



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:19 PM GMT

PDB ID : 1A4Z
Title : ALDEHYDE DEHYDROGENASE FROM BOVINE MITOCHONDRIA
COMPLEX WITH NAD (REDUCED) AND SAMARIUM (III)
Authors : Steinmetz, C.G.; Hurley, T.D.
Deposited on : 1998-02-10
Resolution : 2.75 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

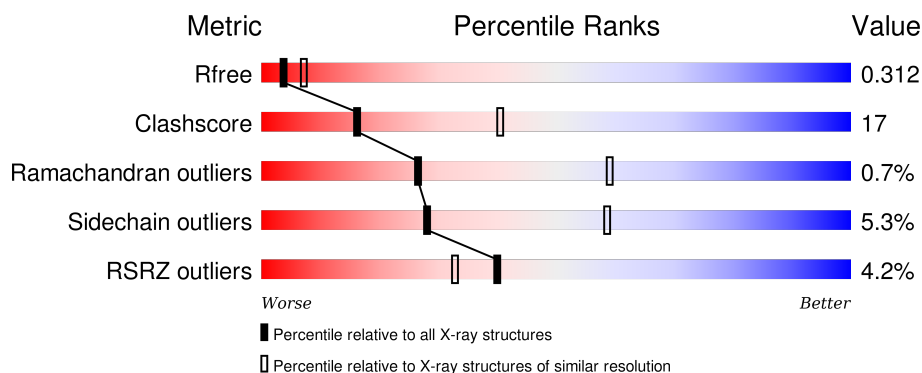
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	499	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>..</div> </div> </div>
1	B	499	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div> </div>
1	C	499	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>..</div> </div> </div>
1	D	499	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15464 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.

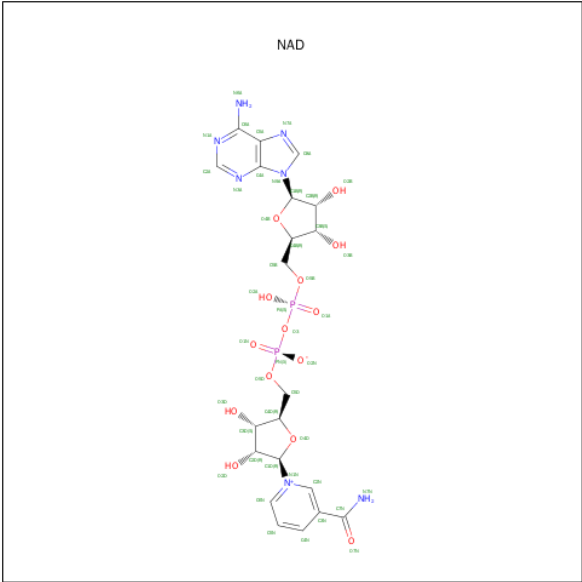
- Molecule 1 is a protein called ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3799	2418	650	714	17			
1	B	493	Total	C	N	O	S	0	0	0
			3799	2418	650	714	17			
1	C	493	Total	C	N	O	S	0	0	0
			3799	2418	650	714	17			
1	D	493	Total	C	N	O	S	0	0	0
			3799	2418	650	714	17			

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

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

- 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		

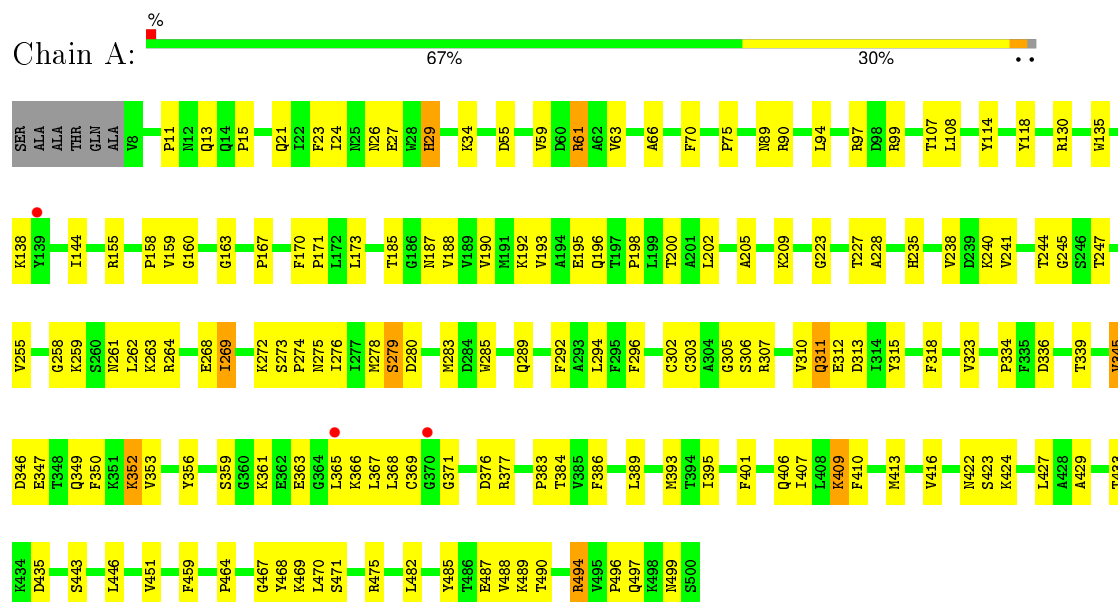
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	23	Total	O	0	0
			23	23		
4	C	18	Total	O	0	0
			18	18		
4	D	21	Total	O	0	0
			21	21		

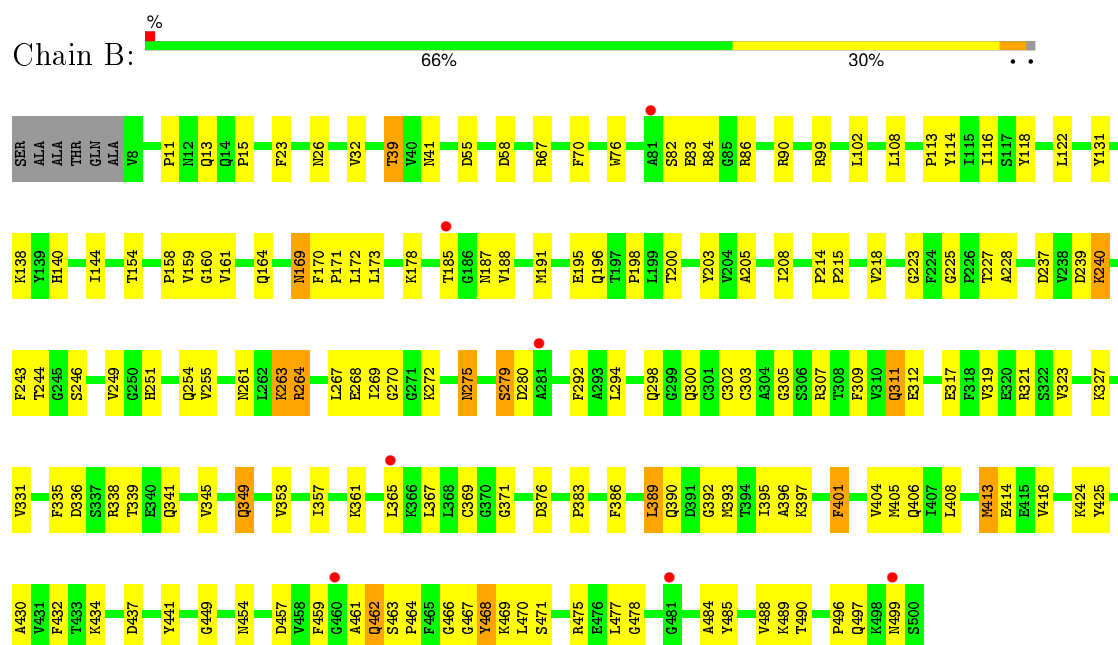
3 Residue-property plots

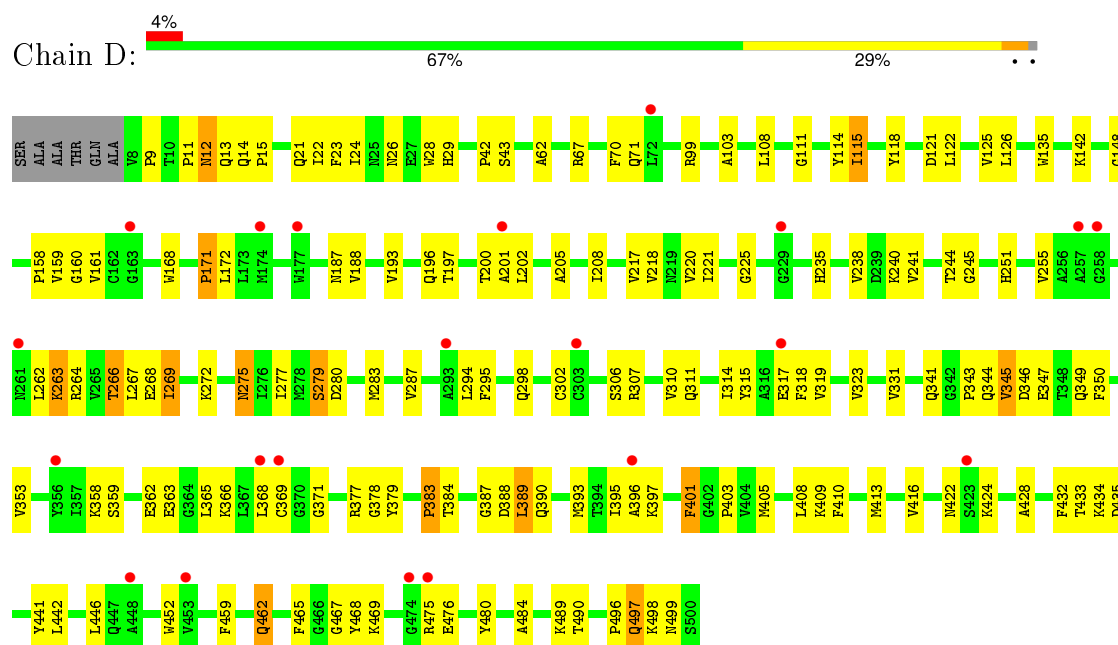
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ALDEHYDE DEHYDROGENASE



• Molecule 1: ALDEHYDE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.60 Å 198.40 Å 91.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.75 77.12 – 2.75	Depositor EDS
% Data completeness (in resolution range)	85.0 (8.00-2.75) 84.7 (77.12-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.73 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.302 0.265 , 0.312	Depositor DCC
R_{free} test set	3354 reflections (7.61%)	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 50110 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	15464	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SM, 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	0.41	0/3884	0.64	0/5268
1	B	0.42	0/3884	0.66	0/5268
1	C	0.39	0/3884	0.63	0/5268
1	D	0.40	0/3884	0.64	0/5268
All	All	0.40	0/15536	0.65	0/21072

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	3799	0	3755	125	0
1	B	3799	0	3755	135	0
1	C	3799	0	3755	147	0
1	D	3799	0	3755	131	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	3	0
3	C	44	0	26	5	0
3	D	44	0	26	7	0
4	A	26	0	0	1	0
4	B	23	0	0	1	0
4	C	18	0	0	0	0
4	D	21	0	0	0	0
All	All	15464	0	15124	511	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 17.

All (511) 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:C:365:LEU:HD13	1:C:395:ILE:HD11	1.44	0.98
1:A:365:LEU:HD22	1:A:389:LEU:HG	1.45	0.94
1:A:365:LEU:HD21	1:A:393:MET:SD	2.07	0.94
1:C:365:LEU:HD11	1:C:393:MET:SD	2.06	0.94
1:A:365:LEU:HD13	1:A:395:ILE:HD11	1.49	0.94
1:C:424:LYS:HD2	1:C:470:LEU:HD12	1.51	0.90
1:D:268:GLU:HG3	1:D:476:GLU:OE2	1.71	0.89
1:C:359:SER:O	1:C:363:GLU:HG2	1.77	0.85
1:B:365:LEU:HD21	1:B:389:LEU:HG	1.59	0.84
1:D:365:LEU:HD21	1:D:393:MET:SD	2.18	0.83
1:A:433:THR:HG22	1:A:435:ASP:H	1.42	0.82
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.64	0.77
1:D:359:SER:O	1:D:363:GLU:HG2	1.85	0.76
1:A:185:THR:HG21	1:A:485:TYR:O	1.86	0.76
1:B:169:ASN:HD21	3:B:501:NAD:H6N	1.51	0.75
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.20	0.75
1:C:311:GLN:HE22	1:C:312:GLU:HG2	1.50	0.74
1:D:433:THR:HG22	1:D:435:ASP:H	1.50	0.74
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.67	0.73
1:B:392:GLY:HA2	1:B:397:LYS:NZ	2.03	0.73
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.69	0.73
1:C:172:LEU:HD21	1:C:200:THR:HB	1.71	0.72
1:B:365:LEU:HD13	1:B:395:ILE:HD11	1.70	0.72
1:D:279:SER:HA	1:D:314:ILE:HD13	1.72	0.72
1:D:344:GLN:NE2	1:D:403:PRO:HD3	2.05	0.71
1:D:188:VAL:HG23	1:D:217:VAL:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.26	0.70
1:C:365:LEU:HD22	1:C:389:LEU:HD22	1.72	0.70
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.72	0.70
1:D:115:ILE:H	1:D:115:ILE:HD13	1.54	0.70
1:B:292:PHE:HE1	1:B:457:ASP:HB2	1.57	0.70
1:B:264:ARG:HD2	1:B:264:ARG:H	1.57	0.70
1:A:409:LYS:NZ	1:A:409:LYS:HB2	2.07	0.70
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.27	0.70
1:D:240:LYS:NZ	1:D:484:ALA:HB1	2.07	0.70
1:C:272:LYS:HD2	1:C:306:SER:HB2	1.73	0.69
1:A:258:GLY:CA	1:B:254:GLN:HG2	2.22	0.69
1:A:361:LYS:HE3	1:A:367:LEU:HD22	1.75	0.69
1:C:283:MET:HB3	1:C:321:ARG:NH1	2.07	0.69
1:D:365:LEU:HD11	1:D:393:MET:SD	2.33	0.69
1:D:389:LEU:HD23	1:D:396:ALA:HB2	1.73	0.69
1:A:227:THR:HG22	1:A:228:ALA:N	2.08	0.68
1:B:279:SER:OG	1:B:311:GLN:HG2	1.93	0.68
1:B:272:LYS:HB2	1:B:425:TYR:CD2	2.29	0.68
1:A:279:SER:OG	1:A:311:GLN:HG2	1.92	0.68
1:D:377:ARG:HG3	1:D:378:GLY:H	1.57	0.68
1:C:372:GLY:O	1:C:382:GLN:HG3	1.94	0.67
1:A:268:GLU:HB3	3:A:501:NAD:N7N	2.10	0.67
1:C:349:GLN:O	1:C:353:VAL:HG23	1.95	0.67
1:C:159:VAL:H	1:C:187:ASN:HD21	1.42	0.66
1:C:365:LEU:HD21	1:C:389:LEU:HA	1.76	0.66
1:D:331:VAL:HG22	1:D:341:GLN:HB3	1.76	0.66
1:A:255:VAL:HG13	1:B:255:VAL:HG13	1.78	0.66
1:A:323:VAL:HG13	1:A:369:CYS:SG	2.35	0.66
1:B:365:LEU:CD1	1:B:395:ILE:HD11	2.25	0.66
1:B:264:ARG:HD2	1:B:264:ARG:N	2.10	0.66
1:C:294:LEU:HD11	1:C:405:MET:HA	1.78	0.66
1:C:252:LEU:O	1:C:255:VAL:HG12	1.96	0.66
1:C:294:LEU:CD1	1:C:405:MET:HA	2.25	0.66
1:B:76:TRP:CH2	1:B:84:ARG:HG2	2.31	0.65
1:D:365:LEU:HD13	1:D:389:LEU:HG	1.78	0.65
1:D:121:ASP:O	1:D:125:VAL:HG23	1.96	0.65
1:D:171:PRO:HG3	1:D:197:THR:HG21	1.79	0.65
1:B:280:ASP:O	1:B:434:LYS:HG3	1.97	0.65
1:D:70:PHE:CZ	1:D:158:PRO:HB2	2.33	0.64
1:C:159:VAL:N	1:C:187:ASN:HD21	1.95	0.64
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HD13	1:A:61:ARG:HD2	1.80	0.64
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.78	0.64
1:D:103:ALA:HB2	1:D:122:LEU:HD12	1.79	0.64
1:C:42:PRO:HB3	1:C:345:VAL:O	1.98	0.64
1:A:490:THR:OG1	1:B:464:PRO:HG2	1.98	0.64
1:A:238:VAL:O	1:A:261:ASN:ND2	2.31	0.64
1:D:148:GLY:O	1:D:498:LYS:HD3	1.98	0.63
1:D:160:GLY:H	1:D:187:ASN:ND2	1.97	0.63
1:D:302:CYS:SG	3:D:501:NAD:C4N	2.87	0.63
1:B:365:LEU:HD11	1:B:393:MET:SD	2.39	0.63
1:C:389:LEU:HD12	1:C:396:ALA:HB2	1.81	0.62
1:C:315:TYR:CE1	1:C:319:VAL:HG21	2.34	0.62
1:A:303:CYS:HG	1:A:459:PHE:HZ	1.47	0.62
1:A:27:GLU:HG3	1:A:29:HIS:CE1	2.34	0.62
1:D:15:PRO:HG2	1:D:108:LEU:HD22	1.81	0.62
1:D:251:HIS:O	1:D:255:VAL:HG23	2.00	0.62
1:C:365:LEU:HD13	1:C:395:ILE:CD1	2.26	0.62
1:C:272:LYS:HG3	1:C:307:ARG:CD	2.30	0.62
1:D:70:PHE:HZ	1:D:158:PRO:HB2	1.65	0.62
1:D:245:GLY:O	1:D:269:ILE:HG22	1.98	0.62
1:C:311:GLN:NE2	1:C:411:LYS:HA	2.15	0.62
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.35	0.61
1:C:241:VAL:HG23	1:C:263:LYS:HG3	1.82	0.61
1:D:358:LYS:O	1:D:362:GLU:HG3	2.00	0.61
1:D:28:TRP:O	1:D:29:HIS:HD2	1.84	0.61
1:B:461:ALA:HA	1:B:477:LEU:HD22	1.81	0.61
1:A:365:LEU:CD2	1:A:389:LEU:HG	2.26	0.60
1:A:99:ARG:HG2	1:A:118:TYR:CE2	2.36	0.60
1:C:70:PHE:CZ	1:C:158:PRO:HB2	2.36	0.60
1:B:159:VAL:N	1:B:187:ASN:HD21	2.00	0.60
1:B:497:GLN:NE2	1:B:499:ASN:HD21	1.99	0.60
1:C:268:GLU:HB3	3:C:501:NAD:H72N	1.67	0.60
1:D:371:GLY:HA2	1:D:384:THR:OG1	2.02	0.60
1:C:294:LEU:HD13	1:C:405:MET:HG3	1.82	0.60
1:C:70:PHE:HZ	1:C:158:PRO:HB2	1.67	0.60
1:B:99:ARG:HG2	1:B:118:TYR:CE2	2.36	0.60
1:D:365:LEU:CD1	1:D:395:ILE:HD11	2.32	0.59
1:B:113:PRO:HB2	1:B:116:ILE:HG12	1.84	0.59
1:B:319:VAL:O	1:B:323:VAL:HG23	2.01	0.59
1:C:361:LYS:NZ	1:C:361:LYS:HB2	2.18	0.59
1:B:102:LEU:HD21	1:B:203:TYR:HD2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LEU:CD1	1:D:405:MET:HA	2.33	0.59
1:C:55:ASP:CG	1:C:227:THR:HG23	2.23	0.59
1:C:365:LEU:CD1	1:C:393:MET:SD	2.87	0.59
1:C:283:MET:HB3	1:C:321:ARG:HH12	1.67	0.59
1:D:12:ASN:O	1:D:15:PRO:HD3	2.02	0.59
1:D:365:LEU:HD12	1:D:395:ILE:HD11	1.85	0.58
1:B:102:LEU:HD21	1:B:203:TYR:CD2	2.38	0.58
1:A:413:MET:HA	1:A:416:VAL:HG12	1.84	0.58
1:A:160:GLY:H	1:A:187:ASN:ND2	2.00	0.58
1:D:159:VAL:N	1:D:187:ASN:HD21	2.00	0.58
1:C:300:GLN:HG2	1:C:401:PHE:O	2.03	0.58
1:B:169:ASN:HD22	1:B:401:PHE:HZ	1.51	0.58
1:A:70:PHE:CE2	1:A:160:GLY:HA2	2.38	0.58
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.39	0.58
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.39	0.58
1:D:205:ALA:HB2	1:D:220:VAL:HG21	1.85	0.58
1:B:323:VAL:HG13	1:B:369:CYS:SG	2.43	0.57
1:B:70:PHE:CE2	1:B:160:GLY:HA2	2.39	0.57
1:D:235:HIS:HB3	1:D:238:VAL:HG23	1.87	0.57
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.04	0.57
1:C:99:ARG:HG3	1:C:122:LEU:HD13	1.87	0.57
1:B:349:GLN:O	1:B:353:VAL:HG23	2.03	0.57
1:D:197:THR:O	1:D:197:THR:HG23	2.05	0.57
1:C:169:ASN:HD21	3:C:501:NAD:H6N	1.68	0.57
1:D:298:GLN:HB3	1:D:344:GLN:NE2	2.19	0.57
1:D:315:TYR:CD1	1:D:409:LYS:HB2	2.40	0.57
1:D:366:LYS:HG3	1:D:368:LEU:HD21	1.85	0.57
1:C:497:GLN:NE2	1:C:499:ASN:HD21	2.03	0.57
1:A:424:LYS:O	1:A:469:LYS:HB2	2.05	0.57
1:D:294:LEU:HD11	1:D:405:MET:HA	1.86	0.56
1:C:311:GLN:NE2	1:C:312:GLU:HG2	2.20	0.56
1:C:238:VAL:O	1:C:261:ASN:ND2	2.38	0.56
1:C:169:ASN:OD1	3:C:501:NAD:H5N	2.05	0.56
1:D:99:ARG:HG2	1:D:118:TYR:CE2	2.39	0.56
1:A:241:VAL:HG23	1:A:263:LYS:HD3	1.87	0.56
1:A:410:PHE:CD2	1:A:416:VAL:HB	2.41	0.56
1:B:365:LEU:HG	1:B:393:MET:CE	2.35	0.56
1:D:365:LEU:CD1	1:D:389:LEU:HG	2.35	0.56
1:D:410:PHE:CD2	1:D:416:VAL:HB	2.41	0.56
1:D:365:LEU:CD2	1:D:393:MET:SD	2.91	0.56
1:D:240:LYS:HZ1	1:D:484:ALA:HB1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:VAL:HG21	1:C:318:PHE:CD2	2.41	0.55
1:C:113:PRO:HB2	1:C:116:ILE:HG12	1.88	0.55
1:C:227:THR:HG22	1:C:228:ALA:N	2.21	0.55
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.41	0.55
1:B:160:GLY:H	1:B:187:ASN:ND2	2.04	0.55
1:C:356:TYR:CG	1:C:400:ILE:HD12	2.40	0.55
1:D:67:ARG:NH2	1:D:161:VAL:HG23	2.22	0.55
1:B:227:THR:HG22	1:B:228:ALA:N	2.22	0.55
1:D:161:VAL:HA	1:D:188:VAL:CG1	2.37	0.55
1:C:413:MET:HA	1:C:416:VAL:HG12	1.88	0.55
1:B:392:GLY:HA2	1:B:397:LYS:HZ3	1.70	0.55
1:A:55:ASP:CG	1:A:227:THR:HG23	2.26	0.55
1:B:365:LEU:HG	1:B:393:MET:SD	2.47	0.54
1:D:196:GLN:HG2	1:D:346:ASP:OD2	2.07	0.54
1:B:395:ILE:HD12	1:B:406:GLN:HG3	1.89	0.54
1:A:409:LYS:HB2	1:A:409:LYS:HZ3	1.72	0.54
1:B:55:ASP:CG	1:B:227:THR:HG23	2.28	0.54
1:D:12:ASN:ND2	1:D:14:GLN:H	2.06	0.54
1:C:8:VAL:HG21	1:C:119:LEU:HD11	1.88	0.54
1:D:244:THR:HA	1:D:268:GLU:O	2.08	0.54
1:B:365:LEU:CD2	1:B:389:LEU:HG	2.34	0.54
1:B:251:HIS:O	1:B:255:VAL:HG23	2.07	0.54
1:B:424:LYS:HB3	1:B:470:LEU:HD13	1.89	0.54
1:C:29:HIS:HD2	1:C:61:ARG:NH2	2.06	0.54
1:B:195:GLU:HB3	1:B:223:GLY:O	2.08	0.54
1:C:365:LEU:HD21	1:C:393:MET:SD	2.48	0.54
1:B:365:LEU:HD21	1:B:389:LEU:HA	1.90	0.54
1:C:244:THR:HG23	3:C:501:NAD:C3N	2.37	0.54
1:A:294:LEU:HD12	1:A:306:SER:HA	1.90	0.54
1:B:365:LEU:HB3	1:B:386:PHE:HD1	1.73	0.54
1:C:410:PHE:CD2	1:C:416:VAL:HB	2.43	0.54
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.07	0.54
1:C:443:SER:HA	1:C:451:VAL:HG11	1.90	0.53
1:A:59:VAL:O	1:A:63:VAL:HG23	2.08	0.53
1:A:433:THR:HG22	1:A:435:ASP:N	2.20	0.53
1:D:280:ASP:O	1:D:434:LYS:HG3	2.08	0.53
1:A:494:ARG:HD3	1:B:454:ASN:O	2.08	0.53
1:A:315:TYR:CD1	1:A:409:LYS:HB3	2.43	0.53
1:D:159:VAL:HG11	1:D:240:LYS:HB2	1.90	0.53
1:C:175:GLN:HG3	1:C:191:MET:CE	2.37	0.53
1:C:198:PRO:O	1:C:202:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:MET:HA	1:D:416:VAL:HG12	1.91	0.53
1:A:349:GLN:O	1:A:353:VAL:HG23	2.09	0.53
1:A:497:GLN:HE21	1:A:499:ASN:HD21	1.56	0.53
1:A:107:THR:HG23	1:A:334:PRO:HB2	1.90	0.53
1:D:442:LEU:O	1:D:446:LEU:HG	2.09	0.53
1:A:336:ASP:HB3	1:A:339:THR:OG1	2.08	0.53
1:B:294:LEU:HD12	1:B:305:GLY:O	2.09	0.53
1:A:258:GLY:HA2	1:B:254:GLN:HG2	1.91	0.53
1:A:247:THR:HA	1:A:269:ILE:HD12	1.91	0.53
1:A:278:MET:SD	1:A:410:PHE:HZ	2.32	0.53
1:C:21:GLN:HB3	1:C:29:HIS:O	2.09	0.53
1:B:70:PHE:CZ	1:B:158:PRO:HB2	2.44	0.53
1:C:497:GLN:HE21	1:C:499:ASN:HD21	1.55	0.53
1:C:115:ILE:HG23	1:C:119:LEU:HD12	1.91	0.53
1:C:183:LEU:HD13	1:C:213:PHE:CE2	2.43	0.53
1:D:365:LEU:CG	1:D:393:MET:SD	2.97	0.53
1:B:169:ASN:ND2	1:B:401:PHE:HZ	2.07	0.53
1:C:261:ASN:HD22	1:C:263:LYS:HB3	1.73	0.53
1:A:196:GLN:HG2	1:A:346:ASP:OD2	2.09	0.53
1:B:23:PHE:CE1	1:B:26:ASN:HA	2.44	0.52
1:A:292:PHE:HE1	1:A:296:PHE:CD1	2.27	0.52
1:A:268:GLU:HB3	3:A:501:NAD:H72N	1.71	0.52
1:B:82:SER:O	1:B:86:ARG:HG2	2.10	0.52
1:B:365:LEU:HB3	1:B:386:PHE:CD1	2.45	0.52
1:C:175:GLN:HG3	1:C:191:MET:HE1	1.91	0.52
1:C:268:GLU:HB3	3:C:501:NAD:N7N	2.23	0.52
1:D:310:VAL:HG21	1:D:318:PHE:CD2	2.43	0.52
1:C:421:ASN:ND2	1:C:447:GLN:HG3	2.25	0.52
1:B:357:ILE:HG22	1:B:361:LYS:HE3	1.91	0.52
1:B:131:TYR:OH	1:B:478:GLY:HA2	2.09	0.52
1:A:244:THR:HG23	3:A:501:NAD:C3N	2.40	0.52
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.32	0.52
1:C:468:TYR:OH	1:D:489:LYS:HB2	2.09	0.52
1:C:168:TRP:HD1	1:C:196:GLN:NE2	2.08	0.52
1:D:99:ARG:HG3	1:D:122:LEU:HD13	1.92	0.52
1:A:15:PRO:HD2	1:A:108:LEU:HD22	1.91	0.52
1:A:389:LEU:HD13	1:A:407:ILE:N	2.25	0.52
1:D:266:THR:O	1:D:267:LEU:HD23	2.10	0.52
1:C:159:VAL:HG12	1:C:187:ASN:ND2	2.25	0.52
1:A:359:SER:O	1:A:363:GLU:HG2	2.10	0.52
1:C:172:LEU:CD2	1:C:200:THR:HB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:HG2	1:A:241:VAL:N	2.25	0.51
1:A:159:VAL:N	1:A:187:ASN:HD21	2.08	0.51
1:D:159:VAL:H	1:D:187:ASN:HD21	1.57	0.51
1:D:401:PHE:CE1	3:D:501:NAD:H2D	2.45	0.51
1:B:401:PHE:CZ	3:B:501:NAD:H2D	2.46	0.51
1:C:361:LYS:HZ3	1:C:361:LYS:HB2	1.75	0.51
1:D:295:PHE:CE2	1:D:383:PRO:HB3	2.46	0.51
1:D:21:GLN:HB3	1:D:29:HIS:O	2.10	0.51
1:B:336:ASP:HB3	1:B:339:THR:OG1	2.10	0.51
1:A:70:PHE:CZ	1:A:158:PRO:HB2	2.45	0.51
1:D:366:LYS:CG	1:D:368:LEU:HD21	2.40	0.51
1:C:160:GLY:H	1:C:187:ASN:ND2	2.08	0.51
1:D:205:ALA:HA	1:D:208:ILE:HD12	1.93	0.51
1:C:389:LEU:CB	1:C:408:LEU:HG	2.41	0.51
1:B:294:LEU:CD1	1:B:405:MET:HA	2.41	0.51
1:B:424:LYS:O	1:B:469:LYS:HB2	2.11	0.51
1:B:365:LEU:CD1	1:B:393:MET:SD	2.99	0.50
1:C:280:ASP:OD1	1:C:433:THR:HG22	2.12	0.50
1:B:338:ARG:HG3	1:B:338:ARG:NH1	2.26	0.50
1:B:272:LYS:HG3	1:B:307:ARG:CD	2.37	0.50
1:D:302:CYS:SG	3:D:501:NAD:C3N	2.99	0.50
1:A:352:LYS:NZ	1:A:356:TYR:HE2	2.09	0.50
1:C:327:LYS:HG3	1:C:369:CYS:SG	2.52	0.50
1:B:11:PRO:HB3	1:B:114:TYR:CE1	2.47	0.50
1:A:244:THR:HA	1:A:268:GLU:O	2.11	0.49
1:C:109:ASP:O	1:C:197:THR:HG22	2.12	0.49
1:C:15:PRO:HD2	1:C:108:LEU:HD13	1.93	0.49
1:A:365:LEU:CD2	1:A:393:MET:SD	2.92	0.49
1:C:272:LYS:HD2	1:C:306:SER:CB	2.42	0.49
1:C:103:ALA:HB2	1:C:122:LEU:HD12	1.95	0.49
1:C:365:LEU:HB3	1:C:386:PHE:HD1	1.76	0.49
1:C:365:LEU:HG	1:C:393:MET:CE	2.42	0.49
1:D:497:GLN:CD	1:D:499:ASN:HD21	2.14	0.49
1:D:390:GLN:O	1:D:393:MET:HG3	2.11	0.49
1:A:241:VAL:CG2	1:A:263:LYS:HD3	2.42	0.49
1:D:408:LEU:N	1:D:408:LEU:HD12	2.27	0.49
1:C:291:HIS:CD2	1:C:325:ARG:HH11	2.31	0.49
1:B:13:GLN:HG2	1:B:335:PHE:CG	2.47	0.49
1:C:15:PRO:HD2	1:C:108:LEU:HD22	1.94	0.49
1:A:366:LYS:HG3	1:A:368:LEU:HD21	1.95	0.49
1:B:309:PHE:CE1	1:B:408:LEU:HD22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:VAL:O	1:D:323:VAL:HG23	2.13	0.49
1:C:243:PHE:HB3	1:C:267:LEU:HD23	1.94	0.49
1:C:63:VAL:HG11	1:C:235:HIS:CE1	2.48	0.49
1:B:140:HIS:CD2	1:C:144:ILE:HG13	2.48	0.49
1:D:103:ALA:HB2	1:D:122:LEU:CD1	2.42	0.48
1:A:366:LYS:CG	1:A:368:LEU:HD21	2.43	0.48
1:C:247:THR:HA	1:C:269:ILE:HD12	1.95	0.48
1:C:245:GLY:O	1:C:269:ILE:HG22	2.13	0.48
1:C:424:LYS:O	1:C:469:LYS:HB2	2.13	0.48
1:A:55:ASP:OD1	1:A:227:THR:HG23	2.13	0.48
1:D:347:GLU:O	1:D:350:PHE:HB3	2.14	0.48
1:A:294:LEU:HD12	1:A:305:GLY:O	2.12	0.48
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.48	0.48
1:B:413:MET:HG3	1:B:414:GLU:N	2.28	0.48
1:C:8:VAL:CG2	1:C:119:LEU:HD11	2.44	0.48
1:C:195:GLU:HG3	1:C:224:PHE:CD1	2.49	0.48
1:C:389:LEU:HB3	1:C:408:LEU:HG	1.95	0.48
1:B:497:GLN:OE1	1:C:78:ARG:HD2	2.14	0.48
1:B:39:THR:CG2	1:B:198:PRO:HD2	2.44	0.48
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.95	0.48
1:A:94:LEU:HD22	1:A:97:ARG:NH1	2.28	0.48
1:B:331:VAL:HG22	1:B:341:GLN:HB3	1.95	0.48
1:C:424:LYS:HD2	1:C:470:LEU:CD1	2.33	0.47
1:D:389:LEU:CD2	1:D:396:ALA:HB2	2.43	0.47
1:C:283:MET:HE1	1:C:321:ARG:HD2	1.94	0.47
1:A:496:PRO:HG3	1:C:441:TYR:HB2	1.96	0.47
1:A:347:GLU:O	1:A:350:PHE:HB3	2.14	0.47
1:A:138:LYS:HE3	1:C:135:TRP:CD1	2.48	0.47
1:D:377:ARG:HG3	1:D:378:GLY:N	2.28	0.47
1:C:122:LEU:O	1:C:126:LEU:HG	2.15	0.47
1:A:26:ASN:HB3	1:A:209:LYS:HG3	1.96	0.47
1:C:430:ALA:HB2	1:C:456:TYR:CD1	2.50	0.47
1:D:275:ASN:HD21	1:D:432:PHE:HE1	1.63	0.47
1:C:283:MET:HE1	1:C:318:PHE:HA	1.96	0.47
1:C:358:LYS:HA	1:C:361:LYS:NZ	2.30	0.47
1:C:36:THR:HG22	1:C:52:ALA:HA	1.96	0.47
1:D:193:VAL:HG11	1:D:201:ALA:CB	2.45	0.47
1:A:170:PHE:HB3	1:A:173:LEU:HB3	1.96	0.47
1:C:251:HIS:ND1	1:D:262:LEU:HD13	2.29	0.47
1:B:159:VAL:H	1:B:187:ASN:HD21	1.61	0.47
1:C:195:GLU:HB3	1:C:223:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ALA:O	1:B:208:ILE:HB	2.15	0.47
1:C:424:LYS:HE3	1:C:425:TYR:CZ	2.50	0.47
1:A:371:GLY:HA2	1:A:384:THR:OG1	2.15	0.47
1:A:144:ILE:CG2	1:B:462:GLN:HB2	2.45	0.47
1:C:62:ALA:CB	1:C:221:ILE:HD11	2.45	0.47
1:A:386:PHE:O	1:A:389:LEU:HD11	2.15	0.47
1:D:393:MET:O	1:D:397:LYS:HG3	2.15	0.46
1:C:244:THR:HA	1:C:268:GLU:O	2.15	0.46
1:C:358:LYS:O	1:C:362:GLU:HG3	2.15	0.46
1:B:269:ILE:HG13	1:B:471:SER:C	2.35	0.46
1:A:155:ARG:HB2	1:A:489:LYS:HB3	1.97	0.46
1:B:338:ARG:HG3	1:B:338:ARG:HH11	1.79	0.46
1:B:239:ASP:O	1:B:263:LYS:HB2	2.16	0.46
1:C:365:LEU:HB3	1:C:386:PHE:CD1	2.50	0.46
1:A:185:THR:HG23	4:A:507:HOH:O	2.15	0.46
1:B:244:THR:HA	1:B:268:GLU:O	2.15	0.46
1:A:193:VAL:HG11	1:A:198:PRO:HA	1.96	0.46
1:B:32:VAL:HG23	1:B:58:ASP:OD1	2.15	0.46
1:A:21:GLN:HB3	1:A:29:HIS:O	2.15	0.46
1:D:22:ILE:HG22	1:D:24:ILE:HG13	1.98	0.46
1:A:352:LYS:HZ2	1:A:356:TYR:HE2	1.59	0.46
1:B:317:GLU:HG2	1:B:321:ARG:HD2	1.98	0.46
1:D:365:LEU:CD1	1:D:393:MET:SD	3.03	0.46
1:C:372:GLY:N	1:C:382:GLN:OE1	2.48	0.46
1:B:67:ARG:NH2	1:B:237:ASP:O	2.48	0.46
1:D:366:LYS:HG3	1:D:368:LEU:CD2	2.46	0.46
1:B:144:ILE:HD11	1:B:154:THR:HG23	1.99	0.45
1:A:227:THR:HG22	1:A:228:ALA:H	1.80	0.45
1:B:392:GLY:HA2	1:B:397:LYS:HZ2	1.77	0.45
1:A:352:LYS:NZ	1:A:356:TYR:CE2	2.82	0.45
1:B:365:LEU:HD11	1:B:389:LEU:HD21	1.98	0.45
1:B:270:GLY:O	1:B:471:SER:HB2	2.16	0.45
1:B:294:LEU:HD21	1:B:404:VAL:O	2.16	0.45
1:D:377:ARG:CG	1:D:378:GLY:H	2.23	0.45
1:A:107:THR:CG2	1:A:334:PRO:HB2	2.47	0.45
1:C:111:GLY:O	1:C:343:PRO:HD2	2.17	0.45
1:D:111:GLY:O	1:D:343:PRO:HD2	2.17	0.45
1:A:365:LEU:CD2	1:A:389:LEU:HA	2.47	0.45
1:B:169:ASN:ND2	1:B:401:PHE:CZ	2.82	0.45
1:A:227:THR:CG2	1:A:228:ALA:N	2.78	0.45
1:B:413:MET:SD	1:B:441:TYR:CD2	3.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:MET:O	1:C:287:VAL:HG23	2.17	0.45
1:C:497:GLN:HE21	1:C:499:ASN:ND2	2.14	0.45
1:D:280:ASP:OD1	1:D:433:THR:HG23	2.17	0.45
1:D:122:LEU:O	1:D:126:LEU:HG	2.17	0.45
1:A:467:GLY:O	1:A:475:ARG:NH2	2.50	0.45
1:B:170:PHE:HB3	1:B:173:LEU:HB3	1.99	0.44
1:D:42:PRO:HB3	1:D:345:VAL:O	2.17	0.44
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.52	0.44
1:A:193:VAL:CG1	1:A:198:PRO:HA	2.47	0.44
1:C:294:LEU:HD13	1:C:405:MET:HA	1.97	0.44
1:A:261:ASN:HD22	1:A:263:LYS:HB3	1.82	0.44
1:B:361:LYS:HE2	1:B:367:LEU:HD22	2.00	0.44
1:A:488:VAL:O	1:B:475:ARG:NH1	2.51	0.44
1:C:170:PHE:HB3	1:C:173:LEU:HB3	2.00	0.44
1:B:39:THR:HG21	1:B:198:PRO:HD2	2.00	0.44
1:A:202:LEU:O	1:A:205:ALA:HB3	2.18	0.44
1:A:389:LEU:HD13	1:A:407:ILE:H	1.83	0.44
1:A:29:HIS:CD2	1:A:29:HIS:N	2.86	0.44
1:B:208:ILE:CD1	1:B:218:VAL:HG11	2.47	0.44
1:B:185:THR:HG21	1:B:485:TYR:O	2.17	0.44
1:B:389:LEU:HD22	1:B:396:ALA:HB2	1.99	0.44
1:A:63:VAL:HG11	1:A:235:HIS:CE1	2.52	0.44
1:A:366:LYS:HG3	1:A:368:LEU:CD2	2.48	0.44
1:A:276:ILE:HD12	1:A:446:LEU:HD11	2.00	0.44
1:A:429:ALA:HB1	1:A:446:LEU:HD13	1.99	0.44
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.18	0.44
1:D:428:ALA:HB1	1:D:452:TRP:CZ3	2.53	0.44
1:A:185:THR:O	1:A:185:THR:HG22	2.17	0.43
1:C:158:PRO:HG3	1:C:185:THR:O	2.17	0.43
1:B:225:GLY:C	1:B:227:THR:H	2.20	0.43
1:B:413:MET:HA	1:B:416:VAL:HG12	1.99	0.43
1:B:389:LEU:CD2	1:B:396:ALA:HB2	2.48	0.43
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.40	0.43
1:A:345:VAL:HG13	1:A:346:ASP:N	2.31	0.43
1:A:273:SER:HA	1:A:274:PRO:HD2	1.89	0.43
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.76	0.43
1:C:32:VAL:HG23	1:C:58:ASP:OD1	2.18	0.43
1:B:311:GLN:NE2	1:B:312:GLU:HG2	2.33	0.43
1:A:245:GLY:O	3:A:501:NAD:H1D	2.17	0.43
1:B:467:GLY:O	1:B:475:ARG:NH2	2.51	0.43
1:A:66:ALA:HB1	1:A:188:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ALA:HB1	1:A:188:VAL:HG12	2.01	0.43
1:C:488:VAL:HG21	1:D:480:TYR:CE2	2.53	0.43
1:B:99:ARG:NH1	1:B:118:TYR:O	2.51	0.43
1:C:205:ALA:O	1:C:208:ILE:HB	2.18	0.43
1:B:357:ILE:HG21	1:B:371:GLY:HA3	2.01	0.43
1:A:285:TRP:O	1:A:289:GLN:HG2	2.19	0.43
1:D:365:LEU:HD23	1:D:365:LEU:HA	1.71	0.43
1:B:298:GLN:O	1:B:300:GLN:HG3	2.19	0.43
1:B:246:SER:OG	1:B:249:VAL:HG23	2.19	0.43
1:A:427:LEU:HB2	1:A:471:SER:HB3	2.01	0.43
1:C:161:VAL:HA	1:C:188:VAL:CG2	2.44	0.43
1:A:389:LEU:HD22	1:A:406:GLN:HB3	2.01	0.43
1:B:390:GLN:HB2	1:B:393:MET:HG3	2.01	0.43
1:D:241:VAL:HG23	1:D:263:LYS:HG3	1.99	0.43
1:C:315:TYR:O	1:C:319:VAL:HG23	2.19	0.43
1:C:11:PRO:HD3	1:C:114:TYR:CE2	2.53	0.43
1:A:23:PHE:CE1	1:A:26:ASN:HA	2.53	0.43
1:C:347:GLU:HB2	1:C:379:TYR:CE1	2.54	0.43
1:A:487:GLU:HG3	1:B:468:TYR:CE1	2.54	0.43
1:A:283:MET:HE1	1:A:318:PHE:HA	2.01	0.43
1:D:349:GLN:O	1:D:353:VAL:HG23	2.19	0.43
1:D:202:LEU:O	1:D:205:ALA:HB3	2.18	0.42
1:A:144:ILE:HD13	1:B:463:SER:HA	2.00	0.42
1:B:496:PRO:HG3	1:D:441:TYR:HB2	2.00	0.42
1:D:70:PHE:CE2	1:D:160:GLY:HA2	2.54	0.42
1:A:135:TRP:CG	1:A:482:LEU:HD11	2.54	0.42
1:B:164:GLN:CD	1:B:178:LYS:HB3	2.39	0.42
1:D:424:LYS:O	1:D:469:LYS:HB2	2.19	0.42
1:B:389:LEU:HD21	1:B:395:ILE:HG13	2.01	0.42
1:B:365:LEU:CG	1:B:393:MET:SD	3.07	0.42
1:A:167:PRO:HD3	1:A:244:THR:O	2.20	0.42
1:D:315:TYR:CE1	1:D:409:LYS:HB2	2.54	0.42
1:A:310:VAL:HG21	1:A:318:PHE:CD1	2.54	0.42
1:C:331:VAL:HG22	1:C:341:GLN:HB3	2.01	0.42
1:B:275:ASN:ND2	1:B:430:ALA:HB3	2.34	0.42
1:C:450:THR:HA	1:D:490:THR:O	2.20	0.42
1:D:368:LEU:HD11	1:D:387:GLY:HA3	2.02	0.42
1:A:280:ASP:OD1	1:A:433:THR:HG23	2.20	0.42
1:C:283:MET:CE	1:C:321:ARG:HD2	2.49	0.42
1:D:238:VAL:O	1:D:263:LYS:HE2	2.19	0.42
1:D:347:GLU:HB2	1:D:379:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LYS:HG3	1:D:307:ARG:CD	2.45	0.42
1:D:9:PRO:HD2	1:D:118:TYR:CZ	2.55	0.42
1:B:70:PHE:CE1	1:B:158:PRO:HB2	2.55	0.42
1:D:467:GLY:O	1:D:475:ARG:NH2	2.52	0.42
1:B:302:CYS:HB3	3:B:501:NAD:C2N	2.49	0.42
1:B:214:PRO:HA	1:B:215:PRO:HD3	1.94	0.42
1:D:11:PRO:HD3	1:D:114:TYR:CE2	2.55	0.42
1:B:154:THR:HA	1:B:489:LYS:O	2.20	0.42
1:B:243:PHE:HB3	1:B:267:LEU:HD23	2.02	0.42
1:A:195:GLU:HB3	1:A:223:GLY:O	2.19	0.42
1:C:311:GLN:HE22	1:C:411:LYS:HA	1.83	0.42
1:D:225:GLY:HA3	3:D:501:NAD:C8A	2.50	0.42
1:C:357:ILE:HD13	1:C:371:GLY:CA	2.49	0.42
1:B:437:ASP:HB3	1:D:496:PRO:CG	2.50	0.42
1:C:39:THR:HG23	1:C:48:ILE:HB	2.00	0.42
1:D:238:VAL:HB	1:D:263:LYS:NZ	2.34	0.41
1:B:164:GLN:O	1:B:191:MET:HG3	2.20	0.41
1:B:240:LYS:NZ	1:B:484:ALA:HB1	2.35	0.41
1:B:449:GLY:HA3	1:B:466:GLY:O	2.20	0.41
1:C:110:ASN:OD1	1:C:112:LYS:HE3	2.19	0.41
1:D:160:GLY:H	1:D:187:ASN:HD22	1.66	0.41
1:A:302:CYS:SG	3:A:501:NAD:C4N	3.08	0.41
1:D:12:ASN:HD22	1:D:12:ASN:C	2.22	0.41
1:D:208:ILE:HD13	1:D:218:VAL:HG11	2.03	0.41
1:C:168:TRP:CD1	1:C:196:GLN:NE2	2.86	0.41
1:C:269:ILE:HB	1:C:270:GLY:H	1.66	0.41
1:A:90:ARG:CZ	1:A:94:LEU:HD21	2.49	0.41
1:D:401:PHE:CZ	3:D:501:NAD:H2D	2.55	0.41
1:C:146:ILE:HA	1:D:462:GLN:HG3	2.02	0.41
1:D:172:LEU:HD21	1:D:200:THR:HB	2.02	0.41
1:A:389:LEU:CD1	1:A:407:ILE:H	2.34	0.41
1:D:323:VAL:HG13	1:D:369:CYS:SG	2.60	0.41
1:C:135:TRP:CG	1:C:482:LEU:HD11	2.55	0.41
1:B:269:ILE:HB	1:B:270:GLY:H	1.74	0.41
1:A:312:GLU:HG3	1:A:313:ASP:N	2.35	0.41
1:A:389:LEU:HD12	1:A:389:LEU:N	2.34	0.41
1:C:146:ILE:HA	1:D:462:GLN:CG	2.51	0.41
1:D:168:TRP:CD1	3:D:501:NAD:O2N	2.73	0.41
1:C:195:GLU:HG3	1:C:224:PHE:CE1	2.55	0.41
1:A:443:SER:HA	1:A:451:VAL:HG11	2.02	0.41
1:A:185:THR:O	1:A:185:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLN:HG2	1:B:401:PHE:O	2.21	0.41
1:B:164:GLN:HB3	1:B:178:LYS:HD2	2.03	0.41
1:C:64:LYS:HE3	1:C:64:LYS:HB2	1.92	0.41
1:D:459:PHE:HE1	1:D:465:PHE:CE1	2.39	0.41
1:C:365:LEU:CG	1:C:393:MET:SD	3.09	0.41
1:D:345:VAL:HG13	1:D:346:ASP:N	2.34	0.41
1:B:185:THR:HG22	1:B:185:THR:O	2.20	0.41
1:B:432:PHE:CD2	1:B:454:ASN:HA	2.56	0.41
1:B:261:ASN:ND2	4:B:515:HOH:O	2.54	0.41
1:A:163:GLY:HA2	1:A:190:VAL:O	2.21	0.41
1:B:172:LEU:HD21	1:B:200:THR:HB	2.02	0.41
1:A:292:PHE:CE1	1:A:296:PHE:CD1	3.07	0.41
1:B:357:ILE:O	1:B:361:LYS:HG3	2.21	0.41
1:B:15:PRO:HD2	1:B:108:LEU:HD13	2.02	0.41
1:D:277:ILE:N	1:D:277:ILE:HD12	2.36	0.41
1:C:9:PRO:HD2	1:C:118:TYR:CZ	2.56	0.41
1:C:291:HIS:NE2	1:C:329:ARG:NH1	2.69	0.40
1:C:159:VAL:HG12	1:C:187:ASN:HD21	1.86	0.40
1:D:263:LYS:H	1:D:263:LYS:HD2	1.87	0.40
1:C:144:ILE:HG23	1:D:462:GLN:HB2	2.03	0.40
1:B:317:GLU:O	1:B:321:ARG:HG3	2.21	0.40
1:D:168:TRP:NE1	3:D:501:NAD:O1N	2.53	0.40
1:A:424:LYS:HB3	1:A:470:LEU:HD12	2.03	0.40
1:C:202:LEU:O	1:C:205:ALA:HB3	2.21	0.40
1:A:135:TRP:CE3	1:A:138:LYS:HB2	2.57	0.40
1:C:315:TYR:CZ	1:C:319:VAL:HG21	2.56	0.40
1:C:347:GLU:CG	1:C:351:LYS:HE3	2.51	0.40
1:C:377:ARG:NH1	1:C:377:ARG:HG2	2.37	0.40
1:D:283:MET:O	1:D:287:VAL:HG23	2.21	0.40
1:B:404:VAL:HG12	1:B:406:GLN:OE1	2.22	0.40
1:D:103:ALA:N	1:D:122:LEU:HD11	2.37	0.40
1:A:475:ARG:NH1	1:B:488:VAL:O	2.55	0.40
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.57	0.40
1:D:62:ALA:HB2	1:D:221:ILE:HD11	2.04	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	491/499 (98%)	461 (94%)	26 (5%)	4 (1%)	24	55
1	B	491/499 (98%)	459 (94%)	29 (6%)	3 (1%)	30	62
1	C	491/499 (98%)	455 (93%)	33 (7%)	3 (1%)	30	62
1	D	491/499 (98%)	453 (92%)	35 (7%)	3 (1%)	30	62
All	All	1964/1996 (98%)	1828 (93%)	123 (6%)	13 (1%)	26	59

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	345	VAL
1	D	345	VAL
1	A	345	VAL
1	A	171	PRO
1	B	345	VAL
1	C	225	GLY
1	A	383	PRO
1	B	383	PRO
1	D	383	PRO
1	B	171	PRO
1	A	269	ILE
1	C	171	PRO
1	D	171	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	398/401 (99%)	375 (94%)	23 (6%)	25	54
1	B	398/401 (99%)	377 (95%)	21 (5%)	28	58
1	C	398/401 (99%)	378 (95%)	20 (5%)	30	61
1	D	398/401 (99%)	377 (95%)	21 (5%)	28	58
All	All	1592/1604 (99%)	1507 (95%)	85 (5%)	28	58

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	29	HIS
1	A	34	LYS
1	A	61	ARG
1	A	75	PRO
1	A	89	ASN
1	A	130	ARG
1	A	192	LYS
1	A	200	THR
1	A	259	LYS
1	A	264	ARG
1	A	275	ASN
1	A	279	SER
1	A	311	GLN
1	A	352	LYS
1	A	376	ASP
1	A	377	ARG
1	A	401	PHE
1	A	409	LYS
1	A	422	ASN
1	A	423	SER
1	A	468	TYR
1	A	494	ARG
1	B	39	THR
1	B	41	ASN
1	B	83	GLU
1	B	90	ARG
1	B	122	LEU
1	B	169	ASN
1	B	196	GLN
1	B	240	LYS
1	B	263	LYS
1	B	264	ARG

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Mol	Chain	Res	Type
1	B	275	ASN
1	B	279	SER
1	B	311	GLN
1	B	327	LYS
1	B	349	GLN
1	B	376	ASP
1	B	389	LEU
1	B	401	PHE
1	B	413	MET
1	B	462	GLN
1	B	468	TYR
1	C	14	GLN
1	C	49	CYS
1	C	64	LYS
1	C	121	ASP
1	C	169	ASN
1	C	196	GLN
1	C	263	LYS
1	C	264	ARG
1	C	269	ILE
1	C	273	SER
1	C	311	GLN
1	C	325	ARG
1	C	348	THR
1	C	369	CYS
1	C	388	ASP
1	C	394	THR
1	C	401	PHE
1	C	433	THR
1	C	462	GLN
1	C	475	ARG
1	D	12	ASN
1	D	13	GLN
1	D	43	SER
1	D	71	GLN
1	D	115	ILE
1	D	142	LYS
1	D	263	LYS
1	D	264	ARG
1	D	266	THR
1	D	269	ILE
1	D	275	ASN

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Mol	Chain	Res	Type
1	D	279	SER
1	D	306	SER
1	D	311	GLN
1	D	317	GLU
1	D	388	ASP
1	D	389	LEU
1	D	401	PHE
1	D	422	ASN
1	D	462	GLN
1	D	497	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41	ASN
1	A	175	GLN
1	A	187	ASN
1	A	261	ASN
1	A	275	ASN
1	A	462	GLN
1	A	497	GLN
1	B	14	GLN
1	B	26	ASN
1	B	41	ASN
1	B	89	ASN
1	B	140	HIS
1	B	187	ASN
1	B	196	GLN
1	B	275	ASN
1	B	311	GLN
1	B	390	GLN
1	B	447	GLN
1	B	497	GLN
1	C	13	GLN
1	C	29	HIS
1	C	175	GLN
1	C	187	ASN
1	C	196	GLN
1	C	254	GLN
1	C	261	ASN
1	C	497	GLN

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Mol	Chain	Res	Type
1	D	12	ASN
1	D	29	HIS
1	D	71	GLN
1	D	89	ASN
1	D	187	ASN
1	D	275	ASN
1	D	300	GLN
1	D	344	GLN
1	D	447	GLN
1	D	497	GLN
1	D	499	ASN

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	501	2	38,48,48	2.02	8 (21%)	47,73,73	2.03	9 (19%)
3	NAD	B	501	2	38,48,48	2.27	9 (23%)	47,73,73	2.30	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	C	501	2	38,48,48	2.16	9 (23%)	47,73,73	1.86	7 (14%)
3	NAD	D	501	2	38,48,48	1.88	6 (15%)	47,73,73	1.97	10 (21%)

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	501	2	-	0/22/62/62	0/5/5/5
3	NAD	B	501	2	-	0/22/62/62	0/5/5/5
3	NAD	C	501	2	-	0/22/62/62	0/5/5/5
3	NAD	D	501	2	-	0/22/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAD	C3N-C7N	-10.90	1.33	1.50
3	A	501	NAD	C3N-C7N	-8.97	1.36	1.50
3	C	501	NAD	C3N-C7N	-8.96	1.36	1.50
3	D	501	NAD	C3N-C7N	-8.37	1.37	1.50
3	C	501	NAD	C4N-C3N	-3.52	1.33	1.39
3	A	501	NAD	C4N-C3N	-2.62	1.34	1.39
3	D	501	NAD	C4N-C3N	-2.60	1.34	1.39
3	B	501	NAD	C5N-C4N	-2.54	1.33	1.38
3	B	501	NAD	C4N-C3N	-2.46	1.35	1.39
3	C	501	NAD	C5N-C4N	-2.40	1.34	1.38
3	B	501	NAD	C2N-C3N	-2.24	1.35	1.39
3	A	501	NAD	C5N-C4N	-2.06	1.34	1.38
3	C	501	NAD	O4D-C1D	2.01	1.43	1.41
3	C	501	NAD	C4A-N3A	2.08	1.38	1.35
3	D	501	NAD	O4B-C1B	2.11	1.43	1.41
3	A	501	NAD	O4B-C1B	2.18	1.44	1.41
3	B	501	NAD	PN-O5D	2.22	1.69	1.59
3	B	501	NAD	C8A-N7A	2.35	1.39	1.34
3	D	501	NAD	C2A-N1A	2.37	1.38	1.33
3	A	501	NAD	C8A-N7A	2.41	1.39	1.34
3	B	501	NAD	C4A-N3A	2.43	1.39	1.35
3	B	501	NAD	C2A-N1A	2.56	1.38	1.33
3	C	501	NAD	O4B-C1B	2.69	1.44	1.41
3	C	501	NAD	C8A-N7A	2.72	1.39	1.34
3	A	501	NAD	C2A-N1A	2.76	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAD	PN-O5D	2.85	1.72	1.59
3	D	501	NAD	C8A-N7A	3.24	1.40	1.34
3	C	501	NAD	C2A-N1A	3.51	1.40	1.33
3	D	501	NAD	C2A-N3A	3.60	1.38	1.32
3	A	501	NAD	C2A-N3A	3.81	1.38	1.32
3	B	501	NAD	C2A-N3A	3.86	1.39	1.32
3	C	501	NAD	C2A-N3A	4.55	1.40	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAD	N3A-C2A-N1A	-10.54	120.82	128.89
3	C	501	NAD	N3A-C2A-N1A	-8.80	122.16	128.89
3	A	501	NAD	N3A-C2A-N1A	-8.08	122.70	128.89
3	D	501	NAD	N3A-C2A-N1A	-7.06	123.49	128.89
3	D	501	NAD	C2B-C1B-N9A	-5.11	106.48	114.29
3	A	501	NAD	O7N-C7N-N7N	-3.45	117.75	122.59
3	D	501	NAD	PN-O3-PA	-3.12	123.97	132.73
3	C	501	NAD	C2B-C1B-N9A	-3.09	109.58	114.29
3	C	501	NAD	C2D-C3D-C4D	-2.88	96.69	102.61
3	B	501	NAD	O7N-C7N-C3N	-2.69	116.65	119.59
3	A	501	NAD	C2B-C1B-N9A	-2.60	110.31	114.29
3	B	501	NAD	C2B-C1B-N9A	-2.59	110.33	114.29
3	B	501	NAD	C4B-O4B-C1B	-2.51	106.96	109.72
3	B	501	NAD	C2B-C3B-C4B	-2.34	97.80	102.61
3	C	501	NAD	O7N-C7N-N7N	-2.29	119.37	122.59
3	D	501	NAD	C2D-C3D-C4D	-2.07	98.36	102.61
3	A	501	NAD	O2N-PN-O3	2.06	114.45	105.09
3	D	501	NAD	O2N-PN-O3	2.09	114.55	105.09
3	D	501	NAD	O2A-PA-O3	2.11	114.65	105.09
3	A	501	NAD	O3-PA-O5B	2.19	108.76	102.94
3	B	501	NAD	O2A-PA-O3	2.33	115.66	105.09
3	B	501	NAD	C3N-C7N-N7N	2.52	120.58	117.82
3	C	501	NAD	C1B-N9A-C4A	2.54	130.76	126.94
3	B	501	NAD	O5B-C5B-C4B	2.58	118.62	109.12
3	D	501	NAD	C3N-C7N-N7N	2.65	120.72	117.82
3	B	501	NAD	O3-PA-O5B	2.82	110.42	102.94
3	B	501	NAD	C2N-C3N-C4N	2.83	121.44	118.29
3	A	501	NAD	C3N-C7N-N7N	2.86	120.94	117.82
3	D	501	NAD	C4D-O4D-C1D	2.93	112.94	109.72
3	C	501	NAD	O2A-PA-O3	2.98	118.62	105.09
3	C	501	NAD	C3N-C7N-N7N	3.02	121.12	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	501	NAD	O3-PN-O5D	3.43	112.03	102.94
3	A	501	NAD	O2A-PA-O3	3.46	120.79	105.09
3	D	501	NAD	O3-PA-O5B	3.87	113.19	102.94
3	D	501	NAD	O4D-C1D-N1N	3.96	112.48	108.13
3	B	501	NAD	O3-PN-O5D	4.29	114.31	102.94
3	B	501	NAD	O4D-C1D-N1N	4.98	113.60	108.13
3	A	501	NAD	O4D-C1D-N1N	6.19	114.94	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAD	5	0
3	B	501	NAD	3	0
3	C	501	NAD	5	0
3	D	501	NAD	7	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	493/499 (98%)	0.30	3 (0%) 90 88	8, 8, 8, 8	0
1	B	493/499 (98%)	0.34	7 (1%) 78 73	8, 8, 8, 8	0
1	C	493/499 (98%)	0.94	52 (10%) 8 5	16, 16, 16, 16	0
1	D	493/499 (98%)	0.68	21 (4%) 39 32	11, 11, 11, 11	0
All	All	1972/1996 (98%)	0.56	83 (4%) 40 33	8, 8, 16, 16	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	LEU	5.5
1	C	375	ALA	4.0
1	D	229	GLY	3.9
1	C	378	GLY	3.9
1	C	250	GLY	3.9
1	C	377	ARG	3.6
1	B	365	LEU	3.3
1	D	368	LEU	3.3
1	D	474	GLY	3.3
1	C	374	ALA	3.1
1	C	396	ALA	3.0
1	D	257	ALA	3.0
1	D	303	CYS	3.0
1	D	261	ASN	2.9
1	A	370	GLY	2.9
1	D	201	ALA	2.8
1	C	48	ILE	2.6
1	C	478	GLY	2.6
1	C	257	ALA	2.6
1	C	471	SER	2.6
1	C	453	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	360	GLY	2.5
1	C	156	HIS	2.5
1	C	376	ASP	2.5
1	D	396	ALA	2.5
1	D	356	TYR	2.5
1	C	431	VAL	2.4
1	A	139	TYR	2.4
1	C	56	LYS	2.4
1	D	163	GLY	2.4
1	A	365	LEU	2.4
1	C	299	GLY	2.3
1	C	32	VAL	2.3
1	C	420	ALA	2.3
1	D	448	ALA	2.3
1	C	467	GLY	2.3
1	D	475	ARG	2.3
1	D	453	VAL	2.3
1	B	481	GLY	2.3
1	C	51	VAL	2.3
1	D	258	GLY	2.3
1	C	254	GLN	2.3
1	C	401	PHE	2.3
1	C	211	ALA	2.2
1	C	470	LEU	2.2
1	C	361	LYS	2.2
1	C	403	PRO	2.2
1	B	281	ALA	2.2
1	C	404	VAL	2.2
1	C	468	TYR	2.2
1	C	303	CYS	2.2
1	B	460	GLY	2.2
1	C	379	TYR	2.2
1	D	72	LEU	2.2
1	D	317	GLU	2.2
1	C	52	ALA	2.2
1	C	389	LEU	2.1
1	D	423	SER	2.1
1	C	333	ASN	2.1
1	C	328	SER	2.1
1	D	174	MET	2.1
1	B	81	ALA	2.1
1	C	103	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	204	VAL	2.1
1	C	307	ARG	2.1
1	B	499	ASN	2.1
1	C	323	VAL	2.1
1	C	235	HIS	2.1
1	D	369	CYS	2.1
1	C	365	LEU	2.0
1	B	185	THR	2.0
1	C	253	ILE	2.0
1	C	17	VAL	2.0
1	C	258	GLY	2.0
1	C	14	GLN	2.0
1	C	425	TYR	2.0
1	D	293	ALA	2.0
1	D	177	TRP	2.0
1	C	463	SER	2.0
1	C	429	ALA	2.0
1	C	347	GLU	2.0
1	C	475	ARG	2.0
1	C	369	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAD	D	501	44/44	0.86	0.31	1.26	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAD	B	501	44/44	0.88	0.21	0.76	11,11,11,11	0
3	NAD	A	501	44/44	0.90	0.21	0.74	11,11,11,11	0
3	NAD	C	501	44/44	0.88	0.26	0.40	12,12,12,12	1
2	SM	A	502	1/1	0.97	0.20	-	18,18,18,18	1
2	SM	B	502	1/1	0.98	0.28	-	19,19,19,19	1
2	SM	D	502	1/1	0.81	0.18	-	17,17,17,17	1
2	SM	C	502	1/1	0.78	0.20	-	15,15,15,15	1

6.5 Other polymers [i](#)

There are no such residues in this entry.