O 38 38	0	0
3	E	71	Total O 71 71	0	0
3	F	85	Total O 85 85	0	0
3	G	47	Total O 47 47	0	0
3	H	47	Total O 47 47	0	0
3	I	80	Total O 80 80	0	0
3	K	42	Total O 42 42	0	0

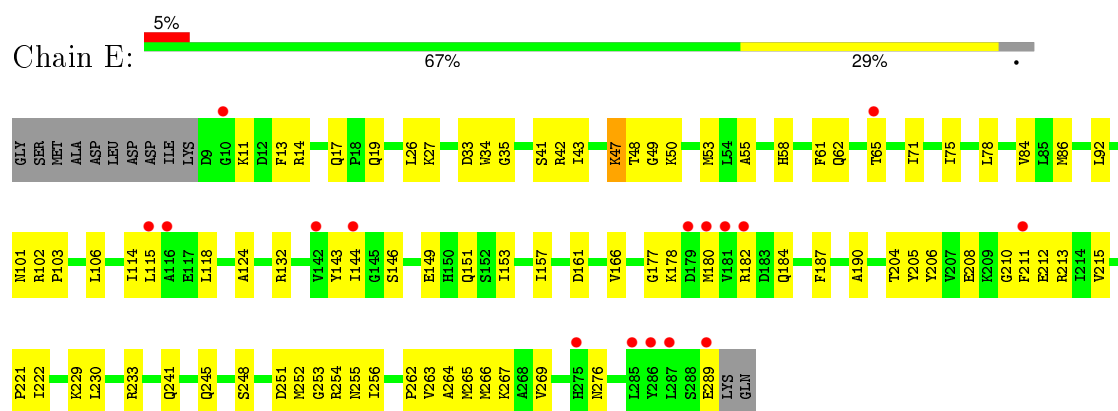




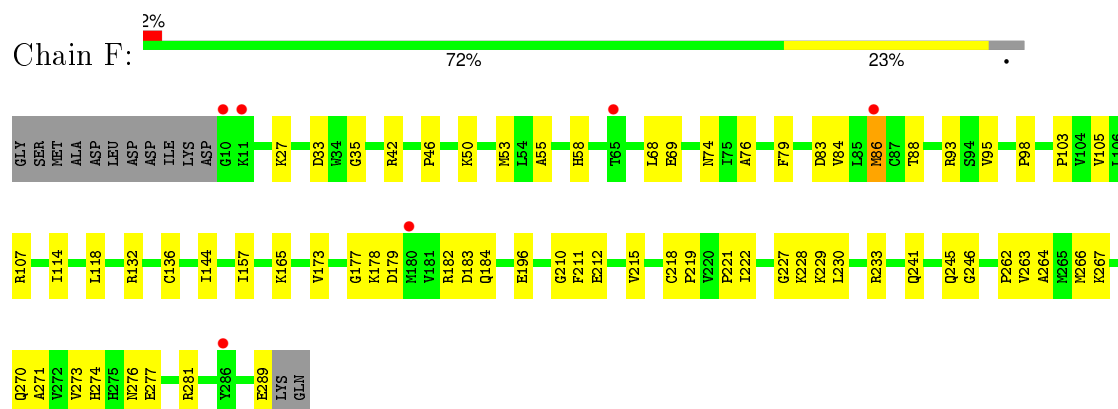
• Molecule 1: Uncharacterized aldolase LsrF



• Molecule 1: Uncharacterized aldolase LsrF

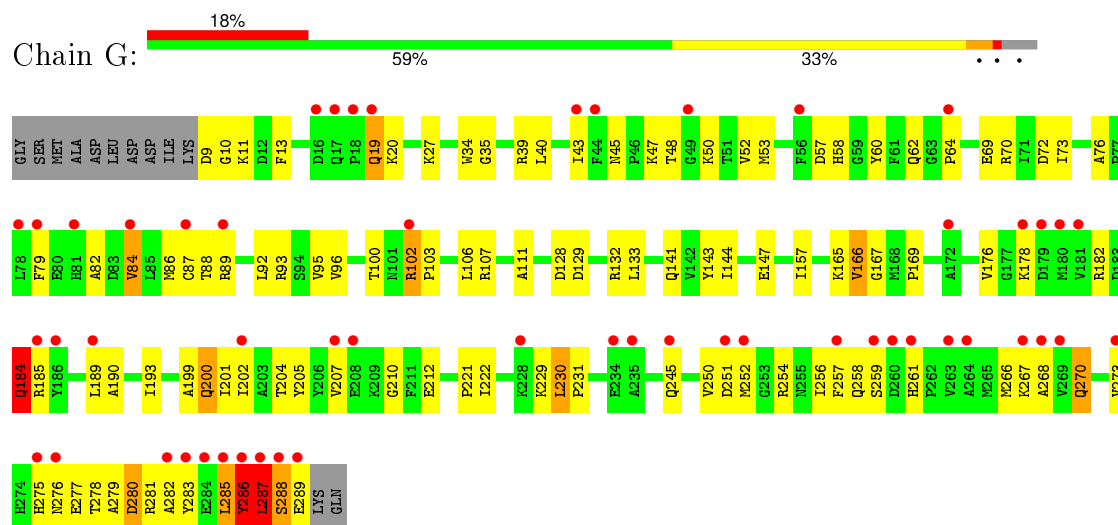


• Molecule 1: Uncharacterized aldolase LsrF

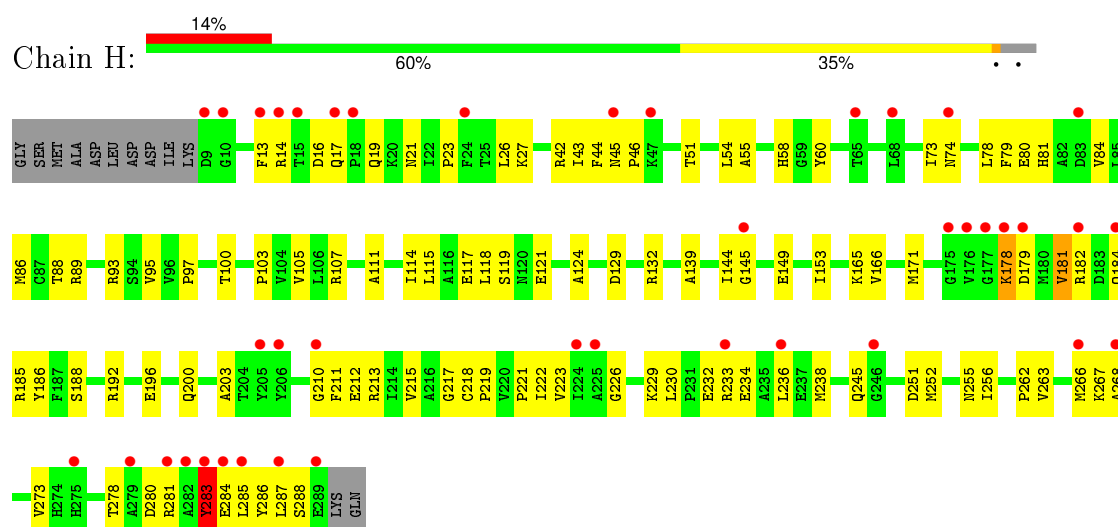




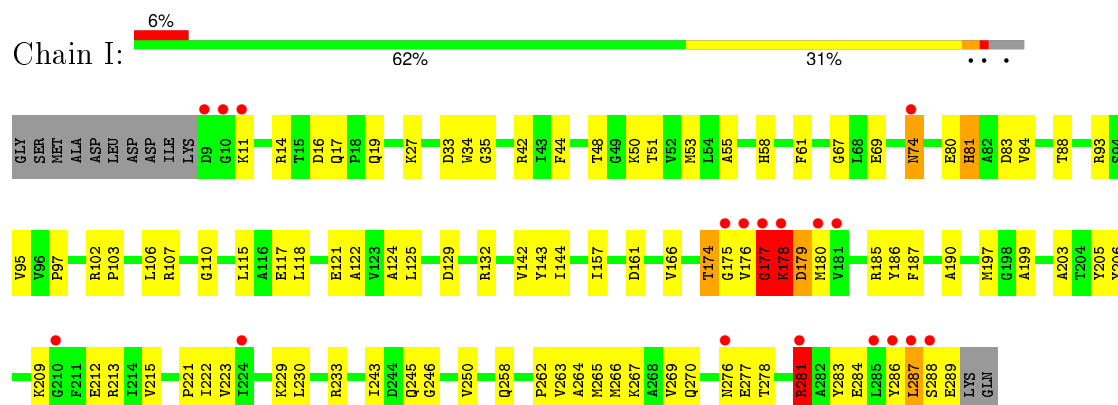
- Molecule 1: Uncharacterized aldolase LsrF



- Molecule 1: Uncharacterized aldolase LsrF

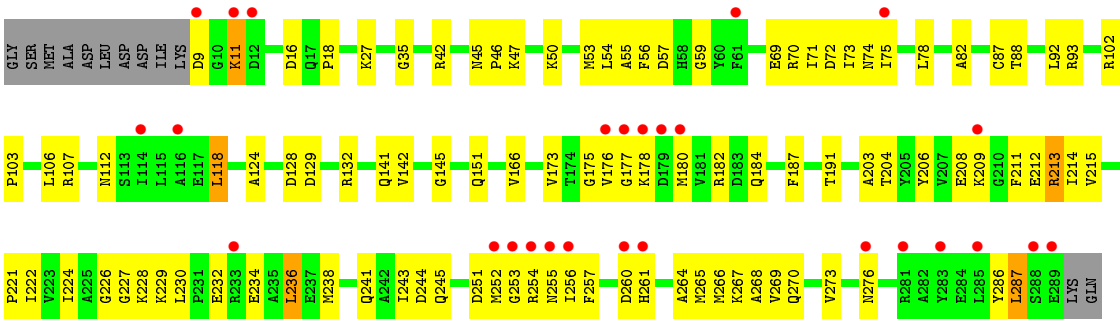


- Molecule 1: Uncharacterized aldolase LsrF



- Molecule 1: Uncharacterized aldolase LsrF





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.62Å 105.74Å 170.40Å 90.00° 101.43° 90.00°	Depositor
Resolution (Å)	49.26 – 2.51 49.26 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.26-2.51) 90.0 (49.26-2.51)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1626)	Depositor
R, $R_{free}$	0.235 , 0.271 0.237 , 0.276	Depositor DCC
$R_{free}$ test set	4585 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.6	EDS
Estimated twinning fraction	0.125 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	2 of 92513 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	22178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 26T

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	0.37	0/2185	0.72	3/2957 (0.1%)
1	B	0.27	0/2185	0.54	0/2957
1	C	0.32	0/2185	0.67	3/2957 (0.1%)
1	D	0.43	0/2185	0.76	2/2957 (0.1%)
1	E	0.29	0/2185	0.58	0/2957
1	F	0.28	0/2177	0.55	0/2946
1	G	0.36	0/2185	0.76	3/2957 (0.1%)
1	H	0.39	1/2185 (0.0%)	0.70	0/2957
1	I	0.41	1/2185 (0.0%)	0.70	4/2957 (0.1%)
1	K	0.33	0/2185	0.73	3/2957 (0.1%)
All	All	0.35	2/21842 (0.0%)	0.68	18/29559 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	4
1	I	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	185	ARG	C-N	10.49	1.58	1.34
1	H	283	TYR	CD1-CE1	-6.17	1.30	1.39

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	287	LEU	CA-CB-CG	-10.14	91.98	115.30
1	I	281	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	K	118	LEU	CA-CB-CG	7.71	133.02	115.30
1	D	287	LEU	CA-CB-CG	-6.43	100.52	115.30
1	G	184	GLN	CA-CB-CG	6.42	127.53	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	280	ASP	Peptide
1	G	285	LEU	Peptide
1	G	286	TYR	Peptide
1	G	287	LEU	Peptide
1	I	178	LYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2146	0	2148	98	0
1	B	2146	0	2148	61	0
1	C	2146	0	2148	76	1
1	D	2146	0	2148	182	1
1	E	2146	0	2148	69	0
1	F	2138	0	2144	54	0
1	G	2146	0	2148	113	0
1	H	2146	0	2148	102	0
1	I	2146	0	2148	88	0
1	K	2146	0	2148	89	0
2	A	13	0	9	1	0
2	B	13	0	9	2	0
2	C	13	0	9	0	0
2	D	13	0	9	4	0
2	E	13	0	9	2	0
2	F	13	0	9	1	0
2	G	13	0	9	2	0
2	H	13	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	13	0	9	3	0
2	K	13	0	9	1	0
3	A	47	0	0	15	0
3	B	73	0	0	14	0
3	C	66	0	0	10	1
3	D	38	0	0	13	0
3	E	71	0	0	17	0
3	F	85	0	0	10	0
3	G	47	0	0	17	0
3	H	47	0	0	14	0
3	I	80	0	0	14	1
3	K	42	0	0	6	0
All	All	22178	0	21566	838	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 838 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:D:256:ILE:HG23	1:D:265:MET:SD	1.30	1.64
1:D:256:ILE:CG2	1:D:265:MET:SD	2.20	1.30
1:G:278:THR:OG1	1:G:281:ARG:CG	1.92	1.18
1:G:278:THR:OG1	1:G:281:ARG:HG2	0.99	1.15
1:B:281:ARG:NH1	3:B:402:HOH:O	1.91	1.01

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:LEU:O	1:D:47:LYS:NZ[2_454]	2.12	0.08
3:C:401:HOH:O	3:I:403:HOH:O[1_455]	2.19	0.01

## 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	279/293 (95%)	267 (96%)	12 (4%)	0	100	100
1	B	279/293 (95%)	269 (96%)	9 (3%)	1 (0%)	39	61
1	C	279/293 (95%)	266 (95%)	11 (4%)	2 (1%)	26	46
1	D	279/293 (95%)	267 (96%)	8 (3%)	4 (1%)	14	24
1	E	279/293 (95%)	268 (96%)	10 (4%)	1 (0%)	39	61
1	F	278/293 (95%)	266 (96%)	11 (4%)	1 (0%)	39	61
1	G	279/293 (95%)	266 (95%)	11 (4%)	2 (1%)	26	46
1	H	279/293 (95%)	265 (95%)	11 (4%)	3 (1%)	17	31
1	I	279/293 (95%)	265 (95%)	10 (4%)	4 (1%)	14	24
1	K	279/293 (95%)	267 (96%)	12 (4%)	0	100	100
All	All	2789/2930 (95%)	2666 (96%)	105 (4%)	18 (1%)	30	50

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	LYS
1	D	178	LYS
1	D	286	TYR
1	E	178	LYS
1	F	178	LYS

### 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	227/237 (96%)	222 (98%)	5 (2%)	60	84
1	B	227/237 (96%)	224 (99%)	3 (1%)	76	92
1	C	227/237 (96%)	224 (99%)	3 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	227/237 (96%)	210 (92%)	17 (8%)	17	31
1	E	227/237 (96%)	224 (99%)	3 (1%)	76	92
1	F	226/237 (95%)	223 (99%)	3 (1%)	76	92
1	G	227/237 (96%)	219 (96%)	8 (4%)	43	70
1	H	227/237 (96%)	223 (98%)	4 (2%)	66	88
1	I	227/237 (96%)	220 (97%)	7 (3%)	47	75
1	K	227/237 (96%)	221 (97%)	6 (3%)	54	81
All	All	2269/2370 (96%)	2210 (97%)	59 (3%)	54	81

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	270	GLN
1	F	182	ARG
1	K	209	LYS
1	D	283	TYR
1	E	47	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	151	GLN
1	F	276	ASN
1	H	81	HIS
1	D	255	ASN
1	E	101	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	26T	A	301	-	10,12,12	5.40	3 (30%)	9,17,17	2.29	6 (66%)
2	26T	B	301	-	10,12,12	5.39	3 (30%)	9,17,17	2.31	6 (66%)
2	26T	C	301	-	10,12,12	5.27	3 (30%)	9,17,17	2.36	7 (77%)
2	26T	D	301	-	10,12,12	5.66	2 (20%)	9,17,17	2.37	6 (66%)
2	26T	E	301	-	10,12,12	5.35	3 (30%)	9,17,17	2.36	7 (77%)
2	26T	F	301	-	10,12,12	5.65	3 (30%)	9,17,17	2.42	7 (77%)
2	26T	G	301	-	10,12,12	5.22	3 (30%)	9,17,17	2.30	6 (66%)
2	26T	H	301	-	10,12,12	5.49	3 (30%)	9,17,17	2.34	6 (66%)
2	26T	I	301	-	10,12,12	5.52	3 (30%)	9,17,17	2.30	6 (66%)
2	26T	K	301	-	10,12,12	5.49	3 (30%)	9,17,17	2.31	6 (66%)

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	26T	A	301	-	-	0/13/14/14	0/0/0/0
2	26T	B	301	-	-	0/13/14/14	0/0/0/0
2	26T	C	301	-	-	0/13/14/14	0/0/0/0
2	26T	D	301	-	-	0/13/14/14	0/0/0/0
2	26T	E	301	-	-	0/13/14/14	0/0/0/0
2	26T	F	301	-	-	0/13/14/14	0/0/0/0
2	26T	G	301	-	-	0/13/14/14	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	26T	H	301	-	-	0/13/14/14	0/0/0/0
2	26T	I	301	-	-	0/13/14/14	0/0/0/0
2	26T	K	301	-	-	0/13/14/14	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	26T	O06-C05	-15.99	1.32	1.43
2	D	301	26T	O06-C05	-15.76	1.32	1.43
2	I	301	26T	O06-C05	-14.99	1.32	1.43
2	K	301	26T	O06-C05	-14.90	1.33	1.43
2	H	301	26T	O06-C05	-14.66	1.33	1.43

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	26T	O06-P07-O10	-3.09	99.28	107.14
2	D	301	26T	O06-P07-O10	-2.99	99.53	107.14
2	D	301	26T	O13-C02-C01	-2.86	115.41	121.01
2	F	301	26T	O13-C02-C01	-2.86	115.42	121.01
2	I	301	26T	O06-P07-O10	-2.83	99.93	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	26T	1	0
2	B	301	26T	2	0
2	D	301	26T	4	0
2	E	301	26T	2	0
2	F	301	26T	1	0
2	G	301	26T	2	0
2	H	301	26T	3	0
2	I	301	26T	3	0
2	K	301	26T	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	281/293 (95%)	0.94	37 (13%) 4 4	31, 50, 104, 156	0
1	B	281/293 (95%)	0.31	7 (2%) 61 65	19, 35, 56, 79	0
1	C	281/293 (95%)	0.78	30 (10%) 8 8	31, 49, 85, 145	0
1	D	281/293 (95%)	1.26	54 (19%) 2 1	37, 61, 113, 137	0
1	E	281/293 (95%)	0.48	16 (5%) 27 31	18, 37, 71, 124	0
1	F	280/293 (95%)	0.25	6 (2%) 67 71	19, 33, 53, 99	0
1	G	281/293 (95%)	1.17	53 (18%) 2 1	33, 58, 109, 201	0
1	H	281/293 (95%)	0.88	41 (14%) 3 3	30, 51, 90, 107	0
1	I	281/293 (95%)	0.44	18 (6%) 23 25	20, 37, 77, 147	0
1	K	281/293 (95%)	0.80	27 (9%) 10 11	28, 49, 88, 119	0
All	All	2809/2930 (95%)	0.73	289 (10%) 9 9	18, 45, 92, 201	0

The worst 5 of 289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	10	GLY	12.0
1	G	287	LEU	9.6
1	H	283	TYR	8.4
1	E	181	VAL	8.3
1	D	287	LEU	7.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	26T	B	301	13/13	0.92	0.22	1.04	39,46,55,56	0
2	26T	E	301	13/13	0.88	0.20	0.68	43,49,72,72	0
2	26T	F	301	13/13	0.87	0.18	0.31	37,63,67,69	0
2	26T	C	301	13/13	0.90	0.20	0.27	31,40,93,93	0
2	26T	A	301	13/13	0.84	0.22	0.15	50,55,86,86	0
2	26T	H	301	13/13	0.90	0.22	0.04	53,58,67,68	0
2	26T	I	301	13/13	0.90	0.17	-0.04	40,55,69,69	0
2	26T	K	301	13/13	0.80	0.23	-0.09	47,58,72,73	0
2	26T	G	301	13/13	0.80	0.19	-0.68	45,60,90,91	0
2	26T	D	301	13/13	0.82	0.18	-0.94	49,66,69,72	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.