



wwPDB X-ray Structure Validation Summary Report

Apr 29, 2014 – 07:05 AM EDT

PDB ID : 4MVJ
Title : 2.85 Angstrom Resolution Crystal Structure of Glyceraldehyde 3-phosphate Dehydrogenase A (gapA) from Escherichia coli Modified by Acetyl Phosphate.
Authors : Minasov, G.; Kuhn, M.; Dubrovskaya, I.; Winsor, J.; Shuvalova, L.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-09-24
Resolution : 2.85 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>

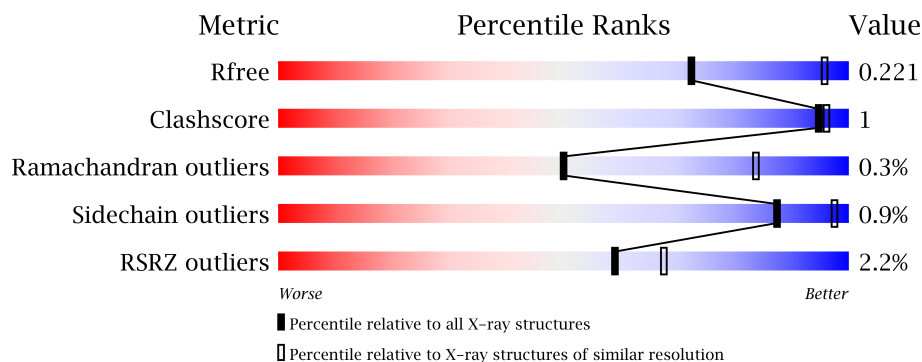
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.85 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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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.

Mol	Chain	Length	Quality of chain
1	A	355	
1	B	355	
1	C	355	
1	K	355	
1	N	355	
2	D	355	
2	L	355	
3	E	355	
4	F	355	
4	J	355	
4	O	355	
5	G	355	
6	H	355	
7	I	355	

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Mol	Chain	Length	Quality of chain
8	M	355	
9	P	355	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	NA	B	402	-	X
11	CL	A	404	-	X
11	CL	B	407	-	X
11	CL	C	407	-	X
11	CL	K	407	-	X
12	PO4	D	408	-	X
12	PO4	D	409	-	X
12	PO4	P	404	-	X
13	POP	F	403	-	X
13	POP	G	406	-	X
13	POP	J	406	-	X
13	POP	M	405	-	X
14	NAD	D	401	-	X
14	NAD	E	401	-	X
14	NAD	I	401	-	X
14	NAD	K	401	-	X
14	NAD	O	401	-	X
14	NAD	P	401	-	X
15	ACT	H	404	-	X
16	PGE	H	405	-	X
18	PG4	J	405	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41155 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 Glyceraldehyde-3-phosphatedehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2509	1576	435	487	11			
1	B	332	Total	C	N	O	S	0	1	0
			2514	1579	436	488	11			
1	C	331	Total	C	N	O	S	0	0	0
			2499	1570	432	486	11			
1	K	331	Total	C	N	O	S	0	1	0
			2509	1576	435	487	11			
1	N	331	Total	C	N	O	S	0	1	0
			2509	1576	435	487	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
A	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
A	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
A	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
A	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
A	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
A	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
A	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
A	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
A	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
A	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
A	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
A	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
A	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
A	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
A	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
A	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
A	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
A	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
A	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
A	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
A	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
A	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
B	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
B	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
B	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
B	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
B	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
B	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
B	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
B	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
B	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
B	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
B	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
B	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
B	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
B	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
B	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
B	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
B	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
B	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
B	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
B	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
B	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
B	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
B	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
B	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
C	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
C	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
C	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
C	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
C	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
C	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
C	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
C	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
C	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
C	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
C	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
C	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
C	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
C	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
C	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
C	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
C	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
C	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
C	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
C	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
C	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
C	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
C	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
K	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
K	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
K	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
K	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
K	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
K	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
K	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
K	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
K	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
K	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
K	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
K	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
K	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
K	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
K	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
K	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
K	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
K	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
K	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
K	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
K	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
K	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
K	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
K	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
N	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
N	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
N	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
N	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
N	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
N	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
N	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
N	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
N	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
N	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
N	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
N	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
N	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
N	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
N	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
N	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
N	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
N	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
N	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
N	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
N	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
N	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
N	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 2 is a protein called Glyceraldehyde-3-phosphatedehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	331	Total	C	N	O	S	0	2	0
			2514	1578	437	488	11			
2	L	331	Total	C	N	O	S	0	1	0
			2506	1574	435	486	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
D	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
D	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
D	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
D	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
D	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
D	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
D	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
D	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
D	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
D	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
D	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
D	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
D	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
D	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
D	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
D	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
D	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
D	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
D	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
D	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
D	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
D	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
L	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
L	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
L	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
L	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
L	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
L	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
L	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
L	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
L	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
L	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
L	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
L	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
L	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
L	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
L	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
L	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
L	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
L	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
L	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
L	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
L	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
L	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
L	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
L	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 3 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	331	Total	C	N	O	S	0	2	0
			2520	1582	434	493	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
E	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
E	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
E	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
E	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
E	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
E	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
E	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
E	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
E	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
E	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
E	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
E	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
E	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
E	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
E	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
E	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
E	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
E	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
E	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
E	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
E	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
E	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
E	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 4 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	3	0
			2531	1588	440	492	11			
4	J	330	Total	C	N	O	S	0	1	0
			2504	1573	434	487	10			
4	O	331	Total	C	N	O	S	0	0	0
			2502	1572	432	487	11			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
F	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
F	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
F	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
F	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
F	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
F	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
F	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
F	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
F	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
F	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
F	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
F	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
F	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
F	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
F	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
F	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
F	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
F	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
F	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
F	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
F	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
F	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
J	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
J	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
J	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
J	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
J	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
J	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
J	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
J	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
J	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
J	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
J	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
J	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
J	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
J	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
J	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
J	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
J	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
J	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
J	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
J	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
J	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
J	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
J	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ALA	-	EXPRESSION TAG	UNP C9QTS9
O	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
O	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
O	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
O	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
O	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
O	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
O	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
O	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
O	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
O	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
O	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
O	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
O	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
O	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
O	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
O	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
O	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
O	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
O	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
O	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
O	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
O	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
O	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
O	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 5 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	331	Total	C	N	O	S	0	2	0
			2520	1582	437	490	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
G	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
G	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
G	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
G	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
G	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
G	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
G	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
G	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
G	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
G	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
G	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
G	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
G	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
G	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
G	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
G	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
G	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
G	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
G	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
G	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
G	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
G	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 6 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	331	Total	C	N	O	S	0	0	0
			2505	1574	432	488	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
H	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
H	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
H	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
H	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
H	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
H	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
H	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
H	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
H	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
H	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
H	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
H	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
H	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
H	-9	THR	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
H	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
H	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
H	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
H	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
H	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
H	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
H	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
H	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 7 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	330	Total	C	N	O	S	0	1	0
			2507	1575	434	488	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
I	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
I	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
I	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
I	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
I	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
I	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
I	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
I	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
I	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
I	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
I	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
I	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
I	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
I	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
I	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
I	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
I	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
I	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
I	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
I	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
I	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
I	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 8 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	331	Total	C	N	O	S	0	1	0
			2508	1575	433	489	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
M	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
M	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
M	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
M	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
M	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
M	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
M	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
M	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
M	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
M	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
M	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
M	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
M	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
M	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
M	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
M	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
M	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
M	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
M	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
M	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
M	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
M	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
M	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 9 is a protein called Glyceraldehyde-3-phosphateDehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	P	330	Total	C	N	O	S	0	1	0
			2507	1575	434	488	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-23	MET	-	EXPRESSION TAG	UNP C9QTS9
P	-22	HIS	-	EXPRESSION TAG	UNP C9QTS9
P	-21	HIS	-	EXPRESSION TAG	UNP C9QTS9
P	-20	HIS	-	EXPRESSION TAG	UNP C9QTS9
P	-19	HIS	-	EXPRESSION TAG	UNP C9QTS9
P	-18	HIS	-	EXPRESSION TAG	UNP C9QTS9
P	-17	HIS	-	EXPRESSION TAG	UNP C9QTS9
P	-16	SER	-	EXPRESSION TAG	UNP C9QTS9
P	-15	SER	-	EXPRESSION TAG	UNP C9QTS9
P	-14	GLY	-	EXPRESSION TAG	UNP C9QTS9
P	-13	VAL	-	EXPRESSION TAG	UNP C9QTS9
P	-12	ASP	-	EXPRESSION TAG	UNP C9QTS9
P	-11	LEU	-	EXPRESSION TAG	UNP C9QTS9
P	-10	GLY	-	EXPRESSION TAG	UNP C9QTS9
P	-9	THR	-	EXPRESSION TAG	UNP C9QTS9
P	-8	GLU	-	EXPRESSION TAG	UNP C9QTS9
P	-7	ASN	-	EXPRESSION TAG	UNP C9QTS9
P	-6	LEU	-	EXPRESSION TAG	UNP C9QTS9
P	-5	TYR	-	EXPRESSION TAG	UNP C9QTS9
P	-4	PHE	-	EXPRESSION TAG	UNP C9QTS9
P	-3	GLN	-	EXPRESSION TAG	UNP C9QTS9
P	-2	SER	-	EXPRESSION TAG	UNP C9QTS9
P	-1	ASN	-	EXPRESSION TAG	UNP C9QTS9
P	0	ALA	-	EXPRESSION TAG	UNP C9QTS9

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	1	Total Na 1 1	0	0
10	D	1	Total Na 1 1	0	0
10	K	1	Total Na 1 1	0	0
10	E	1	Total Na 1 1	0	0
10	H	1	Total Na 1 1	0	0
10	B	2	Total Na 2 2	0	0
10	I	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total 1	Na 1	0	0
10	A	1	Total 1	Na 1	0	0
10	N	1	Total 1	Na 1	0	0
10	M	1	Total 1	Na 1	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

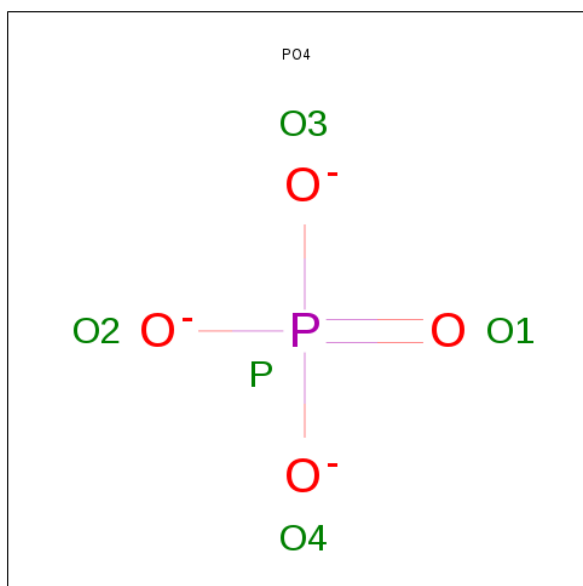
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	2	Total 2	Cl 2	0	0
11	G	4	Total 4	Cl 4	0	0
11	J	2	Total 2	Cl 2	0	0
11	D	5	Total 5	Cl 5	0	0
11	K	6	Total 6	Cl 6	0	0
11	E	5	Total 5	Cl 5	0	0
11	H	1	Total 1	Cl 1	0	0
11	B	6	Total 6	Cl 6	0	0
11	I	2	Total 2	Cl 2	0	0
11	C	5	Total 5	Cl 5	0	0
11	A	4	Total 4	Cl 4	0	0
11	N	1	Total 1	Cl 1	0	0
11	O	2	Total 2	Cl 2	0	0
11	L	1	Total 1	Cl 1	0	0
11	F	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	2	Total	Cl	0	0
			2	2		

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



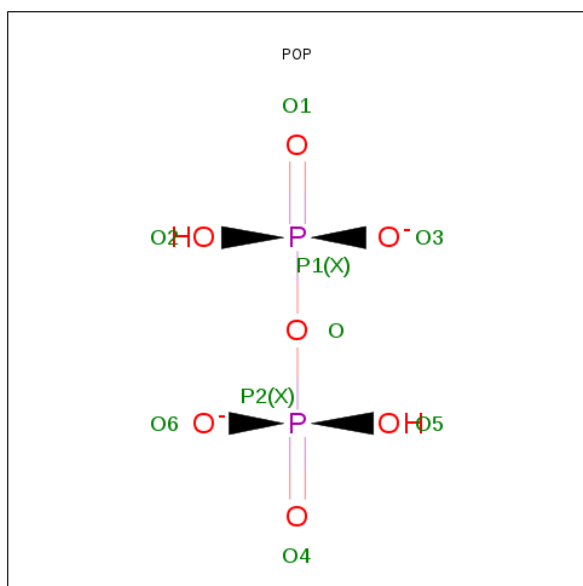
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	A	1	Total	O	P	0	0
			5	4	1		
12	A	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	E	1	Total	O	P	0	0
			5	4	1		
12	F	1	Total	O	P	0	0
			5	4	1		
12	H	1	Total	O	P	0	0
			5	4	1		
12	I	1	Total	O	P	0	0
			5	4	1		

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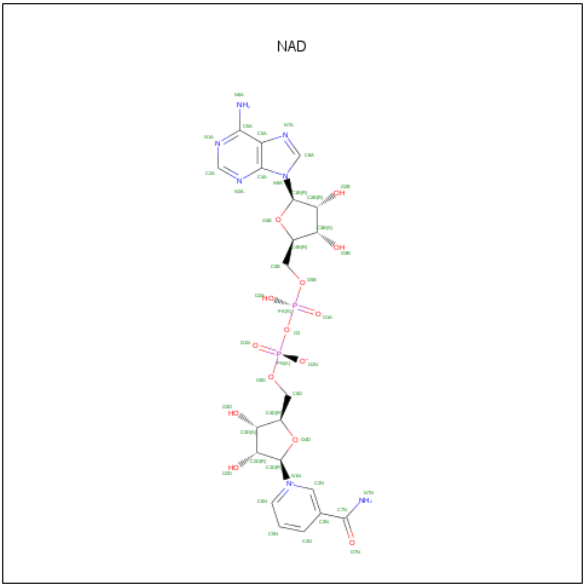
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	J	1	Total	O	P	0	0
			5	4	1		
12	J	1	Total	O	P	0	0
			5	4	1		
12	L	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



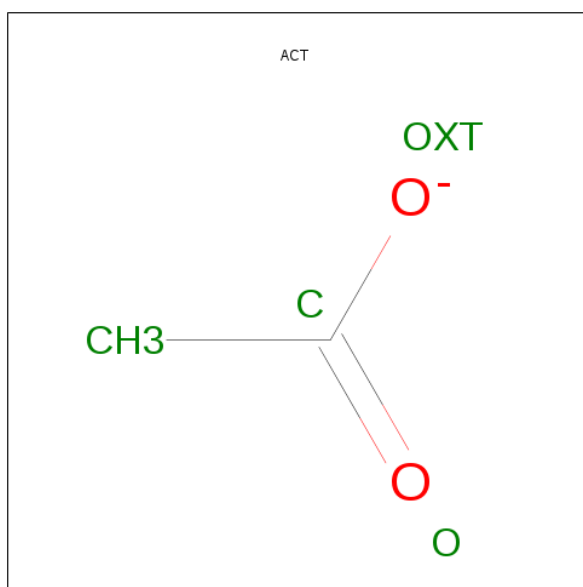
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	P	0	0
			9	7	2		
13	B	1	Total	O	P	0	0
			9	7	2		
13	F	1	Total	O	P	0	0
			9	7	2		
13	G	1	Total	O	P	0	0
			9	7	2		
13	J	1	Total	O	P	0	0
			9	7	2		
13	M	1	Total	O	P	0	0
			9	7	2		

- Molecule 14 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



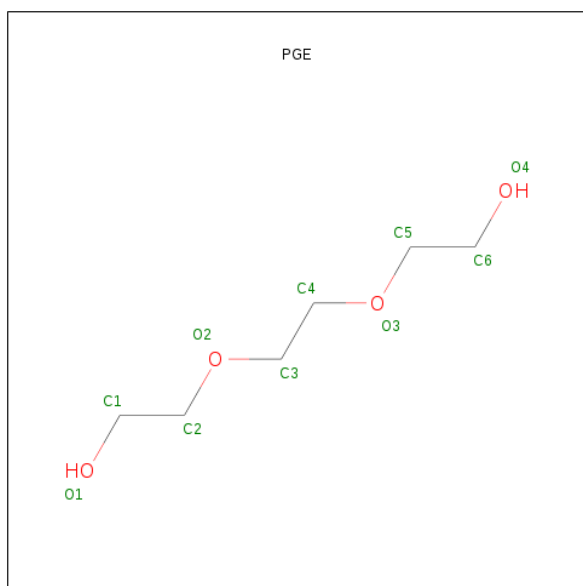
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 15 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



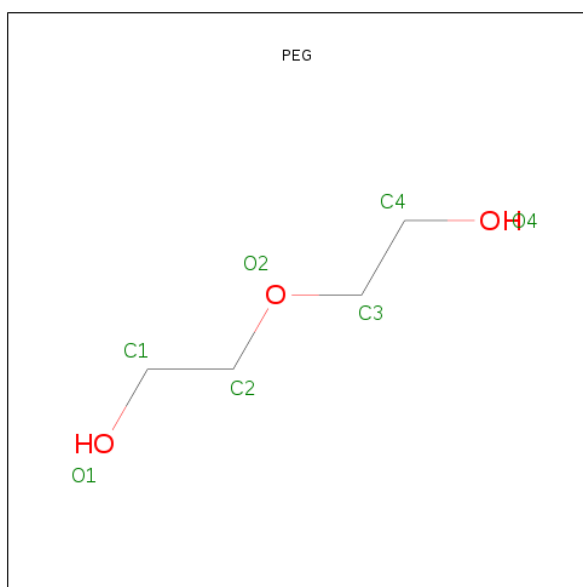
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 16 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



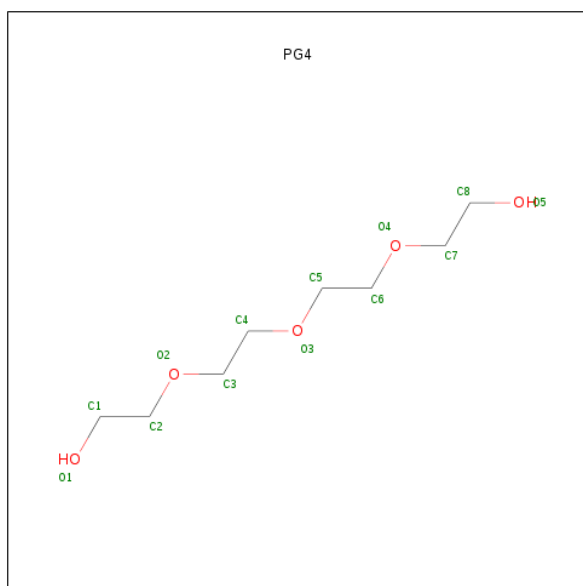
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 17 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



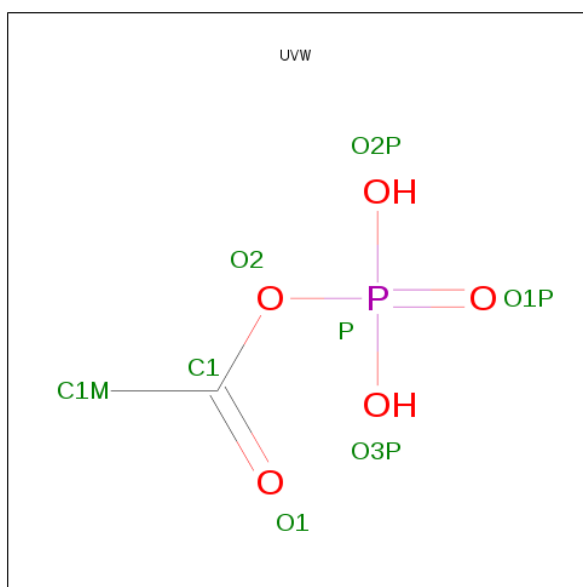
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 18 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	J	1	Total	C	O	0	0
			13	8	5		

- Molecule 19 is ACETYLPHOSPHATE (three-letter code: UVW) (formula: $C_2H_5O_5P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	M	1	Total	C	O	P	0	0
			8	2	5	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	39	Total	O	0	0
			39	39		
20	B	35	Total	O	0	3
			38	38		
20	C	61	Total	O	0	0
			61	61		
20	D	37	Total	O	0	1
			38	38		
20	E	23	Total	O	0	0
			23	23		
20	F	27	Total	O	0	0
			27	27		
20	G	33	Total	O	0	2
			35	35		
20	H	21	Total	O	0	1
			22	22		
20	I	22	Total	O	0	1
			23	23		
20	J	28	Total	O	0	0
			28	28		
20	K	26	Total	O	0	0
			26	26		

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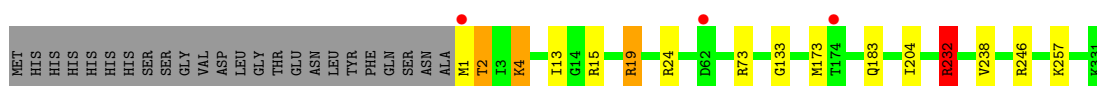
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	L	20	Total 20	O 20	0	0
20	M	24	Total 24	O 24	0	0
20	N	11	Total 11	O 11	0	0
20	O	20	Total 20	O 20	0	0
20	P	16	Total 16	O 16	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

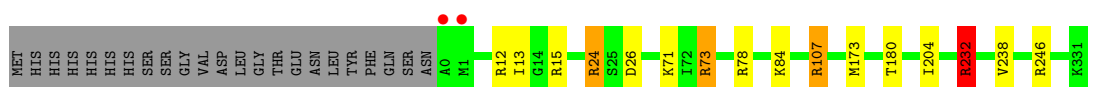
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain A: 



- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain B: 



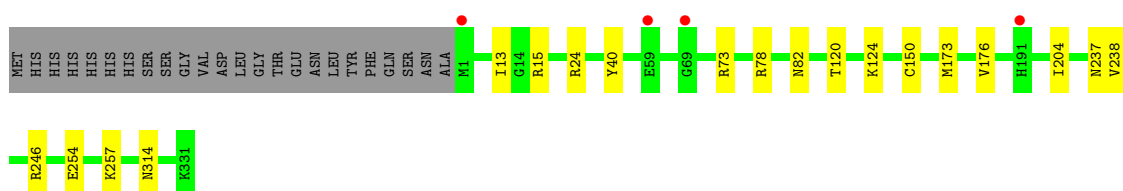
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain C: 



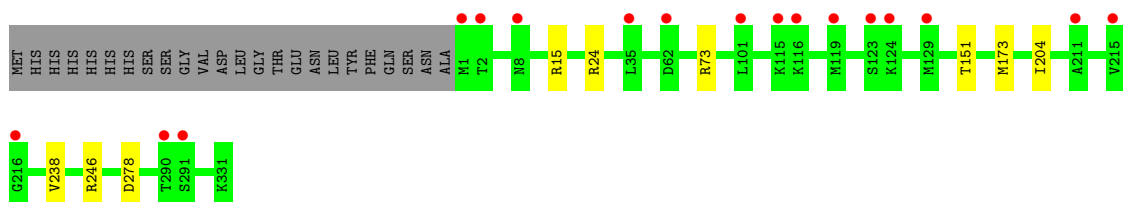
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain K: 



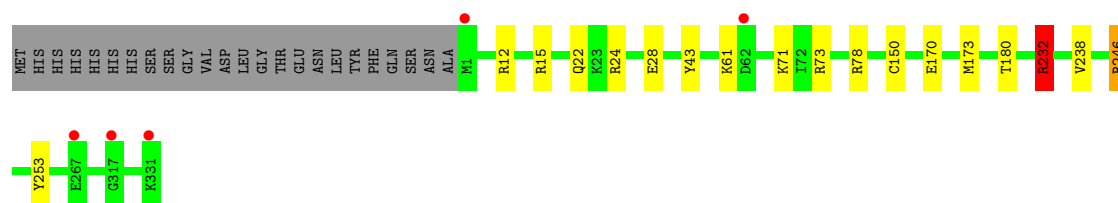
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain N: 



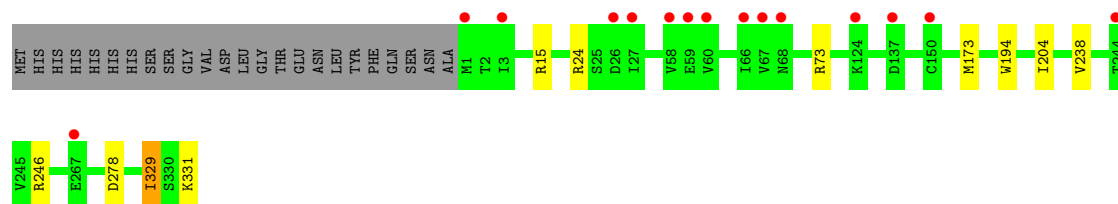
- Molecule 2: Glyceraldehyde-3-phosphatedehydrogenase A

Chain D: 



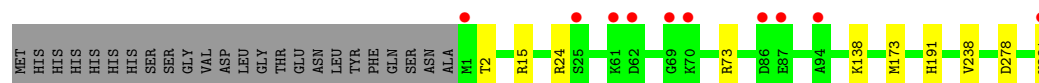
- Molecule 2: Glyceraldehyde-3-phosphatedehydrogenase A

Chain L: 



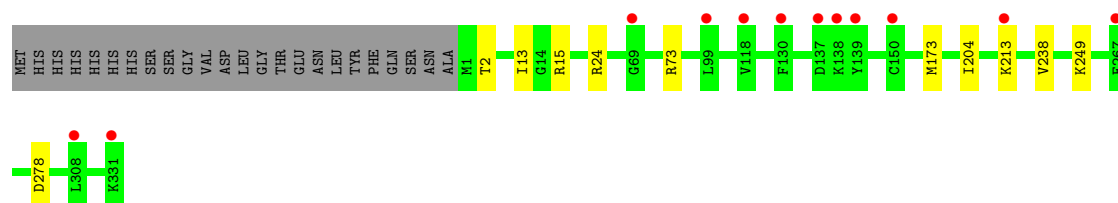
- Molecule 3: Glyceraldehyde-3-phosphateDehydrogenase A

Chain E: 



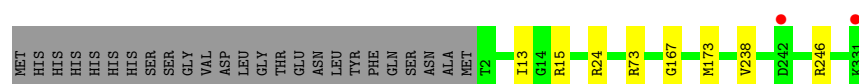
- Molecule 4: Glyceraldehyde-3-phosphateDehydrogenase A

Chain F: 



- Molecule 4: Glyceraldehyde-3-phosphateDehydrogenase A

Chain J: 



- Molecule 4: Glyceraldehyde-3-phosphateDehydrogenase A

Chain O: 



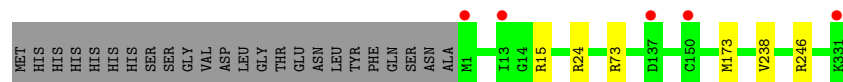
- Molecule 5: Glyceraldehyde-3-phosphateDehydrogenase A

Chain G: 



- Molecule 6: Glyceraldehyde-3-phosphateDehydrogenase A

Chain H: 



- Molecule 7: Glyceraldehyde-3-phosphateDehydrogenase A

Chain I: 



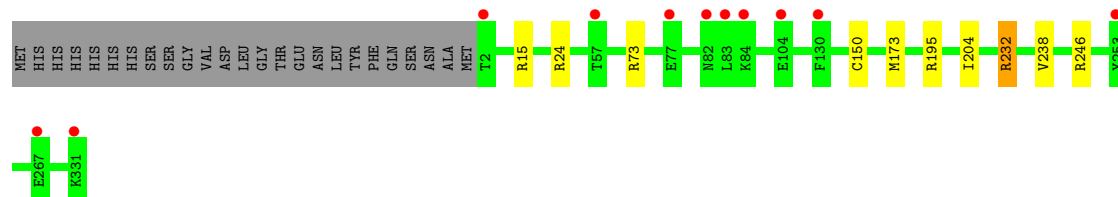
- Molecule 8: Glyceraldehyde-3-phosphateDehydrogenase A

Chain M: 



- Molecule 9: Glyceraldehyde-3-phosphateDehydrogenase A

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.88Å 69.69Å 271.92Å 90.00° 98.80° 90.00°	Depositor
Resolution (Å)	29.91 – 2.85 29.91 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-2.85) 99.9 (29.91-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, R_{free}	0.186 , 0.224 0.184 , 0.221	Depositor DCC
R_{free} test set	6389 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 127140 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	41155	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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: PGE, NAD, CL, NA, PO4, ACT, POP, UVW, PG4, SCY, ALY, PEG

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	0.69	2/2536 (0.1%)	1.90	18/3432 (0.5%)
1	B	0.73	2/2541 (0.1%)	1.70	19/3439 (0.6%)
1	C	0.71	0/2525	0.91	9/3417 (0.3%)
1	K	0.67	3/2536 (0.1%)	1.57	12/3432 (0.3%)
1	N	0.52	0/2536	0.87	9/3432 (0.3%)
2	D	0.68	2/2554 (0.1%)	1.33	17/3457 (0.5%)
2	L	0.57	0/2546	0.91	10/3446 (0.3%)
3	E	0.64	0/2533	0.91	9/3427 (0.3%)
4	F	0.58	0/2545	0.89	7/3443 (0.2%)
4	J	0.59	0/2518	0.89	6/3408 (0.2%)
4	O	0.57	0/2515	0.89	8/3403 (0.2%)
5	G	0.59	0/2537	0.88	8/3432 (0.2%)
6	H	0.59	0/2508	0.89	7/3392 (0.2%)
7	I	0.59	0/2508	1.02	10/3394 (0.3%)
8	M	0.64	0/2534	1.44	14/3429 (0.4%)
9	P	0.55	0/2511	0.97	14/3397 (0.4%)
All	All	0.62	9/40483 (0.0%)	1.17	177/54780 (0.3%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	24	ARG	CZ-NH1	-8.54	1.22	1.33
1	K	24	ARG	CD-NE	-7.65	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	ARG	CZ-NH1	-6.57	1.24	1.33
1	A	19	ARG	CD-NE	-6.46	1.35	1.46
1	K	24	ARG	CZ-NH2	6.18	1.41	1.33

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ARG	NE-CZ-NH1	-56.88	91.86	120.30
1	K	24	ARG	NE-CZ-NH1	-56.64	91.98	120.30
1	K	24	ARG	NE-CZ-NH2	49.91	145.26	120.30
1	A	19	ARG	NE-CZ-NH2	48.79	144.69	120.30
1	B	15	ARG	NE-CZ-NH1	-39.45	100.57	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ARG	Sidechain

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	2509	0	0	6	0
1	B	2514	0	0	6	0
1	C	2499	0	0	6	0
1	K	2509	0	0	8	0
1	N	2509	0	0	2	0
2	D	2514	0	0	7	0
2	L	2506	0	0	2	0
3	E	2520	0	0	1	0
4	F	2531	0	0	2	0
4	J	2504	0	0	1	0
4	O	2502	0	0	4	0
5	G	2520	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	2505	0	0	0	0
7	I	2507	0	0	2	0
8	M	2508	0	0	2	0
9	P	2507	0	0	1	0
10	A	1	0	0	0	0
10	B	2	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	K	1	0	0	0	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
11	A	4	0	0	1	0
11	B	6	0	0	0	0
11	C	5	0	0	0	0
11	D	5	0	0	0	0
11	E	5	0	0	0	0
11	F	1	0	0	0	0
11	G	4	0	0	0	0
11	H	1	0	0	0	0
11	I	2	0	0	0	0
11	J	2	0	0	0	0
11	K	6	0	0	1	0
11	L	1	0	0	0	0
11	M	2	0	0	0	0
11	N	1	0	0	0	0
11	O	2	0	0	0	0
11	P	2	0	0	0	0
12	A	15	0	0	1	0
12	B	5	0	0	0	0
12	D	10	0	0	2	0
12	E	5	0	0	0	0
12	F	5	0	0	0	0
12	H	5	0	0	0	0
12	I	5	0	0	0	0
12	J	10	0	0	0	0
12	L	5	0	0	0	0
12	P	10	0	0	0	0
13	A	9	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	9	0	0	2	0
13	F	9	0	0	2	0
13	G	9	0	0	1	0
13	J	9	0	0	1	0
13	M	9	0	0	2	0
14	C	44	0	26	3	0
14	D	44	0	26	3	0
14	E	44	0	26	1	0
14	I	44	0	26	0	0
14	K	44	0	26	4	0
14	O	44	0	26	3	0
14	P	44	0	26	0	0
15	H	4	0	3	0	0
16	H	10	0	14	0	0
17	H	7	0	10	0	0
18	J	13	0	18	0	0
19	M	8	0	3	0	0
20	A	39	0	0	2	0
20	B	38	0	0	0	0
20	C	61	0	0	1	0
20	D	38	0	0	2	0
20	E	23	0	0	1	0
20	F	27	0	0	1	0
20	G	35	0	0	2	0
20	H	22	0	0	0	0
20	I	23	0	0	1	0
20	J	28	0	0	0	0
20	K	26	0	0	3	0
20	L	20	0	0	1	0
20	M	24	0	0	0	0
20	N	11	0	0	1	0
20	O	20	0	0	1	0
20	P	16	0	0	0	0
All	All	41155	0	230	58	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 1.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:I:104:GLU:OE2	4:O:104:GLU:OE2	1.85	0.94
13:A:409:POP:O2	13:A:409:POP:O4	1.85	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:405:POP:O2	13:M:405:POP:O6	1.91	0.88
2:D:12:ARG:N	14:D:401:NAD:O2A	2.23	0.71
1:B:13:ILE:N	13:B:410:POP:O4	2.24	0.69

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	329/355 (93%)	314 (95%)	14 (4%)	1 (0%)	50	84
1	B	330/355 (93%)	316 (96%)	13 (4%)	1 (0%)	50	84
1	C	328/355 (92%)	315 (96%)	12 (4%)	1 (0%)	50	84
1	K	329/355 (93%)	314 (95%)	14 (4%)	1 (0%)	50	84
1	N	329/355 (93%)	315 (96%)	13 (4%)	1 (0%)	50	84
2	D	331/355 (93%)	317 (96%)	13 (4%)	1 (0%)	50	84
2	L	330/355 (93%)	315 (96%)	14 (4%)	1 (0%)	50	84
3	E	329/355 (93%)	314 (95%)	14 (4%)	1 (0%)	50	84
4	F	330/355 (93%)	316 (96%)	13 (4%)	1 (0%)	50	84
4	J	327/355 (92%)	313 (96%)	12 (4%)	2 (1%)	33	73
4	O	327/355 (92%)	312 (95%)	14 (4%)	1 (0%)	50	84
5	G	329/355 (93%)	315 (96%)	13 (4%)	1 (0%)	50	84
6	H	326/355 (92%)	311 (95%)	14 (4%)	1 (0%)	50	84
7	I	326/355 (92%)	311 (95%)	14 (4%)	1 (0%)	50	84
8	M	329/355 (93%)	313 (95%)	15 (5%)	1 (0%)	50	84
9	P	326/355 (92%)	312 (96%)	13 (4%)	1 (0%)	50	84
All	All	5255/5680 (92%)	5023 (96%)	215 (4%)	17 (0%)	50	84

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	238	VAL
1	A	238	VAL
1	B	238	VAL
2	D	238	VAL
3	E	238	VAL

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	266/286 (93%)	261 (98%)	5 (2%)	69	93
1	B	266/286 (93%)	262 (98%)	4 (2%)	76	95
1	C	265/286 (93%)	263 (99%)	2 (1%)	89	98
1	K	266/286 (93%)	264 (99%)	2 (1%)	89	98
1	N	266/286 (93%)	265 (100%)	1 (0%)	95	99
2	D	268/287 (93%)	265 (99%)	3 (1%)	84	97
2	L	267/287 (93%)	264 (99%)	3 (1%)	84	97
3	E	266/285 (93%)	263 (99%)	3 (1%)	84	97
4	F	267/285 (94%)	263 (98%)	4 (2%)	76	95
4	J	264/285 (93%)	263 (100%)	1 (0%)	95	99
4	O	264/285 (93%)	263 (100%)	1 (0%)	95	99
5	G	266/285 (93%)	265 (100%)	1 (0%)	95	99
6	H	263/284 (93%)	262 (100%)	1 (0%)	95	99
7	I	263/284 (93%)	262 (100%)	1 (0%)	95	99
8	M	266/286 (93%)	263 (99%)	3 (1%)	84	97
9	P	263/284 (93%)	261 (99%)	2 (1%)	89	98
All	All	4246/4567 (93%)	4209 (99%)	37 (1%)	87	97

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	191	HIS
4	F	249	LYS

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Mol	Chain	Res	Type
4	O	173	MET
4	F	2	THR
4	F	173	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

25 non-standard protein/DNA/RNA residues 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
1	ALY	A	46	1	11,11,12	5.64	2 (18%)	10,12,14	3.14	5 (50%)
1	ALY	B	46	1	11,11,12	5.30	3 (27%)	10,12,14	3.46	4 (40%)
1	ALY	C	46	1	11,11,12	5.57	2 (18%)	10,12,14	3.37	5 (50%)
3	ALY	E	249	3	11,11,12	3.69	1 (9%)	10,12,14	3.05	3 (30%)
3	ALY	E	46	3	11,11,12	5.24	1 (9%)	10,12,14	3.14	3 (30%)
4	ALY	F	257	4	11,11,12	5.07	3 (27%)	10,12,14	5.09	5 (50%)
4	ALY	F	46	4	11,11,12	4.46	1 (9%)	10,12,14	3.13	5 (50%)
5	SCY	G	150	5	8,8,9	6.70	2 (25%)	7,9,11	2.93	3 (42%)
5	ALY	G	46	5	11,11,12	4.86	1 (9%)	10,12,14	2.95	4 (40%)
6	SCY	H	150	6	8,8,9	6.94	2 (25%)	7,9,11	3.33	2 (28%)
6	ALY	H	257	6	11,11,12	4.87	4 (36%)	10,12,14	5.13	5 (50%)
6	ALY	H	46	6	11,11,12	5.12	3 (27%)	10,12,14	2.75	4 (40%)
7	ALY	I	249	7	11,11,12	4.24	1 (9%)	10,12,14	2.56	4 (40%)
7	ALY	I	257	7	11,11,12	5.33	3 (27%)	10,12,14	5.37	6 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ALY	I	46	7	11,11,12	5.37	3 (27%)	10,12,14	3.19	5 (50%)
4	ALY	J	257	4	11,11,12	5.65	3 (27%)	10,12,14	5.84	6 (60%)
4	ALY	J	46	4	11,11,12	5.40	2 (18%)	10,12,14	3.04	4 (40%)
1	ALY	K	46	1	11,11,12	5.30	2 (18%)	10,12,14	2.94	4 (40%)
8	ALY	M	257	8	11,11,12	5.57	3 (27%)	10,12,14	5.35	6 (60%)
1	ALY	N	46	1	11,11,12	5.52	2 (18%)	10,12,14	3.05	5 (50%)
4	ALY	O	257	4	11,11,12	5.07	3 (27%)	10,12,14	5.16	6 (60%)
4	ALY	O	46	4	11,11,12	5.36	1 (9%)	10,12,14	3.08	5 (50%)
9	SCY	P	150	9	8,8,9	6.89	2 (25%)	7,9,11	10.68	4 (57%)
9	ALY	P	249	9	11,11,12	3.88	1 (9%)	10,12,14	3.05	3 (30%)
9	ALY	P	46	9	11,11,12	5.02	2 (18%)	10,12,14	3.14	5 (50%)

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
1	ALY	A	46	1	-	2/8/10/12	0/0/0/0
1	ALY	B	46	1	-	2/8/10/12	0/0/0/0
1	ALY	C	46	1	-	2/8/10/12	0/0/0/0
3	ALY	E	249	3	-	2/8/10/12	0/0/0/0
3	ALY	E	46	3	-	2/8/10/12	0/0/0/0
4	ALY	F	257	4	-	0/8/10/12	0/0/0/0
4	ALY	F	46	4	-	2/8/10/12	0/0/0/0
5	SCY	G	150	5	-	1/5/7/9	0/0/0/0
5	ALY	G	46	5	-	2/8/10/12	0/0/0/0
6	SCY	H	150	6	-	1/5/7/9	0/0/0/0
6	ALY	H	257	6	-	0/8/10/12	0/0/0/0
6	ALY	H	46	6	-	2/8/10/12	0/0/0/0
7	ALY	I	249	7	-	2/8/10/12	0/0/0/0
7	ALY	I	257	7	-	0/8/10/12	0/0/0/0
7	ALY	I	46	7	-	2/8/10/12	0/0/0/0
4	ALY	J	257	4	-	2/8/10/12	0/0/0/0
4	ALY	J	46	4	-	2/8/10/12	0/0/0/0
1	ALY	K	46	1	-	2/8/10/12	0/0/0/0
8	ALY	M	257	8	-	2/8/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	N	46	1	-	2/8/10/12	0/0/0/0
4	ALY	O	257	4	-	0/8/10/12	0/0/0/0
4	ALY	O	46	4	-	2/8/10/12	0/0/0/0
9	SCY	P	150	9	-	0/5/7/9	0/0/0/0
9	ALY	P	249	9	-	2/8/10/12	0/0/0/0
9	ALY	P	46	9	-	2/8/10/12	0/0/0/0

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	150	SCY	O-C	19.19	1.24	1.11
9	P	150	SCY	O-C	18.87	1.24	1.11
5	G	150	SCY	O-C	18.59	1.24	1.11
1	A	46	ALY	O-C	18.35	1.24	1.11
4	J	257	ALY	O-C	18.17	1.23	1.11

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	150	SCY	CB-SG-CD	27.93	118.67	100.87
7	I	257	ALY	CE-NZ-CH	14.52	146.13	122.35
4	J	257	ALY	CE-NZ-CH	14.47	146.05	122.35
4	O	257	ALY	CE-NZ-CH	14.08	145.41	122.35
4	F	257	ALY	CE-NZ-CH	13.66	144.72	122.35

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	P	249	ALY	OH-CH-NZ-CE
3	E	46	ALY	OH-CH-NZ-CE
9	P	46	ALY	OH-CH-NZ-CE
4	F	46	ALY	OH-CH-NZ-CE
1	K	46	ALY	OH-CH-NZ-CE

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 94 ligands modelled in this entry, 61 are monoatomic - leaving 33 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$
12	PO4	A	406	-	4,4,4	0.47	0	6,6,6	0.37	0
12	PO4	A	407	-	4,4,4	0.52	0	6,6,6	0.31	0
12	PO4	A	408	-	4,4,4	0.46	0	6,6,6	0.30	0
13	POP	A	409	-	8,8,8	0.82	0	13,13,13	2.07	4 (30%)
12	PO4	B	409	-	4,4,4	0.38	0	6,6,6	0.38	0
13	POP	B	410	-	8,8,8	1.14	0	13,13,13	1.34	2 (15%)
14	NAD	C	401	-	48,48,48	1.51	7 (14%)	73,73,73	1.98	9 (12%)
14	NAD	D	401	-	48,48,48	1.09	4 (8%)	73,73,73	1.94	13 (17%)
12	PO4	D	408	-	4,4,4	0.81	0	6,6,6	0.32	0
12	PO4	D	409	-	4,4,4	0.49	0	6,6,6	0.28	0
14	NAD	E	401	-	48,48,48	1.02	2 (4%)	73,73,73	1.93	11 (15%)
12	PO4	E	408	-	4,4,4	0.34	0	6,6,6	0.32	0
12	PO4	F	402	-	4,4,4	0.20	0	6,6,6	0.28	0
13	POP	F	403	-	8,8,8	0.51	0	13,13,13	1.49	2 (15%)
13	POP	G	406	-	8,8,8	0.78	0	13,13,13	0.67	0
12	PO4	H	403	-	4,4,4	0.35	0	6,6,6	0.29	0
15	ACT	H	404	-	1,3,3	2.10	1 (100%)	0,3,3	0.00	-
16	PGE	H	405	-	9,9,9	0.72	0	8,8,8	0.32	0
17	PEG	H	406	-	6,6,6	0.53	0	5,5,5	0.62	0
14	NAD	I	401	-	48,48,48	1.10	4 (8%)	73,73,73	1.89	9 (12%)
12	PO4	I	405	-	4,4,4	0.67	0	6,6,6	0.30	0
12	PO4	J	403	-	4,4,4	0.47	0	6,6,6	0.29	0
12	PO4	J	404	-	4,4,4	0.41	0	6,6,6	0.28	0
18	PG4	J	405	-	12,12,12	0.63	0	11,11,11	0.23	0
13	POP	J	406	-	8,8,8	0.79	0	13,13,13	1.34	2 (15%)
14	NAD	K	401	-	48,48,48	1.20	4 (8%)	73,73,73	1.96	12 (16%)
12	PO4	L	402	-	4,4,4	0.18	0	6,6,6	0.29	0
19	UVW	M	404	-	7,7,7	3.12	2 (28%)	10,10,10	2.53	3 (30%)
13	POP	M	405	-	8,8,8	0.74	0	13,13,13	1.90	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAD	O	401	-	48,48,48	0.98	4 (8%)	73,73,73	2.09	12 (16%)
14	NAD	P	401	-	48,48,48	1.21	4 (8%)	73,73,73	1.90	12 (16%)
12	PO4	P	404	-	4,4,4	0.25	0	6,6,6	0.30	0
12	PO4	P	405	-	4,4,4	0.36	0	6,6,6	0.29	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
12	PO4	A	406	-	-	0/0/0/0	0/0/0/0
12	PO4	A	407	-	-	0/0/0/0	0/0/0/0
12	PO4	A	408	-	-	0/0/0/0	0/0/0/0
13	POP	A	409	-	-	0/6/6/6	0/0/0/0
12	PO4	B	409	-	-	0/0/0/0	0/0/0/0
13	POP	B	410	-	-	0/6/6/6	0/0/0/0
14	NAD	C	401	-	-	0/30/62/62	0/5/5/5
14	NAD	D	401	-	-	0/30/62/62	0/5/5/5
12	PO4	D	408	-	-	0/0/0/0	0/0/0/0
12	PO4	D	409	-	-	0/0/0/0	0/0/0/0
14	NAD	E	401	-	-	0/30/62/62	0/5/5/5
12	PO4	E	408	-	-	0/0/0/0	0/0/0/0
12	PO4	F	402	-	-	0/0/0/0	0/0/0/0
13	POP	F	403	-	-	0/6/6/6	0/0/0/0
13	POP	G	406	-	-	0/6/6/6	0/0/0/0
12	PO4	H	403	-	-	0/0/0/0	0/0/0/0
15	ACT	H	404	-	-	0/0/0/0	0/0/0/0
16	PGE	H	405	-	-	0/7/7/7	0/0/0/0
17	PEG	H	406	-	-	0/4/4/4	0/0/0/0
14	NAD	I	401	-	-	0/30/62/62	0/5/5/5
12	PO4	I	405	-	-	0/0/0/0	0/0/0/0
12	PO4	J	403	-	-	0/0/0/0	0/0/0/0
12	PO4	J	404	-	-	0/0/0/0	0/0/0/0
18	PG4	J	405	-	-	0/10/10/10	0/0/0/0
13	POP	J	406	-	-	0/6/6/6	0/0/0/0
14	NAD	K	401	-	-	0/30/62/62	0/5/5/5
12	PO4	L	402	-	-	0/0/0/0	0/0/0/0
19	UVW	M	404	-	-	0/3/5/5	0/0/0/0
13	POP	M	405	-	-	0/6/6/6	0/0/0/0
14	NAD	O	401	-	-	0/30/62/62	0/5/5/5
14	NAD	P	401	-	-	0/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PO4	P	404	-	-	0/0/0/0	0/0/0/0
12	PO4	P	405	-	-	0/0/0/0	0/0/0/0

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	404	UVW	O2-C1	7.64	1.47	1.37
14	C	401	NAD	O4D-C1D	4.34	1.46	1.41
14	P	401	NAD	O4D-C1D	4.00	1.46	1.41
14	K	401	NAD	O4D-C1D	3.95	1.46	1.41
14	C	401	NAD	C5A-C4A	3.85	1.49	1.40

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	401	NAD	C5A-C4A-N3A	-8.64	117.56	125.98
14	O	401	NAD	C5A-C4A-N3A	-8.14	118.04	125.98
14	K	401	NAD	C5A-C4A-N3A	-7.95	118.22	125.98
14	I	401	NAD	C5A-C4A-N3A	-7.82	118.35	125.98
14	O	401	NAD	N3A-C2A-N1A	-7.82	122.01	128.89

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 ⓘ

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	331/355 (93%)	-0.38	3 (0%) 81 87	35, 59, 92, 123	0
1	B	332/355 (93%)	-0.45	2 (0%) 86 91	36, 58, 93, 134	0
1	C	331/355 (93%)	-0.51	3 (0%) 81 87	30, 47, 80, 126	0
1	K	331/355 (93%)	-0.44	4 (1%) 75 83	34, 59, 93, 116	0
1	N	331/355 (93%)	0.15	17 (5%) 27 32	54, 97, 150, 182	0
2	D	331/355 (93%)	-0.28	5 (1%) 70 79	27, 65, 97, 153	1 (0%)
2	L	331/355 (93%)	0.10	15 (4%) 32 38	43, 97, 163, 193	0
3	E	331/355 (93%)	-0.38	10 (3%) 48 57	39, 63, 115, 160	0
4	F	331/355 (93%)	0.06	12 (3%) 41 48	45, 86, 124, 159	0
4	J	330/355 (92%)	-0.30	2 (0%) 86 91	35, 80, 126, 159	0
4	O	331/355 (93%)	-0.32	4 (1%) 75 83	42, 66, 106, 126	0
5	G	331/355 (93%)	-0.36	5 (1%) 70 79	40, 64, 102, 133	0
6	H	331/355 (93%)	-0.30	5 (1%) 70 79	43, 70, 102, 134	0
7	I	330/355 (92%)	-0.25	6 (1%) 65 74	34, 80, 124, 158	0
8	M	331/355 (93%)	-0.43	3 (0%) 81 87	40, 59, 98, 129	0
9	P	330/355 (92%)	-0.17	11 (3%) 44 53	45, 83, 123, 159	0
All	All	5294/5680 (93%)	-0.27	107 (2%) 59 71	27, 69, 124, 193	1 (0%)

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	P	82	ASN	7.3
3	E	62	ASP	6.0
1	N	124	LYS	4.6
6	H	150	SCY	4.6
1	B	0	ALA	4.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SCY	G	150	9/10	0.27	2.88	52,58,94,96	0
6	SCY	H	150	9/10	0.40	2.56	58,73,109,115	0
3	ALY	E	249	12/13	0.23	2.53	60,78,121,128	0
1	ALY	K	46	12/13	0.25	2.48	54,62,68,71	0
9	SCY	P	150	9/10	0.22	2.12	68,81,91,105	0
9	ALY	P	46	12/13	0.23	1.58	46,51,60,66	0
9	ALY	P	249	12/13	0.28	1.31	98,125,137,140	0
3	ALY	E	46	12/13	0.22	1.16	53,65,80,84	0
7	ALY	I	249	12/13	0.24	1.11	107,139,150,153	0
4	ALY	O	257	12/13	0.23	1.10	61,67,88,91	0
1	ALY	N	46	12/13	0.21	0.90	59,65,74,75	0
1	ALY	B	46	12/13	0.17	0.87	34,39,55,60	0
7	ALY	I	46	12/13	0.20	0.81	49,59,62,63	0
6	ALY	H	46	12/13	0.19	0.73	41,48,56,58	0
4	ALY	O	46	12/13	0.20	0.73	63,70,90,91	0
1	ALY	C	46	12/13	0.16	0.63	35,42,49,52	0
6	ALY	H	257	12/13	0.19	0.62	70,75,80,85	0
4	ALY	J	257	12/13	0.15	0.36	88,97,100,100	0
5	ALY	G	46	12/13	0.16	0.07	56,63,75,75	0
8	ALY	M	257	12/13	0.17	0.06	55,61,82,86	0
7	ALY	I	257	12/13	0.20	-0.04	80,94,97,97	0
4	ALY	F	257	12/13	0.16	-0.19	56,79,84,84	0
1	ALY	A	46	12/13	0.14	-0.58	55,60,66,67	0
4	ALY	J	46	12/13	0.13	-0.63	35,49,57,60	0
4	ALY	F	46	12/13	0.13	-1.27	58,66,79,79	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	PO4	D	408	5/5	0.47	8.27	24,24,34,51	5
10	NA	B	402	1/1	0.46	7.97	71,71,71,71	0
12	PO4	D	409	5/5	0.45	7.43	62,75,97,102	0
13	POP	G	406	9/9	0.48	6.45	37,49,59,68	9
13	POP	J	406	9/9	0.29	5.99	28,40,44,48	9
12	PO4	P	404	5/5	0.36	5.62	43,45,46,69	5
15	ACT	H	404	4/4	0.35	5.46	65,67,79,80	4
11	CL	C	407	1/1	0.28	5.33	54,54,54,54	1
11	CL	B	407	1/1	0.26	4.74	81,81,81,81	0
13	POP	M	405	9/9	0.35	3.81	30,41,54,56	9
11	CL	K	407	1/1	0.16	3.80	38,38,38,38	1
11	CL	A	404	1/1	0.32	3.77	91,91,91,91	0
14	NAD	K	401	44/44	0.32	3.50	38,53,63,66	44
14	NAD	E	401	44/44	0.39	3.37	38,55,72,83	44
16	PGE	H	405	10/10	0.43	3.26	77,98,114,121	0
14	NAD	O	401	44/44	0.33	2.83	34,58,85,88	44
14	NAD	I	401	44/44	0.35	2.78	32,49,62,69	44
18	PG4	J	405	13/13	0.33	2.69	79,101,107,118	0
13	POP	F	403	9/9	0.39	2.62	41,57,65,74	9
14	NAD	P	401	44/44	0.34	2.29	34,51,58,62	44
14	NAD	D	401	44/44	0.32	2.22	40,56,69,76	44
11	CL	O	402	1/1	0.25	1.94	93,93,93,93	0
12	PO4	B	409	5/5	0.22	1.89	27,34,38,38	5
14	NAD	C	401	44/44	0.25	1.82	52,86,101,113	0
13	POP	A	409	9/9	0.29	1.70	31,41,46,47	9
12	PO4	F	402	5/5	0.29	1.55	49,52,67,76	5
12	PO4	A	408	5/5	0.30	1.45	45,48,51,75	5
11	CL	G	402	1/1	0.28	1.29	87,87,87,87	0
12	PO4	A	407	5/5	0.20	1.29	36,39,67,71	5
11	CL	B	405	1/1	0.18	0.91	82,82,82,82	0
10	NA	H	401	1/1	0.17	0.67	69,69,69,69	0
11	CL	J	402	1/1	0.14	0.63	69,69,69,69	0
11	CL	D	404	1/1	0.18	0.62	70,70,70,70	0
13	POP	B	410	9/9	0.24	0.55	54,91,117,118	0
17	PEG	H	406	7/7	0.19	0.54	80,97,114,116	0
11	CL	H	402	1/1	0.24	0.31	76,76,76,76	0
12	PO4	J	404	5/5	0.22	0.31	40,42,49,65	5
11	CL	E	407	1/1	0.17	0.21	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CL	A	405	1/1	0.22	-0.17	70,70,70,70	0
12	PO4	P	405	5/5	0.20	-0.22	45,52,58,76	5
11	CL	N	402	1/1	0.18	-0.27	65,65,65,65	0
10	NA	E	402	1/1	0.15	-0.38	79,79,79,79	0
12	PO4	L	402	5/5	0.13	-0.38	44,53,61,73	5
11	CL	C	405	1/1	0.14	-0.50	70,70,70,70	0
12	PO4	E	408	5/5	0.17	-0.52	49,68,77,104	5
19	UVW	M	404	8/8	0.19	-0.53	83,101,127,139	0
11	CL	A	402	1/1	0.13	-0.58	66,66,66,66	0
11	CL	B	408	1/1	0.10	-0.64	67,67,67,67	0
11	CL	K	403	1/1	0.12	-0.67	64,64,64,64	0
12	PO4	J	403	5/5	0.14	-0.74	52,58,65,92	5
11	CL	K	408	1/1	0.13	-0.74	86,86,86,86	0
12	PO4	A	406	5/5	0.15	-0.76	62,75,83,121	0
12	PO4	H	403	5/5	0.17	-0.77	53,56,60,80	5
11	CL	L	401	1/1	0.12	-0.89	53,53,53,53	0
11	CL	P	403	1/1	0.11	-0.92	59,59,59,59	0
11	CL	B	406	1/1	0.13	-0.93	80,80,80,80	0
11	CL	E	403	1/1	0.08	-1.07	60,60,60,60	0
12	PO4	I	405	5/5	0.14	-1.09	32,39,46,66	5
11	CL	G	403	1/1	0.10	-1.11	74,74,74,74	0
10	NA	M	401	1/1	0.10	-1.13	85,85,85,85	0
11	CL	D	403	1/1	0.10	-1.15	71,71,71,71	0
10	NA	I	402	1/1	0.07	-1.18	91,91,91,91	0
11	CL	F	401	1/1	0.12	-1.20	79,79,79,79	0
10	NA	K	402	1/1	0.08	-1.23	59,59,59,59	0
11	CL	D	406	1/1	0.09	-1.25	71,71,71,71	0
11	CL	O	403	1/1	0.07	-1.45	61,61,61,61	0
10	NA	G	401	1/1	0.09	-1.51	78,78,78,78	0
10	NA	A	401	1/1	0.09	-1.51	54,54,54,54	0
11	CL	A	403	1/1	0.07	-1.53	71,71,71,71	0
11	CL	E	404	1/1	0.05	-1.54	73,73,73,73	0
11	CL	C	404	1/1	0.05	-1.69	57,57,57,57	0
11	CL	J	401	1/1	0.08	-1.71	67,67,67,67	0
11	CL	M	402	1/1	0.09	-1.74	57,57,57,57	0
10	NA	D	402	1/1	0.12	-1.74	65,65,65,65	0
11	CL	B	404	1/1	0.10	-1.86	71,71,71,71	0
10	NA	B	401	1/1	0.08	-1.89	53,53,53,53	0
11	CL	M	403	1/1	0.05	-1.90	68,68,68,68	0
11	CL	C	403	1/1	0.07	-1.90	52,52,52,52	0
10	NA	N	401	1/1	0.07	-1.90	89,89,89,89	0
11	CL	G	404	1/1	0.05	-2.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	NA	C	402	1/1	0.07	-2.31	67,67,67,67	0
11	CL	I	404	1/1	0.06	-2.34	67,67,67,67	0
11	CL	K	405	1/1	0.05	-2.34	59,59,59,59	0
11	CL	B	403	1/1	0.07	-2.37	51,51,51,51	0
11	CL	D	407	1/1	0.08	-2.42	66,66,66,66	0
11	CL	K	404	1/1	0.07	-2.43	51,51,51,51	0
11	CL	C	406	1/1	0.07	-2.48	46,46,46,46	0
11	CL	D	405	1/1	0.10	-2.85	73,73,73,73	0
11	CL	G	405	1/1	0.08	-3.13	46,46,46,46	0
11	CL	K	406	1/1	0.06	-3.19	70,70,70,70	0
11	CL	E	405	1/1	0.11	-3.38	79,79,79,79	0
11	CL	P	402	1/1	0.05	-3.45	57,57,57,57	0
11	CL	I	403	1/1	0.08	-5.22	88,88,88,88	0
11	CL	E	406	1/1	0.04	-9.89	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.