



Full wwPDB X-ray Structure Validation 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 full wwPDB validation 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>

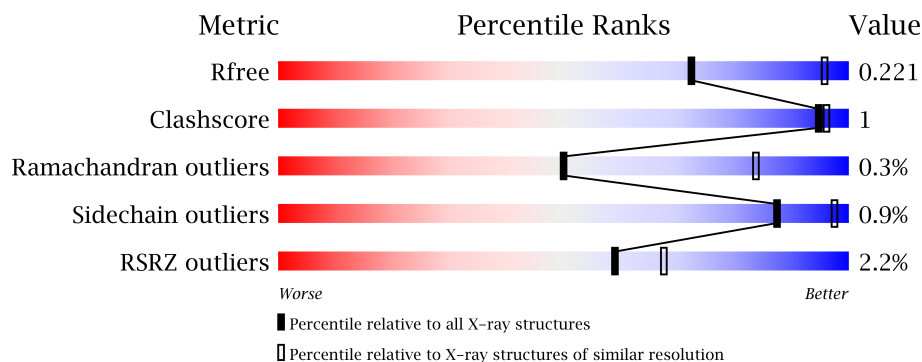
The following versions of software and data (see [references](#)) were used in the production of this report:

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).

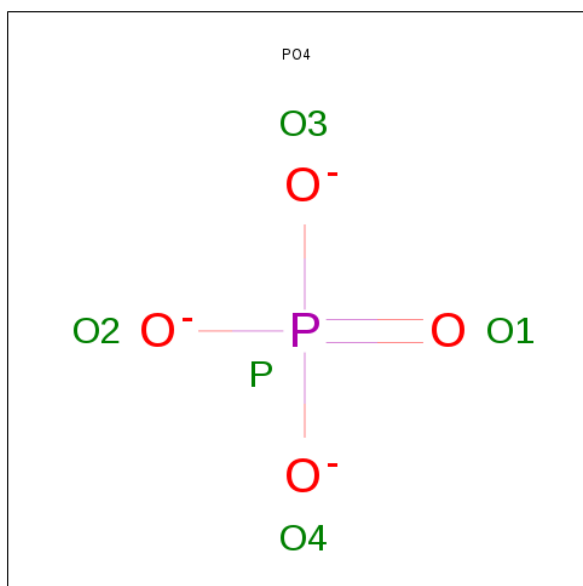
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	2	Total 2	Cl 2	0	0
11	G	4	Total 4	Cl 4	0	0
11	J	2	Total 2	Cl 2	0	0
11	D	5	Total 5	Cl 5	0	0
11	K	6	Total 6	Cl 6	0	0
11	E	5	Total 5	Cl 5	0	0
11	H	1	Total 1	Cl 1	0	0
11	B	6	Total 6	Cl 6	0	0
11	I	2	Total 2	Cl 2	0	0
11	C	5	Total 5	Cl 5	0	0
11	A	4	Total 4	Cl 4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



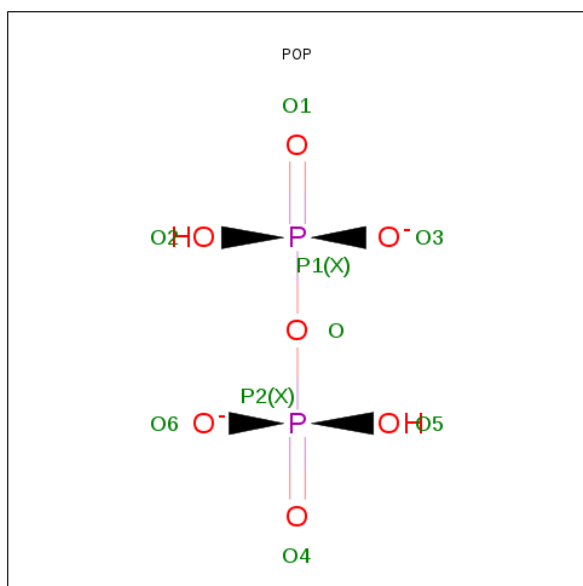
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	A	1	Total	O	P	0	0
			5	4	1		
12	A	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	E	1	Total	O	P	0	0
			5	4	1		
12	F	1	Total	O	P	0	0
			5	4	1		
12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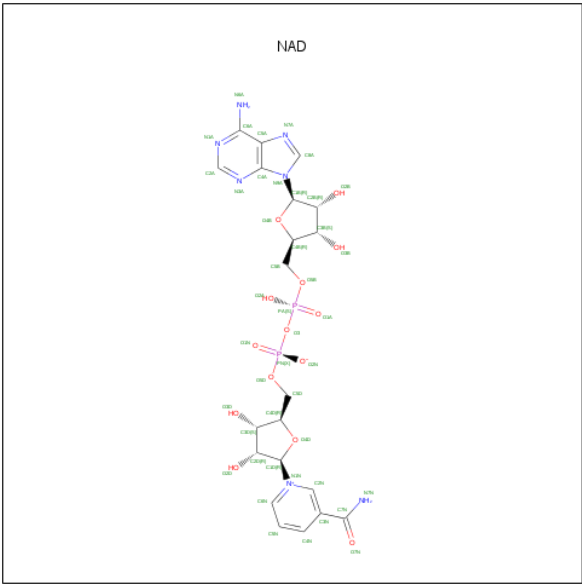
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	J	1	Total	O	P	0	0
			5	4	1		
12	J	1	Total	O	P	0	0
			5	4	1		
12	L	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		

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



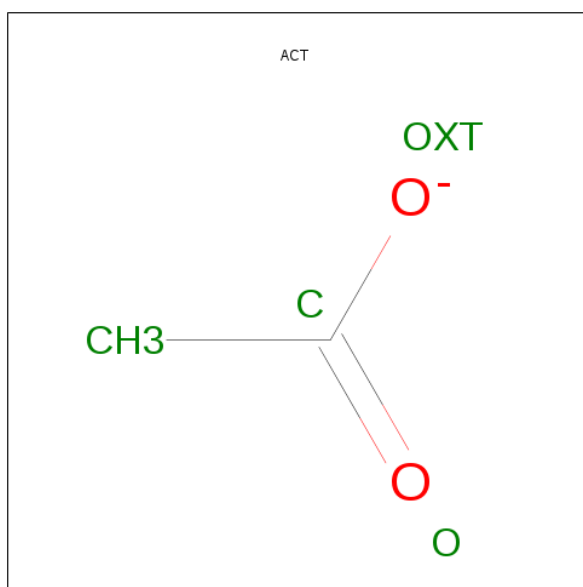
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	P	0	0
			9	7	2		
13	B	1	Total	O	P	0	0
			9	7	2		
13	F	1	Total	O	P	0	0
			9	7	2		
13	G	1	Total	O	P	0	0
			9	7	2		
13	J	1	Total	O	P	0	0
			9	7	2		
13	M	1	Total	O	P	0	0
			9	7	2		

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



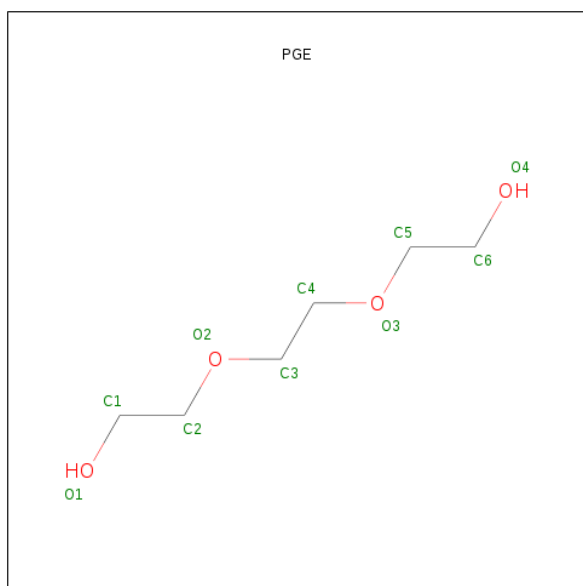
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
14	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2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



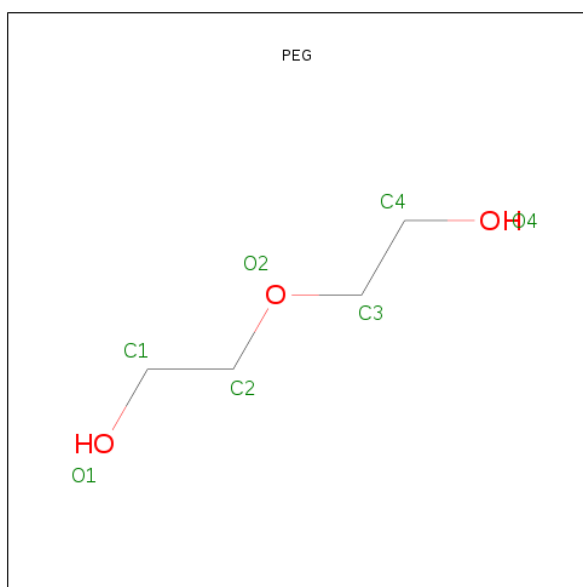
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 16 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



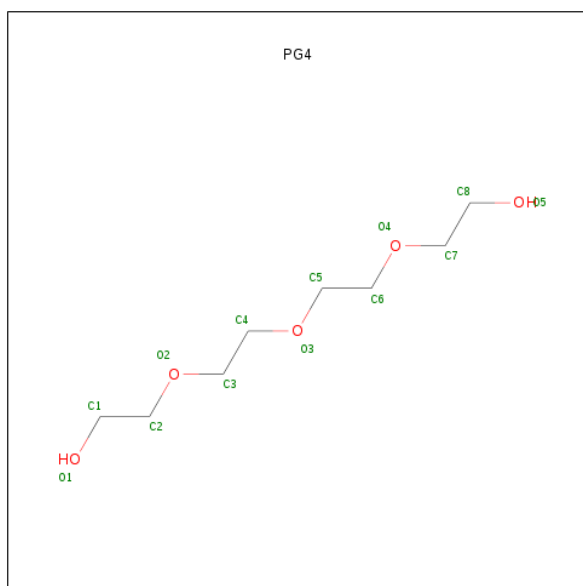
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 17 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



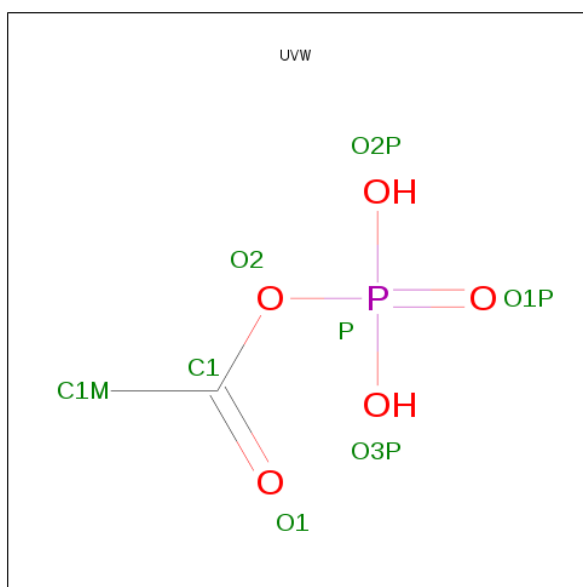
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	H	1	Total	C	O	0	0
			7	4	3		

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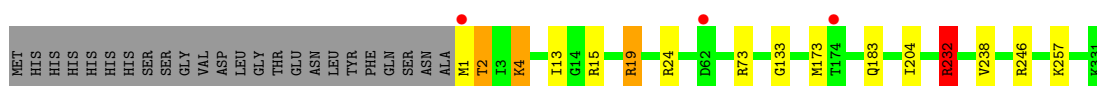
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	L	20	Total 20	O 20	0	0
20	M	24	Total 24	O 24	0	0
20	N	11	Total 11	O 11	0	0
20	O	20	Total 20	O 20	0	0
20	P	16	Total 16	O 16	0	0

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.

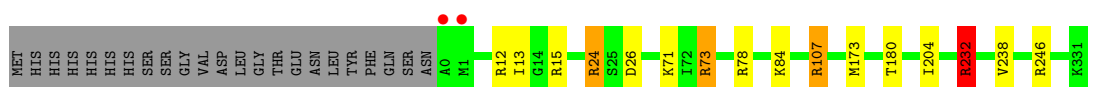
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain A: 



- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain B: 



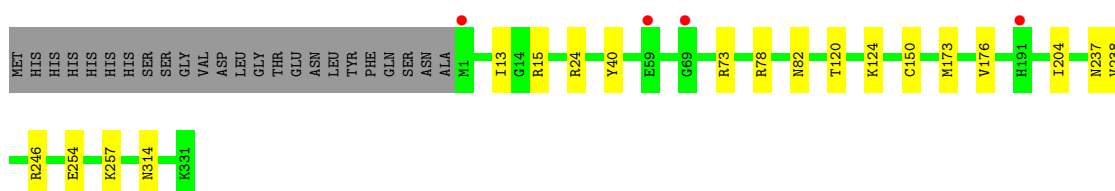
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain C: 



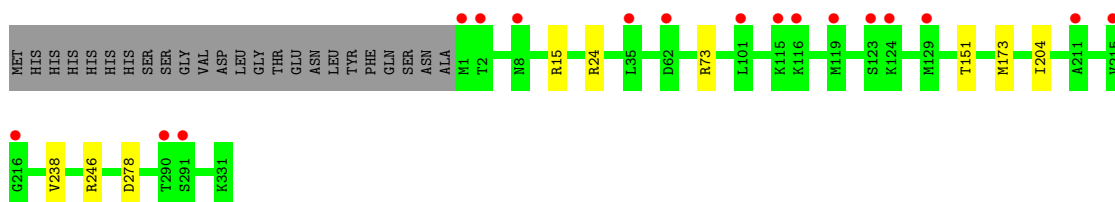
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain K: 



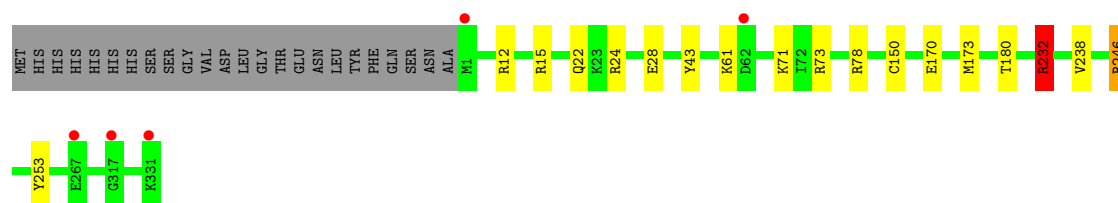
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase A

Chain N: 



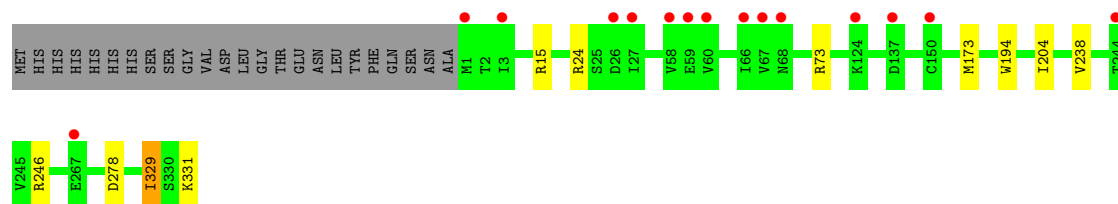
- Molecule 2: Glyceraldehyde-3-phosphatedehydrogenase A

Chain D: 



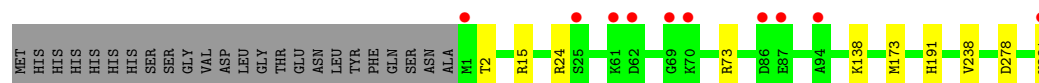
- Molecule 2: Glyceraldehyde-3-phosphatedehydrogenase A

Chain L: 



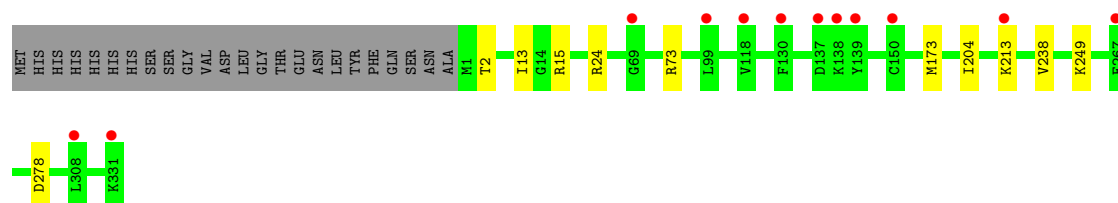
- Molecule 3: Glyceraldehyde-3-phosphateDehydrogenase A

Chain E: 



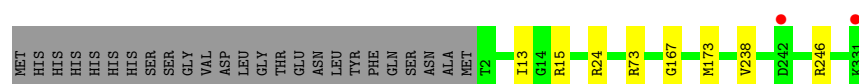
- Molecule 4: Glyceraldehyde-3-phosphateDehydrogenase A

Chain F: 



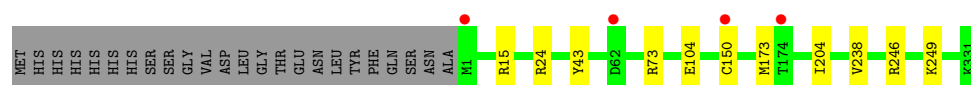
- Molecule 4: Glyceraldehyde-3-phosphateDehydrogenase A

Chain J: 



- Molecule 4: Glyceraldehyde-3-phosphateDehydrogenase A

Chain O: 



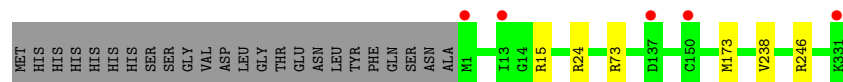
- Molecule 5: Glyceraldehyde-3-phosphateDehydrogenase A

Chain G: 



- Molecule 6: Glyceraldehyde-3-phosphateDehydrogenase A

Chain H: 



- Molecule 7: Glyceraldehyde-3-phosphateDehydrogenase A

Chain I: 



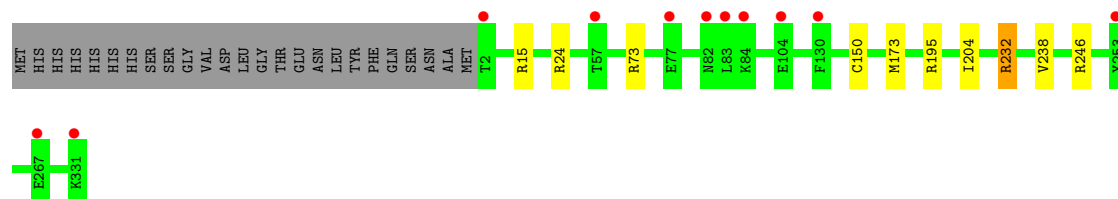
- Molecule 8: Glyceraldehyde-3-phosphateDehydrogenase A

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

All (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
2	D	28	GLU	CD-OE2	-5.84	1.19	1.25
1	B	15	ARG	CZ-NH1	-5.81	1.25	1.33
1	A	15	ARG	CZ-NH1	-5.41	1.26	1.33
2	D	15	ARG	CZ-NH1	-5.07	1.26	1.33

All (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
1	A	15	ARG	NE-CZ-NH1	-39.20	100.70	120.30
2	D	15	ARG	NE-CZ-NH1	-38.98	100.81	120.30
8	M	15	ARG	NE-CZ-NH1	-38.97	100.82	120.30
1	A	15	ARG	NE-CZ-NH2	37.60	139.10	120.30
1	B	15	ARG	NE-CZ-NH2	37.17	138.89	120.30
2	D	15	ARG	NE-CZ-NH2	36.76	138.68	120.30
8	M	15	ARG	NE-CZ-NH2	36.17	138.39	120.30
1	B	107	ARG	NE-CZ-NH1	-34.56	103.02	120.30
1	B	107	ARG	NE-CZ-NH2	29.64	135.12	120.30
1	B	73	ARG	NE-CZ-NH1	-28.29	106.15	120.30
8	M	73	ARG	NE-CZ-NH1	-27.28	106.66	120.30
8	M	73	ARG	NE-CZ-NH2	23.87	132.24	120.30
1	B	73	ARG	NE-CZ-NH2	23.49	132.04	120.30
7	I	246	ARG	NE-CZ-NH2	21.56	131.08	120.30
1	A	19	ARG	CD-NE-CZ	20.49	152.29	123.60
7	I	246	ARG	NE-CZ-NH1	-18.52	111.04	120.30
1	A	232	ARG	NE-CZ-NH1	-16.67	111.97	120.30
1	A	19	ARG	CG-CD-NE	16.15	145.72	111.80
9	P	232	ARG	NE-CZ-NH1	-15.87	112.36	120.30
2	D	232	ARG	NE-CZ-NH1	-15.56	112.52	120.30
8	M	73	ARG	CG-CD-NE	15.26	143.84	111.80
1	B	73	ARG	CG-CD-NE	15.06	143.42	111.80
1	B	232	ARG	NE-CZ-NH1	-14.87	112.87	120.30
4	J	15	ARG	NE-CZ-NH1	12.95	126.78	120.30
9	P	15	ARG	NE-CZ-NH1	12.42	126.51	120.30
4	F	15	ARG	NE-CZ-NH1	12.24	126.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	15	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	K	24	ARG	CD-NE-CZ	12.01	140.42	123.60
7	I	15	ARG	NE-CZ-NH1	11.84	126.22	120.30
2	L	15	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	N	15	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	C	15	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	A	232	ARG	NE-CZ-NH2	11.39	126.00	120.30
1	K	15	ARG	NE-CZ-NH1	11.36	125.98	120.30
4	O	15	ARG	NE-CZ-NH1	11.26	125.93	120.30
5	G	15	ARG	NE-CZ-NH1	11.23	125.91	120.30
3	E	15	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	D	232	ARG	NE-CZ-NH2	11.16	125.88	120.30
1	A	15	ARG	CD-NE-CZ	11.10	139.14	123.60
1	B	73	ARG	CD-NE-CZ	11.09	139.12	123.60
1	B	15	ARG	CD-NE-CZ	11.03	139.05	123.60
1	B	232	ARG	NE-CZ-NH2	10.99	125.80	120.30
9	P	232	ARG	NE-CZ-NH2	10.96	125.78	120.30
2	D	15	ARG	CD-NE-CZ	10.81	138.74	123.60
8	M	15	ARG	CD-NE-CZ	10.71	138.59	123.60
9	P	15	ARG	NE-CZ-NH2	-10.69	114.96	120.30
8	M	73	ARG	CD-NE-CZ	10.53	138.34	123.60
9	P	195	ARG	NE-CZ-NH1	-10.40	115.10	120.30
6	H	15	ARG	NE-CZ-NH2	-10.20	115.20	120.30
2	L	329	ILE	CA-CB-CG1	10.09	130.17	111.00
4	F	15	ARG	NE-CZ-NH2	-10.04	115.28	120.30
7	I	246	ARG	CG-CD-NE	10.04	132.89	111.80
1	B	24	ARG	NE-CZ-NH1	-9.95	115.32	120.30
1	B	24	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	K	15	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	N	15	ARG	NE-CZ-NH2	-9.88	115.36	120.30
4	J	15	ARG	NE-CZ-NH2	-9.88	115.36	120.30
4	O	15	ARG	NE-CZ-NH2	-9.83	115.39	120.30
5	G	15	ARG	NE-CZ-NH2	-9.80	115.40	120.30
3	E	15	ARG	NE-CZ-NH2	-9.80	115.40	120.30
7	I	15	ARG	NE-CZ-NH2	-9.79	115.41	120.30
2	L	15	ARG	NE-CZ-NH2	-9.70	115.45	120.30
7	I	246	ARG	CD-NE-CZ	9.55	136.97	123.60
1	C	15	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	L	329	ILE	CG1-CB-CG2	-9.26	91.02	111.40
1	B	71	LYS	CD-CE-NZ	8.63	131.54	111.70
1	A	73	ARG	NE-CZ-NH1	8.61	124.61	120.30
3	E	73	ARG	NE-CZ-NH1	7.91	124.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	73	ARG	NE-CZ-NH1	7.89	124.25	120.30
6	H	73	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	D	73	ARG	NE-CZ-NH1	7.80	124.20	120.30
8	M	15	ARG	CG-CD-NE	-7.79	95.45	111.80
1	B	15	ARG	CG-CD-NE	-7.74	95.56	111.80
1	A	232	ARG	CD-NE-CZ	7.70	134.38	123.60
4	O	73	ARG	NE-CZ-NH1	7.69	124.14	120.30
4	J	73	ARG	NE-CZ-NH1	7.65	124.12	120.30
9	P	232	ARG	CD-NE-CZ	7.64	134.30	123.60
9	P	195	ARG	NE-CZ-NH2	7.48	124.04	120.30
4	F	73	ARG	NE-CZ-NH1	7.45	124.03	120.30
9	P	73	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	73	ARG	NE-CZ-NH1	7.16	123.88	120.30
2	L	73	ARG	NE-CZ-NH1	7.10	123.85	120.30
5	G	73	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	K	73	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	24	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	73	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	L	329	ILE	CB-CG1-CD1	6.65	132.53	113.90
2	D	28	GLU	CA-CB-CG	6.65	128.03	113.40
7	I	73	ARG	NE-CZ-NH1	6.58	123.59	120.30
5	G	24	ARG	NE-CZ-NH2	-6.52	117.04	120.30
8	M	243	LEU	CA-CB-CG	6.50	130.24	115.30
2	D	61	LYS	CD-CE-NZ	-6.42	96.93	111.70
1	C	73	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	24	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	D	24	ARG	NE-CZ-NH2	-6.38	117.11	120.30
8	M	24	ARG	NE-CZ-NH2	-6.25	117.17	120.30
2	D	78	ARG	NE-CZ-NH1	6.22	123.41	120.30
4	F	24	ARG	NE-CZ-NH2	-6.22	117.19	120.30
6	H	73	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	D	73	ARG	NE-CZ-NH2	-6.14	117.23	120.30
4	F	73	ARG	NE-CZ-NH2	-6.14	117.23	120.30
4	O	73	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	N	24	ARG	NE-CZ-NH2	-5.97	117.31	120.30
9	P	24	ARG	NE-CZ-NH2	-5.95	117.32	120.30
3	E	24	ARG	NE-CZ-NH2	-5.94	117.33	120.30
5	G	73	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	15	ARG	CG-CD-NE	-5.92	99.37	111.80
2	D	15	ARG	CG-CD-NE	-5.91	99.40	111.80
4	O	24	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	N	73	ARG	NE-CZ-NH2	-5.86	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	24	ARG	NE-CZ-NH1	5.83	123.22	120.30
4	J	24	ARG	NE-CZ-NH2	-5.81	117.39	120.30
6	H	246	ARG	NE-CZ-NH2	-5.75	117.43	120.30
4	J	73	ARG	NE-CZ-NH2	-5.72	117.44	120.30
7	I	204	ILE	N-CA-C	-5.68	95.67	111.00
3	E	331	LYS	CG-CD-CE	5.67	128.90	111.90
9	P	73	ARG	NE-CZ-NH2	-5.65	117.47	120.30
9	P	204	ILE	N-CA-C	-5.64	95.76	111.00
5	G	24	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	K	246	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	D	246	ARG	CG-CD-NE	5.63	123.63	111.80
3	E	73	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	246	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	L	73	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	L	24	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	L	246	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	107	ARG	CD-NE-CZ	5.56	131.38	123.60
1	B	204	ILE	N-CA-C	-5.55	96.02	111.00
3	E	331	LYS	CD-CE-NZ	5.54	124.43	111.70
1	B	232	ARG	CD-NE-CZ	5.51	131.32	123.60
8	M	246	ARG	CG-CD-NE	5.51	123.38	111.80
6	H	24	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	24	ARG	NE-CZ-NH2	-5.47	117.56	120.30
7	I	232	ARG	NE-CZ-NH2	-5.47	117.57	120.30
8	M	204	ILE	N-CA-C	-5.43	96.33	111.00
5	G	204	ILE	N-CA-C	-5.42	96.36	111.00
5	G	246	ARG	NE-CZ-NH2	-5.41	117.59	120.30
2	D	71	LYS	CA-CB-CG	-5.40	101.52	113.40
1	N	246	ARG	NE-CZ-NH2	-5.40	117.60	120.30
8	M	24	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	176	VAL	N-CA-C	-5.35	96.57	111.00
1	K	78	ARG	NE-CZ-NH1	5.33	122.97	120.30
9	P	195	ARG	CB-CG-CD	-5.33	97.74	111.60
1	N	246	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	N	204	ILE	N-CA-C	-5.31	96.66	111.00
6	H	246	ARG	NE-CZ-NH1	5.29	122.94	120.30
4	J	246	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	K	204	ILE	N-CA-C	-5.24	96.85	111.00
2	D	78	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	204	ILE	N-CA-C	-5.22	96.90	111.00
4	O	204	ILE	N-CA-C	-5.21	96.92	111.00
4	F	24	ARG	NE-CZ-NH1	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	246	ARG	NE-CZ-NH2	-5.21	117.70	120.30
8	M	176	VAL	N-CA-C	-5.20	96.95	111.00
1	A	24	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	L	204	ILE	N-CA-C	-5.18	97.02	111.00
1	C	204	ILE	N-CA-C	-5.16	97.06	111.00
1	A	246	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	246	ARG	CG-CD-NE	5.15	122.62	111.80
3	E	138	LYS	CB-CG-CD	5.15	124.99	111.60
2	D	232	ARG	CD-NE-CZ	5.13	130.79	123.60
1	C	246	ARG	NE-CZ-NH1	5.12	122.86	120.30
9	P	246	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	N	24	ARG	NE-CZ-NH1	5.11	122.86	120.30
7	I	24	ARG	CG-CD-NE	-5.11	101.07	111.80
9	P	246	ARG	NE-CZ-NH2	-5.11	117.75	120.30
4	F	204	ILE	N-CA-C	-5.10	97.23	111.00
2	D	24	ARG	NE-CZ-NH1	5.07	122.84	120.30
3	E	24	ARG	NE-CZ-NH1	5.07	122.83	120.30
4	O	246	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	K	73	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	K	176	VAL	N-CA-C	-5.00	97.49	111.00

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
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
8:M:13:ILE:N	13:M:405:POP:O4	2.26	0.69
1:K:13:ILE:N	14:K:401:NAD:O2N	2.30	0.65
14:E:401:NAD:O1N	14:E:401:NAD:N7N	2.30	0.63
1:C:62:ASP:N	20:C:522:HOH:O	2.31	0.62
1:A:257:LYS:NZ	12:A:407:PO4:O1	2.36	0.58
1:A:2:THR:O	1:A:4:LYS:NZ	2.38	0.57
2:D:253:TYR:N	20:D:503:HOH:O	2.37	0.56
8:M:73:ARG:NH1	8:M:84:LYS:O	2.37	0.56
4:F:278:ASP:N	20:F:523:HOH:O	2.38	0.55
1:B:73:ARG:NH1	1:B:84:LYS:O	2.39	0.55
1:K:120:THR:O	14:K:401:NAD:H1D	2.06	0.55
1:B:24:ARG:NH2	1:B:26:ASP:OD2	2.41	0.54
5:G:192:LYS:N	20:G:506:HOH:O	2.41	0.53
4:J:13:ILE:N	13:J:406:POP:O6	2.42	0.53
1:K:237:ASN:OD1	1:K:314:ASN:OD1	2.27	0.52
1:K:150:CYS:SG	14:K:401:NAD:H4N	2.49	0.52
1:C:164:ASP:O	5:G:249:LYS:NZ	2.41	0.52
1:C:34:ASP:OD1	14:C:401:NAD:H1B	2.11	0.50
1:A:133:GLY:N	11:A:403:CL:CL	2.83	0.49
5:G:267:GLU:CB	20:G:518:HOH:O	2.61	0.48
4:F:13:ILE:N	13:F:403:POP:O3	2.46	0.48
2:D:170:GLU:OE2	2:D:246:ARG:NH1	2.47	0.48
1:B:12:ARG:N	13:B:410:POP:O4	2.48	0.47
1:C:37:ASP:OD1	1:C:37:ASP:N	2.47	0.47
2:D:150:CYS:SG	14:D:401:NAD:H4N	2.54	0.47
1:A:13:ILE:N	13:A:409:POP:O3	2.47	0.47
14:O:401:NAD:H2D	14:O:401:NAD:H2N	1.41	0.47
14:K:401:NAD:H51N	20:K:519:HOH:O	2.14	0.47
2:L:278:ASP:N	20:L:520:HOH:O	2.47	0.46
1:B:24:ARG:NH2	1:B:26:ASP:OD1	2.48	0.46
2:D:150:CYS:SG	14:D:401:NAD:C4N	3.04	0.46
5:G:13:ILE:N	13:G:406:POP:O5	2.49	0.46
1:N:151:THR:N	20:N:504:HOH:O	2.48	0.46
1:K:40:TYR:CD1	2:L:194:TRP:CE2	3.05	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:150:CYS:SG	14:C:401:NAD:H4N	2.57	0.44
14:O:401:NAD:PN	14:O:401:NAD:H3D	2.56	0.44
1:K:257:LYS:NZ	11:K:404:CL:CL	2.88	0.44
13:F:403:POP:O4	13:F:403:POP:O1	2.36	0.43
1:K:124:LYS:NZ	20:K:507:HOH:O	2.51	0.43
12:D:408:PO4:O3	20:D:537:HOH:O	2.21	0.43
3:E:278:ASP:N	20:E:509:HOH:O	2.50	0.43
7:I:29:ILE:N	20:I:506:HOH:O	2.50	0.43
1:A:232:ARG:NH2	20:A:514:HOH:O	2.52	0.43
9:P:150:SCY:N	9:P:150:SCY:CD	2.82	0.43
1:K:254:GLU:CB	20:K:511:HOH:O	2.67	0.42
1:N:278:ASP:O	4:O:43:TYR:OH	2.36	0.42
2:D:43:TYR:CD1	12:D:409:PO4:O3	2.72	0.42
1:B:180:THR:OG1	1:B:232:ARG:NH1	2.52	0.42
1:A:183:GLN:CB	20:A:512:HOH:O	2.68	0.42
4:O:150:CYS:SG	14:O:401:NAD:C4N	3.08	0.42
4:O:249:LYS:CE	20:O:518:HOH:O	2.68	0.41
2:D:180:THR:OG1	2:D:232:ARG:NH1	2.53	0.41
1:C:150:CYS:SG	14:C:401:NAD:C4N	3.09	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
4	F	238	VAL
5	G	238	VAL
6	H	238	VAL
7	I	238	VAL
4	J	238	VAL
1	K	238	VAL
2	L	238	VAL
8	M	238	VAL
1	N	238	VAL
4	O	238	VAL
9	P	238	VAL
4	J	167	GLY

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

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	4	LYS
1	A	173	MET
1	A	232	ARG
1	B	78	ARG
1	B	107	ARG
1	B	173	MET
1	B	232	ARG
1	C	37	ASP
1	C	173	MET
2	D	22	GLN
2	D	173	MET
2	D	232	ARG
3	E	2	THR
3	E	173	MET

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Mol	Chain	Res	Type
3	E	191	HIS
4	F	2	THR
4	F	173	MET
4	F	213	LYS
4	F	249	LYS
5	G	173	MET
6	H	173	MET
7	I	173	MET
4	J	173	MET
1	K	82	ASN
1	K	173	MET
2	L	173	MET
2	L	329	ILE
2	L	331	LYS
8	M	107	ARG
8	M	173	MET
8	M	243	LEU
1	N	173	MET
4	O	173	MET
9	P	173	MET
9	P	232	ARG

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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
1	C	46	ALY	O-C	17.96	1.23	1.11
1	N	46	ALY	O-C	17.90	1.23	1.11
8	M	257	ALY	O-C	17.74	1.23	1.11
4	O	46	ALY	O-C	17.56	1.23	1.11
4	J	46	ALY	O-C	17.40	1.23	1.11
7	I	46	ALY	O-C	17.29	1.23	1.11
1	K	46	ALY	O-C	17.13	1.23	1.11
1	B	46	ALY	O-C	17.08	1.23	1.11
7	I	257	ALY	O-C	17.06	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	46	ALY	O-C	17.02	1.23	1.11
6	H	46	ALY	O-C	16.30	1.22	1.11
9	P	46	ALY	O-C	16.23	1.22	1.11
4	O	257	ALY	O-C	16.20	1.22	1.11
4	F	257	ALY	O-C	15.99	1.22	1.11
5	G	46	ALY	O-C	15.78	1.22	1.11
6	H	257	ALY	O-C	15.56	1.22	1.11
4	F	46	ALY	O-C	14.44	1.21	1.11
7	I	249	ALY	O-C	13.89	1.20	1.11
9	P	249	ALY	O-C	12.80	1.20	1.11
3	E	249	ALY	O-C	12.02	1.19	1.11
9	P	150	SCY	CB-SG	-4.34	1.76	1.81
6	H	150	SCY	CB-SG	-3.45	1.77	1.81
4	F	257	ALY	CH-NZ	3.25	1.41	1.33
5	G	150	SCY	CB-SG	-3.24	1.77	1.81
8	M	257	ALY	CE-NZ	3.12	1.53	1.46
4	J	257	ALY	CE-NZ	3.09	1.53	1.46
6	H	46	ALY	CE-NZ	3.03	1.53	1.46
4	F	257	ALY	CE-NZ	3.03	1.53	1.46
7	I	257	ALY	CB-CA	-2.90	1.50	1.53
8	M	257	ALY	CH-NZ	2.89	1.41	1.33
4	O	257	ALY	CB-CA	-2.80	1.50	1.53
7	I	46	ALY	CE-NZ	2.78	1.52	1.46
6	H	257	ALY	CH-NZ	2.60	1.40	1.33
6	H	46	ALY	OH-CH	-2.53	1.17	1.23
1	C	46	ALY	CB-CA	2.52	1.57	1.53
1	B	46	ALY	CE-NZ	2.52	1.52	1.46
7	I	257	ALY	CE-NZ	2.40	1.51	1.46
9	P	46	ALY	CE-NZ	2.38	1.51	1.46
4	J	257	ALY	CH-NZ	2.37	1.39	1.33
7	I	46	ALY	OH-CH	-2.32	1.17	1.23
1	K	46	ALY	CA-C	2.31	1.54	1.49
6	H	257	ALY	CE-NZ	2.31	1.51	1.46
1	N	46	ALY	CE-NZ	2.30	1.51	1.46
1	B	46	ALY	OH-CH	-2.26	1.17	1.23
4	O	257	ALY	CE-NZ	2.23	1.51	1.46
4	J	46	ALY	CE-NZ	2.22	1.51	1.46
6	H	257	ALY	CB-CA	2.16	1.56	1.53
1	A	46	ALY	CE-NZ	2.11	1.51	1.46

All (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
6	H	257	ALY	CE-NZ-CH	13.47	144.41	122.35
8	M	257	ALY	CE-NZ-CH	11.87	141.79	122.35
1	B	46	ALY	CE-NZ-CH	8.92	136.95	122.35
1	C	46	ALY	CE-NZ-CH	8.90	136.93	122.35
7	I	46	ALY	CE-NZ-CH	8.68	136.57	122.35
3	E	46	ALY	CE-NZ-CH	8.67	136.54	122.35
4	F	46	ALY	CE-NZ-CH	8.10	135.61	122.35
4	J	46	ALY	CE-NZ-CH	7.95	135.38	122.35
6	H	150	SCY	CB-SG-CD	-7.79	95.91	100.87
4	O	46	ALY	CE-NZ-CH	7.74	135.03	122.35
1	A	46	ALY	CE-NZ-CH	7.74	135.02	122.35
5	G	46	ALY	CE-NZ-CH	7.72	134.99	122.35
1	K	46	ALY	CE-NZ-CH	7.62	134.82	122.35
8	M	257	ALY	CH3-CH-NZ	7.56	127.57	116.15
9	P	46	ALY	CE-NZ-CH	7.28	134.27	122.35
3	E	249	ALY	CE-NZ-CH	7.02	133.84	122.35
9	P	249	ALY	CE-NZ-CH	7.00	133.81	122.35
4	J	257	ALY	CH3-CH-NZ	6.99	126.71	116.15
5	G	150	SCY	CB-SG-CD	-6.69	96.61	100.87
1	N	46	ALY	CE-NZ-CH	5.84	131.92	122.35
8	M	257	ALY	CD-CE-NZ	-5.75	95.08	112.20
4	J	257	ALY	CD-CE-NZ	-5.56	95.65	112.20
6	H	46	ALY	CE-NZ-CH	5.51	131.38	122.35
1	N	46	ALY	CH3-CH-NZ	5.46	124.40	116.15
7	I	257	ALY	OH-CH-NZ	5.03	130.62	121.89
4	F	257	ALY	OH-CH-NZ	4.99	130.54	121.89
6	H	46	ALY	CH3-CH-NZ	4.94	123.61	116.15
3	E	249	ALY	C-CA-N	-4.93	108.90	113.83
6	H	257	ALY	C-CA-N	-4.91	108.92	113.83
6	H	257	ALY	OH-CH-NZ	4.89	130.36	121.89
9	P	249	ALY	C-CA-N	-4.85	108.99	113.83
7	I	249	ALY	CE-NZ-CH	4.76	130.15	122.35
8	M	257	ALY	OH-CH-CH3	-4.70	113.03	122.04
4	O	257	ALY	CD-CE-NZ	-4.55	98.65	112.20
4	O	257	ALY	OH-CH-NZ	4.54	129.76	121.89
9	P	46	ALY	CH3-CH-NZ	4.37	122.76	116.15
7	I	257	ALY	CD-CE-NZ	-4.36	99.23	112.20
1	B	46	ALY	C-CA-N	-4.26	109.58	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	257	ALY	OH-CH-CH3	-4.20	113.99	122.04
4	J	257	ALY	C-CA-N	-4.18	109.66	113.83
4	F	257	ALY	C-CA-N	-4.16	109.67	113.83
4	F	257	ALY	OH-CH-CH3	-4.08	114.22	122.04
4	J	257	ALY	OH-CH-CH3	-4.07	114.24	122.04
7	I	249	ALY	CD-CE-NZ	-4.07	100.09	112.20
8	M	257	ALY	C-CA-N	-3.96	109.87	113.83
1	A	46	ALY	CH3-CH-NZ	3.92	122.08	116.15
4	O	46	ALY	CH3-CH-NZ	3.82	121.92	116.15
7	I	249	ALY	C-CA-N	-3.82	110.02	113.83
1	K	46	ALY	CH3-CH-NZ	3.72	121.77	116.15
4	J	46	ALY	CH3-CH-NZ	3.72	121.76	116.15
8	M	257	ALY	CG-CD-CE	3.71	134.08	113.99
4	F	46	ALY	CH3-CH-NZ	3.65	121.67	116.15
7	I	257	ALY	OH-CH-CH3	-3.56	115.21	122.04
4	J	257	ALY	CG-CD-CE	3.55	133.18	113.99
1	N	46	ALY	OH-CH-CH3	-3.46	115.41	122.04
5	G	46	ALY	CH3-CH-NZ	3.41	121.30	116.15
7	I	257	ALY	C-CA-N	-3.38	110.45	113.83
3	E	46	ALY	CH3-CH-NZ	3.37	121.24	116.15
1	C	46	ALY	CH3-CH-NZ	3.29	121.12	116.15
9	P	249	ALY	CH3-CH-NZ	3.27	121.10	116.15
9	P	46	ALY	C-CA-N	-3.21	110.62	113.83
3	E	249	ALY	CH3-CH-NZ	3.18	120.96	116.15
1	C	46	ALY	C-CA-N	-3.15	110.69	113.83
6	H	257	ALY	CB-CA-N	3.11	119.18	110.35
7	I	46	ALY	CH3-CH-NZ	3.05	120.76	116.15
6	H	46	ALY	OH-CH-CH3	-3.01	116.27	122.04
4	O	257	ALY	C-CA-N	-3.00	110.84	113.83
4	O	257	ALY	OH-CH-CH3	-2.98	116.33	122.04
1	B	46	ALY	CH3-CH-NZ	2.95	120.60	116.15
4	F	257	ALY	CB-CA-N	2.91	118.64	110.35
1	A	46	ALY	OH-CH-CH3	-2.89	116.51	122.04
1	N	46	ALY	C-CA-N	-2.85	110.98	113.83
9	P	46	ALY	OH-CH-CH3	-2.82	116.64	122.04
1	A	46	ALY	C-CA-N	-2.71	111.12	113.83
6	H	150	SCY	OCD-CD-CE	-2.68	114.24	123.22
4	O	46	ALY	C-CA-N	-2.58	111.26	113.83
5	G	46	ALY	OH-CH-CH3	-2.52	117.20	122.04
1	C	46	ALY	CG-CB-CA	2.49	122.58	113.89
1	B	46	ALY	CG-CB-CA	2.48	122.56	113.89
5	G	150	SCY	CA-CB-SG	2.48	118.40	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	46	ALY	OH-CH-CH3	-2.48	117.29	122.04
4	O	46	ALY	OH-CH-CH3	-2.46	117.32	122.04
6	H	46	ALY	CG-CB-CA	2.41	122.31	113.89
7	I	46	ALY	C-CA-N	-2.40	111.43	113.83
4	O	257	ALY	CG-CD-CE	2.40	126.96	113.99
1	K	46	ALY	OH-CH-CH3	-2.38	117.47	122.04
7	I	257	ALY	CG-CD-CE	2.34	126.65	113.99
9	P	150	SCY	C-CA-N	-2.34	111.50	113.83
1	N	46	ALY	CG-CB-CA	2.32	121.98	113.89
7	I	249	ALY	CH3-CH-NZ	2.30	119.63	116.15
4	F	46	ALY	C-CA-N	-2.29	111.54	113.83
4	J	46	ALY	CG-CB-CA	2.28	121.86	113.89
9	P	150	SCY	CA-CB-SG	2.28	117.96	112.89
4	O	46	ALY	CG-CB-CA	2.28	121.85	113.89
1	C	46	ALY	OH-CH-CH3	-2.25	117.74	122.04
9	P	46	ALY	CG-CB-CA	2.24	121.72	113.89
4	J	46	ALY	OH-CH-CH3	-2.24	117.75	122.04
1	K	46	ALY	CG-CB-CA	2.18	121.50	113.89
1	A	46	ALY	CG-CB-CA	2.14	121.37	113.89
4	F	46	ALY	CG-CB-CA	2.13	121.34	113.89
5	G	46	ALY	CG-CB-CA	2.13	121.33	113.89
5	G	150	SCY	OCD-CD-CE	-2.12	116.11	123.22
7	I	46	ALY	CG-CB-CA	2.11	121.26	113.89
9	P	150	SCY	CE-CD-SG	2.10	122.30	113.58
3	E	46	ALY	CG-CB-CA	2.07	121.13	113.89
7	I	46	ALY	OH-CH-CH3	-2.00	118.20	122.04

There are no chirality outliers.

All (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
1	B	46	ALY	OH-CH-NZ-CE
4	O	46	ALY	OH-CH-NZ-CE
3	E	249	ALY	OH-CH-NZ-CE
6	H	46	ALY	OH-CH-NZ-CE
5	G	46	ALY	OH-CH-NZ-CE
4	J	46	ALY	OH-CH-NZ-CE

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Mol	Chain	Res	Type	Atoms
7	I	249	ALY	OH-CH-NZ-CE
1	N	46	ALY	OH-CH-NZ-CE
1	C	46	ALY	OH-CH-NZ-CE
1	A	46	ALY	OH-CH-NZ-CE
9	P	46	ALY	CH3-CH-NZ-CE
4	O	46	ALY	CH3-CH-NZ-CE
7	I	46	ALY	OH-CH-NZ-CE
1	A	46	ALY	CH3-CH-NZ-CE
7	I	46	ALY	CH3-CH-NZ-CE
4	J	46	ALY	CH3-CH-NZ-CE
4	F	46	ALY	CH3-CH-NZ-CE
9	P	249	ALY	CH3-CH-NZ-CE
1	K	46	ALY	CH3-CH-NZ-CE
8	M	257	ALY	OH-CH-NZ-CE
3	E	46	ALY	CH3-CH-NZ-CE
1	N	46	ALY	CH3-CH-NZ-CE
3	E	249	ALY	CH3-CH-NZ-CE
4	J	257	ALY	OH-CH-NZ-CE
5	G	46	ALY	CH3-CH-NZ-CE
7	I	249	ALY	CH3-CH-NZ-CE
1	B	46	ALY	CH3-CH-NZ-CE
6	H	46	ALY	CH3-CH-NZ-CE
1	C	46	ALY	CH3-CH-NZ-CE
8	M	257	ALY	CH3-CH-NZ-CE
4	J	257	ALY	CH3-CH-NZ-CE
5	G	150	SCY	CE-CD-SG-CB
6	H	150	SCY	CE-CD-SG-CB

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%)
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
12	PO4	P	404	-	-	0/0/0/0	0/0/0/0
12	PO4	P	405	-	-	0/0/0/0	0/0/0/0

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	401	NAD	C5A-C4A	3.85	1.49	1.40
14	I	401	NAD	O4D-C1D	3.66	1.45	1.41
14	P	401	NAD	C4A-N9A	-3.50	1.32	1.37
14	K	401	NAD	C4A-N9A	-3.36	1.32	1.37
14	C	401	NAD	O4B-C1B	3.35	1.45	1.41
14	P	401	NAD	C5A-C4A	3.23	1.47	1.40
14	D	401	NAD	C5A-C4A	3.17	1.47	1.40
14	I	401	NAD	C5A-C4A	3.12	1.47	1.40
14	C	401	NAD	C2A-N3A	3.11	1.37	1.32
14	K	401	NAD	C5A-C4A	3.07	1.47	1.40
14	D	401	NAD	O4B-C1B	3.01	1.45	1.41
14	E	401	NAD	C5A-C4A	2.87	1.47	1.40
14	C	401	NAD	PN-O2N	2.86	1.55	1.48
19	M	404	UVW	P-O2	2.81	1.64	1.60
14	O	401	NAD	O4D-C1D	2.80	1.44	1.41
14	C	401	NAD	PN-O1N	2.74	1.55	1.48
14	O	401	NAD	O4B-C1B	2.72	1.44	1.41
14	D	401	NAD	O4D-C1D	2.48	1.44	1.41
14	P	401	NAD	O4B-C1B	2.43	1.44	1.41
14	D	401	NAD	C4A-N9A	-2.32	1.34	1.37
14	O	401	NAD	PA-O3	2.28	1.63	1.59
14	I	401	NAD	O4B-C1B	2.25	1.44	1.41
14	E	401	NAD	C4A-N9A	-2.12	1.34	1.37
14	K	401	NAD	O4B-C1B	2.12	1.43	1.41
14	O	401	NAD	C5A-C4A	2.12	1.45	1.40
15	H	404	ACT	CH3-C	2.10	1.51	1.48
14	I	401	NAD	C2A-N3A	2.08	1.35	1.32
14	C	401	NAD	C2N-C3N	2.04	1.42	1.39

All (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
14	D	401	NAD	C5A-C4A-N3A	-7.66	118.51	125.98
14	E	401	NAD	N3A-C2A-N1A	-7.59	122.21	128.89
14	P	401	NAD	O4D-C1D-N1N	7.44	116.30	108.13
14	D	401	NAD	N3A-C2A-N1A	-7.43	122.36	128.89
14	I	401	NAD	O4D-C1D-N1N	7.18	116.03	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	401	NAD	N3A-C2A-N1A	-7.17	122.58	128.89
14	E	401	NAD	C5A-C4A-N3A	-6.98	119.17	125.98
14	C	401	NAD	O4D-C1D-N1N	6.19	114.94	108.13
14	I	401	NAD	N3A-C2A-N1A	-6.11	123.52	128.89
19	M	404	UVW	O2-C1-O1	-5.91	117.63	122.07
14	D	401	NAD	N3A-C4A-N9A	5.71	135.18	125.39
14	C	401	NAD	N3A-C2A-N1A	-5.66	123.92	128.89
14	P	401	NAD	C5A-C4A-N3A	-5.65	120.47	125.98
14	I	401	NAD	N3A-C4A-N9A	5.64	135.07	125.39
14	K	401	NAD	N3A-C2A-N1A	-5.57	123.99	128.89
14	O	401	NAD	N3A-C4A-N9A	5.47	134.78	125.39
14	K	401	NAD	N3A-C4A-N9A	5.35	134.57	125.39
14	C	401	NAD	N3A-C4A-N9A	5.11	134.16	125.39
14	E	401	NAD	N3A-C4A-N9A	5.05	134.06	125.39
14	E	401	NAD	PN-O3-PA	-4.69	114.30	133.17
14	C	401	NAD	C4A-C5A-N7A	-4.51	105.06	109.41
14	P	401	NAD	N3A-C4A-N9A	4.50	133.12	125.39
14	O	401	NAD	O4D-C1D-N1N	4.39	112.96	108.13
14	D	401	NAD	O4D-C1D-N1N	4.38	112.95	108.13
13	A	409	POP	P2-O-P1	-4.28	119.16	132.02
14	O	401	NAD	C4A-C5A-N7A	-4.25	105.31	109.41
14	K	401	NAD	O2N-PN-O3	-4.19	97.30	108.85
14	E	401	NAD	C3N-C7N-N7N	-4.02	113.30	117.78
13	A	409	POP	O-P2-O4	-3.93	95.95	107.65
13	M	405	POP	P2-O-P1	-3.91	120.28	132.02
14	K	401	NAD	O4D-C1D-N1N	3.85	112.36	108.13
14	K	401	NAD	C4A-C5A-N7A	-3.82	105.72	109.41
14	C	401	NAD	O3-PN-O1N	-3.75	99.70	108.77
14	D	401	NAD	PN-O3-PA	-3.74	118.12	133.17
14	O	401	NAD	C3D-C2D-C1D	3.51	106.42	100.92
14	K	401	NAD	C2D-C1D-N1N	3.46	120.39	113.48
14	O	401	NAD	C2A-N3A-C4A	3.36	122.93	113.27
14	C	401	NAD	C2A-N3A-C4A	3.18	122.43	113.27
14	O	401	NAD	PN-O3-PA	-3.17	120.41	133.17
14	I	401	NAD	PN-O3-PA	-3.17	120.42	133.17
14	E	401	NAD	C4A-C5A-N7A	-3.16	106.35	109.41
19	M	404	UVW	O2-C1-C1M	3.11	119.12	112.10
14	I	401	NAD	C4A-C5A-N7A	-3.05	106.46	109.41
13	F	403	POP	P2-O-P1	-3.05	122.87	132.02
14	E	401	NAD	C2A-N3A-C4A	2.97	121.81	113.27
14	D	401	NAD	C2A-N3A-C4A	2.96	121.80	113.27
19	M	404	UVW	P-O2-C1	2.95	126.12	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	401	NAD	O3-PN-O1N	-2.94	101.66	108.77
13	M	405	POP	O-P1-O1	-2.94	98.91	107.65
14	K	401	NAD	C2A-N3A-C4A	2.87	121.54	113.27
14	K	401	NAD	PN-O3-PA	-2.83	121.79	133.17
14	E	401	NAD	C3D-C2D-C1D	2.76	105.26	100.92
14	O	401	NAD	C2D-C1D-N1N	-2.73	108.03	113.48
13	F	403	POP	O3-P1-O	-2.71	98.03	106.53
14	I	401	NAD	C2A-N3A-C4A	2.71	121.08	113.27
13	M	405	POP	O-P2-O4	-2.66	99.73	107.65
13	M	405	POP	O5-P2-O6	2.63	121.11	110.63
14	O	401	NAD	C8A-N9A-C4A	2.56	109.04	106.96
14	P	401	NAD	C2N-C3N-C4N	2.54	121.16	118.31
14	P	401	NAD	C2A-N3A-C4A	2.43	120.27	113.27
14	C	401	NAD	O2N-PN-O1N	2.42	125.93	118.70
14	K	401	NAD	C3B-C2B-C1B	2.42	104.72	100.92
14	D	401	NAD	C2B-C3B-C4B	2.41	107.44	102.64
14	D	401	NAD	C3N-C7N-N7N	2.39	120.45	117.78
13	B	410	POP	O-P2-O4	-2.38	100.57	107.65
13	M	405	POP	O2-P1-O1	2.38	119.47	110.88
14	P	401	NAD	C8A-N9A-C4A	2.36	108.88	106.96
14	D	401	NAD	C3B-C2B-C1B	2.34	104.59	100.92
14	P	401	NAD	C2A-N1A-C6A	2.33	122.92	118.76
14	P	401	NAD	C3B-C2B-C1B	2.32	104.56	100.92
14	D	401	NAD	C4A-C5A-N7A	-2.29	107.20	109.41
14	C	401	NAD	C3B-C2B-C1B	2.27	104.48	100.92
14	E	401	NAD	C2N-C3N-C4N	2.21	120.79	118.31
14	O	401	NAD	C4B-O4B-C1B	-2.20	107.30	109.72
13	J	406	POP	O-P1-O1	-2.16	101.22	107.65
14	D	401	NAD	O2N-PN-O1N	2.15	125.12	118.70
14	P	401	NAD	C4A-C5A-N7A	-2.11	107.37	109.41
13	B	410	POP	O-P1-O1	-2.11	101.37	107.65
14	I	401	NAD	C8A-N9A-C4A	2.11	108.67	106.96
13	A	409	POP	O3-P1-O	-2.09	99.98	106.53
14	D	401	NAD	O7N-C7N-N7N	-2.09	119.60	122.59
14	D	401	NAD	O3D-C3D-C2D	-2.08	105.12	111.83
14	K	401	NAD	C3N-C7N-N7N	-2.07	115.47	117.78
13	A	409	POP	O5-P2-O	2.07	110.91	104.28
14	K	401	NAD	C2B-C1B-N9A	-2.07	107.71	113.35
14	I	401	NAD	O3D-C3D-C2D	-2.07	105.14	111.83
14	O	401	NAD	C2A-N1A-C6A	2.03	122.38	118.76
13	J	406	POP	O5-P2-O4	2.02	118.19	110.88
14	P	401	NAD	C1B-N9A-C4A	-2.02	123.15	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	401	NAD	C2A-N1A-C6A	2.01	122.33	118.76
14	E	401	NAD	C2D-C1D-N1N	-2.00	109.48	113.48

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%)

All (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

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Mol	Chain	Res	Type	RSRZ
4	F	139	TYR	4.0
3	E	1	MET	3.9
1	N	2	THR	3.8
5	G	59	GLU	3.7
1	N	115	LYS	3.6
1	B	1	MET	3.6
6	H	331	LYS	3.6
3	E	61	LYS	3.5
4	O	174	THR	3.4
4	J	331	LYS	3.4
2	L	150	CYS	3.4
1	K	191[A]	HIS	3.3
2	D	1	MET	3.3
9	P	84	LYS	3.3
7	I	331	LYS	3.3
1	K	59	GLU	3.2
1	A	1	MET	3.2
2	L	1	MET	3.2
2	L	137	ASP	3.2
9	P	331	LYS	3.1
4	F	213	LYS	3.1
2	L	67	VAL	3.1
1	N	1	MET	3.0
1	N	290	THR	3.0
9	P	2	THR	3.0
1	N	62	ASP	3.0
2	L	26	ASP	3.0
1	N	35	LEU	2.9
2	L	68	ASN	2.9
3	E	69	GLY	2.9
4	F	308	LEU	2.8
7	I	23	LYS	2.7
9	P	267	GLU	2.7
3	E	87	GLU	2.7
2	D	317	GLY	2.7
7	I	330	SER	2.7
3	E	86	ASP	2.7
3	E	331	LYS	2.6
4	O	1	MET	2.6
4	F	69	GLY	2.6
2	L	3	ILE	2.6
2	L	267	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
8	M	78	ARG	2.6
3	E	70	LYS	2.6
3	E	25	SER	2.6
4	F	150	CYS	2.6
4	F	267	GLU	2.6
1	N	101	LEU	2.5
1	C	62	ASP	2.5
1	A	174	THR	2.5
2	L	60	VAL	2.5
1	K	69	GLY	2.5
4	O	62	ASP	2.5
1	K	1	MET	2.4
1	N	119	MET	2.4
2	D	331	LYS	2.4
8	M	150	CYS	2.4
2	L	27	ILE	2.4
2	L	124	LYS	2.4
4	F	331	LYS	2.4
1	C	137	ASP	2.4
2	L	59	GLU	2.3
5	G	144	ILE	2.3
2	D	62	ASP	2.3
1	N	211	ALA	2.3
7	I	78	ARG	2.3
9	P	104	GLU	2.3
1	N	116	LYS	2.3
4	F	118	VAL	2.3
1	N	8	ASN	2.3
2	L	58	VAL	2.3
6	H	13	ILE	2.3
6	H	137	ASP	2.3
4	F	138	LYS	2.3
9	P	77	GLU	2.3
9	P	83	LEU	2.3
4	F	99	LEU	2.2
4	F	137[A]	ASP	2.2
1	N	215	VAL	2.2
1	N	129	MET	2.2
9	P	253	TYR	2.2
6	H	1	MET	2.2
1	N	291	SER	2.1
4	J	242	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
7	I	62	ASP	2.1
7	I	71	LYS	2.1
1	N	123	SER	2.1
9	P	130	PHE	2.1
1	C	1	MET	2.1
1	A	62	ASP	2.1
5	G	191[A]	HIS	2.1
9	P	57	THR	2.1
4	F	130	PHE	2.1
2	L	66	ILE	2.1
3	E	94	ALA	2.1
5	G	150	SCY	2.1
5	G	139	TYR	2.0
2	L	244	THR	2.0
4	O	150	CYS	2.0
2	D	267	GLU	2.0
8	M	192	LYS	2.0
1	N	216	GLY	2.0

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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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(\AA^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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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.