



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:28 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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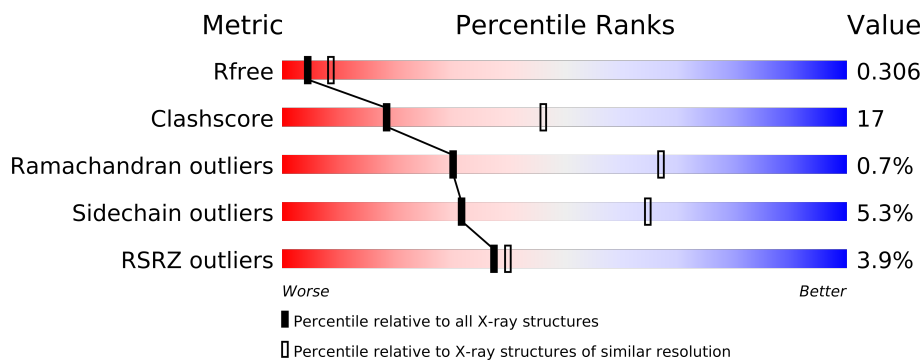
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.75 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))
$R_{free}$	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
1	C	499	
1	D	499	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15464 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 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: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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		



Government	Percentage
Current government	100%
Previous government	0%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.60Å 198.40Å 91.60Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.73Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.230 , 0.302 0.264 , 0.306	Depositor DCC
$R_{free}$ test set	3537 reflections (7.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -0.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Close contacts ⓘ

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	26	5	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (511) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.26	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	27	63
1	B	491/499 (98%)	459 (94%)	29 (6%)	3 (1%)	33	70
1	C	491/499 (98%)	455 (93%)	33 (7%)	3 (1%)	33	70
1	D	491/499 (98%)	453 (92%)	35 (7%)	3 (1%)	33	70
All	All	1964/1996 (98%)	1828 (93%)	123 (6%)	13 (1%)	30	67

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%)	28	60
1	B	398/401 (99%)	377 (95%)	21 (5%)	32	65
1	C	398/401 (99%)	378 (95%)	20 (5%)	34	68
1	D	398/401 (99%)	377 (95%)	21 (5%)	32	65
All	All	1592/1604 (99%)	1507 (95%)	85 (5%)	32	65

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	48,48,48	1.77	6 (12%)	73,73,73	1.86	12 (16%)
3	NAD	B	501	2	48,48,48	2.05	11 (22%)	73,73,73	1.97	15 (20%)
3	NAD	C	501	2	48,48,48	1.90	10 (20%)	73,73,73	1.66	11 (15%)
3	NAD	D	501	2	48,48,48	1.69	8 (16%)	73,73,73	1.87	18 (24%)

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	-	0/30/62/62	0/3/5/5
3	NAD	B	501	2	-	0/30/62/62	0/3/5/5
3	NAD	C	501	2	-	0/30/62/62	0/3/5/5
3	NAD	D	501	2	-	0/30/62/62	0/3/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAD	C3N-C7N	-10.06	1.33	1.50
3	A	501	NAD	C3N-C7N	-8.28	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	NAD	C3N-C7N	-8.27	1.36	1.50
3	D	501	NAD	C3N-C7N	-7.73	1.37	1.50
3	C	501	NAD	C2A-N3A	4.08	1.40	1.32
3	A	501	NAD	PN-O5D	3.75	1.72	1.60
3	C	501	NAD	C4N-C3N	-3.46	1.33	1.39
3	B	501	NAD	C2A-N3A	3.46	1.39	1.32
3	A	501	NAD	C2A-N3A	3.42	1.38	1.32
3	C	501	NAD	C2A-N1A	3.38	1.40	1.33
3	B	501	NAD	PN-O3	3.35	1.67	1.60
3	D	501	NAD	C2A-N3A	3.22	1.38	1.32
3	D	501	NAD	C8A-N7A	3.16	1.40	1.34
3	B	501	NAD	PN-O5D	2.85	1.69	1.60
3	B	501	NAD	C2N-N1N	-2.81	1.31	1.35
3	A	501	NAD	C2A-N1A	2.65	1.39	1.33
3	C	501	NAD	C8A-N7A	2.65	1.39	1.34
3	D	501	NAD	PA-O3	-2.59	1.55	1.59
3	A	501	NAD	C4N-C3N	-2.58	1.34	1.39
3	D	501	NAD	C4N-C3N	-2.56	1.34	1.39
3	B	501	NAD	C2A-N1A	2.47	1.38	1.33
3	B	501	NAD	C4N-C3N	-2.42	1.35	1.39
3	B	501	NAD	C2N-C3N	-2.39	1.35	1.38
3	C	501	NAD	PA-O3	2.36	1.64	1.59
3	C	501	NAD	PN-O5D	2.36	1.67	1.60
3	A	501	NAD	C8A-N7A	2.35	1.39	1.34
3	B	501	NAD	C4A-N3A	2.35	1.39	1.35
3	C	501	NAD	PN-O3	2.31	1.65	1.60
3	B	501	NAD	C5N-C4N	-2.29	1.33	1.39
3	B	501	NAD	C8A-N7A	2.28	1.39	1.34
3	D	501	NAD	C2A-N1A	2.28	1.38	1.33
3	D	501	NAD	C8A-N9A	2.17	1.39	1.36
3	C	501	NAD	C5N-C4N	-2.16	1.34	1.39
3	C	501	NAD	O4B-C1B	2.12	1.44	1.41
3	D	501	NAD	PN-O5D	2.05	1.66	1.60

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAD	N3A-C2A-N1A	-9.43	120.82	128.71
3	C	501	NAD	N3A-C2A-N1A	-7.84	122.16	128.71
3	A	501	NAD	N3A-C2A-N1A	-7.18	122.70	128.71
3	A	501	NAD	O4D-C1D-N1N	6.83	114.94	107.95
3	D	501	NAD	N3A-C2A-N1A	-6.25	123.49	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	NAD	O4D-C1D-C2D	-5.70	98.03	106.77
3	B	501	NAD	O4D-C1D-N1N	5.52	113.60	107.95
3	D	501	NAD	C8A-N9A-C4A	-5.19	102.94	106.90
3	A	501	NAD	C8A-N9A-C4A	-4.60	103.39	106.90
3	D	501	NAD	O4D-C1D-N1N	4.42	112.48	107.95
3	C	501	NAD	O2N-PN-O1N	-4.32	105.70	118.72
3	C	501	NAD	O4D-C1D-C2D	-4.08	100.52	106.77
3	D	501	NAD	O4B-C1B-N9A	3.96	112.12	108.44
3	D	501	NAD	O2N-PN-O1N	-3.81	107.22	118.72
3	B	501	NAD	O4D-C1D-C2D	-3.78	100.98	106.77
3	B	501	NAD	O2N-PN-O1N	-3.69	107.59	118.72
3	A	501	NAD	C2D-C1D-N1N	-3.66	107.66	113.86
3	A	501	NAD	O2N-PN-O1N	-3.65	107.69	118.72
3	A	501	NAD	O7N-C7N-N7N	-3.35	117.75	122.59
3	A	501	NAD	O2A-PA-O3	3.30	120.79	105.14
3	B	501	NAD	O3-PN-O5D	3.23	114.31	101.36
3	C	501	NAD	C2D-C3D-C4D	-2.99	96.69	102.65
3	B	501	NAD	C2D-C1D-N1N	-2.98	108.81	113.86
3	C	501	NAD	C3N-C7N-N7N	2.95	121.12	117.77
3	D	501	NAD	C4D-O4D-C1D	2.94	112.94	109.75
3	C	501	NAD	O2A-PA-O3	2.84	118.62	105.14
3	A	501	NAD	C3N-C7N-N7N	2.79	120.94	117.77
3	B	501	NAD	C2N-C3N-C4N	2.76	121.44	118.31
3	C	501	NAD	C8A-N9A-C4A	-2.66	104.87	106.90
3	A	501	NAD	O3-PN-O5D	2.66	112.03	101.36
3	D	501	NAD	C2B-C1B-N9A	-2.64	106.48	113.27
3	B	501	NAD	O5B-C5B-C4B	2.64	118.62	108.94
3	D	501	NAD	O4B-C1B-C2B	-2.62	102.75	106.77
3	B	501	NAD	O7N-C7N-C3N	-2.60	116.65	119.58
3	D	501	NAD	C3N-C7N-N7N	2.59	120.72	117.77
3	B	501	NAD	C4B-O4B-C1B	-2.57	106.96	109.75
3	B	501	NAD	C3N-C7N-N7N	2.46	120.58	117.77
3	B	501	NAD	C2B-C3B-C4B	-2.44	97.80	102.65
3	B	501	NAD	C3D-C2D-C1D	-2.43	97.10	100.91
3	A	501	NAD	O4D-C1D-C2D	-2.41	103.07	106.77
3	C	501	NAD	C1B-N9A-C4A	2.39	130.76	126.64
3	B	501	NAD	C6N-N1N-C2N	-2.35	119.38	122.04
3	D	501	NAD	C5A-C4A-N9A	2.28	110.46	107.16
3	D	501	NAD	C2D-C1D-N1N	-2.25	110.04	113.86
3	C	501	NAD	O7N-C7N-N7N	-2.23	119.37	122.59
3	C	501	NAD	C6A-C5A-C4A	2.23	121.33	117.25
3	B	501	NAD	O2A-PA-O3	2.22	115.66	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	NAD	O3-PA-O5B	2.19	113.19	103.41
3	D	501	NAD	C2D-C3D-C4D	-2.15	98.36	102.65
3	D	501	NAD	O2N-PN-O3	2.14	114.55	108.79
3	A	501	NAD	O2N-PN-O3	2.10	114.45	108.79
3	D	501	NAD	PN-O3-PA	-2.09	123.97	132.95
3	D	501	NAD	C4A-C5A-N7A	2.03	111.26	109.52
3	C	501	NAD	C4B-O4B-C1B	-2.02	107.55	109.75
3	D	501	NAD	O2A-PA-O3	2.00	114.65	105.14
3	A	501	NAD	C5A-C4A-N9A	2.00	110.05	107.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	493/499 (98%)	0.19	2 (0%) 90 92	8, 8, 8, 8	0
1	B	493/499 (98%)	0.24	3 (0%) 86 89	8, 8, 8, 8	0
1	C	493/499 (98%)	0.91	53 (10%) 6 6	16, 16, 16, 16	0
1	D	493/499 (98%)	0.65	18 (3%) 39 42	11, 11, 11, 11	0
All	All	1972/1996 (98%)	0.50	76 (3%) 37 40	8, 8, 16, 16	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	LEU	5.8
1	C	378	GLY	4.3
1	C	375	ALA	4.1
1	C	377	ARG	3.8
1	C	250	GLY	3.7
1	C	396	ALA	3.7
1	D	368	LEU	3.5
1	B	365	LEU	3.3
1	D	303	CYS	3.3
1	D	229	GLY	3.2
1	C	48	ILE	3.2
1	C	374	ALA	3.0
1	C	360	GLY	3.0
1	C	365	LEU	2.9
1	D	396	ALA	2.9
1	C	400	ILE	2.9
1	C	376	ASP	2.9
1	D	257	ALA	2.8
1	C	17	VAL	2.8
1	C	361	LYS	2.8
1	C	356	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	353	VAL	2.7
1	D	345	VAL	2.7
1	C	404	VAL	2.6
1	C	39	THR	2.6
1	C	299	GLY	2.6
1	D	474	GLY	2.5
1	C	51	VAL	2.5
1	D	356	TYR	2.5
1	C	37	PHE	2.5
1	C	369	CYS	2.5
1	D	353	VAL	2.5
1	D	369	CYS	2.4
1	C	333	ASN	2.4
1	D	261	ASN	2.3
1	D	258	GLY	2.3
1	C	254	GLN	2.3
1	C	14	GLN	2.3
1	C	379	TYR	2.3
1	C	328	SER	2.3
1	C	401	PHE	2.3
1	C	36	THR	2.3
1	C	354	LEU	2.2
1	C	233	ALA	2.2
1	C	204	VAL	2.2
1	D	163	GLY	2.2
1	C	470	LEU	2.2
1	C	156	HIS	2.2
1	D	201	ALA	2.2
1	D	365	LEU	2.2
1	A	365	LEU	2.2
1	C	389	LEU	2.2
1	C	385	VAL	2.1
1	B	390	GLN	2.1
1	C	393	MET	2.1
1	C	431	VAL	2.1
1	D	448	ALA	2.1
1	C	380	PHE	2.1
1	C	235	HIS	2.1
1	C	257	ALA	2.1
1	C	403	PRO	2.1
1	C	177	TRP	2.1
1	C	330	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	224	PHE	2.1
1	C	364	GLY	2.1
1	C	52	ALA	2.1
1	C	349	GLN	2.1
1	C	323	VAL	2.0
1	D	177	TRP	2.0
1	D	317	GLU	2.0
1	C	347	GLU	2.0
1	B	8	VAL	2.0
1	A	370	GLY	2.0
1	C	197	THR	2.0
1	C	211	ALA	2.0
1	C	303	CYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	D	501	44/44	0.31	1.31	11,11,11,11	0
3	NAD	A	501	44/44	0.20	0.57	11,11,11,11	0
3	NAD	B	501	44/44	0.20	0.46	11,11,11,11	0
2	SM	C	502	1/1	0.19	-	15,15,15,15	1
2	SM	A	502	1/1	0.20	-	18,18,18,18	1
2	SM	B	502	1/1	0.27	-	19,19,19,19	1
2	SM	D	502	1/1	0.17	-	17,17,17,17	1
3	NAD	C	501	44/44	0.25	-	12,12,12,12	1



## 6.5 Other polymers ⓘ

There are no such residues in this entry.