wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 06:49 am BST

PDB ID	:	1GT7
Title	:	L-rhamnulose-1-phosphate aldolase from Escherichia coli
Authors	:	Kroemer, M.; Schulz, G.E.
Deposited on	:	2002-01-14
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

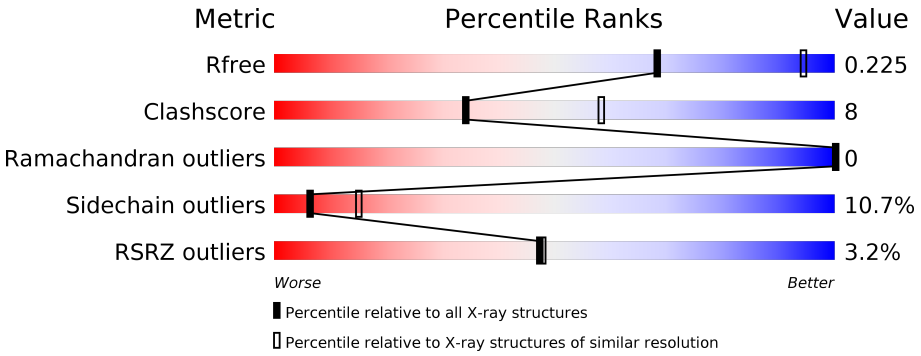
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	274	75% 19% 5%
1	B	274	76% 20%
1	C	274	75% 19% 6%
1	D	274	76% 18% 5%
1	E	274	76% 18% 5%
1	F	274	79% 15% 6%

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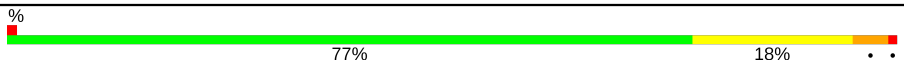
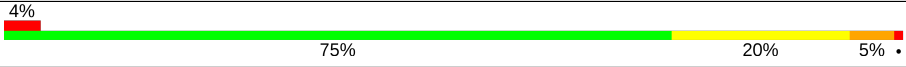
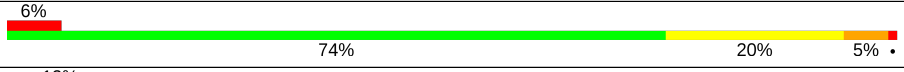
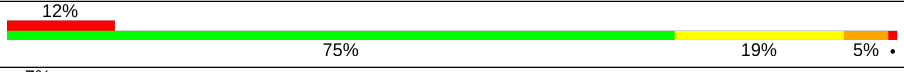
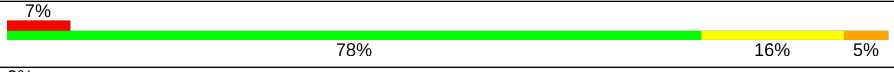
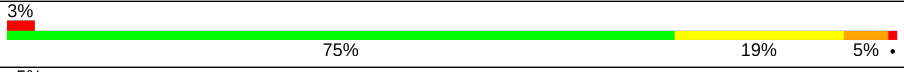
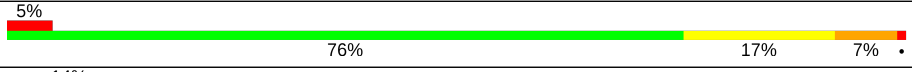
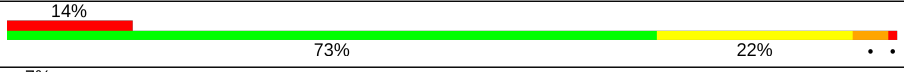
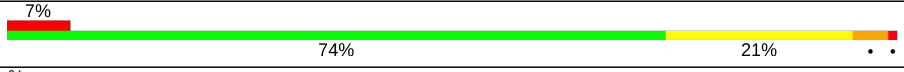
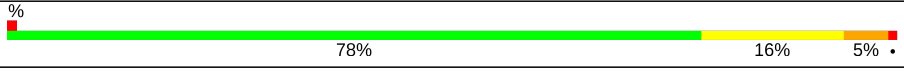
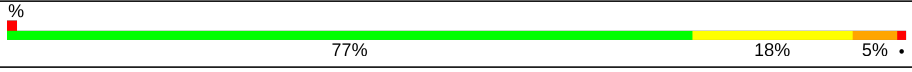
Mol	Chain	Length	Quality of chain
1	G	274	
1	H	274	
1	I	274	
1	J	274	
1	K	274	
1	L	274	
1	M	274	
1	N	274	
1	O	274	
1	P	274	
1	Q	274	
1	R	274	
1	S	274	
1	T	274	

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
3	PGH	A	300	-	X	-	-
3	PGH	B	300	-	X	-	-
3	PGH	C	300	-	X	-	-
3	PGH	D	300	-	X	-	-
3	PGH	E	300	-	X	-	-
3	PGH	F	300	-	X	-	-
3	PGH	G	300	-	X	-	-
3	PGH	H	300	-	X	-	-
3	PGH	I	300	-	X	-	-
3	PGH	J	300	-	X	-	-
3	PGH	K	300	-	X	-	-
3	PGH	L	300	-	X	-	-
3	PGH	M	300	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGH	O	300	-	X	-	-
3	PGH	P	300	-	X	-	-
3	PGH	Q	300	-	X	-	-
3	PGH	R	300	-	X	-	-
3	PGH	S	300	-	X	-	-
3	PGH	T	300	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 46180 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 RHAMNULOSE-1-PHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	B	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	C	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	D	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	E	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	F	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	G	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	H	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	I	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	J	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	K	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	L	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	M	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	N	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	O	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	P	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	R	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	S	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	T	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		
2	Q	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	I	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	T	1	Total	Zn	0	0
			1	1		
2	N	1	Total	Zn	0	0
			1	1		
2	O	1	Total	Zn	0	0
			1	1		

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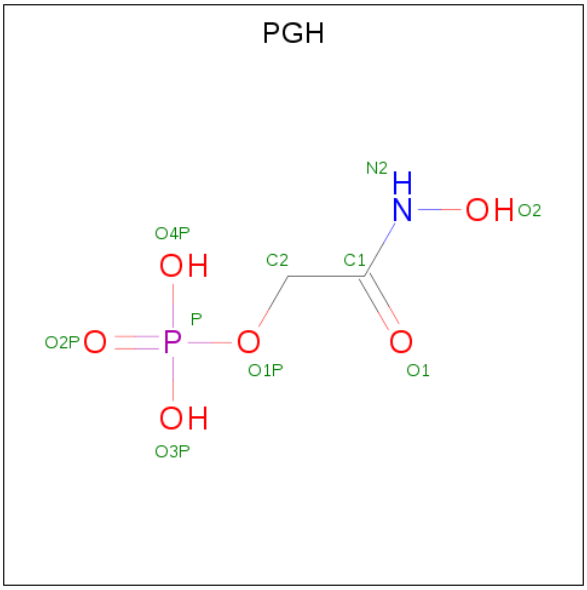
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	S	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	M	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHOGLYCOLOHYDROXAMIC ACID (three-letter code: PGH) (formula: $C_2H_6NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 10 2 1 6 1	0	0
3	B	1	Total C N O P 10 2 1 6 1	0	0
3	C	1	Total C N O P 10 2 1 6 1	0	0
3	D	1	Total C N O P 10 2 1 6 1	0	0
3	E	1	Total C N O P 10 2 1 6 1	0	0
3	F	1	Total C N O P 10 2 1 6 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	H	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	I	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	J	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	K	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	L	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	M	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	N	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	O	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	P	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	Q	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	R	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	S	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	T	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total	O	0	0
			177	177		
4	B	174	Total	O	0	0
			174	174		
4	C	173	Total	O	0	0
			173	173		
4	D	173	Total	O	0	0
			173	173		
4	E	179	Total	O	0	0
			179	179		

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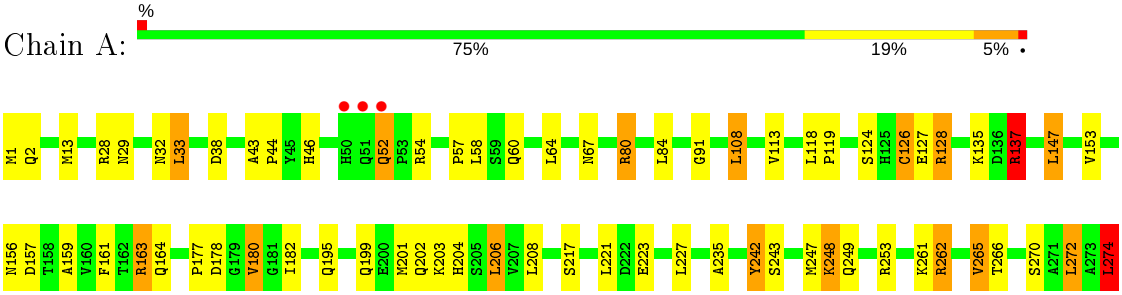
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	174	Total O 174 174	0	0
4	G	176	Total O 176 176	0	0
4	H	171	Total O 171 171	0	0
4	I	177	Total O 177 177	0	0
4	J	178	Total O 178 178	0	0
4	K	177	Total O 177 177	0	0
4	L	167	Total O 167 167	0	0
4	M	183	Total O 183 183	0	0
4	N	170	Total O 170 170	0	0
4	O	175	Total O 175 175	0	0
4	P	167	Total O 167 167	0	0
4	Q	176	Total O 176 176	0	0
4	R	172	Total O 172 172	0	0
4	S	171	Total O 171 171	0	0
4	T	170	Total O 170 170	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.

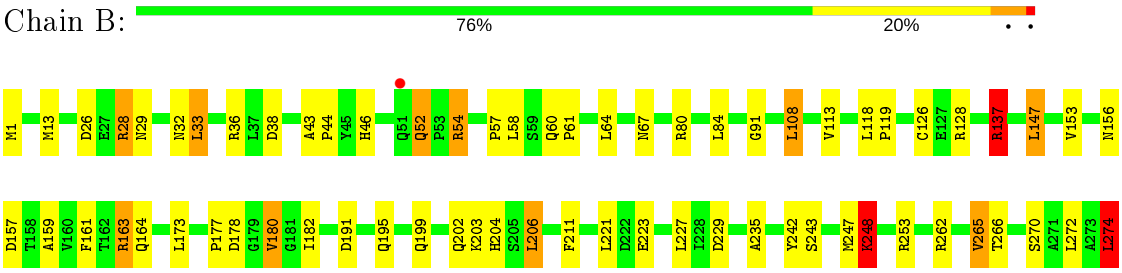
- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain A:



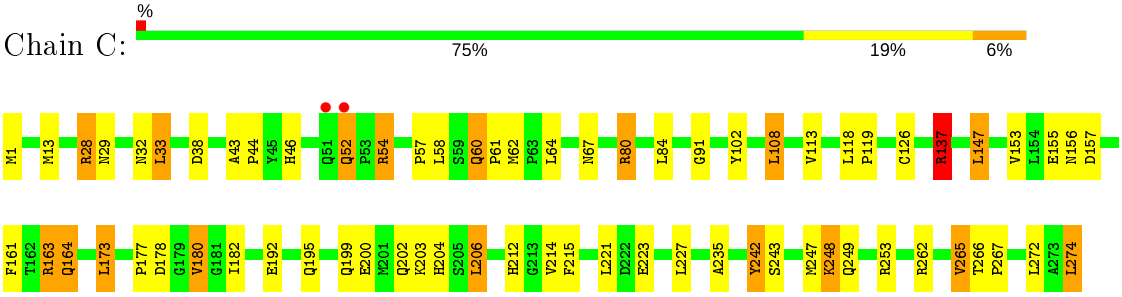
- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain B:



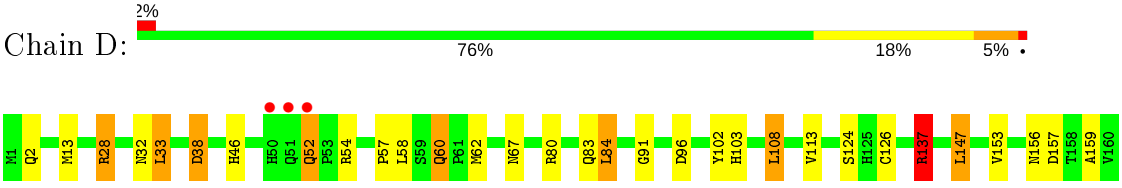
- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

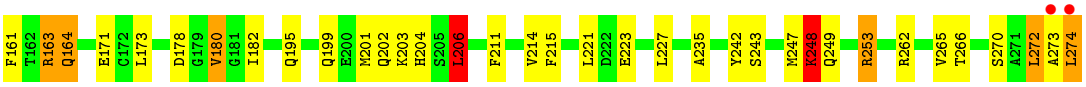
Chain C:



- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

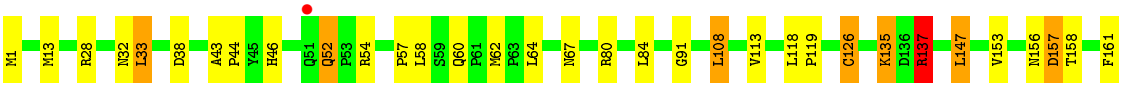
Chain D:

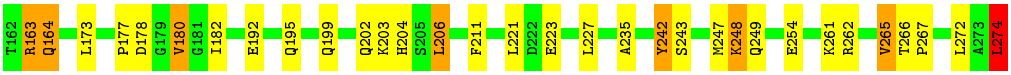




• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

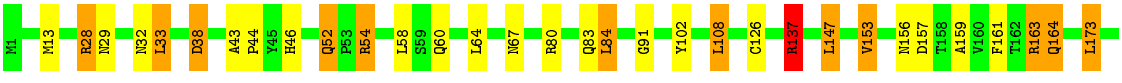
Chain E:





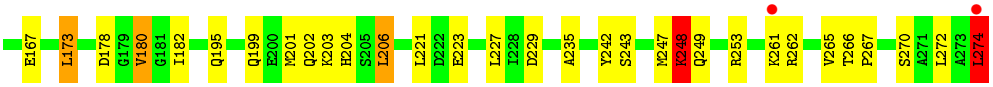
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain F:



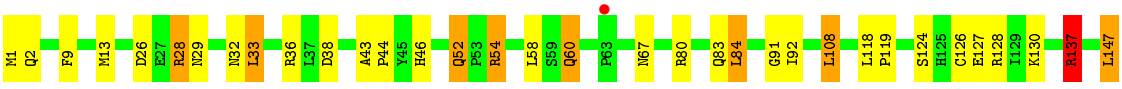
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

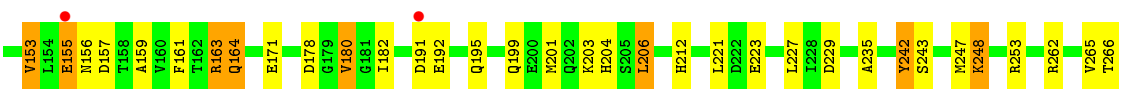
Chain G:



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

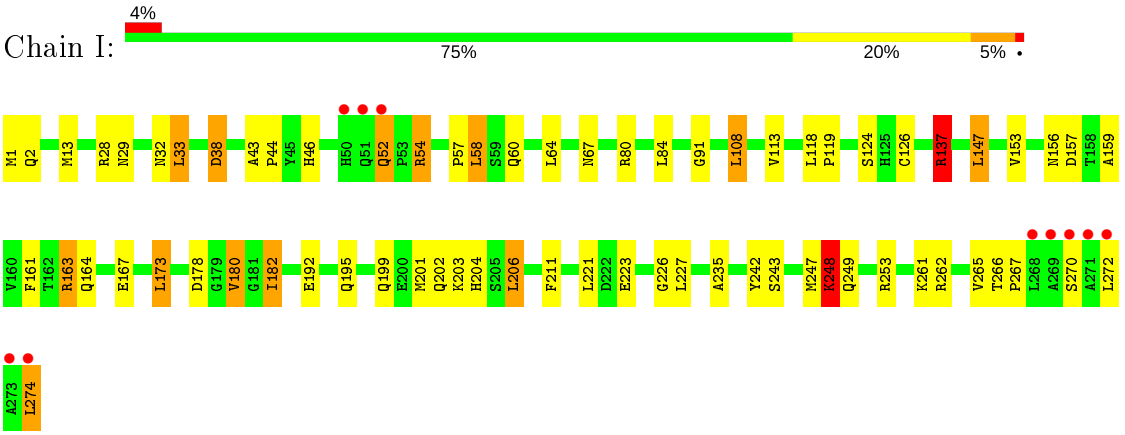
Chain H:





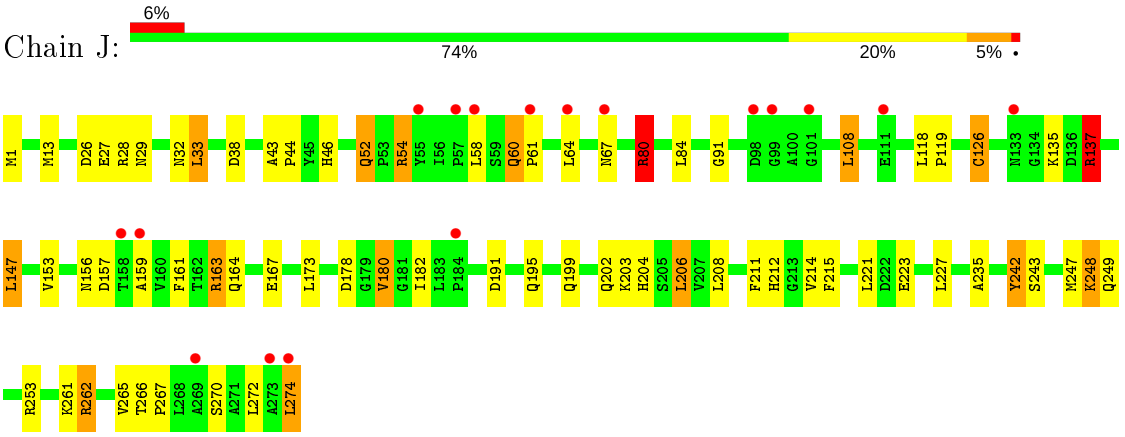
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain I:



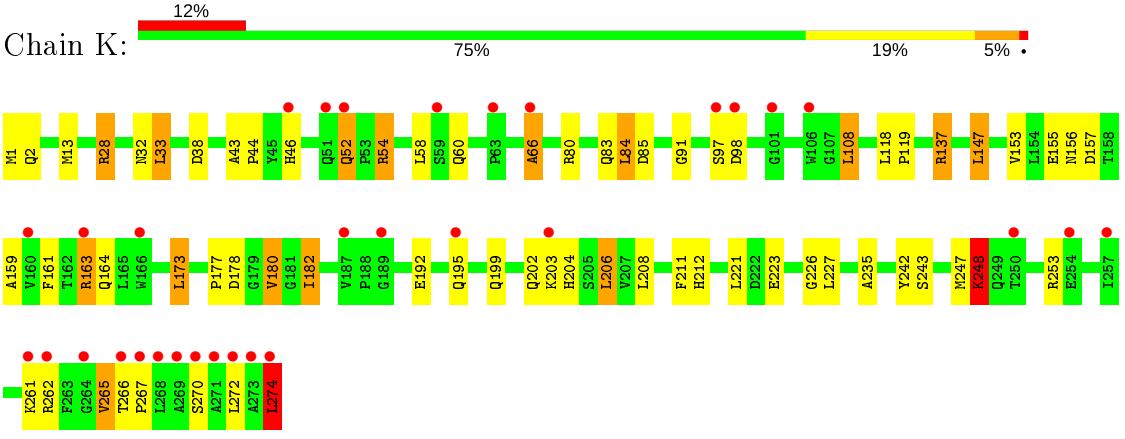
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain J:



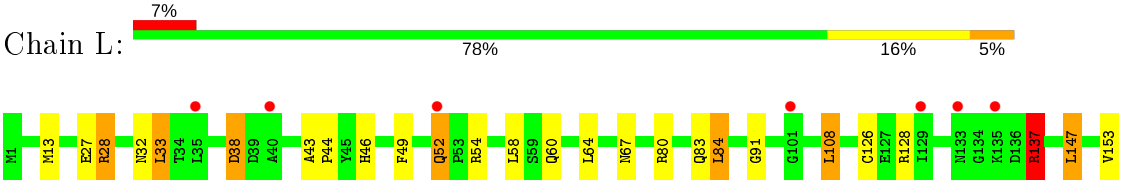
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

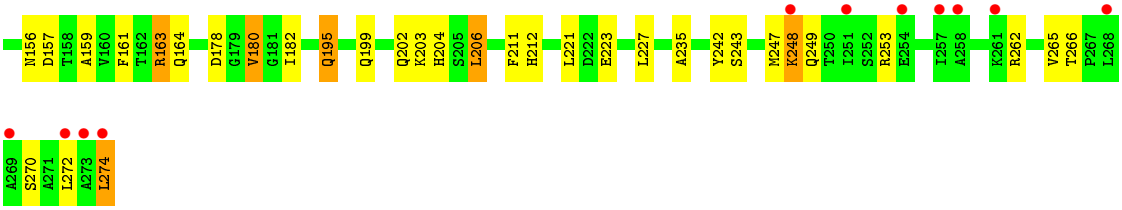
Chain K:



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

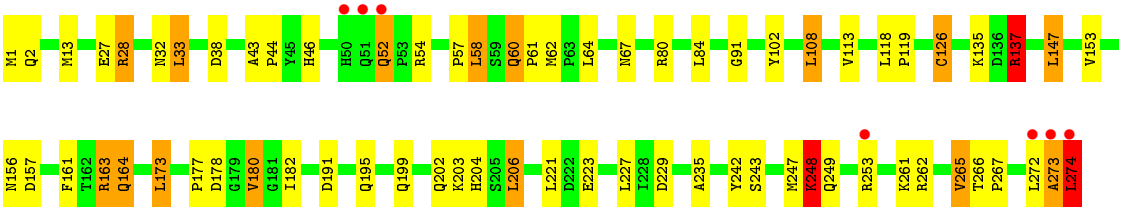
Chain L:





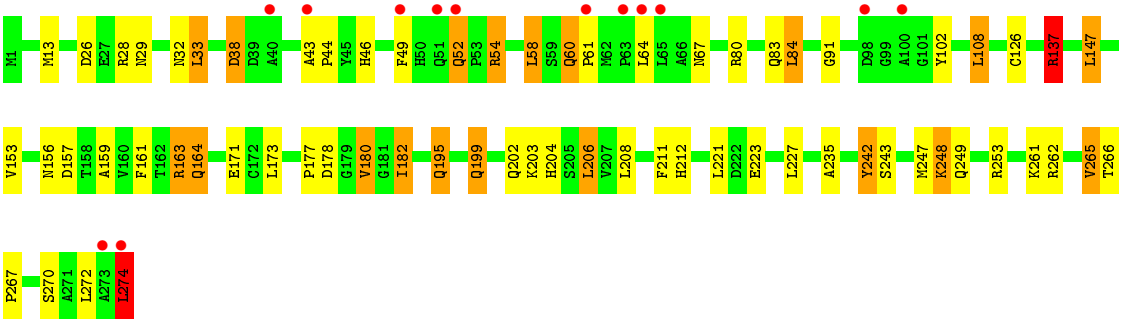
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain M:



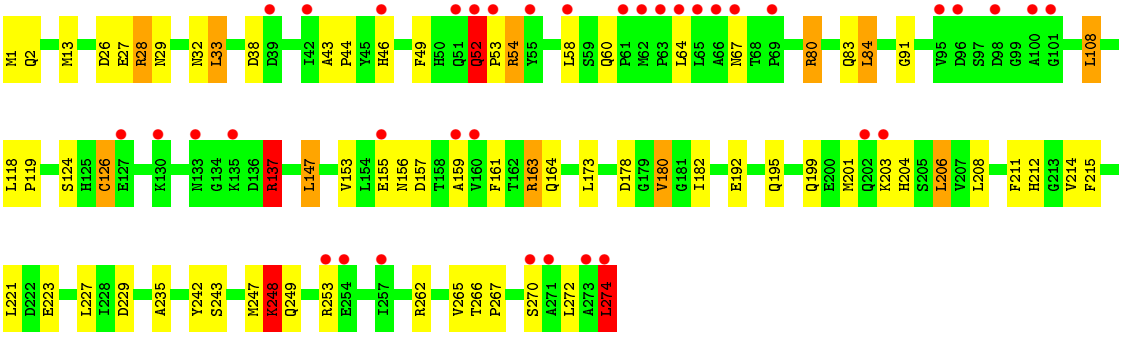
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain N:



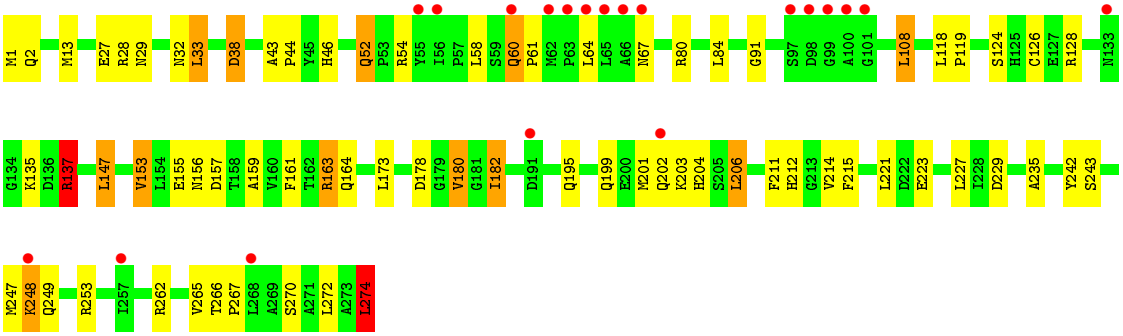
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain O:



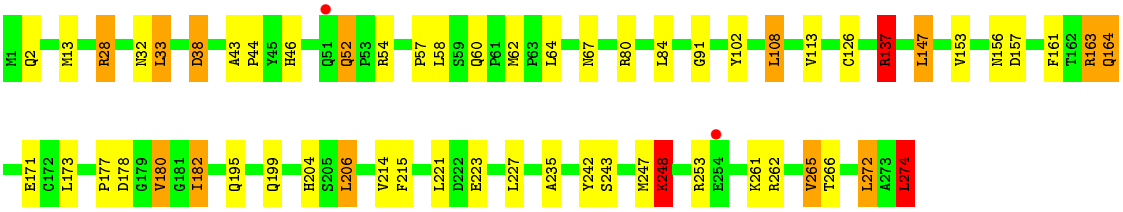
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain P:



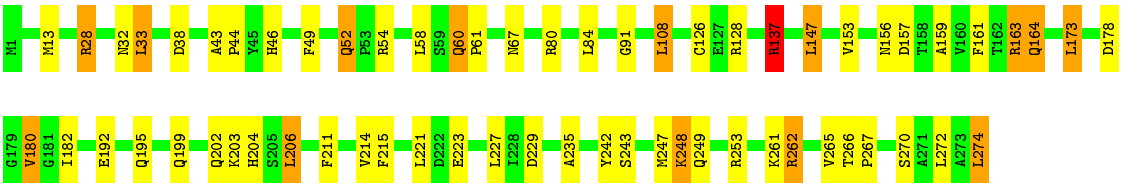
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain Q:



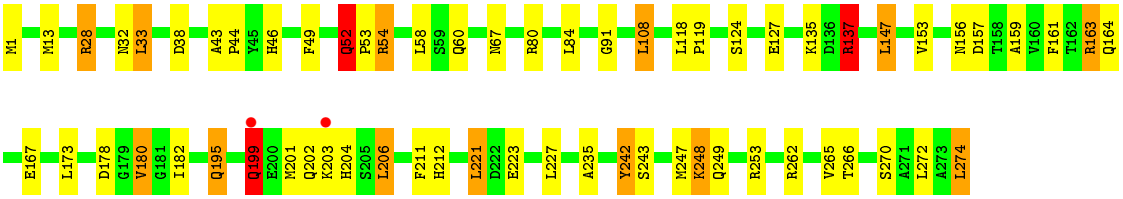
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain R:



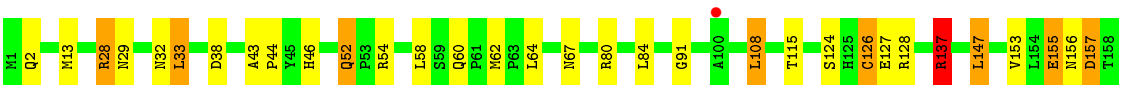
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

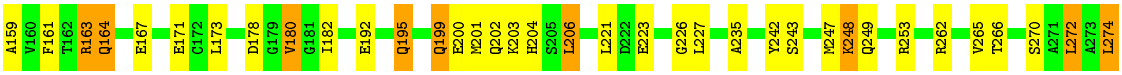
Chain S:



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain T:




A159
V160
F161
T162
R163
Q164
E167
E171
C172
L173
D178
G179
V180
G181
I182
E192
Q195
Q199
E200
M201
Q202
K203
H204
S205
L206
L221
D222
E223
G226
L227
A235
Y242
S243
M247
K248
Q249
R253
R262
V265
T266
S270
A271
L272
A273
L274

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.76Å 225.76Å 285.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.00 – 2.70 44.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.3 (44.00-2.70) 90.3 (44.28-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.235 0.219 , 0.225	Depositor DCC
R_{free} test set	1036 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	46180	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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

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	0.80	1/2178 (0.0%)	1.44	21/2966 (0.7%)
1	B	0.79	1/2178 (0.0%)	1.41	24/2966 (0.8%)
1	C	0.78	0/2178	1.47	27/2966 (0.9%)
1	D	0.81	1/2178 (0.0%)	1.47	24/2966 (0.8%)
1	E	0.77	1/2178 (0.0%)	1.37	21/2966 (0.7%)
1	F	0.76	1/2178 (0.0%)	1.40	24/2966 (0.8%)
1	G	0.76	1/2178 (0.0%)	1.40	21/2966 (0.7%)
1	H	0.82	2/2178 (0.1%)	1.46	30/2966 (1.0%)
1	I	0.81	0/2178	1.37	18/2966 (0.6%)
1	J	0.85	0/2178	1.40	21/2966 (0.7%)
1	K	0.98	1/2178 (0.0%)	1.41	20/2966 (0.7%)
1	L	0.93	0/2178	1.42	18/2966 (0.6%)
1	M	0.80	2/2178 (0.1%)	1.45	23/2966 (0.8%)
1	N	0.85	1/2178 (0.0%)	1.38	23/2966 (0.8%)
1	O	0.98	1/2178 (0.0%)	1.40	23/2966 (0.8%)
1	P	0.91	2/2178 (0.1%)	1.35	20/2966 (0.7%)
1	Q	0.81	1/2178 (0.0%)	1.43	24/2966 (0.8%)
1	R	0.78	0/2178	1.39	24/2966 (0.8%)
1	S	0.77	0/2178	1.39	23/2966 (0.8%)
1	T	0.78	0/2178	1.41	25/2966 (0.8%)
All	All	0.83	16/43560 (0.0%)	1.41	454/59320 (0.8%)

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	D	0	1
1	F	0	1
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	N	0	1
1	P	0	1
1	Q	0	1
All	All	0	7

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	274	LEU	C-OXT	10.31	1.43	1.23
1	P	274	LEU	C-OXT	10.03	1.42	1.23
1	B	274	LEU	C-OXT	9.77	1.42	1.23
1	N	274	LEU	C-OXT	9.67	1.41	1.23
1	K	274	LEU	C-OXT	9.05	1.40	1.23

The worst 5 of 454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	163	ARG	NE-CZ-NH1	20.91	130.76	120.30
1	C	163	ARG	NE-CZ-NH2	-19.36	110.62	120.30
1	D	163	ARG	NE-CZ-NH2	-18.05	111.27	120.30
1	Q	253	ARG	NE-CZ-NH1	17.83	129.22	120.30
1	M	163	ARG	NE-CZ-NH2	-16.75	111.92	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	38	ASP	Mainchain
1	F	38	ASP	Mainchain
1	I	38	ASP	Mainchain
1	L	38	ASP	Mainchain
1	N	38	ASP	Mainchain

5.2 Too-close contacts (i)

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	2124	0	2097	39	0
1	B	2124	0	2097	32	0
1	C	2124	0	2097	33	0
1	D	2124	0	2097	36	2
1	E	2124	0	2097	33	1
1	F	2124	0	2097	30	0
1	G	2124	0	2097	35	0
1	H	2124	0	2097	38	1
1	I	2124	0	2097	38	0
1	J	2124	0	2097	37	0
1	K	2124	0	2097	41	8
1	L	2124	0	2097	33	2
1	M	2124	0	2097	40	2
1	N	2124	0	2097	40	0
1	O	2124	0	2097	39	0
1	P	2124	0	2097	37	0
1	Q	2124	0	2097	30	0
1	R	2124	0	2097	32	0
1	S	2124	0	2097	33	9
1	T	2124	0	2097	44	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	10	0	3	0	0
3	B	10	0	3	0	0
3	C	10	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	3	0	0
3	E	10	0	3	0	0
3	F	10	0	3	0	0
3	G	10	0	3	0	0
3	H	10	0	3	0	0
3	I	10	0	3	0	0
3	J	10	0	3	0	0
3	K	10	0	3	0	0
3	L	10	0	3	0	0
3	M	10	0	3	0	0
3	N	10	0	3	0	0
3	O	10	0	3	0	0
3	P	10	0	3	0	0
3	Q	10	0	3	0	0
3	R	10	0	3	0	0
3	S	10	0	3	0	0
3	T	10	0	3	1	0
4	A	177	0	0	16	0
4	B	174	0	0	14	0
4	C	173	0	0	13	0
4	D	173	0	0	19	0
4	E	179	0	0	15	0
4	F	174	0	0	15	0
4	G	176	0	0	14	0
4	H	171	0	0	18	2
4	I	177	0	0	15	0
4	J	178	0	0	14	0
4	K	177	0	0	22	1
4	L	167	0	0	13	0
4	M	183	0	0	18	0
4	N	170	0	0	16	0
4	O	175	0	0	14	0
4	P	167	0	0	18	0
4	Q	176	0	0	14	0
4	R	172	0	0	15	1
4	S	171	0	0	15	0
4	T	170	0	0	25	0
All	All	46180	0	42000	707	17

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 8.

The worst 5 of 707 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:K:97:SER:CB	4:K:2077:HOH:O	1.66	1.28
1:T:157:ASP:CG	4:T:2105:HOH:O	1.83	1.16
1:K:97:SER:HB3	4:K:2077:HOH:O	1.28	1.15
1:P:163:ARG:NH2	1:P:274:LEU:OXT	1.91	1.03
1:K:163:ARG:NH2	1:K:274:LEU:OXT	1.93	1.02

The worst 5 of 17 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:K:97:SER:OG	1:S:203:LYS:CD[1_655]	1.44	0.76
1:D:274:LEU:CD1	1:M:253:ARG:NH2[5_555]	1.65	0.55
1:K:66:ALA:CB	1:S:199:GLN:NE2[1_655]	1.67	0.53
1:L:195:GLN:NE2	1:L:195:GLN:NE2[5_555]	1.75	0.45
1:K:98:ASP:N	1:S:203:LYS:NZ[1_655]	1.77	0.43

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	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	B	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
1	C	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	D	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	E	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
1	F	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	G	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
1	H	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	I	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	J	272/274 (99%)	262 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	L	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	M	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
1	N	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	O	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
1	P	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
1	Q	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	R	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
1	S	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	T	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
All	All	5440/5480 (99%)	5259 (97%)	181 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	B	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	C	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	D	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	E	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	F	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	G	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	H	228/228 (100%)	205 (90%)	23 (10%)	7	17
1	I	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	J	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	K	228/228 (100%)	203 (89%)	25 (11%)	6	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	M	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	N	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	O	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	P	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	Q	228/228 (100%)	204 (90%)	24 (10%)	7	16
1	R	228/228 (100%)	203 (89%)	25 (11%)	6	14
1	S	228/228 (100%)	202 (89%)	26 (11%)	5	13
1	T	228/228 (100%)	204 (90%)	24 (10%)	7	16
All	All	4560/4560 (100%)	4070 (89%)	490 (11%)	6	15

5 of 490 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	52	GLN
1	L	80	ARG
1	S	161	PHE
1	J	137	ARG
1	K	60	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	156	ASN
1	L	156	ASN
1	S	164	GLN
1	K	164	GLN
1	L	195	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)

Of 40 ligands modelled in this entry, 20 are monoatomic - leaving 20 for Mogul analysis.

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	$\#\|Z\| > 2$
3	PGH	K	300	2	9,9,9	3.44	5 (55%)	10,12,12	2.89	4 (40%)
3	PGH	M	300	2	9,9,9	3.82	5 (55%)	10,12,12	2.71	4 (40%)
3	PGH	P	300	2	9,9,9	3.39	5 (55%)	10,12,12	2.39	3 (30%)
3	PGH	O	300	2	9,9,9	3.88	5 (55%)	10,12,12	2.87	5 (50%)
3	PGH	R	300	2	9,9,9	3.31	5 (55%)	10,12,12	2.05	4 (40%)
3	PGH	A	300	2	9,9,9	3.07	5 (55%)	10,12,12	2.14	5 (50%)
3	PGH	T	300	2	9,9,9	3.61	7 (77%)	10,12,12	2.05	4 (40%)
3	PGH	C	300	2	9,9,9	3.33	5 (55%)	10,12,12	2.11	6 (60%)
3	PGH	E	300	2	9,9,9	3.13	4 (44%)	10,12,12	2.83	6 (60%)
3	PGH	H	300	2	9,9,9	3.49	6 (66%)	10,12,12	2.11	5 (50%)
3	PGH	G	300	2	9,9,9	3.39	6 (66%)	10,12,12	2.11	3 (30%)
3	PGH	J	300	2	9,9,9	3.65	5 (55%)	10,12,12	2.91	6 (60%)
3	PGH	L	300	2	9,9,9	4.05	5 (55%)	10,12,12	2.57	4 (40%)
3	PGH	N	300	2	9,9,9	3.19	5 (55%)	10,12,12	2.88	3 (30%)
3	PGH	B	300	2	9,9,9	3.19	5 (55%)	10,12,12	2.62	5 (50%)
3	PGH	Q	300	2	9,9,9	3.35	5 (55%)	10,12,12	2.42	4 (40%)
3	PGH	D	300	2	9,9,9	3.53	4 (44%)	10,12,12	2.38	4 (40%)
3	PGH	S	300	2	9,9,9	2.97	5 (55%)	10,12,12	2.03	3 (30%)
3	PGH	F	300	2	9,9,9	2.87	5 (55%)	10,12,12	2.49	3 (30%)
3	PGH	I	300	2	9,9,9	2.93	4 (44%)	10,12,12	2.88	3 (30%)

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
3	PGH	K	300	2	-	5/8/8/8	-
3	PGH	M	300	2	-	5/8/8/8	-
3	PGH	P	300	2	-	5/8/8/8	-
3	PGH	O	300	2	-	5/8/8/8	-
3	PGH	R	300	2	-	5/8/8/8	-
3	PGH	A	300	2	-	5/8/8/8	-
3	PGH	T	300	2	-	5/8/8/8	-
3	PGH	C	300	2	-	5/8/8/8	-
3	PGH	E	300	2	-	5/8/8/8	-
3	PGH	H	300	2	-	5/8/8/8	-
3	PGH	G	300	2	-	4/8/8/8	-
3	PGH	J	300	2	-	5/8/8/8	-
3	PGH	L	300	2	-	5/8/8/8	-
3	PGH	N	300	2	-	3/8/8/8	-
3	PGH	B	300	2	-	5/8/8/8	-
3	PGH	Q	300	2	-	3/8/8/8	-
3	PGH	D	300	2	-	5/8/8/8	-
3	PGH	S	300	2	-	5/8/8/8	-
3	PGH	F	300	2	-	5/8/8/8	-
3	PGH	I	300	2	-	5/8/8/8	-

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	300	PGH	O1P-C2	-7.77	1.37	1.43
3	O	300	PGH	O1P-C2	-7.27	1.38	1.43
3	M	300	PGH	P-O1P	7.13	1.83	1.60
3	C	300	PGH	P-O1P	7.02	1.82	1.60
3	T	300	PGH	O1P-C2	-6.64	1.38	1.43

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	300	PGH	O1-C1-N2	6.34	131.06	123.27
3	J	300	PGH	O1-C1-N2	6.32	131.03	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	300	PGH	O1-C1-N2	6.31	131.02	123.27
3	I	300	PGH	O1-C1-N2	6.12	130.78	123.27
3	K	300	PGH	O1-C1-N2	6.06	130.71	123.27

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	300	PGH	N2-C1-C2-O1P
3	J	300	PGH	C2-O1P-P-O3P
3	J	300	PGH	C2-O1P-P-O4P
3	S	300	PGH	N2-C1-C2-O1P
3	S	300	PGH	C2-O1P-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	300	PGH	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^{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	274/274 (100%)	-0.18	3 (1%) 80 82	23, 37, 60, 84	0
1	B	274/274 (100%)	-0.23	1 (0%) 92 93	23, 37, 60, 84	0
1	C	274/274 (100%)	-0.22	2 (0%) 87 89	23, 37, 60, 84	0
1	D	274/274 (100%)	-0.05	5 (1%) 68 70	23, 37, 60, 84	0
1	E	274/274 (100%)	-0.28	1 (0%) 92 93	23, 37, 60, 84	0
1	F	274/274 (100%)	-0.27	0 100 100	23, 37, 60, 84	0
1	G	274/274 (100%)	-0.19	3 (1%) 80 82	23, 37, 60, 84	0
1	H	274/274 (100%)	-0.10	3 (1%) 80 82	23, 37, 60, 84	0
1	I	274/274 (100%)	-0.05	10 (3%) 42 42	23, 37, 60, 84	0
1	J	274/274 (100%)	0.15	17 (6%) 20 19	23, 37, 60, 84	0
1	K	274/274 (100%)	0.52	32 (11%) 4 3	23, 37, 60, 84	0
1	L	274/274 (100%)	0.39	18 (6%) 18 16	23, 37, 60, 84	0
1	M	274/274 (100%)	-0.33	7 (2%) 56 57	23, 37, 60, 84	0
1	N	274/274 (100%)	0.07	13 (4%) 31 30	23, 37, 60, 84	0
1	O	274/274 (100%)	0.54	37 (13%) 3 2	23, 37, 60, 84	0
1	P	274/274 (100%)	0.26	20 (7%) 15 13	23, 37, 60, 84	0
1	Q	274/274 (100%)	-0.14	2 (0%) 87 89	23, 37, 60, 84	0
1	R	274/274 (100%)	-0.09	0 100 100	23, 37, 60, 84	0
1	S	274/274 (100%)	-0.16	2 (0%) 87 89	23, 37, 60, 84	0
1	T	274/274 (100%)	-0.17	1 (0%) 92 93	23, 37, 60, 84	0
All	All	5480/5480 (100%)	-0.03	177 (3%) 47 48	23, 37, 60, 84	0

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	GLN	5.5
1	I	51	GLN	5.5
1	O	274	LEU	5.5
1	Q	51	GLN	4.8
1	M	274	LEU	4.8

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	PGH	L	300	10/10	0.94	0.16	50,52,53,54	0
3	PGH	K	300	10/10	0.95	0.14	50,52,53,54	0
3	PGH	O	300	10/10	0.95	0.15	50,52,53,54	0
3	PGH	I	300	10/10	0.96	0.14	50,52,53,54	0
3	PGH	N	300	10/10	0.96	0.13	50,52,53,54	0
3	PGH	M	300	10/10	0.96	0.13	50,52,53,54	0
3	PGH	P	300	10/10	0.96	0.14	50,52,53,54	0
3	PGH	J	300	10/10	0.96	0.13	50,52,53,54	0
3	PGH	E	300	10/10	0.96	0.16	50,52,53,54	0
2	ZN	K	275	1/1	0.96	0.04	35,35,35,35	0
2	ZN	O	275	1/1	0.97	0.03	35,35,35,35	0
3	PGH	T	300	10/10	0.97	0.17	50,52,53,54	0
3	PGH	C	300	10/10	0.97	0.20	50,52,53,54	0
3	PGH	G	300	10/10	0.97	0.17	50,52,53,54	0
3	PGH	F	300	10/10	0.97	0.16	50,52,53,54	0
3	PGH	Q	300	10/10	0.97	0.17	50,52,53,54	0
3	PGH	S	300	10/10	0.98	0.16	50,52,53,54	0
2	ZN	S	275	1/1	0.98	0.11	33,33,33,33	0
3	PGH	A	300	10/10	0.98	0.18	50,52,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	N	275	1/1	0.98	0.03	35,35,35,35	0
3	PGH	H	300	10/10	0.98	0.16	50,52,53,54	0
3	PGH	B	300	10/10	0.98	0.15	50,52,53,54	0
3	PGH	D	300	10/10	0.98	0.18	50,52,53,54	0
2	ZN	J	275	1/1	0.98	0.03	35,35,35,35	0
2	ZN	D	275	1/1	0.99	0.14	32,32,32,32	0
2	ZN	I	275	1/1	0.99	0.04	34,34,34,34	0
2	ZN	P	275	1/1	0.99	0.05	34,34,34,34	0
2	ZN	M	275	1/1	0.99	0.04	33,33,33,33	0
2	ZN	T	275	1/1	0.99	0.14	33,33,33,33	0
3	PGH	R	300	10/10	0.99	0.16	50,52,53,54	0
2	ZN	H	275	1/1	0.99	0.13	32,32,32,32	0
2	ZN	F	275	1/1	0.99	0.13	34,34,34,34	0
2	ZN	L	275	1/1	0.99	0.04	35,35,35,35	0
2	ZN	C	275	1/1	0.99	0.17	32,32,32,32	0
2	ZN	G	275	1/1	0.99	0.08	34,34,34,34	0
2	ZN	E	275	1/1	0.99	0.11	32,32,32,32	0
2	ZN	Q	275	1/1	1.00	0.14	32,32,32,32	0
2	ZN	A	275	1/1	1.00	0.16	32,32,32,32	0
2	ZN	R	275	1/1	1.00	0.13	32,32,32,32	0
2	ZN	B	275	1/1	1.00	0.12	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.