



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:20 PM UTC

PDB ID : 9FRT / pdb_00009frt
Title : Crystal structure of trans-o-hydroxybenzylidenepyruvate hydratase-aldolase from *Pseudomonas fluorescens* N3
Authors : Milani, M.
Deposited on : 2024-06-19
Resolution : 1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

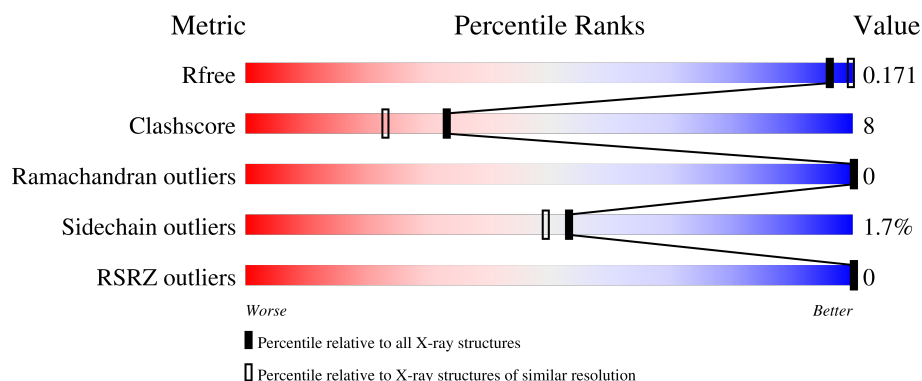
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	346	
1	B	346	
1	C	346	
1	D	346	
1	G	346	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	346	 82% 12% • 5%
1	J	346	 78% 14% • 6%
1	K	346	 81% 13% 6%

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	GOL	A	401	-	-	X	-
2	GOL	C	401	-	-	X	-
3	PO4	B	402	-	X	-	-
3	PO4	C	403	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23793 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 Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	3	0
			2559	1628	435	481	15			
1	B	326	Total	C	N	O	S	0	3	0
			2547	1621	432	479	15			
1	C	327	Total	C	N	O	S	0	7	0
			2575	1643	432	483	17			
1	D	326	Total	C	N	O	S	0	3	0
			2545	1620	431	479	15			
1	G	326	Total	C	N	O	S	0	6	0
			2566	1633	435	482	16			
1	H	327	Total	C	N	O	S	0	1	0
			2543	1616	432	480	15			
1	J	325	Total	C	N	O	S	0	5	0
			2547	1626	430	476	15			
1	K	326	Total	C	N	O	S	0	8	0
			2579	1645	438	480	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP C3KFM9
A	-10	ARG	-	expression tag	UNP C3KFM9
A	-9	GLY	-	expression tag	UNP C3KFM9
A	-8	SER	-	expression tag	UNP C3KFM9
A	-7	HIS	-	expression tag	UNP C3KFM9
A	-6	HIS	-	expression tag	UNP C3KFM9
A	-5	HIS	-	expression tag	UNP C3KFM9
A	-4	HIS	-	expression tag	UNP C3KFM9
A	-3	HIS	-	expression tag	UNP C3KFM9
A	-2	HIS	-	expression tag	UNP C3KFM9
A	-1	GLY	-	expression tag	UNP C3KFM9
A	0	SER	-	expression tag	UNP C3KFM9
B	-11	MET	-	initiating methionine	UNP C3KFM9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	expression tag	UNP C3KFM9
B	-9	GLY	-	expression tag	UNP C3KFM9
B	-8	SER	-	expression tag	UNP C3KFM9
B	-7	HIS	-	expression tag	UNP C3KFM9
B	-6	HIS	-	expression tag	UNP C3KFM9
B	-5	HIS	-	expression tag	UNP C3KFM9
B	-4	HIS	-	expression tag	UNP C3KFM9
B	-3	HIS	-	expression tag	UNP C3KFM9
B	-2	HIS	-	expression tag	UNP C3KFM9
B	-1	GLY	-	expression tag	UNP C3KFM9
B	0	SER	-	expression tag	UNP C3KFM9
C	-11	MET	-	initiating methionine	UNP C3KFM9
C	-10	ARG	-	expression tag	UNP C3KFM9
C	-9	GLY	-	expression tag	UNP C3KFM9
C	-8	SER	-	expression tag	UNP C3KFM9
C	-7	HIS	-	expression tag	UNP C3KFM9
C	-6	HIS	-	expression tag	UNP C3KFM9
C	-5	HIS	-	expression tag	UNP C3KFM9
C	-4	HIS	-	expression tag	UNP C3KFM9
C	-3	HIS	-	expression tag	UNP C3KFM9
C	-2	HIS	-	expression tag	UNP C3KFM9
C	-1	GLY	-	expression tag	UNP C3KFM9
C	0	SER	-	expression tag	UNP C3KFM9
D	-11	MET	-	initiating methionine	UNP C3KFM9
D	-10	ARG	-	expression tag	UNP C3KFM9
D	-9	GLY	-	expression tag	UNP C3KFM9
D	-8	SER	-	expression tag	UNP C3KFM9
D	-7	HIS	-	expression tag	UNP C3KFM9
D	-6	HIS	-	expression tag	UNP C3KFM9
D	-5	HIS	-	expression tag	UNP C3KFM9
D	-4	HIS	-	expression tag	UNP C3KFM9
D	-3	HIS	-	expression tag	UNP C3KFM9
D	-2	HIS	-	expression tag	UNP C3KFM9
D	-1	GLY	-	expression tag	UNP C3KFM9
D	0	SER	-	expression tag	UNP C3KFM9
G	-11	MET	-	initiating methionine	UNP C3KFM9
G	-10	ARG	-	expression tag	UNP C3KFM9
G	-9	GLY	-	expression tag	UNP C3KFM9
G	-8	SER	-	expression tag	UNP C3KFM9
G	-7	HIS	-	expression tag	UNP C3KFM9
G	-6	HIS	-	expression tag	UNP C3KFM9
G	-5	HIS	-	expression tag	UNP C3KFM9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	expression tag	UNP C3KFM9
G	-3	HIS	-	expression tag	UNP C3KFM9
G	-2	HIS	-	expression tag	UNP C3KFM9
G	-1	GLY	-	expression tag	UNP C3KFM9
G	0	SER	-	expression tag	UNP C3KFM9
H	-11	MET	-	initiating methionine	UNP C3KFM9
H	-10	ARG	-	expression tag	UNP C3KFM9
H	-9	GLY	-	expression tag	UNP C3KFM9
H	-8	SER	-	expression tag	UNP C3KFM9
H	-7	HIS	-	expression tag	UNP C3KFM9
H	-6	HIS	-	expression tag	UNP C3KFM9
H	-5	HIS	-	expression tag	UNP C3KFM9
H	-4	HIS	-	expression tag	UNP C3KFM9
H	-3	HIS	-	expression tag	UNP C3KFM9
H	-2	HIS	-	expression tag	UNP C3KFM9
H	-1	GLY	-	expression tag	UNP C3KFM9
H	0	SER	-	expression tag	UNP C3KFM9
J	-11	MET	-	initiating methionine	UNP C3KFM9
J	-10	ARG	-	expression tag	UNP C3KFM9
J	-9	GLY	-	expression tag	UNP C3KFM9
J	-8	SER	-	expression tag	UNP C3KFM9
J	-7	HIS	-	expression tag	UNP C3KFM9
J	-6	HIS	-	expression tag	UNP C3KFM9
J	-5	HIS	-	expression tag	UNP C3KFM9
J	-4	HIS	-	expression tag	UNP C3KFM9
J	-3	HIS	-	expression tag	UNP C3KFM9
J	-2	HIS	-	expression tag	UNP C3KFM9
J	-1	GLY	-	expression tag	UNP C3KFM9
J	0	SER	-	expression tag	UNP C3KFM9
K	-11	MET	-	initiating methionine	UNP C3KFM9
K	-10	ARG	-	expression tag	UNP C3KFM9
K	-9	GLY	-	expression tag	UNP C3KFM9
K	-8	SER	-	expression tag	UNP C3KFM9
K	-7	HIS	-	expression tag	UNP C3KFM9
K	-6	HIS	-	expression tag	UNP C3KFM9
K	-5	HIS	-	expression tag	UNP C3KFM9
K	-4	HIS	-	expression tag	UNP C3KFM9
K	-3	HIS	-	expression tag	UNP C3KFM9
K	-2	HIS	-	expression tag	UNP C3KFM9
K	-1	GLY	-	expression tag	UNP C3KFM9
K	0	SER	-	expression tag	UNP C3KFM9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		

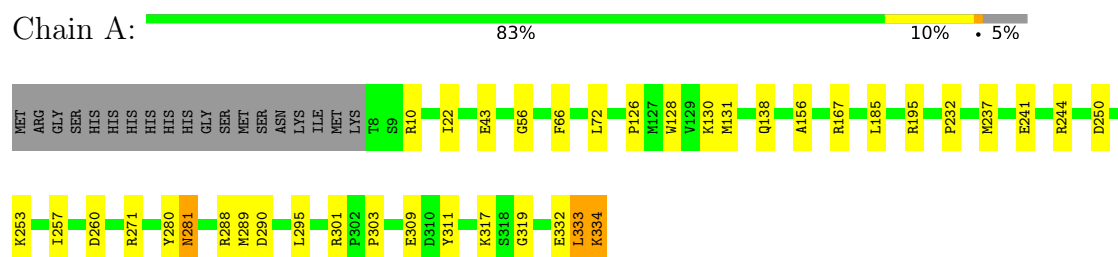
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	390	Total	O	0	5
			395	395		
4	B	389	Total	O	0	2
			391	391		
4	C	412	Total	O	0	2
			414	414		
4	D	415	Total	O	0	4
			419	419		
4	G	369	Total	O	0	1
			370	370		
4	H	384	Total	O	0	0
			384	384		
4	J	422	Total	O	0	3
			425	425		
4	K	399	Total	O	0	7
			406	406		

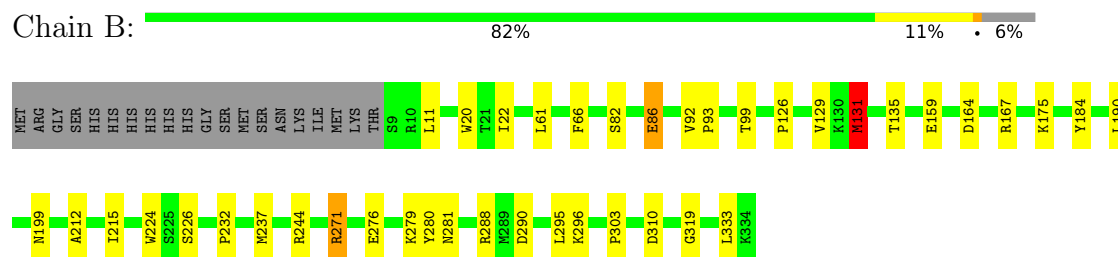
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

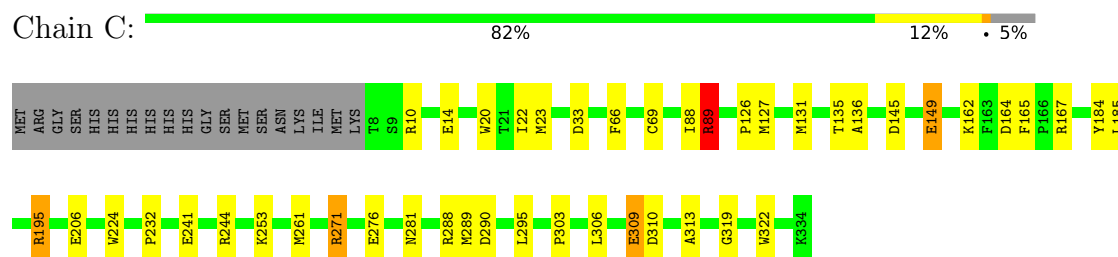
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase



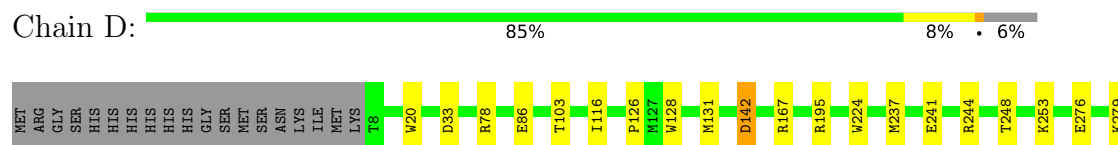
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase



- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase



- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase





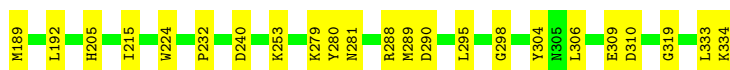
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain G: 81% 12% • 6%



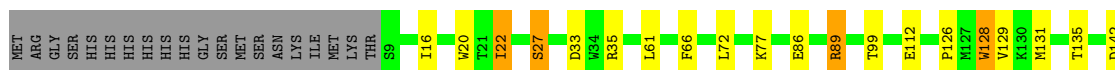
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain H: 82% 12% • 5%



- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain J: 78% 14% • 6%



- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain K: 81% 13% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.70Å 199.89Å 144.15Å 90.00° 133.79° 90.00°	Depositor
Resolution (Å)	36.04 – 1.96 36.04 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.7 (36.04-1.96) 94.8 (36.04-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.139 , 0.168 0.151 , 0.171	Depositor DCC
R_{free} test set	13680 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-h-2*1,1/2*h-1/2*k 0.000 for -h,h+2*1,1/2*h+1/2*k 0.000 for -h-2*1,k,h+1 0.319 for k,h,-1/2*h-1/2*k-l 0.358 for -k,-h,-1/2*h+1/2*k-l 0.000 for -k,h+2*1,-1/2*h+1/2*k 0.000 for -h-2*1,-h,1/2*h+1/2*k+1 0.000 for -h-2*1,h,1/2*h-1/2*k+1 0.000 for k,-h-2*1,-1/2*h-1/2*k 0.000 for -h-2*1,-k,l 0.278 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.503 for H, K, L 0.043 for H, -K, -H-L 0.334 for -K, -H, -1/2H+1/2K-L 0.120 for K, H, -1/2H-1/2K-L	Depositor
Outliers	0 of 277445 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23793	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

¹Intensities estimated from amplitudes.

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

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1185e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL

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	0.77	0/2630	1.10	6/3577 (0.2%)
1	B	0.74	0/2618	1.11	10/3561 (0.3%)
1	C	0.74	0/2658	1.12	10/3616 (0.3%)
1	D	0.74	0/2616	1.11	10/3562 (0.3%)
1	G	0.74	0/2646	1.11	8/3600 (0.2%)
1	H	0.75	0/2608	1.12	8/3548 (0.2%)
1	J	0.76	0/2624	1.09	8/3571 (0.2%)
1	K	0.78	1/2662 (0.0%)	1.10	9/3621 (0.2%)
All	All	0.75	1/21062 (0.0%)	1.11	69/28656 (0.2%)

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	A	0	1
1	C	0	1
1	D	0	1
1	G	0	3
1	J	0	3
1	K	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	326	HIS	CE1-NE2	5.01	1.37	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASN	CA-CB-CG	6.81	119.41	112.60
1	D	281	ASN	CA-CB-CG	6.78	119.38	112.60
1	K	281	ASN	CA-CB-CG	6.69	119.29	112.60
1	B	131	MET	CG-SD-CE	-6.68	86.21	100.90
1	C	23	MET	CB-CA-C	-6.62	98.48	108.61

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ARG	Sidechain
1	C	89	ARG	Sidechain
1	D	195	ARG	Sidechain
1	G	10	ARG	Sidechain
1	G	195	ARG	Sidechain

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	2559	0	2528	45	0
1	B	2547	0	2515	41	0
1	C	2575	0	2557	48	0
1	D	2545	0	2511	36	0
1	G	2566	0	2538	48	0
1	H	2543	0	2503	36	0
1	J	2547	0	2529	57	0
1	K	2579	0	2561	43	0
2	A	6	0	8	6	0
2	B	6	0	8	2	0
2	C	6	0	8	4	0
2	D	6	0	8	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
2	J	6	0	8	0	0
2	K	6	0	8	0	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	0	2	0
3	D	10	0	0	1	0
3	G	10	0	0	1	0
3	H	5	0	0	0	0
3	J	10	0	0	1	0
3	K	15	0	0	1	0
4	A	395	0	0	22	0
4	B	391	0	0	17	0
4	C	414	0	0	22	0
4	D	419	0	0	15	0
4	G	370	0	0	17	0
4	H	384	0	0	15	0
4	J	425	0	0	12	0
4	K	406	0	0	17	0
All	All	23793	0	20306	320	0

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 320 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:190:LEU:HB2	4:K:784:HOH:O	1.22	1.31
1:B:190:LEU:HD23	4:B:785:HOH:O	1.36	1.23
1:D:142:ASP:HB2	4:D:538:HOH:O	1.45	1.17
1:A:72:LEU:HD23	4:A:579:HOH:O	1.57	1.03
1:C:165:PHE:HB2	4:C:504:HOH:O	1.60	1.00

There are no symmetry-related clashes.

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	328/346 (95%)	322 (98%)	6 (2%)	0	100	100
1	B	327/346 (94%)	322 (98%)	5 (2%)	0	100	100
1	C	332/346 (96%)	327 (98%)	5 (2%)	0	100	100
1	D	327/346 (94%)	322 (98%)	5 (2%)	0	100	100
1	G	330/346 (95%)	325 (98%)	5 (2%)	0	100	100
1	H	326/346 (94%)	319 (98%)	7 (2%)	0	100	100
1	J	328/346 (95%)	323 (98%)	5 (2%)	0	100	100
1	K	332/346 (96%)	326 (98%)	6 (2%)	0	100	100
All	All	2630/2768 (95%)	2586 (98%)	44 (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	265/279 (95%)	259 (98%)	6 (2%)	44	38
1	B	264/279 (95%)	261 (99%)	3 (1%)	65	64
1	C	269/279 (96%)	262 (97%)	7 (3%)	40	33
1	D	264/279 (95%)	261 (99%)	3 (1%)	65	64
1	G	267/279 (96%)	263 (98%)	4 (2%)	57	54
1	H	263/279 (94%)	258 (98%)	5 (2%)	50	45
1	J	265/279 (95%)	256 (97%)	9 (3%)	32	23
1	K	268/279 (96%)	265 (99%)	3 (1%)	65	64
All	All	2125/2232 (95%)	2085 (98%)	40 (2%)	53	45

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	22[A]	ILE
1	J	195	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	22[B]	ILE
1	J	89	ARG
1	K	9	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	138	GLN
1	H	281	ASN
1	K	281	ASN
1	J	316	GLN
1	C	199	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
3	PO4	J	402	-	4,4,4	2.42	2 (50%)	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	K	401	-	5,5,5	0.07	0	5,5,5	0.31	0
3	PO4	D	402	-	4,4,4	2.12	1 (25%)	6,6,6	0.99	0
3	PO4	K	402	-	4,4,4	1.30	1 (25%)	6,6,6	0.32	0
3	PO4	K	404	-	4,4,4	0.76	0	6,6,6	0.53	0
3	PO4	C	402	-	4,4,4	1.58	1 (25%)	6,6,6	1.04	0
3	PO4	A	402	-	4,4,4	2.47	3 (75%)	6,6,6	0.85	0
3	PO4	B	402	-	4,4,4	2.95	3 (75%)	6,6,6	1.60	2 (33%)
2	GOL	G	401	-	5,5,5	0.19	0	5,5,5	0.31	0
3	PO4	D	403	-	4,4,4	0.71	0	6,6,6	0.92	0
3	PO4	C	403	-	4,4,4	0.70	0	6,6,6	0.52	0
3	PO4	H	402	-	4,4,4	2.68	3 (75%)	6,6,6	0.91	0
3	PO4	B	403	-	4,4,4	1.14	0	6,6,6	0.52	0
3	PO4	G	402	-	4,4,4	2.34	2 (50%)	6,6,6	1.28	1 (16%)
3	PO4	J	403	-	4,4,4	1.32	1 (25%)	6,6,6	0.63	0
2	GOL	H	401	-	5,5,5	0.20	0	5,5,5	0.64	0
3	PO4	K	403	-	4,4,4	0.77	0	6,6,6	0.82	0
2	GOL	J	401	-	5,5,5	0.22	0	5,5,5	0.34	0
3	PO4	G	403	-	4,4,4	1.22	0	6,6,6	0.66	0
3	PO4	A	403	-	4,4,4	0.75	0	6,6,6	0.75	0
2	GOL	D	401	-	5,5,5	0.14	0	5,5,5	0.35	0
2	GOL	A	401	-	5,5,5	0.26	0	5,5,5	0.68	0
2	GOL	B	401	-	5,5,5	0.19	0	5,5,5	0.37	0
2	GOL	C	401	-	5,5,5	0.31	0	5,5,5	0.39	0

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	GOL	J	401	-	-	4/4/4/4	-
2	GOL	K	401	-	-	2/4/4/4	-
2	GOL	H	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	4/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	B	401	-	-	4/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
2	GOL	G	401	-	-	0/4/4/4	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	PO4	P-O1	4.47	1.61	1.50
3	J	402	PO4	P-O2	-3.58	1.44	1.54
3	H	402	PO4	P-O1	3.57	1.58	1.50
3	D	402	PO4	P-O4	-3.52	1.44	1.54
3	H	402	PO4	P-O3	-3.32	1.45	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	PO4	O4-P-O3	2.66	116.19	107.91
3	G	402	PO4	O4-P-O3	2.34	115.19	107.91
3	B	402	PO4	O3-P-O1	-2.07	103.62	110.95

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	J	401	GOL	O1-C1-C2-C3
2	J	401	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	404	PO4	1	0
3	D	403	PO4	1	0
3	C	403	PO4	2	0
3	B	403	PO4	1	0
3	J	403	PO4	1	0
3	G	403	PO4	1	0
2	A	401	GOL	6	0
2	B	401	GOL	2	0
2	C	401	GOL	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	327/346 (94%)	-1.48	0 100 100	6, 13, 29, 67	3 (0%)
1	B	326/346 (94%)	-1.48	0 100 100	6, 14, 30, 57	3 (0%)
1	C	327/346 (94%)	-1.46	0 100 100	7, 15, 31, 66	7 (2%)
1	D	326/346 (94%)	-1.44	0 100 100	9, 15, 30, 73	3 (0%)
1	G	326/346 (94%)	-1.46	0 100 100	7, 15, 32, 63	6 (1%)
1	H	327/346 (94%)	-1.47	0 100 100	8, 15, 30, 62	1 (0%)
1	J	325/346 (93%)	-1.45	0 100 100	6, 14, 28, 50	5 (1%)
1	K	326/346 (94%)	-1.47	0 100 100	6, 14, 28, 52	8 (2%)
All	All	2610/2768 (94%)	-1.46	0 100 100	6, 14, 30, 73	36 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	401	6/6	0.98	0.05	18,23,25,26	6
2	GOL	D	401	6/6	0.98	0.05	19,23,31,35	6
2	GOL	G	401	6/6	0.98	0.05	19,22,24,25	6
2	GOL	H	401	6/6	0.98	0.05	19,24,27,29	6
3	PO4	C	403	5/5	0.98	0.06	87,90,92,94	0
2	GOL	B	401	6/6	0.99	0.05	22,28,30,31	6
2	GOL	J	401	6/6	0.99	0.05	20,26,31,36	6
2	GOL	K	401	6/6	0.99	0.05	23,32,36,36	6
3	PO4	A	403	5/5	0.99	0.09	38,39,43,47	0
3	PO4	B	403	5/5	0.99	0.06	34,36,45,51	0
2	GOL	C	401	6/6	0.99	0.05	20,26,29,36	6
3	PO4	D	403	5/5	0.99	0.06	33,34,52,54	0
3	PO4	G	403	5/5	0.99	0.05	29,36,41,48	0
3	PO4	J	403	5/5	0.99	0.04	43,48,56,61	0
3	PO4	K	403	5/5	0.99	0.06	26,38,47,59	0
3	PO4	K	404	5/5	0.99	0.04	39,44,52,58	0
3	PO4	G	402	5/5	1.00	0.02	12,13,14,15	0
3	PO4	C	402	5/5	1.00	0.02	15,15,16,17	0
3	PO4	H	402	5/5	1.00	0.02	11,12,13,14	0
3	PO4	J	402	5/5	1.00	0.02	13,15,17,19	0
3	PO4	B	402	5/5	1.00	0.02	11,12,15,15	0
3	PO4	K	402	5/5	1.00	0.02	12,12,14,15	0
3	PO4	D	402	5/5	1.00	0.01	11,13,15,18	0
3	PO4	A	402	5/5	1.00	0.02	11,12,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.