



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:36 AM GMT

PDB ID : 3QW2
Title : L-myo-inositol 1-phosphate synthase from Archaeoglobus mutant N255A
Authors : Neelon, K.; Roberts, M.F.; Stec, B.
Deposited on : 2011-02-26
Resolution : 2.59 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>

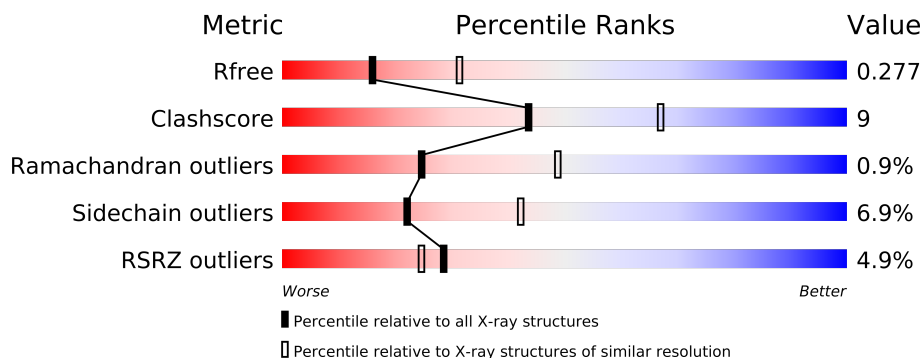
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.59 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	392	
1	B	392	
1	C	392	
1	D	392	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	393	-	X
5	SO4	C	394	-	X
5	SO4	C	397	-	X
6	K	C	398	-	X
6	K	D	397	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13061 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 Myo-inositol-1-phosphatesynthase (Ino1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			
1	B	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			
1	C	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			
1	D	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			

There are 4 discrepancies between the modelled and reference sequences:

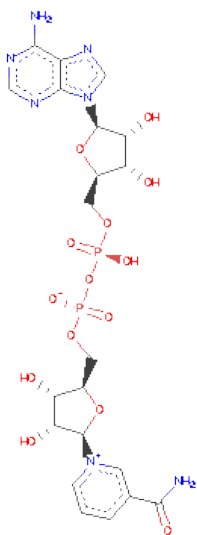
Chain	Residue	Modelled	Actual	Comment	Reference
A	255	ALA	ASN	ENGINEERED MUTATION	UNP O28480
B	255	ALA	ASN	ENGINEERED MUTATION	UNP O28480
C	255	ALA	ASN	ENGINEERED MUTATION	UNP O28480
D	255	ALA	ASN	ENGINEERED MUTATION	UNP O28480

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



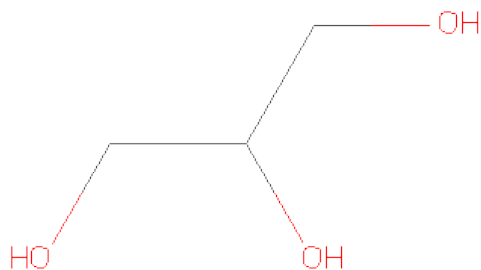
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	D	1	Total	K	0	0
			1	1		
6	C	1	Total	K	0	0
			1	1		

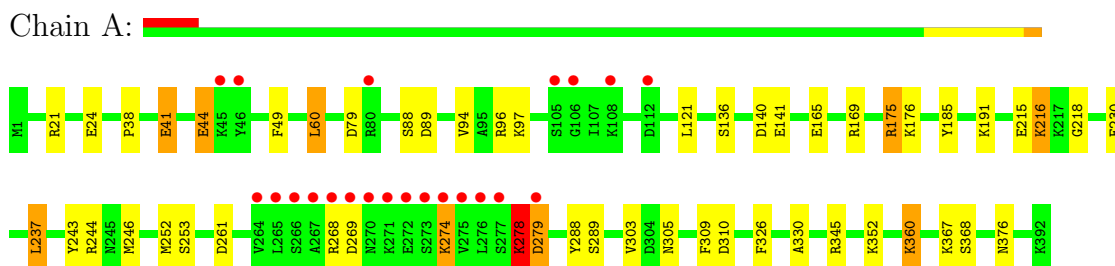
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	115	Total 115	O 115	0	0
7	B	100	Total 100	O 100	0	0
7	C	138	Total 138	O 138	0	0
7	D	133	Total 133	O 133	0	0

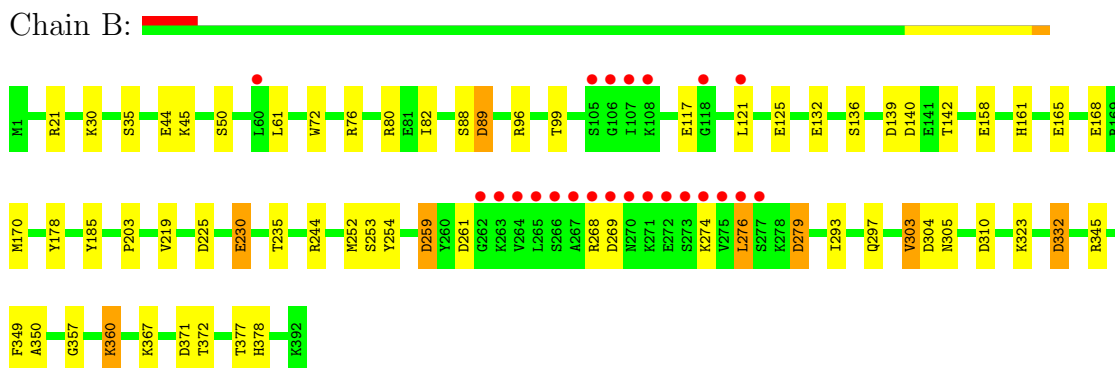
3 Residue-property plots

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: Myo-inositol-1-phosphatesynthase (Ino1)



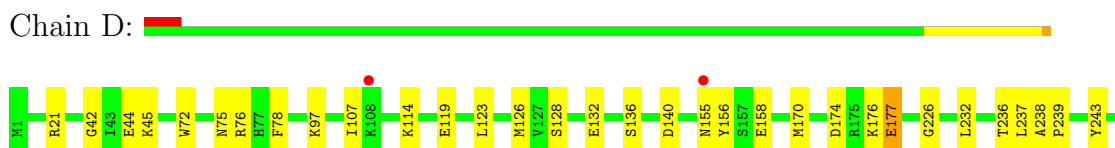
- Molecule 1: Myo-inositol-1-phosphatesynthase (Ino1)

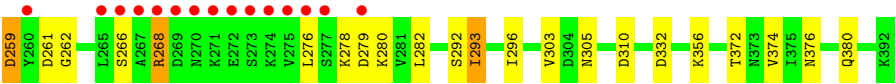


- Molecule 1: Myo-inositol-1-phosphatesynthase (Ino1)



- Molecule 1: Myo-inositol-1-phosphatesynthase (Ino1)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.51Å 88.04Å 103.73Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	103.14 – 2.59 38.71 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.3 (103.14-2.59) 96.4 (38.71-2.59)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.267 0.193 , 0.277	Depositor DCC
R_{free} test set	2506 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 6.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49234 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13061	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: PO4, GOL, K, SO4, NAD

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	0.72	0/3152	0.78	1/4253 (0.0%)
1	B	0.73	0/3152	0.78	2/4253 (0.0%)
1	C	0.73	0/3152	0.79	2/4253 (0.0%)
1	D	0.74	0/3152	0.78	1/4253 (0.0%)
All	All	0.73	0/12608	0.79	6/17012 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	LEU	CA-CB-CG	6.21	129.58	115.30
1	B	61	LEU	CA-CB-CG	6.09	129.30	115.30
1	C	61	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	60	LEU	CA-CB-CG	5.68	128.37	115.30
1	D	276	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	74	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3081	0	0	27	0
1	B	3081	0	0	32	0
1	C	3081	0	0	19	0
1	D	3081	0	0	31	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	4	0
3	C	44	0	26	1	0
3	D	44	0	26	3	0
4	A	6	0	8	1	0
4	B	6	0	8	2	0
5	A	5	0	0	0	0
5	B	10	0	0	2	0
5	C	15	0	0	2	0
5	D	10	0	0	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	115	0	0	9	0
7	B	100	0	0	12	0
7	C	138	0	0	13	0
7	D	133	0	0	16	0
All	All	13061	0	120	111	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 9.

All (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:126:MET:SD	7:D:466:HOH:O	2.16	1.01
1:D:259:ASP:CB	7:D:484:HOH:O	2.23	0.84
1:A:121:LEU:O	1:A:176:LYS:NZ	2.13	0.81
1:C:169:ARG:NH2	7:C:405:HOH:O	2.12	0.81
1:B:21:ARG:CD	7:B:460:HOH:O	2.33	0.77
1:C:260:TYR:CD1	7:C:469:HOH:O	2.38	0.77
1:A:243:TYR:OH	1:B:378:HIS:CD2	2.45	0.70
1:C:260:TYR:CG	7:C:469:HOH:O	2.46	0.69
1:A:49:PHE:CD1	7:A:423:HOH:O	2.44	0.69
1:A:253:SER:CB	7:A:399:HOH:O	2.41	0.69
1:B:121:LEU:CB	7:B:430:HOH:O	2.40	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:C:400:HOH:O	1:D:237:LEU:CD2	2.42	0.67
1:C:378:HIS:CD2	1:D:243:TYR:OH	2.48	0.65
1:A:269:ASP:OD2	7:A:473:HOH:O	2.14	0.65
1:A:141:GLU:OE2	1:A:352:LYS:NZ	2.31	0.64
1:C:215:GLU:CG	7:C:445:HOH:O	2.45	0.64
1:C:107:ILE:CD1	7:C:520:HOH:O	2.46	0.63
1:B:293:ILE:CB	7:D:512:HOH:O	2.47	0.62
1:B:230:GLU:OE2	1:B:253:SER:CB	2.48	0.62
1:B:80:ARG:CD	7:B:463:HOH:O	2.49	0.61
1:D:42:GLY:N	7:D:421:HOH:O	2.33	0.60
1:D:226:GLY:O	3:D:396:NAD:H5N	2.01	0.60
3:D:396:NAD:C4N	7:D:524:HOH:O	2.50	0.60
1:A:244:ARG:NH1	7:A:443:HOH:O	2.37	0.58
1:B:274:LYS:NZ	4:B:397:GOL:O1	2.37	0.57
1:B:244:ARG:NH1	7:B:492:HOH:O	2.37	0.57
1:D:72:TRP:NE1	1:D:78:PHE:O	2.37	0.57
1:A:345:ARG:NH1	7:A:423:HOH:O	2.38	0.57
1:C:80:ARG:NH2	7:C:514:HOH:O	2.38	0.57
1:D:177:GLU:CG	7:D:458:HOH:O	2.54	0.56
1:C:373:ASN:N	5:C:397:SO4:O2	2.38	0.56
1:A:175:ARG:CA	1:A:175:ARG:NE	2.69	0.56
1:B:30:LYS:N	7:B:470:HOH:O	2.38	0.56
1:B:261:ASP:CB	7:B:479:HOH:O	2.54	0.56
1:B:82:ILE:CG2	7:B:491:HOH:O	2.53	0.55
1:A:360:LYS:CD	7:A:470:HOH:O	2.54	0.54
1:D:97:LYS:CE	1:D:119:GLU:OE1	2.56	0.54
1:A:21:ARG:NH1	1:A:89:ASP:OD1	2.41	0.53
1:C:226:GLY:O	3:C:396:NAD:H5N	2.08	0.53
1:A:305:ASN:ND2	1:A:330:ALA:O	2.43	0.52
1:A:97:LYS:NZ	7:A:502:HOH:O	2.43	0.51
1:C:274:LYS:NZ	7:C:424:HOH:O	2.42	0.51
1:B:372:THR:OG1	5:B:394:SO4:O1	2.29	0.51
3:D:396:NAD:H4N	7:D:524:HOH:O	2.10	0.50
1:C:283:GLU:CG	7:C:428:HOH:O	2.59	0.49
3:B:396:NAD:H2D	4:B:397:GOL:O3	2.12	0.49
1:B:323:LYS:NZ	7:B:408:HOH:O	2.45	0.49
1:A:237:LEU:CD1	7:B:451:HOH:O	2.60	0.49
1:B:125:GLU:CB	7:B:430:HOH:O	2.61	0.49
1:D:114:LYS:NZ	7:D:420:HOH:O	2.46	0.48
1:B:72:TRP:O	1:B:76:ARG:N	2.46	0.48
1:B:225:ASP:O	1:B:367:LYS:N	2.46	0.48
1:B:349:PHE:O	1:B:350:ALA:C	2.51	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:TYR:N	1:A:288:TYR:CD1	2.80	0.48
1:B:89:ASP:N	1:B:89:ASP:OD2	2.47	0.48
1:A:230:GLU:OE1	1:A:278:LYS:NZ	2.46	0.48
1:B:360:LYS:CG	7:B:483:HOH:O	2.62	0.48
1:C:296:ILE:CB	7:C:502:HOH:O	2.62	0.48
1:D:376:ASN:C	1:D:376:ASN:OD1	2.52	0.48
1:D:45:LYS:CE	7:D:423:HOH:O	2.61	0.47
1:D:123:LEU:CD2	1:D:126:MET:CE	2.93	0.47
1:B:367:LYS:NZ	2:B:395:PO4:O3	2.47	0.47
1:D:280:LYS:CG	7:D:444:HOH:O	2.62	0.46
1:A:274:LYS:NZ	4:A:397:GOL:H11	2.31	0.46
1:D:75:ASN:O	1:D:76:ARG:C	2.54	0.46
1:B:279:ASP:N	1:B:279:ASP:OD2	2.50	0.45
1:D:174:ASP:OD2	1:D:176:LYS:NZ	2.50	0.45
1:B:35:SER:OG	1:B:345:ARG:NH1	2.50	0.45
1:B:117:GLU:N	1:B:117:GLU:OE2	2.50	0.44
1:C:237:LEU:CB	7:C:400:HOH:O	2.65	0.44
1:D:238:ALA:N	1:D:239:PRO:CD	2.80	0.44
1:A:376:ASN:C	1:A:376:ASN:OD1	2.56	0.44
1:B:254:TYR:OH	1:B:297:GLN:CG	2.66	0.44
1:A:215:GLU:O	1:A:218:GLY:N	2.50	0.44
1:D:262:GLY:N	7:D:505:HOH:O	2.50	0.44
1:D:372:THR:OG1	5:D:393:SO4:O4	2.36	0.44
1:A:367:LYS:NZ	2:A:395:PO4:O3	2.50	0.44
1:A:44:GLU:OE1	1:A:44:GLU:N	2.51	0.44
1:D:21:ARG:NH1	7:D:425:HOH:O	2.51	0.43
1:D:156:TYR:CD1	1:D:156:TYR:C	2.91	0.43
1:A:230:GLU:CG	7:A:399:HOH:O	2.66	0.43
1:A:38:PRO:O	1:A:41:GLU:CG	2.67	0.43
1:B:332:ASP:OD2	3:B:396:NAD:C7N	2.67	0.43
1:C:315:LYS:NZ	7:C:483:HOH:O	2.52	0.42
1:B:371:ASP:N	5:B:393:SO4:O3	2.53	0.42
1:D:279:ASP:O	1:D:282:LEU:N	2.51	0.42
1:D:107:ILE:CD1	7:D:498:HOH:O	2.68	0.42
1:B:303:VAL:CG1	1:B:304:ASP:N	2.82	0.42
1:C:122:SER:N	1:C:125:GLU:OE2	2.53	0.42
3:B:396:NAD:PN	7:B:479:HOH:O	2.77	0.42
1:B:139:ASP:N	1:B:142:THR:OG1	2.52	0.42
1:D:123:LEU:CA	1:D:126:MET:CE	2.98	0.42
1:B:185:TYR:OH	3:B:396:NAD:N1A	2.53	0.42
1:C:80:ARG:NH2	5:C:394:SO4:O3	2.52	0.42
1:A:252:MET:CE	1:A:309:PHE:O	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:ARG:NH1	7:A:431:HOH:O	2.52	0.41
1:D:155:ASN:CB	7:D:491:HOH:O	2.68	0.41
1:D:232:LEU:O	1:D:236:THR:OG1	2.37	0.41
1:B:219:VAL:O	1:B:357:GLY:N	2.53	0.41
1:C:225:ASP:O	1:C:367:LYS:N	2.54	0.41
1:B:235:THR:OG1	1:B:377:THR:OG1	2.39	0.41
1:C:231:THR:OG1	2:C:395:PO4:O4	2.39	0.41
1:D:293:ILE:CG2	7:D:514:HOH:O	2.68	0.41
1:D:374:VAL:O	1:D:380:GLN:NE2	2.54	0.41
1:C:278:LYS:N	7:C:442:HOH:O	2.52	0.41
1:D:279:ASP:CB	1:D:292:SER:CB	2.99	0.41
1:A:279:ASP:OD2	1:A:279:ASP:N	2.54	0.41
1:A:185:TYR:OH	3:A:396:NAD:N1A	2.54	0.40
1:D:278:LYS:CE	7:D:426:HOH:O	2.69	0.40
1:B:161:HIS:NE2	1:B:178:TYR:O	2.55	0.40
1:D:128:SER:O	1:D:132:GLU:CG	2.70	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	390/392 (100%)	362 (93%)	24 (6%)	4 (1%)	22	45
1	B	390/392 (100%)	368 (94%)	20 (5%)	2 (0%)	38	67
1	C	390/392 (100%)	363 (93%)	21 (5%)	6 (2%)	15	30
1	D	390/392 (100%)	364 (93%)	24 (6%)	2 (0%)	38	67
All	All	1560/1568 (100%)	1457 (93%)	89 (6%)	14 (1%)	25	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	267	ALA
1	C	278	LYS

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Mol	Chain	Res	Type
1	A	216	LYS
1	A	274	LYS
1	A	278	LYS
1	C	259	ASP
1	C	364	PHE
1	A	303	VAL
1	B	259	ASP
1	B	303	VAL
1	C	303	VAL
1	D	303	VAL
1	D	268	ARG
1	C	118	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	324/324 (100%)	299 (92%)	25 (8%)	18	35
1	B	324/324 (100%)	298 (92%)	26 (8%)	17	33
1	C	324/324 (100%)	301 (93%)	23 (7%)	21	40
1	D	324/324 (100%)	308 (95%)	16 (5%)	35	62
All	All	1296/1296 (100%)	1206 (93%)	90 (7%)	22	42

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	41	GLU
1	A	44	GLU
1	A	60	LEU
1	A	79	ASP
1	A	88	SER
1	A	94	VAL
1	A	136	SER
1	A	140	ASP
1	A	165	GLU

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Mol	Chain	Res	Type
1	A	169	ARG
1	A	175	ARG
1	A	191	LYS
1	A	216	LYS
1	A	237	LEU
1	A	246	MET
1	A	261	ASP
1	A	268	ARG
1	A	278	LYS
1	A	279	ASP
1	A	289	SER
1	A	310	ASP
1	A	326	PHE
1	A	360	LYS
1	A	368	SER
1	B	44	GLU
1	B	45	LYS
1	B	50	SER
1	B	88	SER
1	B	89	ASP
1	B	96	ARG
1	B	99	THR
1	B	132	GLU
1	B	136	SER
1	B	140	ASP
1	B	158	GLU
1	B	165	GLU
1	B	168	GLU
1	B	170	MET
1	B	203	PRO
1	B	230	GLU
1	B	252	MET
1	B	259	ASP
1	B	268	ARG
1	B	269	ASP
1	B	276	LEU
1	B	279	ASP
1	B	305	ASN
1	B	310	ASP
1	B	332	ASP
1	B	360	LYS
1	C	21	ARG

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Mol	Chain	Res	Type
1	C	41	GLU
1	C	60	LEU
1	C	61	LEU
1	C	62	SER
1	C	70	GLU
1	C	108	LYS
1	C	112	ASP
1	C	135	LYS
1	C	153	LEU
1	C	158	GLU
1	C	172	ASP
1	C	259	ASP
1	C	261	ASP
1	C	274	LYS
1	C	276	LEU
1	C	280	LYS
1	C	289	SER
1	C	296	ILE
1	C	305	ASN
1	C	310	ASP
1	C	332	ASP
1	C	367	LYS
1	D	44	GLU
1	D	136	SER
1	D	140	ASP
1	D	158	GLU
1	D	170	MET
1	D	177	GLU
1	D	259	ASP
1	D	261	ASP
1	D	266	SER
1	D	268	ARG
1	D	293	ILE
1	D	296	ILE
1	D	305	ASN
1	D	310	ASP
1	D	332	ASP
1	D	356	LYS

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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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$
5	SO4	A	393	-	4,4,4	0.12	0	6,6,6	0.50	0
2	PO4	A	395	-	4,4,4	0.76	0	6,6,6	0.33	0
3	NAD	A	396	-	48,48,48	1.57	6 (12%)	73,73,73	1.91	11 (15%)
4	GOL	A	397	-	5,5,5	0.38	0	5,5,5	0.19	0
5	SO4	B	393	-	4,4,4	0.17	0	6,6,6	0.28	0
5	SO4	B	394	-	4,4,4	0.23	0	6,6,6	0.56	0
2	PO4	B	395	-	4,4,4	0.45	0	6,6,6	0.32	0
3	NAD	B	396	-	48,48,48	1.59	5 (10%)	73,73,73	1.78	8 (10%)
4	GOL	B	397	-	5,5,5	0.43	0	5,5,5	0.16	0
5	SO4	C	393	-	4,4,4	0.25	0	6,6,6	0.46	0
5	SO4	C	394	-	4,4,4	0.19	0	6,6,6	0.14	0
2	PO4	C	395	-	4,4,4	0.78	0	6,6,6	0.32	0
3	NAD	C	396	6	48,48,48	1.46	4 (8%)	73,73,73	1.63	12 (16%)
5	SO4	C	397	-	4,4,4	0.17	0	6,6,6	0.51	0
5	SO4	D	393	-	4,4,4	0.39	0	6,6,6	0.55	0
5	SO4	D	394	-	4,4,4	0.19	0	6,6,6	0.32	0
2	PO4	D	395	-	4,4,4	0.45	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	D	396	6	48,48,48	1.50	4 (8%)	73,73,73	1.82	11 (15%)

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
5	SO4	A	393	-	-	0/0/0/0	0/0/0/0
2	PO4	A	395	-	-	0/0/0/0	0/0/0/0
3	NAD	A	396	-	-	0/30/62/62	0/3/5/5
4	GOL	A	397	-	-	0/4/4/4	0/0/0/0
5	SO4	B	393	-	-	0/0/0/0	0/0/0/0
5	SO4	B	394	-	-	0/0/0/0	0/0/0/0
2	PO4	B	395	-	-	0/0/0/0	0/0/0/0
3	NAD	B	396	-	-	0/30/62/62	0/3/5/5
4	GOL	B	397	-	-	0/4/4/4	0/0/0/0
5	SO4	C	393	-	-	0/0/0/0	0/0/0/0
5	SO4	C	394	-	-	0/0/0/0	0/0/0/0
2	PO4	C	395	-	-	0/0/0/0	0/0/0/0
3	NAD	C	396	6	-	0/30/62/62	0/3/5/5
5	SO4	C	397	-	-	0/0/0/0	0/0/0/0
5	SO4	D	393	-	-	0/0/0/0	0/0/0/0
5	SO4	D	394	-	-	0/0/0/0	0/0/0/0
2	PO4	D	395	-	-	0/0/0/0	0/0/0/0
3	NAD	D	396	6	-	0/30/62/62	0/3/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	396	NAD	O7N-C7N	7.67	1.42	1.24
3	A	396	NAD	O7N-C7N	7.23	1.41	1.24
3	D	396	NAD	O7N-C7N	7.15	1.40	1.24
3	C	396	NAD	O7N-C7N	6.85	1.40	1.24
3	D	396	NAD	C2A-N3A	4.10	1.40	1.32
3	C	396	NAD	C2A-N1A	3.35	1.40	1.33
3	A	396	NAD	C2N-N1N	3.30	1.39	1.35
3	B	396	NAD	C2A-N3A	3.21	1.38	1.32
3	C	396	NAD	C2A-N3A	3.07	1.38	1.32
3	A	396	NAD	C2A-N3A	3.02	1.38	1.32
3	B	396	NAD	PN-O3	2.65	1.65	1.60
3	D	396	NAD	C2A-N1A	2.62	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	396	NAD	C2A-N1A	2.62	1.39	1.33
3	B	396	NAD	PA-O3	2.58	1.64	1.59
3	B	396	NAD	C2A-N1A	2.55	1.38	1.33
3	D	396	NAD	PN-O3	2.23	1.65	1.60
3	A	396	NAD	PN-O3	2.19	1.64	1.60
3	A	396	NAD	PA-O3	2.18	1.63	1.59
3	C	396	NAD	C2N-N1N	2.04	1.37	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	396	NAD	N3A-C2A-N1A	-11.48	119.11	128.71
3	B	396	NAD	N3A-C2A-N1A	-10.60	119.85	128.71
3	D	396	NAD	N3A-C2A-N1A	-10.23	120.16	128.71
3	C	396	NAD	N3A-C2A-N1A	-8.42	121.67	128.71
3	A	396	NAD	O7N-C7N-N7N	-4.58	115.98	122.59
3	D	396	NAD	N3A-C4A-N9A	4.31	133.22	125.43
3	B	396	NAD	N3A-C4A-N9A	4.14	132.90	125.43
3	B	396	NAD	O4D-C1D-N1N	3.90	111.94	107.95
3	A	396	NAD	N3A-C4A-N9A	3.87	132.42	125.43
3	C	396	NAD	C2D-C1D-N1N	-3.87	107.31	113.86
3	A	396	NAD	O7N-C7N-C3N	3.43	123.45	119.58
3	D	396	NAD	O4B-C1B-N9A	3.11	111.33	108.44
3	D	396	NAD	C5A-C4A-N3A	-3.11	118.93	125.70
3	C	396	NAD	O4D-C1D-N1N	3.09	111.12	107.95
3	C	396	NAD	C3N-C7N-N7N	3.00	121.19	117.77
3	D	396	NAD	PN-O3-PA	-2.87	120.64	132.95
3	D	396	NAD	O7N-C7N-C3N	-2.84	116.38	119.58
3	C	396	NAD	C3D-C2D-C1D	2.83	105.34	100.91
3	C	396	NAD	N3A-C4A-N9A	2.74	130.38	125.43
3	D	396	NAD	C2A-N3A-C4A	2.73	121.79	114.01
3	D	396	NAD	C4A-C5A-N7A	-2.57	107.32	109.52
3	D	396	NAD	C2N-C3N-C4N	2.57	121.22	118.31
3	B	396	NAD	C5A-C4A-N3A	-2.56	120.14	125.70
3	A	396	NAD	C3N-C7N-N7N	2.46	120.57	117.77
3	B	396	NAD	C4A-C5A-N7A	-2.44	107.43	109.52
3	D	396	NAD	C3N-C7N-N7N	2.33	120.42	117.77
3	A	396	NAD	N7A-C8A-N9A	-2.30	107.85	114.36
3	B	396	NAD	C3D-C2D-C1D	2.30	104.51	100.91
3	A	396	NAD	C2A-N3A-C4A	2.29	120.52	114.01
3	C	396	NAD	C4D-O4D-C1D	-2.27	107.28	109.75
3	A	396	NAD	C1B-N9A-C4A	-2.24	122.77	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	396	NAD	O5D-PN-O1N	-2.24	99.12	108.61
3	B	396	NAD	N7A-C8A-N9A	-2.22	108.09	114.36
3	C	396	NAD	O2N-PN-O3	2.21	114.74	108.79
3	C	396	NAD	C4B-O4B-C1B	2.20	112.14	109.75
3	B	396	NAD	C2A-N3A-C4A	2.20	120.27	114.01
3	A	396	NAD	C3D-C2D-C1D	2.18	104.31	100.91
3	A	396	NAD	O2A-PA-O3	2.13	115.26	105.14
3	C	396	NAD	C8A-N9A-C1B	2.13	130.57	126.38
3	A	396	NAD	C5A-C4A-N3A	-2.11	121.10	125.70
3	C	396	NAD	C1B-N9A-C4A	-2.11	122.99	126.64
3	D	396	NAD	C6N-N1N-C2N	-2.04	119.73	122.04

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	392/392 (100%)	0.25	22 (5%)	24 20	13, 26, 63, 100	0
1	B	392/392 (100%)	0.21	23 (5%)	22 18	11, 27, 58, 93	0
1	C	392/392 (100%)	0.18	16 (4%)	35 32	10, 22, 55, 94	0
1	D	392/392 (100%)	0.08	17 (4%)	34 30	11, 21, 55, 98	0
All	All	1568/1568 (100%)	0.18	78 (4%)	28 24	10, 24, 58, 100	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	275	VAL	13.8
1	C	273	SER	12.2
1	D	277	SER	9.7
1	D	269	ASP	8.6
1	C	276	LEU	8.1
1	D	270	ASN	7.8
1	A	275	VAL	7.5
1	C	277	SER	7.2
1	D	275	VAL	7.1
1	A	269	ASP	7.0
1	D	276	LEU	6.9
1	B	275	VAL	6.6
1	D	272	GLU	6.6
1	B	276	LEU	6.4
1	D	266	SER	6.4
1	D	273	SER	6.3
1	A	270	ASN	6.2
1	C	272	GLU	6.0
1	A	276	LEU	6.0
1	A	277	SER	5.9
1	C	271	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	267	ALA	5.8
1	A	274	LYS	5.7
1	D	279	ASP	5.2
1	B	271	LYS	5.2
1	A	272	GLU	4.9
1	B	268	ARG	4.9
1	D	271	LYS	4.5
1	C	268	ARG	4.5
1	B	277	SER	4.5
1	A	108	LYS	4.3
1	D	260	TYR	4.2
1	B	269	ASP	4.2
1	A	273	SER	4.1
1	B	266	SER	4.0
1	D	267	ALA	4.0
1	B	267	ALA	3.9
1	B	270	ASN	3.9
1	C	270	ASN	3.9
1	A	265	LEU	3.9
1	C	274	LYS	3.8
1	D	268	ARG	3.8
1	A	268	ARG	3.7
1	B	274	LYS	3.6
1	D	274	LYS	3.6
1	B	264	VAL	3.6
1	C	264	VAL	3.3
1	A	266	SER	3.3
1	A	264	VAL	3.2
1	A	267	ALA	3.2
1	C	266	SER	3.2
1	C	269	ASP	3.1
1	A	106	GLY	3.0
1	A	271	LYS	3.0
1	B	107	ILE	3.0
1	B	272	GLU	3.0
1	B	60	LEU	2.9
1	B	105	SER	2.8
1	B	265	LEU	2.8
1	A	45	LYS	2.8
1	A	46	TYR	2.6
1	A	105	SER	2.6
1	B	106	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	155	ASN	2.4
1	A	279	ASP	2.4
1	C	105	SER	2.4
1	B	121	LEU	2.3
1	A	112	ASP	2.3
1	B	108	LYS	2.3
1	D	265	LEU	2.3
1	B	273	SER	2.3
1	B	118	GLY	2.3
1	C	278	LYS	2.2
1	C	106	GLY	2.2
1	B	263	LYS	2.2
1	A	80	ARG	2.2
1	D	108	LYS	2.2
1	B	262	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
6	K	C	398	1/1	0.44	6.84	90,90,90,90	0
5	SO4	A	393	5/5	0.25	2.97	57,58,59,59	0
5	SO4	C	397	5/5	0.22	2.91	73,73,75,75	0
6	K	D	397	1/1	0.24	2.64	88,88,88,88	0
5	SO4	C	394	5/5	0.26	2.40	91,92,92,93	0
5	SO4	B	394	5/5	0.17	0.78	63,64,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	397	6/6	0.35	0.59	70,71,72,72	0
4	GOL	B	397	6/6	0.27	0.46	64,65,66,67	0
5	SO4	B	393	5/5	0.14	0.46	63,63,65,65	0
3	NAD	C	396	44/44	0.17	0.18	23,40,52,53	0
5	SO4	C	393	5/5	0.17	0.13	60,61,62,63	0
5	SO4	D	393	5/5	0.13	-0.05	57,58,58,60	0
3	NAD	B	396	44/44	0.16	-0.10	22,38,50,51	0
2	PO4	C	395	5/5	0.16	-0.31	17,18,21,21	0
3	NAD	A	396	44/44	0.15	-0.38	29,37,42,43	0
6	K	A	394	1/1	0.12	-0.38	45,45,45,45	0
3	NAD	D	396	44/44	0.12	-0.61	11,30,44,45	0
2	PO4	D	395	5/5	0.15	-0.65	18,18,19,20	0
2	PO4	A	395	5/5	0.16	-0.88	18,18,22,22	0
5	SO4	D	394	5/5	0.11	-1.01	50,50,51,52	0
2	PO4	B	395	5/5	0.13	-1.44	19,21,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.