



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:33 AM EDT

PDB ID : 2CZC / pdb_00002czc
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from *Pyrococcus horikoshii* OT3
Authors : Ito, K.; Arai, R.; Kamo-Uchikubo, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-13
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

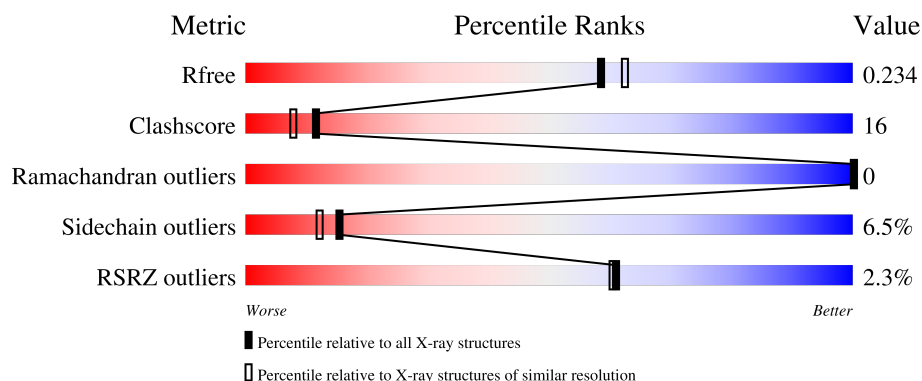
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	76% 19% 5%
1	B	334	75% 22% .
1	C	334	68% 28% .
1	D	334	65% 29% 5% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	601	-	X	X	-
2	PO4	A	602	-	X	-	X
2	PO4	B	603	-	X	X	X
2	PO4	C	604	-	X	X	-
2	PO4	D	605	-	X	X	X

2 Entry composition [i](#)

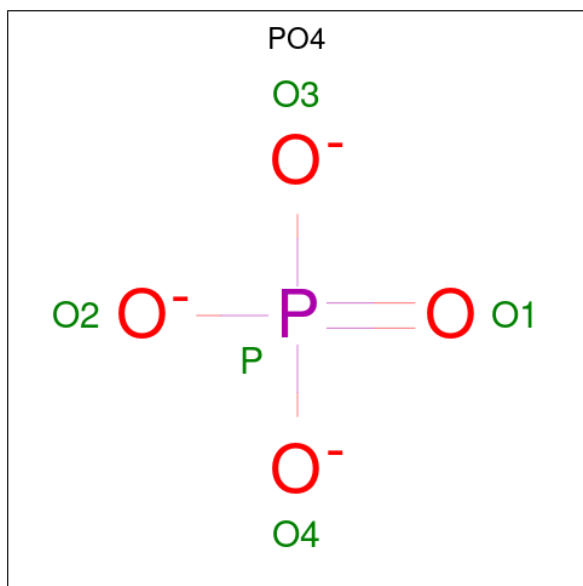
There are 4 unique types of molecules in this entry. The entry contains 11153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2627	1681	443	495	8			
1	B	333	Total	C	N	O	S	0	0	0
			2619	1676	442	494	7			
1	C	333	Total	C	N	O	S	0	0	0
			2619	1676	442	494	7			
1	D	332	Total	C	N	O	S	0	0	0
			2609	1670	440	492	7			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



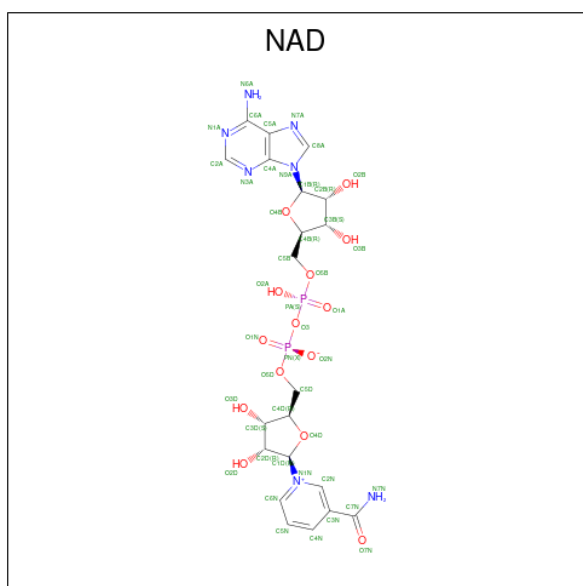
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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	147	Total	O	0	0
			147	147		
4	B	126	Total	O	0	0
			126	126		

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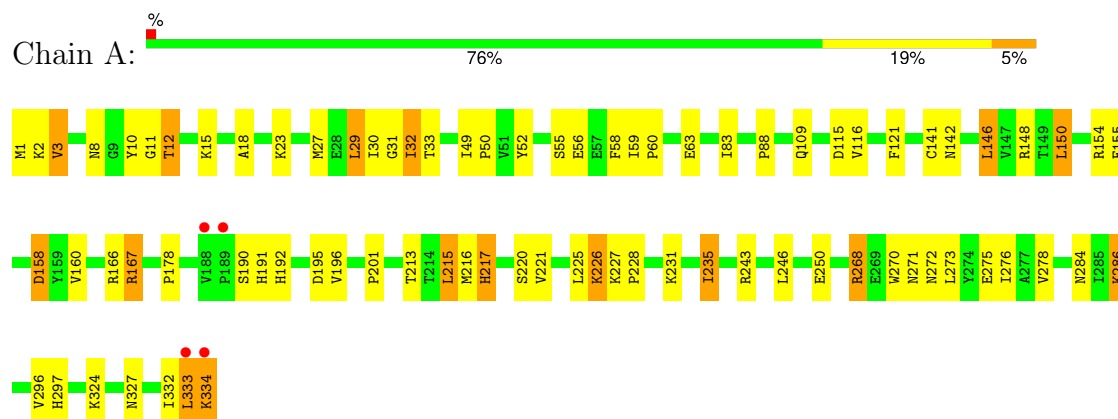
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	113	Total 113	O 113	0	0
4	D	92	Total 92	O 92	0	0

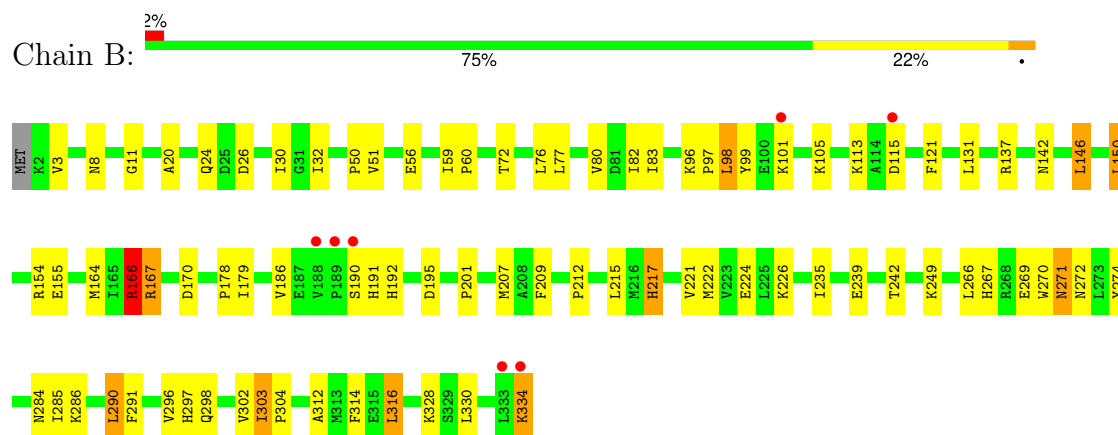
3 Residue-property plots [i](#)

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

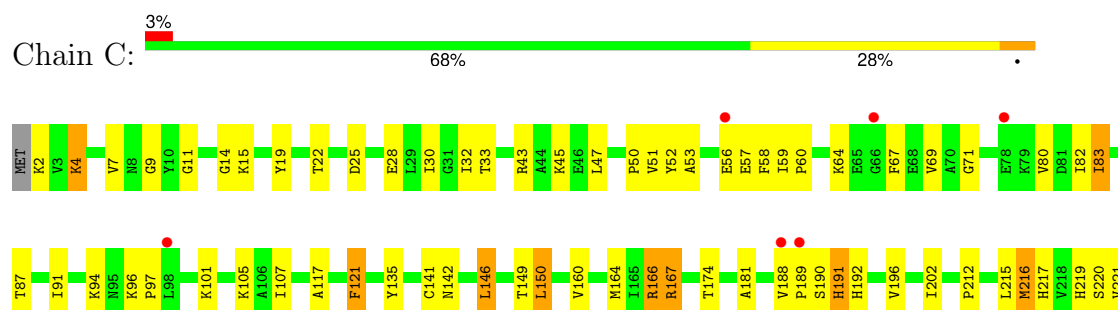
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

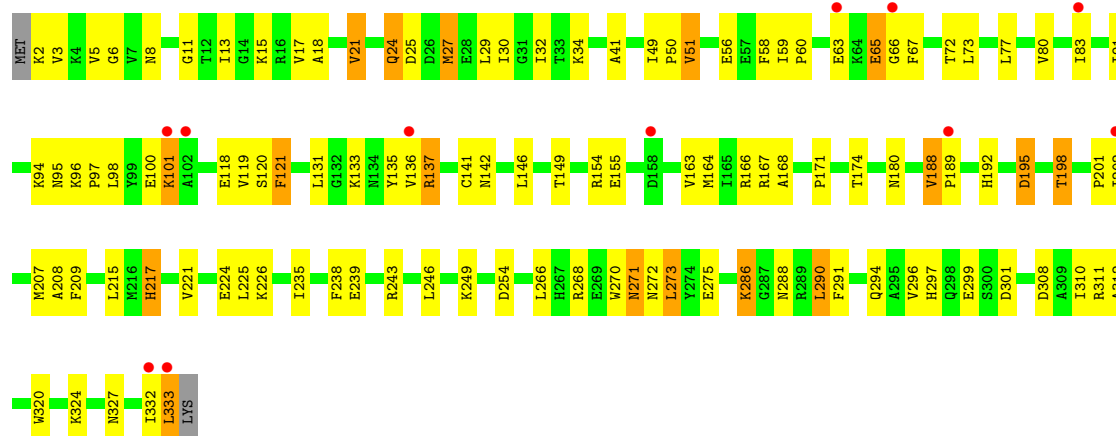


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.69Å 127.19Å 161.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.00 49.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.2 (49.96-2.00) 88.3 (49.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.241 0.200 , 0.234	Depositor DCC
R_{free} test set	8869 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11153	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 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.54	0/2677	0.98	5/3624 (0.1%)
1	B	0.53	0/2669	1.00	8/3614 (0.2%)
1	C	0.52	0/2669	0.98	7/3614 (0.2%)
1	D	0.53	0/2659	0.97	6/3603 (0.2%)
All	All	0.53	0/10674	0.98	26/14455 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	LEU	N-CA-C	8.86	120.63	110.97
1	B	215	LEU	N-CA-C	8.63	120.61	111.03
1	C	215	LEU	N-CA-C	8.41	120.36	111.03
1	B	221	VAL	N-CA-C	6.98	117.94	108.17
1	C	166	ARG	N-CA-C	6.82	121.16	110.17
1	A	116	VAL	N-CA-C	6.73	120.45	111.17
1	D	121	PHE	N-CA-C	6.66	120.38	109.06
1	D	221	VAL	N-CA-C	6.55	117.29	108.11
1	B	121	PHE	N-CA-C	6.29	119.75	109.06
1	A	121	PHE	N-CA-C	6.08	119.40	109.06
1	B	166	ARG	N-CA-C	5.97	119.79	110.17
1	C	121	PHE	N-CA-C	5.88	118.80	108.75
1	C	221	VAL	N-CA-C	5.65	116.08	108.17
1	C	332	ILE	CA-C-N	5.51	132.06	121.54
1	C	332	ILE	C-N-CA	5.51	132.06	121.54
1	B	217	HIS	N-CA-C	-5.49	102.63	110.59
1	D	217	HIS	N-CA-C	-5.38	102.56	110.52
1	B	26	ASP	N-CA-C	-5.28	106.70	112.72
1	B	226	LYS	N-CA-C	-5.25	107.04	113.50
1	A	217	HIS	N-CA-C	-5.23	102.72	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	GLU	N-CA-C	-5.17	102.81	110.46
1	B	80	VAL	N-CA-C	5.16	116.80	108.85
1	A	221	VAL	N-CA-C	5.16	115.39	108.17
1	C	259	ILE	N-CA-C	-5.13	105.49	110.42
1	A	158	ASP	N-CA-C	-5.08	106.78	113.12
1	D	288	ASN	N-CA-C	-5.02	106.90	112.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2667	71	0
1	B	2619	0	2655	72	0
1	C	2619	0	2655	99	0
1	D	2609	0	2642	110	0
2	A	10	0	0	3	0
2	B	5	0	0	4	0
2	C	5	0	0	6	0
2	D	5	0	0	5	0
3	A	44	0	26	6	0
3	B	44	0	26	3	0
3	C	44	0	26	6	0
3	D	44	0	25	5	0
4	A	147	0	0	7	0
4	B	126	0	0	5	0
4	C	113	0	0	4	0
4	D	92	0	0	5	0
All	All	11153	0	10722	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:SER:OG	1:D:137:ARG:HD2	1.33	1.29
1:D:142:ASN:HD22	2:D:605:PO4:P	1.83	1.01
1:A:286:LYS:HE3	1:D:189:PRO:HD2	1.42	1.00
1:A:333:LEU:O	1:A:334:LYS:HD3	1.61	0.99
1:B:154:ARG:HH21	1:B:201:PRO:HG2	1.27	0.98
1:D:320:TRP:O	1:D:324:LYS:HG2	1.65	0.95
1:D:142:ASN:ND2	2:D:605:PO4:O2	2.07	0.87
1:D:167:ARG:HG3	1:D:217:HIS:CE1	2.10	0.87
1:D:120:SER:HG	1:D:137:ARG:HD2	1.37	0.85
1:A:243:ARG:HD3	1:A:327:ASN:OD1	1.79	0.82
1:B:192:HIS:HE1	2:B:603:PO4:O2	1.63	0.82
1:D:120:SER:OG	1:D:137:ARG:CD	2.24	0.81
1:B:166:ARG:NH2	2:B:603:PO4:O3	2.14	0.80
1:C:4:LYS:HE2	1:C:28:GLU:OE1	1.81	0.80
1:B:142:ASN:ND2	2:B:603:PO4:O2	2.11	0.79
1:A:3:VAL:CG1	1:A:27:MET:HG2	2.13	0.79
1:C:56:GLU:O	1:C:59:ILE:HG22	1.82	0.79
1:C:107:ILE:HD11	1:C:313:MET:HE1	1.65	0.79
1:D:238:PHE:HB3	1:D:246:LEU:HD11	1.64	0.78
1:A:333:LEU:O	1:A:334:LYS:CD	2.30	0.78
1:C:190:SER:OG	1:C:192:HIS:HD2	1.66	0.78
1:D:120:SER:HB2	1:D:198:THR:HG23	1.65	0.76
1:B:97:PRO:O	1:B:101:LYS:HD3	1.85	0.76
1:A:284:ASN:HD22	1:D:188:VAL:HG13	1.50	0.76
1:B:303:ILE:HG13	1:B:304:PRO:HD3	1.70	0.74
1:B:334:LYS:HD3	4:B:639:HOH:O	1.87	0.74
1:A:216:MET:HB3	1:A:296:VAL:O	1.87	0.74
1:A:12:THR:HG23	3:A:501:NAD:O1A	1.87	0.73
1:B:113:LYS:HE2	1:B:115:ASP:OD2	1.88	0.73
1:C:167:ARG:HH11	1:C:298:GLN:HG3	1.53	0.73
1:C:97:PRO:O	1:C:101:LYS:HE2	1.89	0.72
1:B:154:ARG:NH2	1:B:201:PRO:HG2	2.03	0.72
1:D:202:ILE:HD12	1:D:202:ILE:O	1.90	0.72
1:D:98:LEU:O	1:D:101:LYS:HD3	1.90	0.72
1:B:166:ARG:HG3	1:B:209:PHE:O	1.90	0.72
1:D:195:ASP:O	1:D:198:THR:HG22	1.91	0.71
1:B:190:SER:OG	1:B:192:HIS:HD2	1.73	0.71
1:A:56:GLU:CD	1:A:56:GLU:H	1.98	0.71
1:B:191:HIS:CD2	4:B:682:HOH:O	2.44	0.71
1:C:245:LEU:CD1	1:C:275:GLU:HG3	2.21	0.71
1:D:142:ASN:ND2	2:D:605:PO4:O1	2.25	0.70
1:D:56:GLU:HG2	1:D:72:THR:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:SER:CB	1:D:137:ARG:HD2	2.21	0.70
1:D:167:ARG:HG3	1:D:217:HIS:HE1	1.56	0.69
1:C:64:LYS:O	1:C:64:LYS:HD3	1.93	0.69
1:A:327:ASN:HD22	1:A:334:LYS:NZ	1.90	0.69
1:D:24:GLN:HG3	1:D:311:ARG:NH1	2.08	0.69
1:A:327:ASN:HD22	1:A:334:LYS:HZ3	1.40	0.68
1:D:271:ASN:HB3	4:D:664:HOH:O	1.92	0.68
1:B:272:ASN:HA	1:B:297:HIS:CE1	2.29	0.68
1:B:303:ILE:HG13	1:B:304:PRO:CD	2.25	0.67
1:C:59:ILE:N	1:C:60:PRO:HD2	2.08	0.67
1:D:32:ILE:C	1:D:32:ILE:HD12	2.19	0.66
1:D:83:ILE:HD12	1:D:83:ILE:O	1.96	0.65
1:D:273:LEU:HD13	1:D:275:GLU:O	1.95	0.65
1:C:216:MET:HG3	1:C:256:THR:HB	1.79	0.65
1:C:80:VAL:HG21	1:C:83:ILE:HG23	1.77	0.65
1:D:59:ILE:N	1:D:60:PRO:HD2	2.11	0.65
1:B:249:LYS:HE2	4:B:606:HOH:O	1.97	0.65
1:C:196:VAL:HG11	1:C:202:ILE:HD11	1.79	0.65
1:A:284:ASN:ND2	1:D:188:VAL:HG13	2.11	0.64
1:D:80:VAL:HG21	1:D:83:ILE:HG23	1.79	0.64
1:D:149:THR:HG21	1:D:294:GLN:OE1	1.97	0.64
1:A:333:LEU:C	1:A:334:LYS:HD2	2.22	0.64
1:D:120:SER:CB	1:D:198:THR:HG23	2.28	0.64
1:A:227:LYS:HG3	1:A:228:PRO:HD2	1.80	0.64
1:A:88:PRO:HD3	3:A:501:NAD:O4B	1.98	0.63
1:B:272:ASN:HA	1:B:297:HIS:HE1	1.63	0.63
1:C:7:VAL:CG1	1:C:32:ILE:HG22	2.27	0.63
1:D:142:ASN:ND2	2:D:605:PO4:P	2.65	0.63
1:C:2:LYS:HD3	1:C:25:ASP:O	1.99	0.63
1:A:59:ILE:N	1:A:60:PRO:HD2	2.14	0.62
1:D:3:VAL:CG1	1:D:27:MET:HB3	2.29	0.62
1:B:217:HIS:HB2	1:B:296:VAL:CG1	2.28	0.62
1:D:2:LYS:HE2	1:D:25:ASP:O	1.99	0.62
1:D:27:MET:HE1	1:D:310:ILE:HD13	1.82	0.62
1:C:142:ASN:ND2	2:C:604:PO4:O4	2.29	0.62
1:A:333:LEU:C	1:A:334:LYS:CD	2.73	0.61
1:D:195:ASP:CG	4:D:681:HOH:O	2.42	0.61
1:D:27:MET:HE1	1:D:310:ILE:CD1	2.30	0.61
1:C:273:LEU:HD13	1:C:275:GLU:O	2.00	0.61
1:C:245:LEU:HD11	1:C:333:LEU:HD12	1.83	0.61
4:A:610:HOH:O	1:D:249:LYS:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ILE:HD12	1:C:83:ILE:O	2.01	0.61
1:C:58:PHE:C	1:C:60:PRO:HD2	2.26	0.60
1:D:192:HIS:CE1	1:D:208:ALA:HB2	2.36	0.60
1:D:238:PHE:CB	1:D:246:LEU:HD11	2.32	0.60
1:C:309:ALA:C	1:C:313:MET:HE2	2.27	0.60
1:C:107:ILE:CD1	1:C:313:MET:HE1	2.31	0.60
1:C:146:LEU:O	1:C:150:LEU:HB2	2.02	0.60
1:B:186:VAL:HG22	4:B:624:HOH:O	2.02	0.59
1:B:212:PRO:O	1:C:212:PRO:HG2	2.03	0.59
1:D:188:VAL:HA	1:D:189:PRO:C	2.27	0.59
1:A:220:SER:OG	1:D:207:MET:HE2	2.02	0.59
1:B:3:VAL:HG21	1:B:316:LEU:HD21	1.85	0.59
1:D:217:HIS:HB2	1:D:296:VAL:CG1	2.33	0.59
1:A:324:LYS:NZ	1:A:324:LYS:HB3	2.17	0.58
1:C:245:LEU:HD12	1:C:275:GLU:HG3	1.84	0.58
1:C:167:ARG:HG3	1:C:217:HIS:CE1	2.38	0.58
1:D:290:LEU:HD22	1:D:291:PHE:N	2.19	0.58
1:B:77:LEU:CD1	1:B:98:LEU:HD12	2.34	0.58
1:D:13:ILE:HD11	3:D:504:NAD:C3N	2.33	0.58
1:C:192:HIS:HE1	2:C:604:PO4:O4	1.87	0.58
1:D:59:ILE:HG22	1:D:63:GLU:OE2	2.04	0.58
1:B:271:ASN:O	1:B:271:ASN:ND2	2.37	0.57
1:B:137:ARG:O	1:B:137:ARG:HG3	2.04	0.57
1:D:18:ALA:O	1:D:21:VAL:HG13	2.05	0.57
1:D:131:LEU:HA	1:D:312:ALA:O	2.05	0.57
1:B:217:HIS:HB2	1:B:296:VAL:HG13	1.87	0.57
1:B:32:ILE:HD12	1:B:32:ILE:C	2.30	0.57
1:C:11:GLY:O	1:C:15:LYS:HG2	2.04	0.57
1:B:222:MET:HE3	1:B:224:GLU:HG2	1.89	0.55
1:C:51:VAL:O	1:C:69:VAL:HG23	2.05	0.55
1:B:20:ALA:HB2	1:B:303:ILE:HD13	1.87	0.55
1:A:271:ASN:ND2	1:A:271:ASN:O	2.38	0.55
1:C:309:ALA:O	1:C:313:MET:HE2	2.05	0.55
1:A:30:ILE:O	1:A:50:PRO:CG	2.55	0.55
1:C:107:ILE:CG1	1:C:313:MET:HE1	2.37	0.55
1:C:190:SER:OG	1:C:192:HIS:CD2	2.54	0.55
1:A:272:ASN:HA	1:A:297:HIS:CE1	2.43	0.54
1:B:235:ILE:O	1:B:239:GLU:HG3	2.07	0.54
1:C:149:THR:HG21	1:C:294:GLN:OE1	2.07	0.54
1:B:164:MET:HE2	1:B:164:MET:HA	1.90	0.54
1:C:141:CYS:HB3	3:C:503:NAD:H5N	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:SER:CB	1:D:137:ARG:CD	2.85	0.54
1:B:167:ARG:HG3	1:B:217:HIS:CE1	2.43	0.54
1:D:56:GLU:OE1	1:D:59:ILE:HG13	2.07	0.53
1:A:192:HIS:HE1	2:A:601:PO4:O3	1.91	0.53
1:C:181:ALA:O	1:C:212:PRO:HD3	2.09	0.53
1:B:105:LYS:HD2	1:B:314:PHE:CZ	2.43	0.53
1:A:142:ASN:OD1	2:A:601:PO4:O3	2.26	0.53
1:C:167:ARG:HD3	1:C:298:GLN:NE2	2.23	0.53
1:A:167:ARG:HD2	1:A:167:ARG:C	2.33	0.53
1:D:154:ARG:HE	1:D:201:PRO:HG2	1.72	0.53
1:D:17:VAL:O	1:D:21:VAL:HG12	2.09	0.53
1:B:314:PHE:HB3	1:B:316:LEU:HD13	1.90	0.53
1:C:107:ILE:HD11	1:C:313:MET:CE	2.38	0.52
1:B:166:ARG:HB3	1:B:217:HIS:ND1	2.24	0.52
1:D:201:PRO:O	1:D:202:ILE:HG23	2.08	0.52
1:D:271:ASN:ND2	1:D:271:ASN:O	2.39	0.52
1:B:274:TYR:HE1	1:B:303:ILE:HG12	1.75	0.52
1:C:43:ARG:CZ	1:C:47:LEU:HD21	2.39	0.52
1:C:96:LYS:N	1:C:97:PRO:HD2	2.24	0.52
1:D:91:ILE:HG22	1:D:95:ASN:ND2	2.25	0.52
3:C:503:NAD:O2B	4:C:715:HOH:O	2.19	0.52
1:A:334:LYS:HG2	1:A:334:LYS:OXT	2.10	0.52
1:B:207:MET:HE2	1:C:220:SER:OG	2.09	0.51
1:B:314:PHE:CB	1:B:316:LEU:HD13	2.40	0.51
1:C:45:LYS:HE2	1:C:67:PHE:CZ	2.45	0.51
1:A:286:LYS:HE3	1:D:189:PRO:CD	2.28	0.51
1:B:8:ASN:OD1	3:B:502:NAD:H2A	2.09	0.51
1:A:30:ILE:O	1:A:50:PRO:HG2	2.10	0.51
1:C:69:VAL:HG22	1:C:71:GLY:H	1.74	0.51
1:D:98:LEU:HA	1:D:101:LYS:HD2	1.92	0.51
1:A:167:ARG:HD2	1:A:167:ARG:O	2.10	0.51
1:D:163:VAL:C	1:D:164:MET:HE2	2.36	0.51
1:B:146:LEU:O	1:B:150:LEU:HB2	2.10	0.50
1:B:167:ARG:HD3	1:B:298:GLN:NE2	2.26	0.50
1:C:87:THR:HG22	3:C:503:NAD:C2A	2.42	0.50
4:C:672:HOH:O	1:D:271:ASN:HB3	2.11	0.50
1:B:284:ASN:ND2	1:C:188:VAL:HB	2.25	0.50
1:C:30:ILE:O	1:C:50:PRO:HG2	2.10	0.50
1:C:43:ARG:NH1	1:C:47:LEU:HD21	2.27	0.50
1:C:82:ILE:HD11	1:C:107:ILE:HG13	1.92	0.50
1:D:96:LYS:N	1:D:97:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ILE:N	1:C:60:PRO:CD	2.75	0.50
1:C:196:VAL:CG1	1:C:202:ILE:HD11	2.42	0.50
1:D:11:GLY:O	1:D:15:LYS:HG2	2.11	0.50
1:A:167:ARG:HB2	1:A:213:THR:O	2.11	0.50
1:C:192:HIS:HE1	2:C:604:PO4:P	2.35	0.50
1:C:53:ALA:H	1:C:69:VAL:HG21	1.77	0.50
1:C:270:TRP:O	1:C:271:ASN:CG	2.55	0.50
1:C:238:PHE:HA	1:C:241:THR:HG23	1.93	0.50
1:D:65:GLU:HG3	1:D:66:GLY:H	1.77	0.49
1:C:105:LYS:HD2	1:C:314:PHE:CZ	2.47	0.49
1:B:166:ARG:HB3	1:B:217:HIS:CE1	2.47	0.49
1:B:274:TYR:CE1	1:B:303:ILE:HG12	2.47	0.49
1:D:18:ALA:O	1:D:21:VAL:CG1	2.60	0.49
1:D:51:VAL:HG11	1:D:67:PHE:CE1	2.48	0.49
1:C:32:ILE:C	1:C:32:ILE:HD12	2.38	0.49
1:D:118:GLU:OE1	1:D:133:LYS:HB3	2.13	0.49
1:A:158:ASP:HB2	1:A:226:LYS:HB3	1.95	0.48
1:B:269:GLU:CD	1:B:269:GLU:H	2.21	0.48
1:B:242:THR:HA	1:B:334:LYS:OXT	2.12	0.48
1:B:3:VAL:CG2	1:B:316:LEU:HD21	2.44	0.48
1:A:3:VAL:HG13	1:A:27:MET:HG2	1.95	0.48
1:B:266:LEU:O	1:B:267:HIS:HB2	2.14	0.48
3:A:501:NAD:C5N	4:A:682:HOH:O	2.62	0.47
1:C:33:THR:HA	1:C:52:TYR:O	2.14	0.47
1:D:94:LYS:O	1:D:97:PRO:HD2	2.14	0.47
1:D:202:ILE:HD12	1:D:202:ILE:C	2.38	0.47
1:C:167:ARG:HD3	1:C:298:GLN:CD	2.39	0.47
1:C:266:LEU:O	1:C:267:HIS:HB2	2.14	0.47
1:A:30:ILE:O	1:A:50:PRO:HG3	2.14	0.47
1:C:30:ILE:O	1:C:50:PRO:CG	2.62	0.47
1:D:30:ILE:HG13	1:D:80:VAL:HG12	1.95	0.47
1:A:178:PRO:HB3	1:C:174:THR:HB	1.96	0.47
1:B:179:ILE:CD1	1:D:168:ALA:HB3	2.45	0.47
1:C:300:SER:O	1:C:303:ILE:HG12	2.14	0.47
1:C:82:ILE:HG13	1:C:105:LYS:O	2.15	0.47
1:C:271:ASN:HB3	4:C:652:HOH:O	2.13	0.47
1:D:270:TRP:O	1:D:271:ASN:CG	2.58	0.47
1:A:215:LEU:HD13	1:D:180:ASN:HD21	1.79	0.47
1:A:246:LEU:N	1:A:246:LEU:HD22	2.30	0.47
1:C:269:GLU:H	1:C:269:GLU:CD	2.23	0.47
1:A:166:ARG:HA	1:A:217:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:ND1	1:A:195:ASP:OD1	2.49	0.46
1:C:166:ARG:HD2	2:C:604:PO4:O4	2.15	0.46
1:D:6:GLY:O	1:D:83:ILE:HA	2.15	0.46
1:D:208:ALA:C	1:D:209:PHE:CD1	2.93	0.46
1:C:82:ILE:HG13	1:C:105:LYS:C	2.41	0.46
1:D:30:ILE:O	1:D:50:PRO:HG2	2.15	0.46
1:A:8:ASN:HB2	1:A:83:ILE:HD11	1.96	0.46
1:A:32:ILE:HG23	1:A:49:ILE:HG21	1.96	0.46
1:A:220:SER:HG	1:D:207:MET:HE2	1.80	0.46
1:A:270:TRP:O	1:A:271:ASN:CG	2.58	0.46
1:D:286:LYS:NZ	1:D:286:LYS:HB3	2.30	0.46
1:B:11:GLY:HA3	3:B:502:NAD:O5B	2.15	0.46
1:D:29:LEU:HD23	1:D:49:ILE:HD12	1.97	0.46
1:C:192:HIS:CE1	2:C:604:PO4:O4	2.67	0.46
1:C:91:ILE:CD1	1:C:94:LYS:HZ1	2.29	0.46
1:A:148:ARG:HD2	1:A:276:ILE:HG12	1.98	0.46
1:B:59:ILE:N	1:B:60:PRO:HD2	2.30	0.46
1:C:244:VAL:O	1:C:334:LYS:HE3	2.16	0.46
1:A:10:TYR:CD2	1:A:32:ILE:HG13	2.51	0.45
1:D:51:VAL:HG11	1:D:67:PHE:HE1	1.79	0.45
1:A:141:CYS:SG	2:A:601:PO4:O2	2.73	0.45
1:C:19:TYR:O	1:C:22:THR:HB	2.16	0.45
1:C:11:GLY:HA3	3:C:503:NAD:O5B	2.16	0.45
1:B:270:TRP:O	1:B:271:ASN:CG	2.60	0.45
1:C:64:LYS:HD3	1:C:64:LYS:C	2.42	0.45
1:B:30:ILE:O	1:B:50:PRO:HG2	2.15	0.45
1:C:56:GLU:HG3	1:C:57:GLU:N	2.31	0.45
1:B:20:ALA:O	1:B:24:GLN:HG2	2.16	0.45
1:C:9:GLY:O	1:C:14:GLY:HA3	2.16	0.45
1:C:249:LYS:H	1:C:281:GLU:CD	2.25	0.45
1:D:121:PHE:CD1	1:D:121:PHE:C	2.95	0.45
1:B:96:LYS:HB3	1:B:97:PRO:HD3	1.98	0.45
1:C:191:HIS:ND1	1:C:191:HIS:C	2.75	0.45
1:D:272:ASN:HA	1:D:297:HIS:CE1	2.51	0.45
1:D:5:VAL:HG21	1:D:27:MET:CE	2.47	0.45
1:B:83:ILE:HG21	1:B:99:TYR:CD1	2.52	0.45
1:C:237:ILE:O	1:C:241:THR:CG2	2.65	0.44
1:C:275:GLU:H	1:C:275:GLU:CD	2.24	0.44
1:A:109:GLN:HB3	3:A:501:NAD:H1D	1.98	0.44
1:D:13:ILE:CD1	3:D:504:NAD:C3N	2.95	0.44
1:D:273:LEU:CD1	1:D:275:GLU:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:N	1:A:60:PRO:CD	2.80	0.44
1:A:215:LEU:HD13	1:D:180:ASN:ND2	2.33	0.44
1:C:4:LYS:HD3	1:C:30:ILE:HD11	2.00	0.44
1:C:142:ASN:HB2	2:C:604:PO4:O2	2.18	0.44
1:D:3:VAL:HG13	1:D:27:MET:HB3	1.97	0.44
1:D:332:ILE:O	1:D:333:LEU:HB2	2.18	0.44
1:A:271:ASN:HB3	4:A:654:HOH:O	2.17	0.44
1:A:327:ASN:ND2	1:A:334:LYS:HZ3	2.13	0.44
1:C:53:ALA:N	1:C:69:VAL:HG21	2.33	0.44
1:C:272:ASN:HA	1:C:297:HIS:CE1	2.53	0.44
1:C:310:ILE:HA	1:C:313:MET:CE	2.48	0.44
4:A:742:HOH:O	1:B:271:ASN:HB3	2.18	0.43
1:C:7:VAL:HG12	1:C:32:ILE:HG22	1.99	0.43
1:C:237:ILE:O	1:C:241:THR:HG22	2.19	0.43
1:A:190:SER:OG	1:A:192:HIS:HD2	2.01	0.43
3:A:501:NAD:C2B	4:A:749:HOH:O	2.65	0.43
1:B:167:ARG:NH1	1:B:170:ASP:OD2	2.49	0.43
1:C:242:THR:HA	1:C:334:LYS:O	2.18	0.43
1:D:266:LEU:HB3	1:D:268:ARG:HG2	2.00	0.43
1:A:146:LEU:O	1:A:150:LEU:HB2	2.18	0.43
1:C:4:LYS:HE3	1:C:4:LYS:HA	2.00	0.43
1:D:100:GLU:HG2	1:D:135:TYR:OH	2.19	0.43
1:D:65:GLU:HG3	1:D:66:GLY:N	2.33	0.43
1:A:31:GLY:HA2	1:A:50:PRO:HG2	2.01	0.43
1:D:34:LYS:HD3	1:D:41:ALA:HB2	2.00	0.43
1:D:333:LEU:O	4:D:691:HOH:O	2.21	0.43
1:B:192:HIS:CE1	2:B:603:PO4:O2	2.55	0.43
1:D:24:GLN:HB3	1:D:27:MET:CG	2.49	0.43
1:D:137:ARG:NH1	1:D:198:THR:HG21	2.34	0.43
3:D:504:NAD:O2B	4:D:696:HOH:O	2.21	0.43
1:A:332:ILE:HG22	1:A:334:LYS:HB3	2.01	0.42
1:C:249:LYS:N	1:C:281:GLU:OE1	2.52	0.42
1:D:59:ILE:CG2	1:D:63:GLU:OE2	2.67	0.42
1:A:31:GLY:CA	1:A:50:PRO:HG2	2.49	0.42
1:B:303:ILE:HD11	1:B:330:LEU:HD13	2.02	0.42
1:A:192:HIS:O	1:A:196:VAL:HG23	2.18	0.42
1:C:121:PHE:CD1	1:C:121:PHE:C	2.97	0.42
1:D:235:ILE:O	1:D:239:GLU:HG3	2.19	0.42
1:D:327:ASN:HA	1:D:332:ILE:HD12	2.01	0.42
1:D:120:SER:CB	1:D:198:THR:CG2	2.97	0.42
1:B:59:ILE:HD11	1:B:72:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:OD1	3:A:501:NAD:H2A	2.18	0.42
1:A:268:ARG:NH2	1:A:275:GLU:OE1	2.52	0.42
1:B:178:PRO:HB3	1:D:174:THR:HB	2.00	0.42
1:C:327:ASN:HA	1:C:332:ILE:HB	2.00	0.42
1:D:59:ILE:N	1:D:60:PRO:CD	2.80	0.42
1:D:141:CYS:SG	2:D:605:PO4:O2	2.75	0.42
1:A:231:LYS:O	1:A:235:ILE:HG23	2.20	0.42
1:D:268:ARG:NH2	1:D:275:GLU:OE1	2.51	0.42
1:C:229:LEU:HD21	1:C:234:VAL:HG22	2.00	0.42
1:D:27:MET:HE1	1:D:310:ILE:HD12	2.02	0.42
1:A:142:ASN:HD21	1:A:217:HIS:CD2	2.38	0.42
1:A:18:ALA:HB1	1:A:29:LEU:HD11	2.01	0.42
1:A:246:LEU:HD13	1:A:278:VAL:HB	2.01	0.42
1:B:101:LYS:N	1:B:101:LYS:CD	2.83	0.42
1:B:286:LYS:NZ	1:C:189:PRO:HD3	2.34	0.42
1:B:302:VAL:HG22	4:B:702:HOH:O	2.20	0.42
1:D:59:ILE:O	1:D:63:GLU:HG3	2.19	0.42
1:D:73:LEU:O	1:D:77:LEU:HG	2.20	0.42
1:A:334:LYS:OXT	1:A:334:LYS:CG	2.68	0.41
1:D:8:ASN:OD1	3:D:504:NAD:H2A	2.19	0.41
1:B:167:ARG:HD3	1:B:298:GLN:CD	2.45	0.41
1:A:58:PHE:C	1:A:60:PRO:HD2	2.45	0.41
1:C:164:MET:SD	1:C:219:HIS:CD2	3.13	0.41
1:D:58:PHE:C	1:D:60:PRO:HD2	2.44	0.41
1:A:33:THR:HA	1:A:52:TYR:O	2.20	0.41
1:A:250:GLU:HG3	4:A:715:HOH:O	2.19	0.41
1:C:52:TYR:HA	1:C:69:VAL:CG2	2.51	0.41
1:C:216:MET:HA	1:C:298:GLN:OE1	2.20	0.41
1:D:155:GLU:O	1:D:226:LYS:HD2	2.20	0.41
1:A:11:GLY:O	1:A:15:LYS:HG2	2.21	0.41
1:B:314:PHE:HB3	1:B:316:LEU:CD1	2.51	0.41
3:C:503:NAD:O2B	4:C:714:HOH:O	2.21	0.41
1:A:154:ARG:HD2	1:A:201:PRO:O	2.20	0.41
1:C:117:ALA:HB1	1:C:135:TYR:O	2.21	0.41
3:D:504:NAD:O2B	4:D:695:HOH:O	2.21	0.41
1:B:82:ILE:HG13	1:B:105:LYS:O	2.21	0.41
1:B:131:LEU:HA	1:B:312:ALA:O	2.21	0.41
1:B:166:ARG:HG3	1:B:166:ARG:H	1.69	0.41
1:B:207:MET:HE2	1:C:220:SER:HG	1.84	0.41
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.84	0.41
1:C:217:HIS:CD2	1:C:298:GLN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:SER:HA	1:D:137:ARG:CD	2.50	0.41
1:D:171:PRO:HD2	1:D:299:GLU:OE2	2.21	0.41
1:D:243:ARG:NH1	1:D:308:ASP:OD1	2.46	0.41
1:D:24:GLN:HB3	1:D:27:MET:HG2	2.02	0.41
1:D:217:HIS:HB2	1:D:296:VAL:HG13	2.00	0.41
1:A:271:ASN:HB3	4:A:742:HOH:O	2.20	0.40
1:A:327:ASN:CB	1:A:334:LYS:HZ3	2.34	0.40
1:A:59:ILE:O	1:A:63:GLU:HG3	2.21	0.40
1:B:298:GLN:O	3:B:502:NAD:H4N	2.21	0.40
1:B:285:ILE:HD13	1:B:290:LEU:HA	2.03	0.40
1:B:222:MET:HG3	1:B:291:PHE:CE2	2.56	0.40
1:C:141:CYS:HB3	3:C:503:NAD:C5N	2.50	0.40
1:D:119:VAL:O	1:D:136:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	332/334 (99%)	318 (96%)	14 (4%)	0	100	100
1	B	331/334 (99%)	319 (96%)	12 (4%)	0	100	100
1	C	331/334 (99%)	317 (96%)	14 (4%)	0	100	100
1	D	330/334 (99%)	316 (96%)	14 (4%)	0	100	100
All	All	1324/1336 (99%)	1270 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/282 (100%)	259 (92%)	23 (8%)	10	7
1	B	281/282 (100%)	265 (94%)	16 (6%)	18	15
1	C	281/282 (100%)	267 (95%)	14 (5%)	22	20
1	D	280/282 (99%)	260 (93%)	20 (7%)	13	10
All	All	1124/1128 (100%)	1051 (94%)	73 (6%)	15	12

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	3	VAL
1	A	12	THR
1	A	23	LYS
1	A	29	LEU
1	A	32	ILE
1	A	55	SER
1	A	115	ASP
1	A	146	LEU
1	A	150	LEU
1	A	155	GLU
1	A	160	VAL
1	A	167	ARG
1	A	215	LEU
1	A	225	LEU
1	A	226	LYS
1	A	235	ILE
1	A	268	ARG
1	A	273	LEU
1	A	286	LYS
1	A	333	LEU
1	A	334	LYS
1	B	51	VAL

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Mol	Chain	Res	Type
1	B	56	GLU
1	B	76	LEU
1	B	98	LEU
1	B	146	LEU
1	B	150	LEU
1	B	155	GLU
1	B	166	ARG
1	B	167	ARG
1	B	195	ASP
1	B	271	ASN
1	B	290	LEU
1	B	303	ILE
1	B	316	LEU
1	B	328	LYS
1	B	334	LYS
1	C	4	LYS
1	C	83	ILE
1	C	146	LEU
1	C	150	LEU
1	C	160	VAL
1	C	167	ARG
1	C	191	HIS
1	C	216	MET
1	C	241	THR
1	C	273	LEU
1	C	275	GLU
1	C	286	LYS
1	C	288	ASN
1	C	316	LEU
1	D	21	VAL
1	D	24	GLN
1	D	27	MET
1	D	51	VAL
1	D	101	LYS
1	D	137	ARG
1	D	146	LEU
1	D	166	ARG
1	D	188	VAL
1	D	195	ASP
1	D	198	THR
1	D	224	GLU
1	D	225	LEU

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Mol	Chain	Res	Type
1	D	254	ASP
1	D	271	ASN
1	D	273	LEU
1	D	286	LYS
1	D	290	LEU
1	D	301	ASP
1	D	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	109	GLN
1	A	142	ASN
1	A	192	HIS
1	A	267	HIS
1	A	284	ASN
1	A	294	GLN
1	A	306	ASN
1	A	327	ASN
1	B	109	GLN
1	B	192	HIS
1	B	203	ASN
1	B	267	HIS
1	B	284	ASN
1	B	306	ASN
1	C	74	ASN
1	C	192	HIS
1	D	109	GLN
1	D	267	HIS
1	D	306	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	502	-	46,48,48	1.71	8 (17%)	64,73,73	1.90	15 (23%)
2	PO4	A	601	-	4,4,4	2.03	3 (75%)	6,6,6	1.38	2 (33%)
2	PO4	C	604	-	4,4,4	2.02	3 (75%)	6,6,6	1.25	1 (16%)
3	NAD	C	503	-	46,48,48	1.57	5 (10%)	64,73,73	2.11	10 (15%)
3	NAD	A	501	-	46,48,48	1.73	7 (15%)	64,73,73	1.69	13 (20%)
2	PO4	D	605	-	4,4,4	2.04	3 (75%)	6,6,6	1.30	1 (16%)
2	PO4	A	602	-	4,4,4	2.01	3 (75%)	6,6,6	1.26	1 (16%)
3	NAD	D	504	-	46,48,48	2.85	18 (39%)	64,73,73	2.58	24 (37%)
2	PO4	B	603	-	4,4,4	2.00	3 (75%)	6,6,6	1.28	1 (16%)

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	D	504	-	-	13/30/62/62	0/5/5/5
3	NAD	A	501	-	-	12/30/62/62	0/5/5/5
3	NAD	C	503	-	-	6/30/62/62	0/5/5/5
3	NAD	B	502	-	-	5/30/62/62	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504	NAD	PA-O3	-9.51	1.49	1.59
3	C	503	NAD	O7N-C7N	6.67	1.36	1.24
3	B	502	NAD	O7N-C7N	6.62	1.36	1.24
3	A	501	NAD	O7N-C7N	6.61	1.36	1.24
3	D	504	NAD	O7N-C7N	6.56	1.36	1.24
3	B	502	NAD	C2N-N1N	5.35	1.40	1.35
3	D	504	NAD	C2N-N1N	5.31	1.40	1.35
3	D	504	NAD	C5A-N7A	-5.03	1.29	1.39
3	A	501	NAD	C2N-N1N	4.99	1.40	1.35
3	D	504	NAD	C4A-N9A	-4.97	1.27	1.37
3	D	504	NAD	C8A-N9A	-4.60	1.29	1.37
3	D	504	NAD	C5A-C4A	-4.55	1.31	1.39
3	C	503	NAD	C2N-N1N	4.21	1.39	1.35
3	D	504	NAD	C2A-N1A	-3.62	1.27	1.33
3	A	501	NAD	C5A-N7A	-3.52	1.32	1.39
3	D	504	NAD	O5B-C5B	-3.48	1.31	1.44
3	D	504	NAD	PA-O5B	-3.30	1.46	1.59
3	C	503	NAD	C5A-N7A	-3.22	1.33	1.39
3	A	501	NAD	C4A-N9A	-3.21	1.31	1.37
3	D	504	NAD	O4D-C1D	3.18	1.45	1.40
3	A	501	NAD	C8A-N9A	-3.16	1.32	1.37
3	B	502	NAD	C5A-N7A	-3.07	1.33	1.39
3	D	504	NAD	PA-O1A	-2.96	1.40	1.50
3	D	504	NAD	O4B-C4B	-2.90	1.38	1.45
3	B	502	NAD	C8A-N9A	-2.88	1.32	1.37
3	D	504	NAD	C5A-C6A	-2.86	1.33	1.41
3	B	502	NAD	O4D-C1D	2.80	1.44	1.40
3	A	501	NAD	O4D-C1D	2.78	1.44	1.40
3	C	503	NAD	C4A-N9A	-2.77	1.31	1.37
3	B	502	NAD	C4A-N9A	-2.66	1.32	1.37
3	D	504	NAD	C5B-C4B	-2.60	1.43	1.51
3	D	504	NAD	C6N-N1N	2.48	1.41	1.35
3	B	502	NAD	C6N-N1N	2.39	1.40	1.35
2	D	605	PO4	P-O2	2.38	1.61	1.54
2	A	601	PO4	P-O3	2.36	1.61	1.54
2	A	602	PO4	P-O3	2.34	1.61	1.54
2	D	605	PO4	P-O3	2.33	1.61	1.54
2	C	604	PO4	P-O2	2.33	1.61	1.54
2	A	601	PO4	P-O2	2.33	1.61	1.54
2	A	602	PO4	P-O2	2.33	1.61	1.54
2	C	604	PO4	P-O3	2.33	1.61	1.54
3	D	504	NAD	C6A-N6A	-2.32	1.28	1.34
2	B	603	PO4	P-O2	2.31	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	PO4	P-O3	2.30	1.61	1.54
3	A	501	NAD	C6N-N1N	2.28	1.40	1.35
3	D	504	NAD	C3B-C4B	-2.28	1.47	1.53
2	D	605	PO4	P-O4	-2.14	1.48	1.54
2	A	601	PO4	P-O4	-2.13	1.48	1.54
2	C	604	PO4	P-O4	-2.12	1.48	1.54
2	B	603	PO4	P-O4	-2.12	1.48	1.54
3	B	502	NAD	PN-O3	2.11	1.61	1.59
2	A	602	PO4	P-O4	-2.09	1.48	1.54
3	C	503	NAD	C8A-N9A	-2.00	1.34	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	504	NAD	O4B-C1B-C2B	-7.99	89.52	106.62
3	C	503	NAD	C1B-N9A-C8A	7.83	144.47	127.09
3	C	503	NAD	C4A-N9A-C1B	-7.27	109.64	126.63
3	D	504	NAD	O4B-C1B-N9A	-7.11	94.44	108.09
3	D	504	NAD	C5A-C4A-N9A	7.04	113.49	105.81
3	C	503	NAD	N3A-C2A-N1A	-6.04	119.44	128.58
3	B	502	NAD	N3A-C2A-N1A	-5.48	120.28	128.58
3	D	504	NAD	C5A-C4A-N3A	-5.18	119.58	126.72
3	D	504	NAD	C4A-C5A-N7A	-5.17	104.67	110.58
3	A	501	NAD	N3A-C2A-N1A	-4.96	121.07	128.58
3	D	504	NAD	O4B-C4B-C5B	4.85	124.86	109.33
3	B	502	NAD	C5A-C4A-N3A	-4.69	120.26	126.72
3	B	502	NAD	C4A-N9A-C8A	4.68	110.66	105.74
3	C	503	NAD	C2A-N1A-C6A	4.50	126.12	118.73
3	C	503	NAD	C4D-O4D-C1D	-4.45	105.85	109.92
3	C	503	NAD	O4D-C4D-C5D	-4.43	95.14	109.33
3	B	502	NAD	N9A-C8A-N7A	-4.34	107.77	113.94
3	A	501	NAD	C4A-N9A-C1B	-4.25	116.69	126.63
3	D	504	NAD	O2A-PA-O5B	-4.21	88.47	107.57
3	B	502	NAD	N3A-C4A-N9A	4.14	134.22	127.17
3	A	501	NAD	C4A-N9A-C8A	4.12	110.06	105.74
3	B	502	NAD	C2A-N3A-C4A	4.06	121.75	111.83
3	B	502	NAD	C4B-O4B-C1B	-3.72	101.25	109.47
3	A	501	NAD	N9A-C8A-N7A	-3.61	108.81	113.94
3	D	504	NAD	C6A-C5A-C4A	3.58	122.07	117.18
3	B	502	NAD	C2B-C1B-N9A	-3.56	104.46	113.30
3	A	501	NAD	C4B-O4B-C1B	-3.41	101.94	109.47
3	D	504	NAD	O7N-C7N-C3N	3.32	123.66	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	504	NAD	O2B-C2B-C1B	3.16	120.98	110.10
3	B	502	NAD	C5A-N7A-C8A	3.09	108.31	103.45
3	D	504	NAD	O3B-C3B-C4B	3.03	119.78	111.08
3	D	504	NAD	C3N-C7N-N7N	-2.92	114.14	117.74
3	A	501	NAD	O4B-C1B-N9A	-2.78	102.76	108.09
3	D	504	NAD	N9A-C8A-N7A	-2.77	110.01	113.94
3	C	503	NAD	C3B-C2B-C1B	-2.76	96.25	101.46
3	A	501	NAD	C1B-N9A-C8A	2.75	133.21	127.09
3	D	504	NAD	O3-PA-O1A	2.73	118.91	110.70
3	D	504	NAD	C4N-C3N-C7N	-2.64	113.86	121.06
3	A	501	NAD	C2A-N3A-C4A	2.58	118.12	111.83
3	A	501	NAD	C4D-O4D-C1D	-2.55	107.59	109.92
3	D	504	NAD	C5A-N7A-C8A	2.54	107.44	103.45
3	D	504	NAD	C6N-N1N-C2N	-2.51	119.74	121.88
3	D	504	NAD	O2B-C2B-C3B	-2.50	103.81	111.82
3	B	502	NAD	C4A-C5A-N7A	-2.49	107.73	110.58
3	C	503	NAD	C5A-C4A-N9A	2.44	108.47	105.81
2	A	601	PO4	O4-P-O1	2.41	119.49	110.95
3	C	503	NAD	C6A-C5A-N7A	2.40	136.71	132.09
3	D	504	NAD	C1B-N9A-C8A	2.35	132.30	127.09
2	B	603	PO4	O4-P-O1	2.33	119.18	110.95
2	D	605	PO4	O4-P-O1	2.32	119.14	110.95
3	B	502	NAD	C4A-N9A-C1B	-2.31	121.23	126.63
2	C	604	PO4	O4-P-O1	2.26	118.94	110.95
3	A	501	NAD	C3B-C2B-C1B	-2.24	97.22	101.46
3	A	501	NAD	C2A-N1A-C6A	2.24	122.41	118.73
2	A	602	PO4	O4-P-O1	2.22	118.82	110.95
3	B	502	NAD	O7N-C7N-C3N	2.22	122.31	119.60
3	A	501	NAD	C5A-N7A-C8A	2.17	106.86	103.45
3	D	504	NAD	N6A-C6A-N1A	2.12	123.10	118.38
3	D	504	NAD	C2N-C3N-C7N	2.11	125.55	119.46
3	A	501	NAD	C2B-C3B-C4B	2.10	106.67	102.61
3	D	504	NAD	C4A-N9A-C1B	-2.10	121.73	126.63
3	B	502	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
3	B	502	NAD	O4B-C4B-C5B	-2.09	102.65	109.33
3	D	504	NAD	C2A-N3A-C4A	2.06	116.87	111.83
2	A	601	PO4	O3-P-O2	-2.05	101.55	107.91
3	C	503	NAD	O7N-C7N-C3N	2.02	122.07	119.60
3	D	504	NAD	C2N-C3N-C4N	2.00	120.59	118.26
3	B	502	NAD	O4B-C4B-C3B	2.00	109.12	105.15

There are no chirality outliers.

All (36) torsion outliers are listed below:

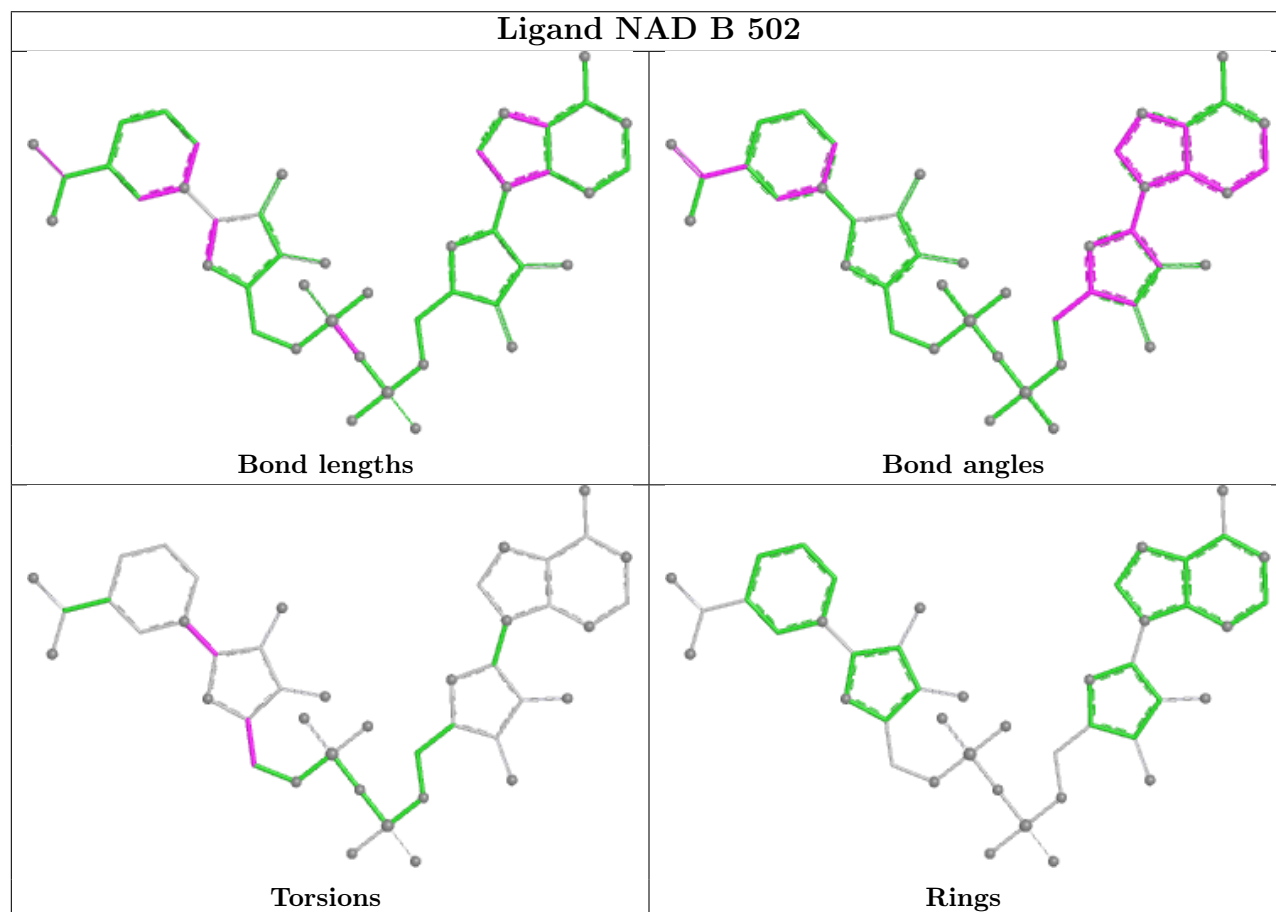
Mol	Chain	Res	Type	Atoms
3	A	501	NAD	C5B-O5B-PA-O2A
3	A	501	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C6N
3	B	502	NAD	C2D-C1D-N1N-C2N
3	B	502	NAD	C2D-C1D-N1N-C6N
3	C	503	NAD	O4D-C1D-N1N-C2N
3	D	504	NAD	C5B-O5B-PA-O2A
3	D	504	NAD	C5B-O5B-PA-O3
3	D	504	NAD	C2B-C1B-N9A-C8A
3	D	504	NAD	O4D-C1D-N1N-C2N
3	A	501	NAD	O4B-C4B-C5B-O5B
3	D	504	NAD	O4B-C4B-C5B-O5B
3	D	504	NAD	C3B-C4B-C5B-O5B
3	A	501	NAD	O4D-C4D-C5D-O5D
3	D	504	NAD	O4D-C4D-C5D-O5D
3	A	501	NAD	C3B-C4B-C5B-O5B
3	C	503	NAD	C2B-C1B-N9A-C8A
3	C	503	NAD	O4D-C4D-C5D-O5D
3	A	501	NAD	C5B-O5B-PA-O1A
3	A	501	NAD	C5B-O5B-PA-O3
3	A	501	NAD	C5D-O5D-PN-O1N
3	D	504	NAD	C5B-O5B-PA-O1A
3	D	504	NAD	C5D-O5D-PN-O1N
3	C	503	NAD	C2B-C1B-N9A-C4A
3	A	501	NAD	O4D-C1D-N1N-C6N
3	B	502	NAD	O4D-C4D-C5D-O5D
3	C	503	NAD	O4D-C1D-N1N-C6N
3	D	504	NAD	O4D-C1D-N1N-C6N
3	C	503	NAD	O4B-C1B-N9A-C8A
3	A	501	NAD	PN-O3-PA-O2A
3	A	501	NAD	C2B-C1B-N9A-C8A
3	D	504	NAD	C2B-C1B-N9A-C4A
3	A	501	NAD	C3D-C4D-C5D-O5D
3	D	504	NAD	C3D-C4D-C5D-O5D
3	D	504	NAD	PN-O3-PA-O2A

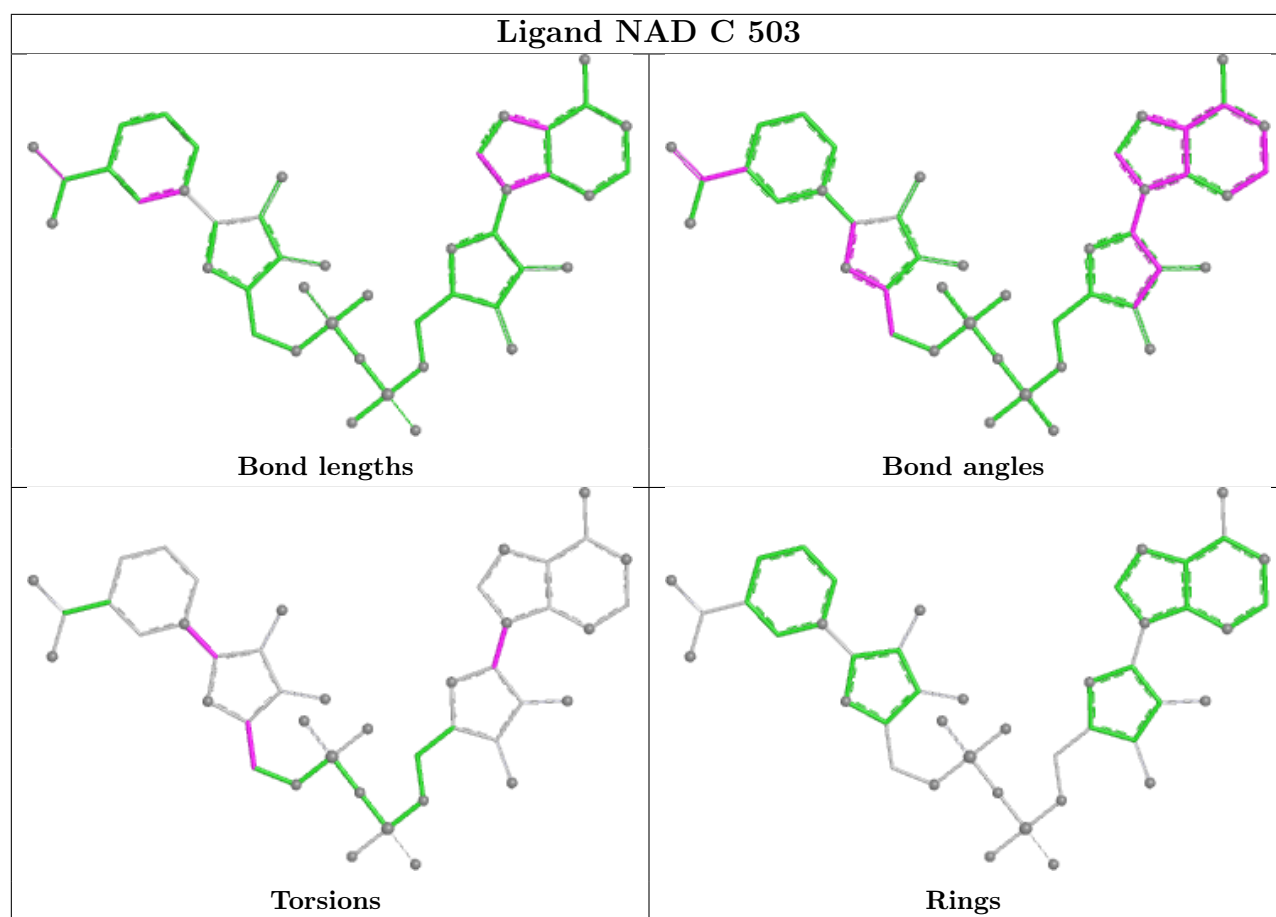
There are no ring outliers.

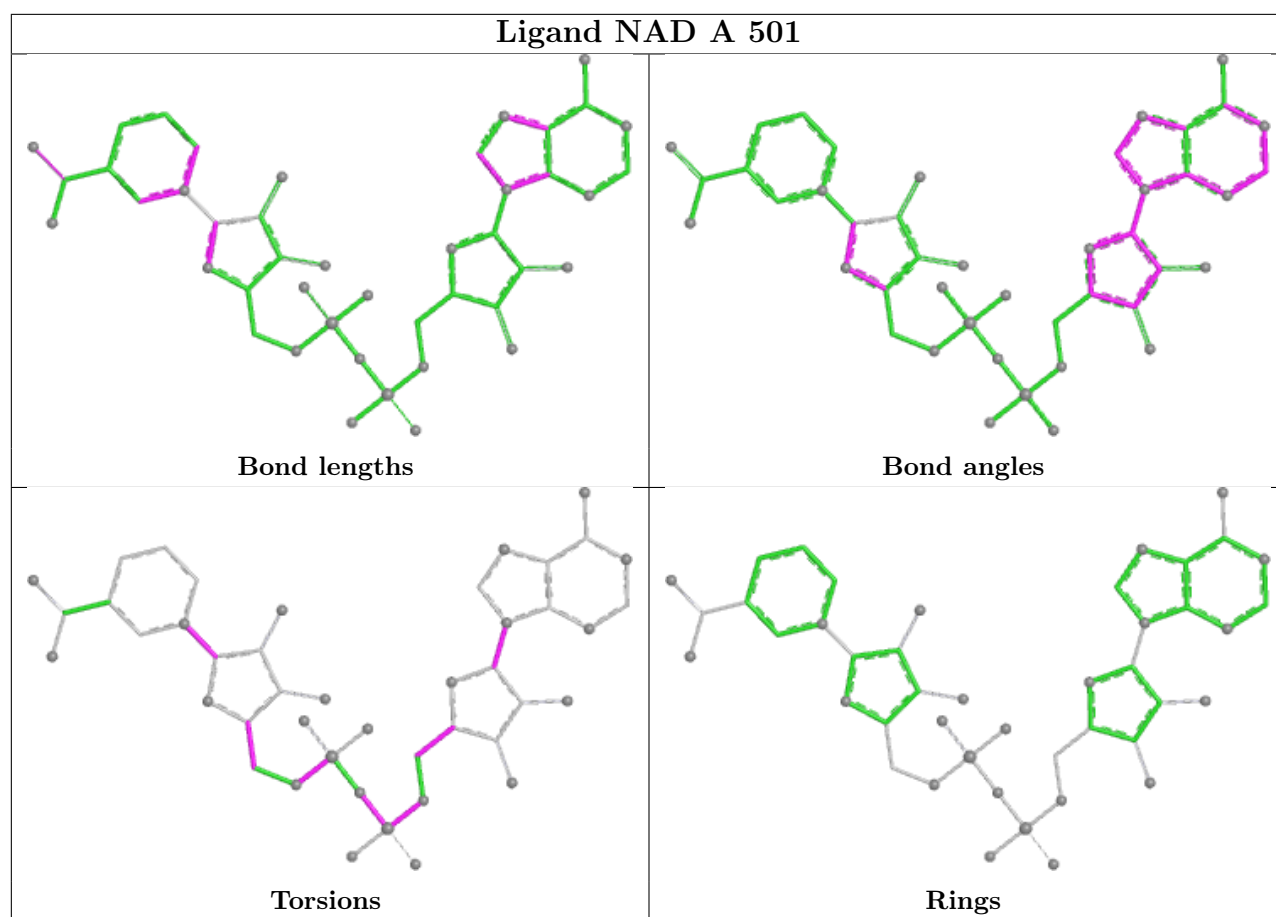
8 monomers are involved in 38 short contacts:

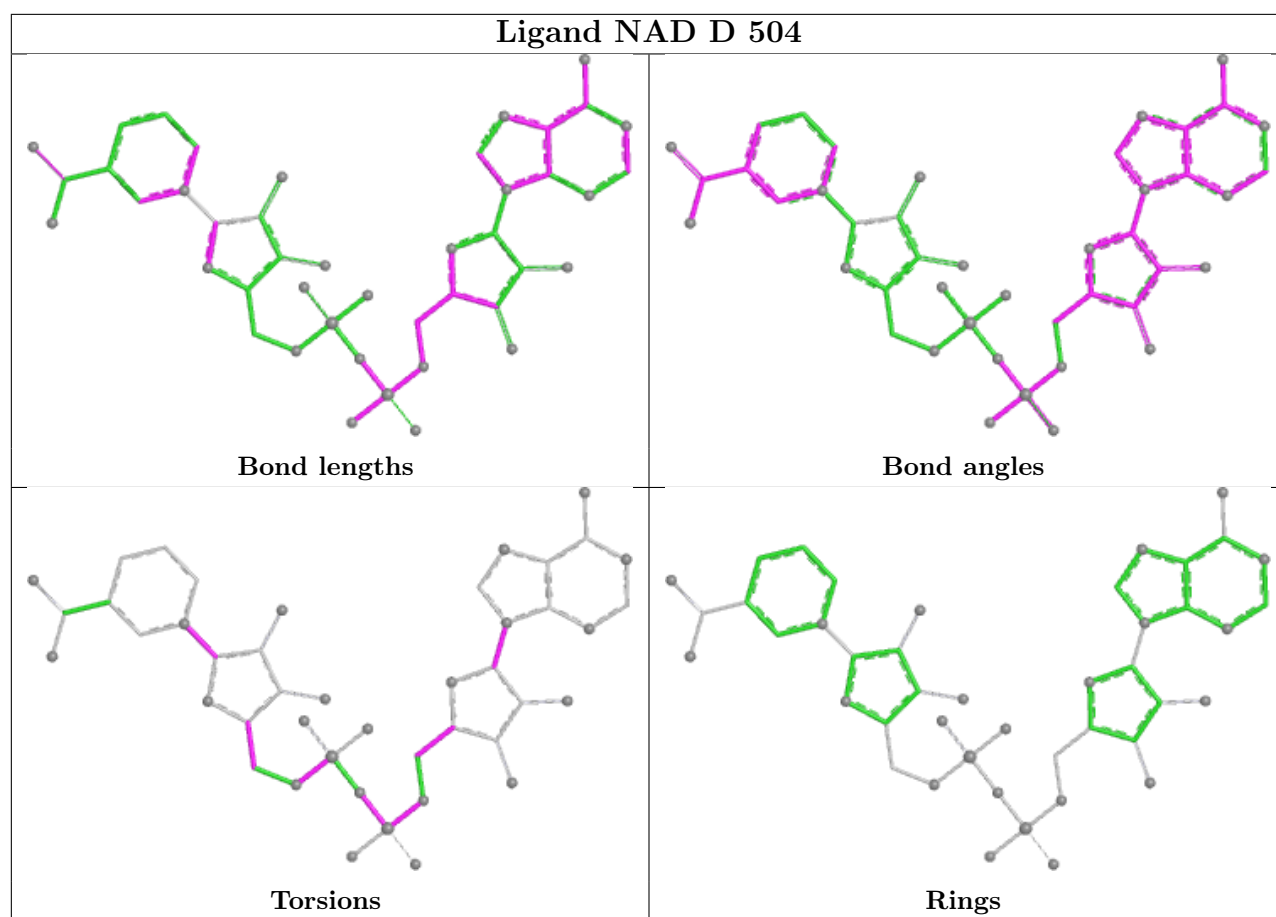
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	NAD	3	0
2	A	601	PO4	3	0
2	C	604	PO4	6	0
3	C	503	NAD	6	0
3	A	501	NAD	6	0
2	D	605	PO4	5	0
3	D	504	NAD	5	0
2	B	603	PO4	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.06	4 (1%) 76 76	16, 25, 39, 52	0
1	B	333/334 (99%)	-0.02	7 (2%) 63 63	14, 25, 43, 52	0
1	C	333/334 (99%)	0.19	9 (2%) 56 55	16, 29, 46, 59	0
1	D	332/334 (99%)	0.35	11 (3%) 49 48	16, 31, 47, 57	0
All	All	1332/1336 (99%)	0.12	31 (2%) 61 60	14, 28, 44, 59	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	LYS	5.1
1	D	333	LEU	4.3
1	D	63	GLU	3.6
1	A	189	PRO	3.6
1	D	66	GLY	3.4
1	C	56	GLU	3.2
1	D	189	PRO	3.2
1	B	334	LYS	3.1
1	B	333	LEU	3.1
1	C	189	PRO	3.0
1	B	115	ASP	3.0
1	D	101	LYS	3.0
1	C	333	LEU	3.0
1	A	333	LEU	2.9
1	C	332	ILE	2.8
1	C	188	VAL	2.6
1	D	332	ILE	2.5
1	B	189	PRO	2.5
1	C	288	ASN	2.5
1	B	101	LYS	2.4
1	B	188	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	2.3
1	D	83	ILE	2.2
1	D	158	ASP	2.1
1	C	66	GLY	2.1
1	D	202	ILE	2.1
1	B	190	SER	2.1
1	C	78	GLU	2.1
1	D	136	VAL	2.0
1	D	102	ALA	2.0
1	C	98	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

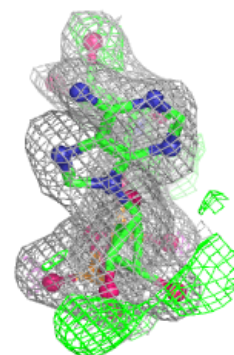
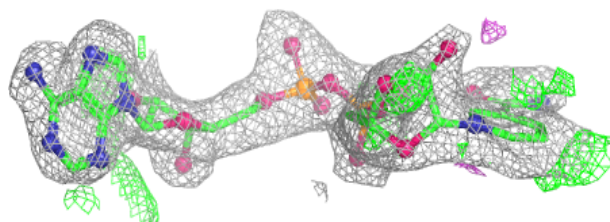
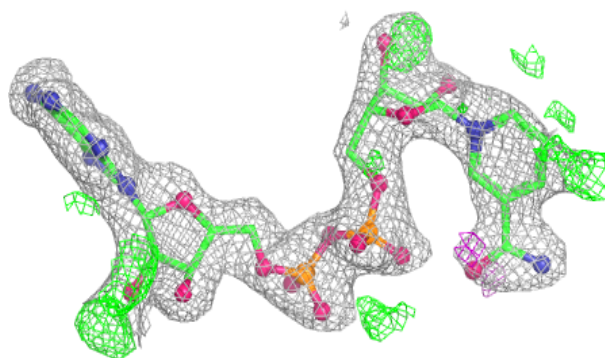
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	B	603	5/5	0.41	0.73	49,49,50,56	5
2	PO4	A	602	5/5	0.64	0.90	53,53,54,62	5
2	PO4	D	605	5/5	0.74	0.77	59,60,60,69	5
2	PO4	A	601	5/5	0.84	0.77	53,54,54,63	5
2	PO4	C	604	5/5	0.85	0.70	54,54,55,63	5
3	NAD	D	504	44/44	0.85	0.14	22,30,33,38	44
3	NAD	C	503	44/44	0.86	0.15	30,35,40,42	44
3	NAD	A	501	44/44	0.87	0.14	20,29,37,40	44
3	NAD	B	502	44/44	0.87	0.14	23,29,34,39	44

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

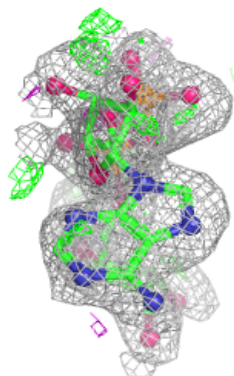
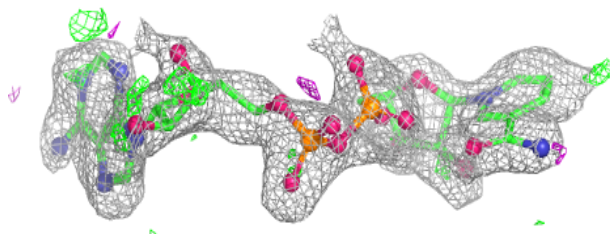
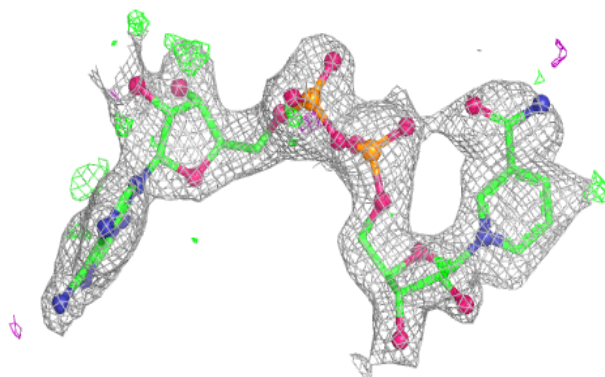
Electron density around NAD D 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



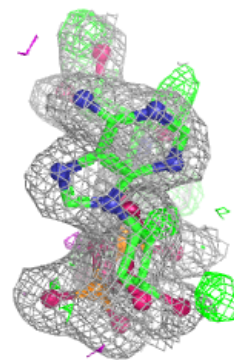
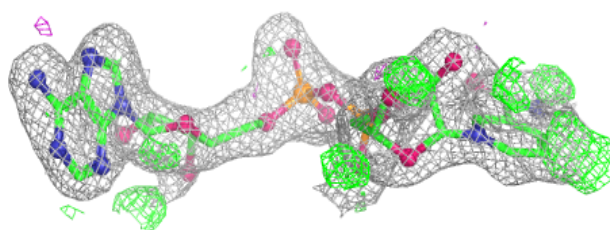
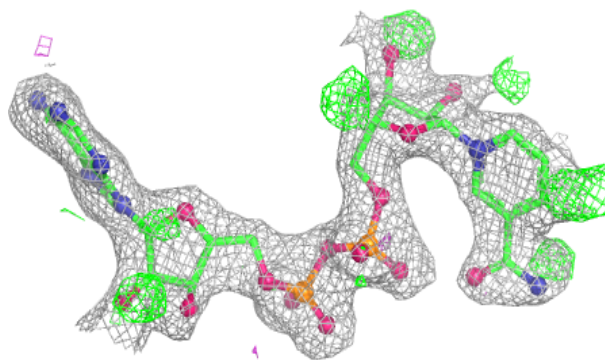
Electron density around NAD C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

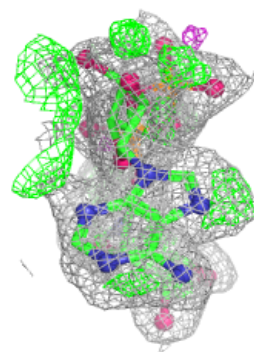
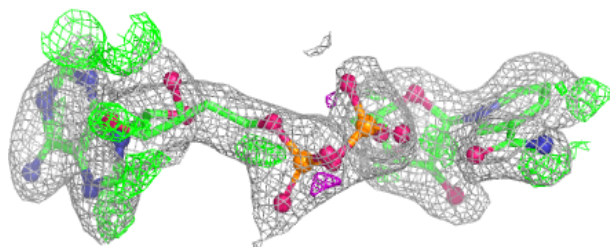
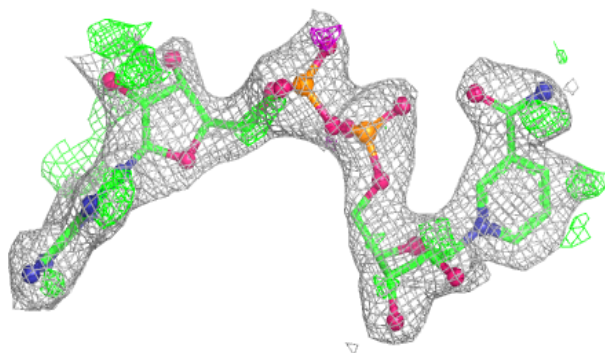


Electron density around NAD A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD B 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.