



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:56 PM GMT

PDB ID : 4F7W
Title : Crystal structure of Klebsiella pneumoniae pantothenate kinase in complex with N-pentylpantothenamide
Authors : Li, B.; Tempel, W.; Smil, D.; Bolshan, Y.; Hong, B.S.; Park, H.W.; Structural Genomics Consortium (SGC)
Deposited on : 2012-05-16
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

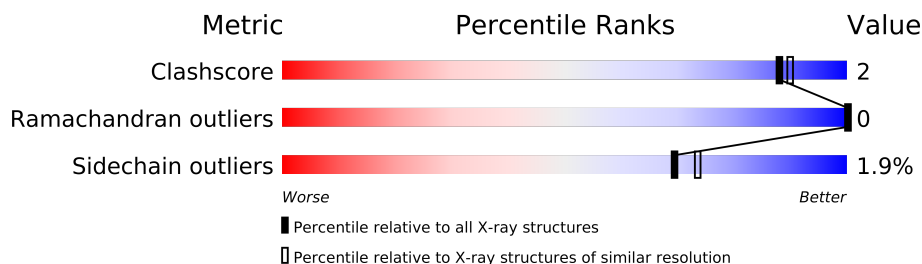
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	334	
1	B	334	
1	C	334	
1	D	334	
1	E	334	
1	F	334	
1	G	334	
1	H	334	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21299 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2499	1600	431	461	7			
1	C	309	Total	C	N	O	S	0	1	0
			2502	1602	431	462	7			
1	B	309	Total	C	N	O	S	0	0	0
			2499	1600	431	461	7			
1	D	308	Total	C	N	O	S	0	1	0
			2494	1596	430	461	7			
1	E	304	Total	C	N	O	S	0	0	0
			2463	1578	426	453	6			
1	F	309	Total	C	N	O	S	0	1	0
			2507	1604	433	463	7			
1	G	308	Total	C	N	O	S	0	1	0
			2494	1596	430	461	7			
1	H	303	Total	C	N	O	S	0	2	0
			2458	1576	422	454	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	EXPRESSION TAG	UNP B5XYG3
A	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
A	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
A	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
A	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
A	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
A	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
A	990	SER	-	EXPRESSION TAG	UNP B5XYG3
A	991	SER	-	EXPRESSION TAG	UNP B5XYG3
A	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
A	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
A	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
A	995	ASN	-	EXPRESSION TAG	UNP B5XYG3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
A	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
A	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
A	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
A	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
C	983	MET	-	EXPRESSION TAG	UNP B5XYG3
C	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
C	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
C	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
C	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
C	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
C	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
C	990	SER	-	EXPRESSION TAG	UNP B5XYG3
C	991	SER	-	EXPRESSION TAG	UNP B5XYG3
C	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
C	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
C	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
C	995	ASN	-	EXPRESSION TAG	UNP B5XYG3
C	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
C	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
C	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
C	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
C	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
B	983	MET	-	EXPRESSION TAG	UNP B5XYG3
B	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
B	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
B	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
B	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
B	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
B	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
B	990	SER	-	EXPRESSION TAG	UNP B5XYG3
B	991	SER	-	EXPRESSION TAG	UNP B5XYG3
B	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
B	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
B	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
B	995	ASN	-	EXPRESSION TAG	UNP B5XYG3
B	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
B	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
B	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
B	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
B	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
D	983	MET	-	EXPRESSION TAG	UNP B5XYG3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
D	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
D	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
D	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
D	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
D	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
D	990	SER	-	EXPRESSION TAG	UNP B5XYG3
D	991	SER	-	EXPRESSION TAG	UNP B5XYG3
D	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
D	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
D	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
D	995	ASN	-	EXPRESSION TAG	UNP B5XYG3
D	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
D	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
D	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
D	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
D	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
E	983	MET	-	EXPRESSION TAG	UNP B5XYG3
E	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
E	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
E	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
E	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
E	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
E	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
E	990	SER	-	EXPRESSION TAG	UNP B5XYG3
E	991	SER	-	EXPRESSION TAG	UNP B5XYG3
E	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
E	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
E	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
E	995	ASN	-	EXPRESSION TAG	UNP B5XYG3
E	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
E	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
E	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
E	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
E	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
F	983	MET	-	EXPRESSION TAG	UNP B5XYG3
F	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
F	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
F	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
F	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
F	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
F	989	HIS	-	EXPRESSION TAG	UNP B5XYG3

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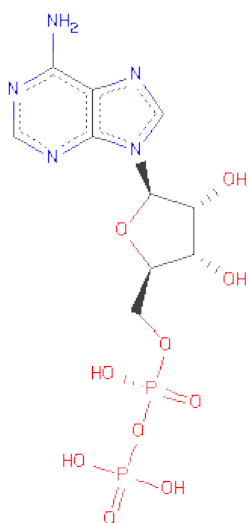
Chain	Residue	Modelled	Actual	Comment	Reference
F	990	SER	-	EXPRESSION TAG	UNP B5XYG3
F	991	SER	-	EXPRESSION TAG	UNP B5XYG3
F	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
F	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
F	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
F	995	ASN	-	EXPRESSION TAG	UNP B5XYG3
F	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
F	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
F	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
F	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
F	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
G	983	MET	-	EXPRESSION TAG	UNP B5XYG3
G	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
G	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
G	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
G	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
G	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
G	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
G	990	SER	-	EXPRESSION TAG	UNP B5XYG3
G	991	SER	-	EXPRESSION TAG	UNP B5XYG3
G	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
G	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
G	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
G	995	ASN	-	EXPRESSION TAG	UNP B5XYG3
G	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
G	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
G	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
G	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
G	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3
H	983	MET	-	EXPRESSION TAG	UNP B5XYG3
H	984	HIS	-	EXPRESSION TAG	UNP B5XYG3
H	985	HIS	-	EXPRESSION TAG	UNP B5XYG3
H	986	HIS	-	EXPRESSION TAG	UNP B5XYG3
H	987	HIS	-	EXPRESSION TAG	UNP B5XYG3
H	988	HIS	-	EXPRESSION TAG	UNP B5XYG3
H	989	HIS	-	EXPRESSION TAG	UNP B5XYG3
H	990	SER	-	EXPRESSION TAG	UNP B5XYG3
H	991	SER	-	EXPRESSION TAG	UNP B5XYG3
H	992	GLY	-	EXPRESSION TAG	UNP B5XYG3
H	993	ARG	-	EXPRESSION TAG	UNP B5XYG3
H	994	GLU	-	EXPRESSION TAG	UNP B5XYG3
H	995	ASN	-	EXPRESSION TAG	UNP B5XYG3

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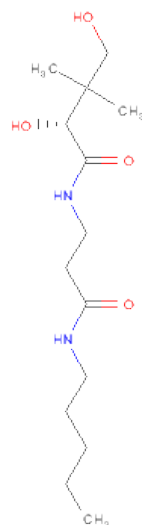
Chain	Residue	Modelled	Actual	Comment	Reference
H	996	LEU	-	EXPRESSION TAG	UNP B5XYG3
H	997	TYR	-	EXPRESSION TAG	UNP B5XYG3
H	998	PHE	-	EXPRESSION TAG	UNP B5XYG3
H	999	GLN	-	EXPRESSION TAG	UNP B5XYG3
H	1000	GLY	-	EXPRESSION TAG	UNP B5XYG3

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is (2R)-2,4-DIHYDROXY-3,3-DIMETHYL-N-[3-OXO-3-(PENTYLAMINO)PROPYL]BUTANAMIDE (three-letter code: PN4) (formula: C₁₄H₂₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	14	2	4		
3	C	1	Total	C	N	O	0	0
			20	14	2	4		
3	B	1	Total	C	N	O	0	0
			20	14	2	4		
3	D	1	Total	C	N	O	0	0
			20	14	2	4		
3	E	1	Total	C	N	O	0	0
			20	14	2	4		
3	F	1	Total	C	N	O	0	0
			20	14	2	4		
3	G	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	6	Total	X	0	0
			6	6		
4	D	8	Total	X	0	0
			8	8		
4	H	4	Total	X	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total 7	X 7	0	0
4	C	7	Total 7	X 7	0	0
4	A	1	Total 1	X 1	0	0
4	F	7	Total 7	X 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total 131	O 131	0	0
5	C	146	Total 146	O 146	0	0
5	B	126	Total 126	O 126	0	0
5	D	140	Total 140	O 140	0	0
5	E	83	Total 83	O 83	0	0
5	F	128	Total 128	O 128	0	0
5	G	130	Total 130	O 130	0	0
5	H	103	Total 103	O 103	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.

Note EDS failed to run properly.

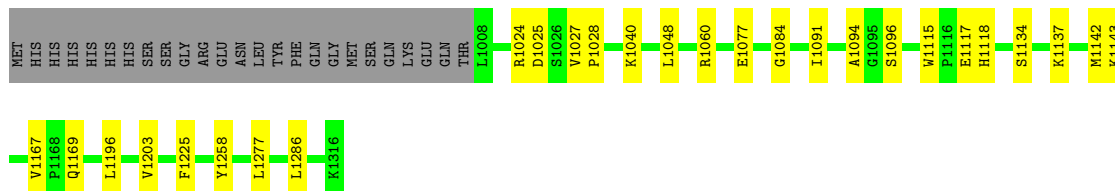
- Molecule 1: Pantothenate kinase

Chain A: 



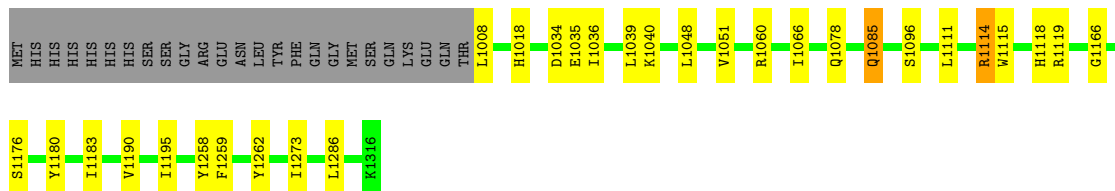
- Molecule 1: Pantothenate kinase

Chain C: 



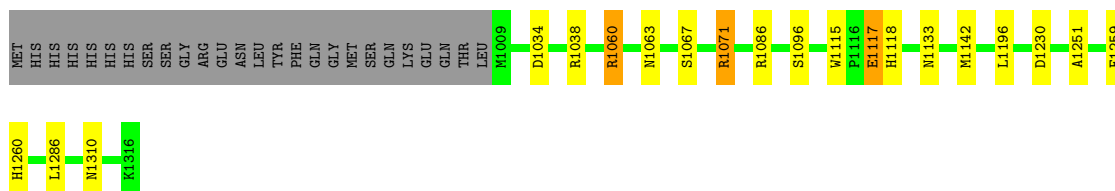
- Molecule 1: Pantothenate kinase

Chain B: 



- Molecule 1: Pantothenate kinase

Chain D: 



- Molecule 1: Pantothenate kinase

	F1244	MET
	L1245	HIS
	K1246	HIS
	F1247	HIS
	R1248	HIS
	K1264	HIS
	D1272	SER
	S1276	ARG
	K1316	GLU
		ASN
		LEU
		PHE
		GLN
		GLY
		MET
		SER
		GLN
		LYS
		GLI
		GLN
		THR
		L1008
		R1024
		ASP
		SER
		VAL
		PRO
		MET
		T1030
		T1037
		I1066
		Q1085
		R1086
		H1120
		G1166
		V1167
		T1171
		D1187
		P1193
		D1194
		I1195
		D1230
		E1233
		V1240

- Chain F:

S1304		MET
	N1310	HIS
		HIS
	K1316	HIS
		HIS
		HIS
		SER
		SER
		GLY
		ARG
		GLU
		ASN
		LEU
		TYR
		PHE
		GLN
		GLY
		MET
		SER
		GLN
		LYS
		GLU
		GLN
		THR
		L1008
		R1024
		T1030
		S1047
		R1060
		R1071
		A1094
		G1095
		S1096
		W1115
		H1118
		T1125
		V1203
		P1232
		L1235
		Y1288
		F1289
		L1286
		M1301

- Chain G: 

● Molecule 1: Pantothenate kinase

Chain H:

Chain H:

L1196	MET
L1236	HIS
L1281	HIS
L1286	HIS
R1296	SER
Q1311	ARG
R1316	GLY
	GLU
	ASN
	LEU
	TYR
	PHE
	GLN
	GLY
	MET
	SER
	LYS
	GLU
	GLN
	THR
	L1008
	Q1014
	W1020
	L1023
	ARG
	ASP
	SER
	VAL
	PRO
	MET
	T1030
	L1031
	T1032
	S1047
	T1082
	Q1085
	S1096
	W1115
	H1118
	K1143
	T1171
	D1187

4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.84Å 130.82Å 192.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 2.10	Depositor
% Data completeness (in resolution range)	99.9 (39.65-2.10)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.185 , 0.226	Depositor
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.017	Xtriage
Estimated twinning fraction	0.090 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 187327 reflections (0.001%)	Xtriage
Total number of atoms	21299	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, PN4, ADP

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	0.62	0/2558	0.67	0/3471
1	B	0.63	0/2558	0.68	0/3471
1	C	0.67	1/2564 (0.0%)	0.70	0/3479
1	D	0.67	1/2556 (0.0%)	0.71	3/3468 (0.1%)
1	E	0.61	0/2520	0.66	1/3417 (0.0%)
1	F	0.65	0/2566	0.71	2/3482 (0.1%)
1	G	0.64	0/2556	0.71	1/3468 (0.0%)
1	H	0.63	0/2521	0.68	1/3419 (0.0%)
All	All	0.64	2/20399 (0.0%)	0.69	8/27675 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1117	GLU	CD-OE1	6.08	1.32	1.25
1	C	1117	GLU	CD-OE1	5.79	1.32	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1296	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	1230	ASP	CB-CG-OD1	5.61	123.35	118.30
1	E	1230	ASP	CB-CG-OD1	5.50	123.25	118.30
1	F	1301	MET	CA-CB-CG	5.47	122.59	113.30
1	D	1071	ARG	NE-CZ-NH1	5.41	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2499	0	2501	13	0
1	B	2499	0	2501	21	0
1	C	2502	0	2506	14	0
1	D	2494	0	2493	12	0
1	E	2463	0	2466	10	0
1	F	2507	0	2506	10	0
1	G	2494	0	2495	8	0
1	H	2458	0	2462	10	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
3	A	20	0	28	5	0
3	B	20	0	28	7	0
3	C	20	0	27	3	0
3	D	20	0	28	0	0
3	E	20	0	28	4	0
3	F	20	0	28	3	0
3	G	20	0	28	0	0
4	A	1	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	8	0	0	0	0
4	F	7	0	0	0	0
4	G	6	0	0	0	0
4	H	4	0	0	0	0
5	A	131	0	0	2	0
5	B	126	0	0	0	0
5	C	146	0	0	0	0
5	D	140	0	0	1	0
5	E	83	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	128	0	0	2	0
5	G	130	0	0	1	0
5	H	103	0	0	0	0
All	All	21299	0	20221	96	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 96 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1258:TYR:CE1	3:A:1402:PN4:HAA	1.80	1.17
1:C:1258:TYR:HD2	3:C:1402:PN4:HAA	1.18	1.08
1:A:1258:TYR:HE1	3:A:1402:PN4:HAA	1.15	0.99
1:C:1258:TYR:CD2	3:C:1402:PN4:HAA	2.11	0.83
1:D:1133:ASN:HA	1:D:1142:MET:HE1	1.64	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	307/334 (92%)	300 (98%)	7 (2%)	0	100	100
1	B	307/334 (92%)	302 (98%)	5 (2%)	0	100	100
1	C	308/334 (92%)	300 (97%)	8 (3%)	0	100	100
1	D	307/334 (92%)	299 (97%)	8 (3%)	0	100	100
1	E	300/334 (90%)	294 (98%)	6 (2%)	0	100	100
1	F	308/334 (92%)	304 (99%)	4 (1%)	0	100	100
1	G	307/334 (92%)	300 (98%)	7 (2%)	0	100	100
1	H	301/334 (90%)	289 (96%)	12 (4%)	0	100	100
All	All	2445/2672 (92%)	2388 (98%)	57 (2%)	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	278/301 (92%)	276 (99%)	2 (1%)	91	94
1	B	278/301 (92%)	270 (97%)	8 (3%)	55	57
1	C	279/301 (93%)	275 (99%)	4 (1%)	78	83
1	D	278/301 (92%)	271 (98%)	7 (2%)	60	63
1	E	273/301 (91%)	265 (97%)	8 (3%)	55	57
1	F	279/301 (93%)	276 (99%)	3 (1%)	84	88
1	G	278/301 (92%)	273 (98%)	5 (2%)	71	75
1	H	274/301 (91%)	269 (98%)	5 (2%)	71	75
All	All	2217/2408 (92%)	2175 (98%)	42 (2%)	69	73

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1196	LEU
1	E	1086	ARG
1	H	1032	THR
1	D	1259	PHE
1	E	1037	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1205	GLN
1	E	1019	GLN
1	H	1063	ASN
1	D	1310	ASN
1	F	1014	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 55 ligands modelled in this entry, 40 are unknown - leaving 15 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$
2	ADP	A	1401	-	29,29,29	1.29	3 (10%)	45,45,45	1.84	6 (13%)
3	PN4	A	1402	-	19,19,19	0.70	0	24,24,24	0.78	0
2	ADP	B	1401	-	29,29,29	1.18	2 (6%)	45,45,45	1.82	7 (15%)
3	PN4	B	1402	-	19,19,19	0.99	1 (5%)	24,24,24	1.03	2 (8%)
2	ADP	C	1401	-	29,29,29	1.25	2 (6%)	45,45,45	1.71	6 (13%)
3	PN4	C	1402	-	19,19,19	1.12	2 (10%)	24,24,24	0.88	1 (4%)
2	ADP	D	1401	-	29,29,29	1.18	2 (6%)	45,45,45	1.61	5 (11%)
3	PN4	D	1402	-	19,19,19	1.37	2 (10%)	24,24,24	1.00	2 (8%)
2	ADP	E	1401	-	29,29,29	1.24	3 (10%)	45,45,45	1.84	10 (22%)
3	PN4	E	1402	-	19,19,19	0.57	0	24,24,24	0.89	1 (4%)
2	ADP	F	1401	-	29,29,29	1.25	3 (10%)	45,45,45	1.62	7 (15%)
3	PN4	F	1402	-	19,19,19	0.96	1 (5%)	24,24,24	1.02	1 (4%)
2	ADP	G	1401	-	29,29,29	1.45	4 (13%)	45,45,45	1.76	9 (20%)
3	PN4	G	1402	-	19,19,19	1.31	2 (10%)	24,24,24	1.33	2 (8%)
2	ADP	H	1401	-	29,29,29	1.35	4 (13%)	45,45,45	1.82	10 (22%)

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	ADP	A	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	A	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	B	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	B	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	C	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	C	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	D	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	D	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	E	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	E	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	F	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	F	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	G	1401	-	-	0/16/32/32	0/1/3/3
3	PN4	G	1402	-	-	0/25/25/25	0/0/0/0
2	ADP	H	1401	-	-	0/16/32/32	0/1/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1401	ADP	C4-N9	-4.04	1.31	1.37
2	C	1401	ADP	C4-N9	-3.99	1.31	1.37
2	G	1401	ADP	C4-N9	-3.90	1.32	1.37
3	D	1402	PN4	CAW-CAV	3.79	1.59	1.55
2	G	1401	ADP	O4'-C1'	3.73	1.47	1.41

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	ADP	N3-C2-N1	-7.35	122.56	128.71
2	H	1401	ADP	N3-C2-N1	-6.95	122.90	128.71
2	A	1401	ADP	N3-C2-N1	-6.94	122.91	128.71
2	G	1401	ADP	N3-C2-N1	-6.90	122.94	128.71
2	E	1401	ADP	N3-C2-N1	-6.75	123.07	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.