



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PL6
Title : Human SDH/NADH/inhibitor complex
Authors : Pauly, T.A.; Ekstrom, J.L.; Beebe, D.A.; Chrnyk, B.; Cunningham, D.; Griffor, M.; Kamath, A.; Lee, S.E.; Madura, R.; McGuire, D.; Subashi, T.; Wasilko, D.; Watts, P.; Mylari, B.L.; Oates, P.J.; Adams, P.D.; Rath, V.L.
Deposited on : 2003-06-07
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

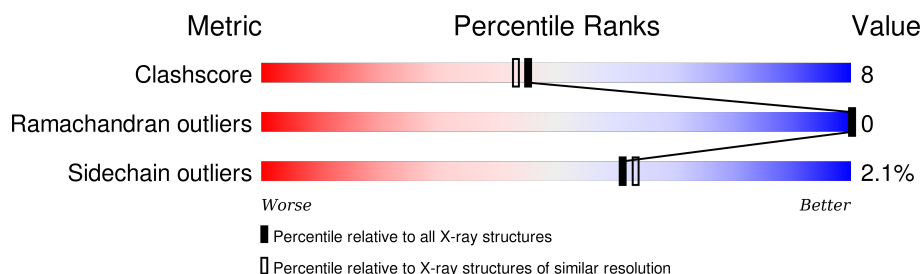
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	356	 88% 11% •
1	B	356	 87% 12% •
1	C	356	 88% 11% •
1	D	356	 88% 11% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12337 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sorbitol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	Se	0	5	0
			2716	1724	473	498	11	10			
1	B	356	Total	C	N	O	S	Se	0	5	0
			2716	1724	473	498	11	10			
1	C	356	Total	C	N	O	S	Se	0	5	0
			2716	1724	473	498	11	10			
1	D	356	Total	C	N	O	S	Se	0	5	0
			2716	1724	473	498	11	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	107	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	185	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	194	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	238	GLN	LEU	SEE REMARK 999	UNP Q00796
A	278	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	309	MSE	MET	MODIFIED RESIDUE	UNP Q00796
A	346	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	38	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	107	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	185	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	194	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	238	GLN	LEU	SEE REMARK 999	UNP Q00796
B	278	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	309	MSE	MET	MODIFIED RESIDUE	UNP Q00796
B	346	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	38	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	65	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	107	MSE	MET	MODIFIED RESIDUE	UNP Q00796

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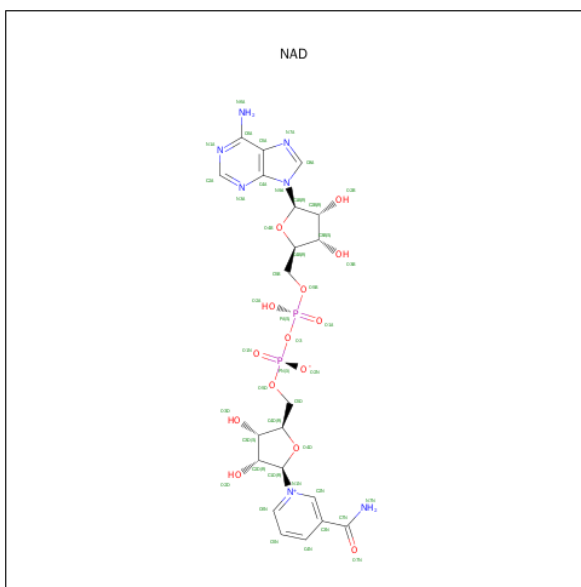
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Chain	Residue	Modelled	Actual	Comment	Reference
C	185	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	194	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	238	GLN	LEU	SEE REMARK 999	UNP Q00796
C	278	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	309	MSE	MET	MODIFIED RESIDUE	UNP Q00796
C	346	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	38	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	65	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	107	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	185	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	194	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	238	GLN	LEU	SEE REMARK 999	UNP Q00796
D	278	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	309	MSE	MET	MODIFIED RESIDUE	UNP Q00796
D	346	MSE	MET	MODIFIED RESIDUE	UNP Q00796

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

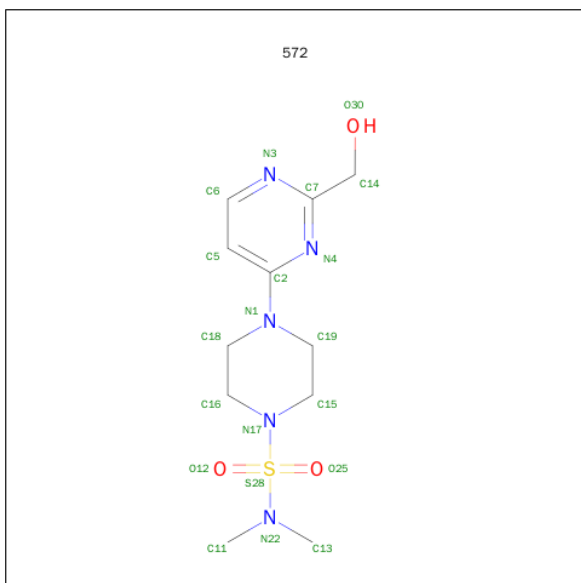
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 4-[2-(HYDROXYMETHYL)PYRIMIDIN-4-YL]-N,N-DIMETHYLPIPERAZINE-1-SULFONAMIDE (three-letter code: 572) (formula: $C_{11}H_{19}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
4	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
4	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
4	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 5 is water.

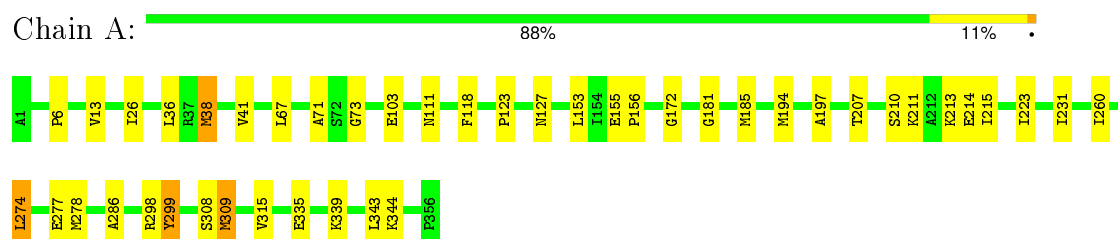
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	317	Total	O	0	0
			317	317		
5	B	290	Total	O	0	0
			290	290		
5	C	283	Total	O	0	0
			283	283		
5	D	323	Total	O	0	0
			323	323		

3 Residue-property plots

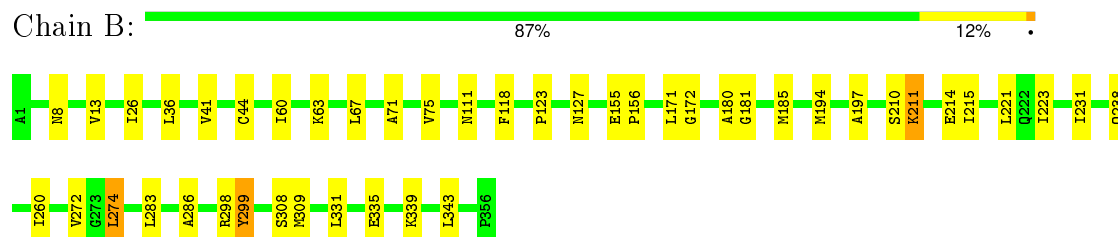
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

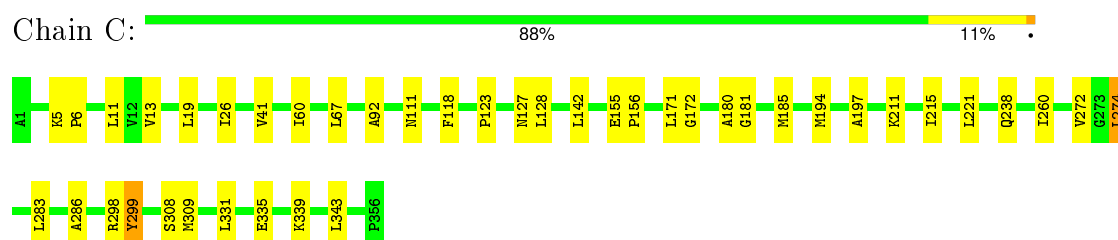
• Molecule 1: Sorbitol dehydrogenase



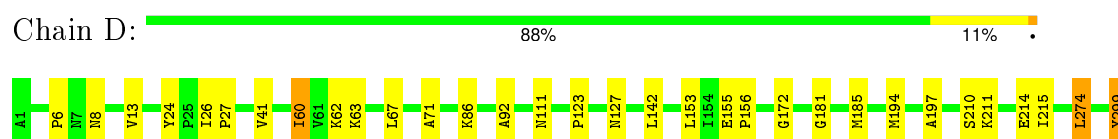
• Molecule 1: Sorbitol dehydrogenase



• Molecule 1: Sorbitol dehydrogenase



• Molecule 1: Sorbitol dehydrogenase



S308	K309	Y315	E335	K338	K339	G340	L343	K344	L347	P356
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	134.81Å 134.81Å 225.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.84 – 2.00	Depositor
% Data completeness (in resolution range)	92.2 (57.84-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12337	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 572, ZN, 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	0.39	0/2765	0.69	0/3732
1	B	0.38	0/2765	0.68	0/3732
1	C	0.38	0/2765	0.68	0/3732
1	D	0.40	0/2765	0.69	0/3732
All	All	0.39	0/11060	0.69	0/14928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2716	0	2768	54	0
1	B	2716	0	2768	52	0
1	C	2716	0	2768	49	0
1	D	2716	0	2768	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	1	0
3	C	44	0	26	1	0
3	D	44	0	26	0	0
4	A	20	0	19	0	0
4	B	20	0	19	1	0
4	C	20	0	19	1	0
4	D	20	0	19	0	0
5	A	317	0	0	8	0
5	B	290	0	0	6	0
5	C	283	0	0	4	0
5	D	323	0	0	7	0
All	All	12337	0	11252	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLY:HA2	1:B:309[A]:MSE:HE3	1.26	1.17
1:C:309[A]:MSE:HE3	1:D:172:GLY:HA2	1.26	1.15
1:C:197:ALA:CB	1:D:309[A]:MSE:HE1	1.77	1.15
1:C:172:GLY:HA2	1:D:309[A]:MSE:HE3	1.18	1.14
1:A:309[A]:MSE:HE3	1:B:172:GLY:HA2	1.13	1.12
1:A:309[A]:MSE:HE1	1:B:197:ALA:CB	1.79	1.12
1:C:309[A]:MSE:HE1	1:D:197:ALA:CB	1.81	1.11
1:A:309[A]:MSE:CE	1:B:197:ALA:HB2	1.82	1.09
1:A:197:ALA:CB	1:B:309[A]:MSE:HE1	1.81	1.09
1:C:197:ALA:HB2	1:D:309[A]:MSE:CE	1.81	1.08
1:C:309[A]:MSE:CE	1:D:197:ALA:HB2	1.84	1.06
1:A:38:MSE:HE2	1:A:38:MSE:HA	1.35	1.06
1:A:197:ALA:HB2	1:B:309[A]:MSE:CE	1.85	1.05
1:A:197:ALA:HB2	1:B:309[A]:MSE:HE1	1.02	1.01
1:A:309[A]:MSE:HE1	1:B:197:ALA:HB2	1.01	1.00
1:A:309[A]:MSE:CE	1:B:172:GLY:HA2	1.91	0.99
1:C:309[A]:MSE:HE1	1:D:197:ALA:HB2	1.00	0.98
1:C:197:ALA:HB2	1:D:309[A]:MSE:HE1	1.00	0.98
1:C:172:GLY:HA2	1:D:309[A]:MSE:CE	1.92	0.97
1:C:309[A]:MSE:CE	1:D:172:GLY:HA2	1.95	0.96
1:A:172:GLY:HA2	1:B:309[A]:MSE:CE	1.96	0.94
1:C:331:LEU:HD21	5:C:1812:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MSE:CE	1:A:38:MSE:HA	2.12	0.79
1:D:309[A]:MSE:HA	1:D:309[A]:MSE:HE2	1.64	0.78
1:A:309[A]:MSE:HE3	1:B:172:GLY:CA	2.06	0.76
1:C:172:GLY:CA	1:D:309[A]:MSE:HE3	2.10	0.75
1:C:6:PRO:HG2	1:C:26:ILE:CD1	2.18	0.74
1:D:309[A]:MSE:CA	1:D:309[A]:MSE:HE2	2.17	0.74
1:A:309[A]:MSE:HA	1:A:309[A]:MSE:HE2	1.69	0.74
1:B:331:LEU:HD21	5:B:1785:HOH:O	1.89	0.72
1:D:309[A]:MSE:N	1:D:309[A]:MSE:HE2	2.05	0.72
1:A:309[A]:MSE:CA	1:A:309[A]:MSE:HE2	2.20	0.71
1:A:309[A]:MSE:N	1:A:309[A]:MSE:HE2	2.05	0.71
1:B:185[B]:MSE:HE1	1:B:211:LYS:HD2	1.71	0.71
1:A:274:LEU:HD22	5:A:1620:HOH:O	1.90	0.70
1:A:6:PRO:HG2	1:A:26:ILE:CD1	2.22	0.70
1:B:309[A]:MSE:N	1:B:309[A]:MSE:HE2	2.06	0.69
1:C:309[A]:MSE:N	1:C:309[A]:MSE:HE2	2.06	0.69
1:A:339:LYS:HE3	5:A:1335:HOH:O	1.94	0.68
1:D:274:LEU:HD22	5:D:1988:HOH:O	1.96	0.64
1:B:309[A]:MSE:CA	1:B:309[A]:MSE:HE2	2.28	0.64
1:B:309[A]:MSE:HE2	1:B:309[A]:MSE:HA	1.80	0.63
1:C:309[A]:MSE:CA	1:C:309[A]:MSE:HE2	2.29	0.62
1:D:6:PRO:HG2	1:D:26:ILE:CD1	2.28	0.62
1:A:185[B]:MSE:SE	1:A:343:LEU:HD21	2.50	0.62
1:C:308:SER:C	1:C:309[A]:MSE:HE2	2.20	0.62
1:C:309[A]:MSE:HE3	1:D:172:GLY:CA	2.16	0.62
1:A:172:GLY:CA	1:B:309[A]:MSE:HE3	2.16	0.62
1:B:308:SER:C	1:B:309[A]:MSE:HE2	2.21	0.61
1:A:309[A]:MSE:HE1	1:B:197:ALA:CA	2.31	0.61
1:C:309[A]:MSE:HE2	1:C:309[A]:MSE:HA	1.82	0.61
1:A:185[B]:MSE:HE2	1:A:215:ILE:HD11	1.83	0.61
1:C:197:ALA:CA	1:D:309[A]:MSE:HE1	2.31	0.61
1:C:274:LEU:HD22	5:C:1958:HOH:O	1.99	0.61
1:C:185[B]:MSE:HE1	1:C:211:LYS:HD2	1.82	0.60
1:D:13[A]:VAL:CG2	1:D:67:LEU:HD11	2.32	0.60
1:D:339:LYS:HE3	5:D:1315:HOH:O	2.02	0.59
1:B:221:LEU:HD21	1:B:238:GLN:NE2	2.18	0.59
1:B:221:LEU:CD2	1:B:238:GLN:HE22	2.15	0.59
1:A:277:GLU:O	1:A:278:MSE:HE2	2.03	0.59
1:D:308:SER:C	1:D:309[A]:MSE:HE2	2.23	0.58
1:D:13[A]:VAL:HG23	1:D:67:LEU:HD11	1.85	0.58
1:D:185[B]:MSE:HE2	1:D:215:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13[A]:VAL:CG2	1:A:67:LEU:HD11	2.33	0.58
1:A:308:SER:C	1:A:309[A]:MSE:HE2	2.23	0.58
1:A:185[A]:MSE:HA	1:A:185[A]:MSE:HE2	1.83	0.58
1:D:63:LYS:HE3	5:D:1280:HOH:O	2.03	0.58
1:D:6:PRO:HG2	1:D:26:ILE:HD12	1.86	0.58
1:A:197:ALA:CA	1:B:309[A]:MSE:HE1	2.35	0.57
1:B:185[B]:MSE:SE	1:B:343:LEU:HD21	2.54	0.57
1:C:185[B]:MSE:SE	5:C:1448:HOH:O	2.73	0.56
1:B:210:SER:O	1:B:214:GLU:HG3	2.05	0.56
1:D:185[B]:MSE:SE	5:D:1489:HOH:O	2.75	0.55
1:C:185[A]:MSE:HA	1:C:185[A]:MSE:HE2	1.87	0.55
1:C:309[A]:MSE:HE1	1:D:197:ALA:CA	2.36	0.55
1:D:185[B]:MSE:SE	1:D:343:LEU:HD21	2.57	0.54
1:C:185[B]:MSE:SE	1:C:343:LEU:HD21	2.57	0.54
1:A:185[B]:MSE:SE	5:A:1418:HOH:O	2.76	0.53
1:B:181:GLY:O	1:B:185[B]:MSE:HG3	2.09	0.53
1:C:181:GLY:O	1:C:185[B]:MSE:HG3	2.09	0.53
1:C:185[B]:MSE:HE2	1:C:215:ILE:CD1	2.39	0.52
1:A:13[A]:VAL:HG23	1:A:67:LEU:HD11	1.92	0.52
1:B:13[A]:VAL:CG2	1:B:67:LEU:HD11	2.40	0.52
1:C:6:PRO:HG2	1:C:26:ILE:HD12	1.91	0.52
1:D:185[A]:MSE:HA	1:D:185[A]:MSE:HE2	1.92	0.51
1:B:185[B]:MSE:SE	5:B:1474:HOH:O	2.78	0.51
1:A:210:SER:O	1:A:214:GLU:HG3	2.10	0.51
1:B:339:LYS:HE3	5:B:1496:HOH:O	2.10	0.51
1:A:207:THR:HG22	5:A:1899:HOH:O	2.10	0.50
1:B:185[A]:MSE:HA	1:B:185[A]:MSE:HE2	1.93	0.50
1:D:185[B]:MSE:HE1	1:D:211:LYS:HD2	1.93	0.50
1:C:6:PRO:HG2	1:C:26:ILE:HD11	1.92	0.50
1:A:309[B]:MSE:HE2	1:A:315:VAL:HG11	1.95	0.49
1:B:185[B]:MSE:HE2	1:B:215:ILE:CD1	2.43	0.49
1:A:36:LEU:CB	1:A:38:MSE:HE3	2.43	0.49
1:B:274:LEU:HD22	5:B:1658:HOH:O	2.10	0.49
1:B:331:LEU:HD11	5:B:1785:HOH:O	2.13	0.49
1:B:185[B]:MSE:SE	1:B:343:LEU:CD2	3.11	0.49
1:B:221:LEU:CD2	1:B:238:GLN:NE2	2.76	0.48
1:A:185[B]:MSE:HE1	1:A:211:LYS:HD2	1.96	0.48
1:D:181:GLY:O	1:D:185[B]:MSE:HG3	2.14	0.48
1:A:181:GLY:O	1:A:185[B]:MSE:HG3	2.13	0.48
1:B:221:LEU:HG	1:B:238:GLN:HE22	1.79	0.47
1:D:210:SER:O	1:D:214:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:HD21	1:D:344:LYS:HG2	1.96	0.47
1:A:309[B]:MSE:SE	1:B:171:LEU:HD21	2.65	0.47
1:B:41:VAL:HG22	1:B:71:ALA:HB2	1.96	0.47
1:A:38:MSE:HE2	1:A:73:GLY:HA3	1.98	0.46
1:C:221:LEU:CD2	1:C:238:GLN:HE22	2.28	0.46
1:C:185[B]:MSE:SE	1:C:343:LEU:CD2	3.14	0.46
1:D:111:ASN:HB3	1:D:299:TYR:O	2.16	0.46
1:B:8:ASN:HB2	1:B:26:ILE:HD13	1.98	0.45
1:A:38:MSE:CE	1:A:38:MSE:CA	2.89	0.45
1:A:36:LEU:HB3	1:A:38:MSE:HE3	1.98	0.45
1:A:335:GLU:O	1:A:339:LYS:HG2	2.16	0.45
1:C:274:LEU:HG	4:C:409:572:H181	1.98	0.45
5:A:1530:HOH:O	1:B:194:MSE:HE1	2.17	0.45
1:C:41:VAL:HG11	1:C:128:LEU:HG	1.98	0.45
1:A:185[B]:MSE:HE2	1:A:215:ILE:CD1	2.46	0.45
1:A:41:VAL:HG22	1:A:71:ALA:HB2	1.98	0.45
1:C:155:GLU:HB3	1:C:156:PRO:CD	2.47	0.45
1:D:309[B]:MSE:HE2	1:D:315:VAL:HG11	1.98	0.45
1:B:155:GLU:HB3	1:B:156:PRO:CD	2.47	0.45
1:A:111:ASN:HB3	1:A:299:TYR:O	2.17	0.45
1:D:185[B]:MSE:HE2	1:D:215:ILE:CD1	2.46	0.45
1:D:92:ALA:HB2	1:D:142:LEU:HD21	1.98	0.45
1:B:335:GLU:O	1:B:339:LYS:HG2	2.17	0.45
1:C:171:LEU:HD21	1:D:309[B]:MSE:SE	2.67	0.44
1:C:5:LYS:HE3	5:C:2133:HOH:O	2.16	0.44
1:D:41:VAL:HG22	1:D:71:ALA:HB2	1.98	0.44
1:C:335:GLU:O	1:C:339:LYS:HG2	2.17	0.44
1:B:260:ILE:HG23	1:B:286:ALA:HB2	1.99	0.44
1:B:118:PHE:CZ	1:B:298:ARG:HD2	2.53	0.43
1:C:260:ILE:HG23	1:C:286:ALA:HB2	1.99	0.43
1:C:111:ASN:HB3	1:C:299:TYR:O	2.18	0.43
1:A:260:ILE:HG23	1:A:286:ALA:HB2	1.99	0.43
1:B:180:ALA:HA	1:B:185[A]:MSE:HE3	2.00	0.43
1:B:13[A]:VAL:HG23	1:B:67:LEU:HD11	1.99	0.43
1:B:63:LYS:HE3	5:B:1284:HOH:O	2.18	0.43
1:C:13[A]:VAL:CG2	1:C:67:LEU:HD11	2.48	0.43
1:C:194:MSE:HE1	5:D:1788:HOH:O	2.19	0.42
1:D:335:GLU:O	1:D:339:LYS:HG2	2.19	0.42
1:A:153:LEU:HD21	1:A:344:LYS:HG2	2.01	0.42
1:B:221:LEU:CG	1:B:238:GLN:HE22	2.32	0.42
1:A:103:GLU:HG2	5:A:1959:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD12	1:A:231:ILE:HD12	2.02	0.42
1:C:272:VAL:O	3:C:408:NAD:H2N	2.18	0.42
1:D:309[A]:MSE:CA	1:D:309[A]:MSE:CE	2.93	0.42
1:A:309[A]:MSE:CE	1:A:309[A]:MSE:CA	2.95	0.42
1:C:118:PHE:CZ	1:C:298:ARG:HD2	2.55	0.41
1:A:13[B]:VAL:HG13	1:A:13[B]:VAL:O	2.20	0.41
1:B:272:VAL:O	3:B:406:NAD:H2N	2.20	0.41
1:B:223:ILE:HD12	1:B:231:ILE:HD12	2.02	0.41
1:A:194:MSE:HE1	5:A:1837:HOH:O	2.20	0.41
1:B:111:ASN:HB3	1:B:299:TYR:O	2.20	0.41
1:A:213:LYS:HE2	5:A:1359:HOH:O	2.20	0.41
1:C:309[A]:MSE:CE	1:C:309[A]:MSE:HA	2.48	0.41
1:C:180:ALA:HA	1:C:185[A]:MSE:HE3	2.02	0.41
1:D:26:ILE:HA	1:D:27:PRO:HD3	1.97	0.41
1:C:221:LEU:HD21	1:C:238:GLN:NE2	2.36	0.41
1:A:155:GLU:HB3	1:A:156:PRO:CD	2.50	0.41
1:C:11:LEU:HD11	1:C:19:LEU:HG	2.02	0.41
1:C:185[B]:MSE:HE2	1:C:215:ILE:HD13	2.01	0.41
1:C:92:ALA:HB2	1:C:142:LEU:HD21	2.03	0.41
1:D:347:LEU:HA	1:D:347:LEU:HD23	1.90	0.41
1:B:36:LEU:HD23	1:B:75:VAL:HA	2.03	0.41
1:D:194:MSE:HE1	5:D:1894:HOH:O	2.20	0.41
1:B:44:CYS:SG	4:B:407:572:H6	2.60	0.41
1:D:60:ILE:HG13	1:D:62:LYS:HG3	2.02	0.41
1:D:86:LYS:HE2	5:D:1772:HOH:O	2.21	0.41
1:D:155:GLU:HB3	1:D:156:PRO:CD	2.51	0.40
1:D:8:ASN:HB3	1:D:24:TYR:O	2.22	0.40
1:D:338:LYS:C	1:D:340:GLY:H	2.24	0.40
1:A:118:PHE:CE1	1:A:298:ARG:HD2	2.57	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	359/356 (101%)	351 (98%)	8 (2%)	0	100	100
1	B	359/356 (101%)	349 (97%)	10 (3%)	0	100	100
1	C	359/356 (101%)	349 (97%)	10 (3%)	0	100	100
1	D	359/356 (101%)	348 (97%)	11 (3%)	0	100	100
All	All	1436/1424 (101%)	1397 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/282 (105%)	288 (98%)	7 (2%)	57	58
1	B	295/282 (105%)	288 (98%)	7 (2%)	57	58
1	C	295/282 (105%)	289 (98%)	6 (2%)	63	65
1	D	295/282 (105%)	290 (98%)	5 (2%)	68	71
All	All	1180/1128 (105%)	1155 (98%)	25 (2%)	61	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	MSE
1	A	123	PRO
1	A	127	ASN
1	A	274	LEU
1	A	299	TYR
1	A	309[A]	MSE
1	A	309[B]	MSE
1	B	60	ILE
1	B	123	PRO
1	B	127	ASN
1	B	211	LYS
1	B	274	LEU
1	B	283	LEU

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Mol	Chain	Res	Type
1	B	299	TYR
1	C	60	ILE
1	C	123	PRO
1	C	127	ASN
1	C	274	LEU
1	C	283	LEU
1	C	299	TYR
1	D	60	ILE
1	D	123	PRO
1	D	127	ASN
1	D	274	LEU
1	D	299	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	B	127	ASN
1	B	222	GLN
1	B	238	GLN
1	C	127	ASN
1	C	238	GLN
1	C	355	ASN
1	D	127	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
3	NAD	A	404	-	38,48,48	2.09	7 (18%)	47,73,73	1.77	7 (14%)
4	572	A	405	2	21,21,21	4.47	11 (52%)	27,30,30	2.13	8 (29%)
3	NAD	B	406	-	38,48,48	2.04	8 (21%)	47,73,73	1.80	6 (12%)
4	572	B	407	2	21,21,21	4.44	12 (57%)	27,30,30	2.07	9 (33%)
3	NAD	C	408	-	38,48,48	2.01	7 (18%)	47,73,73	1.76	6 (12%)
4	572	C	409	2	21,21,21	4.42	11 (52%)	27,30,30	2.07	9 (33%)
3	NAD	D	410	-	38,48,48	2.08	8 (21%)	47,73,73	1.77	7 (14%)
4	572	D	411	2	21,21,21	4.50	11 (52%)	27,30,30	2.15	9 (33%)

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
3	NAD	A	404	-	-	0/22/62/62	0/5/5/5
4	572	A	405	2	-	0/16/28/28	0/2/2/2
3	NAD	B	406	-	-	0/22/62/62	0/5/5/5
4	572	B	407	2	-	0/16/28/28	0/2/2/2
3	NAD	C	408	-	-	0/22/62/62	0/5/5/5
4	572	C	409	2	-	0/16/28/28	0/2/2/2
3	NAD	D	410	-	-	0/22/62/62	0/5/5/5
4	572	D	411	2	-	0/16/28/28	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	NAD	O4B-C1B	-2.94	1.37	1.41
3	D	410	NAD	O4B-C1B	-2.80	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	NAD	C6N-C5N	-2.78	1.32	1.38
3	D	410	NAD	C6N-C5N	-2.74	1.32	1.38
3	A	404	NAD	C6N-C5N	-2.70	1.32	1.38
3	C	408	NAD	C6N-C5N	-2.69	1.32	1.38
3	D	410	NAD	PN-O1N	-2.45	1.42	1.51
3	B	406	NAD	PN-O1N	-2.41	1.42	1.51
4	B	407	572	C18-C16	-2.33	1.41	1.51
4	C	409	572	C18-C16	-2.33	1.41	1.51
4	A	405	572	C18-C16	-2.30	1.42	1.51
3	C	408	NAD	PN-O1N	-2.29	1.42	1.51
4	D	411	572	C18-C16	-2.27	1.42	1.51
3	A	404	NAD	PN-O1N	-2.22	1.43	1.51
3	B	406	NAD	C3N-C7N	-2.18	1.47	1.50
4	B	407	572	C7-N3	2.06	1.36	1.33
4	C	409	572	C6-N3	2.08	1.39	1.34
3	D	410	NAD	C2A-N1A	2.10	1.37	1.33
3	C	408	NAD	C2A-N1A	2.11	1.37	1.33
4	A	405	572	C6-N3	2.13	1.39	1.34
4	A	405	572	C18-N1	2.14	1.50	1.46
4	D	411	572	C6-N3	2.15	1.39	1.34
4	B	407	572	C6-N3	2.18	1.39	1.34
4	B	407	572	C18-N1	2.20	1.50	1.46
4	D	411	572	C18-N1	2.23	1.50	1.46
3	B	406	NAD	C2A-N1A	2.26	1.38	1.33
4	C	409	572	C18-N1	2.33	1.50	1.46
4	A	405	572	C2-N4	2.86	1.38	1.34
4	D	411	572	C2-N4	2.93	1.38	1.34
4	C	409	572	C5-C2	2.96	1.46	1.39
4	B	407	572	C5-C2	2.96	1.46	1.39
4	B	407	572	C2-N4	2.98	1.38	1.34
4	C	409	572	C2-N4	2.99	1.38	1.34
4	A	405	572	C5-C2	3.01	1.46	1.39
4	D	411	572	C5-C2	3.02	1.46	1.39
3	C	408	NAD	C6N-N1N	3.09	1.43	1.35
3	D	410	NAD	C6N-N1N	3.11	1.43	1.35
3	B	406	NAD	C6N-N1N	3.14	1.43	1.35
4	D	411	572	C15-N17	3.18	1.51	1.47
3	A	404	NAD	C6N-N1N	3.32	1.44	1.35
4	A	405	572	C15-N17	3.36	1.51	1.47
4	B	407	572	C15-N17	3.69	1.52	1.47
4	C	409	572	C15-N17	3.81	1.52	1.47
3	D	410	NAD	C2N-C3N	5.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	NAD	C2N-C3N	5.21	1.46	1.39
3	C	408	NAD	C2N-C3N	5.21	1.46	1.39
3	A	404	NAD	C2N-C3N	5.31	1.47	1.39
3	A	404	NAD	C5N-C4N	5.49	1.50	1.38
3	B	406	NAD	C5N-C4N	5.51	1.50	1.38
3	C	408	NAD	C5N-C4N	5.59	1.50	1.38
3	D	410	NAD	C5N-C4N	5.64	1.50	1.38
4	C	409	572	S28-N17	6.36	1.72	1.59
4	B	407	572	S28-N17	6.37	1.72	1.59
4	A	405	572	S28-N17	6.61	1.72	1.59
4	D	411	572	S28-N17	6.63	1.72	1.59
3	C	408	NAD	C4N-C3N	7.21	1.51	1.39
3	B	406	NAD	C4N-C3N	7.33	1.51	1.39
3	D	410	NAD	C4N-C3N	7.39	1.52	1.39
3	A	404	NAD	C4N-C3N	7.54	1.52	1.39
4	C	409	572	S28-N22	7.95	1.75	1.59
4	D	411	572	S28-N22	8.04	1.75	1.59
4	B	407	572	S28-N22	8.04	1.75	1.59
4	A	405	572	S28-N22	8.08	1.75	1.59
4	B	407	572	C16-N17	8.48	1.57	1.47
4	C	409	572	C16-N17	8.48	1.57	1.47
4	A	405	572	C16-N17	8.79	1.57	1.47
4	C	409	572	O12-S28	8.82	1.62	1.42
4	D	411	572	C16-N17	8.96	1.57	1.47
4	B	407	572	O12-S28	9.11	1.62	1.42
4	A	405	572	O12-S28	9.25	1.62	1.42
4	D	411	572	O12-S28	9.33	1.63	1.42
4	A	405	572	O25-S28	9.82	1.64	1.42
4	D	411	572	O25-S28	9.85	1.64	1.42
4	B	407	572	O25-S28	9.96	1.64	1.42
4	C	409	572	O25-S28	10.07	1.64	1.42

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	406	NAD	C5N-C4N-C3N	-6.52	112.14	120.33
3	C	408	NAD	C5N-C4N-C3N	-6.43	112.25	120.33
3	D	410	NAD	C5N-C4N-C3N	-6.23	112.51	120.33
3	A	404	NAD	C5N-C4N-C3N	-6.21	112.52	120.33
3	D	410	NAD	O3-PN-O5D	-4.35	91.39	102.94
3	B	406	NAD	O3-PN-O5D	-4.34	91.41	102.94
3	A	404	NAD	O3-PN-O5D	-4.34	91.42	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	408	NAD	O3-PN-O5D	-4.19	91.83	102.94
4	B	407	572	C11-N22-S28	-3.86	109.85	118.12
4	D	411	572	C11-N22-S28	-3.82	109.94	118.12
4	C	409	572	C11-N22-S28	-3.79	109.99	118.12
4	A	405	572	C11-N22-S28	-3.77	110.04	118.12
4	A	405	572	O12-S28-O25	-3.09	115.44	121.32
4	D	411	572	O12-S28-O25	-3.05	115.51	121.32
3	B	406	NAD	O7N-C7N-C3N	-2.96	116.35	119.59
4	C	409	572	O12-S28-O25	-2.78	116.04	121.32
4	B	407	572	O12-S28-O25	-2.76	116.06	121.32
3	D	410	NAD	O7N-C7N-C3N	-2.53	116.83	119.59
3	A	404	NAD	O7N-C7N-C3N	-2.51	116.84	119.59
3	C	408	NAD	O7N-C7N-C3N	-2.43	116.93	119.59
4	A	405	572	C5-C2-N4	-2.41	119.81	123.47
4	D	411	572	C5-C2-N4	-2.39	119.84	123.47
4	C	409	572	C5-C2-N4	-2.33	119.93	123.47
4	B	407	572	C5-C2-N4	-2.28	120.02	123.47
4	B	407	572	N3-C7-N4	-2.04	123.35	126.30
4	D	411	572	N3-C7-N4	-2.02	123.38	126.30
4	C	409	572	N3-C7-N4	-2.01	123.40	126.30
3	D	410	NAD	O3B-C3B-C2B	2.01	118.36	111.83
4	C	409	572	C5-C2-N1	2.01	124.88	121.57
4	B	407	572	C5-C2-N1	2.07	124.98	121.57
3	A	404	NAD	O3B-C3B-C2B	2.11	118.68	111.83
4	A	405	572	C5-C2-N1	2.21	125.19	121.57
4	D	411	572	C5-C2-N1	2.27	125.30	121.57
4	C	409	572	O25-S28-N22	2.32	112.14	108.88
4	B	407	572	C18-C16-N17	2.45	111.00	109.02
4	C	409	572	C18-C16-N17	2.47	111.02	109.02
3	D	410	NAD	PN-O3-PA	2.47	139.66	132.73
4	B	407	572	O25-S28-N22	2.54	112.45	108.88
3	A	404	NAD	PN-O3-PA	2.58	139.97	132.73
4	A	405	572	O25-S28-N22	2.62	112.56	108.88
4	D	411	572	O25-S28-N22	2.66	112.62	108.88
3	C	408	NAD	PN-O3-PA	2.77	140.51	132.73
4	A	405	572	C18-C16-N17	2.83	111.32	109.02
4	D	411	572	C18-C16-N17	2.90	111.37	109.02
3	B	406	NAD	PN-O3-PA	2.93	140.96	132.73
4	B	407	572	C6-N3-C7	3.00	117.75	115.67
4	A	405	572	C6-N3-C7	3.08	117.80	115.67
4	D	411	572	C6-N3-C7	3.13	117.84	115.67
4	C	409	572	C6-N3-C7	3.14	117.85	115.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	NAD	C6N-C5N-C4N	3.85	125.25	119.44
3	D	410	NAD	C6N-C5N-C4N	3.87	125.29	119.44
3	B	406	NAD	C6N-C5N-C4N	3.94	125.39	119.44
3	C	408	NAD	C6N-C5N-C4N	3.96	125.42	119.44
3	C	408	NAD	C3N-C7N-N7N	4.52	122.77	117.82
3	A	404	NAD	C3N-C7N-N7N	4.58	122.83	117.82
3	B	406	NAD	C3N-C7N-N7N	4.70	122.96	117.82
3	D	410	NAD	C3N-C7N-N7N	4.72	122.99	117.82
4	C	409	572	C7-N4-C2	5.72	120.45	115.68
4	B	407	572	C7-N4-C2	5.77	120.49	115.68
4	A	405	572	C7-N4-C2	6.01	120.69	115.68
4	D	411	572	C7-N4-C2	6.09	120.76	115.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	NAD	1	0
4	B	407	572	1	0
3	C	408	NAD	1	0
4	C	409	572	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.