



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 09:33 PM EDT

PDB ID : 1T2F
Title : Human B lactate dehydrogenase complexed with NAD⁺ and 4-hydroxy-1,2,5-oxadiazole-3-carboxylic acid
Authors : Cameron, A.; Read, J.; Tranter, R.; Winter, V.J.; Sessions, R.B.; Brady, R.L.; Vivas, L.; Easton, A.; Kendrick, H.; Croft, S.L.; Barros, D.; Lavandera, J.L.; Martin, J.J.; Risco, F.; Garcia-Ochoa, S.; Gamo, F.J.; Sanz, L.; Leon, L.; Ruiz, J.R.; Gabarro, R.; Mallo, A.; De Las Heras, F.G.
Deposited on : 2004-04-21
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

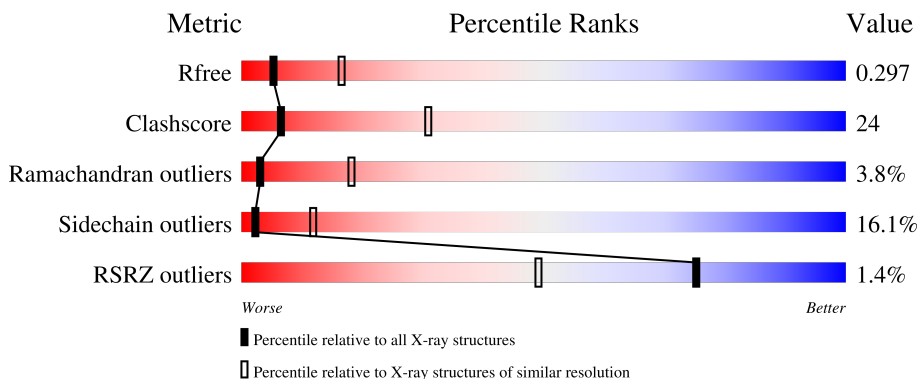
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)


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	333	
1	B	333	
1	C	333	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35

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Mol	Chain	Length	Quality of chain
1	D	333	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '50%', a yellow segment in the middle labeled '38%', and a red segment on the right labeled '10%'. A small red square is positioned at the very beginning of the bar, and a small black dot is at the very end.</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10665 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 L-lactate dehydrogenase B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2555	1627	430	484	14	51	0	0
1	B	332	2555	1627	430	484	14	71	0	0
1	C	332	2555	1627	430	484	14	65	0	0
1	D	332	2555	1627	430	484	14	78	0	0

There are 4 discrepancies between the modelled and reference sequences:

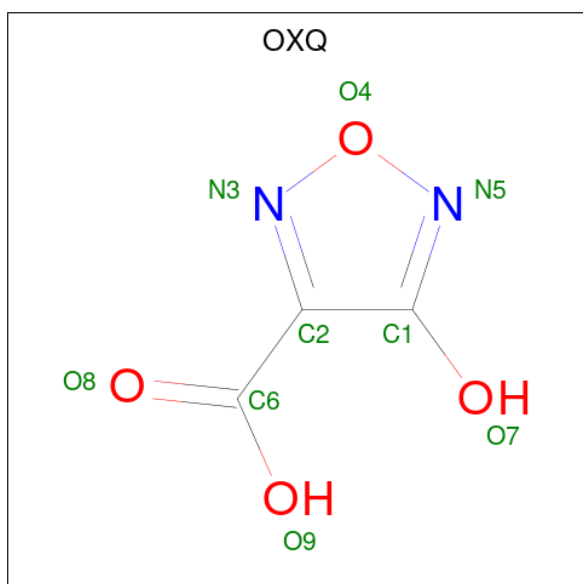
Chain	Residue	Modelled	Actual	Comment	Reference
A	332	PHE	ASP	engineered mutation	UNP P07195
B	332	PHE	ASP	engineered mutation	UNP P07195
C	332	PHE	ASP	engineered mutation	UNP P07195
D	332	PHE	ASP	engineered mutation	UNP P07195

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is 4-HYDROXY-1,2,5-OXADIAZOLE-3-CARBOXYLIC ACID (three-letter code: OXQ) (formula: C₃H₂N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	3	2	4		
3	B	1	Total	C	N	O	0	0
			9	3	2	4		
3	C	1	Total	C	N	O	0	0
			9	3	2	4		
3	D	1	Total	C	N	O	0	0
			9	3	2	4		

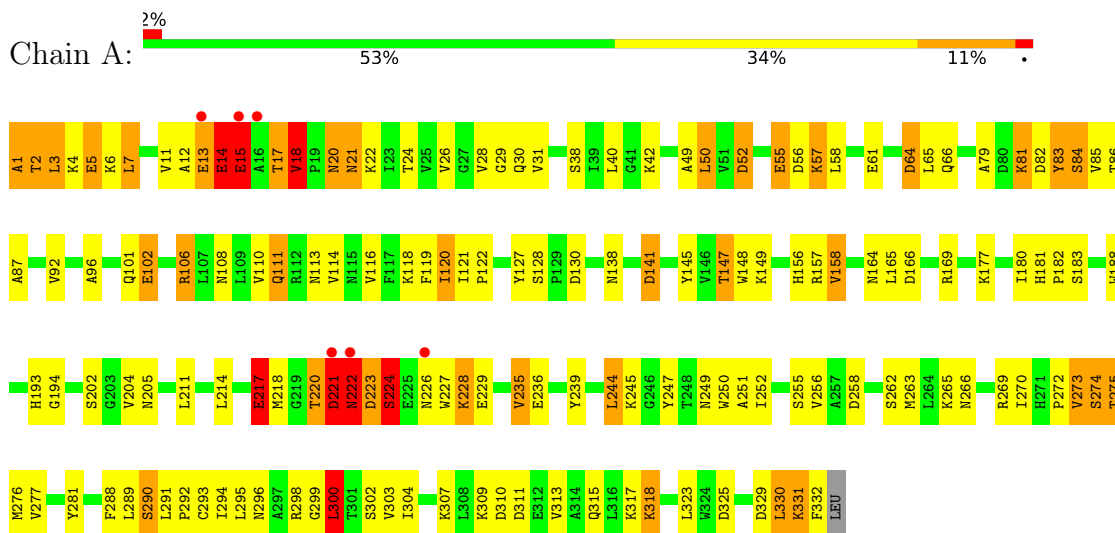
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	76	Total	O	0	0
			76	76		
4	C	48	Total	O	0	0
			48	48		
4	D	43	Total	O	0	0
			43	43		

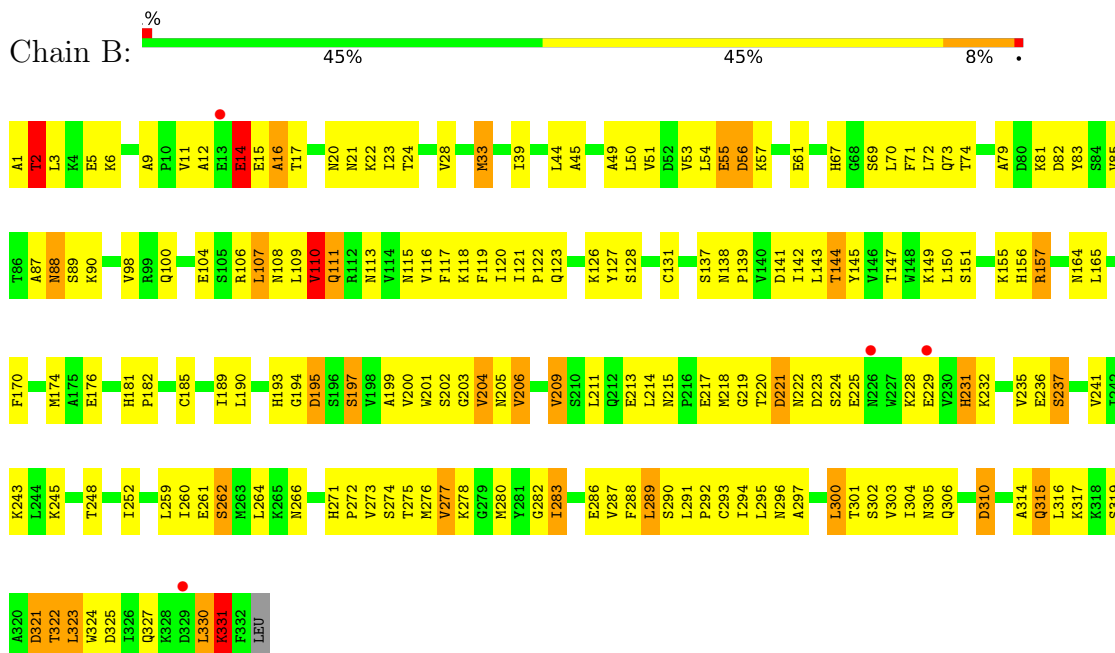
3 Residue-property plots [i](#)

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.

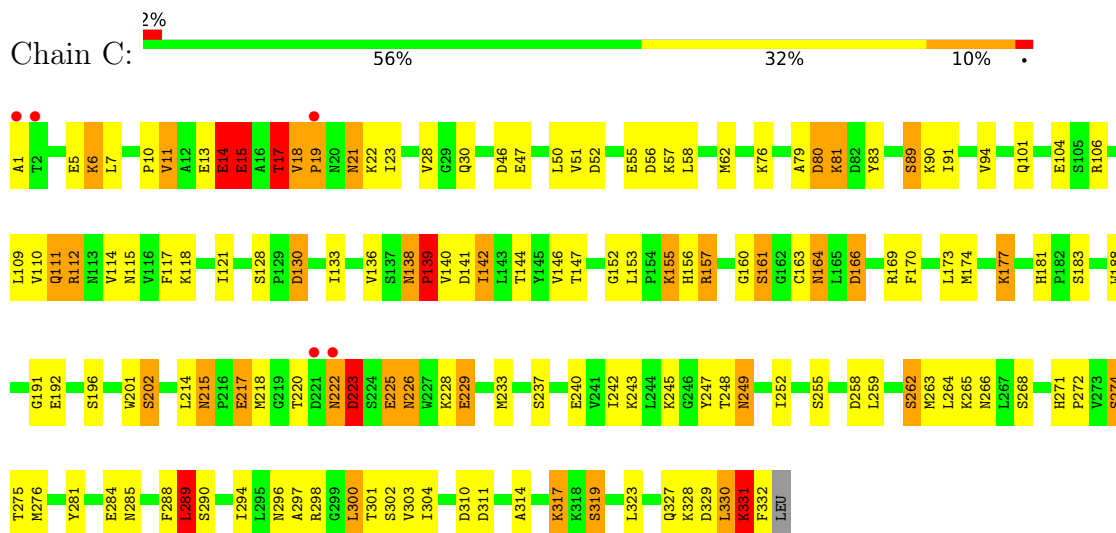
- Molecule 1: L-lactate dehydrogenase B chain



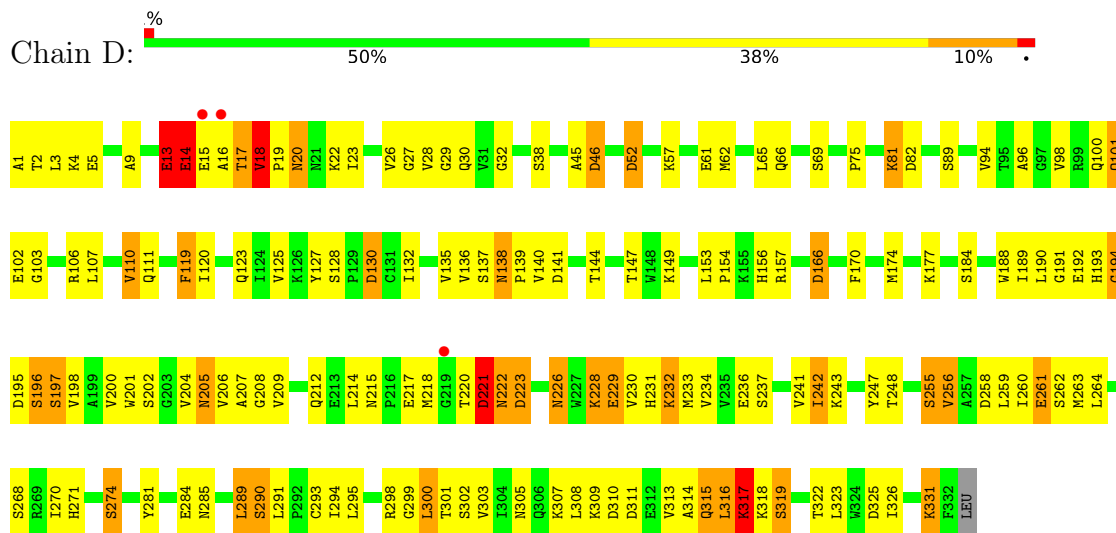
- Molecule 1: L-lactate dehydrogenase B chain



- Molecule 1: L-lactate dehydrogenase B chain



• Molecule 1: L-lactate dehydrogenase B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.40Å 160.44Å 59.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.00 28.90 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.88-3.00) 90.3 (28.90-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.215 , 0.321 0.201 , 0.297	Depositor DCC
R_{free} test set	1247 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	0.292	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10665	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0889e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXQ, 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	1.26	8/2597 (0.3%)	1.28	18/3520 (0.5%)
1	B	1.19	6/2597 (0.2%)	1.19	24/3520 (0.7%)
1	C	1.24	8/2597 (0.3%)	1.28	29/3520 (0.8%)
1	D	1.49	13/2597 (0.5%)	1.52	36/3520 (1.0%)
All	All	1.30	35/10388 (0.3%)	1.32	107/14080 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	1	3
1	C	2	2
1	D	4	0
All	All	8	7

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	GLU	CA-CB	-33.15	0.81	1.53
1	D	119	PHE	CB-CG	29.10	2.00	1.51
1	A	222	ASN	CA-CB	27.49	2.24	1.53
1	D	318	LYS	CA-CB	-27.04	0.94	1.53
1	D	217	GLU	CB-CG	-26.53	1.01	1.52
1	B	217	GLU	CA-CB	-26.11	0.96	1.53
1	A	221	ASP	CA-CB	-23.00	1.03	1.53
1	B	221	ASP	CA-CB	-19.59	1.10	1.53
1	D	229	GLU	CB-CG	-18.69	1.16	1.52
1	C	317	LYS	CG-CD	16.33	2.08	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	LYS	CA-CB	-16.11	1.18	1.53
1	C	229	GLU	CB-CG	16.04	1.82	1.52
1	B	145	TYR	CB-CG	15.21	1.74	1.51
1	D	214	LEU	CA-CB	-15.10	1.19	1.53
1	D	13	GLU	CB-CG	14.89	1.80	1.52
1	D	4	LYS	CG-CD	-12.71	1.09	1.52
1	A	14	GLU	CA-CB	12.37	1.81	1.53
1	D	284	GLU	CA-CB	-12.26	1.26	1.53
1	A	228	LYS	CB-CG	-12.07	1.20	1.52
1	B	14	GLU	CA-CB	-12.00	1.27	1.53
1	B	225	GLU	CA-CB	-11.14	1.29	1.53
1	C	217	GLU	CA-CB	-9.23	1.33	1.53
1	C	331	LYS	CA-CB	9.10	1.74	1.53
1	A	217	GLU	CA-CB	-7.97	1.36	1.53
1	D	221	ASP	CA-CB	7.70	1.70	1.53
1	A	118	LYS	CB-CG	7.58	1.73	1.52
1	A	331	LYS	CA-CB	-7.02	1.38	1.53
1	D	81	LYS	CG-CD	7.01	1.76	1.52
1	D	307	LYS	CB-CG	6.82	1.71	1.52
1	D	228	LYS	CB-CG	-6.72	1.34	1.52
1	C	298	ARG	CA-CB	6.22	1.67	1.53
1	D	317	LYS	CA-CB	-5.71	1.41	1.53
1	C	101	GLN	CA-CB	-5.08	1.42	1.53
1	C	228	LYS	CA-CB	-5.05	1.42	1.53
1	A	298	ARG	CB-CG	-5.04	1.39	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	27.37	173.62	113.40
1	D	318	LYS	CA-CB-CG	27.25	173.35	113.40
1	D	119	PHE	CB-CG-CD2	20.86	135.40	120.80
1	A	221	ASP	N-CA-CB	20.71	147.88	110.60
1	D	331	LYS	N-CA-CB	20.29	147.12	110.60
1	C	6	LYS	CA-CB-CG	19.84	157.04	113.40
1	D	119	PHE	CB-CG-CD1	-19.63	107.06	120.80
1	D	221	ASP	CB-CA-C	19.38	149.16	110.40
1	D	317	LYS	CA-CB-CG	18.01	153.02	113.40
1	D	222	ASN	CB-CA-C	17.33	145.05	110.40
1	B	217	GLU	CB-CA-C	16.04	142.49	110.40
1	A	221	ASP	CB-CA-C	-14.65	81.10	110.40
1	C	6	LYS	CB-CA-C	14.12	138.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ASN	CB-CA-C	-14.10	82.20	110.40
1	C	331	LYS	CB-CA-C	13.30	137.01	110.40
1	C	331	LYS	N-CA-CB	-12.98	87.23	110.60
1	D	22	LYS	CB-CA-C	12.81	136.01	110.40
1	C	284	GLU	CA-CB-CG	12.76	141.47	113.40
1	D	214	LEU	CB-CA-C	12.23	133.43	110.20
1	C	14	GLU	N-CA-CB	-11.29	90.27	110.60
1	D	222	ASN	N-CA-CB	-11.21	90.42	110.60
1	B	145	TYR	CB-CG-CD2	11.08	127.65	121.00
1	C	14	GLU	CB-CA-C	-11.02	88.37	110.40
1	A	222	ASN	CA-CB-CG	-10.45	90.40	113.40
1	B	220	THR	N-CA-CB	-10.44	90.47	110.30
1	B	145	TYR	CB-CG-CD1	-10.24	114.85	121.00
1	B	14	GLU	N-CA-CB	10.15	128.88	110.60
1	A	119	PHE	CB-CA-C	-9.62	91.15	110.40
1	B	217	GLU	N-CA-CB	-9.58	93.36	110.60
1	B	14	GLU	CA-CB-CG	9.32	133.91	113.40
1	B	225	GLU	N-CA-CB	-9.12	94.19	110.60
1	B	225	GLU	CB-CA-C	9.08	128.57	110.40
1	D	317	LYS	CB-CA-C	9.07	128.54	110.40
1	A	119	PHE	N-CA-CB	-8.85	94.68	110.60
1	D	229	GLU	CA-CB-CG	-8.84	93.96	113.40
1	B	310	ASP	CB-CG-OD2	8.81	126.23	118.30
1	C	217	GLU	CB-CA-C	8.80	128.00	110.40
1	C	6	LYS	N-CA-CB	-8.71	94.93	110.60
1	D	228	LYS	CA-CB-CG	8.65	132.44	113.40
1	D	229	GLU	CB-CG-CD	-8.60	90.98	114.20
1	D	141	ASP	CB-CG-OD2	8.38	125.84	118.30
1	B	6	LYS	CA-CB-CG	-8.37	95.00	113.40
1	D	82	ASP	CB-CG-OD2	8.12	125.61	118.30
1	C	228	LYS	N-CA-CB	8.01	125.01	110.60
1	D	130	ASP	CB-CG-OD2	7.98	125.48	118.30
1	D	318	LYS	N-CA-CB	7.94	124.89	110.60
1	D	46	ASP	CB-CG-OD2	7.77	125.29	118.30
1	C	229	GLU	CA-CB-CG	-7.72	96.41	113.40
1	B	243	LYS	CB-CA-C	7.64	125.69	110.40
1	C	14	GLU	CA-CB-CG	7.47	129.84	113.40
1	C	155	LYS	N-CA-CB	-7.29	97.49	110.60
1	C	317	LYS	CG-CD-CE	-7.26	90.13	111.90
1	A	141	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	52	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	155	LYS	CB-CA-C	6.95	124.30	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	LYS	CB-CG-CD	6.91	129.56	111.60
1	C	80	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	243	LYS	N-CA-CB	-6.61	98.70	110.60
1	D	221	ASP	CA-CB-CG	6.59	127.90	113.40
1	C	317	LYS	CB-CG-CD	-6.58	94.48	111.60
1	B	325	ASP	CB-CG-OD2	6.55	124.20	118.30
1	D	52	ASP	CB-CG-OD2	6.54	124.18	118.30
1	B	221	ASP	CB-CA-C	6.53	123.45	110.40
1	B	221	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	310	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	6	LYS	CB-CG-CD	-6.44	94.86	111.60
1	D	307	LYS	CA-CB-CG	-6.28	99.59	113.40
1	C	130	ASP	CB-CG-OD2	6.26	123.94	118.30
1	D	284	GLU	N-CA-CB	-6.22	99.40	110.60
1	D	222	ASN	CA-CB-CG	6.20	127.04	113.40
1	A	14	GLU	N-CA-CB	-6.09	99.64	110.60
1	B	155	LYS	N-CA-CB	6.08	121.55	110.60
1	C	223	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	64	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	284	GLU	CA-CB-CG	-6.07	100.05	113.40
1	C	228	LYS	CB-CA-C	6.04	122.47	110.40
1	D	101	GLN	CA-CB-CG	5.93	126.44	113.40
1	D	258	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	101	GLN	CB-CA-C	5.85	122.11	110.40
1	C	284	GLU	CB-CA-C	5.85	122.10	110.40
1	B	220	THR	CA-CB-CG2	5.83	120.56	112.40
1	A	300	LEU	CA-CB-CG	5.81	128.66	115.30
1	D	221	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	56	ASP	CB-CG-OD2	5.67	123.41	118.30
1	D	223	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	329	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	310	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	228	LYS	CA-CB-CG	5.49	125.47	113.40
1	D	214	LEU	N-CA-CB	-5.47	99.46	110.40
1	B	195	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	221	ASP	N-CA-CB	-5.44	100.81	110.60
1	D	325	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	331	LYS	CB-CA-C	-5.40	99.59	110.40
1	A	119	PHE	CA-CB-CG	-5.31	101.15	113.90
1	C	112	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	139	PRO	N-CD-CG	-5.30	95.26	103.20
1	B	82	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	LEU	CA-CB-CG	5.25	127.38	115.30
1	C	166	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	259	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	317	LYS	N-CA-CB	5.16	119.89	110.60
1	A	298	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	14	GLU	CA-CB-CG	5.10	124.61	113.40
1	A	4	LYS	CA-CB-CG	5.08	124.57	113.40
1	B	321	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	217	GLU	CB-CA-C	-5.04	100.32	110.40
1	B	82	ASP	CB-CG-OD1	5.00	122.80	118.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	221	ASP	CA
1	B	222	ASN	CA
1	C	6	LYS	CA
1	C	284	GLU	CA
1	D	221	ASP	CA
1	D	222	ASN	CA
1	D	317	LYS	CA
1	D	318	LYS	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	15	GLU	Peptide
1	B	1	ALA	Peptide
1	B	139	PRO	Peptide
1	B	222	ASN	Peptide
1	C	138	ASN	Peptide
1	C	17	THR	Peptide

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2555	0	2627	126	4
1	B	2555	0	2627	149	4
1	C	2555	0	2627	113	3
1	D	2555	0	2627	109	3
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	4	0
2	D	44	0	26	4	0
3	A	9	0	0	1	0
3	B	9	0	0	1	0
3	C	9	0	0	3	0
3	D	9	0	0	2	0
4	A	66	0	0	17	0
4	B	76	0	0	34	0
4	C	48	0	0	27	0
4	D	43	0	0	13	0
All	All	10665	0	10612	485	7

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 24.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ILE:HB	4:C:452:HOH:O	1.29	1.24
1:B:324:TRP:HB3	4:B:456:HOH:O	1.38	1.23
1:C:152:GLY:HA3	4:C:454:HOH:O	1.42	1.18
1:C:302:SER:HB2	4:C:452:HOH:O	1.49	1.12
1:A:229:GLU:HG3	4:A:456:HOH:O	1.48	1.10
1:C:14:GLU:HA	1:C:15:GLU:HB3	1.25	1.09
1:C:163:CYS:HB2	4:C:435:HOH:O	1.55	1.04
1:B:149:LYS:NZ	1:B:286:GLU:OE1	1.93	1.01
1:A:329:ASP:HB2	4:A:452:HOH:O	1.61	0.98
1:D:75:PRO:HA	4:D:451:HOH:O	1.62	0.98
1:B:306:GLN:HB3	4:B:472:HOH:O	1.64	0.97
1:A:318:LYS:HZ2	1:A:318:LYS:HB3	1.28	0.97
1:A:309:LYS:HG3	4:A:463:HOH:O	1.66	0.93
1:B:327:GLN:HA	1:B:330:LEU:HD22	1.48	0.92
1:C:17:THR:HB	4:C:442:HOH:O	1.70	0.92
1:B:115:ASN:HB3	4:B:451:HOH:O	1.69	0.92
1:B:202:SER:HB2	4:B:469:HOH:O	1.69	0.90
1:C:14:GLU:CA	1:C:15:GLU:HB3	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:O	1:B:293:CYS:SG	2.33	0.85
1:B:121:ILE:HD12	1:B:147:THR:HG23	1.58	0.85
1:C:18:VAL:HG22	4:C:424:HOH:O	1.74	0.85
1:A:22:LYS:NZ	1:A:85:VAL:O	2.08	0.84
1:A:229:GLU:HB3	4:A:455:HOH:O	1.76	0.84
1:A:166:ASP:HA	4:A:460:HOH:O	1.76	0.84
1:C:152:GLY:CA	4:C:454:HOH:O	2.10	0.84
1:A:318:LYS:HB3	1:A:318:LYS:NZ	1.93	0.83
1:C:217:GLU:O	1:C:220:THR:HG22	1.79	0.83
1:A:329:ASP:C	4:A:452:HOH:O	2.17	0.82
1:C:14:GLU:HA	1:C:15:GLU:CB	2.07	0.82
1:D:196:SER:HB2	1:D:319:SER:OG	1.79	0.82
1:D:138:ASN:HD22	1:D:140:VAL:N	1.79	0.81
1:A:82:ASP:OD1	1:A:84:SER:OG	2.00	0.79
1:A:110:VAL:O	1:A:114:VAL:HG23	1.83	0.79
1:B:113:ASN:O	1:B:116:VAL:HB	1.84	0.78
1:B:138:ASN:ND2	4:B:480:HOH:O	1.94	0.78
1:A:329:ASP:CB	4:A:452:HOH:O	2.21	0.78
1:A:262:SER:OG	1:A:269:ARG:NH2	2.17	0.78
1:A:204:VAL:O	4:A:428:HOH:O	2.01	0.78
1:B:165:LEU:O	1:B:165:LEU:HD12	1.84	0.78
1:B:266:ASN:HD22	1:B:297:ALA:H	1.29	0.77
1:D:281:TYR:CE2	1:D:308:LEU:HD12	2.20	0.76
1:A:223:ASP:O	1:A:224:SER:O	2.03	0.76
1:A:330:LEU:N	4:A:452:HOH:O	2.18	0.76
1:B:201:TRP:HB3	1:B:218:MET:SD	2.27	0.75
1:B:56:ASP:HB2	4:B:452:HOH:O	1.87	0.74
1:B:22:LYS:HZ2	1:B:49:ALA:HB2	1.51	0.74
1:B:229:GLU:OE1	4:B:444:HOH:O	2.06	0.74
1:C:110:VAL:O	1:C:111:GLN:C	2.26	0.73
1:C:19:PRO:O	4:C:424:HOH:O	2.06	0.73
1:C:161:SER:HB2	4:C:427:HOH:O	1.87	0.73
1:D:1:ALA:N	1:D:5:GLU:OE1	2.22	0.73
1:B:111:GLN:O	4:B:417:HOH:O	2.05	0.73
1:B:181:HIS:CE1	4:B:454:HOH:O	2.42	0.73
1:C:121:ILE:HD12	1:C:147:THR:HG23	1.71	0.72
1:A:3:LEU:HD11	1:B:211:LEU:HD13	1.72	0.71
1:A:169:ARG:HD2	4:A:460:HOH:O	1.90	0.71
1:C:21:ASN:HD22	1:C:90:LYS:NZ	1.87	0.70
1:D:100:GLN:NE2	3:D:408:OXQ:O4	2.23	0.70
1:A:127:TYR:CZ	4:A:459:HOH:O	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:NZ	1:B:85:VAL:O	2.24	0.70
1:B:98:VAL:H	1:B:113:ASN:HD21	1.38	0.70
1:D:222:ASN:HA	4:D:418:HOH:O	1.91	0.70
1:C:15:GLU:HB2	4:C:449:HOH:O	1.91	0.70
1:A:147:THR:HG22	1:A:158:VAL:HG11	1.73	0.70
1:B:252:ILE:HD13	2:B:403:NAD:O7N	1.90	0.70
1:A:21:ASN:ND2	4:A:442:HOH:O	2.25	0.70
1:D:138:ASN:HD22	1:D:140:VAL:H	1.39	0.70
1:C:266:ASN:HD22	1:C:297:ALA:H	1.39	0.69
1:D:309:LYS:O	1:D:313:VAL:HG23	1.93	0.69
1:C:294:ILE:HG22	1:C:294:ILE:O	1.91	0.69
1:D:255:SER:O	1:D:256:VAL:C	2.31	0.69
1:D:198:VAL:HG21	1:D:316:LEU:HD13	1.75	0.68
1:D:212:GLN:O	1:D:215:ASN:C	2.32	0.68
1:B:106:ARG:HB2	4:B:467:HOH:O	1.93	0.68
1:D:138:ASN:ND2	1:D:140:VAL:H	1.91	0.68
1:D:17:THR:O	1:D:19:PRO:HD3	1.93	0.67
1:A:30:GLN:NE2	1:A:247:TYR:CZ	2.62	0.67
1:C:290:SER:HB3	4:C:435:HOH:O	1.94	0.67
1:B:296:ASN:ND2	4:B:475:HOH:O	2.29	0.66
1:D:232:LYS:NZ	1:D:236:GLU:OE2	2.16	0.66
1:B:98:VAL:HA	4:B:458:HOH:O	1.95	0.66
1:C:157:ARG:HD3	4:C:428:HOH:O	1.96	0.66
1:D:128:SER:N	4:D:434:HOH:O	2.29	0.66
1:A:82:ASP:C	1:A:84:SER:H	2.00	0.66
1:D:135:VAL:HG12	1:D:135:VAL:O	1.96	0.66
1:B:170:PHE:CD1	1:B:189:ILE:HD11	2.32	0.65
1:A:181:HIS:HD2	1:A:183:SER:H	1.45	0.65
1:B:28:VAL:HG23	1:B:28:VAL:O	1.96	0.64
1:C:275:THR:O	1:C:288:PHE:HA	1.98	0.64
1:B:113:ASN:O	1:B:116:VAL:N	2.30	0.64
1:B:205:ASN:O	1:B:206:VAL:HG23	1.97	0.64
1:C:163:CYS:HA	1:C:166:ASP:OD2	1.98	0.64
1:A:265:LYS:HG3	4:C:450:HOH:O	1.98	0.63
1:A:188:TRP:HZ3	1:A:272:PRO:HD3	1.64	0.63
1:A:49:ALA:C	1:A:50:LEU:HD23	2.18	0.63
1:B:21:ASN:OD1	1:B:90:LYS:NZ	2.30	0.63
1:D:100:GLN:NE2	4:D:419:HOH:O	2.01	0.63
1:C:1:ALA:HB3	1:C:5:GLU:CD	2.20	0.62
1:C:28:VAL:HG11	1:C:50:LEU:HD13	1.82	0.62
1:D:127:TYR:N	4:D:434:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD23	1:A:50:LEU:N	2.14	0.62
1:C:17:THR:HA	4:C:442:HOH:O	1.98	0.62
1:A:111:GLN:HG3	4:A:467:HOH:O	2.00	0.61
2:A:401:NAD:C4N	3:A:402:OXQ:C1	2.78	0.61
1:A:111:GLN:HB3	4:A:438:HOH:O	2.00	0.61
1:B:314:ALA:HA	4:B:440:HOH:O	2.00	0.61
1:D:241:VAL:HG11	1:D:248:THR:HG22	1.81	0.61
1:B:23:ILE:HD12	1:B:45:ALA:HB2	1.82	0.61
1:D:270:ILE:HA	1:D:293:CYS:O	2.00	0.61
1:B:87:ALA:HA	1:B:127:TYR:O	2.00	0.61
1:B:266:ASN:ND2	1:B:296:ASN:HB2	2.16	0.61
1:A:3:LEU:CD1	1:B:211:LEU:HD13	2.30	0.60
1:B:23:ILE:HD11	1:B:264:LEU:HD11	1.84	0.60
1:D:268:SER:HA	1:D:295:LEU:O	2.00	0.60
1:C:192:GLU:HB3	1:C:196:SER:OG	2.02	0.60
1:A:116:VAL:O	1:A:120:ILE:HG23	2.02	0.60
1:C:196:SER:OG	1:C:319:SER:OG	2.19	0.60
1:A:156:HIS:HB2	1:A:300:LEU:O	2.01	0.60
1:C:290:SER:CB	4:C:435:HOH:O	2.50	0.60
1:A:38:SER:O	1:A:42:LYS:HG3	2.02	0.59
1:B:61:GLU:OE2	4:B:422:HOH:O	2.15	0.59
1:D:89:SER:N	1:D:128:SER:OG	2.34	0.59
1:D:274:SER:HA	1:D:289:LEU:O	2.02	0.59
1:B:44:LEU:HD21	1:B:261:GLU:HG3	1.84	0.59
1:B:50:LEU:HB2	1:B:79:ALA:HB2	1.84	0.59
1:C:242:ILE:HG21	4:C:444:HOH:O	2.03	0.59
1:A:177:LYS:HG2	4:A:451:HOH:O	2.03	0.59
1:C:91:ILE:HD12	1:C:264:LEU:HD21	1.84	0.59
1:A:265:LYS:HE2	4:C:450:HOH:O	2.02	0.59
1:C:138:ASN:ND2	3:C:406:OXQ:N5	2.51	0.59
1:B:45:ALA:O	1:B:74:THR:HG23	2.03	0.59
1:A:42:LYS:NZ	1:A:42:LYS:HB3	2.18	0.58
1:D:153:LEU:O	1:D:154:PRO:C	2.41	0.58
1:C:18:VAL:O	1:C:18:VAL:HG13	2.03	0.58
1:D:110:VAL:HG13	1:D:111:GLN:H	1.68	0.58
1:C:52:ASP:OD2	2:C:405:NAD:O3B	2.13	0.58
1:A:1:ALA:O	1:A:5:GLU:HB2	2.02	0.58
1:B:206:VAL:O	1:B:209:VAL:HG13	2.04	0.58
1:B:223:ASP:HB2	4:B:470:HOH:O	2.03	0.58
1:C:110:VAL:HG13	1:C:111:GLN:N	2.18	0.58
1:B:9:ALA:HB2	1:D:305:ASN:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:PHE:CE2	1:B:143:LEU:HB3	2.38	0.58
1:C:58:LEU:HG	1:C:79:ALA:HB1	1.84	0.58
1:D:52:ASP:OD2	2:D:407:NAD:O3B	2.19	0.58
1:B:11:VAL:HG23	1:D:303:VAL:HG23	1.86	0.57
1:D:192:GLU:OE1	1:D:196:SER:OG	2.17	0.57
1:A:40:LEU:HD11	1:A:65:LEU:HD13	1.87	0.57
1:C:21:ASN:HD22	1:C:90:LYS:HZ2	1.53	0.57
1:C:136:VAL:HG22	1:C:161:SER:HB3	1.87	0.56
1:A:250:TRP:CZ2	1:B:33:MET:HB3	2.40	0.56
1:D:27:GLY:O	1:D:32:GLY:HA3	2.05	0.56
1:D:300:LEU:HD12	1:D:300:LEU:C	2.26	0.56
1:B:203:GLY:O	1:B:204:VAL:C	2.43	0.56
1:D:201:TRP:HB3	1:D:218:MET:SD	2.46	0.56
1:A:82:ASP:O	1:A:84:SER:N	2.39	0.56
1:B:300:LEU:HD12	1:B:300:LEU:C	2.26	0.56
1:A:28:VAL:O	1:A:57:LYS:NZ	2.37	0.56
1:B:327:GLN:O	1:B:330:LEU:HB2	2.06	0.56
1:D:13:GLU:O	1:D:14:GLU:O	2.24	0.56
1:B:305:ASN:OD1	1:D:9:ALA:HB2	2.06	0.55
1:A:293:CYS:HA	1:A:302:SER:O	2.07	0.55
1:D:140:VAL:O	1:D:144:THR:OG1	2.13	0.55
1:B:294:ILE:HD12	1:B:302:SER:OG	2.06	0.55
1:C:255:SER:O	1:C:258:ASP:HB3	2.06	0.55
1:D:106:ARG:NH1	1:D:194:GLY:HA2	2.22	0.55
1:D:226:ASN:HD22	1:D:226:ASN:N	2.04	0.54
1:B:190:LEU:HD12	1:B:200:VAL:HG21	1.89	0.54
1:C:17:THR:O	1:C:18:VAL:HG12	2.07	0.54
1:B:100:GLN:CB	4:B:463:HOH:O	2.56	0.54
1:C:262:SER:OG	1:C:271:HIS:HE1	1.90	0.54
1:B:149:LYS:HZ1	1:B:286:GLU:CD	2.02	0.54
1:D:17:THR:O	1:D:19:PRO:CD	2.56	0.54
1:A:110:VAL:O	1:A:114:VAL:CG2	2.55	0.54
1:D:132:ILE:HG21	1:D:263:MET:SD	2.47	0.54
1:A:265:LYS:CE	4:C:450:HOH:O	2.55	0.54
1:A:295:LEU:CD2	1:A:300:LEU:HD22	2.38	0.54
1:B:303:VAL:HG12	1:B:304:ILE:N	2.23	0.54
1:C:169:ARG:O	1:C:173:LEU:HG	2.08	0.54
1:C:330:LEU:O	1:C:331:LYS:O	2.24	0.54
1:C:10:PRO:HD3	4:C:420:HOH:O	2.07	0.54
1:D:138:ASN:ND2	1:D:140:VAL:N	2.49	0.54
1:A:252:ILE:O	1:A:256:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLU:O	1:B:262:SER:C	2.45	0.53
1:B:286:GLU:CG	4:B:460:HOH:O	2.56	0.53
1:C:259:LEU:O	1:C:263:MET:HG3	2.08	0.53
1:D:191:GLY:C	1:D:289:LEU:HD22	2.28	0.53
1:D:314:ALA:O	1:D:317:LYS:N	2.41	0.53
1:A:181:HIS:CD2	1:A:183:SER:OG	2.62	0.53
1:B:22:LYS:HG2	1:B:89:SER:HA	1.90	0.53
1:B:113:ASN:O	1:B:116:VAL:CB	2.56	0.53
1:B:219:GLY:N	4:B:470:HOH:O	2.40	0.53
1:C:28:VAL:CG1	1:C:50:LEU:HD13	2.37	0.53
1:A:204:VAL:HG12	1:A:211:LEU:HD12	1.91	0.53
1:A:130:ASP:HA	1:A:157:ARG:HH12	1.73	0.53
1:B:100:GLN:HB3	4:B:463:HOH:O	2.09	0.53
1:D:196:SER:CB	1:D:319:SER:OG	2.53	0.53
1:A:13:GLU:O	1:A:15:GLU:HB2	2.09	0.53
1:B:271:HIS:O	1:B:273:VAL:N	2.42	0.52
1:A:17:THR:O	1:A:18:VAL:HG12	2.10	0.52
1:A:165:LEU:O	1:A:166:ASP:C	2.46	0.52
1:B:28:VAL:HG23	1:B:57:LYS:HD3	1.91	0.52
1:A:294:ILE:HB	1:A:302:SER:HB2	1.90	0.52
1:B:147:THR:O	1:B:151:SER:OG	2.18	0.52
1:C:164:ASN:HD22	1:C:272:PRO:HD2	1.75	0.52
1:C:327:GLN:HA	1:C:330:LEU:HD22	1.91	0.52
1:D:196:SER:O	1:D:197:SER:C	2.46	0.52
1:A:58:LEU:HD11	1:A:79:ALA:HB1	1.91	0.52
1:D:295:LEU:HA	1:D:299:GLY:O	2.09	0.52
1:A:18:VAL:CG1	1:A:18:VAL:O	2.58	0.52
1:B:69:SER:O	1:B:72:LEU:N	2.39	0.51
1:B:118:LYS:NZ	1:B:331:LYS:O	2.43	0.51
1:B:306:GLN:CB	4:B:472:HOH:O	2.40	0.51
1:A:256:VAL:HG12	1:A:256:VAL:O	2.10	0.51
1:C:138:ASN:HD21	3:C:406:OXQ:C1	2.22	0.51
1:C:181:HIS:CD2	1:C:183:SER:H	2.28	0.51
1:B:231:HIS:O	1:B:235:VAL:HG23	2.10	0.51
1:C:296:ASN:ND2	1:C:301:THR:OG1	2.42	0.51
1:D:205:ASN:ND2	1:D:208:GLY:H	2.08	0.51
1:B:73:GLN:NE2	1:D:261:GLU:OE2	2.39	0.51
1:B:292:PRO:C	1:B:293:CYS:SG	2.89	0.51
1:A:156:HIS:CB	1:A:300:LEU:O	2.58	0.51
1:A:180:ILE:HG22	1:D:294:ILE:HG12	1.93	0.51
1:B:117:PHE:CD2	1:B:143:LEU:HD22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ASP:CG	1:C:130:ASP:O	2.48	0.51
1:A:223:ASP:O	1:A:224:SER:C	2.49	0.51
1:B:24:THR:OG1	1:B:49:ALA:HB3	2.11	0.51
1:B:164:ASN:HA	1:B:272:PRO:HG2	1.92	0.51
1:B:193:HIS:HD2	4:B:480:HOH:O	1.94	0.51
1:C:136:VAL:O	2:C:405:NAD:H2N	2.10	0.51
1:B:316:LEU:O	1:B:319:SER:HB2	2.11	0.51
1:C:160:GLY:HA3	1:C:274:SER:HB3	1.93	0.51
1:B:39:ILE:HD11	1:B:260:ILE:HD13	1.93	0.51
1:B:107:LEU:C	1:B:109:LEU:H	2.14	0.50
1:A:82:ASP:C	1:A:84:SER:N	2.65	0.50
1:B:83:TYR:CE2	1:B:120:ILE:HG23	2.47	0.50
1:B:83:TYR:CZ	1:B:120:ILE:HG23	2.47	0.50
1:B:113:ASN:OD1	1:B:138:ASN:O	2.29	0.50
1:C:18:VAL:O	1:C:18:VAL:CG1	2.60	0.50
1:A:247:TYR:N	1:A:247:TYR:CD2	2.80	0.50
1:A:156:HIS:HB3	1:C:11:VAL:HG12	1.94	0.50
1:B:53:VAL:HG13	2:B:403:NAD:C2A	2.42	0.50
1:B:54:LEU:O	1:B:55:GLU:C	2.50	0.50
1:B:315:GLN:NE2	4:B:474:HOH:O	2.45	0.50
1:C:220:THR:HG23	1:C:220:THR:O	2.12	0.50
1:B:23:ILE:HG22	1:B:24:THR:N	2.26	0.50
1:C:181:HIS:HD2	1:C:183:SER:HB3	1.77	0.50
1:D:192:GLU:HG3	1:D:323:LEU:HD21	1.92	0.50
1:D:300:LEU:HD12	1:D:300:LEU:O	2.12	0.50
1:A:147:THR:HG22	1:A:158:VAL:CG1	2.41	0.49
1:B:170:PHE:CG	1:B:189:ILE:HD11	2.46	0.49
1:C:22:LYS:HB3	1:C:89:SER:HA	1.94	0.49
1:D:2:THR:HG22	1:D:5:GLU:OE2	2.12	0.49
1:A:164:ASN:HD22	1:A:272:PRO:HD2	1.76	0.49
1:B:120:ILE:O	1:B:123:GLN:N	2.45	0.49
1:C:240:GLU:HG3	4:C:425:HOH:O	2.12	0.49
1:D:212:GLN:O	1:D:215:ASN:N	2.45	0.49
1:C:152:GLY:N	4:C:454:HOH:O	2.35	0.49
1:C:294:ILE:O	1:C:294:ILE:CG2	2.60	0.49
1:B:28:VAL:HB	1:B:33:MET:SD	2.52	0.49
1:C:110:VAL:O	1:C:111:GLN:O	2.29	0.49
1:D:274:SER:HA	1:D:290:SER:HA	1.95	0.49
1:B:194:GLY:N	4:B:433:HOH:O	2.44	0.49
1:C:249:ASN:HA	1:C:252:ILE:HG22	1.94	0.49
1:D:18:VAL:HG22	4:D:430:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ASN:C	1:D:20:ASN:HD22	2.16	0.49
1:C:156:HIS:HB2	1:C:300:LEU:O	2.13	0.49
1:D:110:VAL:HG13	1:D:111:GLN:N	2.28	0.49
1:A:235:VAL:HG12	1:A:236:GLU:N	2.28	0.49
1:B:203:GLY:N	4:B:469:HOH:O	2.45	0.49
1:B:215:ASN:O	1:B:215:ASN:ND2	2.46	0.49
1:B:117:PHE:CG	1:B:143:LEU:HD22	2.48	0.48
1:D:188:TRP:CH2	1:D:270:ILE:HG22	2.48	0.48
1:A:24:THR:HG21	1:A:86:THR:CG2	2.43	0.48
1:B:252:ILE:HD13	2:B:403:NAD:C7N	2.43	0.48
1:D:315:GLN:HG3	4:D:424:HOH:O	2.13	0.48
1:A:26:VAL:HG12	1:A:96:ALA:HB2	1.96	0.48
1:D:262:SER:OG	1:D:271:HIS:HE1	1.96	0.48
1:A:30:GLN:NE2	1:A:247:TYR:OH	2.47	0.48
1:B:149:LYS:NZ	4:B:446:HOH:O	2.35	0.48
1:B:292:PRO:O	1:B:293:CYS:SG	2.72	0.48
1:D:220:THR:O	1:D:221:ASP:O	2.31	0.48
1:A:31:VAL:HA	1:A:249:ASN:HB2	1.94	0.48
1:D:29:GLY:O	1:D:30:GLN:C	2.51	0.48
1:A:281:TYR:HB3	1:A:313:VAL:HG13	1.95	0.48
1:B:195:ASP:HA	1:B:235:VAL:HG13	1.95	0.48
1:B:303:VAL:CG1	1:B:304:ILE:N	2.77	0.48
1:A:236:GLU:HA	1:A:239:TYR:HD1	1.79	0.48
1:B:277:VAL:HB	1:B:283:ILE:HD13	1.96	0.48
1:A:274:SER:HA	1:A:289:LEU:O	2.14	0.48
1:A:295:LEU:HA	1:A:299:GLY:O	2.13	0.48
1:B:144:THR:O	1:B:147:THR:N	2.45	0.47
1:D:138:ASN:HD22	1:D:139:PRO:HA	1.78	0.47
2:D:407:NAD:C4N	3:D:408:OXQ:C1	2.92	0.47
1:A:64:ASP:OD2	1:B:245:LYS:NZ	2.45	0.47
1:A:87:ALA:HA	1:A:127:TYR:O	2.14	0.47
1:A:269:ARG:HG2	1:D:184:SER:OG	2.14	0.47
1:A:318:LYS:NZ	1:A:318:LYS:CB	2.72	0.47
1:B:2:THR:HG22	1:B:5:GLU:H	1.80	0.47
1:C:252:ILE:HD13	2:C:405:NAD:O7N	2.14	0.47
1:A:13:GLU:O	1:A:14:GLU:C	2.53	0.47
1:B:23:ILE:CG2	1:B:24:THR:N	2.77	0.47
1:D:232:LYS:O	1:D:236:GLU:HG2	2.14	0.47
1:B:259:LEU:HD23	1:B:271:HIS:CD2	2.49	0.47
1:C:164:ASN:ND2	1:C:272:PRO:HD2	2.30	0.47
1:A:86:THR:O	1:A:87:ALA:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:NAD:O1A	4:B:424:HOH:O	2.21	0.47
1:D:2:THR:HG23	1:D:5:GLU:H	1.79	0.47
1:D:206:VAL:O	1:D:207:ALA:HB3	2.15	0.46
1:C:110:VAL:O	1:C:114:VAL:HG23	2.15	0.46
1:A:55:GLU:HG3	1:A:81:LYS:HD3	1.96	0.46
1:C:140:VAL:HG21	1:C:161:SER:OG	2.15	0.46
1:A:217:GLU:O	1:A:224:SER:CB	2.64	0.46
1:B:15:GLU:O	1:B:16:ALA:HB2	2.15	0.46
1:B:149:LYS:O	1:B:150:LEU:C	2.53	0.46
1:B:241:VAL:HG11	1:B:248:THR:HG22	1.97	0.46
1:C:191:GLY:HA2	1:C:289:LEU:HD22	1.97	0.46
1:D:170:PHE:CD2	1:D:189:ILE:HD11	2.50	0.46
1:C:201:TRP:O	1:C:202:SER:C	2.53	0.46
1:A:83:TYR:O	1:A:127:TYR:CD1	2.69	0.46
1:A:245:LYS:HG3	1:A:247:TYR:O	2.16	0.46
1:A:273:VAL:O	1:A:290:SER:HA	2.15	0.46
1:A:275:THR:O	1:A:277:VAL:HG13	2.16	0.46
1:B:277:VAL:O	1:B:280:MET:HB2	2.15	0.46
1:C:112:ARG:HG3	4:C:445:HOH:O	2.14	0.46
1:A:40:LEU:CD1	1:A:65:LEU:HD13	2.46	0.46
1:C:51:VAL:HG11	1:C:83:TYR:CZ	2.50	0.46
1:A:3:LEU:O	1:A:7:LEU:N	2.48	0.46
1:A:101:GLN:O	1:A:102:GLU:C	2.55	0.46
1:B:324:TRP:CE3	1:B:327:GLN:HB3	2.51	0.45
1:C:157:ARG:CD	4:C:428:HOH:O	2.62	0.45
1:D:26:VAL:HB	1:D:94:VAL:HA	1.97	0.45
1:D:291:LEU:O	1:D:293:CYS:SG	2.54	0.45
1:A:204:VAL:CG1	1:A:211:LEU:HD12	2.46	0.45
1:B:50:LEU:HB2	1:B:79:ALA:CB	2.45	0.45
1:B:288:PHE:O	1:B:289:LEU:HD23	2.16	0.45
1:C:303:VAL:HG12	1:C:304:ILE:N	2.31	0.45
1:A:57:LYS:O	1:A:58:LEU:C	2.55	0.45
1:B:282:GLY:CA	4:B:464:HOH:O	2.64	0.45
1:B:193:HIS:CD2	4:B:480:HOH:O	2.69	0.45
1:A:169:ARG:HG2	1:B:67:HIS:HB3	1.99	0.45
1:A:220:THR:O	1:A:222:ASN:N	2.50	0.45
1:C:21:ASN:HD22	1:C:90:LYS:HZ3	1.62	0.45
1:D:106:ARG:O	1:D:139:PRO:HD3	2.16	0.45
1:B:275:THR:HA	4:B:466:HOH:O	2.16	0.45
1:B:282:GLY:HA3	4:B:464:HOH:O	2.16	0.45
1:C:259:LEU:HD23	1:C:271:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:N	1:A:122:PRO:CD	2.80	0.45
1:A:130:ASP:HA	1:A:157:ARG:NH1	2.30	0.45
1:A:145:TYR:HB2	1:A:288:PHE:CD2	2.52	0.45
1:C:94:VAL:HG11	1:C:117:PHE:CZ	2.52	0.45
1:D:5:GLU:HB3	4:D:433:HOH:O	2.17	0.45
1:B:156:HIS:HB2	1:B:300:LEU:O	2.17	0.45
1:C:311:ASP:O	1:C:314:ALA:HB3	2.17	0.45
1:D:136:VAL:O	1:D:137:SER:C	2.55	0.45
1:A:61:GLU:O	1:A:65:LEU:HG	2.17	0.45
1:A:255:SER:O	1:A:258:ASP:N	2.49	0.45
1:B:276:MET:HG2	1:B:288:PHE:CE1	2.52	0.45
1:A:106:ARG:NH1	1:A:194:GLY:HA2	2.32	0.44
1:D:190:LEU:HB3	1:D:290:SER:O	2.16	0.44
1:A:20:ASN:HD21	1:C:21:ASN:HD21	1.65	0.44
1:B:236:GLU:O	1:B:237:SER:C	2.55	0.44
1:C:294:ILE:HD12	4:C:452:HOH:O	2.17	0.44
1:A:244:LEU:HB3	1:B:56:ASP:O	2.17	0.44
1:C:14:GLU:CA	1:C:15:GLU:CB	2.79	0.44
1:C:142:ILE:O	1:C:146:VAL:HG23	2.18	0.44
1:D:101:GLN:O	1:D:103:GLY:N	2.51	0.44
1:B:321:ASP:O	1:B:322:THR:C	2.56	0.44
1:D:294:ILE:CD1	1:D:302:SER:OG	2.66	0.44
1:C:160:GLY:HA3	1:C:274:SER:CB	2.47	0.44
1:D:46:ASP:C	1:D:46:ASP:OD1	2.55	0.44
1:D:154:PRO:HB3	1:D:156:HIS:CE1	2.53	0.44
1:C:215:ASN:O	1:C:215:ASN:CG	2.56	0.44
1:A:165:LEU:HD11	1:A:251:ALA:HB1	1.98	0.44
1:B:87:ALA:O	1:B:88:ASN:C	2.55	0.44
1:C:106:ARG:HG3	4:C:423:HOH:O	2.17	0.44
1:D:135:VAL:O	1:D:140:VAL:HG23	2.18	0.44
1:A:113:ASN:ND2	1:A:138:ASN:O	2.45	0.44
1:B:203:GLY:O	1:B:205:ASN:N	2.51	0.44
1:B:301:THR:O	1:B:302:SER:HB3	2.18	0.44
1:C:133:ILE:HG21	1:C:147:THR:HG21	1.98	0.44
1:D:128:SER:C	4:D:434:HOH:O	2.56	0.44
1:D:242:ILE:HG22	1:D:243:LYS:N	2.33	0.44
1:D:125:VAL:C	4:D:434:HOH:O	2.57	0.43
1:A:12:ALA:HB2	1:C:156:HIS:CG	2.53	0.43
1:A:218:MET:HE2	1:A:227:TRP:CD2	2.53	0.43
1:C:47:GLU:CD	1:C:76:LYS:HD3	2.39	0.43
1:D:23:ILE:HD12	1:D:45:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG12	1:A:236:GLU:HG2	2.00	0.43
1:B:286:GLU:HG3	4:B:460:HOH:O	2.17	0.43
4:B:455:HOH:O	1:D:15:GLU:HA	2.17	0.43
1:C:110:VAL:CG1	1:C:111:GLN:N	2.81	0.43
1:A:127:TYR:CE1	4:A:459:HOH:O	2.70	0.43
1:A:293:CYS:SG	1:A:300:LEU:HD11	2.59	0.43
1:B:100:GLN:HB3	1:B:104:GLU:HB3	2.01	0.43
1:C:170:PHE:CE1	1:C:174:MET:CE	3.01	0.43
1:D:62:MET:HG2	1:D:66:GLN:NE2	2.33	0.43
1:A:24:THR:HB	1:A:92:VAL:HG13	2.00	0.43
1:A:277:VAL:HG11	1:A:291:LEU:HD11	1.99	0.43
1:C:19:PRO:HG3	1:C:47:GLU:OE1	2.18	0.43
1:D:230:VAL:O	1:D:234:VAL:HG23	2.19	0.43
1:D:247:TYR:HB2	4:D:420:HOH:O	2.18	0.43
1:A:277:VAL:CG1	1:A:291:LEU:HD11	2.49	0.43
1:B:100:GLN:HB2	4:B:463:HOH:O	2.18	0.43
1:C:30:GLN:CD	1:C:247:TYR:CZ	2.92	0.43
1:C:222:ASN:O	1:C:223:ASP:O	2.37	0.43
1:D:132:ILE:HD13	1:D:157:ARG:HA	2.01	0.43
1:B:106:ARG:HD3	1:B:138:ASN:ND2	2.33	0.42
1:C:215:ASN:O	1:C:218:MET:HB3	2.18	0.42
1:D:69:SER:HB3	4:D:445:HOH:O	2.18	0.42
1:D:120:ILE:O	1:D:123:GLN:HB2	2.18	0.42
1:C:22:LYS:C	1:C:23:ILE:HG13	2.39	0.42
1:C:265:LYS:HD3	4:C:408:HOH:O	2.18	0.42
1:D:300:LEU:C	1:D:300:LEU:CD1	2.87	0.42
1:A:20:ASN:HD21	1:C:21:ASN:ND2	2.18	0.42
1:A:50:LEU:N	1:A:50:LEU:CD2	2.82	0.42
1:B:69:SER:O	1:B:71:PHE:N	2.53	0.42
1:D:170:PHE:CG	1:D:189:ILE:HD11	2.54	0.42
1:A:28:VAL:HG12	1:A:50:LEU:HD13	2.02	0.42
1:A:65:LEU:O	1:A:66:GLN:C	2.58	0.42
1:B:2:THR:HG22	1:B:5:GLU:N	2.34	0.42
1:B:115:ASN:HB2	4:B:417:HOH:O	2.19	0.42
1:B:165:LEU:HD12	1:B:165:LEU:C	2.40	0.42
1:B:174:MET:SD	1:B:185:CYS:HB3	2.60	0.42
1:C:1:ALA:HB3	1:C:5:GLU:CG	2.49	0.42
1:C:153:LEU:HD22	1:C:157:ARG:HH12	1.83	0.42
1:B:2:THR:HG22	1:B:5:GLU:HB2	2.01	0.42
1:B:12:ALA:HB1	1:D:298:ARG:NH2	2.35	0.42
1:B:119:PHE:CD1	1:B:119:PHE:C	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:CG	1:B:266:ASN:O	2.56	0.42
1:B:300:LEU:C	1:B:300:LEU:CD1	2.88	0.42
1:D:153:LEU:C	1:D:154:PRO:O	2.56	0.42
1:A:273:VAL:HG23	1:A:300:LEU:CD2	2.50	0.42
1:C:255:SER:O	1:C:258:ASP:CB	2.68	0.42
1:A:141:ASP:HB3	1:A:288:PHE:O	2.19	0.42
1:B:321:ASP:O	1:B:324:TRP:N	2.53	0.42
1:D:2:THR:HG22	1:D:5:GLU:CD	2.40	0.42
1:B:83:TYR:OH	1:B:120:ILE:HG12	2.20	0.42
1:B:126:LYS:HD3	1:B:127:TYR:CE1	2.54	0.42
1:C:177:LYS:HE2	1:C:226:ASN:ND2	2.35	0.41
1:D:2:THR:HG22	1:D:5:GLU:CG	2.50	0.41
1:D:166:ASP:OD2	1:D:193:HIS:CE1	2.73	0.41
1:D:294:ILE:HD12	1:D:302:SER:OG	2.19	0.41
1:B:274:SER:HA	1:B:290:SER:HA	2.01	0.41
1:C:220:THR:O	1:C:220:THR:CG2	2.68	0.41
1:A:263:MET:HA	1:A:296:ASN:O	2.20	0.41
1:B:142:ILE:HG13	1:B:323:LEU:CD1	2.51	0.41
1:D:301:THR:O	1:D:302:SER:HB3	2.20	0.41
1:D:260:ILE:HG22	1:D:264:LEU:HD12	2.03	0.41
1:A:56:ASP:OD1	4:A:404:HOH:O	2.21	0.41
1:D:65:LEU:O	1:D:66:GLN:C	2.57	0.41
1:A:329:ASP:O	1:A:330:LEU:C	2.58	0.41
1:B:156:HIS:CD2	1:B:157:ARG:HG2	2.55	0.41
1:C:118:LYS:HE2	1:C:332:PHE:HB3	2.01	0.41
1:D:260:ILE:CG2	1:D:264:LEU:HD12	2.51	0.41
2:D:407:NAD:H3B	4:D:443:HOH:O	2.21	0.41
1:B:110:VAL:HG22	1:B:111:GLN:N	2.35	0.41
1:B:121:ILE:HB	1:B:122:PRO:HD3	2.03	0.41
1:B:149:LYS:CE	1:B:286:GLU:OE1	2.68	0.41
1:C:109:LEU:HB2	1:C:139:PRO:HD2	2.03	0.41
1:C:164:ASN:HD22	1:C:164:ASN:HA	1.78	0.41
1:C:225:GLU:O	1:C:226:ASN:CG	2.58	0.41
1:D:18:VAL:HA	1:D:19:PRO:HD2	1.76	0.41
1:A:292:PRO:HB2	1:A:304:ILE:HB	2.03	0.41
1:A:294:ILE:HD11	1:A:304:ILE:HD11	2.03	0.41
1:B:106:ARG:O	1:B:109:LEU:HD12	2.21	0.41
1:B:138:ASN:OD1	3:B:404:OXQ:N5	2.54	0.41
1:B:199:ALA:O	1:B:201:TRP:N	2.54	0.41
1:C:55:GLU:CG	1:C:81:LYS:HD3	2.51	0.41
1:D:2:THR:O	1:D:5:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:O	1:B:209:VAL:CG1	2.69	0.40
1:C:118:LYS:NZ	1:C:332:PHE:HB3	2.35	0.40
1:C:240:GLU:CG	4:C:425:HOH:O	2.69	0.40
1:D:96:ALA:HB1	2:D:407:NAD:C4A	2.51	0.40
1:D:197:SER:HB2	1:D:231:HIS:HE1	1.85	0.40
1:A:28:VAL:HG22	1:A:52:ASP:OD2	2.21	0.40
1:A:270:ILE:HA	1:A:293:CYS:O	2.22	0.40
1:D:57:LYS:NZ	1:D:61:GLU:OE2	2.53	0.40
1:D:197:SER:O	1:D:231:HIS:NE2	2.53	0.40
1:A:24:THR:CG2	1:A:86:THR:HG22	2.51	0.40
1:D:241:VAL:CG1	1:D:248:THR:HG22	2.48	0.40
1:A:29:GLY:O	1:A:30:GLN:C	2.60	0.40
1:C:18:VAL:O	1:C:19:PRO:C	2.60	0.40
1:C:144:THR:HG22	1:C:288:PHE:CD1	2.57	0.40
1:C:188:TRP:CD1	1:C:188:TRP:N	2.89	0.40
2:C:405:NAD:C5N	3:C:406:OXQ:N3	2.85	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:CA	1:B:14:GLU:OE2[1_554]	1.19	1.01
1:C:14:GLU:OE1	1:D:149:LYS:NZ[1_554]	1.69	0.51
1:A:148:TRP:O	1:B:14:GLU:OE1[1_554]	1.75	0.45
1:A:149:LYS:C	1:B:14:GLU:OE2[1_554]	1.78	0.42
1:C:14:GLU:OE2	1:D:149:LYS:NZ[1_554]	1.82	0.38
1:C:14:GLU:CD	1:D:149:LYS:NZ[1_554]	1.94	0.26
1:A:149:LYS:O	1:B:14:GLU:OE2[1_554]	2.02	0.18

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	330/333 (99%)	272 (82%)	45 (14%)	13 (4%)	3	17
1	B	330/333 (99%)	264 (80%)	51 (16%)	15 (4%)	2	14
1	C	330/333 (99%)	275 (83%)	45 (14%)	10 (3%)	4	24
1	D	330/333 (99%)	269 (82%)	49 (15%)	12 (4%)	3	19
All	All	1320/1332 (99%)	1080 (82%)	190 (14%)	50 (4%)	3	18

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	221	ASP
1	A	222	ASN
1	A	224	SER
1	A	226	ASN
1	B	16	ALA
1	B	70	LEU
1	B	110	VAL
1	B	197	SER
1	B	237	SER
1	C	15	GLU
1	C	139	PRO
1	C	331	LYS
1	D	14	GLU
1	D	204	VAL
1	D	221	ASP
1	A	13	GLU
1	A	20	ASN
1	A	331	LYS
1	B	2	THR
1	B	55	GLU
1	B	204	VAL
1	B	213	GLU
1	C	223	ASP
1	D	194	GLY
1	A	193	HIS
1	B	14	GLU
1	B	221	ASP
1	C	104	GLU
1	D	13	GLU
1	D	102	GLU
1	D	200	VAL
1	A	17	THR

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Mol	Chain	Res	Type
1	A	18	VAL
1	A	102	GLU
1	B	144	THR
1	C	226	ASN
1	A	83	TYR
1	B	331	LYS
1	C	18	VAL
1	C	19	PRO
1	C	222	ASN
1	C	249	ASN
1	D	16	ALA
1	D	28	VAL
1	D	18	VAL
1	D	110	VAL
1	B	182	PRO
1	B	206	VAL
1	D	256	VAL

5.3.2 Protein sidechains [i](#)

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	288/289 (100%)	236 (82%)	52 (18%)	1 9
1	B	288/289 (100%)	248 (86%)	40 (14%)	3 16
1	C	288/289 (100%)	241 (84%)	47 (16%)	2 11
1	D	288/289 (100%)	241 (84%)	47 (16%)	2 11
All	All	1152/1156 (100%)	966 (84%)	186 (16%)	2 12

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LEU
1	A	5	GLU
1	A	6	LYS

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Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	VAL
1	A	14	GLU
1	A	15	GLU
1	A	18	VAL
1	A	21	ASN
1	A	50	LEU
1	A	55	GLU
1	A	57	LYS
1	A	81	LYS
1	A	84	SER
1	A	106	ARG
1	A	108	ASN
1	A	111	GLN
1	A	120	ILE
1	A	128	SER
1	A	147	THR
1	A	158	VAL
1	A	182	PRO
1	A	202	SER
1	A	205	ASN
1	A	214	LEU
1	A	217	GLU
1	A	220	THR
1	A	221	ASP
1	A	222	ASN
1	A	223	ASP
1	A	224	SER
1	A	228	LYS
1	A	235	VAL
1	A	244	LEU
1	A	266	ASN
1	A	273	VAL
1	A	274	SER
1	A	275	THR
1	A	276	MET
1	A	290	SER
1	A	300	LEU
1	A	303	VAL
1	A	307	LYS
1	A	311	ASP
1	A	315	GLN

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Mol	Chain	Res	Type
1	A	317	LYS
1	A	318	LYS
1	A	323	LEU
1	A	325	ASP
1	A	330	LEU
1	A	332	PHE
1	B	2	THR
1	B	3	LEU
1	B	17	THR
1	B	20	ASN
1	B	33	MET
1	B	51	VAL
1	B	56	ASP
1	B	81	LYS
1	B	88	ASN
1	B	107	LEU
1	B	108	ASN
1	B	110	VAL
1	B	111	GLN
1	B	128	SER
1	B	131	CYS
1	B	137	SER
1	B	141	ASP
1	B	157	ARG
1	B	176	GLU
1	B	197	SER
1	B	209	VAL
1	B	214	LEU
1	B	224	SER
1	B	228	LYS
1	B	231	HIS
1	B	232	LYS
1	B	262	SER
1	B	277	VAL
1	B	278	LYS
1	B	283	ILE
1	B	287	VAL
1	B	289	LEU
1	B	295	LEU
1	B	300	LEU
1	B	310	ASP
1	B	315	GLN

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Mol	Chain	Res	Type
1	B	317	LYS
1	B	322	THR
1	B	323	LEU
1	B	330	LEU
1	C	6	LYS
1	C	7	LEU
1	C	11	VAL
1	C	13	GLU
1	C	14	GLU
1	C	15	GLU
1	C	17	THR
1	C	21	ASN
1	C	46	ASP
1	C	57	LYS
1	C	62	MET
1	C	80	ASP
1	C	81	LYS
1	C	89	SER
1	C	111	GLN
1	C	115	ASN
1	C	128	SER
1	C	141	ASP
1	C	142	ILE
1	C	155	LYS
1	C	157	ARG
1	C	161	SER
1	C	164	ASN
1	C	177	LYS
1	C	202	SER
1	C	214	LEU
1	C	215	ASN
1	C	225	GLU
1	C	229	GLU
1	C	233	MET
1	C	237	SER
1	C	243	LYS
1	C	245	LYS
1	C	248	THR
1	C	262	SER
1	C	268	SER
1	C	274	SER
1	C	276	MET

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Mol	Chain	Res	Type
1	C	281	TYR
1	C	285	ASN
1	C	289	LEU
1	C	300	LEU
1	C	317	LYS
1	C	319	SER
1	C	323	LEU
1	C	330	LEU
1	C	331	LYS
1	D	3	LEU
1	D	14	GLU
1	D	17	THR
1	D	18	VAL
1	D	20	ASN
1	D	38	SER
1	D	81	LYS
1	D	98	VAL
1	D	107	LEU
1	D	119	PHE
1	D	130	ASP
1	D	138	ASN
1	D	147	THR
1	D	166	ASP
1	D	174	MET
1	D	177	LYS
1	D	195	ASP
1	D	196	SER
1	D	197	SER
1	D	202	SER
1	D	205	ASN
1	D	209	VAL
1	D	221	ASP
1	D	223	ASP
1	D	226	ASN
1	D	228	LYS
1	D	229	GLU
1	D	232	LYS
1	D	233	MET
1	D	237	SER
1	D	242	ILE
1	D	255	SER
1	D	261	GLU

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Mol	Chain	Res	Type
1	D	274	SER
1	D	285	ASN
1	D	289	LEU
1	D	290	SER
1	D	300	LEU
1	D	310	ASP
1	D	311	ASP
1	D	315	GLN
1	D	316	LEU
1	D	317	LYS
1	D	319	SER
1	D	322	THR
1	D	326	ILE
1	D	331	LYS

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

Mol	Chain	Res	Type
1	A	21	ASN
1	A	30	GLN
1	A	108	ASN
1	A	164	ASN
1	A	181	HIS
1	A	205	ASN
1	A	231	HIS
1	A	266	ASN
1	B	20	ASN
1	B	113	ASN
1	B	156	HIS
1	B	164	ASN
1	B	181	HIS
1	B	212	GLN
1	B	266	ASN
1	B	271	HIS
1	B	306	GLN
1	B	315	GLN
1	C	21	ASN
1	C	108	ASN
1	C	115	ASN
1	C	181	HIS
1	C	205	ASN
1	C	212	GLN

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Mol	Chain	Res	Type
1	C	266	ASN
1	C	271	HIS
1	C	327	GLN
1	D	20	ASN
1	D	66	GLN
1	D	113	ASN
1	D	138	ASN
1	D	156	HIS
1	D	181	HIS
1	D	186	HIS
1	D	205	ASN
1	D	226	ASN
1	D	266	ASN
1	D	271	HIS
1	D	315	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	B	403	-	42,48,48	2.05	5 (11%)	50,73,73	2.05	11 (22%)
3	OXQ	D	408	-	5,9,9	1.71	2 (40%)	4,12,12	2.40	1 (25%)
3	OXQ	A	402	-	5,9,9	1.31	1 (20%)	4,12,12	1.67	1 (25%)
2	NAD	D	407	-	42,48,48	2.15	4 (9%)	50,73,73	1.58	10 (20%)
3	OXQ	B	404	-	5,9,9	1.56	1 (20%)	4,12,12	2.22	2 (50%)
2	NAD	C	405	-	42,48,48	1.82	7 (16%)	50,73,73	2.01	10 (20%)
2	NAD	A	401	-	42,48,48	2.00	5 (11%)	50,73,73	1.60	9 (18%)
3	OXQ	C	406	-	5,9,9	1.49	1 (20%)	4,12,12	1.18	0

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	B	403	-	-	11/26/62/62	0/5/5/5
3	OXQ	D	408	-	-	3/3/4/4	0/1/1/1
3	OXQ	A	402	-	-	2/3/4/4	0/1/1/1
2	NAD	D	407	-	-	10/26/62/62	0/5/5/5
3	OXQ	B	404	-	-	2/3/4/4	0/1/1/1
2	NAD	C	405	-	-	6/26/62/62	0/5/5/5
2	NAD	A	401	-	-	4/26/62/62	0/5/5/5
3	OXQ	C	406	-	-	2/3/4/4	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	NAD	O7N-C7N	10.24	1.43	1.24
2	D	407	NAD	O7N-C7N	9.79	1.42	1.24
2	A	401	NAD	O7N-C7N	9.21	1.41	1.24
2	C	405	NAD	O7N-C7N	7.28	1.38	1.24
2	D	407	NAD	C2A-N3A	6.28	1.42	1.32
2	A	401	NAD	C2A-N3A	5.31	1.40	1.32
2	C	405	NAD	C2A-N3A	3.93	1.38	1.32
2	D	407	NAD	C2A-N1A	3.88	1.41	1.33
2	B	403	NAD	C2A-N3A	3.41	1.37	1.32
2	A	401	NAD	C2A-N1A	3.30	1.40	1.33
2	C	405	NAD	C2A-N1A	3.24	1.39	1.33
2	C	405	NAD	C2D-C1D	-3.21	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	OXQ	O9-C6	-3.13	1.21	1.30
2	B	403	NAD	C2A-N1A	3.01	1.39	1.33
2	A	401	NAD	C2D-C1D	-2.88	1.49	1.53
3	C	406	OXQ	O9-C6	-2.83	1.21	1.30
3	D	408	OXQ	O9-C6	-2.70	1.22	1.30
2	D	407	NAD	C2N-N1N	2.68	1.38	1.35
2	C	405	NAD	O4B-C1B	-2.37	1.37	1.41
3	A	402	OXQ	O9-C6	-2.33	1.23	1.30
3	D	408	OXQ	C2-C6	-2.33	1.47	1.51
2	A	401	NAD	O4D-C4D	-2.32	1.39	1.45
2	B	403	NAD	C3N-C7N	2.26	1.54	1.50
2	C	405	NAD	C2B-C1B	-2.13	1.50	1.53
2	B	403	NAD	C2N-N1N	2.07	1.37	1.35
2	C	405	NAD	O3D-C3D	-2.05	1.38	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	NAD	N3A-C2A-N1A	-7.73	116.60	128.68
2	C	405	NAD	C1B-N9A-C4A	-5.77	116.51	126.64
2	C	405	NAD	C3N-C7N-N7N	5.20	123.99	117.75
2	C	405	NAD	O7N-C7N-N7N	-5.08	115.36	122.58
2	C	405	NAD	N3A-C2A-N1A	-4.76	121.23	128.68
2	D	407	NAD	PN-O3-PA	-4.73	116.60	132.83
2	B	403	NAD	C1B-N9A-C4A	-4.59	118.57	126.64
2	C	405	NAD	PN-O3-PA	-4.56	117.19	132.83
2	A	401	NAD	N3A-C2A-N1A	-4.46	121.70	128.68
2	B	403	NAD	O7N-C7N-N7N	-4.29	116.48	122.58
3	D	408	OXQ	C1-C2-C6	-4.27	123.84	131.26
2	B	403	NAD	PN-O3-PA	-4.16	118.54	132.83
2	B	403	NAD	O7N-C7N-C3N	4.06	124.49	119.63
2	D	407	NAD	N3A-C2A-N1A	-4.01	122.42	128.68
2	D	407	NAD	O4B-C1B-C2B	-3.94	101.17	106.93
2	B	403	NAD	O3D-C3D-C4D	-3.60	100.65	111.05
2	A	401	NAD	O4D-C1D-C2D	-3.38	101.99	106.93
2	D	407	NAD	O4D-C1D-C2D	-3.33	102.06	106.93
2	A	401	NAD	PN-O3-PA	-3.23	121.74	132.83
2	A	401	NAD	O2N-PN-O1N	3.22	128.16	112.24
2	A	401	NAD	O4B-C1B-C2B	-3.17	102.30	106.93
3	B	404	OXQ	O8-C6-C2	3.16	127.23	120.73
3	B	404	OXQ	O9-C6-O8	-3.04	116.60	123.35
2	A	401	NAD	C3D-C2D-C1D	-2.91	96.60	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	OXQ	C1-C2-C6	-2.89	126.24	131.26
2	B	403	NAD	O3B-C3B-C2B	-2.86	102.56	111.82
2	C	405	NAD	C5A-C6A-N6A	2.84	124.66	120.35
2	A	401	NAD	C3B-C2B-C1B	2.68	105.01	100.98
2	D	407	NAD	C3B-C2B-C1B	-2.62	97.03	100.98
2	C	405	NAD	O2N-PN-O1N	2.60	125.10	112.24
2	C	405	NAD	C4A-C5A-N7A	-2.48	106.81	109.40
2	B	403	NAD	C3D-C2D-C1D	-2.44	97.30	100.98
2	B	403	NAD	C2A-N1A-C6A	2.42	122.89	118.75
2	C	405	NAD	C3N-C2N-N1N	2.40	122.77	120.43
2	D	407	NAD	O2N-PN-O1N	2.37	123.94	112.24
2	A	401	NAD	O3D-C3D-C2D	-2.35	104.23	111.82
2	D	407	NAD	O2B-C2B-C3B	2.24	119.08	111.82
2	A	401	NAD	O2B-C2B-C3B	-2.19	104.75	111.82
2	D	407	NAD	C3N-C7N-N7N	2.18	120.37	117.75
2	C	405	NAD	O4B-C4B-C5B	2.14	116.41	109.37
2	B	403	NAD	O2D-C2D-C3D	2.08	118.55	111.82
2	B	403	NAD	O4D-C1D-C2D	-2.05	103.94	106.93
2	D	407	NAD	C5A-C6A-N6A	-2.04	117.26	120.35
2	D	407	NAD	O3D-C3D-C4D	-2.01	105.23	111.05

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	403	NAD	C5D-O5D-PN-O3
2	B	403	NAD	O4D-C4D-C5D-O5D
2	B	403	NAD	O4D-C1D-N1N-C2N
2	B	403	NAD	O4D-C1D-N1N-C6N
2	C	405	NAD	O4B-C4B-C5B-O5B
2	C	405	NAD	O4D-C1D-N1N-C2N
2	C	405	NAD	O4D-C1D-N1N-C6N
2	C	405	NAD	C2D-C1D-N1N-C2N
2	C	405	NAD	C2D-C1D-N1N-C6N
2	D	407	NAD	C5B-O5B-PA-O1A
2	D	407	NAD	O4B-C4B-C5B-O5B
2	D	407	NAD	C3B-C4B-C5B-O5B
2	D	407	NAD	O4D-C1D-N1N-C2N
2	D	407	NAD	O4D-C1D-N1N-C6N
2	D	407	NAD	C2D-C1D-N1N-C2N
2	D	407	NAD	C2D-C1D-N1N-C6N
3	A	402	OXQ	C1-C2-C6-O9

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Mol	Chain	Res	Type	Atoms
3	A	402	OXQ	C1-C2-C6-O8
3	B	404	OXQ	C1-C2-C6-O9
3	B	404	OXQ	C1-C2-C6-O8
3	C	406	OXQ	C1-C2-C6-O9
3	C	406	OXQ	C1-C2-C6-O8
3	D	408	OXQ	C1-C2-C6-O9
3	D	408	OXQ	C1-C2-C6-O8
2	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	B	403	NAD	O4B-C4B-C5B-O5B
2	B	403	NAD	C3B-C4B-C5B-O5B
2	B	403	NAD	C3D-C4D-C5D-O5D
2	A	401	NAD	O4D-C4D-C5D-O5D
2	C	405	NAD	C3B-C4B-C5B-O5B
3	D	408	OXQ	N3-C2-C6-O8
2	B	403	NAD	C5B-O5B-PA-O2A
2	B	403	NAD	C5D-O5D-PN-O1N
2	B	403	NAD	C5D-O5D-PN-O2N
2	D	407	NAD	C5B-O5B-PA-O2A
2	B	403	NAD	C2D-C1D-N1N-C2N
2	D	407	NAD	C5B-O5B-PA-O3
2	D	407	NAD	PA-O3-PN-O1N
2	A	401	NAD	C3D-C4D-C5D-O5D

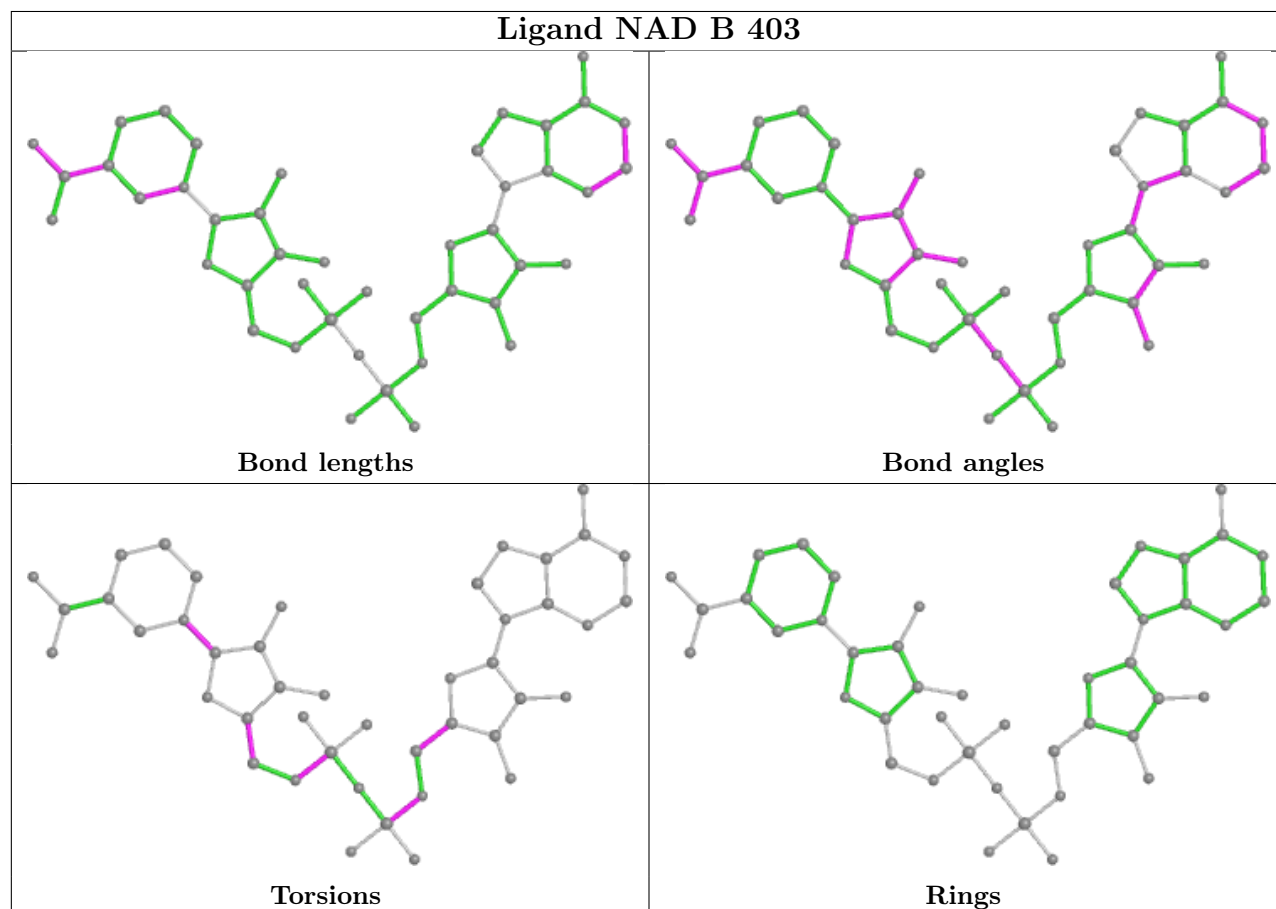
There are no ring outliers.

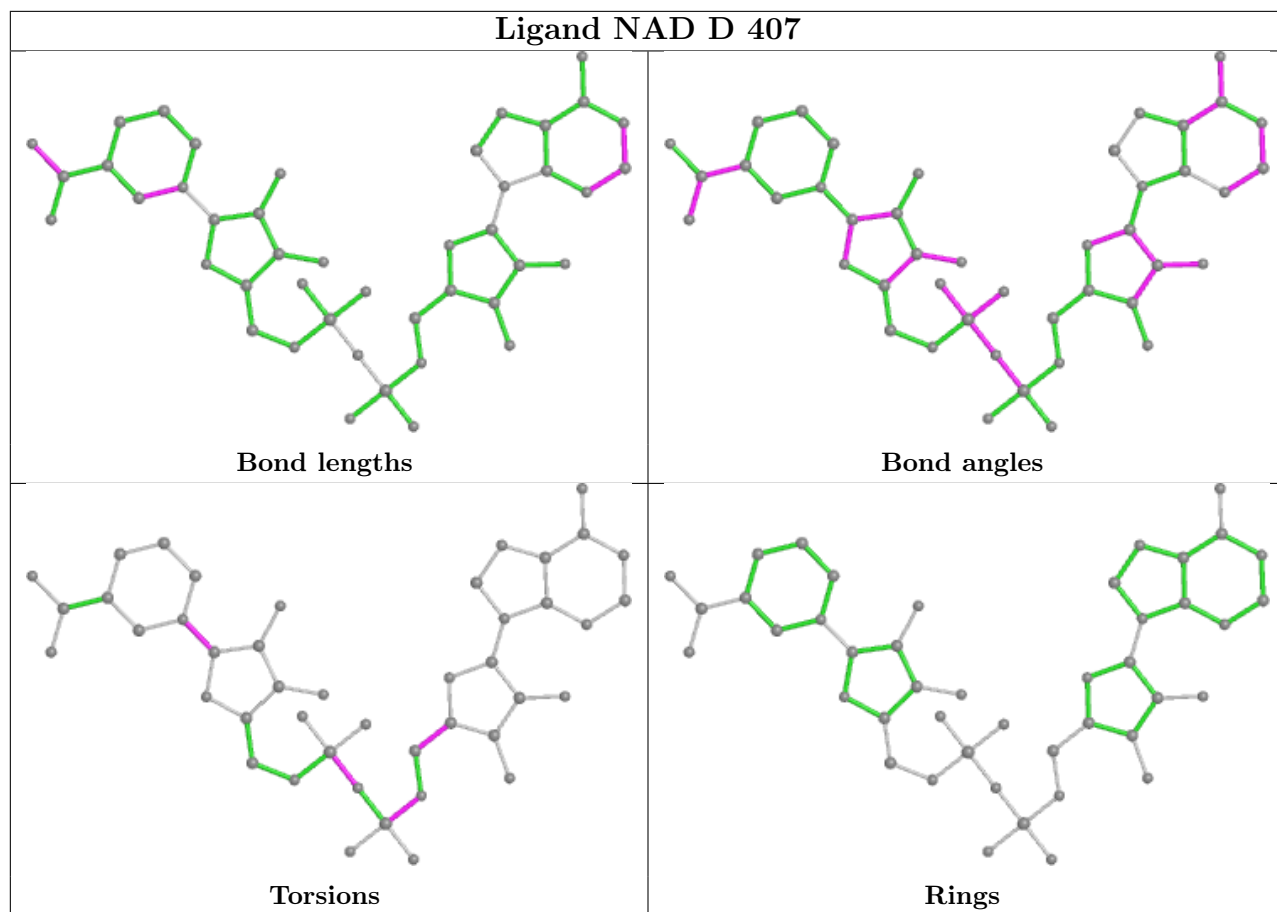
8 monomers are involved in 17 short contacts:

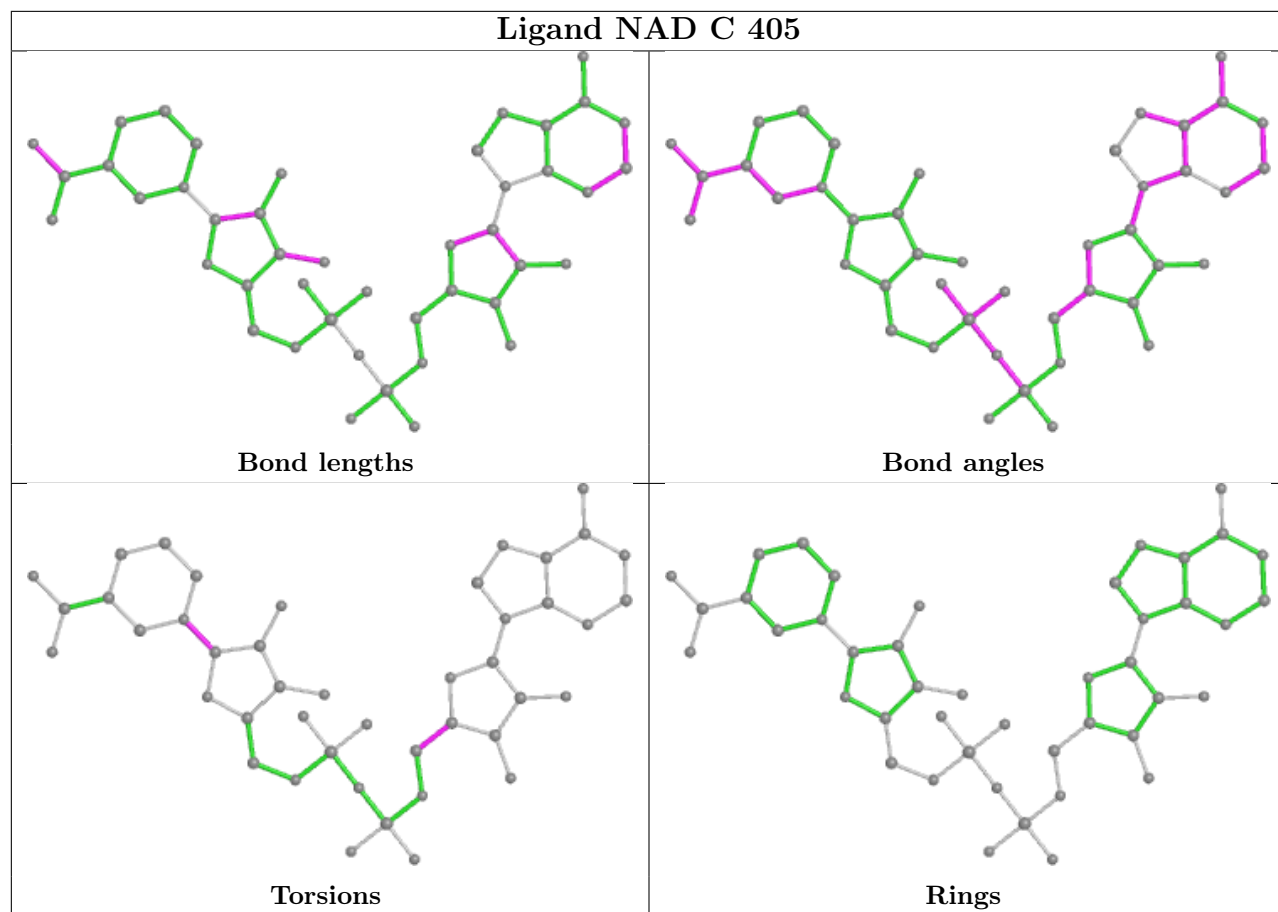
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	NAD	4	0
3	D	408	OXQ	2	0
3	A	402	OXQ	1	0
2	D	407	NAD	4	0
3	B	404	OXQ	1	0
2	C	405	NAD	4	0
2	A	401	NAD	1	0
3	C	406	OXQ	3	0

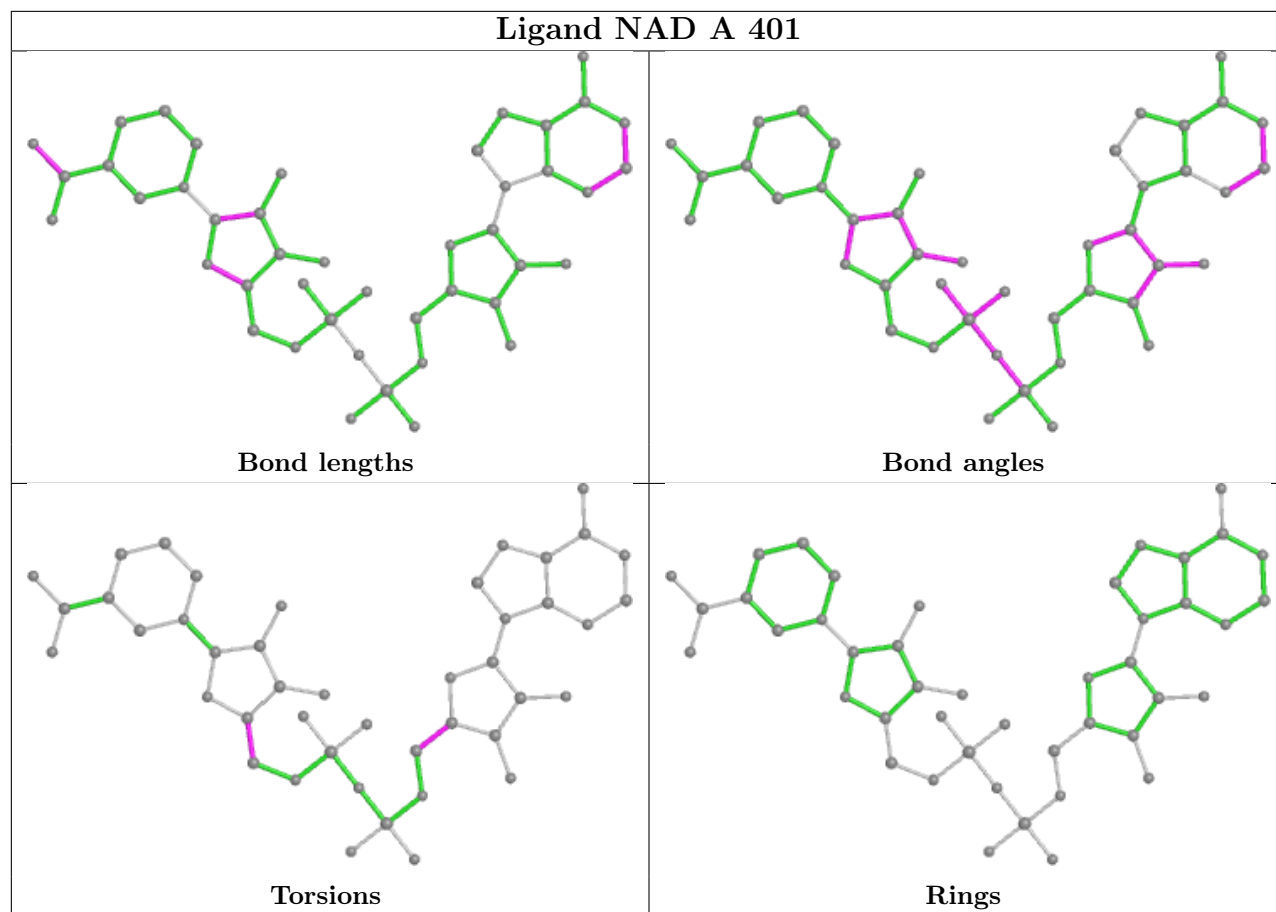
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	332/333 (99%)	-0.38	6 (1%) 68 40	37, 50, 82, 93	11 (3%)
1	B	332/333 (99%)	-0.09	4 (1%) 79 54	38, 61, 85, 90	15 (4%)
1	C	332/333 (99%)	-0.28	5 (1%) 73 46	37, 54, 84, 92	14 (4%)
1	D	332/333 (99%)	-0.31	3 (0%) 84 63	37, 53, 85, 93	18 (5%)
All	All	1328/1332 (99%)	-0.27	18 (1%) 75 49	37, 54, 84, 93	58 (4%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	ASN	6.1
1	D	15	GLU	4.4
1	C	221	ASP	3.6
1	A	221	ASP	3.4
1	D	219	GLY	3.1
1	A	226	ASN	3.1
1	A	16	ALA	2.8
1	C	2	THR	2.8
1	A	13	GLU	2.7
1	B	229	GLU	2.6
1	C	1	ALA	2.5
1	B	329	ASP	2.4
1	B	13	GLU	2.3
1	A	222	ASN	2.3
1	B	226	ASN	2.2
1	D	16	ALA	2.2
1	A	15	GLU	2.1
1	C	19	PRO	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 monosaccharides in this entry.

6.4 Ligands [i](#)

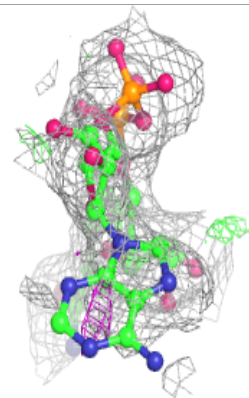
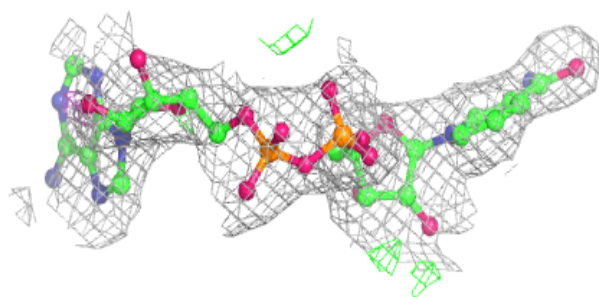
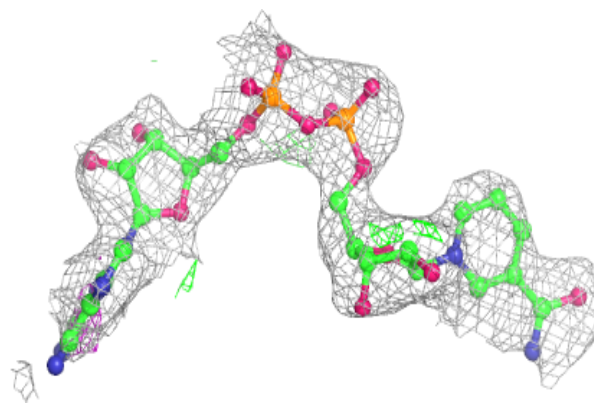
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	B	403	44/44	0.90	0.21	46,61,84,87	0
3	OXQ	B	404	9/9	0.92	0.19	53,56,60,62	0
2	NAD	D	407	44/44	0.93	0.16	33,42,47,49	0
3	OXQ	A	402	9/9	0.93	0.21	63,64,65,65	0
2	NAD	C	405	44/44	0.93	0.18	33,43,52,57	0
2	NAD	A	401	44/44	0.94	0.16	29,40,50,51	0
3	OXQ	C	406	9/9	0.95	0.16	56,58,59,59	0
3	OXQ	D	408	9/9	0.97	0.18	63,65,67,68	0

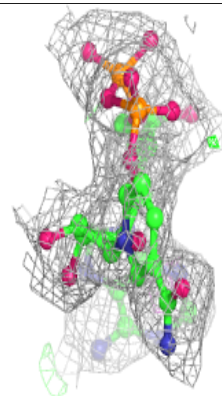
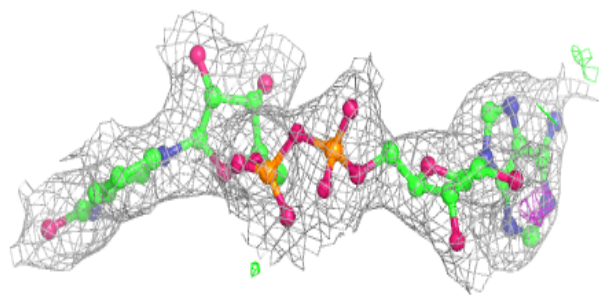
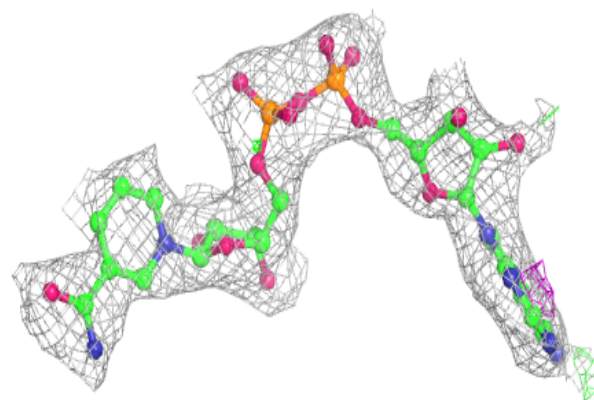
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 403:

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

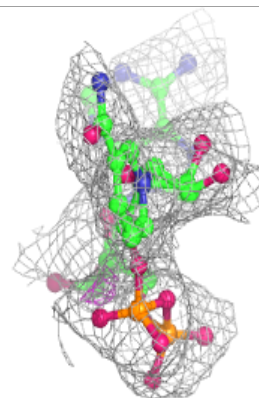
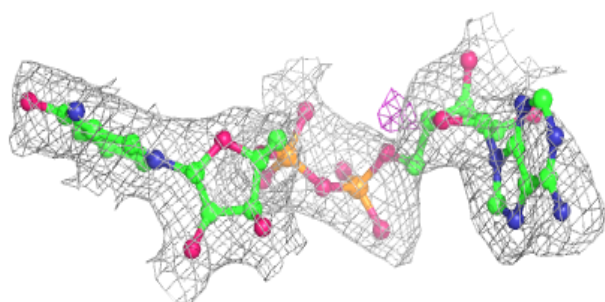
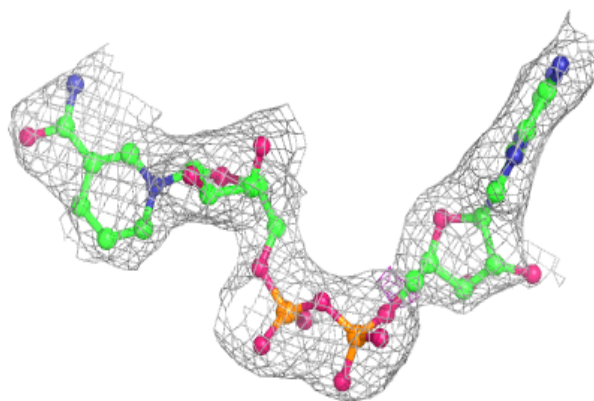
**Electron density around NAD D 407:**

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

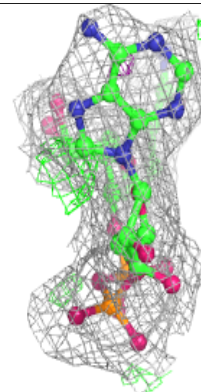
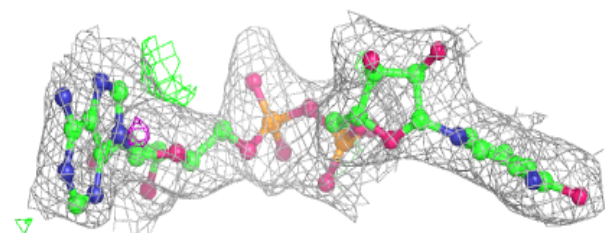
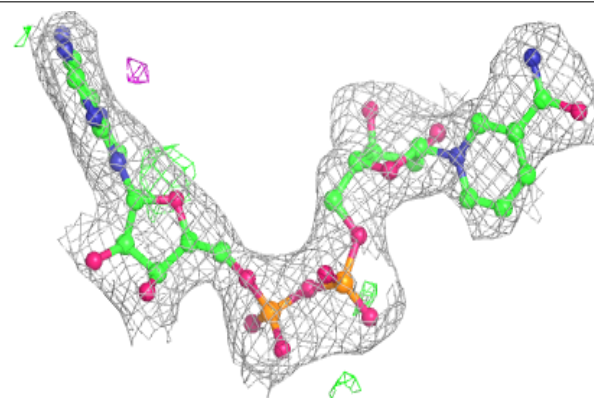


Electron density around NAD C 405:

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

**Electron density around NAD A 401:**

$2mF_o-DF_c$ (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.