



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2018 – 01:07 PM EDT

PDB ID : 6B5H
Title : ALDH1A2 liganded with NAD and 1-(4-cyanophenyl)-N-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1H-pyrazole-4-carboxamide (compound CM121)
Authors : Chen, Y.; Zhu, J.-Y.; Schonbrunn, E.
Deposited on : 2017-09-29
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031021
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

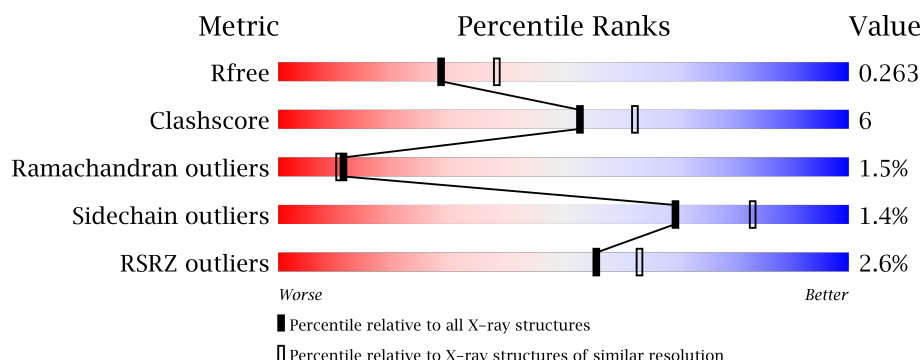
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	493	<div> <div>0.0%</div> <div>88%</div> <div>12%</div> </div>
1	B	493	<div> <div>5%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	C	493	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	D	493	<div> <div>0.0%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition ⓘ

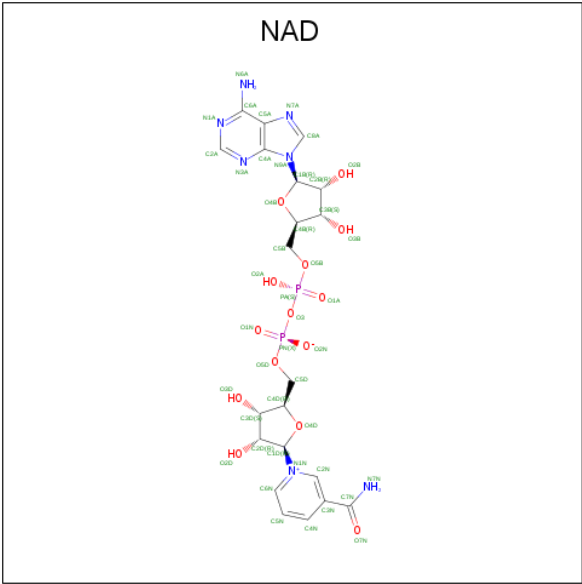
There are 4 unique types of molecules in this entry. The entry contains 15902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinal dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	B	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	C	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	D	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



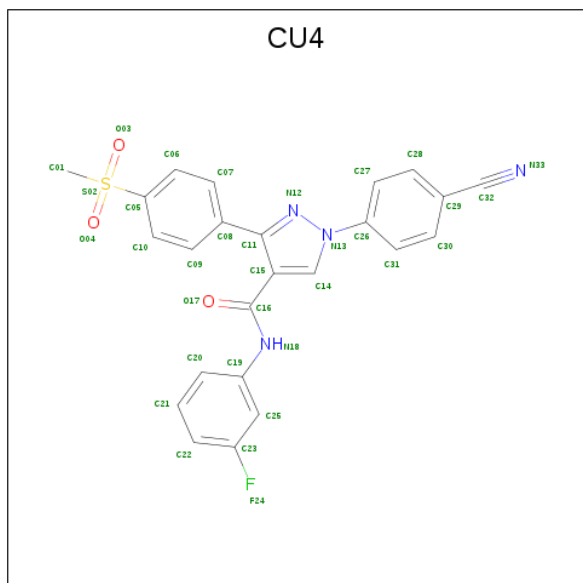
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	B	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

- Molecule 3 is 1-(4-cyanophenyl)-N-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1H-pyrazole-4-carboxamide (three-letter code: CU4) (formula: C₂₄H₁₇FN₄O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
3	B	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
3	C	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
3	D	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	74	Total	O	0	0
			74	74		
4	C	64	Total	O	0	0
			64	64		

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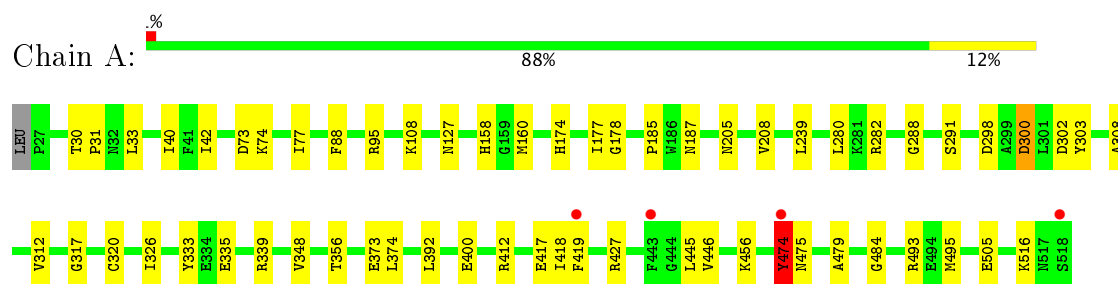
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	122	Total 122	O 122	0	0

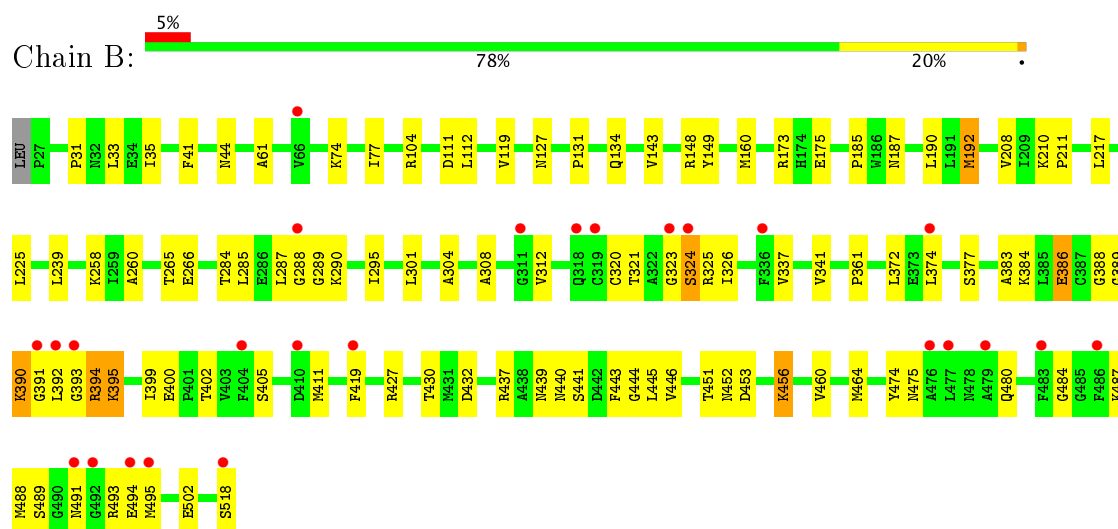
3 Residue-property plots [i](#)

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

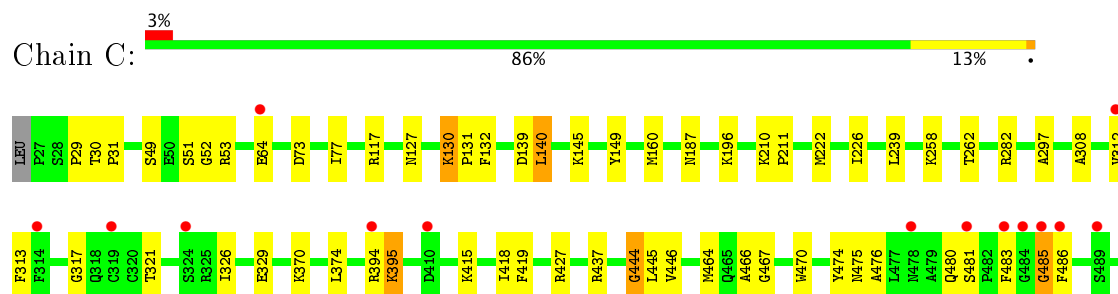
• Molecule 1: Retinal dehydrogenase 2

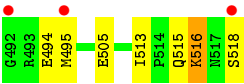


• Molecule 1: Retinal dehydrogenase 2

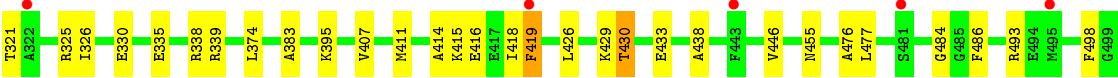
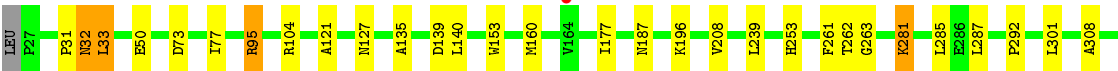
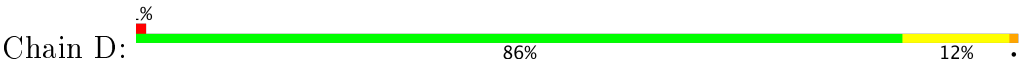


• Molecule 1: Retinal dehydrogenase 2





● Molecule 1: Retinal dehydrogenase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.85Å 141.86Å 164.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.82 – 2.30 82.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.82-2.30) 99.8 (82.38-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_2575	Depositor
R, R_{free}	0.206 , 0.264 0.206 , 0.263	Depositor DCC
R_{free} test set	1776 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15902	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5281e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

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: CU4, 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	0.25	0/3884	0.42	0/5254
1	B	0.26	0/3884	0.44	0/5254
1	C	0.26	0/3884	0.43	0/5254
1	D	0.25	0/3884	0.42	0/5254
All	All	0.26	0/15536	0.43	0/21016

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	3803	0	3779	41	0
1	B	3803	0	3779	66	0
1	C	3803	0	3777	44	0
1	D	3803	0	3779	38	0
2	A	44	0	24	4	0
2	B	44	0	24	3	0
2	C	44	0	23	3	0
2	D	44	0	21	3	0
3	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	1	0
3	C	33	0	0	0	0
3	D	33	0	0	0	0
4	A	122	0	0	0	0
4	B	74	0	0	1	0
4	C	64	0	0	2	0
4	D	122	0	0	0	0
All	All	15902	0	15206	180	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 6.

All (180) 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:B:453:ASP:HB3	1:B:456:LYS:HD2	1.50	0.93
1:C:370:LYS:HZ1	1:C:419:PHE:H	1.22	0.86
1:A:320:CYS:HG	1:A:419:PHE:HZ	0.88	0.84
1:A:417:GLU:OE2	1:A:419:PHE:HE1	1.60	0.84
1:A:320:CYS:SG	2:A:601:NAD:H2D	2.17	0.84
1:A:417:GLU:CD	1:A:419:PHE:HE1	1.81	0.83
1:D:383:ALA:HB2	1:D:411:MET:HE1	1.64	0.78
1:C:370:LYS:NZ	1:C:419:PHE:H	1.83	0.76
1:C:187:ASN:HD21	2:C:601:NAD:H5N	1.52	0.74
1:A:417:GLU:CD	1:A:419:PHE:CE1	2.59	0.74
1:C:494:GLU:HG3	1:C:495:MET:HG2	1.70	0.74
1:B:388:GLY:HA3	1:B:402:THR:HA	1.69	0.73
1:B:187:ASN:HD21	2:B:601:NAD:H5N	1.54	0.72
1:B:74:LYS:NZ	4:B:701:HOH:O	2.22	0.72
1:B:77:ILE:HD13	1:B:239:LEU:HD22	1.72	0.71
1:D:77:ILE:HD13	1:D:239:LEU:HD22	1.72	0.71
1:B:320:CYS:SG	2:B:601:NAD:H2D	2.30	0.71
1:C:474:TYR:O	1:C:476:ALA:N	2.21	0.71
1:A:77:ILE:HD13	1:A:239:LEU:HD22	1.73	0.69
1:A:374:LEU:HD13	1:A:418:ILE:HG12	1.74	0.68
1:C:427:ARG:O	1:C:437:ARG:NH2	2.27	0.68
1:A:320:CYS:SG	1:A:419:PHE:HZ	2.08	0.67
1:C:77:ILE:HD13	1:C:239:LEU:HD22	1.78	0.66
1:A:187:ASN:HD21	2:A:601:NAD:H5N	1.61	0.65
1:B:518:SER:HA	1:D:95:ARG:HH11	1.61	0.65
1:D:177:ILE:HG12	1:D:505:GLU:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:LEU:HD13	1:D:418:ILE:HG12	1.80	0.64
1:D:135:ALA:O	1:D:140:LEU:HD12	1.99	0.63
1:D:31:PRO:O	1:D:33:LEU:N	2.32	0.61
1:B:320:CYS:HG	1:B:419:PHE:HZ	1.47	0.61
1:A:288:GLY:HA2	1:A:445:LEU:HD22	1.82	0.59
1:B:489:SER:O	1:B:489:SER:OG	2.14	0.59
1:C:64:GLU:N	1:C:64:GLU:OE2	2.32	0.59
1:B:111:ASP:OD1	1:B:148:ARG:NH2	2.33	0.59
1:C:445:LEU:HD12	1:C:485:GLY:HA2	1.85	0.59
1:A:479:ALA:HA	1:A:495:MET:HE3	1.85	0.58
1:B:337:VAL:O	1:B:341:VAL:HG12	2.03	0.58
1:B:386:GLU:OE2	1:B:405:SER:OG	2.18	0.58
1:C:467:GLY:HA3	1:C:485:GLY:H	1.67	0.58
1:A:298:ASP:OD2	1:A:456:LYS:NZ	2.36	0.57
1:A:348:VAL:HG11	1:A:356:THR:HG22	1.86	0.57
1:A:392:LEU:HD13	1:A:400:GLU:HG3	1.85	0.57
1:B:285:LEU:HB3	1:B:287:LEU:HD21	1.86	0.57
1:C:444:GLY:O	1:C:486:PHE:HB2	2.05	0.56
1:A:187:ASN:ND2	2:A:601:NAD:H5N	2.21	0.56
1:B:160:MET:HA	1:D:160:MET:HA	1.87	0.56
1:B:288:GLY:HA2	1:B:445:LEU:HD22	1.87	0.55
1:B:372:LEU:HD21	1:B:390:LYS:HB3	1.89	0.55
1:D:498:PHE:HA	1:D:501:ARG:HG3	1.89	0.55
1:C:513:ILE:HD11	1:C:516:LYS:HB2	1.87	0.54
1:D:430:THR:HG22	1:D:433:GLU:H	1.72	0.54
1:B:287:LEU:HB2	1:B:489:SER:HA	1.89	0.54
1:C:258:LYS:HD3	1:C:282:ARG:HB2	1.87	0.54
1:B:389:GLY:O	1:B:390:LYS:HB3	2.06	0.54
1:D:484:GLY:HA3	1:D:493:ARG:HD3	1.90	0.54
1:B:295:ILE:HD12	1:B:304:ALA:HB1	1.89	0.53
1:B:452:ASN:ND2	1:D:455:ASN:OD1	2.42	0.53
1:A:335:GLU:HG2	1:A:339:ARG:HE	1.73	0.53
1:D:187:ASN:HD21	2:D:601:NAD:H5N	1.73	0.53
1:B:443:PHE:HD1	1:B:489:SER:HB2	1.73	0.53
1:A:417:GLU:HG2	1:A:419:PHE:HD1	1.75	0.52
1:A:291:SER:HB3	1:A:446:VAL:HG12	1.90	0.52
1:B:173:ARG:NH1	1:B:175:GLU:OE2	2.43	0.52
1:B:430:THR:HG22	1:B:432:ASP:H	1.75	0.52
1:B:388:GLY:HA2	1:B:400:GLU:OE1	2.10	0.51
1:C:130:LYS:HD2	1:C:131:PRO:HD2	1.92	0.51
1:A:302:ASP:OD1	1:A:339:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ASN:HB3	3:B:602:CU4:N12	2.26	0.51
1:A:160:MET:HA	1:C:160:MET:HA	1.93	0.51
1:D:330:GLU:HB2	1:D:429:LYS:HG2	1.92	0.51
1:B:308:ALA:HB1	1:B:326:ILE:HD13	1.92	0.50
1:D:321:THR:HG22	1:D:446:VAL:HG21	1.93	0.50
1:D:253:HIS:O	1:D:281:LYS:NZ	2.45	0.50
1:B:258:LYS:HZ3	1:B:260:ALA:HB2	1.77	0.50
1:C:464:MET:O	1:D:507:LYS:NZ	2.44	0.50
1:B:266:GLU:H	1:B:266:GLU:CD	2.14	0.50
1:B:265:THR:HG1	1:B:443:PHE:HE1	1.58	0.50
1:D:335:GLU:OE2	1:D:339:ARG:NH2	2.37	0.50
1:B:427:ARG:O	1:B:437:ARG:NH1	2.39	0.49
1:B:321:THR:HG22	1:B:446:VAL:HG11	1.95	0.49
1:D:419:PHE:CZ	2:D:601:NAD:H2D	2.48	0.49
1:A:73:ASP:OD1	1:A:74:LYS:N	2.46	0.49
1:C:196:LYS:NZ	1:C:262:THR:OG1	2.44	0.49
1:B:390:LYS:HZ1	1:B:392:LEU:H	1.61	0.48
1:B:321:THR:O	1:B:474:TYR:OH	2.17	0.48
1:D:121:ALA:HB2	1:D:140:LEU:HD13	1.94	0.48
1:C:321:THR:HG22	1:C:446:VAL:HG21	1.95	0.48
1:A:484:GLY:HA3	1:A:493:ARG:HD3	1.95	0.48
1:B:393:GLY:O	1:B:395:LYS:N	2.46	0.48
1:D:335:GLU:OE1	1:D:338:ARG:NH2	2.42	0.48
1:A:417:GLU:HG2	1:A:419:PHE:CD1	2.49	0.48
1:C:149:TYR:CE1	1:C:480:GLN:HG3	2.49	0.48
1:B:390:LYS:HB2	1:B:399:ILE:HG23	1.96	0.47
1:B:208:VAL:HG13	1:B:239:LEU:HD13	1.96	0.47
1:A:308:ALA:HB1	1:A:326:ILE:HD13	1.97	0.47
1:D:153:TRP:CG	1:D:500:LEU:HD11	2.49	0.47
1:B:112:LEU:HB3	1:B:225:LEU:HD22	1.95	0.47
1:C:312:VAL:O	1:C:317:GLY:HA2	2.15	0.47
1:B:460:VAL:O	1:B:464:MET:HG2	2.15	0.47
1:C:470:TRP:HD1	1:D:510:THR:HB	1.79	0.47
1:A:30:THR:HB	1:A:33:LEU:HD13	1.97	0.46
1:B:324:SER:OG	1:B:325:ARG:N	2.47	0.46
1:B:374:LEU:HA	1:B:377:SER:HB3	1.97	0.46
1:B:143:VAL:HG21	1:B:190:LEU:HG	1.97	0.46
1:B:289:GLY:HA3	1:B:443:PHE:HB3	1.98	0.46
1:C:187:ASN:ND2	2:C:601:NAD:H5N	2.27	0.46
1:C:419:PHE:CZ	2:C:601:NAD:H2D	2.51	0.46
1:B:383:ALA:HB2	1:B:411:MET:HE1	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:NZ	1:D:262:THR:OG1	2.47	0.45
1:B:439:ASN:O	1:B:441:SER:N	2.49	0.45
1:C:505:GLU:HG2	1:D:486:PHE:CE1	2.52	0.45
1:A:282:ARG:NH2	1:A:505:GLU:OE1	2.50	0.45
1:B:323:GLY:O	1:B:325:ARG:N	2.50	0.45
2:A:601:NAD:H8A	2:A:601:NAD:H2B	1.88	0.44
1:C:73:ASP:O	1:C:77:ILE:HG12	2.18	0.44
1:B:493:ARG:HA	1:B:493:ARG:HD3	1.89	0.44
1:C:145:LYS:NZ	4:C:702:HOH:O	2.38	0.44
1:B:41:PHE:CZ	1:B:44:ASN:HA	2.52	0.44
1:A:158:HIS:CG	1:C:160:MET:HE2	2.52	0.44
1:B:372:LEU:HD21	1:B:390:LYS:CB	2.48	0.44
1:A:300:ASP:HB3	1:A:303:TYR:HB3	2.00	0.44
1:B:61:ALA:HA	1:B:361:PRO:HG3	2.00	0.44
1:C:312:VAL:HG23	1:C:313:PHE:CD2	2.53	0.44
1:C:297:ALA:N	1:C:329:GLU:OE1	2.39	0.44
1:B:487:LYS:HB3	1:B:488:MET:H	1.52	0.44
1:C:308:ALA:O	1:C:312:VAL:HG22	2.17	0.44
1:B:131:PRO:HB2	1:B:134:GLN:HG2	1.99	0.43
1:B:210:LYS:NZ	1:B:211:PRO:O	2.49	0.43
1:D:308:ALA:HB1	1:D:326:ILE:HD13	1.99	0.43
1:D:73:ASP:O	1:D:77:ILE:HG12	2.17	0.43
1:A:177:ILE:N	1:A:205:ASN:OD1	2.51	0.43
1:B:484:GLY:HA3	1:B:493:ARG:HD3	2.00	0.43
1:D:263:GLY:O	1:D:287:LEU:HA	2.19	0.43
1:C:415:LYS:HE2	1:C:415:LYS:HB3	1.83	0.43
1:B:149:TYR:CE1	1:B:480:GLN:HG3	2.54	0.42
1:A:417:GLU:OE2	1:A:419:PHE:CE1	2.52	0.42
1:A:312:VAL:O	1:A:317:GLY:HA2	2.19	0.42
1:A:333:TYR:CD1	1:A:427:ARG:HB3	2.55	0.42
1:B:104:ARG:HD2	1:B:104:ARG:HA	1.82	0.42
1:B:494:GLU:HG2	1:B:495:MET:H	1.84	0.42
1:C:444:GLY:O	1:C:466:ALA:HA	2.20	0.42
1:B:284:THR:HG21	1:B:502:GLU:HG3	2.00	0.42
1:B:393:GLY:C	1:B:395:LYS:H	2.22	0.42
1:D:104:ARG:HA	1:D:104:ARG:HD2	1.85	0.42
1:C:395:LYS:HG3	4:C:723:HOH:O	2.20	0.42
1:B:35:ILE:HD13	1:B:217:LEU:HD13	2.02	0.41
1:C:210:LYS:HE3	1:C:211:PRO:O	2.20	0.41
1:B:312:VAL:HG23	1:B:324:SER:H	1.84	0.41
1:A:280:LEU:HB2	1:B:488:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:MET:O	1:C:226:ILE:HG12	2.20	0.41
1:D:292:PRO:HG3	1:D:438:ALA:HB1	2.02	0.41
1:D:32:ASN:OD1	1:D:33:LEU:N	2.53	0.41
1:A:474:TYR:HA	1:A:475:ASN:HA	1.69	0.41
1:B:192:MET:HE2	1:B:192:MET:HB3	1.92	0.41
1:A:95:ARG:HH21	1:C:518:SER:HA	1.86	0.41
1:D:208:VAL:HG13	1:D:239:LEU:HD13	2.03	0.41
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.82	0.41
1:A:88:PHE:CE2	1:A:178:GLY:HA2	2.54	0.41
1:A:479:ALA:HA	1:A:495:MET:CE	2.51	0.41
1:B:287:LEU:O	2:B:601:NAD:O2D	2.37	0.41
1:C:30:THR:HA	1:C:31:PRO:HD3	1.93	0.41
1:A:288:GLY:HA3	1:A:320:CYS:SG	2.60	0.41
1:B:301:LEU:HA	1:B:301:LEU:HD23	1.85	0.41
1:D:127:ASN:ND2	1:D:127:ASN:O	2.53	0.41
1:A:40:ILE:HG22	1:A:42:ILE:HG13	2.02	0.41
1:A:208:VAL:HG13	1:A:239:LEU:HD13	2.02	0.41
1:B:33:LEU:HD11	1:B:119:VAL:HG13	2.03	0.41
1:C:515:GLN:O	1:C:516:LYS:HB3	2.21	0.41
1:A:373:GLU:CD	1:A:412:ARG:HH22	2.24	0.41
1:B:451:THR:OG1	1:B:452:ASN:N	2.52	0.41
1:C:29:PRO:HG3	1:C:132:PHE:CG	2.55	0.41
1:C:49:SER:HB2	1:C:52:GLY:H	1.86	0.41
1:C:308:ALA:HB1	1:C:326:ILE:HD13	2.03	0.41
1:C:374:LEU:HD13	1:C:418:ILE:HG12	2.04	0.40
1:D:325:ARG:HD3	1:D:414:ALA:O	2.21	0.40
1:C:117:ARG:HG3	1:C:140:LEU:HD22	2.03	0.40
1:D:263:GLY:C	2:D:601:NAD:H1D	2.41	0.40
1:C:51:SER:OG	1:C:53:ARG:HG3	2.20	0.40
1:D:261:PHE:HB3	1:D:285:LEU:HD23	2.03	0.40
1:D:407:VAL:HB	1:D:426:LEU:HG	2.02	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	490/493 (99%)	469 (96%)	16 (3%)	5 (1%)	17	19
1	B	490/493 (99%)	455 (93%)	23 (5%)	12 (2%)	6	5
1	C	490/493 (99%)	455 (93%)	29 (6%)	6 (1%)	14	15
1	D	490/493 (99%)	463 (94%)	20 (4%)	7 (1%)	12	12
All	All	1960/1972 (99%)	1842 (94%)	88 (4%)	30 (2%)	11	11

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	PRO
1	B	386	GLU
1	C	475	ASN
1	D	32	ASN
1	A	516	LYS
1	B	324	SER
1	B	394	ARG
1	B	444	GLY
1	B	491	ASN
1	D	416	GLU
1	A	31	PRO
1	B	384	LYS
1	B	440	ASN
1	C	481	SER
1	C	483	PHE
1	D	476	ALA
1	D	477	LEU
1	A	300	ASP
1	A	474	TYR
1	C	444	GLY
1	C	485	GLY
1	C	516	LYS
1	D	33	LEU
1	D	430	THR
1	B	390	LYS
1	B	395	LYS
1	D	516	LYS
1	B	185	PRO
1	B	391	GLY
1	A	185	PRO

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	401/402 (100%)	397 (99%)	4 (1%)	78	89
1	B	401/402 (100%)	396 (99%)	5 (1%)	74	86
1	C	401/402 (100%)	395 (98%)	6 (2%)	67	82
1	D	401/402 (100%)	394 (98%)	7 (2%)	63	79
All	All	1604/1608 (100%)	1582 (99%)	22 (1%)	69	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	127	ASN
1	A	174	HIS
1	A	474	TYR
1	B	127	ASN
1	B	192	MET
1	B	290	LYS
1	B	394	ARG
1	B	456	LYS
1	C	127	ASN
1	C	130	LYS
1	C	139	ASP
1	C	140	LEU
1	C	394	ARG
1	C	395	LYS
1	D	50	GLU
1	D	95	ARG
1	D	139	ASP
1	D	281	LYS
1	D	395	LYS
1	D	415	LYS
1	D	419	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	B	359	GLN
1	D	515	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	601	-	40,48,48	4.08	13 (32%)	44,73,73	1.98	9 (20%)
3	CU4	A	602	-	35,36,36	2.78	11 (31%)	44,52,52	2.05	9 (20%)
2	NAD	B	601	-	40,48,48	4.00	13 (32%)	44,73,73	1.95	6 (13%)
3	CU4	B	602	-	35,36,36	2.71	11 (31%)	44,52,52	1.86	8 (18%)
2	NAD	C	601	-	40,48,48	3.96	13 (32%)	44,73,73	1.87	5 (11%)
3	CU4	C	602	-	35,36,36	2.69	10 (28%)	44,52,52	1.90	7 (15%)
2	NAD	D	601	-	40,48,48	3.94	13 (32%)	44,73,73	1.98	5 (11%)
3	CU4	D	602	-	35,36,36	2.68	9 (25%)	44,52,52	1.90	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	601	-	-	0/22/62/62	0/5/5/5
3	CU4	A	602	-	-	0/22/24/24	0/4/4/4
2	NAD	B	601	-	-	0/22/62/62	0/5/5/5
3	CU4	B	602	-	-	0/22/24/24	0/4/4/4
2	NAD	C	601	-	-	0/22/62/62	0/5/5/5
3	CU4	C	602	-	-	0/22/24/24	0/4/4/4
2	NAD	D	601	-	-	0/22/62/62	0/5/5/5
3	CU4	D	602	-	-	0/22/24/24	0/4/4/4

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	CU4	C08-C11	-6.71	1.41	1.49
2	D	601	NAD	O4B-C4B	-6.68	1.30	1.45
2	A	601	NAD	O4D-C4D	-6.54	1.30	1.45
2	C	601	NAD	O4B-C4B	-6.37	1.30	1.45
2	A	601	NAD	O4B-C4B	-6.26	1.31	1.45
2	D	601	NAD	O4D-C4D	-6.21	1.31	1.45
2	B	601	NAD	O4B-C4B	-6.17	1.31	1.45
2	B	601	NAD	O4D-C4D	-6.11	1.31	1.45
2	C	601	NAD	O4D-C4D	-5.98	1.31	1.45
3	C	602	CU4	C08-C11	-5.97	1.42	1.49
3	B	602	CU4	C08-C11	-5.96	1.42	1.49
3	D	602	CU4	C08-C11	-5.95	1.42	1.49
3	A	602	CU4	C29-C32	-5.93	1.30	1.44
3	C	602	CU4	C29-C32	-5.92	1.30	1.44
3	B	602	CU4	C29-C32	-5.91	1.30	1.44
3	D	602	CU4	C29-C32	-5.88	1.30	1.44
3	A	602	CU4	N12-N13	-5.52	1.29	1.39
3	B	602	CU4	N12-N13	-5.43	1.29	1.39
3	C	602	CU4	N12-N13	-5.33	1.29	1.39
3	D	602	CU4	N12-N13	-5.30	1.30	1.39
3	A	602	CU4	C26-N13	-4.10	1.36	1.44
3	D	602	CU4	C26-N13	-3.89	1.36	1.44
3	C	602	CU4	C26-N13	-3.89	1.36	1.44
3	B	602	CU4	C26-N13	-3.88	1.36	1.44
3	B	602	CU4	C15-C16	-3.66	1.42	1.50
3	A	602	CU4	C15-C16	-3.66	1.42	1.50
3	C	602	CU4	C15-C16	-3.60	1.42	1.50
3	D	602	CU4	C15-C16	-3.48	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	O3D-C3D	-3.09	1.35	1.43
2	D	601	NAD	O3D-C3D	-3.07	1.35	1.43
2	B	601	NAD	O3D-C3D	-2.99	1.35	1.43
2	B	601	NAD	O3B-C3B	-2.93	1.35	1.43
2	A	601	NAD	O3B-C3B	-2.91	1.35	1.43
2	D	601	NAD	O3B-C3B	-2.84	1.36	1.43
2	A	601	NAD	O3D-C3D	-2.81	1.36	1.43
2	C	601	NAD	O3B-C3B	-2.80	1.36	1.43
2	C	601	NAD	C5A-C4A	-2.40	1.35	1.40
2	A	601	NAD	C5A-C4A	-2.32	1.35	1.40
2	B	601	NAD	C5A-C4A	-2.31	1.35	1.40
2	D	601	NAD	C5A-C4A	-2.30	1.35	1.40
3	A	602	CU4	F24-C23	-2.29	1.30	1.36
3	C	602	CU4	F24-C23	-2.27	1.31	1.36
3	B	602	CU4	F24-C23	-2.26	1.31	1.36
3	D	602	CU4	F24-C23	-2.25	1.31	1.36
3	B	602	CU4	C22-C23	2.00	1.41	1.37
3	A	602	CU4	C01-S02	2.04	1.83	1.75
3	D	602	CU4	C25-C23	2.05	1.41	1.37
3	C	602	CU4	C25-C23	2.06	1.41	1.37
3	A	602	CU4	C25-C23	2.08	1.41	1.37
3	B	602	CU4	C01-S02	2.15	1.83	1.75
3	C	602	CU4	C01-S02	2.16	1.83	1.75
3	A	602	CU4	C06-C05	2.18	1.42	1.38
2	A	601	NAD	O2D-C2D	2.19	1.48	1.43
3	B	602	CU4	C25-C23	2.19	1.41	1.37
2	C	601	NAD	O2D-C2D	2.25	1.48	1.43
2	D	601	NAD	O2D-C2D	2.29	1.48	1.43
2	B	601	NAD	O2D-C2D	2.32	1.48	1.43
2	C	601	NAD	C6A-N6A	2.33	1.43	1.34
2	A	601	NAD	C6A-N6A	2.36	1.43	1.34
2	B	601	NAD	C6A-N6A	2.37	1.43	1.34
2	D	601	NAD	C6A-N6A	2.39	1.43	1.34
2	B	601	NAD	O2B-C2B	2.50	1.49	1.43
2	D	601	NAD	C2A-N3A	2.52	1.36	1.32
2	C	601	NAD	C2A-N3A	2.55	1.36	1.32
2	A	601	NAD	C2A-N3A	2.65	1.36	1.32
2	A	601	NAD	O2B-C2B	2.69	1.49	1.43
2	B	601	NAD	C2A-N3A	2.74	1.36	1.32
2	C	601	NAD	O2B-C2B	2.76	1.49	1.43
2	D	601	NAD	O2B-C2B	3.04	1.50	1.43
2	D	601	NAD	C3N-C7N	3.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	C3N-C7N	3.40	1.55	1.50
2	B	601	NAD	C3N-C7N	3.52	1.56	1.50
2	A	601	NAD	C3N-C7N	3.60	1.56	1.50
3	D	602	CU4	O04-S02	5.81	1.60	1.43
3	A	602	CU4	O03-S02	5.82	1.60	1.43
3	B	602	CU4	O04-S02	5.83	1.60	1.43
3	C	602	CU4	O04-S02	5.83	1.60	1.43
3	C	602	CU4	O03-S02	5.88	1.61	1.43
3	D	602	CU4	O03-S02	5.89	1.61	1.43
3	B	602	CU4	O03-S02	5.90	1.61	1.43
3	A	602	CU4	O04-S02	6.01	1.61	1.43
2	D	601	NAD	C7N-N7N	6.09	1.44	1.33
2	C	601	NAD	C7N-N7N	6.09	1.44	1.33
2	A	601	NAD	C7N-N7N	6.14	1.45	1.33
2	B	601	NAD	C7N-N7N	6.16	1.45	1.33
2	D	601	NAD	O4D-C1D	14.34	1.61	1.41
2	C	601	NAD	O4D-C1D	14.53	1.61	1.41
2	D	601	NAD	O4B-C1B	14.77	1.61	1.41
2	B	601	NAD	O4D-C1D	14.78	1.61	1.41
2	A	601	NAD	O4B-C1B	15.01	1.62	1.41
2	C	601	NAD	O4B-C1B	15.04	1.62	1.41
2	B	601	NAD	O4B-C1B	15.13	1.62	1.41
2	A	601	NAD	O4D-C1D	15.49	1.62	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	N3A-C2A-N1A	-10.20	120.13	128.86
2	B	601	NAD	N3A-C2A-N1A	-10.18	120.15	128.86
2	C	601	NAD	N3A-C2A-N1A	-9.99	120.31	128.86
2	D	601	NAD	N3A-C2A-N1A	-9.87	120.41	128.86
3	C	602	CU4	O04-S02-O03	-5.55	107.82	117.84
3	A	602	CU4	O04-S02-O03	-5.37	108.14	117.84
3	B	602	CU4	O04-S02-O03	-5.35	108.18	117.84
3	D	602	CU4	O04-S02-O03	-5.31	108.24	117.84
2	D	601	NAD	C4D-O4D-C1D	-4.41	105.23	109.83
2	D	601	NAD	C4B-O4B-C1B	-3.57	106.11	109.83
2	B	601	NAD	C4D-O4D-C1D	-3.51	106.16	109.83
2	B	601	NAD	C4B-O4B-C1B	-2.80	106.91	109.83
3	D	602	CU4	C22-C23-C25	-2.76	119.66	123.29
2	A	601	NAD	C4D-O4D-C1D	-2.76	106.95	109.83
3	C	602	CU4	C22-C23-C25	-2.73	119.70	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	CU4	C22-C23-C25	-2.68	119.76	123.29
2	A	601	NAD	PN-O3-PA	-2.66	123.67	132.63
3	B	602	CU4	C22-C23-C25	-2.54	119.95	123.29
2	C	601	NAD	C4D-O4D-C1D	-2.52	107.20	109.83
2	D	601	NAD	PN-O3-PA	-2.49	124.26	132.63
2	C	601	NAD	PN-O3-PA	-2.46	124.37	132.63
2	A	601	NAD	C4B-O4B-C1B	-2.23	107.50	109.83
2	B	601	NAD	C5B-C4B-C3B	-2.18	107.08	115.29
2	B	601	NAD	PN-O3-PA	-2.13	125.47	132.63
2	C	601	NAD	N6A-C6A-N1A	-2.10	114.21	118.57
3	D	602	CU4	O17-C16-C15	-2.08	117.11	120.98
2	A	601	NAD	O7N-C7N-N7N	-2.01	119.68	122.60
2	A	601	NAD	C2N-C3N-C4N	2.01	120.57	118.26
2	A	601	NAD	C2D-C3D-C4D	2.15	106.74	102.62
3	B	602	CU4	C15-C16-N18	2.22	120.46	116.12
2	A	601	NAD	C5A-C6A-N6A	2.39	125.34	120.47
2	A	601	NAD	C3N-C7N-N7N	2.45	120.60	117.76
2	B	601	NAD	C5A-C6A-N6A	2.49	125.54	120.47
2	D	601	NAD	C5A-C6A-N6A	2.64	125.85	120.47
2	C	601	NAD	C5A-C6A-N6A	2.64	125.85	120.47
3	A	602	CU4	C15-C16-N18	2.79	121.56	116.12
3	B	602	CU4	O04-S02-C05	2.79	110.55	108.29
3	C	602	CU4	C15-C16-N18	2.80	121.59	116.12
3	D	602	CU4	C15-C16-N18	3.18	122.32	116.12
3	B	602	CU4	O03-S02-C05	3.36	111.01	108.29
3	B	602	CU4	C19-C25-C23	3.46	121.07	117.97
3	A	602	CU4	C11-N12-N13	3.56	109.23	105.44
3	D	602	CU4	C01-S02-C05	3.57	108.83	104.59
3	A	602	CU4	C06-C05-S02	3.61	123.08	119.60
3	A	602	CU4	C19-C25-C23	3.66	121.24	117.97
3	D	602	CU4	O03-S02-C05	3.73	111.31	108.29
3	C	602	CU4	O03-S02-C05	3.83	111.39	108.29
3	A	602	CU4	O04-S02-C05	3.93	111.47	108.29
3	C	602	CU4	C19-C25-C23	3.97	121.52	117.97
3	C	602	CU4	C11-N12-N13	4.01	109.71	105.44
3	D	602	CU4	O04-S02-C05	4.04	111.56	108.29
3	D	602	CU4	C11-N12-N13	4.04	109.75	105.44
3	D	602	CU4	C19-C25-C23	4.19	121.72	117.97
3	B	602	CU4	C11-N12-N13	4.39	110.12	105.44
3	A	602	CU4	O03-S02-C05	4.48	111.91	108.29
3	B	602	CU4	C01-S02-C05	4.84	110.33	104.59
3	A	602	CU4	C01-S02-C05	5.11	110.65	104.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	CU4	C01-S02-C05	5.57	111.20	104.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	4	0
2	B	601	NAD	3	0
3	B	602	CU4	1	0
2	C	601	NAD	3	0
2	D	601	NAD	3	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 ⓘ

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	492/493 (99%)	0.05	4 (0%) 86 89	22, 35, 49, 65	0
1	B	492/493 (99%)	0.45	25 (5%) 28 35	22, 49, 74, 86	0
1	C	492/493 (99%)	0.27	17 (3%) 44 51	26, 46, 61, 77	0
1	D	492/493 (99%)	0.06	6 (1%) 79 83	20, 34, 49, 64	0
All	All	1968/1972 (99%)	0.21	52 (2%) 56 63	20, 40, 67, 86	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	391	GLY	9.3
1	B	492	GLY	6.5
1	B	477	LEU	5.7
1	A	518	SER	5.3
1	B	311	GLY	5.1
1	B	476	ALA	4.4
1	C	394	ARG	4.3
1	B	393	GLY	4.3
1	A	474	TYR	4.2
1	B	419	PHE	3.9
1	B	410	ASP	3.5
1	B	483	PHE	3.5
1	C	492	GLY	3.4
1	B	374	LEU	3.3
1	A	419	PHE	3.3
1	B	491	ASN	3.3
1	C	312	VAL	3.2
1	C	484	GLY	3.2
1	B	288	GLY	3.1
1	B	392	LEU	3.1
1	C	483	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	518	SER	2.9
1	B	319	CYS	2.8
1	D	419	PHE	2.8
1	D	495	MET	2.7
1	C	495	MET	2.7
1	C	481	SER	2.7
1	B	479	ALA	2.7
1	C	478	ASN	2.7
1	D	322	ALA	2.6
1	B	323	GLY	2.6
1	C	319	CYS	2.6
1	C	518	SER	2.5
1	A	443	PHE	2.5
1	C	410	ASP	2.5
1	B	318	GLN	2.4
1	C	64	GLU	2.4
1	C	324	SER	2.3
1	C	314	PHE	2.2
1	D	481	SER	2.2
1	D	443	PHE	2.2
1	C	486	PHE	2.2
1	B	494	GLU	2.2
1	B	495	MET	2.2
1	B	324	SER	2.2
1	D	164	VAL	2.1
1	C	489	SER	2.1
1	C	485	GLY	2.1
1	B	404	PHE	2.1
1	B	66	VAL	2.1
1	B	336	PHE	2.0
1	B	486	PHE	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CU4	B	602	33/33	0.72	0.38	58,73,83,83	0
2	NAD	D	601	44/44	0.87	0.24	24,48,64,66	0
3	CU4	D	602	33/33	0.87	0.29	40,50,60,70	0
3	CU4	A	602	33/33	0.88	0.24	44,52,58,62	0
3	CU4	C	602	33/33	0.90	0.25	50,61,68,74	0
2	NAD	B	601	44/44	0.91	0.19	39,59,69,71	0
2	NAD	C	601	44/44	0.92	0.17	36,50,64,65	0
2	NAD	A	601	44/44	0.93	0.17	25,43,57,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.