



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 1HLP / pdb_00001hlp
Title : STRUCTURAL FEATURES STABILIZING HALOPHILIC MALATE DEHYDROGENASE FROM AN ARCHAEABACTERIUM
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Deposited on : 1994-10-04
Resolution : 3.20 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

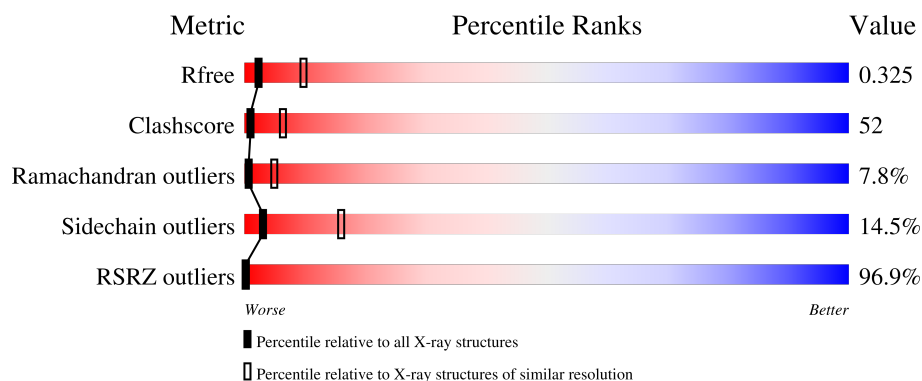
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	303	96% 33% 48% 17% .
1	B	303	98% 32% 50% 15% .

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	NAD	B	330	-	-	-	X

2 Entry composition [i](#)

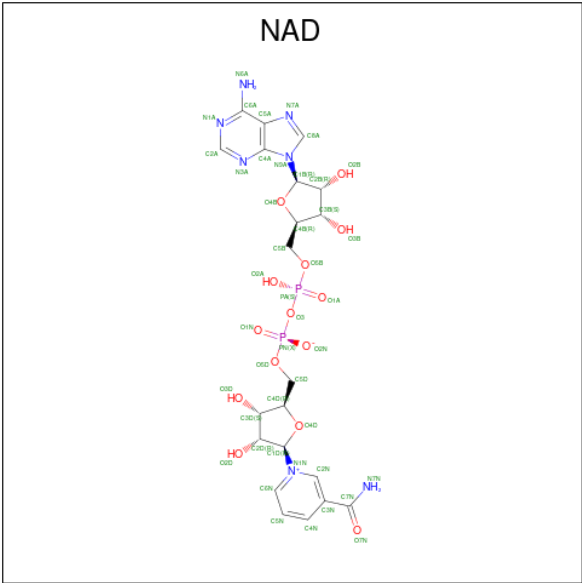
There are 2 unique types of molecules in this entry. The entry contains 4690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2301	1415	393	489	4			
1	B	303	Total	C	N	O	S	0	0	0
			2301	1415	393	489	4			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

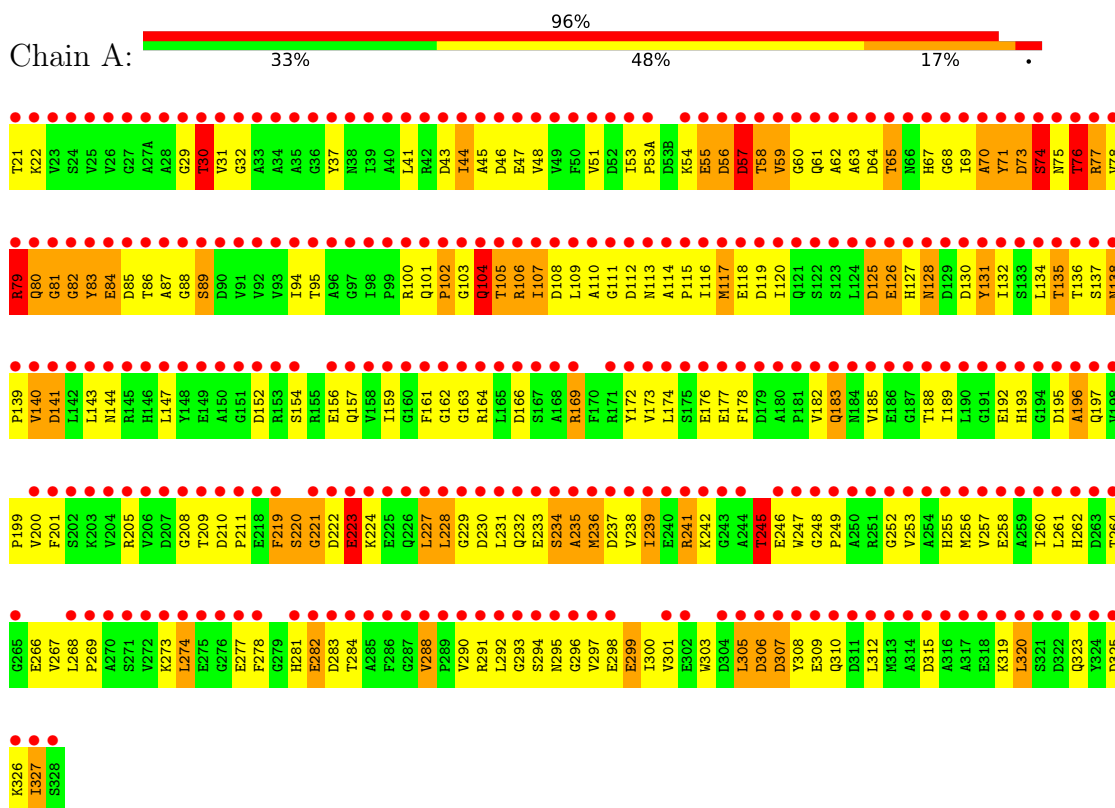


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

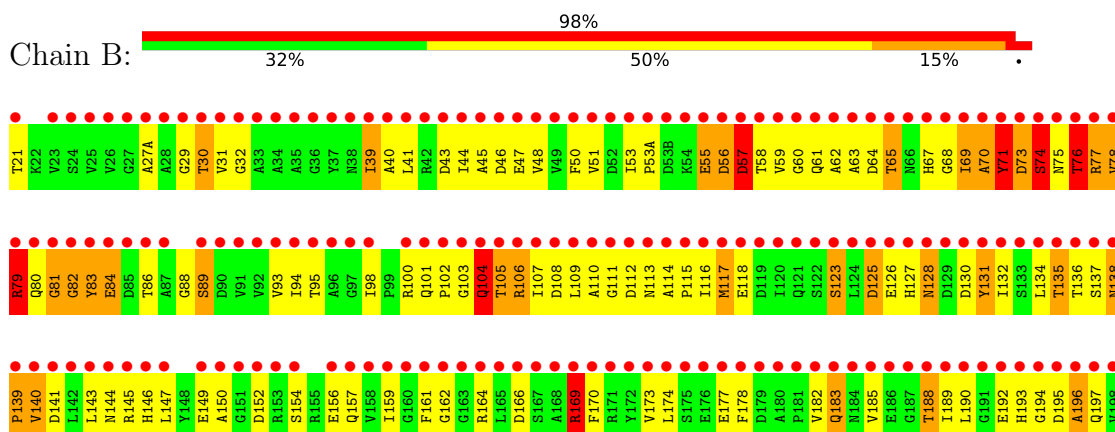
3 Residue-property plots

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: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



P199	G265	K326
V200	E266	I327
F201	V267	S328
S202	L268	
F203	P269	
V204	A270	
R205	S271	
V206	V272	
D207	K273	
G208	L274	
T209	E275	
D210	G276	
P211	E277	
E218	F278	
F219	G279	
S220	H281	
G221	E282	
D222	D283	
E223	T284	
K224	A285	
E225	F286	
G226	G287	
L227	V288	
L228	P289	
G229	V290	
D230	R291	
L231	L292	
Q232	G293	
E233	S294	
S234	N295	
A235	G296	
M236	V297	
D237	E298	
V238	E299	
T239	I300	
E240	V301	
R241	E302	
K242	V303	
G243	D304	
A244	L305	
T245	D306	
E246	D307	
W247	Y308	
G248	E309	
F249	Q310	
A250	D311	
R251	L312	
G252	M313	
V253	A314	
A254	D315	
H255	A316	
M256	A317	
V257	E318	
E258	K319	
A259	L320	
I260	S321	
L261	D322	
H262	Q323	
D263	Y324	
T264	D325	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.60Å 130.60Å 123.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 10.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	84.0 (10.00-3.20) 73.2 (10.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.83Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.280 0.315 , 0.325	Depositor DCC
R_{free} test set	3012 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	1.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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:
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	0.90	1/2338 (0.0%)	1.32	24/3175 (0.8%)
1	B	0.89	0/2338	1.32	23/3175 (0.7%)
All	All	0.90	1/4676 (0.0%)	1.32	47/6350 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	THR	CA-CB	6.01	1.61	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PHE	N-CA-C	-14.13	95.88	111.28
1	B	219	PHE	N-CA-C	-13.77	96.28	111.28
1	A	138	ASN	N-CA-C	12.40	130.15	113.77
1	A	57	ASP	N-CA-C	-12.04	96.71	111.40
1	B	57	ASP	N-CA-C	-11.38	98.85	111.14
1	B	83	TYR	N-CA-C	-10.51	99.62	111.71
1	B	138	ASN	N-CA-C	9.81	131.49	109.81
1	A	326	LYS	N-CA-C	-9.25	101.19	111.28
1	B	326	LYS	N-CA-C	-9.12	101.31	111.07
1	A	221	GLY	N-CA-C	-8.75	92.45	113.18
1	A	83	TYR	N-CA-C	-8.73	101.67	111.71
1	A	224	LYS	N-CA-C	-8.62	102.02	112.54
1	A	223	GLU	N-CA-C	8.57	129.05	110.80
1	B	74	SER	N-CA-C	8.09	128.03	110.80
1	A	74	SER	N-CA-C	8.01	127.87	110.80
1	A	222	ASP	N-CA-C	-7.97	97.67	109.15
1	B	221	GLY	N-CA-C	-7.70	94.92	113.18
1	A	237	ASP	N-CA-C	-7.65	102.94	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	LYS	N-CA-C	-7.55	103.33	112.54
1	B	139	PRO	N-CA-C	-7.42	105.30	114.20
1	B	223	GLU	N-CA-C	7.41	126.58	110.80
1	A	125	ASP	N-CA-C	-7.06	100.60	110.35
1	A	312	LEU	N-CA-C	-6.85	103.05	111.40
1	B	76	THR	N-CA-C	6.78	120.72	109.46
1	B	78	VAL	N-CA-C	6.52	116.41	108.06
1	A	76	THR	N-CA-C	6.30	119.92	109.46
1	B	237	ASP	N-CA-C	-6.28	104.49	111.71
1	A	245	THR	N-CA-C	-6.21	100.20	109.15
1	A	241	ARG	N-CA-C	6.14	117.98	111.28
1	B	40	ALA	N-CA-C	6.10	117.93	111.28
1	A	306	ASP	N-CA-C	-5.98	102.78	110.19
1	B	245	THR	N-CA-C	-5.84	99.62	108.67
1	B	117	MET	N-CA-C	-5.61	104.38	111.11
1	A	264	THR	N-CA-C	5.60	119.37	112.54
1	A	176	GLU	N-CA-C	-5.46	105.33	111.28
1	B	169	ARG	N-CA-C	-5.44	105.25	111.07
1	B	231	LEU	N-CA-C	5.41	119.42	111.04
1	A	117	MET	N-CA-C	-5.35	105.45	111.28
1	B	39	ILE	N-CA-C	-5.25	105.21	110.30
1	B	138	ASN	CA-C-N	-5.24	114.31	120.12
1	B	138	ASN	C-N-CA	-5.24	114.31	120.12
1	A	220	SER	N-CA-C	-5.22	99.69	110.80
1	A	325	ASP	N-CA-C	-5.11	107.11	113.55
1	B	125	ASP	N-CA-C	-5.09	101.85	109.79
1	A	288	VAL	N-CA-CB	-5.07	107.36	111.67
1	A	246	GLU	N-CA-C	5.05	118.87	111.34
1	B	312	LEU	N-CA-C	-5.01	105.73	111.14

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	2301	0	2165	233	0
1	B	2301	0	2165	261	0
2	A	44	0	26	10	0
2	B	44	0	26	12	0
All	All	4690	0	4382	474	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 52.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HB	1:B:77:ARG:HB2	1.50	0.94
1:B:291:ARG:HG2	1:B:298:GLU:HB2	1.51	0.92
1:A:249:PRO:O	1:A:253:VAL:HG23	1.70	0.92
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.32	0.90
1:A:62:ALA:H	1:A:79:ARG:HH12	1.19	0.90
1:A:29:GLY:HA3	2:A:330:NAD:O5B	1.73	0.89
1:B:29:GLY:HA3	2:B:330:NAD:O5B	1.73	0.88
1:B:79:ARG:HH11	1:B:79:ARG:HB3	1.39	0.87
1:B:32:GLY:HA2	1:B:95:THR:HG21	1.54	0.86
1:A:63:ALA:H	1:A:79:ARG:NH2	1.74	0.86
1:B:249:PRO:O	1:B:253:VAL:HG23	1.77	0.85
1:A:291:ARG:HG2	1:A:298:GLU:HB2	1.56	0.85
1:B:189:ILE:HD11	1:B:231:LEU:HD21	1.58	0.83
1:A:69:ILE:HG13	1:A:70:ALA:H	1.43	0.83
1:A:79:ARG:HD2	1:A:79:ARG:H	1.43	0.82
1:A:182:VAL:HG21	1:B:70:ALA:HB1	1.60	0.82
1:A:189:ILE:HD11	1:A:231:LEU:HD21	1.61	0.82
1:B:113:ASN:HA	1:B:116:ILE:HD12	1.60	0.82
1:A:48:VAL:HB	1:A:77:ARG:HB2	1.62	0.82
1:B:78:VAL:HG12	1:B:80:GLN:HG3	1.60	0.81
1:B:65:THR:HB	1:B:77:ARG:CZ	2.11	0.80
1:A:65:THR:HB	1:A:77:ARG:CZ	2.11	0.80
1:A:65:THR:HG23	1:B:247:TRP:CD1	2.17	0.80
1:A:114:ALA:HB3	1:A:115:PRO:HD3	1.63	0.79
1:A:177:GLU:HG2	1:A:227:LEU:HD11	1.62	0.79
1:A:62:ALA:HB3	1:A:79:ARG:NH1	1.98	0.79
1:B:136:THR:HB	2:B:330:NAD:H2N	1.63	0.78
1:B:290:VAL:HG21	1:B:297:VAL:HG22	1.66	0.78
1:B:183:GLN:HA	1:B:183:GLN:HE21	1.50	0.77
1:B:69:ILE:HG13	1:B:70:ALA:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ALA:H	1:B:79:ARG:NH2	1.83	0.76
1:B:43:ASP:HA	1:B:75:ASN:ND2	2.01	0.75
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.51	0.75
1:A:65:THR:HB	1:A:77:ARG:NH1	2.01	0.75
1:A:228:LEU:HG	1:A:232:GLN:OE1	1.86	0.74
1:A:43:ASP:HA	1:A:75:ASN:HD22	1.52	0.74
1:B:94:ILE:HB	1:B:135:THR:HB	1.70	0.73
1:B:62:ALA:HB3	1:B:79:ARG:NH1	2.03	0.73
1:B:62:ALA:H	1:B:79:ARG:HH12	1.34	0.73
1:A:77:ARG:HD2	1:A:77:ARG:O	1.89	0.73
1:A:169:ARG:HD2	1:A:236:MET:HE1	1.69	0.72
1:A:62:ALA:N	1:A:79:ARG:HH12	1.86	0.72
1:B:21:THR:OG1	1:B:45:ALA:HA	1.89	0.72
1:A:242:LYS:HE2	1:B:64:ASP:OD2	1.89	0.72
1:A:319:LYS:HG2	1:A:323:GLN:OE1	1.89	0.71
1:A:247:TRP:CD1	1:B:65:THR:HG23	2.25	0.71
1:B:59:VAL:HA	1:B:79:ARG:HG3	1.72	0.70
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.05	0.70
1:B:136:THR:O	2:B:330:NAD:H2N	1.91	0.70
1:B:177:GLU:HG2	1:B:227:LEU:HD11	1.72	0.70
1:B:78:VAL:CG1	1:B:80:GLN:HG3	2.22	0.70
1:A:238:VAL:HG13	1:A:239:ILE:HG12	1.73	0.70
1:B:77:ARG:HD2	1:B:77:ARG:O	1.91	0.70
1:B:65:THR:HB	1:B:77:ARG:NH1	2.06	0.69
1:B:192:GLU:HG3	1:B:320:LEU:HD11	1.73	0.69
1:B:138:ASN:C	1:B:140:VAL:H	2.00	0.69
1:B:273:LYS:HD2	1:B:284:THR:O	1.91	0.69
1:A:56:ASP:OD1	1:B:241:ARG:HD2	1.92	0.69
1:A:59:VAL:HA	1:A:79:ARG:HG3	1.75	0.68
1:A:169:ARG:HD3	1:B:67:HIS:ND1	2.08	0.68
1:A:136:THR:O	2:A:330:NAD:H2N	1.94	0.68
1:A:256:MET:HG2	1:A:268:LEU:HD13	1.76	0.68
1:B:128:ASN:N	1:B:128:ASN:HD22	1.92	0.68
1:A:136:THR:HB	2:A:330:NAD:H2N	1.76	0.67
1:A:32:GLY:HA2	1:A:95:THR:HG21	1.76	0.67
1:A:234:SER:C	1:A:236:MET:H	2.01	0.67
1:A:257:VAL:HA	1:A:260:ILE:HD12	1.76	0.67
1:B:257:VAL:HA	1:B:260:ILE:HD12	1.77	0.67
1:B:236:MET:O	1:B:239:ILE:HG13	1.95	0.67
1:B:199:PRO:HG3	1:B:228:LEU:HD11	1.77	0.66
1:A:69:ILE:HG13	1:A:70:ALA:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASP:O	1:A:115:PRO:HD2	1.95	0.66
1:B:189:ILE:CD1	1:B:231:LEU:HD21	2.24	0.66
1:B:231:LEU:O	1:B:236:MET:HE3	1.95	0.66
1:A:138:ASN:C	1:A:140:VAL:H	2.02	0.65
1:B:69:ILE:HB	1:B:74:SER:OG	1.97	0.65
1:A:62:ALA:H	1:A:79:ARG:NH1	1.93	0.65
1:B:238:VAL:HG13	1:B:239:ILE:HG12	1.78	0.65
1:B:115:PRO:O	1:B:118:GLU:HB2	1.97	0.64
1:B:166:ASP:OD2	1:B:193:HIS:HD2	1.80	0.64
1:A:54:LYS:O	1:A:56:ASP:N	2.31	0.64
1:A:113:ASN:HA	1:A:116:ILE:HD12	1.80	0.64
1:A:59:VAL:HG13	1:A:79:ARG:HG3	1.80	0.63
1:B:268:LEU:O	1:B:290:VAL:HG12	1.97	0.63
1:B:306:ASP:O	1:B:310:GLN:HG3	1.98	0.63
1:A:104:GLN:O	1:A:108:ASP:HB2	1.97	0.63
1:A:268:LEU:HD12	1:A:292:LEU:HD12	1.79	0.63
1:B:31:VAL:HG12	2:B:330:NAD:PN	2.38	0.63
1:B:79:ARG:H	1:B:79:ARG:HD2	1.64	0.63
1:B:319:LYS:HG2	1:B:323:GLN:OE1	1.98	0.63
1:A:138:ASN:O	1:A:140:VAL:HG12	1.99	0.63
1:A:241:ARG:HD2	1:B:56:ASP:OD1	1.99	0.63
1:B:59:VAL:HG12	1:B:59:VAL:O	1.99	0.62
1:B:268:LEU:HD12	1:B:292:LEU:HD12	1.81	0.62
1:B:112:ASP:O	1:B:115:PRO:HD2	2.00	0.62
1:A:138:ASN:C	1:A:140:VAL:N	2.58	0.62
1:B:62:ALA:N	1:B:79:ARG:HH12	1.97	0.62
1:B:233:GLU:O	1:B:235:ALA:N	2.33	0.62
1:A:59:VAL:HG12	1:A:59:VAL:O	1.99	0.61
1:A:51:VAL:HG21	1:A:86:THR:CG2	2.29	0.61
1:B:43:ASP:HA	1:B:75:ASN:HD22	1.65	0.61
1:B:65:THR:HB	1:B:77:ARG:NH2	2.15	0.61
1:B:219:PHE:O	1:B:221:GLY:N	2.34	0.61
1:B:69:ILE:HG13	1:B:70:ALA:N	2.15	0.61
1:B:88:GLY:H	1:B:128:ASN:HB3	1.64	0.61
1:B:266:GLU:O	1:B:291:ARG:HA	2.00	0.61
1:B:78:VAL:HB	1:B:80:GLN:HE21	1.65	0.60
1:B:105:THR:O	1:B:107:ILE:N	2.33	0.60
1:B:197:GLN:HE22	1:B:232:GLN:HG3	1.65	0.60
1:A:79:ARG:C	1:A:81:GLY:H	2.09	0.60
1:B:51:VAL:HG21	1:B:86:THR:CG2	2.32	0.60
1:A:43:ASP:HA	1:A:75:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ALA:HB3	1:B:115:PRO:HD3	1.84	0.59
1:A:273:LYS:HD2	1:A:284:THR:O	2.02	0.59
1:B:138:ASN:C	1:B:140:VAL:N	2.59	0.59
1:B:107:ILE:HG22	1:B:327:ILE:CD1	2.33	0.59
1:A:21:THR:OG1	1:A:45:ALA:HA	2.03	0.59
1:A:62:ALA:CB	1:A:79:ARG:NH1	2.65	0.59
1:B:104:GLN:HG3	1:B:109:LEU:HB2	1.83	0.59
1:A:21:THR:O	1:A:46:ASP:HB2	2.02	0.59
1:A:209:THR:O	1:A:211:PRO:HD3	2.03	0.59
1:B:136:THR:HB	2:B:330:NAD:C2N	2.33	0.59
1:B:267:VAL:HA	1:B:290:VAL:O	2.02	0.59
1:A:47:GLU:HA	1:A:76:THR:O	2.03	0.59
1:B:107:ILE:O	1:B:110:ALA:HB3	2.01	0.59
1:B:125:ASP:O	1:B:126:GLU:HG2	2.03	0.59
1:A:189:ILE:CD1	1:A:231:LEU:HD21	2.33	0.58
1:B:140:VAL:HG21	1:B:161:PHE:O	2.03	0.58
1:B:139:PRO:HD2	1:B:143:LEU:HD21	1.83	0.58
1:B:235:ALA:C	1:B:236:MET:HE2	2.29	0.58
1:A:51:VAL:HG22	1:A:81:GLY:O	2.03	0.58
1:B:27(A):ALA:CB	1:B:50:PHE:HB3	2.34	0.58
1:B:128:ASN:N	1:B:128:ASN:ND2	2.52	0.58
1:B:228:LEU:HG	1:B:232:GLN:OE1	2.04	0.58
1:B:211:PRO:HB3	1:B:219:PHE:CE2	2.39	0.57
1:B:230:ASP:HA	1:B:234:SER:HB2	1.85	0.57
1:A:94:ILE:HB	1:A:135:THR:HB	1.85	0.57
1:B:107:ILE:HG22	1:B:327:ILE:HD11	1.87	0.57
1:B:58:THR:O	1:B:79:ARG:NH1	2.38	0.57
1:B:59:VAL:C	1:B:79:ARG:CZ	2.78	0.57
1:A:273:LYS:HE3	1:A:283:ASP:HA	1.87	0.56
1:A:58:THR:O	1:A:79:ARG:NH1	2.39	0.56
1:A:69:ILE:HD12	1:A:74:SER:HB2	1.86	0.56
1:A:268:LEU:O	1:A:290:VAL:HG12	2.05	0.56
1:B:47:GLU:HA	1:B:76:THR:O	2.06	0.56
1:A:30:THR:HG23	2:A:330:NAD:O1N	2.04	0.56
1:A:306:ASP:O	1:A:310:GLN:HG3	2.05	0.56
1:B:59:VAL:HA	1:B:79:ARG:CG	2.36	0.56
1:B:182:VAL:O	1:B:182:VAL:HG22	2.05	0.56
1:B:293:GLY:O	1:B:295:ASN:N	2.39	0.56
1:B:305:LEU:HD12	1:B:305:LEU:H	1.71	0.56
1:A:117:MET:HB3	1:A:147:LEU:HG	1.87	0.56
1:B:62:ALA:H	1:B:79:ARG:NH1	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:MET:HG2	1:B:268:LEU:HD13	1.88	0.56
1:A:107:ILE:CG2	1:A:327:ILE:HD13	2.35	0.56
1:B:113:ASN:HA	1:B:116:ILE:CD1	2.33	0.55
1:B:78:VAL:HB	1:B:80:GLN:NE2	2.21	0.55
1:A:107:ILE:HG22	1:A:327:ILE:HD13	1.88	0.55
1:B:132:ILE:HD12	1:B:132:ILE:H	1.71	0.55
1:A:233:GLU:O	1:A:235:ALA:N	2.40	0.55
1:A:301:VAL:HG12	1:A:303:TRP:CD1	2.41	0.55
1:A:62:ALA:HA	1:A:65:THR:OG1	2.07	0.55
1:A:65:THR:HB	1:A:77:ARG:NH2	2.21	0.55
1:A:69:ILE:HB	1:A:74:SER:OG	2.07	0.55
1:A:162:GLY:HA2	2:A:330:NAD:O7N	2.07	0.54
1:B:166:ASP:O	1:B:169:ARG:HB2	2.08	0.54
1:B:278:PHE:HE2	1:B:305:LEU:HD11	1.72	0.54
1:A:78:VAL:HB	1:A:80:GLN:HE21	1.72	0.54
1:B:80:GLN:O	1:B:81:GLY:C	2.50	0.54
1:B:201:PHE:CZ	1:B:228:LEU:HD13	2.42	0.54
1:A:37:TYR:HB2	1:A:65:THR:CG2	2.38	0.54
1:A:65:THR:CB	1:A:77:ARG:NH1	2.69	0.54
1:A:107:ILE:HG22	1:A:327:ILE:CD1	2.37	0.54
1:B:77:ARG:O	1:B:78:VAL:HG23	2.07	0.54
1:A:298:GLU:O	1:A:299:GLU:HB3	2.07	0.54
1:B:62:ALA:HA	1:B:65:THR:OG1	2.07	0.54
1:B:138:ASN:O	1:B:140:VAL:HG12	2.06	0.54
1:A:51:VAL:HG21	1:A:86:THR:HG22	1.89	0.54
1:A:62:ALA:N	1:A:79:ARG:NH1	2.52	0.54
1:A:290:VAL:HG21	1:A:297:VAL:HG22	1.90	0.54
1:A:64:ASP:HB2	1:B:238:VAL:HG23	1.90	0.54
1:B:53:ILE:HG23	2:B:330:NAD:C4A	2.38	0.54
1:A:63:ALA:HB2	1:A:79:ARG:HH21	1.73	0.54
1:B:134:LEU:HD22	1:B:253:VAL:HG13	1.90	0.54
1:A:31:VAL:HG13	1:A:95:THR:HB	1.90	0.53
1:A:65:THR:O	1:A:68:GLY:N	2.41	0.53
1:A:113:ASN:HA	1:A:116:ILE:CD1	2.38	0.53
1:A:230:ASP:HA	1:A:234:SER:OG	2.07	0.53
1:A:84:GLU:HA	1:A:127:HIS:CE1	2.43	0.53
1:A:140:VAL:HG13	1:A:141:ASP:H	1.74	0.53
1:B:134:LEU:HD21	1:B:161:PHE:HB2	1.89	0.53
1:B:190:LEU:HB3	1:B:287:GLY:O	2.09	0.53
1:B:298:GLU:O	1:B:299:GLU:HB3	2.09	0.53
1:A:78:VAL:HG12	1:A:80:GLN:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:O	1:B:147:LEU:HB2	2.08	0.53
1:A:166:ASP:OD2	1:A:193:HIS:HD2	1.91	0.52
1:B:77:ARG:HD2	1:B:77:ARG:C	2.33	0.52
1:B:211:PRO:C	1:B:219:PHE:H	2.18	0.52
1:B:31:VAL:HG12	2:B:330:NAD:O2N	2.10	0.52
1:A:164:ARG:HD3	1:A:268:LEU:HD22	1.90	0.52
1:A:88:GLY:H	1:A:128:ASN:HB3	1.74	0.52
1:B:83:TYR:CD2	1:B:123:SER:HB2	2.45	0.52
1:B:86:THR:O	1:B:89:SER:HB2	2.10	0.52
1:B:236:MET:SD	1:B:239:ILE:HD11	2.50	0.52
1:A:236:MET:O	1:A:239:ILE:HG13	2.10	0.52
1:B:223:GLU:OE1	1:B:223:GLU:HA	2.10	0.52
1:A:236:MET:HA	1:A:238:VAL:HG12	1.91	0.52
1:A:136:THR:HB	2:A:330:NAD:C2N	2.40	0.52
1:B:274:LEU:HD13	1:B:277:GLU:HB2	1.91	0.52
1:B:100:ARG:NH2	1:B:102:PRO:O	2.43	0.51
1:B:169:ARG:HD2	1:B:236:MET:HE1	1.92	0.51
1:B:59:VAL:HG13	1:B:79:ARG:HG3	1.91	0.51
1:A:64:ASP:OD2	1:B:242:LYS:HE2	2.11	0.51
1:B:195:ASP:O	1:B:196:ALA:CB	2.59	0.51
1:B:201:PHE:HZ	1:B:228:LEU:HD13	1.74	0.51
1:B:270:ALA:HB3	1:B:290:VAL:HG11	1.92	0.51
1:A:107:ILE:O	1:A:110:ALA:HB3	2.11	0.51
1:A:293:GLY:O	1:A:295:ASN:N	2.43	0.51
1:B:115:PRO:HA	1:B:118:GLU:CD	2.36	0.51
1:A:31:VAL:HG12	2:A:330:NAD:PN	2.51	0.51
1:A:80:GLN:O	1:A:81:GLY:C	2.53	0.51
1:A:144:ASN:O	1:A:147:LEU:HB2	2.11	0.51
1:A:292:LEU:HA	1:A:296:GLY:O	2.10	0.51
1:A:134:LEU:HA	1:A:159:ILE:O	2.10	0.51
1:B:174:LEU:O	1:B:178:PHE:HD1	1.93	0.51
1:A:134:LEU:HD21	1:A:161:PHE:HB2	1.92	0.50
1:A:139:PRO:HD2	1:A:143:LEU:HD21	1.93	0.50
1:B:31:VAL:HG13	1:B:95:THR:HB	1.92	0.50
1:A:195:ASP:O	1:A:196:ALA:CB	2.60	0.50
1:A:267:VAL:HA	1:A:290:VAL:O	2.11	0.50
1:B:21:THR:O	1:B:46:ASP:HB2	2.11	0.50
1:B:88:GLY:N	1:B:128:ASN:HB3	2.26	0.50
1:B:241:ARG:NH1	1:B:241:ARG:HG3	2.27	0.50
1:A:63:ALA:N	1:A:79:ARG:NH2	2.53	0.50
1:A:169:ARG:HD3	1:B:67:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:CB	1:B:80:GLN:HE21	2.24	0.50
1:A:59:VAL:HA	1:A:79:ARG:CG	2.41	0.50
1:B:62:ALA:N	1:B:79:ARG:NH1	2.60	0.50
1:B:63:ALA:HB2	1:B:79:ARG:HH21	1.77	0.50
1:B:211:PRO:HA	1:B:219:PHE:CZ	2.46	0.50
1:B:234:SER:C	1:B:236:MET:H	2.19	0.50
1:B:95:THR:O	2:B:330:NAD:H51N	2.11	0.50
1:B:264:THR:OG1	1:B:266:GLU:HG3	2.12	0.50
1:B:201:PHE:HA	1:B:204:VAL:HG23	1.94	0.49
1:B:62:ALA:CB	1:B:79:ARG:NH1	2.74	0.49
1:B:106:ARG:O	1:B:109:LEU:HB3	2.12	0.49
1:A:305:LEU:HD12	1:A:305:LEU:H	1.78	0.49
1:A:22:LYS:HA	1:A:47:GLU:O	2.12	0.49
1:B:32:GLY:HA2	1:B:95:THR:CG2	2.34	0.49
1:B:62:ALA:HB1	1:B:77:ARG:HD3	1.94	0.49
1:B:241:ARG:HG3	1:B:241:ARG:HH11	1.77	0.49
1:A:154:SER:OG	1:A:156:GLU:HG2	2.11	0.49
1:A:86:THR:O	1:A:89:SER:HB2	2.13	0.49
1:B:27(A):ALA:HB1	1:B:50:PHE:HB3	1.94	0.49
1:B:53:ILE:HB	1:B:53(A):PRO:HD2	1.95	0.49
1:B:136:THR:HG22	1:B:161:PHE:HB3	1.95	0.49
1:B:209:THR:O	1:B:211:PRO:HD3	2.13	0.49
1:B:100:ARG:HG2	1:B:101:GLN:N	2.27	0.49
1:A:115:PRO:O	1:A:118:GLU:HB2	2.12	0.48
1:B:305:LEU:HB3	1:B:309:GLU:OE1	2.12	0.48
1:A:105:THR:O	1:A:106:ARG:C	2.56	0.48
1:B:130:ASP:O	1:B:131:TYR:C	2.56	0.48
1:B:154:SER:OG	1:B:156:GLU:HG2	2.13	0.48
1:B:197:GLN:NE2	1:B:232:GLN:HG3	2.28	0.48
1:B:205:ARG:HG3	1:B:210:ASP:OD2	2.13	0.48
1:A:77:ARG:HD2	1:A:77:ARG:C	2.37	0.48
1:B:103:GLY:C	1:B:105:THR:H	2.22	0.48
1:B:281:HIS:O	1:B:282:GLU:HG3	2.13	0.48
1:A:134:LEU:CD2	1:A:161:PHE:HB2	2.44	0.48
1:A:169:ARG:CD	1:A:236:MET:HE1	2.42	0.48
1:B:253:VAL:O	1:B:257:VAL:HG23	2.13	0.48
1:A:197:GLN:NE2	1:A:232:GLN:HG3	2.29	0.48
1:A:199:PRO:HG3	1:A:228:LEU:HD21	1.96	0.48
1:B:84:GLU:HA	1:B:127:HIS:CE1	2.49	0.48
1:B:169:ARG:O	1:B:173:VAL:HG22	2.14	0.48
1:A:108:ASP:O	1:A:111:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:O	1:A:236:MET:HE3	2.13	0.48
1:B:58:THR:C	1:B:60:GLY:H	2.22	0.48
1:B:59:VAL:O	1:B:79:ARG:NH2	2.47	0.48
1:B:258:GLU:O	1:B:262:HIS:HB2	2.14	0.48
1:A:67:HIS:HE1	1:B:235:ALA:O	1.97	0.47
1:A:143:LEU:HD22	1:A:143:LEU:H	1.79	0.47
1:A:197:GLN:HE22	1:A:232:GLN:HG3	1.79	0.47
1:A:199:PRO:HG3	1:A:228:LEU:HD11	1.95	0.47
1:A:44:ILE:CD1	1:A:261:LEU:HD12	2.44	0.47
1:B:59:VAL:C	1:B:79:ARG:NH2	2.72	0.47
1:B:111:GLY:O	1:B:114:ALA:HB3	2.13	0.47
1:B:134:LEU:HA	1:B:159:ILE:O	2.13	0.47
1:B:79:ARG:C	1:B:81:GLY:H	2.21	0.47
1:B:189:ILE:HD11	1:B:231:LEU:CD2	2.39	0.47
1:A:128:ASN:N	1:A:128:ASN:HD22	2.10	0.47
1:A:256:MET:O	1:A:260:ILE:HG13	2.15	0.47
1:A:201:PHE:CZ	1:A:228:LEU:HD13	2.49	0.47
1:B:309:GLU:O	1:B:312:LEU:N	2.46	0.47
1:A:105:THR:O	1:A:107:ILE:N	2.47	0.47
1:A:164:ARG:N	1:A:269:PRO:HG2	2.29	0.47
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.80	0.47
1:A:100:ARG:NH2	1:A:103:GLY:O	2.48	0.47
1:A:192:GLU:HG3	1:A:320:LEU:HD11	1.95	0.47
1:A:219:PHE:O	1:A:221:GLY:N	2.46	0.47
1:A:230:ASP:HA	1:A:234:SER:CB	2.44	0.47
1:B:69:ILE:O	1:B:71:TYR:N	2.48	0.47
1:B:164:ARG:N	1:B:269:PRO:HG2	2.28	0.47
1:B:117:MET:HB3	1:B:147:LEU:HG	1.96	0.47
1:A:69:ILE:CG1	1:A:70:ALA:H	2.22	0.47
1:A:101:GLN:HB3	1:A:102:PRO:HD2	1.97	0.47
1:A:211:PRO:C	1:A:219:PHE:H	2.22	0.47
1:B:83:TYR:CE2	1:B:123:SER:HB2	2.49	0.47
1:A:60:GLY:C	1:A:79:ARG:HH22	2.23	0.47
1:A:132:ILE:HA	1:A:157:GLN:HB3	1.96	0.46
1:A:59:VAL:HG22	1:A:79:ARG:HG3	1.98	0.46
1:A:106:ARG:O	1:A:107:ILE:C	2.59	0.46
1:A:234:SER:C	1:A:236:MET:N	2.66	0.46
1:B:281:HIS:C	1:B:282:GLU:HG3	2.40	0.46
1:B:221:GLY:HA2	1:B:224:LYS:HE3	1.98	0.46
1:A:125:ASP:O	1:A:126:GLU:HG2	2.15	0.46
1:A:164:ARG:HG3	1:A:164:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:N	1:A:79:ARG:HH22	2.14	0.46
1:A:100:ARG:HG2	1:A:101:GLN:N	2.30	0.46
1:A:305:LEU:HB3	1:A:309:GLU:OE1	2.16	0.46
1:A:104:GLN:HG3	1:A:109:LEU:HB2	1.97	0.46
1:A:130:ASP:O	1:A:131:TYR:C	2.59	0.46
1:B:205:ARG:HG2	1:B:209:THR:O	2.15	0.46
1:B:134:LEU:CD2	1:B:161:PHE:HB2	2.46	0.46
1:B:174:LEU:CB	1:B:185:VAL:HG11	2.46	0.46
1:A:85:ASP:C	1:A:87:ALA:H	2.24	0.45
1:A:307:ASP:HA	1:A:310:GLN:HB2	1.98	0.45
1:B:230:ASP:HA	1:B:234:SER:CB	2.47	0.45
1:A:245:THR:OG1	2:A:330:NAD:H6N	2.16	0.45
1:B:132:ILE:HA	1:B:157:GLN:HB3	1.98	0.45
1:B:236:MET:HE2	1:B:236:MET:N	2.32	0.45
1:B:136:THR:O	1:B:137:SER:C	2.59	0.45
1:B:143:LEU:HD22	1:B:143:LEU:H	1.82	0.45
1:B:164:ARG:HD3	1:B:268:LEU:HD22	1.99	0.45
1:B:236:MET:HA	1:B:238:VAL:HG12	1.98	0.45
1:B:62:ALA:HB1	1:B:77:ARG:CD	2.46	0.45
1:B:103:GLY:O	1:B:105:THR:N	2.47	0.45
1:B:195:ASP:O	1:B:196:ALA:HB3	2.17	0.45
1:B:59:VAL:O	1:B:59:VAL:CG1	2.64	0.45
1:B:82:GLY:C	1:B:84:GLU:N	2.68	0.45
1:A:128:ASN:N	1:A:128:ASN:ND2	2.64	0.45
1:B:60:GLY:C	1:B:79:ARG:HH22	2.25	0.45
1:A:64:ASP:OD2	1:B:246:GLU:HB3	2.17	0.45
1:A:73:ASP:HA	1:B:183:GLN:OE1	2.17	0.45
1:A:205:ARG:HD2	1:A:208:GLY:HA2	1.98	0.45
1:B:218:GLU:C	1:B:220:SER:N	2.72	0.45
1:A:172:TYR:O	1:A:173:VAL:C	2.60	0.45
1:B:301:VAL:HG12	1:B:303:TRP:CD1	2.52	0.45
1:A:94:ILE:O	1:A:94:ILE:HG22	2.17	0.45
1:B:247:TRP:O	1:B:248:GLY:C	2.59	0.45
1:A:87:ALA:HB2	1:A:127:HIS:HB3	1.99	0.44
1:A:162:GLY:O	1:A:163:GLY:C	2.60	0.44
1:B:79:ARG:HB3	1:B:79:ARG:NH1	2.18	0.44
1:B:305:LEU:HD12	1:B:305:LEU:N	2.33	0.44
1:A:77:ARG:O	1:A:78:VAL:HG23	2.18	0.44
1:A:274:LEU:HD13	1:A:277:GLU:HB2	1.99	0.44
1:B:104:GLN:O	1:B:105:THR:C	2.60	0.44
1:A:174:LEU:HB3	1:A:185:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASP:O	1:B:111:GLY:N	2.51	0.44
1:A:61:GLN:OE1	1:B:242:LYS:NZ	2.48	0.44
1:A:174:LEU:CB	1:A:185:VAL:HG11	2.48	0.44
1:A:223:GLU:CD	1:A:223:GLU:H	2.25	0.44
1:A:140:VAL:O	1:A:141:ASP:C	2.61	0.44
1:A:274:LEU:HD12	1:A:277:GLU:O	2.18	0.44
1:B:101:GLN:HB3	1:B:102:PRO:HD2	2.00	0.44
1:B:211:PRO:HA	1:B:219:PHE:CE1	2.53	0.44
1:A:59:VAL:C	1:A:79:ARG:NH2	2.75	0.44
1:A:183:GLN:OE1	1:B:73:ASP:HA	2.17	0.44
1:A:290:VAL:HG23	1:A:297:VAL:HG13	1.99	0.44
1:B:51:VAL:HG21	1:B:86:THR:HG22	1.99	0.44
1:B:51:VAL:HG22	1:B:81:GLY:O	2.18	0.44
1:B:62:ALA:CB	1:B:77:ARG:HD3	2.48	0.44
1:B:113:ASN:HB2	1:B:143:LEU:HD11	2.00	0.44
1:B:174:LEU:HB3	1:B:185:VAL:HG11	2.00	0.44
1:A:139:PRO:HB2	1:A:143:LEU:CD2	2.47	0.44
1:A:29:GLY:O	1:A:32:GLY:N	2.50	0.44
1:A:277:GLU:O	1:A:278:PHE:HB2	2.18	0.44
1:A:78:VAL:CG1	1:A:79:ARG:N	2.81	0.44
1:A:62:ALA:HB3	1:A:79:ARG:CZ	2.48	0.43
1:A:63:ALA:H	1:A:79:ARG:HH22	1.58	0.43
1:A:100:ARG:NH2	1:A:102:PRO:O	2.52	0.43
1:A:230:ASP:HA	1:A:234:SER:HB2	2.01	0.43
1:A:193:HIS:CE1	2:A:330:NAD:O7N	2.71	0.43
1:B:114:ALA:O	1:B:118:GLU:HG3	2.18	0.43
1:A:79:ARG:C	1:A:81:GLY:N	2.76	0.43
1:A:277:GLU:H	1:A:277:GLU:CD	2.27	0.43
1:A:252:GLY:O	1:A:255:HIS:HB3	2.19	0.43
1:B:59:VAL:O	1:B:79:ARG:CZ	2.67	0.43
1:B:107:ILE:CG2	1:B:327:ILE:HD13	2.48	0.43
1:B:202:SER:HA	1:B:218:GLU:OE1	2.19	0.43
1:A:57:ASP:OD1	1:A:57:ASP:N	2.51	0.43
1:B:60:GLY:CA	1:B:79:ARG:NH2	2.81	0.43
1:B:69:ILE:CG1	1:B:70:ALA:H	2.23	0.43
1:B:117:MET:HG3	1:B:143:LEU:HD12	1.99	0.43
1:A:62:ALA:HB1	1:A:77:ARG:HD3	1.99	0.43
1:A:281:HIS:O	1:A:282:GLU:HG3	2.19	0.43
1:B:188:THR:HG22	1:B:189:ILE:H	1.83	0.43
1:B:201:PHE:HA	1:B:204:VAL:CG2	2.47	0.43
1:B:292:LEU:HA	1:B:296:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:HG21	1:B:70:ALA:CB	2.41	0.43
1:A:242:LYS:NZ	1:B:61:GLN:OE1	2.44	0.43
1:B:108:ASP:O	1:B:109:LEU:C	2.60	0.43
1:A:174:LEU:O	1:A:178:PHE:HD1	2.02	0.43
1:A:201:PHE:HZ	1:A:228:LEU:HD13	1.84	0.43
1:A:136:THR:HG22	1:A:161:PHE:HB3	2.01	0.42
1:B:227:LEU:C	1:B:229:GLY:N	2.74	0.42
1:B:139:PRO:HB2	1:B:143:LEU:CD2	2.49	0.42
1:B:234:SER:C	1:B:236:MET:N	2.77	0.42
1:B:307:ASP:O	1:B:308:TYR:C	2.62	0.42
1:A:115:PRO:HA	1:A:118:GLU:CD	2.45	0.42
1:B:83:TYR:OH	2:B:330:NAD:N1A	2.53	0.42
1:A:62:ALA:HB1	1:A:77:ARG:CD	2.49	0.42
1:A:136:THR:O	1:A:137:SER:C	2.63	0.42
1:B:210:ASP:HA	1:B:211:PRO:HD3	1.74	0.42
1:B:55:GLU:O	1:B:55:GLU:HG3	2.18	0.42
1:B:146:HIS:O	1:B:150:ALA:CB	2.67	0.42
1:A:56:ASP:O	1:B:241:ARG:CB	2.67	0.42
1:A:78:VAL:HB	1:A:80:GLN:NE2	2.35	0.42
1:A:266:GLU:O	1:A:291:ARG:HA	2.20	0.42
1:B:277:GLU:CD	1:B:277:GLU:H	2.28	0.42
1:B:162:GLY:HA2	2:B:330:NAD:O7N	2.20	0.42
1:B:276:GLY:O	1:B:277:GLU:C	2.62	0.42
1:A:83:TYR:OH	2:A:330:NAD:N1A	2.53	0.42
1:B:194:GLY:O	1:B:195:ASP:C	2.61	0.42
1:B:300:ILE:HD12	1:B:300:ILE:H	1.85	0.42
1:A:53:ILE:HB	1:A:53(A):PRO:HD2	2.02	0.42
1:A:105:THR:O	1:A:105:THR:HG23	2.20	0.42
1:A:119:ASP:O	1:A:120:ILE:C	2.62	0.42
1:B:65:THR:CB	1:B:77:ARG:NH1	2.80	0.42
1:B:274:LEU:HD12	1:B:277:GLU:O	2.20	0.42
1:A:104:GLN:O	1:A:105:THR:C	2.62	0.42
1:A:223:GLU:OE1	1:A:223:GLU:HA	2.19	0.42
1:B:39:ILE:HD11	1:B:93:VAL:HG21	2.02	0.42
1:A:210:ASP:HA	1:A:211:PRO:HD3	1.69	0.41
1:B:63:ALA:N	1:B:79:ARG:NH2	2.62	0.41
1:A:307:ASP:O	1:A:308:TYR:C	2.63	0.41
1:B:278:PHE:CE1	1:B:302:GLU:HA	2.55	0.41
1:B:145:ARG:O	1:B:149:GLU:HG2	2.19	0.41
1:B:146:HIS:O	1:B:150:ALA:HB3	2.20	0.41
1:A:58:THR:C	1:A:60:GLY:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:HB3	1:A:284:THR:HG21	2.01	0.41
1:A:301:VAL:HG12	1:A:303:TRP:HD1	1.83	0.41
1:A:73:ASP:O	1:A:74:SER:CB	2.67	0.41
1:A:248:GLY:HA2	1:B:68:GLY:HA2	2.02	0.41
1:B:69:ILE:HD13	1:B:69:ILE:HG21	1.89	0.41
1:B:105:THR:O	1:B:106:ARG:C	2.64	0.41
1:B:170:PHE:O	1:B:173:VAL:HG23	2.21	0.41
1:A:59:VAL:O	1:A:59:VAL:CG1	2.68	0.41
1:A:60:GLY:CA	1:A:79:ARG:NH2	2.84	0.41
1:A:235:ALA:O	1:B:67:HIS:HE1	2.03	0.41
1:A:241:ARG:H	1:A:241:ARG:HG2	1.69	0.41
1:A:247:TRP:HA	1:A:247:TRP:CE3	2.55	0.41
1:B:131:TYR:O	1:B:131:TYR:CG	2.73	0.41
1:B:211:PRO:C	1:B:219:PHE:N	2.78	0.41
1:B:98:ILE:O	1:B:109:LEU:HD11	2.21	0.41
1:A:234:SER:O	1:A:236:MET:N	2.53	0.41
1:A:258:GLU:O	1:A:262:HIS:HB2	2.21	0.41
1:B:43:ASP:O	1:B:43:ASP:CG	2.63	0.41
1:A:59:VAL:C	1:A:79:ARG:CZ	2.94	0.40
1:B:219:PHE:N	1:B:219:PHE:CD1	2.88	0.40
1:A:79:ARG:O	1:A:81:GLY:N	2.49	0.40
1:A:82:GLY:C	1:A:84:GLU:N	2.77	0.40
1:B:57:ASP:OD1	1:B:57:ASP:N	2.54	0.40
1:A:114:ALA:O	1:A:118:GLU:HG3	2.20	0.40
1:B:51:VAL:HG13	1:B:81:GLY:O	2.22	0.40
1:A:60:GLY:N	1:A:79:ARG:NH2	2.69	0.40
1:A:290:VAL:CG2	1:A:297:VAL:HG13	2.51	0.40
1:A:300:ILE:H	1:A:300:ILE:HD12	1.85	0.40
1:B:29:GLY:O	1:B:32:GLY:N	2.47	0.40
1:B:100:ARG:NH2	1:B:103:GLY:O	2.55	0.40
1:B:138:ASN:HB2	2:B:330:NAD:O2D	2.21	0.40
1:B:140:VAL:HG13	1:B:141:ASP:H	1.86	0.40
1:A:227:LEU:C	1:A:229:GLY:N	2.79	0.40
1:B:140:VAL:HG11	2:B:330:NAD:H72N	1.87	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	301/303 (99%)	230 (76%)	46 (15%)	25 (8%)	0	4
1	B	301/303 (99%)	232 (77%)	47 (16%)	22 (7%)	1	6
All	All	602/606 (99%)	462 (77%)	93 (15%)	47 (8%)	1	5

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	55	GLU
1	A	70	ALA
1	A	71	TYR
1	A	106	ARG
1	A	131	TYR
1	A	140	VAL
1	A	152	ASP
1	A	196	ALA
1	A	234	SER
1	A	294	SER
1	B	30	THR
1	B	70	ALA
1	B	81	GLY
1	B	104	GLN
1	B	106	ARG
1	B	131	TYR
1	B	140	VAL
1	B	152	ASP
1	B	196	ALA
1	B	234	SER
1	B	294	SER
1	A	81	GLY
1	A	82	GLY
1	A	200	VAL

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Mol	Chain	Res	Type
1	B	71	TYR
1	B	79	ARG
1	B	82	GLY
1	B	220	SER
1	A	73	ASP
1	A	80	GLN
1	A	104	GLN
1	B	105	THR
1	B	299	GLU
1	A	56	ASP
1	A	105	THR
1	A	107	ILE
1	A	220	SER
1	A	299	GLU
1	B	73	ASP
1	A	235	ALA
1	B	56	ASP
1	B	250	ALA
1	A	79	ARG
1	A	59	VAL
1	B	221	GLY
1	B	69	ILE

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	244/244 (100%)	207 (85%)	37 (15%)	3	14
1	B	244/244 (100%)	210 (86%)	34 (14%)	3	17
All	All	488/488 (100%)	417 (86%)	71 (14%)	3	16

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	44	ILE
1	A	55	GLU
1	A	57	ASP
1	A	58	THR
1	A	65	THR
1	A	71	TYR
1	A	74	SER
1	A	76	THR
1	A	77	ARG
1	A	79	ARG
1	A	84	GLU
1	A	89	SER
1	A	102	PRO
1	A	104	GLN
1	A	126	GLU
1	A	128	ASN
1	A	135	THR
1	A	141	ASP
1	A	169	ARG
1	A	183	GLN
1	A	188	THR
1	A	223	GLU
1	A	227	LEU
1	A	228	LEU
1	A	236	MET
1	A	239	ILE
1	A	245	THR
1	A	274	LEU
1	A	282	GLU
1	A	288	VAL
1	A	305	LEU
1	A	307	ASP
1	A	315	ASP
1	A	320	LEU
1	A	327	ILE
1	B	30	THR
1	B	41	LEU
1	B	44	ILE
1	B	55	GLU
1	B	57	ASP
1	B	65	THR

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Mol	Chain	Res	Type
1	B	71	TYR
1	B	74	SER
1	B	76	THR
1	B	77	ARG
1	B	79	ARG
1	B	84	GLU
1	B	89	SER
1	B	104	GLN
1	B	123	SER
1	B	128	ASN
1	B	135	THR
1	B	169	ARG
1	B	183	GLN
1	B	188	THR
1	B	219	PHE
1	B	223	GLU
1	B	227	LEU
1	B	228	LEU
1	B	232	GLN
1	B	239	ILE
1	B	240	GLU
1	B	241	ARG
1	B	274	LEU
1	B	282	GLU
1	B	288	VAL
1	B	305	LEU
1	B	307	ASP
1	B	320	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	80	GLN
1	A	128	ASN
1	A	138	ASN
1	A	157	GLN
1	A	183	GLN
1	A	184	ASN
1	A	193	HIS
1	A	281	HIS
1	B	75	ASN

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Mol	Chain	Res	Type
1	B	80	GLN
1	B	128	ASN
1	B	138	ASN
1	B	157	GLN
1	B	183	GLN
1	B	184	ASN
1	B	193	HIS
1	B	197	GLN
1	B	281	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	A	330	-	46,48,48	1.29	5 (10%)	64,73,73	2.29	15 (23%)
2	NAD	B	330	-	46,48,48	2.13	7 (15%)	64,73,73	2.40	22 (34%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	330	-	-	7/30/62/62	0/5/5/5
2	NAD	B	330	-	-	8/30/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	NAD	PN-O3	8.20	1.68	1.59
2	B	330	NAD	PA-O3	7.27	1.67	1.59
2	B	330	NAD	C2N-N1N	5.94	1.41	1.35
2	A	330	NAD	C2N-N1N	4.94	1.40	1.35
2	A	330	NAD	C6N-N1N	2.56	1.41	1.35
2	A	330	NAD	O4D-C1D	2.55	1.44	1.40
2	B	330	NAD	C5A-N7A	-2.38	1.34	1.39
2	A	330	NAD	C8A-N7A	2.27	1.36	1.31
2	B	330	NAD	O4D-C1D	2.25	1.43	1.40
2	A	330	NAD	C5A-N7A	-2.22	1.35	1.39
2	B	330	NAD	C8A-N7A	2.22	1.35	1.31
2	B	330	NAD	C6N-N1N	2.06	1.40	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	330	NAD	C4D-O4D-C1D	-9.94	100.83	109.92
2	B	330	NAD	C4D-O4D-C1D	-9.17	101.53	109.92
2	B	330	NAD	C5A-C4A-N3A	-6.92	117.19	126.72
2	A	330	NAD	C5A-C4A-N3A	-5.86	118.65	126.72
2	A	330	NAD	C6A-C5A-N7A	-5.72	121.07	132.09
2	B	330	NAD	O2B-C2B-C3B	-4.15	98.50	111.82
2	A	330	NAD	C4B-O4B-C1B	-3.93	100.78	109.47
2	B	330	NAD	O4B-C1B-N9A	3.90	115.58	108.09
2	A	330	NAD	O4B-C1B-N9A	3.75	115.29	108.09
2	A	330	NAD	O3-PN-O1N	-3.67	99.68	110.70
2	B	330	NAD	N3A-C4A-N9A	3.59	133.27	127.17
2	A	330	NAD	N3A-C2A-N1A	-3.55	123.21	128.58
2	B	330	NAD	N3A-C2A-N1A	-3.53	123.24	128.58
2	B	330	NAD	C2A-N3A-C4A	3.53	120.45	111.83
2	B	330	NAD	O7N-C7N-C3N	-3.47	115.35	119.60
2	B	330	NAD	N9A-C8A-N7A	-3.40	109.11	113.94
2	B	330	NAD	C6A-C5A-C4A	3.31	121.70	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	NAD	C6A-C5A-N7A	-3.30	125.72	132.09
2	A	330	NAD	C2B-C1B-N9A	3.22	121.30	113.30
2	A	330	NAD	C6N-N1N-C2N	-3.17	119.18	121.88
2	A	330	NAD	C2A-N3A-C4A	3.07	119.33	111.83
2	A	330	NAD	C6A-C5A-C4A	3.07	121.37	117.18
2	B	330	NAD	C6N-N1N-C2N	-2.95	119.37	121.88
2	A	330	NAD	N3A-C4A-N9A	2.80	131.92	127.17
2	B	330	NAD	O5D-PN-O1N	-2.75	98.04	108.94
2	B	330	NAD	C6N-C5N-C4N	2.56	123.13	119.45
2	A	330	NAD	C4A-N9A-C8A	2.47	108.33	105.74
2	B	330	NAD	C4A-N9A-C8A	2.44	108.30	105.74
2	B	330	NAD	C4N-C3N-C7N	-2.43	114.43	121.06
2	B	330	NAD	C5N-C6N-N1N	-2.41	117.10	120.38
2	B	330	NAD	C4A-N9A-C1B	-2.37	121.10	126.63
2	B	330	NAD	C2B-C1B-N9A	2.36	119.17	113.30
2	B	330	NAD	O2B-C2B-C1B	2.24	117.82	110.10
2	B	330	NAD	C4B-O4B-C1B	-2.12	104.78	109.47
2	A	330	NAD	N9A-C8A-N7A	-2.10	110.95	113.94
2	B	330	NAD	C5A-N7A-C8A	2.08	106.72	103.45
2	A	330	NAD	O3-PA-O1A	-2.06	104.51	110.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

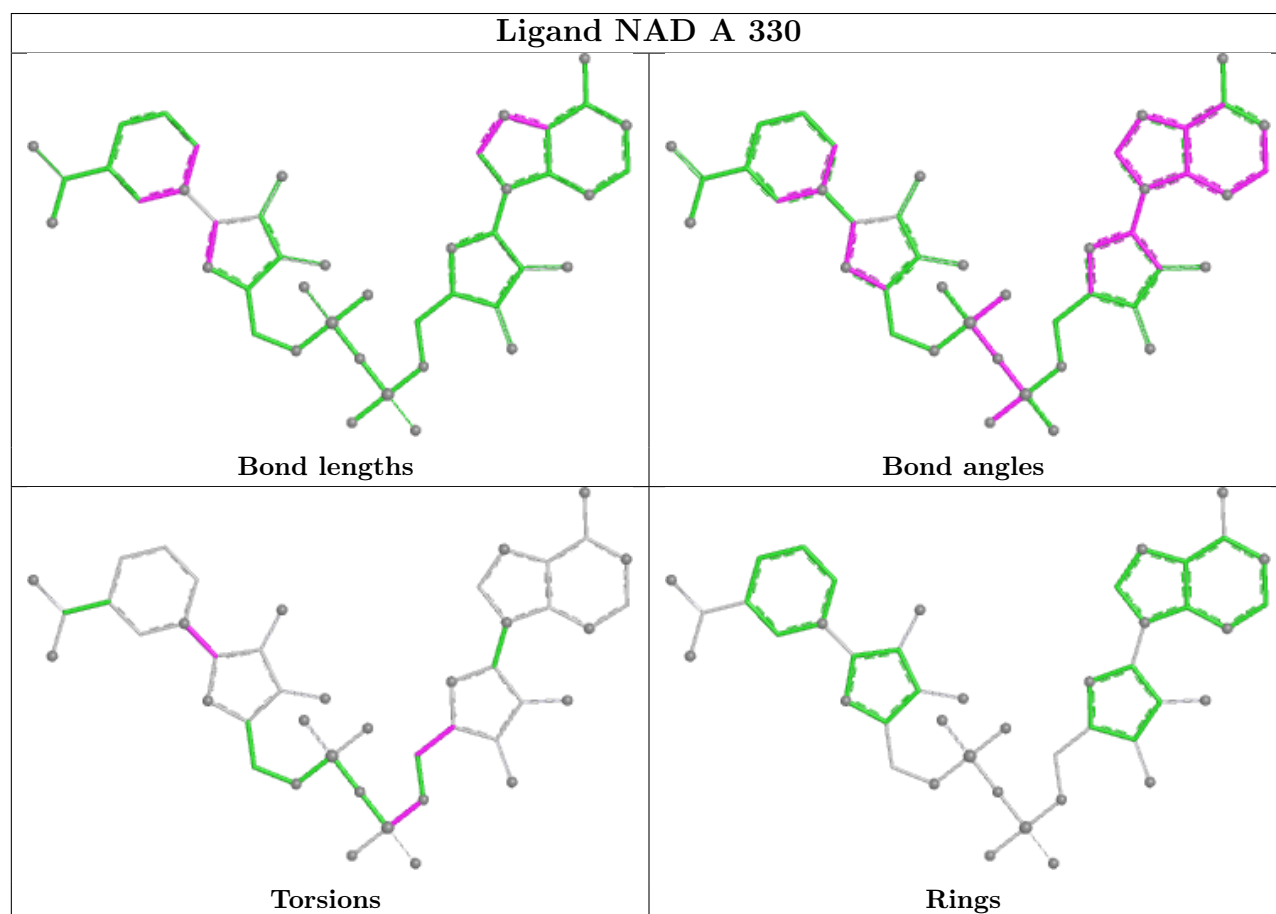
Mol	Chain	Res	Type	Atoms
2	A	330	NAD	O4D-C1D-N1N-C2N
2	A	330	NAD	O4D-C1D-N1N-C6N
2	A	330	NAD	C2D-C1D-N1N-C2N
2	A	330	NAD	C2D-C1D-N1N-C6N
2	B	330	NAD	O4D-C1D-N1N-C2N
2	B	330	NAD	O4D-C1D-N1N-C6N
2	B	330	NAD	C2D-C1D-N1N-C2N
2	A	330	NAD	O4B-C4B-C5B-O5B
2	A	330	NAD	C3B-C4B-C5B-O5B
2	B	330	NAD	PN-O3-PA-O5B
2	A	330	NAD	C5B-O5B-PA-O1A
2	B	330	NAD	O4B-C4B-C5B-O5B
2	B	330	NAD	C2D-C1D-N1N-C6N
2	B	330	NAD	O4B-C1B-N9A-C8A
2	B	330	NAD	C2B-C1B-N9A-C8A

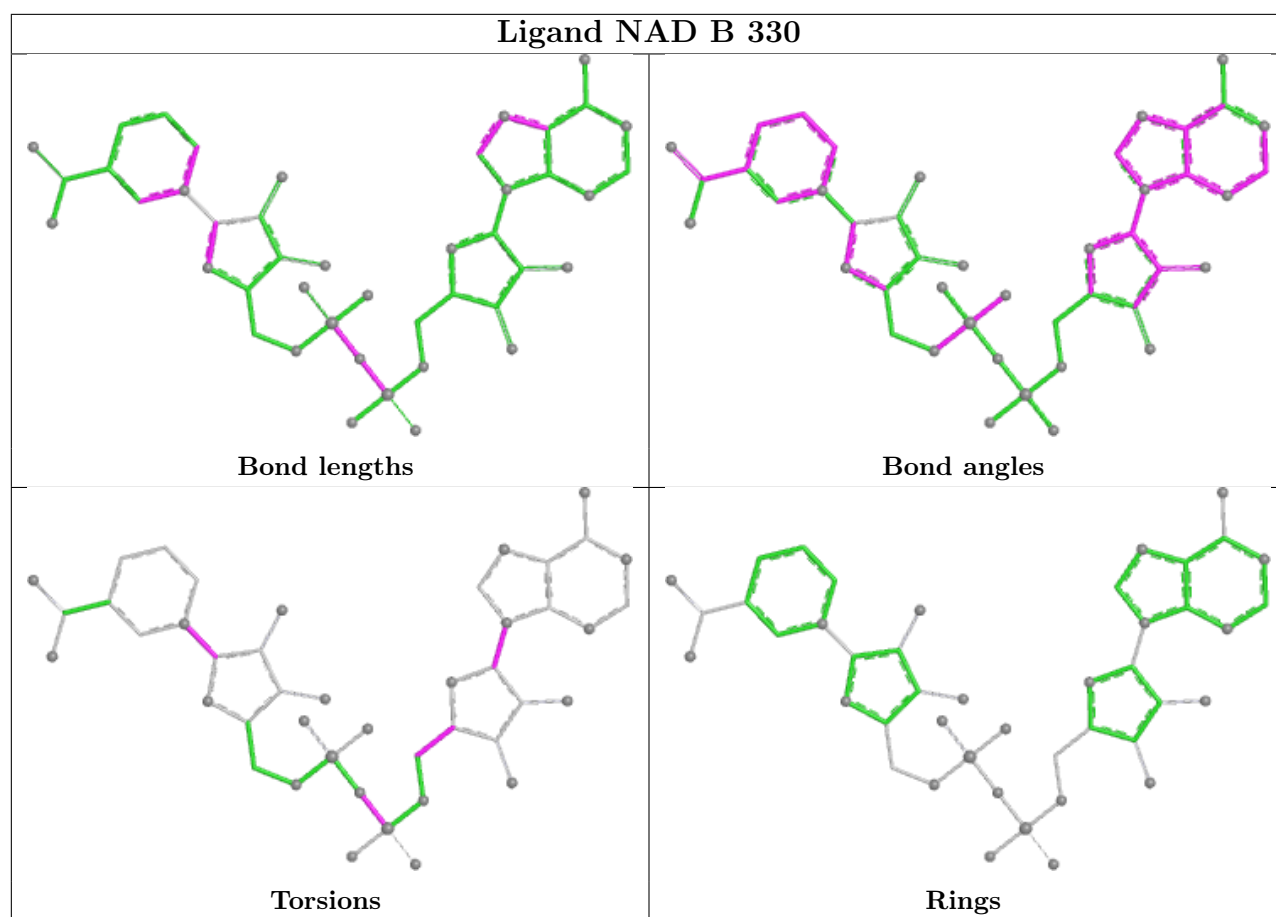
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	NAD	10	0
2	B	330	NAD	12	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	303/303 (100%)	5.99	291 (96%) 0 0	2, 16, 35, 46	0
1	B	303/303 (100%)	5.31	296 (97%) 0 0	2, 16, 35, 46	0
All	All	606/606 (100%)	5.65	587 (96%) 0 0	2, 16, 35, 46	0

All (587) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	GLY	19.2
1	A	254	ALA	15.2
1	A	208	GLY	13.2
1	A	314	ALA	12.7
1	A	105	THR	12.6
1	A	68	GLY	12.5
1	A	252	GLY	11.7
1	A	183	GLN	11.6
1	B	52	ASP	11.1
1	B	173	VAL	10.9
1	A	259	ALA	10.8
1	B	259	ALA	10.8
1	A	262	HIS	10.8
1	A	73	ASP	10.7
1	B	168	ALA	10.6
1	B	118	GLU	10.5
1	A	247	TRP	10.5
1	A	263	ASP	10.4
1	B	267	VAL	10.4
1	A	45	ALA	10.3
1	B	325	ASP	10.3
1	A	76	THR	10.2
1	B	119	ASP	10.2
1	B	150	ALA	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	184	ASN	10.0
1	A	250	ALA	10.0
1	A	122	SER	9.8
1	A	274	LEU	9.8
1	A	287	GLY	9.7
1	A	123	SER	9.6
1	B	262	HIS	9.6
1	A	288	VAL	9.5
1	A	74	SER	9.5
1	A	167	SER	9.5
1	B	242	LYS	9.4
1	A	209	THR	9.3
1	A	187	GLY	9.3
1	A	188	THR	9.2
1	A	37	TYR	9.1
1	B	306	ASP	9.0
1	B	175	SER	9.0
1	A	312	LEU	9.0
1	B	237	ASP	9.0
1	A	109	LEU	8.9
1	A	233	GLU	8.9
1	B	238	VAL	8.9
1	A	51	VAL	8.8
1	A	186	GLU	8.8
1	B	218	GLU	8.8
1	A	210	ASP	8.7
1	B	311	ASP	8.7
1	B	322	ASP	8.7
1	B	314	ALA	8.7
1	B	80	GLN	8.7
1	A	164	ARG	8.7
1	B	296	GLY	8.7
1	A	205	ARG	8.6
1	A	27	GLY	8.5
1	B	122	SER	8.5
1	A	202	SER	8.5
1	A	229	GLY	8.5
1	A	270	ALA	8.4
1	A	316	ALA	8.4
1	B	324	TYR	8.4
1	B	167	SER	8.4
1	B	287	GLY	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	135	THR	8.3
1	A	38	ASN	8.2
1	B	328	SER	8.2
1	A	90	ASP	8.2
1	B	211	PRO	8.2
1	A	185	VAL	8.1
1	B	27	GLY	8.1
1	A	235	ALA	8.1
1	B	231	LEU	8.1
1	A	194	GLY	8.0
1	A	295	ASN	8.0
1	A	285	ALA	8.0
1	A	257	VAL	8.0
1	A	104	GLN	7.9
1	B	81	GLY	7.9
1	B	58	THR	7.9
1	B	125	ASP	7.9
1	B	258	GLU	7.9
1	A	304	ASP	7.9
1	A	27(A)	ALA	7.9
1	A	95	THR	7.9
1	B	146	HIS	7.8
1	B	49	VAL	7.8
1	B	182	VAL	7.8
1	B	62	ALA	7.8
1	A	181	PRO	7.8
1	B	180	ALA	7.7
1	A	115	PRO	7.7
1	A	44	ILE	7.7
1	A	292	LEU	7.7
1	A	144	ASN	7.7
1	A	197	GLN	7.6
1	A	218	GLU	7.6
1	B	41	LEU	7.6
1	B	236	MET	7.6
1	B	172	TYR	7.6
1	B	79	ARG	7.6
1	B	185	VAL	7.5
1	B	191	GLY	7.5
1	A	224	LYS	7.5
1	A	132	ILE	7.5
1	A	79	ARG	7.5

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Mol	Chain	Res	Type	RSRZ
1	B	109	LEU	7.5
1	A	22	LYS	7.5
1	B	274	LEU	7.4
1	A	62	ALA	7.4
1	A	141	ASP	7.4
1	B	87	ALA	7.4
1	A	301	VAL	7.4
1	B	152	ASP	7.4
1	A	168	ALA	7.4
1	B	199	PRO	7.4
1	B	84	GLU	7.3
1	B	232	GLN	7.3
1	B	92	VAL	7.3
1	B	123	SER	7.3
1	A	308	TYR	7.3
1	A	242	LYS	7.3
1	A	315	ASP	7.3
1	B	254	ALA	7.2
1	A	238	VAL	7.2
1	A	66	ASN	7.2
1	A	150	ALA	7.2
1	A	222	ASP	7.2
1	A	47	GLU	7.2
1	B	176	GLU	7.2
1	B	264	THR	7.2
1	B	270	ALA	7.2
1	A	64	ASP	7.1
1	A	283	ASP	7.1
1	A	25	VAL	7.1
1	B	68	GLY	7.1
1	B	312	LEU	7.1
1	B	281	HIS	7.1
1	A	46	ASP	7.1
1	A	60	GLY	7.1
1	A	261	LEU	7.1
1	A	204	VAL	7.1
1	A	32	GLY	7.1
1	A	151	GLY	7.1
1	B	266	GLU	7.1
1	A	86	THR	7.1
1	B	93	VAL	7.1
1	B	210	ASP	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	55	GLU	7.0
1	B	78	VAL	7.0
1	A	200	VAL	7.0
1	A	165	LEU	7.0
1	A	309	GLU	7.0
1	A	231	LEU	7.0
1	B	86	THR	7.0
1	B	108	ASP	7.0
1	A	219	PHE	7.0
1	A	133	SER	6.9
1	A	41	LEU	6.9
1	A	93	VAL	6.9
1	A	234	SER	6.9
1	B	271	SER	6.9
1	A	85	ASP	6.9
1	A	130	ASP	6.9
1	A	157	GLN	6.9
1	A	176	GLU	6.9
1	B	245	THR	6.9
1	A	307	ASP	6.9
1	A	160	GLY	6.8
1	A	26	VAL	6.8
1	A	230	ASP	6.8
1	B	104	GLN	6.8
1	B	252	GLY	6.8
1	A	179	ASP	6.8
1	A	125	ASP	6.8
1	B	292	LEU	6.8
1	A	96	ALA	6.8
1	A	113	ASN	6.8
1	B	105	THR	6.7
1	A	248	GLY	6.7
1	B	38	ASN	6.7
1	A	111	GLY	6.7
1	A	80	GLN	6.6
1	B	197	GLN	6.6
1	B	189	ILE	6.6
1	A	243	GLY	6.6
1	B	209	THR	6.6
1	A	107	ILE	6.6
1	B	64	ASP	6.6
1	A	148	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	293	GLY	6.6
1	A	255	HIS	6.6
1	B	116	ILE	6.6
1	A	84	GLU	6.6
1	A	118	GLU	6.6
1	B	298	GLU	6.6
1	B	305	LEU	6.5
1	A	101	GLN	6.5
1	A	131	TYR	6.5
1	B	103	GLY	6.5
1	B	260	ILE	6.5
1	B	27(A)	ALA	6.5
1	A	126	GLU	6.5
1	A	159	ILE	6.5
1	B	308	TYR	6.5
1	B	115	PRO	6.5
1	B	219	PHE	6.5
1	A	134	LEU	6.5
1	A	260	ILE	6.5
1	B	24	SER	6.4
1	B	202	SER	6.4
1	B	151	GLY	6.4
1	B	239	ILE	6.4
1	B	82	GLY	6.4
1	A	306	ASP	6.4
1	B	126	GLU	6.4
1	B	114	ALA	6.4
1	A	237	ASP	6.3
1	B	29	GLY	6.3
1	A	23	VAL	6.3
1	A	282	GLU	6.3
1	B	131	TYR	6.3
1	A	67	HIS	6.3
1	B	21	THR	6.3
1	B	51	VAL	6.3
1	B	309	GLU	6.3
1	A	48	VAL	6.3
1	A	322	ASP	6.3
1	A	136	THR	6.2
1	A	281	HIS	6.2
1	A	91	VAL	6.2
1	A	211	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	83	TYR	6.2
1	B	253	VAL	6.2
1	B	44	ILE	6.2
1	A	163	GLY	6.2
1	A	286	PHE	6.2
1	B	160	GLY	6.2
1	B	144	ASN	6.1
1	A	291	ARG	6.1
1	B	250	ALA	6.1
1	B	269	PRO	6.1
1	A	192	GLU	6.1
1	A	191	GLY	6.1
1	B	127	HIS	6.1
1	A	162	GLY	6.1
1	A	193	HIS	6.1
1	B	71	TYR	6.1
1	B	222	ASP	6.1
1	B	255	HIS	6.1
1	A	180	ALA	6.1
1	A	298	GLU	6.1
1	A	138	ASN	6.1
1	A	258	GLU	6.0
1	B	316	ALA	6.0
1	A	323	GLN	6.0
1	B	318	GLU	6.0
1	A	89	SER	6.0
1	A	171	ARG	6.0
1	B	66	ASN	6.0
1	A	149	GLU	6.0
1	A	120	ILE	6.0
1	A	28	ALA	6.0
1	A	127	HIS	5.9
1	A	137	SER	5.9
1	A	83	TYR	5.9
1	B	73	ASP	5.9
1	A	290	VAL	5.9
1	A	189	ILE	5.9
1	B	30	THR	5.9
1	A	75	ASN	5.9
1	A	198	VAL	5.9
1	A	156	GLU	5.9
1	B	113	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	271	SER	5.8
1	A	294	SER	5.8
1	A	65	THR	5.8
1	A	284	THR	5.8
1	A	108	ASP	5.8
1	A	114	ALA	5.8
1	A	317	ALA	5.8
1	A	59	VAL	5.8
1	B	192	GLU	5.8
1	A	77	ARG	5.7
1	A	158	VAL	5.7
1	B	286	PHE	5.7
1	B	46	ASP	5.7
1	A	190	LEU	5.7
1	A	53(A)	PRO	5.6
1	A	273	LYS	5.6
1	A	146	HIS	5.6
1	B	102	PRO	5.6
1	B	34	ALA	5.6
1	B	74	SER	5.6
1	B	224	LYS	5.6
1	B	310	GLN	5.6
1	B	233	GLU	5.6
1	A	21	THR	5.6
1	A	129	ASP	5.5
1	B	124	LEU	5.5
1	B	186	GLU	5.5
1	B	297	VAL	5.5
1	B	163	GLY	5.5
1	A	81	GLY	5.5
1	B	97	GLY	5.5
1	B	95	THR	5.4
1	A	239	ILE	5.4
1	B	179	ASP	5.4
1	B	225	GLU	5.4
1	A	24	SER	5.4
1	A	227	LEU	5.4
1	B	134	LEU	5.4
1	B	26	VAL	5.4
1	B	169	ARG	5.4
1	A	311	ASP	5.4
1	B	307	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	198	VAL	5.4
1	B	226	GLN	5.3
1	A	110	ALA	5.3
1	B	317	ALA	5.3
1	A	29	GLY	5.3
1	B	107	ILE	5.3
1	A	121	GLN	5.3
1	A	256	MET	5.3
1	B	251	ARG	5.3
1	A	161	PHE	5.3
1	B	243	GLY	5.3
1	A	61	GLN	5.3
1	B	284	THR	5.3
1	B	138	ASN	5.3
1	B	120	ILE	5.3
1	B	137	SER	5.2
1	A	40	ALA	5.2
1	B	263	ASP	5.2
1	A	128	ASN	5.2
1	B	166	ASP	5.2
1	A	53	ILE	5.1
1	A	175	SER	5.1
1	B	164	ARG	5.1
1	B	207	ASP	5.1
1	B	154	SER	5.1
1	A	236	MET	5.1
1	B	321	SER	5.1
1	A	106	ARG	5.1
1	A	318	GLU	5.1
1	A	172	TYR	5.1
1	B	156	GLU	5.0
1	A	196	ALA	5.0
1	B	57	ASP	5.0
1	B	205	ARG	5.0
1	B	178	PHE	5.0
1	A	302	GLU	5.0
1	B	230	ASP	5.0
1	A	320	LEU	5.0
1	B	157	GLN	5.0
1	B	56	ASP	4.9
1	A	119	ASP	4.9
1	B	183	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	158	VAL	4.9
1	A	94	ILE	4.9
1	B	288	VAL	4.9
1	B	36	GLY	4.9
1	B	162	GLY	4.8
1	A	264	THR	4.8
1	B	128	ASN	4.8
1	A	116	ILE	4.8
1	B	153	ARG	4.8
1	A	206	VAL	4.8
1	B	320	LEU	4.8
1	B	101	GLN	4.8
1	B	240	GLU	4.8
1	A	195	ASP	4.8
1	B	65	THR	4.8
1	B	59	VAL	4.8
1	A	39	ILE	4.8
1	A	102	PRO	4.8
1	A	173	VAL	4.8
1	A	265	GLY	4.7
1	A	58	THR	4.7
1	A	166	ASP	4.7
1	B	206	VAL	4.7
1	B	25	VAL	4.7
1	B	133	SER	4.7
1	A	56	ASP	4.7
1	A	269	PRO	4.6
1	B	326	LYS	4.6
1	A	140	VAL	4.6
1	B	129	ASP	4.6
1	B	313	MET	4.6
1	B	184	ASN	4.6
1	A	203	LYS	4.6
1	B	327	ILE	4.6
1	A	145	ARG	4.6
1	B	60	GLY	4.6
1	A	253	VAL	4.6
1	B	188	THR	4.6
1	A	153	ARG	4.6
1	A	225	GLU	4.6
1	B	77	ARG	4.6
1	A	232	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	121	GLN	4.5
1	A	69	ILE	4.5
1	A	142	LEU	4.5
1	A	223	GLU	4.5
1	A	124	LEU	4.5
1	A	70	ALA	4.5
1	B	75	ASN	4.5
1	A	112	ASP	4.4
1	A	296	GLY	4.4
1	B	40	ALA	4.4
1	B	43	ASP	4.4
1	B	96	ALA	4.4
1	B	54	LYS	4.4
1	A	49	VAL	4.4
1	B	208	GLY	4.4
1	B	85	ASP	4.4
1	B	299	GLU	4.4
1	A	97	GLY	4.4
1	B	69	ILE	4.4
1	B	50	PHE	4.3
1	A	147	LEU	4.3
1	B	323	GLN	4.3
1	A	57	ASP	4.3
1	B	53	ILE	4.3
1	A	52	ASP	4.3
1	B	100	ARG	4.3
1	A	117	MET	4.2
1	A	42	ARG	4.2
1	A	50	PHE	4.2
1	B	194	GLY	4.2
1	A	321	SER	4.2
1	A	34	ALA	4.2
1	A	221	GLY	4.2
1	A	324	TYR	4.2
1	A	251	ARG	4.2
1	B	227	LEU	4.2
1	B	244	ALA	4.2
1	B	276	GLY	4.2
1	B	315	ASP	4.1
1	B	301	VAL	4.1
1	A	326	LYS	4.1
1	B	136	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	282	GLU	4.1
1	B	161	PHE	4.1
1	B	319	LYS	4.1
1	B	181	PRO	4.1
1	A	325	ASP	4.1
1	B	31	VAL	4.1
1	B	140	VAL	4.1
1	B	204	VAL	4.1
1	A	78	VAL	4.1
1	A	71	TYR	4.1
1	A	152	ASP	4.0
1	B	39	ILE	4.0
1	A	55	GLU	4.0
1	B	63	ALA	4.0
1	A	226	GLN	4.0
1	A	54	LYS	4.0
1	A	88	GLY	4.0
1	B	67	HIS	4.0
1	B	234	SER	4.0
1	A	177	GLU	4.0
1	A	246	GLU	4.0
1	B	304	ASP	4.0
1	A	63	ALA	3.9
1	A	319	LYS	3.9
1	B	221	GLY	3.9
1	B	177	GLU	3.9
1	A	249	PRO	3.9
1	A	328	SER	3.9
1	B	203	LYS	3.9
1	B	228	LEU	3.9
1	B	45	ALA	3.9
1	B	42	ARG	3.8
1	B	223	GLU	3.8
1	A	87	ALA	3.8
1	B	277	GLU	3.8
1	B	165	LEU	3.8
1	B	300	ILE	3.7
1	A	143	LEU	3.7
1	B	190	LEU	3.7
1	B	200	VAL	3.7
1	B	130	ASP	3.7
1	B	294	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	247	TRP	3.7
1	B	170	PHE	3.7
1	B	117	MET	3.6
1	A	278	PHE	3.6
1	A	35	ALA	3.6
1	A	169	ARG	3.6
1	A	92	VAL	3.6
1	B	35	ALA	3.6
1	A	33	ALA	3.6
1	A	139	PRO	3.6
1	A	244	ALA	3.6
1	B	196	ALA	3.6
1	B	111	GLY	3.5
1	B	257	VAL	3.5
1	A	154	SER	3.5
1	A	82	GLY	3.5
1	A	297	VAL	3.5
1	B	141	ASP	3.5
1	A	313	MET	3.5
1	B	256	MET	3.5
1	B	272	VAL	3.5
1	B	37	TYR	3.4
1	B	261	LEU	3.4
1	B	193	HIS	3.4
1	B	289	PRO	3.4
1	B	268	LEU	3.4
1	B	76	THR	3.4
1	B	249	PRO	3.4
1	A	182	VAL	3.4
1	A	310	GLN	3.4
1	B	47	GLU	3.4
1	A	98	ILE	3.4
1	B	290	VAL	3.3
1	B	89	SER	3.3
1	B	53(B)	ASP	3.3
1	B	90	ASP	3.3
1	B	110	ALA	3.3
1	B	235	ALA	3.3
1	B	302	GLU	3.3
1	B	187	GLY	3.3
1	B	171	ARG	3.2
1	A	207	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	3.2
1	B	94	ILE	3.2
1	B	295	ASN	3.2
1	B	220	SER	3.2
1	A	30	THR	3.2
1	B	145	ARG	3.1
1	A	99	PRO	3.1
1	B	248	GLY	3.1
1	B	291	ARG	3.1
1	A	327	ILE	3.1
1	A	31	VAL	3.1
1	B	303	TRP	3.1
1	B	273	LYS	3.1
1	B	98	ILE	3.1
1	B	132	ILE	3.1
1	B	23	VAL	3.0
1	B	28	ALA	3.0
1	B	135	THR	3.0
1	B	285	ALA	3.0
1	A	100	ARG	2.9
1	A	241	ARG	2.9
1	B	279	GLY	2.9
1	B	265	GLY	2.9
1	B	195	ASP	2.9
1	B	48	VAL	2.8
1	B	53(A)	PRO	2.8
1	B	241	ARG	2.8
1	B	201	PHE	2.8
1	A	228	LEU	2.8
1	A	36	GLY	2.8
1	A	289	PRO	2.7
1	A	240	GLU	2.7
1	A	275	GLU	2.7
1	B	70	ALA	2.7
1	B	149	GLU	2.6
1	B	61	GLN	2.6
1	B	106	ARG	2.6
1	A	276	GLY	2.6
1	B	174	LEU	2.6
1	B	229	GLY	2.6
1	A	277	GLU	2.5
1	A	268	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	VAL	2.5
1	B	32	GLY	2.5
1	A	103	GLY	2.4
1	B	33	ALA	2.4
1	B	91	VAL	2.4
1	A	174	LEU	2.3
1	B	143	LEU	2.2
1	B	112	ASP	2.2
1	B	147	LEU	2.2
1	A	201	PHE	2.2
1	B	159	ILE	2.2
1	B	246	GLU	2.2
1	A	43	ASP	2.1
1	B	142	LEU	2.1
1	B	275	GLU	2.1
1	B	139	PRO	2.0
1	A	305	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.

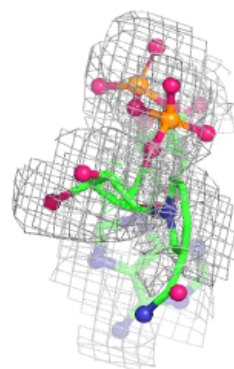
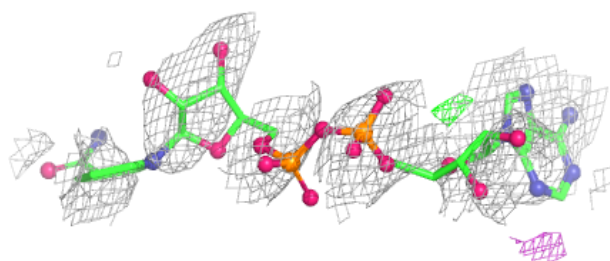
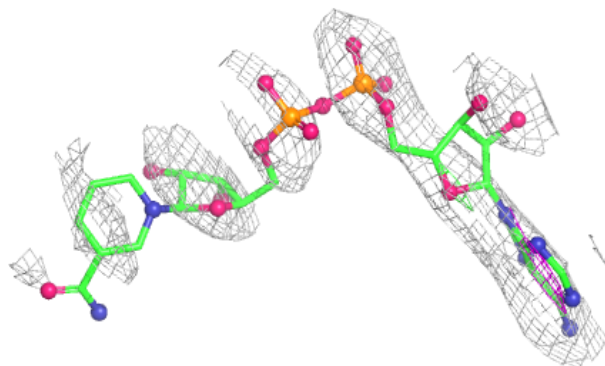
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	330	44/44	0.44	0.42	21,31,36,39	0
2	NAD	A	330	44/44	0.52	0.34	20,29,34,36	0

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.

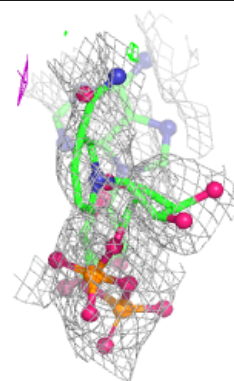
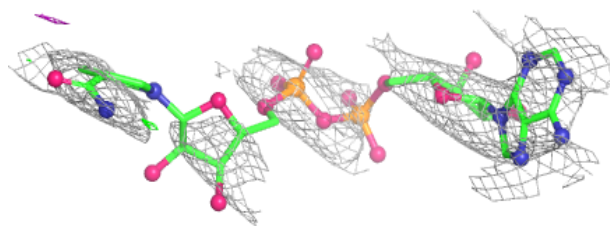
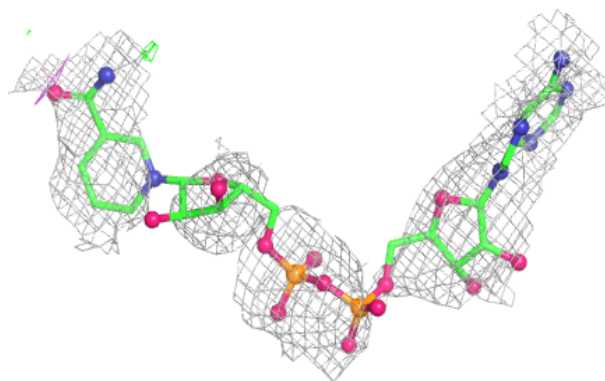
Electron density around NAD B 330:

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



Electron density around NAD A 330:

$2mF_o-DF_c$ (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.