



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:37 AM GMT

PDB ID : 1CW3
Title : HUMAN MITOCHONDRIAL ALDEHYDE DEHYDROGENASE COM-
PLEXED WITH NAD⁺ AND MN²⁺
Authors : Ni, L.; Zhou, J.; Hurley, T.D.; Weiner, H.
Deposited on : 1999-08-25
Resolution : 2.58 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

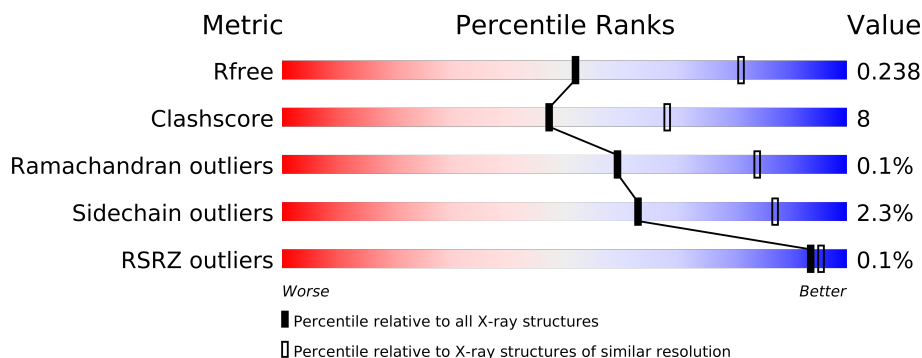
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.58 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	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	B	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	C	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	D	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	E	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	F	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	G	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	H	494	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31839 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 MITOCHONDRIAL ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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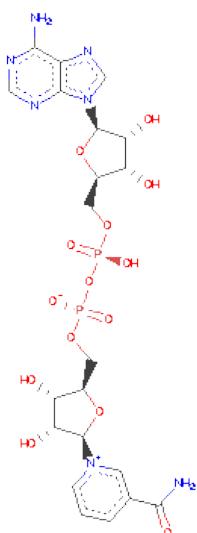
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

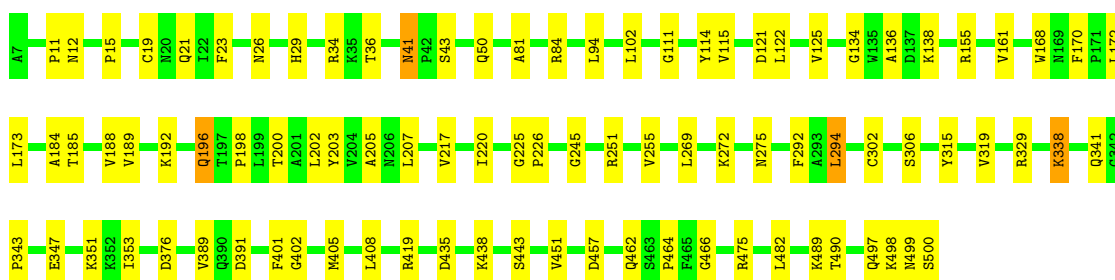
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	118	Total	O	0	0
			118	118		
5	C	127	Total	O	0	0
			127	127		
5	D	147	Total	O	0	0
			147	147		
5	E	132	Total	O	0	0
			132	132		
5	F	140	Total	O	0	0
			140	140		
5	G	148	Total	O	0	0
			148	148		
5	H	148	Total	O	0	0
			148	148		

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.

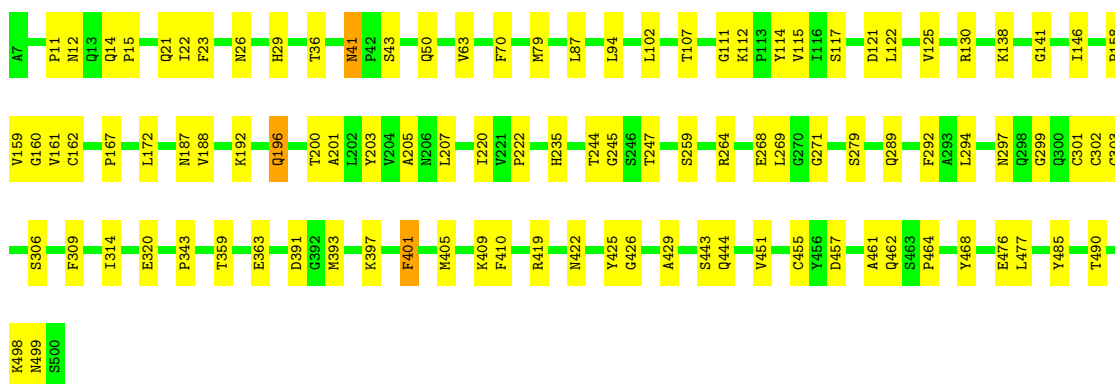
• Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain A:



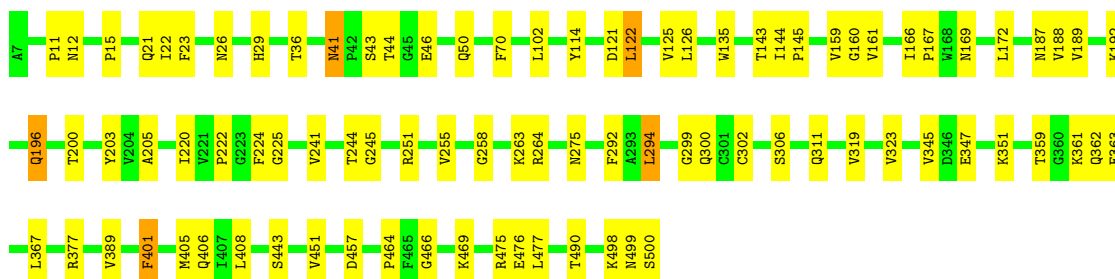
• Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain B:



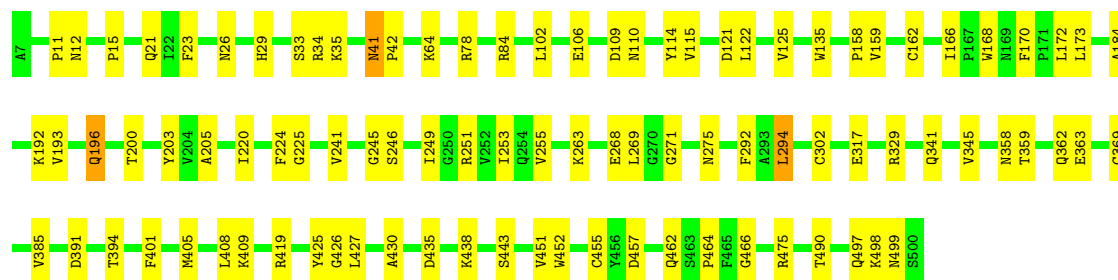
• Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain C:



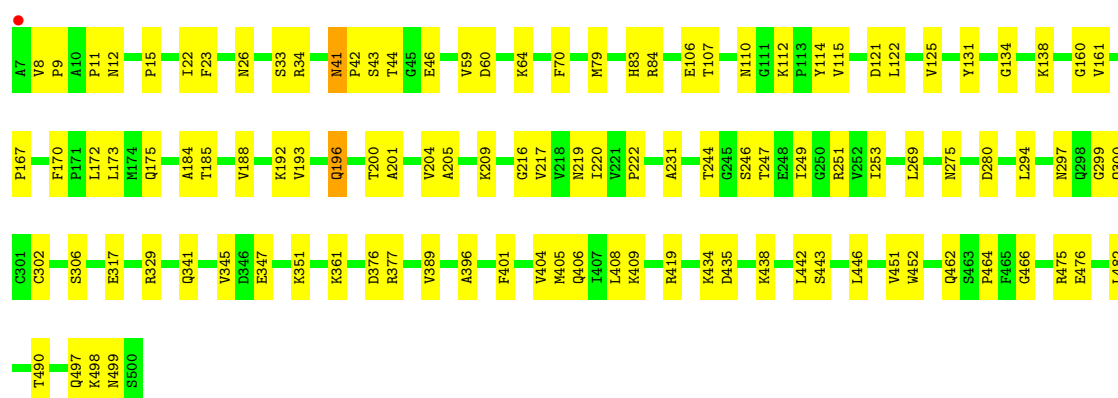
- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain D:



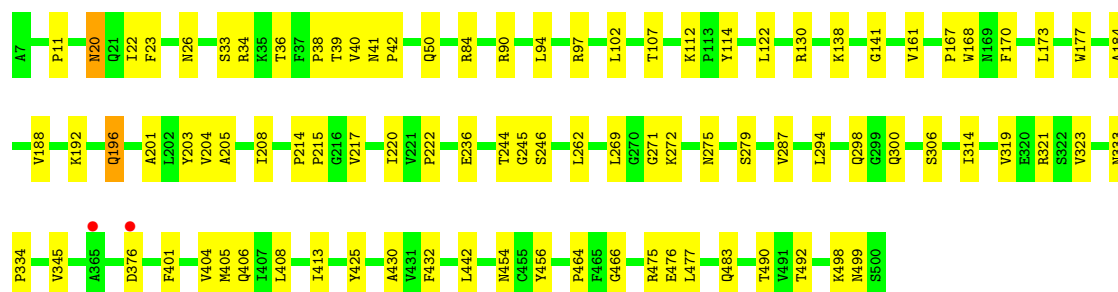
- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain E:



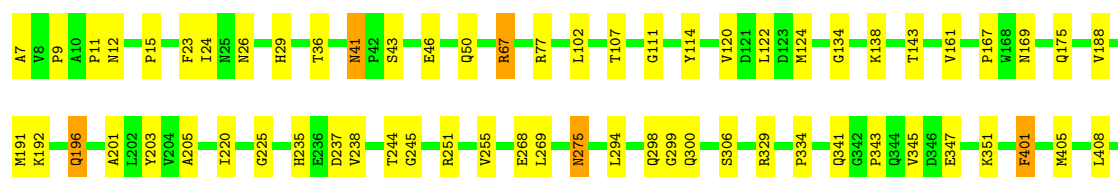
- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain F:



- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

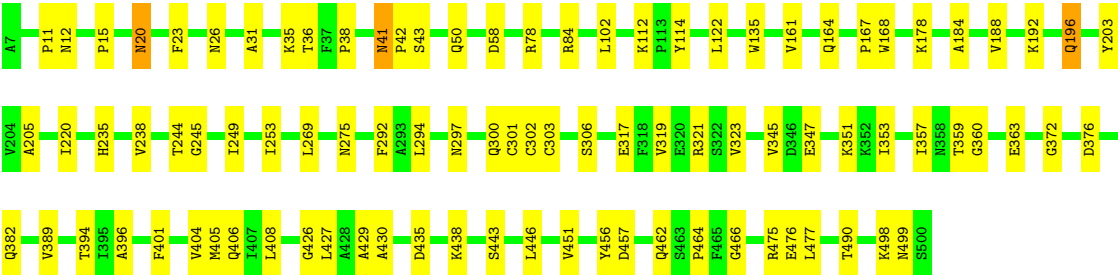
Chain G:





● Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.40Å 176.30Å 102.00Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	45.00 – 2.58 44.03 – 2.58	Depositor EDS
% Data completeness (in resolution range)	91.6 (45.00-2.58) 91.4 (44.03-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.175 , 0.242 0.177 , 0.238	Depositor DCC
R_{free} test set	7234 reflections (7.03%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 2.0	EDS
Estimated twinning fraction	0.149 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 102859 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31839	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, 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	0.36	0/3882	0.61	0/5267
1	B	0.37	0/3882	0.61	0/5267
1	C	0.37	0/3882	0.61	0/5267
1	D	0.38	0/3882	0.63	0/5267
1	E	0.36	0/3882	0.60	0/5267
1	F	0.37	0/3882	0.60	0/5267
1	G	0.37	0/3882	0.61	0/5267
1	H	0.38	0/3882	0.61	0/5267
All	All	0.37	0/31056	0.61	0/42136

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	3798	0	3745	63	0
1	B	3798	0	3745	72	0
1	C	3798	0	3745	61	0
1	D	3798	0	3745	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3798	0	3745	69	0
1	F	3798	0	3745	65	0
1	G	3798	0	3745	57	0
1	H	3798	0	3745	66	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	26	3	0
4	B	44	0	26	2	0
4	C	44	0	26	7	0
4	D	44	0	26	5	0
4	E	44	0	26	3	0
4	F	44	0	26	4	0
4	G	44	0	26	4	0
4	H	44	0	26	6	0
5	A	127	0	0	5	0
5	B	118	0	0	5	0
5	C	127	0	0	2	0
5	D	147	0	0	7	0
5	E	132	0	0	5	0
5	F	140	0	0	5	0
5	G	148	0	0	2	0
5	H	148	0	0	3	0
All	All	31839	0	30168	488	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 8.

All (488) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:347:GLU:HG2	1:C:351:LYS:HE2	1.53	0.89
1:F:196:GLN:H	1:F:196:GLN:HE21	1.28	0.81
1:A:196:GLN:H	1:A:196:GLN:HE21	1.28	0.81
1:G:196:GLN:H	1:G:196:GLN:HE21	1.29	0.80
1:A:347:GLU:HG2	1:A:351:LYS:HE2	1.64	0.79
1:C:361:LYS:HE2	1:C:367:LEU:HD22	1.62	0.79
1:H:196:GLN:HE21	1:H:196:GLN:H	1.31	0.79
1:F:404:VAL:HG12	1:F:406:GLN:HE22	1.50	0.77
1:H:360:GLY:HA2	5:H:8553:HOH:O	1.84	0.75
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.69	0.75
1:E:196:GLN:H	1:E:196:GLN:HE21	1.33	0.74
1:C:44:THR:HG22	1:C:377:ARG:HH21	1.53	0.74
4:D:4502:NAD:H6N	4:D:4502:NAD:O2N	1.88	0.73
1:A:391:ASP:OD2	1:A:419:ARG:HD2	1.89	0.73
5:E:9052:HOH:O	1:F:483:GLN:HB3	1.88	0.73
1:B:196:GLN:H	1:B:196:GLN:HE21	1.39	0.70
1:E:347:GLU:HG2	1:E:351:LYS:HE2	1.73	0.70
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.73	0.70
1:E:205:ALA:HB2	1:E:220:ILE:HD12	1.71	0.69
1:E:302:CYS:SG	5:E:9224:HOH:O	2.48	0.69
1:H:363:GLU:HB2	5:H:8553:HOH:O	1.92	0.69
1:F:102:LEU:HD21	1:F:203:TYR:HD2	1.57	0.69
1:E:404:VAL:HG12	1:E:406:GLN:HE22	1.57	0.69
1:D:294:LEU:HD22	1:D:405:MET:HB2	1.73	0.69
1:A:251:ARG:NH2	1:B:259:SER:O	2.25	0.68
1:E:404:VAL:HG12	1:E:406:GLN:NE2	2.09	0.68
1:B:41:ASN:HD22	1:B:43:SER:H	1.42	0.67
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.76	0.67
1:D:196:GLN:H	1:D:196:GLN:HE21	1.43	0.66
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.31	0.65
1:H:36:THR:HB	1:H:50:GLN:HG3	1.79	0.65
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.78	0.64
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.32	0.64
4:A:1502:NAD:O2N	4:A:1502:NAD:H6N	1.97	0.64
1:A:36:THR:HB	1:A:50:GLN:HG3	1.81	0.63
1:C:196:GLN:HE21	1:C:196:GLN:H	1.46	0.63
1:C:464:PRO:HG2	1:D:490:THR:OG1	1.98	0.63
1:F:404:VAL:HG12	1:F:406:GLN:NE2	2.14	0.62
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.34	0.62
1:A:115:VAL:HG23	5:A:1513:HOH:O	2.00	0.61
1:F:36:THR:HB	1:F:50:GLN:HG3	1.83	0.61
1:G:300:GLN:HE22	1:G:345:VAL:H	1.49	0.60
1:E:216:GLY:HA2	1:E:219:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:6502:NAD:O2N	4:F:6502:NAD:H6N	2.01	0.60
1:D:35:LYS:HA	1:H:359:THR:OG1	2.02	0.60
1:F:102:LEU:HD21	1:F:203:TYR:CD2	2.35	0.60
1:C:362:GLN:HE22	1:G:50:GLN:NE2	1.99	0.60
1:G:41:ASN:HD22	1:G:43:SER:H	1.49	0.59
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.37	0.59
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.37	0.59
1:H:302:CYS:HB3	4:H:8502:NAD:C7N	2.33	0.59
1:C:401:PHE:CZ	4:C:3502:NAD:H2D	2.37	0.59
1:D:33:SER:O	1:D:34:ARG:HB2	2.02	0.59
1:E:121:ASP:O	1:E:125:VAL:HG23	2.03	0.59
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.85	0.59
1:H:347:GLU:HG2	1:H:351:LYS:HE2	1.84	0.58
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.85	0.58
1:B:41:ASN:ND2	1:B:43:SER:H	2.00	0.58
1:A:226:PRO:HG3	5:A:1529:HOH:O	2.01	0.58
1:B:294:LEU:HD12	1:B:306:SER:HA	1.84	0.58
1:B:391:ASP:OD2	1:B:419:ARG:HD2	2.03	0.58
1:D:109:ASP:HB3	5:D:4521:HOH:O	2.03	0.58
1:C:241:VAL:HG23	1:C:263:LYS:HD3	1.86	0.58
1:E:294:LEU:HD12	1:E:306:SER:HA	1.86	0.57
1:D:462:GLN:NE2	5:D:4506:HOH:O	2.37	0.57
1:A:138:LYS:HE3	1:C:135:TRP:CD1	2.40	0.56
1:A:294:LEU:HD22	1:A:405:MET:HB2	1.87	0.56
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.06	0.56
1:B:201:ALA:HB2	5:B:2600:HOH:O	2.03	0.56
1:A:198:PRO:O	1:A:202:LEU:HG	2.05	0.56
1:A:102:LEU:HD21	1:A:203:TYR:HD2	1.70	0.56
1:C:359:THR:O	1:C:363:GLU:HG3	2.06	0.56
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.41	0.56
1:F:20:ASN:HD22	1:F:20:ASN:N	2.04	0.55
1:G:329:ARG:HE	1:G:341:GLN:HB2	1.71	0.55
1:G:12:ASN:O	1:G:15:PRO:HD3	2.07	0.55
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.88	0.55
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.88	0.55
1:D:369:CYS:SG	1:D:385:VAL:HG23	2.46	0.55
1:F:20:ASN:HD22	1:F:20:ASN:H	1.54	0.55
1:E:41:ASN:C	1:E:41:ASN:HD22	2.10	0.55
1:G:294:LEU:HD13	1:G:405:MET:HA	1.87	0.55
1:G:430:ALA:HB2	1:G:456:TYR:CD1	2.41	0.55
1:B:111:GLY:O	1:B:343:PRO:HD2	2.07	0.55
1:H:302:CYS:SG	1:H:427:LEU:HD21	2.47	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:41:ASN:HD21	1:C:43:SER:HB2	1.72	0.55
1:A:500:SER:OXT	1:D:158:PRO:HD3	2.07	0.54
1:A:294:LEU:HD12	1:A:306:SER:HA	1.89	0.54
1:A:12:ASN:O	1:A:15:PRO:HD3	2.08	0.54
1:B:247:THR:HA	1:B:269:LEU:HD13	1.89	0.54
1:F:214:PRO:HD2	1:F:217:VAL:HG21	1.90	0.54
1:B:401:PHE:CZ	4:B:2502:NAD:H2D	2.41	0.54
1:B:41:ASN:HD22	1:B:41:ASN:C	2.10	0.54
1:F:39:THR:HA	5:F:9249:HOH:O	2.06	0.54
1:E:497:GLN:OE1	1:H:78:ARG:HD2	2.08	0.54
1:H:372:GLY:H	1:H:382:GLN:HE21	1.55	0.54
1:E:115:VAL:HG23	5:E:9012:HOH:O	2.08	0.54
1:B:112:LYS:HE2	1:B:297:ASN:OD1	2.08	0.54
1:E:79:MET:SD	1:E:83:HIS:HD2	2.30	0.54
1:A:172:LEU:HD21	1:A:200:THR:HB	1.90	0.54
1:H:161:VAL:HA	1:H:188:VAL:HG23	1.89	0.53
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.88	0.53
1:H:319:VAL:O	1:H:323:VAL:HG23	2.09	0.53
1:G:294:LEU:HD12	1:G:306:SER:HA	1.91	0.53
1:A:443:SER:HA	1:A:451:VAL:HG11	1.89	0.53
1:B:279:SER:HA	1:B:314:ILE:HD13	1.90	0.53
1:F:319:VAL:O	1:F:323:VAL:HG23	2.09	0.53
1:E:302:CYS:HB3	4:E:5502:NAD:C7N	2.39	0.53
1:F:246:SER:HB3	4:F:6502:NAD:O4D	2.09	0.53
4:H:8502:NAD:O2N	4:H:8502:NAD:H6N	2.08	0.53
1:F:22:ILE:HG12	1:F:222:PRO:HD2	1.90	0.53
1:E:247:THR:HA	1:E:269:LEU:HD13	1.91	0.53
1:A:302:CYS:SG	5:A:1621:HOH:O	2.59	0.53
1:G:401:PHE:CZ	4:G:7502:NAD:H2D	2.44	0.53
1:C:12:ASN:O	1:C:15:PRO:HD3	2.09	0.53
1:D:408:LEU:N	1:D:408:LEU:HD12	2.24	0.52
1:G:268:GLU:HB3	4:G:7502:NAD:N7N	2.24	0.52
1:H:167:PRO:HD3	1:H:244:THR:O	2.09	0.52
1:C:319:VAL:O	1:C:323:VAL:HG23	2.09	0.52
1:D:84:ARG:NH1	1:D:184:ALA:O	2.43	0.52
1:F:130:ARG:HD2	5:F:9075:HOH:O	2.09	0.52
1:G:430:ALA:HB2	1:G:456:TYR:CE1	2.44	0.52
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.44	0.52
1:E:300:GLN:HE22	1:E:345:VAL:H	1.57	0.52
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.43	0.52
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.90	0.52
1:E:361:LYS:HA	5:E:9047:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:LYS:HD2	1:A:306:SER:OG	2.10	0.52
1:G:464:PRO:HG2	1:H:490:THR:OG1	2.10	0.52
1:B:102:LEU:HD21	1:B:203:TYR:HD2	1.75	0.52
1:G:7:ALA:O	1:G:9:PRO:HD3	2.10	0.51
1:F:294:LEU:HD12	1:F:306:SER:HA	1.92	0.51
1:C:36:THR:HB	1:C:50:GLN:HG3	1.91	0.51
1:H:196:GLN:H	1:H:196:GLN:NE2	2.06	0.51
1:E:172:LEU:HD21	1:E:200:THR:HB	1.91	0.51
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.45	0.51
1:C:251:ARG:O	1:C:255:VAL:HG23	2.10	0.51
1:B:498:LYS:HG2	1:B:499:ASN:N	2.24	0.51
1:C:172:LEU:HD21	1:C:200:THR:HB	1.93	0.51
1:F:204:VAL:O	1:F:208:ILE:HG13	2.10	0.51
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.11	0.51
1:E:246:SER:HB3	4:E:5502:NAD:O4D	2.11	0.51
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.92	0.51
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.45	0.51
1:B:12:ASN:O	1:B:15:PRO:HD3	2.11	0.51
1:E:134:GLY:O	1:E:138:LYS:HD2	2.11	0.51
1:F:196:GLN:N	1:F:196:GLN:HE21	2.04	0.51
1:E:12:ASN:O	1:E:15:PRO:HD3	2.11	0.51
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.46	0.51
1:C:121:ASP:O	1:C:125:VAL:HG23	2.12	0.50
1:D:172:LEU:HD21	1:D:200:THR:HB	1.93	0.50
1:E:249:ILE:O	1:E:253:ILE:HG12	2.11	0.50
1:B:289:GLN:HE21	1:B:455:CYS:HA	1.76	0.50
1:C:498:LYS:HG2	1:C:499:ASN:N	2.26	0.50
1:E:41:ASN:ND2	1:E:43:SER:H	2.10	0.50
1:G:294:LEU:CD1	1:G:405:MET:HA	2.41	0.50
1:B:115:VAL:HG23	5:B:2542:HOH:O	2.11	0.50
1:A:498:LYS:HG2	1:A:499:ASN:N	2.27	0.50
1:D:292:PHE:HE1	1:D:457:ASP:HB2	1.77	0.50
1:H:498:LYS:HG2	1:H:499:ASN:N	2.25	0.50
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.94	0.50
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.10	0.50
1:A:196:GLN:HE21	1:A:196:GLN:N	2.06	0.50
1:A:225:GLY:HA3	4:A:1502:NAD:C8A	2.41	0.50
1:G:443:SER:HA	1:G:451:VAL:HG11	1.92	0.50
1:H:353:ILE:O	1:H:357:ILE:HG13	2.12	0.50
1:E:443:SER:HA	1:E:451:VAL:HG11	1.94	0.49
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.12	0.49
1:F:201:ALA:HB2	5:F:9086:HOH:O	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:102:LEU:HD21	1:G:203:TYR:HD2	1.77	0.49
1:F:294:LEU:HD13	1:F:405:MET:HA	1.94	0.49
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.47	0.49
1:H:408:LEU:N	1:H:408:LEU:HD12	2.27	0.49
4:F:6502:NAD:O2N	4:F:6502:NAD:C6N	2.60	0.49
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.95	0.49
1:E:84:ARG:NH1	1:E:184:ALA:O	2.46	0.49
1:G:134:GLY:O	1:G:138:LYS:HD2	2.12	0.49
1:A:338:LYS:HB2	5:A:1614:HOH:O	2.12	0.49
1:E:112:LYS:HE2	1:E:297:ASN:OD1	2.13	0.49
1:A:41:ASN:HD22	1:A:41:ASN:C	2.16	0.49
1:D:359:THR:O	1:D:363:GLU:HG3	2.12	0.49
1:B:22:ILE:HG12	1:B:222:PRO:HD2	1.95	0.49
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.94	0.49
1:C:258:GLY:O	1:D:251:ARG:HG2	2.13	0.48
1:F:138:LYS:HD3	1:H:135:TRP:CE2	2.48	0.48
1:A:389:VAL:HB	1:A:408:LEU:HG	1.95	0.48
1:D:435:ASP:HB3	1:D:438:LYS:HD2	1.95	0.48
1:G:67:ARG:HD2	1:G:237:ASP:OD2	2.12	0.48
1:H:294:LEU:HD12	1:H:306:SER:HA	1.95	0.48
1:F:300:GLN:HE22	1:F:345:VAL:H	1.61	0.48
1:H:36:THR:CB	1:H:50:GLN:HG3	2.43	0.48
1:B:159:VAL:CG1	1:B:162:CYS:SG	3.01	0.48
1:C:292:PHE:HE1	1:C:457:ASP:HB2	1.78	0.48
1:C:302:CYS:SG	4:C:3502:NAD:C3N	3.01	0.48
1:H:435:ASP:HB3	1:H:438:LYS:HD2	1.94	0.48
1:G:498:LYS:HG2	1:G:499:ASN:N	2.27	0.48
1:E:167:PRO:HD3	1:E:244:THR:HB	1.96	0.48
1:D:251:ARG:O	1:D:255:VAL:HG23	2.13	0.48
1:F:36:THR:CB	1:F:50:GLN:HG3	2.43	0.48
4:H:8502:NAD:O2N	4:H:8502:NAD:H5N	2.13	0.48
1:B:172:LEU:HD21	1:B:200:THR:HB	1.95	0.48
1:E:452:TRP:HD1	1:F:492:THR:HB	1.79	0.48
1:D:12:ASN:O	1:D:15:PRO:HD3	2.13	0.48
1:B:422:ASN:HB3	5:B:2589:HOH:O	2.13	0.48
1:A:315:TYR:O	1:A:319:VAL:HG23	2.13	0.48
1:B:79:MET:HE1	1:B:87:LEU:HD12	1.94	0.48
1:C:245:GLY:HA2	4:C:3502:NAD:O4D	2.13	0.48
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.95	0.48
1:D:246:SER:HB3	4:D:4502:NAD:O4D	2.13	0.47
1:H:168:TRP:NE1	4:H:8502:NAD:O2N	2.47	0.47
1:A:408:LEU:HD12	1:A:408:LEU:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.96	0.47
1:B:294:LEU:CD1	1:B:405:MET:HA	2.44	0.47
1:E:131:TYR:CE1	1:E:462:GLN:HB3	2.50	0.47
1:E:41:ASN:HD22	1:E:43:SER:H	1.61	0.47
1:A:251:ARG:O	1:A:255:VAL:HG23	2.15	0.47
1:E:161:VAL:HA	1:E:188:VAL:HG23	1.96	0.47
1:C:167:PRO:HD3	1:C:244:THR:O	2.14	0.47
1:H:404:VAL:HG12	1:H:406:GLN:OE1	2.14	0.47
1:B:301:CYS:SG	1:B:303:CYS:SG	3.13	0.47
1:E:464:PRO:HG2	1:F:490:THR:OG1	2.14	0.47
1:C:21:GLN:HB3	1:C:29:HIS:O	2.15	0.47
1:E:464:PRO:HA	1:E:476:GLU:O	2.15	0.47
1:A:84:ARG:NH1	1:A:184:ALA:O	2.48	0.47
1:H:300:GLN:HE22	1:H:345:VAL:H	1.63	0.47
1:E:251:ARG:HG2	1:F:262:LEU:HD11	1.97	0.47
1:G:41:ASN:ND2	1:G:43:SER:H	2.12	0.47
1:A:41:ASN:ND2	1:A:43:SER:H	2.13	0.47
1:H:164:GLN:OE1	1:H:178:LYS:HB3	2.15	0.47
1:H:41:ASN:C	1:H:41:ASN:HD22	2.18	0.47
1:H:84:ARG:NH1	1:H:184:ALA:O	2.48	0.47
1:H:196:GLN:HE21	1:H:196:GLN:N	2.07	0.46
1:B:159:VAL:HG12	1:B:187:ASN:OD1	2.15	0.46
1:H:292:PHE:HE1	1:H:457:ASP:HB2	1.80	0.46
1:H:20:ASN:HD22	1:H:20:ASN:H	1.63	0.46
1:F:167:PRO:HD3	1:F:244:THR:O	2.15	0.46
1:H:41:ASN:ND2	1:H:43:SER:H	2.12	0.46
1:D:452:TRP:HB3	1:D:455:CYS:O	2.15	0.46
1:H:38:PRO:HD3	1:H:50:GLN:HE22	1.81	0.46
1:G:225:GLY:HA3	4:G:7502:NAD:C8A	2.45	0.46
1:B:393:MET:O	1:B:397:LYS:HG3	2.14	0.46
1:D:159:VAL:CG1	1:D:162:CYS:SG	3.03	0.46
1:D:170:PHE:HB3	1:D:173:LEU:HB3	1.96	0.46
1:G:347:GLU:O	1:G:351:LYS:HG2	2.15	0.46
1:F:432:PHE:HA	1:F:454:ASN:OD1	2.15	0.46
1:G:41:ASN:C	1:G:41:ASN:HD22	2.19	0.46
1:E:106:GLU:O	1:E:110:ASN:HB3	2.16	0.46
1:G:111:GLY:O	1:G:343:PRO:HD2	2.16	0.46
1:E:280:ASP:O	1:E:434:LYS:HE2	2.15	0.46
1:G:435:ASP:HB3	1:G:438:LYS:HD2	1.98	0.46
1:C:224:PHE:HD1	5:C:3512:HOH:O	1.98	0.46
1:H:443:SER:HA	1:H:451:VAL:HG11	1.97	0.46
1:E:435:ASP:HB3	1:E:438:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:359:THR:O	1:B:363:GLU:HG3	2.16	0.46
1:B:292:PHE:HE1	1:B:457:ASP:HB2	1.79	0.46
1:H:294:LEU:HD22	1:H:405:MET:HB2	1.96	0.46
1:F:245:GLY:O	1:F:269:LEU:HA	2.16	0.46
1:A:94:LEU:HB3	1:A:207:LEU:HD22	1.98	0.46
1:A:155:ARG:NH2	1:B:444:GLN:HG3	2.31	0.46
1:H:12:ASN:O	1:H:15:PRO:HD3	2.16	0.46
1:E:209:LYS:HA	5:E:9025:HOH:O	2.15	0.46
1:C:36:THR:CB	1:C:50:GLN:HG3	2.46	0.46
1:E:188:VAL:HG12	1:E:217:VAL:HA	1.97	0.46
1:G:298:GLN:HA	5:G:9410:HOH:O	2.16	0.45
1:G:107:THR:HG23	1:G:334:PRO:HB2	1.98	0.45
1:D:302:CYS:HB3	4:D:4502:NAD:O7N	2.15	0.45
1:D:225:GLY:HA3	4:D:4502:NAD:C8A	2.46	0.45
1:D:498:LYS:HG2	1:D:499:ASN:N	2.30	0.45
1:E:442:LEU:O	1:E:446:LEU:HG	2.15	0.45
1:A:168:TRP:NE1	4:A:1502:NAD:O2N	2.49	0.45
1:C:144:ILE:HA	1:C:145:PRO:HD3	1.62	0.45
1:E:175:GLN:HE22	1:E:204:VAL:HG21	1.81	0.45
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.51	0.45
1:G:167:PRO:HD3	1:G:244:THR:O	2.16	0.45
1:C:44:THR:CG2	1:C:377:ARG:HH21	2.24	0.45
1:F:168:TRP:NE1	4:F:6502:NAD:O2N	2.49	0.45
1:B:464:PRO:HA	1:B:476:GLU:O	2.17	0.45
1:C:469:LYS:HA	5:D:4538:HOH:O	2.16	0.45
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.98	0.45
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.51	0.45
1:G:452:TRP:HB3	1:G:455:CYS:O	2.16	0.45
1:D:329:ARG:HE	1:D:341:GLN:HB2	1.80	0.45
1:E:389:VAL:CG1	1:E:396:ALA:HB2	2.46	0.45
1:B:117:SER:HA	1:B:121:ASP:HB2	1.99	0.45
1:H:294:LEU:CD1	1:H:405:MET:HA	2.46	0.45
1:B:141:GLY:HA3	1:C:143:THR:OG1	2.15	0.45
1:H:430:ALA:HB2	1:H:456:TYR:CE1	2.52	0.45
1:H:112:LYS:HE2	1:H:297:ASN:OD1	2.17	0.45
1:B:302:CYS:HB3	4:B:2502:NAD:C2N	2.46	0.45
1:B:107:THR:HG23	1:B:112:LYS:O	2.17	0.45
1:D:394:THR:HG21	1:H:35:LYS:HG3	1.97	0.45
1:A:292:PHE:HE1	1:A:457:ASP:HB2	1.82	0.45
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.99	0.45
1:G:120:VAL:O	1:G:124:MET:HG3	2.17	0.45
1:H:20:ASN:HD22	1:H:20:ASN:N	2.14	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.52	0.45
1:B:36:THR:HB	1:B:50:GLN:HG3	1.99	0.45
1:A:111:GLY:O	1:A:343:PRO:HD2	2.17	0.45
1:D:358:ASN:OD1	1:H:50:GLN:HG2	2.16	0.44
1:D:271:GLY:HA2	1:D:425:TYR:CD2	2.52	0.44
1:D:391:ASP:OD2	1:D:419:ARG:HD2	2.17	0.44
4:H:8502:NAD:O2N	4:H:8502:NAD:C5N	2.65	0.44
1:C:225:GLY:HA3	4:C:3502:NAD:C8A	2.48	0.44
1:F:271:GLY:HA2	1:F:425:TYR:CD2	2.52	0.44
1:D:102:LEU:HD21	1:D:203:TYR:CD2	2.52	0.44
1:B:429:ALA:HB3	1:B:451:VAL:HG22	1.99	0.44
1:D:275:ASN:ND2	1:D:430:ALA:HB3	2.32	0.44
1:B:294:LEU:HD13	1:B:405:MET:HA	1.99	0.44
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.53	0.44
1:D:106:GLU:O	1:D:110:ASN:HB3	2.16	0.44
1:D:121:ASP:O	1:D:125:VAL:HG23	2.17	0.44
1:F:298:GLN:NE2	5:F:9073:HOH:O	2.50	0.44
1:H:429:ALA:HB1	1:H:446:LEU:HD13	1.99	0.44
1:B:271:GLY:HA2	1:B:425:TYR:CD2	2.52	0.44
1:B:294:LEU:O	1:B:299:GLY:HA2	2.17	0.44
1:C:169:ASN:HD21	4:C:3502:NAD:C5N	2.31	0.44
1:C:255:VAL:HG13	1:D:255:VAL:HG13	1.99	0.44
1:B:167:PRO:HD3	1:B:244:THR:O	2.18	0.44
4:H:8502:NAD:O2N	4:H:8502:NAD:C6N	2.65	0.44
1:F:294:LEU:HD22	1:F:405:MET:HB2	2.00	0.44
1:A:435:ASP:HB3	1:A:438:LYS:HD2	2.00	0.44
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.53	0.44
1:B:130:ARG:HD2	5:B:2517:HOH:O	2.17	0.44
1:C:294:LEU:HD12	1:C:306:SER:HA	1.99	0.44
1:F:107:THR:HG23	1:F:112:LYS:O	2.17	0.44
1:G:498:LYS:HE2	1:G:498:LYS:HB3	1.78	0.44
1:B:309:PHE:HB3	1:B:410:PHE:CD2	2.53	0.44
1:E:329:ARG:HE	1:E:341:GLN:HB2	1.82	0.44
1:A:81:ALA:HB1	1:A:136:ALA:O	2.18	0.44
1:H:294:LEU:HD13	1:H:405:MET:HA	2.00	0.43
1:C:306:SER:O	1:C:406:GLN:HB2	2.19	0.43
1:F:173:LEU:HD11	1:F:177:TRP:HE1	1.83	0.43
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.18	0.43
1:A:121:ASP:O	1:A:125:VAL:HG23	2.19	0.43
1:C:443:SER:HA	1:C:451:VAL:HG11	2.00	0.43
1:F:84:ARG:NH1	1:F:184:ALA:O	2.51	0.43
1:G:235:HIS:HB3	1:G:238:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:430:ALA:HB2	1:F:456:TYR:CE1	2.54	0.43
1:H:235:HIS:HB3	1:H:238:VAL:HG23	2.01	0.43
1:F:33:SER:O	1:F:34:ARG:HB2	2.19	0.43
1:E:70:PHE:CZ	1:E:160:GLY:HA2	2.52	0.43
1:G:408:LEU:N	1:G:408:LEU:HD12	2.33	0.43
1:B:264:ARG:HD2	1:B:264:ARG:H	1.83	0.43
1:F:287:VAL:HG21	1:F:321:ARG:HD3	2.00	0.43
1:F:214:PRO:HA	1:F:215:PRO:HD3	1.92	0.43
1:E:251:ARG:HA	1:F:262:LEU:HD21	2.00	0.43
1:G:201:ALA:HB2	5:G:9126:HOH:O	2.18	0.43
1:A:391:ASP:OD2	1:A:419:ARG:CD	2.64	0.43
1:F:38:PRO:HD3	1:F:50:GLN:HE22	1.84	0.43
1:C:300:GLN:HE22	1:C:345:VAL:H	1.65	0.43
1:G:36:THR:HB	1:G:50:GLN:HG3	2.00	0.43
1:A:245:GLY:O	1:A:269:LEU:HA	2.19	0.43
1:B:461:ALA:HA	1:B:477:LEU:HD22	2.01	0.43
1:G:489:LYS:NZ	1:H:446:LEU:O	2.47	0.43
1:E:466:GLY:HA3	1:E:475:ARG:HD3	2.01	0.43
1:C:311:GLN:HG3	5:C:3534:HOH:O	2.17	0.43
1:F:413:ILE:HD11	1:F:442:LEU:HG	2.01	0.43
1:E:452:TRP:CD1	1:F:492:THR:HB	2.53	0.43
1:B:63:VAL:HG11	1:B:235:HIS:CE1	2.54	0.43
1:E:185:THR:HG23	1:E:482:LEU:HD22	2.00	0.43
1:H:476:GLU:O	1:H:477:LEU:HB2	2.19	0.43
1:D:168:TRP:NE1	4:D:4502:NAD:O2N	2.51	0.43
1:C:102:LEU:HD21	1:C:203:TYR:HD2	1.84	0.43
1:B:297:ASN:HA	5:B:2558:HOH:O	2.18	0.42
1:C:70:PHE:CZ	1:C:160:GLY:HA2	2.53	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.53	0.42
1:A:102:LEU:HD21	1:A:203:TYR:CD2	2.51	0.42
1:A:329:ARG:HE	1:A:341:GLN:HB2	1.83	0.42
1:E:193:VAL:HG11	1:E:201:ALA:CB	2.49	0.42
1:H:245:GLY:O	1:H:269:LEU:HA	2.19	0.42
1:H:102:LEU:HD21	1:H:203:TYR:CD2	2.54	0.42
1:E:294:LEU:HD13	1:E:405:MET:HA	2.00	0.42
1:F:279:SER:HA	1:F:314:ILE:HD13	2.01	0.42
1:A:36:THR:CB	1:A:50:GLN:HG3	2.47	0.42
1:B:121:ASP:O	1:B:125:VAL:HG23	2.19	0.42
1:B:244:THR:OG1	1:B:268:GLU:HB2	2.19	0.42
1:F:476:GLU:O	1:F:477:LEU:HB2	2.19	0.42
1:F:272:LYS:HD2	1:F:306:SER:OG	2.19	0.42
1:D:394:THR:HG21	1:H:35:LYS:CG	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:462:GLN:HE21	1:B:146:ILE:HG13	1.84	0.42
1:F:408:LEU:HD12	1:F:408:LEU:N	2.33	0.42
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.35	0.42
1:E:42:PRO:HG3	1:E:345:VAL:O	2.19	0.42
1:C:498:LYS:HE2	1:C:498:LYS:HB3	1.80	0.42
1:E:8:VAL:HA	1:E:9:PRO:HD3	1.96	0.42
1:B:158:PRO:HD3	1:C:500:SER:OXT	2.20	0.42
1:B:476:GLU:O	1:B:477:LEU:HB2	2.19	0.42
1:F:112:LYS:HE2	1:F:112:LYS:HB3	1.83	0.42
1:F:170:PHE:HB3	1:F:173:LEU:HB3	2.01	0.42
1:E:409:LYS:O	1:E:419:ARG:NH1	2.49	0.42
1:A:489:LYS:HB2	1:B:468:TYR:OH	2.20	0.42
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.55	0.42
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.54	0.42
1:A:41:ASN:HD22	1:A:43:SER:H	1.67	0.42
1:D:409:LYS:O	1:D:419:ARG:NH1	2.51	0.42
1:B:11:PRO:HB3	1:B:114:TYR:CE1	2.54	0.42
1:D:497:GLN:HB3	5:D:4615:HOH:O	2.19	0.42
1:E:498:LYS:HG2	1:E:499:ASN:N	2.34	0.42
1:H:466:GLY:HA3	1:H:475:ARG:HD3	2.02	0.42
1:F:94:LEU:HD22	1:F:97:ARG:NH1	2.35	0.42
1:H:317:GLU:HG2	1:H:321:ARG:HH11	1.84	0.42
1:E:44:THR:HG22	1:E:377:ARG:NH1	2.35	0.41
1:C:389:VAL:HB	1:C:408:LEU:HG	2.02	0.41
1:C:22:ILE:HG12	1:C:222:PRO:HD2	2.02	0.41
1:F:466:GLY:HA3	1:F:475:ARG:HD3	2.02	0.41
1:G:24:ILE:HB	1:G:29:HIS:CD2	2.55	0.41
1:D:249:ILE:O	1:D:253:ILE:HG12	2.20	0.41
1:D:41:ASN:C	1:D:41:ASN:HD22	2.23	0.41
1:D:42:PRO:HB3	1:D:345:VAL:O	2.20	0.41
1:D:166:ILE:HD11	1:D:193:VAL:HG12	2.01	0.41
1:G:77:ARG:HH11	1:G:77:ARG:HG3	1.85	0.41
1:E:33:SER:O	1:E:34:ARG:HB2	2.20	0.41
1:D:302:CYS:SG	1:D:427:LEU:HD21	2.60	0.41
1:B:36:THR:CB	1:B:50:GLN:HG3	2.50	0.41
1:G:251:ARG:O	1:G:255:VAL:HG23	2.20	0.41
1:C:196:GLN:NE2	1:C:196:GLN:H	2.17	0.41
1:A:353:ILE:HD13	1:A:402:GLY:HA3	2.01	0.41
1:E:170:PHE:HB3	1:E:173:LEU:HB3	2.02	0.41
1:E:22:ILE:HG12	1:E:222:PRO:HD2	2.03	0.41
1:G:464:PRO:HA	1:G:476:GLU:O	2.20	0.41
1:B:187:ASN:ND2	1:B:485:TYR:HB3	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:21:GLN:HB3	1:D:29:HIS:O	2.19	0.41
1:D:443:SER:HA	1:D:451:VAL:HG11	2.03	0.41
4:E:5502:NAD:O2N	4:E:5502:NAD:H6N	2.21	0.41
1:D:498:LYS:HB3	1:D:498:LYS:HE2	1.92	0.41
1:B:443:SER:HA	1:B:451:VAL:HG11	2.02	0.41
1:B:138:LYS:HE3	1:D:135:TRP:CD1	2.55	0.41
1:G:196:GLN:N	1:G:196:GLN:HE21	2.07	0.41
1:B:244:THR:HA	1:B:268:GLU:O	2.21	0.41
1:F:141:GLY:HA3	1:G:143:THR:OG1	2.20	0.41
1:G:175:GLN:HG3	1:G:191:MET:SD	2.60	0.41
1:B:94:LEU:HB3	1:B:207:LEU:HD22	2.02	0.41
1:C:166:ILE:HB	1:C:167:PRO:HD2	2.02	0.41
1:H:178:LYS:HD3	5:H:8535:HOH:O	2.20	0.41
1:H:249:ILE:O	1:H:253:ILE:HG12	2.21	0.41
1:A:170:PHE:HB3	1:A:173:LEU:HB3	2.02	0.41
1:F:40:VAL:HB	5:F:9248:HOH:O	2.19	0.41
1:C:362:GLN:NE2	1:G:50:GLN:NE2	2.68	0.41
1:C:302:CYS:SG	4:C:3502:NAD:C4N	3.09	0.41
1:C:302:CYS:SG	4:C:3502:NAD:C7N	3.09	0.41
1:B:294:LEU:HD22	1:B:405:MET:HB2	2.01	0.41
1:B:409:LYS:O	1:B:419:ARG:NH1	2.54	0.41
1:G:169:ASN:HD21	4:G:7502:NAD:C5N	2.33	0.41
1:G:268:GLU:OE1	1:G:476:GLU:HG3	2.21	0.41
1:E:107:THR:HG23	1:E:112:LYS:O	2.21	0.41
1:E:131:TYR:CZ	1:E:462:GLN:HA	2.56	0.41
1:H:164:GLN:CD	1:H:178:LYS:HB3	2.41	0.41
1:H:430:ALA:HB2	1:H:456:TYR:CD1	2.56	0.41
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.56	0.41
1:H:301:CYS:SG	1:H:303:CYS:SG	3.13	0.41
1:D:224:PHE:HB3	5:D:4581:HOH:O	2.21	0.41
1:A:185:THR:HG23	1:A:482:LEU:HD22	2.03	0.41
1:D:245:GLY:O	1:D:269:LEU:HA	2.21	0.41
1:G:413:ILE:HD11	1:G:442:LEU:HG	2.03	0.41
1:A:134:GLY:O	1:A:138:LYS:HD2	2.21	0.41
1:C:294:LEU:O	1:C:299:GLY:HA2	2.21	0.41
1:E:389:VAL:HB	1:E:408:LEU:HG	2.03	0.41
1:F:11:PRO:HB3	1:F:114:TYR:CE1	2.55	0.41
1:A:21:GLN:HB3	1:A:29:HIS:O	2.21	0.41
1:D:268:GLU:HB3	5:D:4592:HOH:O	2.21	0.41
1:E:294:LEU:O	1:E:299:GLY:HA2	2.21	0.40
1:D:35:LYS:HG3	1:H:394:THR:HG21	2.02	0.40
1:H:42:PRO:HB3	1:H:345:VAL:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:115:VAL:HG23	5:D:4589:HOH:O	2.21	0.40
1:H:389:VAL:CG1	1:H:396:ALA:HB2	2.52	0.40
1:E:59:VAL:HG21	1:E:231:ALA:HB3	2.03	0.40
1:C:159:VAL:HG12	1:C:187:ASN:OD1	2.22	0.40
1:H:31:ALA:HA	1:H:58:ASP:OD1	2.20	0.40
1:F:430:ALA:HB2	1:F:456:TYR:CD1	2.56	0.40
1:C:122:LEU:O	1:C:126:LEU:HG	2.21	0.40
1:B:70:PHE:CZ	1:B:160:GLY:HA2	2.56	0.40
1:B:21:GLN:HB3	1:B:29:HIS:O	2.20	0.40
1:F:498:LYS:HG2	1:F:499:ASN:N	2.36	0.40
1:A:294:LEU:HD13	1:A:405:MET:HA	2.03	0.40
1:G:294:LEU:O	1:G:299:GLY:HA2	2.21	0.40
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.86	0.40
1:H:41:ASN:HD22	1:H:43:SER:H	1.68	0.40
1:A:497:GLN:NE2	1:D:78:ARG:HD2	2.36	0.40
1:E:60:ASP:O	1:E:64:LYS:HG3	2.20	0.40
1:A:161:VAL:HA	1:A:188:VAL:HG23	2.03	0.40
1:C:264:ARG:H	1:C:264:ARG:HD2	1.86	0.40
1:B:245:GLY:O	1:B:269:LEU:HA	2.22	0.40
1:F:42:PRO:HB3	1:F:345:VAL:O	2.20	0.40
1:A:188:VAL:HG12	1:A:217:VAL:HA	2.04	0.40
1:A:19:CYS:HA	5:A:1505:HOH:O	2.20	0.40
1:C:476:GLU:O	1:C:477:LEU:HB2	2.20	0.40
1:F:333:ASN:HA	1:F:334:PRO:HD2	1.95	0.40
1:G:245:GLY:O	1:G:269:LEU:HA	2.21	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	492/494 (100%)	470 (96%)	22 (4%)	0	100	100
1	B	492/494 (100%)	475 (96%)	16 (3%)	1 (0%)	56	81
1	C	492/494 (100%)	469 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	492/494 (100%)	468 (95%)	23 (5%)	1 (0%)	56	81
1	E	492/494 (100%)	473 (96%)	19 (4%)	0	100	100
1	F	492/494 (100%)	473 (96%)	19 (4%)	0	100	100
1	G	492/494 (100%)	470 (96%)	22 (4%)	0	100	100
1	H	492/494 (100%)	472 (96%)	19 (4%)	1 (0%)	56	81
All	All	3936/3952 (100%)	3770 (96%)	163 (4%)	3 (0%)	59	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	426	GLY
1	D	426	GLY
1	H	426	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/399 (100%)	388 (97%)	11 (3%)	56	83
1	B	399/399 (100%)	391 (98%)	8 (2%)	68	90
1	C	399/399 (100%)	390 (98%)	9 (2%)	63	87
1	D	399/399 (100%)	390 (98%)	9 (2%)	63	87
1	E	399/399 (100%)	390 (98%)	9 (2%)	63	87
1	F	399/399 (100%)	389 (98%)	10 (2%)	60	85
1	G	399/399 (100%)	391 (98%)	8 (2%)	68	90
1	H	399/399 (100%)	390 (98%)	9 (2%)	63	87
All	All	3192/3192 (100%)	3119 (98%)	73 (2%)	63	87

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG

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Mol	Chain	Res	Type
1	A	41	ASN
1	A	122	LEU
1	A	189	VAL
1	A	192	LYS
1	A	196	GLN
1	A	275	ASN
1	A	294	LEU
1	A	338	LYS
1	A	376	ASP
1	A	401	PHE
1	B	14	GLN
1	B	41	ASN
1	B	122	LEU
1	B	192	LYS
1	B	196	GLN
1	B	320	GLU
1	B	401	PHE
1	B	462	GLN
1	C	41	ASN
1	C	46	GLU
1	C	122	LEU
1	C	189	VAL
1	C	192	LYS
1	C	196	GLN
1	C	275	ASN
1	C	294	LEU
1	C	401	PHE
1	D	41	ASN
1	D	64	LYS
1	D	122	LEU
1	D	192	LYS
1	D	196	GLN
1	D	294	LEU
1	D	317	GLU
1	D	362	GLN
1	D	401	PHE
1	E	41	ASN
1	E	46	GLU
1	E	122	LEU
1	E	192	LYS
1	E	196	GLN
1	E	275	ASN

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Mol	Chain	Res	Type
1	E	317	GLU
1	E	376	ASP
1	E	401	PHE
1	F	20	ASN
1	F	41	ASN
1	F	90	ARG
1	F	122	LEU
1	F	192	LYS
1	F	196	GLN
1	F	236	GLU
1	F	275	ASN
1	F	376	ASP
1	F	401	PHE
1	G	41	ASN
1	G	46	GLU
1	G	67	ARG
1	G	122	LEU
1	G	192	LYS
1	G	196	GLN
1	G	275	ASN
1	G	401	PHE
1	H	20	ASN
1	H	41	ASN
1	H	122	LEU
1	H	192	LYS
1	H	196	GLN
1	H	275	ASN
1	H	376	ASP
1	H	401	PHE
1	H	462	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	26	ASN
1	A	29	HIS
1	A	41	ASN
1	A	83	HIS
1	A	175	GLN
1	A	196	GLN
1	A	275	ASN

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Mol	Chain	Res	Type
1	A	300	GLN
1	A	462	GLN
1	B	13	GLN
1	B	26	ASN
1	B	41	ASN
1	B	175	GLN
1	B	196	GLN
1	B	289	GLN
1	C	14	GLN
1	C	26	ASN
1	C	29	HIS
1	C	41	ASN
1	C	89	ASN
1	C	196	GLN
1	C	275	ASN
1	C	300	GLN
1	C	358	ASN
1	C	462	GLN
1	D	14	GLN
1	D	26	ASN
1	D	41	ASN
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	344	GLN
1	D	462	GLN
1	E	13	GLN
1	E	14	GLN
1	E	25	ASN
1	E	26	ASN
1	E	41	ASN
1	E	83	HIS
1	E	89	ASN
1	E	175	GLN
1	E	196	GLN
1	E	219	ASN
1	E	275	ASN
1	E	300	GLN
1	E	349	GLN
1	E	406	GLN
1	E	462	GLN
1	F	13	GLN

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Mol	Chain	Res	Type
1	F	20	ASN
1	F	26	ASN
1	F	29	HIS
1	F	41	ASN
1	F	50	GLN
1	F	175	GLN
1	F	196	GLN
1	F	275	ASN
1	F	300	GLN
1	F	406	GLN
1	G	14	GLN
1	G	26	ASN
1	G	41	ASN
1	G	50	GLN
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	G	349	GLN
1	G	447	GLN
1	H	14	GLN
1	H	20	ASN
1	H	26	ASN
1	H	41	ASN
1	H	50	GLN
1	H	89	ASN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	GLN
1	H	382	GLN

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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAD	A	1502	2	48,48,48	1.33	5 (10%)	73,73,73	2.07	20 (27%)
4	NAD	B	2502	2	48,48,48	1.29	5 (10%)	73,73,73	1.75	9 (12%)
4	NAD	C	3502	2	48,48,48	1.22	5 (10%)	73,73,73	1.69	9 (12%)
4	NAD	D	4502	2	48,48,48	1.38	5 (10%)	73,73,73	1.92	14 (19%)
4	NAD	E	5502	2	48,48,48	1.36	4 (8%)	73,73,73	2.13	22 (30%)
4	NAD	F	6502	2	48,48,48	1.38	4 (8%)	73,73,73	2.14	20 (27%)
4	NAD	G	7502	2	48,48,48	1.35	4 (8%)	73,73,73	1.71	12 (16%)
4	NAD	H	8502	2	48,48,48	1.42	4 (8%)	73,73,73	2.31	21 (28%)

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
4	NAD	A	1502	2	-	0/30/62/62	0/3/5/5
4	NAD	B	2502	2	-	0/30/62/62	0/3/5/5
4	NAD	C	3502	2	-	0/30/62/62	0/3/5/5
4	NAD	D	4502	2	-	0/30/62/62	0/3/5/5
4	NAD	E	5502	2	-	0/30/62/62	0/3/5/5
4	NAD	F	6502	2	-	0/30/62/62	0/3/5/5
4	NAD	G	7502	2	-	0/30/62/62	0/3/5/5
4	NAD	H	8502	2	-	0/30/62/62	0/3/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	8502	NAD	C2N-N1N	6.08	1.43	1.35
4	F	6502	NAD	C2N-N1N	5.75	1.42	1.35
4	A	1502	NAD	C2N-N1N	5.61	1.42	1.35
4	E	5502	NAD	C2N-N1N	5.54	1.42	1.35
4	D	4502	NAD	C2N-N1N	5.54	1.42	1.35
4	G	7502	NAD	C2N-N1N	5.16	1.41	1.35
4	B	2502	NAD	C2N-N1N	4.97	1.41	1.35
4	C	3502	NAD	C2N-N1N	4.89	1.41	1.35
4	H	8502	NAD	O4D-C1D	3.65	1.47	1.41
4	G	7502	NAD	C4A-N9A	-3.52	1.32	1.37
4	D	4502	NAD	O4B-C1B	3.45	1.46	1.41
4	E	5502	NAD	C4A-N9A	-3.37	1.32	1.37
4	F	6502	NAD	O4D-C1D	3.32	1.46	1.41
4	A	1502	NAD	O4D-C1D	3.32	1.46	1.41
4	F	6502	NAD	C4A-N9A	-3.24	1.33	1.37
4	B	2502	NAD	C4A-N9A	-3.13	1.33	1.37
4	D	4502	NAD	O4D-C1D	3.12	1.46	1.41
4	H	8502	NAD	C4A-N9A	-3.11	1.33	1.37
4	E	5502	NAD	O4D-C1D	3.10	1.46	1.41
4	H	8502	NAD	O4B-C1B	2.99	1.45	1.41
4	D	4502	NAD	C4A-N9A	-2.84	1.33	1.37
4	G	7502	NAD	C2B-C1B	-2.82	1.49	1.53
4	C	3502	NAD	C4A-N9A	-2.76	1.33	1.37
4	A	1502	NAD	O4B-C1B	2.65	1.45	1.41
4	E	5502	NAD	O4B-C1B	2.55	1.45	1.41
4	G	7502	NAD	O4B-C1B	2.53	1.45	1.41
4	A	1502	NAD	C4A-N9A	-2.50	1.34	1.37
4	B	2502	NAD	O4B-C1B	2.40	1.45	1.41
4	C	3502	NAD	O4D-C1D	2.38	1.45	1.41
4	C	3502	NAD	O4B-C1B	2.36	1.45	1.41
4	B	2502	NAD	O4D-C1D	2.33	1.44	1.41
4	D	4502	NAD	C2B-C1B	-2.24	1.50	1.53
4	F	6502	NAD	O4B-C1B	2.23	1.44	1.41
4	A	1502	NAD	C2N-C3N	2.08	1.41	1.38
4	C	3502	NAD	C5A-N7A	-2.01	1.32	1.40
4	B	2502	NAD	C5A-N7A	-2.01	1.32	1.40

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5502	NAD	N3A-C2A-N1A	-8.37	121.71	128.71
4	F	6502	NAD	N3A-C2A-N1A	-8.19	121.86	128.71
4	B	2502	NAD	N3A-C2A-N1A	-7.66	122.31	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4502	NAD	N3A-C2A-N1A	-7.17	122.72	128.71
4	H	8502	NAD	N3A-C2A-N1A	-7.01	122.85	128.71
4	C	3502	NAD	N3A-C2A-N1A	-6.98	122.87	128.71
4	A	1502	NAD	N3A-C2A-N1A	-6.94	122.91	128.71
4	A	1502	NAD	N3A-C4A-N9A	6.75	137.63	125.43
4	B	2502	NAD	N3A-C4A-N9A	6.67	137.47	125.43
4	H	8502	NAD	O4B-C1B-N9A	6.64	114.62	108.44
4	H	8502	NAD	N3A-C4A-N9A	6.60	137.36	125.43
4	D	4502	NAD	O4B-C1B-N9A	6.38	114.38	108.44
4	H	8502	NAD	O4D-C1D-N1N	6.28	114.37	107.95
4	D	4502	NAD	N3A-C4A-N9A	6.13	136.51	125.43
4	E	5502	NAD	O4B-C1B-N9A	6.01	114.03	108.44
4	G	7502	NAD	N3A-C2A-N1A	-5.92	123.76	128.71
4	G	7502	NAD	N3A-C4A-N9A	5.82	135.94	125.43
4	F	6502	NAD	N3A-C4A-N9A	5.82	135.93	125.43
4	C	3502	NAD	N3A-C4A-N9A	5.80	135.91	125.43
4	C	3502	NAD	O4B-C1B-N9A	5.48	113.53	108.44
4	E	5502	NAD	N3A-C4A-N9A	5.29	134.99	125.43
4	F	6502	NAD	C6N-N1N-C2N	-5.01	116.38	122.04
4	A	1502	NAD	C6N-N1N-C2N	-4.75	116.67	122.04
4	H	8502	NAD	C2N-N1N-C1D	4.63	130.81	119.33
4	F	6502	NAD	O4B-C1B-N9A	4.62	112.73	108.44
4	G	7502	NAD	O4D-C1D-C2D	-4.60	99.72	106.77
4	A	1502	NAD	C2D-C1D-N1N	4.43	121.35	113.86
4	E	5502	NAD	O5D-C5D-C4D	4.32	124.79	108.94
4	A	1502	NAD	C5A-C4A-N3A	-4.30	116.33	125.70
4	G	7502	NAD	O4B-C1B-N9A	4.18	112.33	108.44
4	H	8502	NAD	C4N-C3N-C7N	-3.99	110.50	121.10
4	B	2502	NAD	O4D-C1D-C2D	-3.85	100.87	106.77
4	B	2502	NAD	C5A-C4A-N3A	-3.78	117.46	125.70
4	D	4502	NAD	C5A-C4A-N3A	-3.75	117.54	125.70
4	H	8502	NAD	C5A-C4A-N3A	-3.72	117.59	125.70
4	B	2502	NAD	O4B-C1B-N9A	3.66	111.84	108.44
4	C	3502	NAD	C5A-C4A-N3A	-3.65	117.76	125.70
4	D	4502	NAD	C6N-N1N-C2N	-3.64	117.92	122.04
4	E	5502	NAD	PN-O5D-C5D	3.62	132.76	120.24
4	H	8502	NAD	C6N-N1N-C2N	-3.56	118.02	122.04
4	F	6502	NAD	C2N-N1N-C1D	3.55	128.12	119.33
4	F	6502	NAD	C5A-C4A-N3A	-3.54	117.99	125.70
4	H	8502	NAD	O5D-C5D-C4D	3.54	121.92	108.94
4	F	6502	NAD	C4D-O4D-C1D	3.53	113.59	109.75
4	H	8502	NAD	C4A-C5A-N7A	3.54	112.55	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6502	NAD	C4N-C3N-C7N	-3.42	112.01	121.10
4	A	1502	NAD	C2N-N1N-C1D	3.40	127.76	119.33
4	H	8502	NAD	C6N-N1N-C1D	-3.36	111.01	119.33
4	B	2502	NAD	C4A-C5A-N7A	3.35	112.39	109.52
4	E	5502	NAD	C5A-C4A-N3A	-3.31	118.49	125.70
4	E	5502	NAD	C6N-N1N-C2N	-3.25	118.37	122.04
4	F	6502	NAD	O4D-C1D-C2D	-3.23	101.82	106.77
4	A	1502	NAD	C3N-C7N-N7N	-3.23	114.10	117.77
4	E	5502	NAD	C4N-C3N-C7N	-3.19	112.61	121.10
4	G	7502	NAD	C5A-C4A-N3A	-3.14	118.87	125.70
4	H	8502	NAD	C2N-C3N-C7N	3.11	128.60	119.35
4	A	1502	NAD	O4B-C1B-N9A	3.10	111.33	108.44
4	G	7502	NAD	O4D-C1D-N1N	3.10	111.13	107.95
4	H	8502	NAD	O4D-C1D-C2D	-3.09	102.03	106.77
4	H	8502	NAD	C2D-C1D-N1N	3.09	119.09	113.86
4	A	1502	NAD	O4D-C1D-C2D	-3.03	102.12	106.77
4	F	6502	NAD	C3N-C7N-N7N	-3.01	114.34	117.77
4	A	1502	NAD	C2N-C3N-C4N	2.96	121.66	118.31
4	A	1502	NAD	C6A-C5A-C4A	2.93	122.62	117.25
4	B	2502	NAD	C6A-C5A-C4A	2.92	122.61	117.25
4	E	5502	NAD	O4D-C1D-C2D	-2.91	102.32	106.77
4	H	8502	NAD	O4D-C4D-C5D	2.86	119.58	109.36
4	C	3502	NAD	O4D-C1D-C2D	-2.84	102.42	106.77
4	A	1502	NAD	C5N-C6N-N1N	2.82	125.19	120.43
4	F	6502	NAD	C5N-C6N-N1N	2.81	125.18	120.43
4	C	3502	NAD	C6A-C5A-C4A	2.81	122.40	117.25
4	F	6502	NAD	C3D-C2D-C1D	2.79	105.28	100.91
4	A	1502	NAD	C3D-C2D-C1D	2.76	105.23	100.91
4	D	4502	NAD	C4A-C5A-N7A	2.76	111.88	109.52
4	A	1502	NAD	C4N-C3N-C7N	-2.75	113.80	121.10
4	A	1502	NAD	O5D-C5D-C4D	2.74	118.98	108.94
4	G	7502	NAD	C4A-C5A-N7A	2.71	111.85	109.52
4	E	5502	NAD	C2N-C3N-C4N	2.70	121.36	118.31
4	E	5502	NAD	C1B-N9A-C4A	-2.68	122.00	126.64
4	H	8502	NAD	C6A-C5A-C4A	2.67	122.15	117.25
4	E	5502	NAD	C8A-N9A-C1B	2.64	131.58	126.38
4	G	7502	NAD	C1B-N9A-C4A	-2.63	122.09	126.64
4	E	5502	NAD	C2N-N1N-C1D	2.62	125.83	119.33
4	D	4502	NAD	C6A-C5A-C4A	2.60	122.02	117.25
4	F	6502	NAD	C6A-C5A-C4A	2.57	121.96	117.25
4	F	6502	NAD	C2D-C1D-N1N	2.55	118.18	113.86
4	F	6502	NAD	C2N-C3N-C7N	2.55	126.93	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5502	NAD	C3D-C2D-C1D	2.52	104.85	100.91
4	E	5502	NAD	C4A-C5A-N7A	2.50	111.67	109.52
4	E	5502	NAD	C3N-C7N-N7N	-2.50	114.92	117.77
4	D	4502	NAD	C3N-C7N-N7N	-2.50	114.93	117.77
4	H	8502	NAD	C3D-C2D-C1D	2.49	104.81	100.91
4	A	1502	NAD	C2A-N3A-C4A	2.49	121.10	114.01
4	G	7502	NAD	C6A-C5A-C4A	2.44	121.73	117.25
4	C	3502	NAD	O4D-C1D-N1N	2.42	110.43	107.95
4	F	6502	NAD	C2N-C3N-C4N	2.41	121.04	118.31
4	D	4502	NAD	C2N-N1N-C1D	2.38	125.24	119.33
4	A	1502	NAD	C4D-O4D-C1D	2.35	112.30	109.75
4	A	1502	NAD	O4D-C4D-C5D	2.34	117.72	109.36
4	D	4502	NAD	C4N-C3N-C7N	-2.34	114.88	121.10
4	E	5502	NAD	C4D-O4D-C1D	2.31	112.26	109.75
4	B	2502	NAD	C2A-N3A-C4A	2.25	120.43	114.01
4	A	1502	NAD	O7N-C7N-C3N	2.25	122.11	119.58
4	H	8502	NAD	C2N-C3N-C4N	2.25	120.86	118.31
4	F	6502	NAD	O5D-C5D-C4D	2.25	117.18	108.94
4	D	4502	NAD	C2A-N3A-C4A	2.25	120.40	114.01
4	E	5502	NAD	C2N-C3N-C7N	2.24	126.03	119.35
4	D	4502	NAD	O5D-C5D-C4D	2.24	117.17	108.94
4	D	4502	NAD	C2N-C3N-C4N	2.23	120.84	118.31
4	D	4502	NAD	C5N-C6N-N1N	2.22	124.18	120.43
4	A	1502	NAD	O4D-C1D-N1N	2.20	110.21	107.95
4	F	6502	NAD	C2A-N3A-C4A	2.20	120.29	114.01
4	E	5502	NAD	O2N-PN-O1N	-2.20	112.10	118.72
4	F	6502	NAD	O7N-C7N-C3N	2.19	122.05	119.58
4	G	7502	NAD	O3B-C3B-C4B	-2.17	104.69	111.08
4	B	2502	NAD	C2D-C1D-N1N	2.16	117.52	113.86
4	E	5502	NAD	C6A-C5A-C4A	2.14	121.18	117.25
4	H	8502	NAD	C2A-N3A-C4A	2.10	120.00	114.01
4	E	5502	NAD	C2A-N3A-C4A	2.08	119.93	114.01
4	C	3502	NAD	C2A-N3A-C4A	2.08	119.92	114.01
4	E	5502	NAD	C5A-C6A-N6A	2.06	125.38	120.72
4	H	8502	NAD	O2N-PN-O3	2.06	114.34	108.79
4	G	7502	NAD	C6N-N1N-C2N	-2.05	119.72	122.04
4	F	6502	NAD	O4D-C4D-C5D	2.03	116.61	109.36
4	G	7502	NAD	O5B-C5B-C4B	2.03	116.39	108.94
4	C	3502	NAD	C4N-C3N-C7N	-2.03	115.72	121.10
4	H	8502	NAD	PN-O3-PA	-2.02	124.25	132.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/494 (100%)	-0.50	0 100 100	11, 28, 42, 61	0
1	B	494/494 (100%)	-0.45	0 100 100	8, 30, 48, 70	0
1	C	494/494 (100%)	-0.45	0 100 100	8, 29, 48, 70	0
1	D	494/494 (100%)	-0.54	0 100 100	9, 25, 41, 68	0
1	E	494/494 (100%)	-0.49	1 (0%) 93 95	13, 30, 47, 72	0
1	F	494/494 (100%)	-0.38	2 (0%) 90 91	13, 33, 53, 73	0
1	G	494/494 (100%)	-0.53	0 100 100	11, 29, 45, 59	0
1	H	494/494 (100%)	-0.57	0 100 100	11, 26, 40, 70	0
All	All	3952/3952 (100%)	-0.49	3 (0%) 93 95	8, 29, 47, 73	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	7	ALA	3.1
1	F	365	ALA	3.1
1	F	376	ASP	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAD	B	2502	44/44	0.16	1.77	20,48,74,75	0
4	NAD	A	1502	44/44	0.15	1.68	25,47,70,74	0
4	NAD	H	8502	44/44	0.14	1.54	11,45,69,72	0
4	NAD	D	4502	44/44	0.13	1.15	9,28,60,62	0
4	NAD	C	3502	44/44	0.14	1.12	17,35,61,65	0
4	NAD	F	6502	44/44	0.15	0.85	23,53,71,74	0
4	NAD	E	5502	44/44	0.14	0.83	29,47,71,73	0
4	NAD	G	7502	44/44	0.13	0.53	22,37,61,62	0
3	MG	H	8501	1/1	0.11	-0.31	31,31,31,31	0
3	MG	C	3501	1/1	0.09	-1.26	37,37,37,37	0
3	MG	F	6501	1/1	0.07	-1.65	33,33,33,33	0
3	MG	D	4501	1/1	0.08	-1.76	24,24,24,24	0
3	MG	E	5501	1/1	0.07	-1.77	38,38,38,38	0
3	MG	G	7501	1/1	0.08	-1.88	32,32,32,32	0
3	MG	A	1501	1/1	0.07	-2.14	27,27,27,27	0
3	MG	B	2501	1/1	0.04	-5.05	23,23,23,23	0
2	MN	H	8503	1/1	0.03	-	35,35,35,35	1
2	MN	B	2503	1/1	0.12	-	43,43,43,43	1
2	MN	A	1503	1/1	0.18	-	42,42,42,42	1
2	MN	F	6503	1/1	0.14	-	59,59,59,59	1
2	MN	G	7503	1/1	0.12	-	36,36,36,36	1
2	MN	D	4503	1/1	0.17	-	28,28,28,28	1
2	MN	E	5503	1/1	0.06	-	40,40,40,40	1
2	MN	C	3503	1/1	0.10	-	33,33,33,33	1

6.5 Other polymers ⓘ

There are no such residues in this entry.