



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:32 PM UTC

PDB ID : 1T2F / pdb_00001t2f
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:

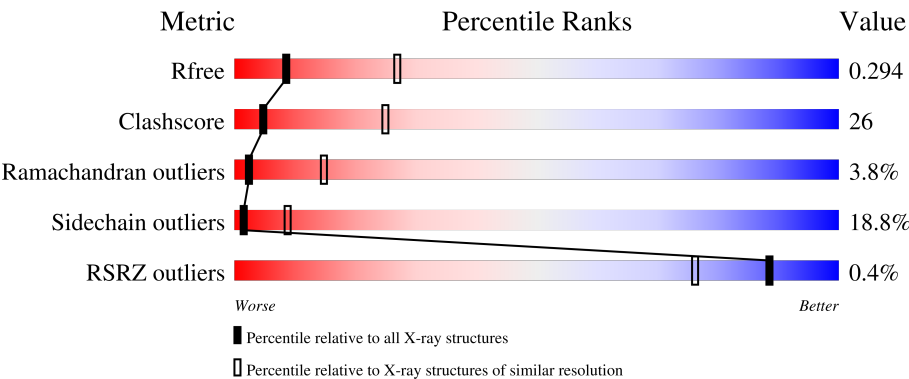
MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal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

1 Overall quality at a glance i

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	333	 47% 38% 12%

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
3	OXQ	D	408	-	X	-	-

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
1	A	332	Total	C	N	O	S	51	0	0
			2555	1627	430	484	14			
1	B	332	Total	C	N	O	S	71	0	0
			2555	1627	430	484	14			
1	C	332	Total	C	N	O	S	65	0	0
			2555	1627	430	484	14			
1	D	332	Total	C	N	O	S	78	0	0
			2555	1627	430	484	14			

There are 4 discrepancies between the modelled and reference sequences:

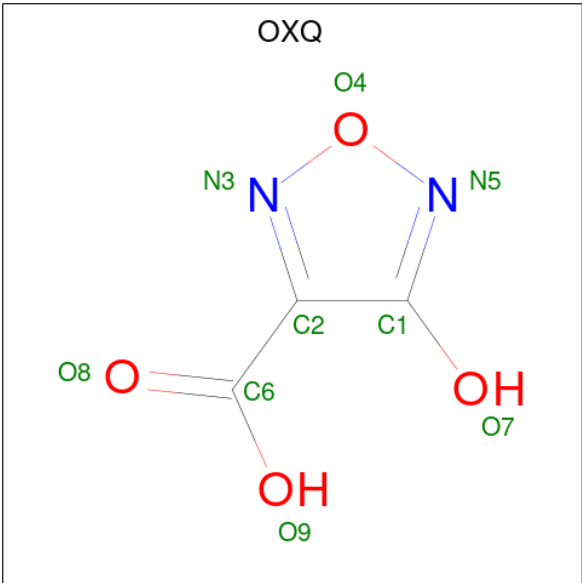
Chain	Residue	Modelled	Actual	Comment	Reference
A	332	PHE	ASP	engineered mutation	UNP P07195
B	332	PHE	ASP	engineered mutation	UNP P07195
C	332	PHE	ASP	engineered mutation	UNP P07195
D	332	PHE	ASP	engineered mutation	UNP P07195

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (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		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-HYDROXY-1,2,5-OXADIAZOLE-3-CARBOXYLIC ACID (CCD ID: 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		

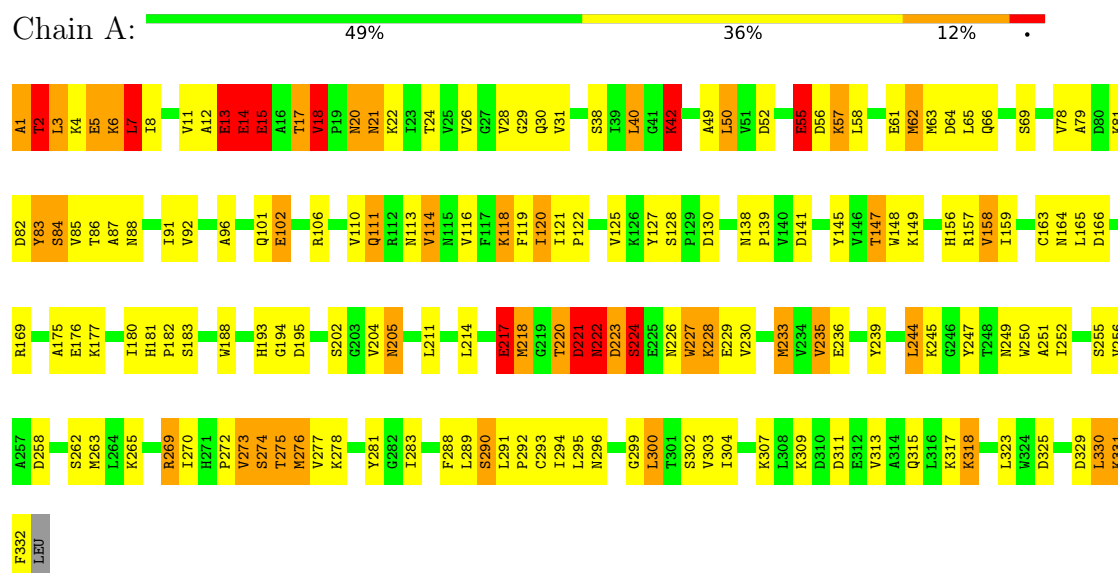
- Molecule 4 is water.

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		

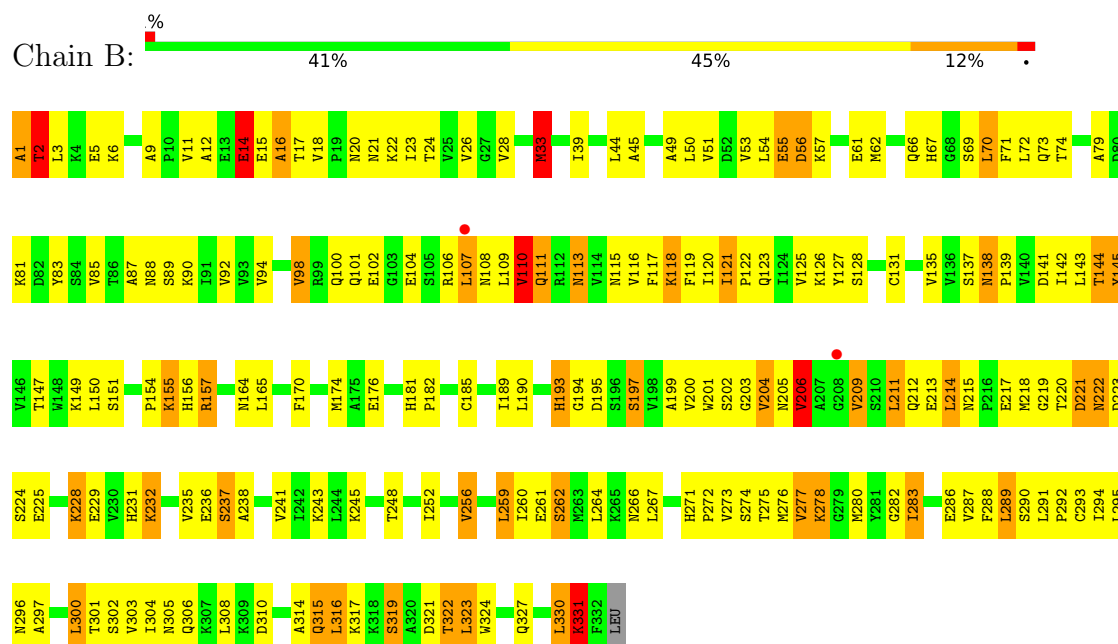
3 Residue-property plots

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.

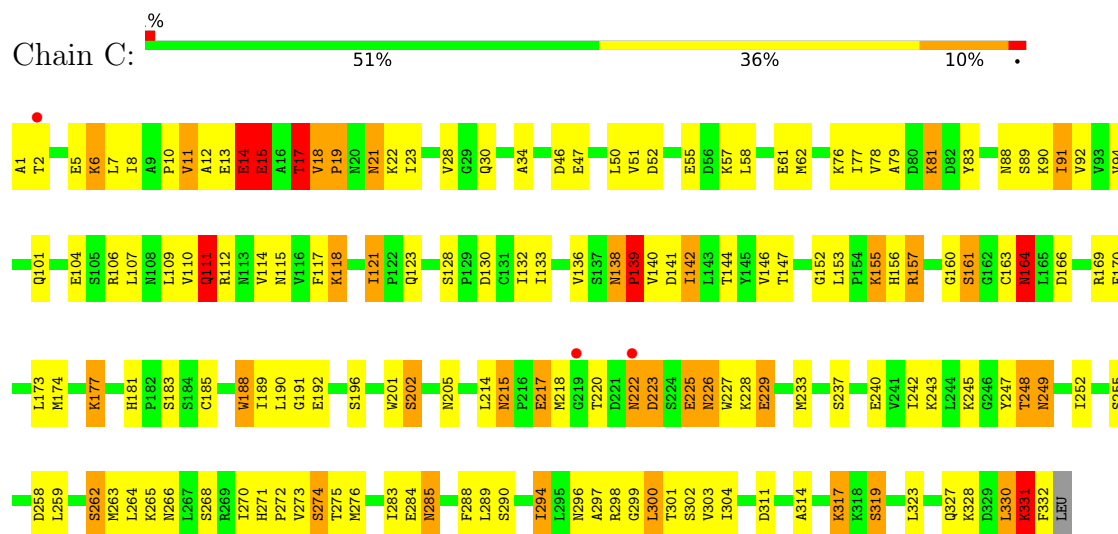
• Molecule 1: L-lactate dehydrogenase B chain



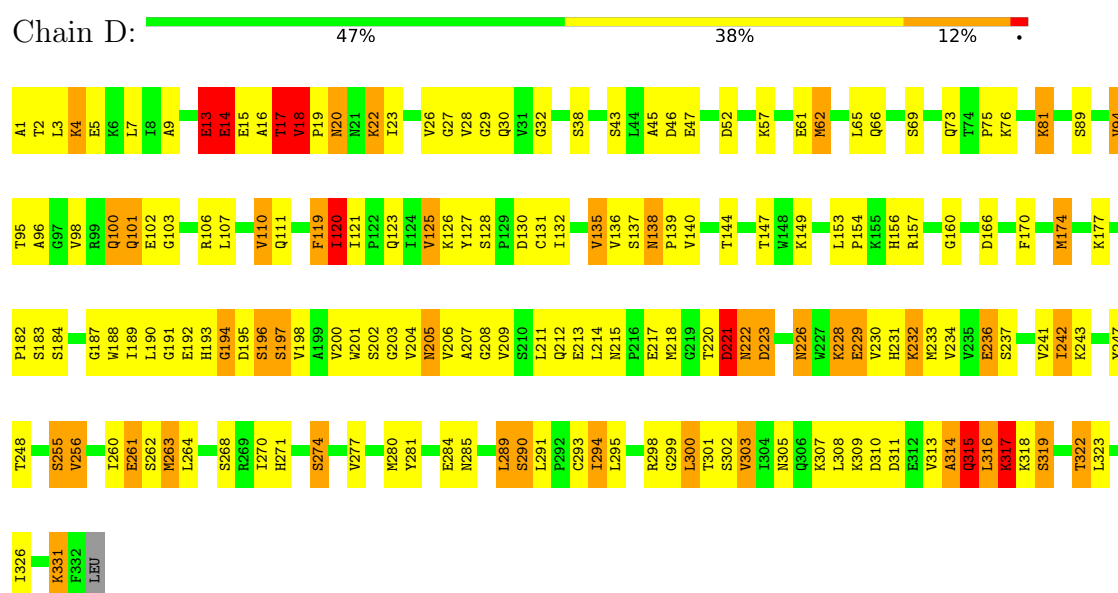
• Molecule 1: L-lactate dehydrogenase B chain



• 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 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.88-3.00) 90.4 (29.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.215 , 0.321 (Not available) , 0.294	Depositor DCC
R_{free} test set	1247 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	1.69	13/2597 (0.5%)	1.81	22/3520 (0.6%)
1	B	1.51	9/2597 (0.3%)	1.41	25/3520 (0.7%)
1	C	1.57	16/2597 (0.6%)	1.55	37/3520 (1.1%)
1	D	1.67	19/2597 (0.7%)	1.74	41/3520 (1.2%)
All	All	1.61	57/10388 (0.5%)	1.64	125/14080 (0.9%)

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 (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	GLU	CA-CB	-42.87	0.81	1.53
1	A	222	ASN	CA-CB	42.10	2.24	1.53
1	D	318	LYS	CA-CB	-34.91	0.94	1.53
1	B	217	GLU	CA-CB	-31.95	0.96	1.53
1	A	221	ASP	CA-CB	-29.65	1.03	1.53
1	B	221	ASP	CA-CB	-25.22	1.10	1.53
1	D	214	LEU	CA-CB	-22.04	1.19	1.53
1	D	119	PHE	CB-CG	21.81	2.00	1.50
1	B	331	LYS	CA-CB	-20.69	1.18	1.53
1	C	317	LYS	CG-CD	18.51	2.08	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	GLU	CA-CB	17.41	1.81	1.53
1	D	217	GLU	CB-CG	-16.90	1.01	1.52
1	B	14	GLU	CA-CB	-15.33	1.27	1.53
1	D	284	GLU	CA-CB	-14.92	1.26	1.53
1	D	4	LYS	CG-CD	-14.40	1.09	1.52
1	B	225	GLU	CA-CB	-13.60	1.29	1.53
1	A	217	GLU	CA-CB	-13.50	1.36	1.52
1	C	331	LYS	CA-CB	12.12	1.74	1.53
1	D	229	GLU	CB-CG	-11.94	1.16	1.52
1	C	217	GLU	CA-CB	-11.09	1.33	1.53
1	A	228	LYS	CB-CG	-10.83	1.20	1.52
1	B	145	TYR	CB-CG	10.37	1.74	1.51
1	D	221	ASP	CA-CB	10.31	1.70	1.53
1	C	229	GLU	CB-CG	10.06	1.82	1.52
1	D	13	GLU	CB-CG	9.33	1.80	1.52
1	C	62	MET	SD-CE	-9.24	1.56	1.79
1	C	298	ARG	CA-CB	9.18	1.67	1.53
1	A	331	LYS	CA-CB	-8.85	1.38	1.53
1	D	81	LYS	CG-CD	7.94	1.76	1.52
1	D	317	LYS	CA-CB	-7.71	1.41	1.53
1	A	62	MET	SD-CE	-7.15	1.61	1.79
1	A	118	LYS	CB-CG	6.86	1.73	1.52
1	C	228	LYS	CA-CB	-6.77	1.42	1.53
1	D	101	GLN	CA-CB	-6.59	1.43	1.53
1	C	101	GLN	CA-CB	-6.57	1.42	1.53
1	C	248	THR	CA-CB	6.53	1.65	1.53
1	D	307	LYS	CB-CG	6.17	1.71	1.52
1	A	63	MET	SD-CE	6.11	1.94	1.79
1	D	228	LYS	CB-CG	-6.01	1.34	1.52
1	C	2	THR	CA-CB	6.00	1.63	1.53
1	B	155	LYS	CA-CB	-5.95	1.44	1.53
1	C	121	ILE	CA-CB	-5.77	1.51	1.54
1	B	33	MET	SD-CE	-5.64	1.65	1.79
1	C	34	ALA	CA-CB	-5.49	1.44	1.53
1	C	91	ILE	CA-CB	-5.48	1.46	1.54
1	A	2	THR	CA-CB	5.48	1.62	1.53
1	D	331	LYS	CA-CB	5.34	1.59	1.53
1	A	125	VAL	CA-CB	5.34	1.61	1.54
1	A	159	ILE	CA-CB	-5.25	1.47	1.54
1	D	95	THR	CA-CB	-5.20	1.46	1.53
1	A	233	MET	SD-CE	5.19	1.92	1.79
1	C	283	ILE	CA-CB	5.18	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	VAL	CA-CB	-5.16	1.47	1.54
1	D	22	LYS	CA-CB	-5.13	1.44	1.53
1	D	17	THR	CA-CB	5.04	1.61	1.53
1	B	92	VAL	CA-C	-5.03	1.46	1.52
1	D	263	MET	SD-CE	5.01	1.92	1.79

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	61.02	173.62	112.60
1	D	318	LYS	CA-CB-CG	29.63	173.35	114.10
1	D	331	LYS	N-CA-CB	23.24	147.12	109.94
1	A	222	ASN	CA-CB-CG	-22.20	90.40	112.60
1	A	221	ASP	N-CA-CB	22.13	147.88	110.49
1	C	6	LYS	CA-CB-CG	21.47	157.04	114.10
1	D	221	ASP	CB-CA-C	19.47	149.16	110.42
1	D	317	LYS	CA-CB-CG	19.46	153.02	114.10
1	D	222	ASN	CB-CA-C	17.40	145.05	110.42
1	C	6	LYS	CB-CA-C	16.12	138.64	111.23
1	D	22	LYS	CB-CA-C	15.84	136.01	109.72
1	D	221	ASP	CA-CB-CG	15.30	127.90	112.60
1	B	217	GLU	CB-CA-C	15.24	142.49	110.32
1	A	221	ASP	CB-CA-C	-14.73	81.10	110.42
1	D	222	ASN	CA-CB-CG	14.44	127.04	112.60
1	A	222	ASN	CB-CA-C	-14.18	82.20	110.42
1	D	214	LEU	CB-CA-C	14.14	133.43	110.81
1	C	331	LYS	N-CA-CB	-13.76	87.23	110.49
1	C	284	GLU	CA-CB-CG	13.69	141.47	114.10
1	C	331	LYS	CB-CA-C	13.36	137.01	110.42
1	B	220	THR	N-CA-CB	-13.19	90.47	110.39
1	D	229	GLU	CB-CG-CD	-12.72	90.98	112.60
1	A	119	PHE	CA-CB-CG	-12.65	101.15	113.80
1	A	119	PHE	CB-CA-C	-12.34	91.15	111.02
1	C	14	GLU	N-CA-CB	-11.96	90.27	110.49
1	D	222	ASN	N-CA-CB	-11.87	90.42	110.49
1	C	6	LYS	N-CA-CB	-11.18	94.93	111.25
1	D	317	LYS	CB-CA-C	11.08	128.54	110.81
1	C	14	GLU	CB-CA-C	-11.08	88.37	110.42
1	B	14	GLU	N-CA-CB	10.88	128.88	110.49
1	B	225	GLU	N-CA-CB	-10.62	94.19	110.44
1	B	225	GLU	CB-CA-C	10.31	128.57	110.01
1	B	222	ASN	N-CA-C	10.18	123.56	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	PHE	N-CA-CB	-10.15	94.68	110.92
1	C	228	LYS	N-CA-CB	10.12	125.01	109.94
1	D	229	GLU	CA-CB-CG	-10.07	93.96	114.10
1	B	217	GLU	N-CA-CB	-9.98	93.36	110.32
1	B	14	GLU	CA-CB-CG	9.91	133.91	114.10
1	A	227	TRP	N-CA-C	9.72	121.56	110.97
1	B	6	LYS	CA-CB-CG	-9.55	95.00	114.10
1	C	317	LYS	CG-CD-CE	-9.21	90.13	111.30
1	D	228	LYS	CA-CB-CG	9.17	132.44	114.10
1	C	229	GLU	CA-CB-CG	-8.85	96.41	114.10
1	C	111	GLN	N-CA-C	-8.73	100.37	111.02
1	D	119	PHE	CB-CG-CD2	8.65	135.40	120.70
1	D	318	LYS	N-CA-CB	8.52	124.89	110.49
1	C	217	GLU	CB-CA-C	8.38	128.00	110.32
1	C	155	LYS	N-CA-CB	-8.32	97.49	110.30
1	B	155	LYS	CB-CA-C	8.11	124.30	110.84
1	D	119	PHE	CA-CB-CG	-8.03	105.77	113.80
1	D	119	PHE	CB-CG-CD1	-8.03	107.06	120.70
1	C	328	LYS	CB-CG-CD	7.94	129.56	111.30
1	C	14	GLU	CA-CB-CG	7.87	129.84	114.10
1	B	243	LYS	CB-CA-C	7.82	125.69	110.67
1	A	217	GLU	CB-CA-C	-7.62	100.32	111.91
1	B	243	LYS	N-CA-CB	-7.47	98.70	110.28
1	D	101	GLN	CB-CA-C	7.46	122.11	109.80
1	C	317	LYS	CB-CG-CD	-7.31	94.48	111.30
1	C	228	LYS	CB-CA-C	7.29	122.47	110.81
1	D	307	LYS	CA-CB-CG	-7.25	99.59	114.10
1	D	314	ALA	N-CA-C	-7.18	103.39	111.07
1	B	6	LYS	CB-CG-CD	-7.15	94.86	111.30
1	D	284	GLU	N-CA-CB	-7.04	99.40	110.46
1	C	284	GLU	CB-CA-C	7.03	122.10	110.92
1	D	214	LEU	N-CA-CB	-7.03	99.46	109.94
1	D	284	GLU	CA-CB-CG	-7.02	100.05	114.10
1	D	131	CYS	N-CA-C	7.01	120.45	110.14
1	B	155	LYS	N-CA-CB	6.96	121.55	109.72
1	D	331	LYS	CB-CA-C	-6.69	99.59	110.77
1	D	317	LYS	N-CA-CB	6.68	119.89	109.94
1	C	12	ALA	CA-C-O	6.67	122.53	118.33
1	B	319	SER	N-CA-C	-6.60	103.77	110.97
1	C	227	TRP	N-CA-C	6.58	119.27	111.71
1	B	221	ASP	CB-CA-C	6.55	123.45	110.42
1	B	259	LEU	N-CA-C	-6.37	104.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLU	N-CA-C	6.32	118.69	111.11
1	B	256	VAL	N-CA-C	-6.29	104.37	110.72
1	D	101	GLN	CA-CB-CG	6.17	126.44	114.10
1	C	285	ASN	N-CA-C	6.07	117.81	109.18
1	A	14	GLU	N-CA-CB	-5.93	99.64	109.72
1	B	220	THR	CA-CB-CG2	5.92	120.56	110.50
1	D	217	GLU	CB-CG-CD	5.79	122.44	112.60
1	C	61	GLU	N-CA-C	-5.79	104.41	112.45
1	C	188	TRP	N-CA-C	5.79	118.90	109.24
1	A	42	LYS	N-CA-C	-5.78	106.22	113.28
1	D	221	ASP	N-CA-CB	-5.73	100.81	110.49
1	C	228	LYS	CA-CB-CG	5.68	125.47	114.10
1	A	7	LEU	N-CA-C	-5.68	106.48	113.41
1	D	160	GLY	N-CA-C	-5.66	102.40	112.54
1	C	205	ASN	N-CA-C	5.65	116.73	108.14
1	B	308	LEU	N-CA-C	5.62	117.69	108.52
1	A	114	VAL	N-CA-C	-5.60	104.90	110.62
1	A	88	ASN	N-CA-C	5.58	119.39	112.58
1	C	273	VAL	N-CA-C	5.57	117.84	108.81
1	C	132	ILE	N-CA-C	-5.57	100.42	108.71
1	B	232	LYS	CB-CA-C	5.56	119.60	110.88
1	D	95	THR	CB-CA-C	-5.53	102.12	111.02
1	C	164	ASN	N-CA-C	-5.53	105.17	111.14
1	C	88	ASN	CA-C-N	5.44	128.44	120.71
1	C	88	ASN	C-N-CA	5.44	128.44	120.71
1	A	69	SER	N-CA-C	5.43	117.28	111.36
1	A	40	LEU	N-CA-C	5.41	117.25	111.36
1	C	270	ILE	N-CA-C	5.38	116.73	108.71
1	C	298	ARG	CB-CA-C	5.37	119.71	110.79
1	B	18	VAL	CB-CA-C	-5.37	105.62	110.88
1	B	228	LYS	CB-CG-CD	5.37	123.64	111.30
1	D	94	VAL	CB-CA-C	-5.36	104.45	111.25
1	B	98	VAL	N-CA-C	-5.35	101.36	108.96
1	D	211	LEU	N-CA-C	-5.35	106.75	113.28
1	C	328	LYS	CG-CD-CE	5.33	123.55	111.30
1	D	62	MET	N-CA-C	-5.32	105.38	111.07
1	C	139	PRO	N-CD-CG	-5.30	95.26	103.20
1	B	193	HIS	N-CA-C	5.29	117.79	111.71
1	D	214	LEU	N-CA-C	-5.26	104.80	111.11
1	A	14	GLU	CA-CB-CG	5.26	124.61	114.10
1	A	4	LYS	CA-CB-CG	5.24	124.57	114.10
1	C	284	GLU	N-CA-CB	5.23	117.77	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	GLY	N-CA-C	5.23	119.01	112.73
1	D	322	THR	N-CA-C	-5.21	105.05	111.40
1	A	6	LYS	N-CA-C	5.19	117.87	109.83
1	D	120	ILE	CB-CA-C	-5.15	105.30	112.04
1	D	13	GLU	CA-CB-CG	-5.13	103.84	114.10
1	C	299	GLY	N-CA-C	-5.11	106.40	111.56
1	A	217	GLU	N-CA-CB	5.06	118.48	110.49
1	D	315	GLN	N-CA-C	5.05	117.44	111.33

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	139	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2555	0	2627	163	4
1	C	2555	0	2627	114	3
1	D	2555	0	2627	117	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	15	0
All	All	10665	0	10612	521	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 26.

All (521) 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:329:ASP:C	4:A:452:HOH:O	2.17	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: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:C:110:VAL:O	1:C:111:GLN:C	2.26	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:229:GLU:OE1	4:B:444:HOH:O	2.06	0.74
1:B:22:LYS:HZ2	1:B:49:ALA:HB2	1.52	0.73
1:D:255:SER:O	1:D:256:VAL:C	2.31	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:D:212:GLN:O	1:D:215:ASN:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:82:ASP:C	1:A:84:SER:H	2.00	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:C:21:ASN:HD22	1:C:90:LYS:HZ2	1.40	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:198:VAL:HG21	1:D:316:LEU:HD13	1.75	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:A:49:ALA:C	1:A:50:LEU:HD23	2.18	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:1:ALA:HB3	1:C:5:GLU:CD	2.20	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: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:B:22:LYS:NZ	1:B:85:VAL:O	2.24	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:D:153:LEU:O	1:D:154:PRO:C	2.41	0.63
1:B:277:VAL:O	1:B:280:MET:HE3	1.98	0.63
1:B:21:ASN:OD1	1:B:90:LYS:NZ	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLN:NE2	4:D:419:HOH:O	2.01	0.63
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
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:D:300:LEU:HD12	1:D:300:LEU:C	2.26	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:B:300:LEU:HD12	1:B:300:LEU:C	2.26	0.61
1:B:203:GLY:O	1:B:204:VAL:C	2.43	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:B:149:LYS:HZ1	1:B:286:GLU:CD	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:GLU:O	1:B:262:SER:C	2.45	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:D:191:GLY:C	1:D:289:LEU:HD22	2.28	0.58
1:B:9:ALA:HB2	1:D:305:ASN:OD1	2.04	0.58
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:A:40:LEU:HD11	1:A:65:LEU:HD13	1.87	0.57
1:A:165:LEU:O	1:A:166:ASP:C	2.46	0.57
1:D:196:SER:O	1:D:197:SER:C	2.46	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: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:A:28:VAL:O	1:A:57:LYS:NZ	2.37	0.56
1:B:292:PRO:C	1:B:293:CYS:SG	2.89	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:A:223:ASP:O	1:A:224:SER:C	2.49	0.55
1:B:305:ASN:OD1	1:D:9:ALA:HB2	2.06	0.55
1:C:130:ASP:CG	1:C:130:ASP:O	2.48	0.55
1:A:82:ASP:C	1:A:84:SER:N	2.65	0.55
1:A:293:CYS:HA	1:A:302:SER:O	2.07	0.55
1:B:107:LEU:C	1:B:109:LEU:H	2.14	0.55
1:D:140:VAL:O	1:D:144:THR:OG1	2.13	0.55
1:B:54:LEU:O	1:B:55:GLU:C	2.50	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:D:17:THR:O	1:D:19:PRO:CD	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:192:GLU:OE1	1:D:196:SER:OG	2.17	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
1:D:20:ASN:C	1:D:20:ASN:HD22	2.16	0.54
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: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:D:29:GLY:O	1:D:30:GLN:C	2.51	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: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: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:A:13:GLU:O	1:A:14:GLU:C	2.53	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:D:291:LEU:O	1:D:293:CYS:SG	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:O	1:A:87:ALA:C	2.54	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: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
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:C:201:TRP:O	1:C:202:SER:C	2.53	0.51
1:B:39:ILE:HD11	1:B:260:ILE:HD13	1.93	0.51
1:B:83:TYR:CE2	1:B:120:ILE:HG23	2.47	0.50
1:A:101:GLN:O	1:A:102:GLU:C	2.55	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:A:276:MET:HE1	1:A:278:LYS:HB2	1.92	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:57:LYS:O	1:A:58:LEU:C	2.55	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: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: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:23:ILE:HG22	1:B:24:THR:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LYS:O	1:B:150:LEU:C	2.53	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:D:136:VAL:O	1:D:137:SER:C	2.55	0.49
1:B:28:VAL:HB	1:B:33:MET:SD	2.52	0.49
1:B:236:GLU:O	1:B:237:SER:C	2.55	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:B:321:ASP:O	1:B:322:THR:C	2.56	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
1:A:64:ASP:OD2	1:B:245:LYS:NZ	2.45	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: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:C:215:ASN:O	1:C:215:ASN:CG	2.56	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:87:ALA:O	1:B:88:ASN:C	2.55	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:128:SER:C	4:D:434:HOH:O	2.56	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:D:125:VAL:C	4:D:434:HOH:O	2.57	0.48
1:B:292:PRO:O	1:B:293:CYS:SG	2.72	0.48
1:C:47:GLU:CD	1:C:76:LYS:HD3	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HA	1:A:299:GLY:O	2.13	0.48
1:A:235:VAL:HG12	1:A:236:GLU:N	2.28	0.47
1:B:62:MET:HE3	1:B:66:GLN:OE1	2.14	0.47
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: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:C:30:GLN:CD	1:C:247:TYR:CZ	2.92	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:D:174:MET:HE1	1:D:187:GLY:HA3	1.97	0.47
1:B:23:ILE:CG2	1:B:24:THR:N	2.77	0.47
1:D:300:LEU:C	1:D:300:LEU:CD1	2.87	0.47
1:A:65:LEU:O	1:A:66:GLN:C	2.58	0.47
1:D:232:LYS:O	1:D:236:GLU:HG2	2.14	0.47
1:B:165:LEU:HD12	1:B:165:LEU:C	2.40	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:B:119:PHE:CD1	1:B:119:PHE:C	2.91	0.47
1:B:266:ASN:CG	1:B:266:ASN:O	2.56	0.47
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:153:LEU:C	1:D:154:PRO:O	2.56	0.47
1:B:300:LEU:C	1:B:300:LEU:CD1	2.88	0.47
1:D:46:ASP:C	1:D:46:ASP:OD1	2.55	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:D:2:THR:HG22	1:D:5:GLU:CD	2.40	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:241:VAL:HG11	1:B:248:THR:HG22	1.97	0.46
1:C:22:LYS:C	1:C:23:ILE:HG13	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:65:LEU:O	1:D:66:GLN:C	2.57	0.46
1:A:40:LEU:CD1	1:A:65:LEU:HD13	2.46	0.46
1:A:218:MET:HE2	1:A:227:TRP:CD2	2.51	0.46
1:A:329:ASP:O	1:A:330:LEU:C	2.58	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: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:C:225:GLU:O	1:C:226:ASN:CG	2.58	0.45
1:D:26:VAL:HB	1:D:94:VAL:HA	1.97	0.45
1:A:82:ASP:CG	1:A:84:SER:HG	2.18	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: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: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:18:VAL:O	1:C:19:PRO:C	2.60	0.45
1:C:259:LEU:HD23	1:C:271:HIS:CD2	2.52	0.45
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: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:C:294:ILE:HD12	4:C:452:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HB3	1:B:56:ASP:O	2.17	0.44
1:B:110:VAL:O	1:B:111:GLN:C	2.60	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:A:29:GLY:O	1:A:30:GLN:C	2.60	0.44
1:C:189:ILE:C	1:C:190:LEU:HD23	2.42	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:154:PRO:HB3	1:D:156:HIS:CE1	2.53	0.44
1:B:144:THR:O	1:B:145:TYR:C	2.61	0.44
1:A:165:LEU:HD11	1:A:251:ALA:HB1	1.98	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:A:163:CYS:O	1:A:164:ASN:C	2.58	0.44
1:B:203:GLY:O	1:B:205:ASN:N	2.51	0.44
1:C:133:ILE:HG21	1:C:147:THR:HG21	1.98	0.44
1:D:242:ILE:HG22	1:D:243:LYS:N	2.33	0.44
1:A:12:ALA:HB2	1:C:156:HIS:CG	2.53	0.43
1:D:23:ILE:HD12	1:D:45:ALA:HB2	1.99	0.43
1:A:235:VAL:HG12	1:A:236:GLU:HG2	2.00	0.43
1:B:69:SER:O	1:B:70:LEU:C	2.62	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:B:154:PRO:O	1:B:155:LYS:C	2.62	0.43
1:B:212:GLN:C	1:B:214:LEU:H	2.27	0.43
1:D:62:MET:HG2	1:D:66:GLN:NE2	2.33	0.43
1:D:73:GLN:C	4:D:421:HOH:O	2.61	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:301:THR:O	1:B:302:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:MET:HE3	1:B:33:MET:HA	2.01	0.43
1:B:100:GLN:HB2	4:B:463:HOH:O	2.18	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:D:223:ASP:C	1:D:223:ASP:OD1	2.61	0.42
1:C:265:LYS:HD3	4:C:408:HOH:O	2.18	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:B:2:THR:HG22	1:B:5:GLU:N	2.34	0.42
1:B:107:LEU:C	1:B:109:LEU:N	2.77	0.42
1:B:115:ASN:HB2	4:B:417:HOH:O	2.19	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:C:191:GLY:O	1:C:192:GLU:C	2.63	0.42
1:A:116:VAL:C	1:A:118:LYS:N	2.78	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: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:B:276:MET:HE1	1:B:278:LYS:HB3	2.01	0.42
1:B:314:ALA:O	1:B:315:GLN:C	2.63	0.41
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:47:GLU:CD	1:D:76:LYS:HD3	2.45	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:A:1:ALA:C	1:A:2:THR:O	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:GLN:O	1:D:213:GLU:C	2.63	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:A:138:ASN:HA	1:A:139:PRO:C	2.45	0.41
1:B:101:GLN:O	1:B:102:GLU:C	2.64	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:182:PRO:O	1:D:183:SER:C	2.63	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:B:237:SER:O	1:B:238:ALA:C	2.63	0.41
1:C:77:ILE:C	1:C:78:VAL:HG13	2.46	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:D:1:ALA:H2	1:D:5:GLU:CD	2.28	0.41
1:D:18:VAL:HA	1:D:19:PRO:HD2	1.76	0.41
1:A:194:GLY:O	1:A:195:ASP:C	2.64	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
1:A:62:MET:HE2	1:A:62:MET:HB3	1.87	0.40
1:A:205:ASN:ND2	1:A:205:ASN:C	2.79	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:CG2	1:A:86:THR:HG22	2.51	0.40
1:D:126:LYS:C	4:D:434:HOH:O	2.64	0.40
1:D:241:VAL:CG1	1:D:248:THR:HG22	2.48	0.40
1:B:1:ALA:O	1:B:2:THR:C	2.65	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
1:A:116:VAL:C	1:A:118:LYS:H	2.29	0.40
1:A:175:ALA:O	1:A:176:GLU:C	2.64	0.40
1:A:218:MET:HE2	1:A:227:TRP:CE2	2.56	0.40
1:A:318:LYS:HZ3	1:A:318:LYS:C	2.29	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%)	2	14
1	B	330/333 (99%)	264 (80%)	51 (16%)	15 (4%)	2	12
1	C	330/333 (99%)	275 (83%)	45 (14%)	10 (3%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	330/333 (99%)	269 (82%)	49 (15%)	12 (4%)	2	16
All	All	1320/1332 (99%)	1080 (82%)	190 (14%)	50 (4%)	2	15

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
1	A	18	VAL
1	A	102	GLU
1	B	144	THR

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Mol	Chain	Res	Type
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 ⓘ

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%)	230 (80%)	58 (20%)	1	7
1	B	288/289 (100%)	237 (82%)	51 (18%)	2	10
1	C	288/289 (100%)	240 (83%)	48 (17%)	2	12
1	D	288/289 (100%)	228 (79%)	60 (21%)	1	7
All	All	1152/1156 (100%)	935 (81%)	217 (19%)	1	9

All (217) 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
1	A	7	LEU
1	A	8	ILE
1	A	11	VAL

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Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	15	GLU
1	A	18	VAL
1	A	21	ASN
1	A	42	LYS
1	A	50	LEU
1	A	55	GLU
1	A	57	LYS
1	A	78	VAL
1	A	84	SER
1	A	91	ILE
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	218	MET
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	230	VAL
1	A	233	MET
1	A	235	VAL
1	A	244	LEU
1	A	269	ARG
1	A	273	VAL
1	A	274	SER
1	A	275	THR
1	A	276	MET
1	A	283	ILE
1	A	290	SER
1	A	300	LEU
1	A	303	VAL

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Mol	Chain	Res	Type
1	A	307	LYS
1	A	311	ASP
1	A	315	GLN
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	26	VAL
1	B	33	MET
1	B	51	VAL
1	B	56	ASP
1	B	81	LYS
1	B	94	VAL
1	B	107	LEU
1	B	108	ASN
1	B	110	VAL
1	B	111	GLN
1	B	113	ASN
1	B	118	LYS
1	B	121	ILE
1	B	125	VAL
1	B	128	SER
1	B	131	CYS
1	B	135	VAL
1	B	137	SER
1	B	138	ASN
1	B	141	ASP
1	B	157	ARG
1	B	176	GLU
1	B	197	SER
1	B	206	VAL
1	B	209	VAL
1	B	211	LEU
1	B	214	LEU
1	B	224	SER
1	B	228	LYS

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Mol	Chain	Res	Type
1	B	232	LYS
1	B	256	VAL
1	B	262	SER
1	B	267	LEU
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
1	B	316	LEU
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	8	ILE
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	81	LYS
1	C	107	LEU
1	C	111	GLN
1	C	115	ASN
1	C	118	LYS
1	C	123	GLN
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

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Mol	Chain	Res	Type
1	C	177	LYS
1	C	185	CYS
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
1	C	285	ASN
1	C	294	ILE
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	4	LYS
1	D	7	LEU
1	D	14	GLU
1	D	17	THR
1	D	18	VAL
1	D	20	ASN
1	D	22	LYS
1	D	38	SER
1	D	43	SER
1	D	81	LYS
1	D	98	VAL
1	D	100	GLN
1	D	107	LEU
1	D	119	PHE
1	D	120	ILE
1	D	121	ILE
1	D	125	VAL

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Mol	Chain	Res	Type
1	D	130	ASP
1	D	135	VAL
1	D	138	ASN
1	D	147	THR
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	236	GLU
1	D	237	SER
1	D	242	ILE
1	D	255	SER
1	D	261	GLU
1	D	274	SER
1	D	277	VAL
1	D	280	MET
1	D	285	ASN
1	D	289	LEU
1	D	290	SER
1	D	294	ILE
1	D	300	LEU
1	D	303	VAL
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 (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	30	GLN
1	A	100	GLN
1	A	108	ASN
1	A	164	ASN
1	A	181	HIS
1	A	186	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	226	ASN
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	123	GLN
1	C	164	ASN
1	C	181	HIS
1	C	186	HIS
1	C	205	ASN
1	C	212	GLN
1	C	215	ASN
1	C	266	ASN
1	C	271	HIS
1	C	327	GLN
1	D	20	ASN
1	D	30	GLN
1	D	66	GLN
1	D	108	ASN
1	D	113	ASN
1	D	115	ASN
1	D	123	GLN

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Mol	Chain	Res	Type
1	D	138	ASN
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 oligosaccharides 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
3	OXQ	B	404	-	9,9,9	2.16	3 (33%)	12,12,12	1.49	3 (25%)
2	NAD	A	401	-	46,48,48	1.89	6 (13%)	64,73,73	1.79	14 (21%)
2	NAD	B	403	-	46,48,48	2.01	7 (15%)	64,73,73	2.06	15 (23%)
3	OXQ	C	406	-	9,9,9	1.63	2 (22%)	12,12,12	1.43	1 (8%)
3	OXQ	D	408	-	9,9,9	1.91	3 (33%)	12,12,12	1.78	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXQ	A	402	-	9,9,9	1.76	3 (33%)	12,12,12	1.95	2 (16%)
2	NAD	D	407	-	46,48,48	2.07	5 (10%)	64,73,73	1.82	18 (28%)
2	NAD	C	405	-	46,48,48	1.66	5 (10%)	64,73,73	1.97	15 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXQ	B	404	-	-	0/4/4/4	0/1/1/1
2	NAD	A	401	-	-	4/30/62/62	0/5/5/5
2	NAD	B	403	-	-	11/30/62/62	0/5/5/5
3	OXQ	C	406	-	-	0/4/4/4	0/1/1/1
3	OXQ	D	408	-	-	4/4/4/4	0/1/1/1
3	OXQ	A	402	-	-	4/4/4/4	0/1/1/1
2	NAD	D	407	-	-	10/30/62/62	0/5/5/5
2	NAD	C	405	-	-	6/30/62/62	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	NAD	O7N-C7N	10.54	1.43	1.24
2	D	407	NAD	O7N-C7N	10.08	1.42	1.24
2	A	401	NAD	O7N-C7N	9.48	1.41	1.24
2	C	405	NAD	O7N-C7N	7.50	1.38	1.24
2	D	407	NAD	C2A-N3A	4.67	1.42	1.33
2	D	407	NAD	C2A-N1A	4.04	1.41	1.33
2	A	401	NAD	C2A-N3A	3.79	1.40	1.33
3	B	404	OXQ	O9-C6	-3.51	1.21	1.30
3	B	404	OXQ	C1-N5	3.44	1.34	1.31
2	A	401	NAD	C2A-N1A	3.44	1.40	1.33
2	C	405	NAD	C2A-N1A	3.38	1.39	1.33
2	D	407	NAD	C5A-N7A	-3.33	1.33	1.39
3	A	402	OXQ	O7-C1	-3.31	1.23	1.33
3	D	408	OXQ	O7-C1	-3.30	1.23	1.33
3	B	404	OXQ	O7-C1	-3.21	1.23	1.33
3	C	406	OXQ	O9-C6	-3.18	1.21	1.30
2	B	403	NAD	C2A-N1A	3.14	1.39	1.33
3	C	406	OXQ	O7-C1	-3.07	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C8A-N7A	3.05	1.37	1.31
3	D	408	OXQ	O9-C6	-3.03	1.22	1.30
2	D	407	NAD	C2N-N1N	2.95	1.38	1.35
3	A	402	OXQ	O9-C6	-2.63	1.23	1.30
2	C	405	NAD	C2A-N3A	2.53	1.38	1.33
2	A	401	NAD	C5A-N7A	-2.38	1.34	1.39
2	A	401	NAD	O4D-C4D	-2.33	1.39	1.45
2	B	403	NAD	C2N-N1N	2.27	1.37	1.35
2	B	403	NAD	C3N-C7N	2.27	1.54	1.50
2	C	405	NAD	C2N-N1N	2.14	1.37	1.35
2	B	403	NAD	C2A-N3A	2.06	1.37	1.33
3	D	408	OXQ	C1-N5	2.05	1.33	1.31
2	B	403	NAD	C4A-N3A	2.03	1.38	1.34
2	B	403	NAD	C8A-N7A	2.03	1.35	1.31
3	A	402	OXQ	C1-N5	2.02	1.33	1.31
2	C	405	NAD	C8A-N7A	2.00	1.35	1.31

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	NAD	N3A-C2A-N1A	-7.91	116.60	128.58
2	A	401	NAD	C5A-C4A-N3A	-5.32	119.40	126.72
2	C	405	NAD	C3N-C7N-N7N	5.08	123.99	117.74
2	B	403	NAD	O4B-C1B-N9A	5.06	117.81	108.09
2	C	405	NAD	O7N-C7N-N7N	-5.02	115.36	122.62
2	C	405	NAD	N9A-C8A-N7A	-4.91	106.98	113.94
2	C	405	NAD	N3A-C2A-N1A	-4.86	121.23	128.58
2	D	407	NAD	C5A-C4A-N3A	-4.85	120.04	126.72
2	A	401	NAD	C4D-O4D-C1D	-4.69	105.63	109.92
2	A	401	NAD	N3A-C2A-N1A	-4.55	121.70	128.58
2	D	407	NAD	O4B-C1B-N9A	4.47	116.67	108.09
2	C	405	NAD	C4A-N9A-C1B	-4.33	116.51	126.63
2	B	403	NAD	O7N-C7N-N7N	-4.24	116.48	122.62
3	A	402	OXQ	N5-O4-N3	-4.22	106.25	111.49
2	B	403	NAD	N9A-C8A-N7A	-4.15	108.04	113.94
2	D	407	NAD	N3A-C2A-N1A	-4.07	122.42	128.58
2	B	403	NAD	O7N-C7N-C3N	4.00	124.49	119.60
3	A	402	OXQ	O4-N5-C1	3.99	108.24	104.28
2	D	407	NAD	N9A-C8A-N7A	-3.91	108.39	113.94
2	D	407	NAD	N3A-C4A-N9A	3.80	133.63	127.17
2	B	403	NAD	O3D-C3D-C4D	-3.63	100.65	111.08
2	D	407	NAD	C5A-N7A-C8A	3.51	108.97	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	407	NAD	C6A-C5A-C4A	3.48	121.93	117.18
2	B	403	NAD	C4A-N9A-C1B	-3.45	118.57	126.63
2	C	405	NAD	C5A-N7A-C8A	3.44	108.86	103.45
3	D	408	OXQ	N5-O4-N3	-3.40	107.27	111.49
2	A	401	NAD	O2N-PN-O1N	3.38	128.16	112.44
3	C	406	OXQ	O4-N5-C1	3.37	107.63	104.28
2	B	403	NAD	C2A-N3A-C4A	3.32	119.94	111.83
2	C	405	NAD	C4A-N9A-C8A	3.32	109.22	105.74
2	C	405	NAD	C4A-C5A-N7A	-3.30	106.81	110.58
2	C	405	NAD	C1B-N9A-C8A	3.22	134.24	127.09
2	A	401	NAD	C6A-C5A-C4A	3.20	121.55	117.18
2	A	401	NAD	C2A-N3A-C4A	3.20	119.65	111.83
2	A	401	NAD	N3A-C4A-N9A	3.15	132.52	127.17
3	B	404	OXQ	O9-C6-O8	-3.06	116.60	123.90
2	B	403	NAD	C4A-N9A-C8A	2.93	108.81	105.74
2	B	403	NAD	O3B-C3B-C2B	-2.89	102.56	111.82
2	C	405	NAD	O2N-PN-O1N	2.72	125.10	112.44
3	D	408	OXQ	O4-N5-C1	2.59	106.86	104.28
2	D	407	NAD	O4B-C1B-C2B	-2.54	101.17	106.62
2	B	403	NAD	C2A-N1A-C6A	2.53	122.89	118.73
2	D	407	NAD	C2A-N3A-C4A	2.53	118.01	111.83
3	B	404	OXQ	O8-C6-C2	2.49	127.23	120.92
2	D	407	NAD	O2N-PN-O1N	2.47	123.94	112.44
2	A	401	NAD	O3-PN-O1N	-2.45	103.34	110.70
2	D	407	NAD	C5A-C6A-N6A	-2.44	117.26	123.29
2	B	403	NAD	C2B-C1B-N9A	-2.40	107.33	113.30
2	B	403	NAD	C1B-N9A-C8A	2.40	132.41	127.09
2	A	401	NAD	O3D-C3D-C2D	-2.37	104.23	111.82
2	D	407	NAD	C3B-C2B-C1B	-2.34	97.03	101.46
2	B	403	NAD	C5A-N7A-C8A	2.34	107.12	103.45
3	B	404	OXQ	N5-O4-N3	-2.33	108.60	111.49
2	D	407	NAD	C4A-N9A-C8A	2.30	108.15	105.74
2	D	407	NAD	O2B-C2B-C3B	2.27	119.08	111.82
2	C	405	NAD	O4B-C1B-N9A	2.25	112.41	108.09
2	C	405	NAD	C2A-N3A-C4A	2.24	117.30	111.83
2	D	407	NAD	C4B-O4B-C1B	-2.23	104.55	109.47
3	D	408	OXQ	C1-C2-N3	2.21	111.81	108.72
2	C	405	NAD	O4B-C4B-C5B	2.21	116.41	109.33
2	A	401	NAD	O2B-C2B-C3B	-2.21	104.75	111.82
2	A	401	NAD	O3-PA-O1A	-2.15	104.24	110.70
3	D	408	OXQ	C6-C2-N3	2.14	124.34	119.71
2	D	407	NAD	C3N-C7N-N7N	2.13	120.37	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	407	NAD	C4A-C5A-N7A	-2.12	108.16	110.58
2	C	405	NAD	C5A-C4A-N9A	2.12	108.12	105.81
2	B	403	NAD	O2D-C2D-C3D	2.10	118.55	111.82
2	C	405	NAD	C6N-N1N-C1D	2.10	123.84	119.73
2	A	401	NAD	C5A-C4A-N9A	2.08	108.08	105.81
2	D	407	NAD	O3D-C3D-C4D	-2.04	105.23	111.08
2	A	401	NAD	N9A-C8A-N7A	-2.02	111.07	113.94
2	A	401	NAD	O4B-C1B-C2B	-2.02	102.30	106.62

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	403	NAD	C5D-O5D-PN-O2N
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	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	C5B-O5B-PA-O3
2	D	407	NAD	O4B-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
3	A	402	OXQ	N3-C2-C6-O9
3	A	402	OXQ	C1-C2-C6-O8
3	A	402	OXQ	N3-C2-C6-O8
3	D	408	OXQ	C1-C2-C6-O9
3	D	408	OXQ	N3-C2-C6-O9
3	D	408	OXQ	C1-C2-C6-O8
3	D	408	OXQ	N3-C2-C6-O8
2	D	407	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	O4D-C4D-C5D-O5D
2	B	403	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	B	403	NAD	C3B-C4B-C5B-O5B
2	B	403	NAD	C3D-C4D-C5D-O5D

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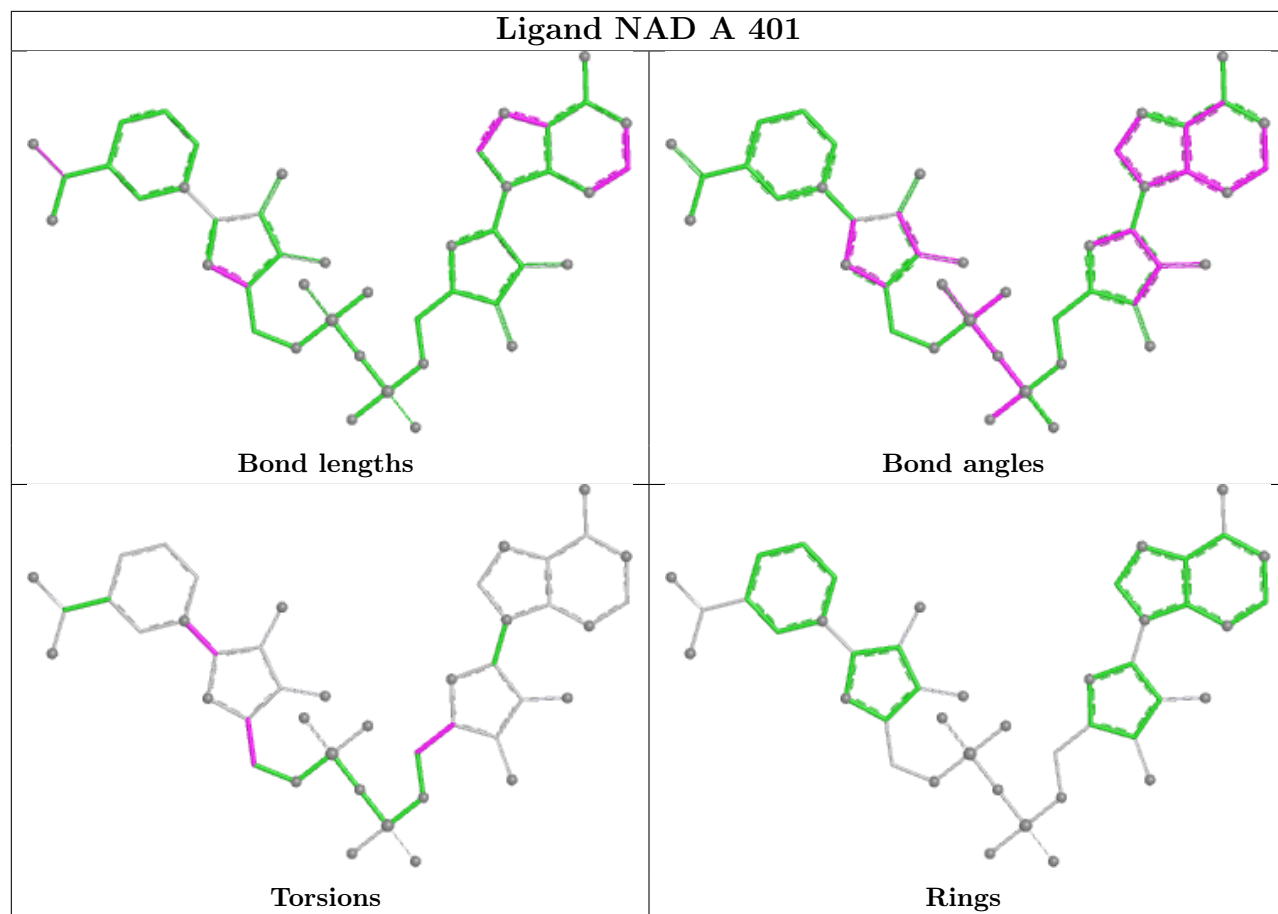
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4B-C4B-C5B-O5B
2	C	405	NAD	O4B-C4B-C5B-O5B
2	C	405	NAD	C3B-C4B-C5B-O5B
2	B	403	NAD	C5B-O5B-PA-O2A
2	B	403	NAD	C5D-O5D-PN-O3
2	B	403	NAD	C5D-O5D-PN-O1N
2	D	407	NAD	C5B-O5B-PA-O2A
2	B	403	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C2N
2	D	407	NAD	PA-O3-PN-O1N

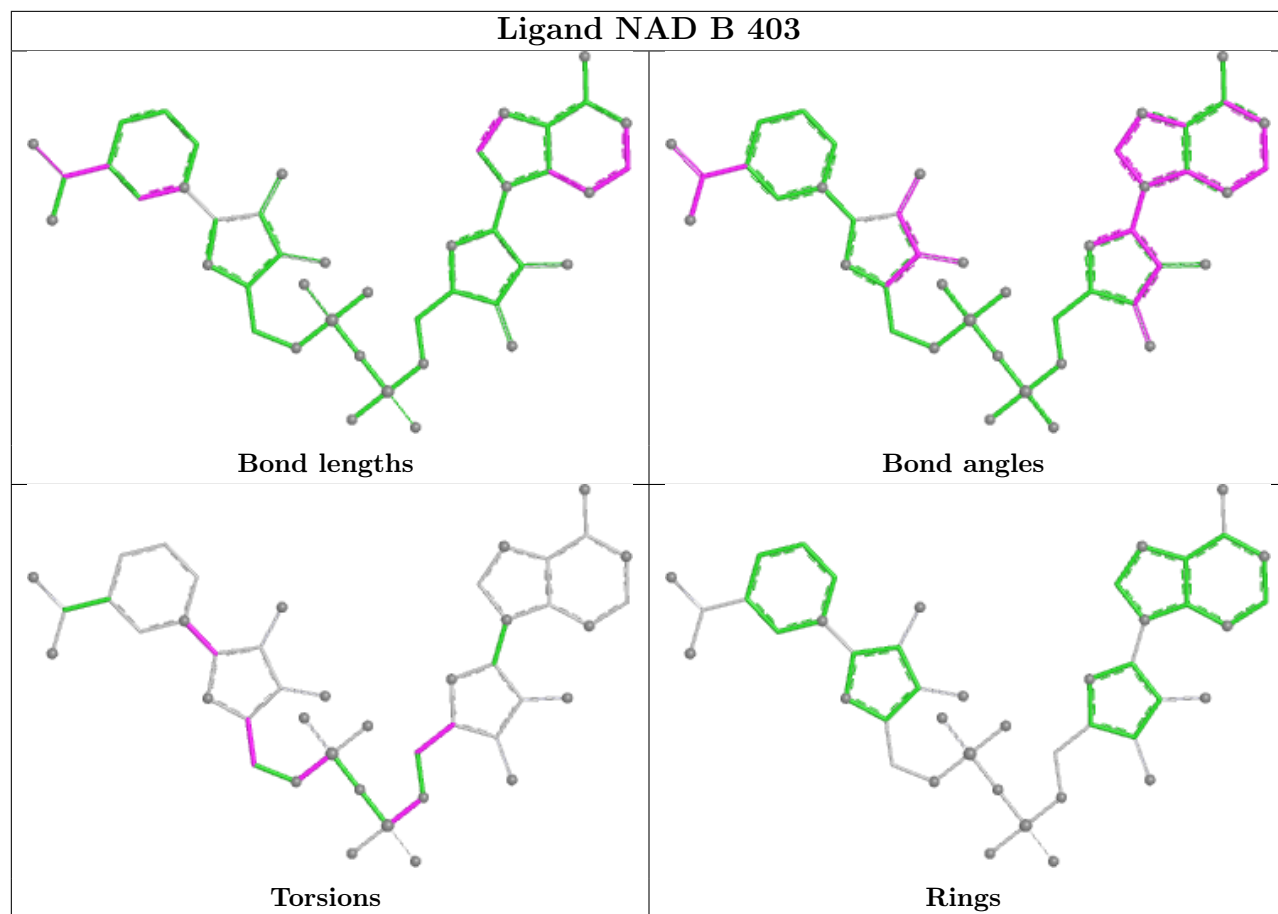
There are no ring outliers.

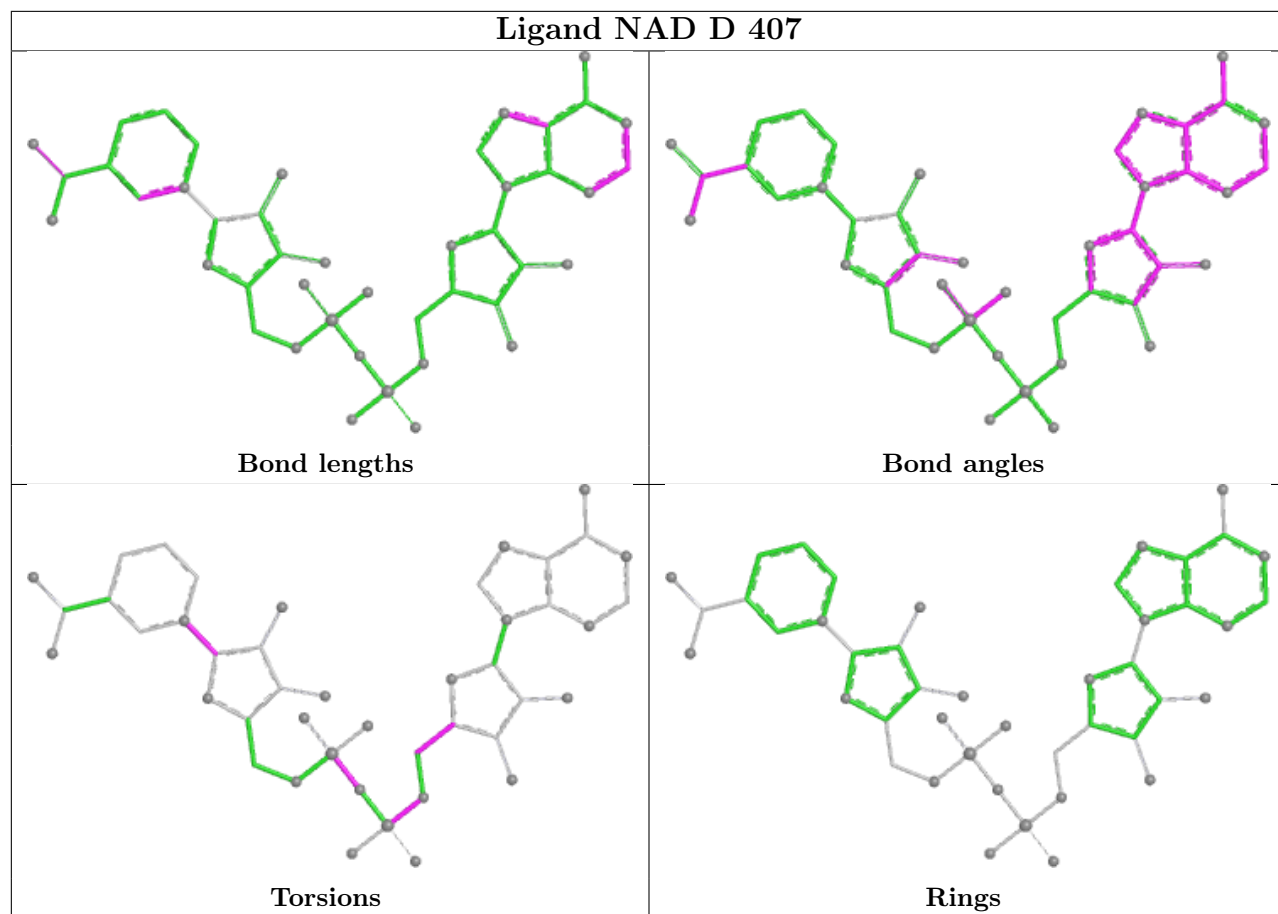
8 monomers are involved in 17 short contacts:

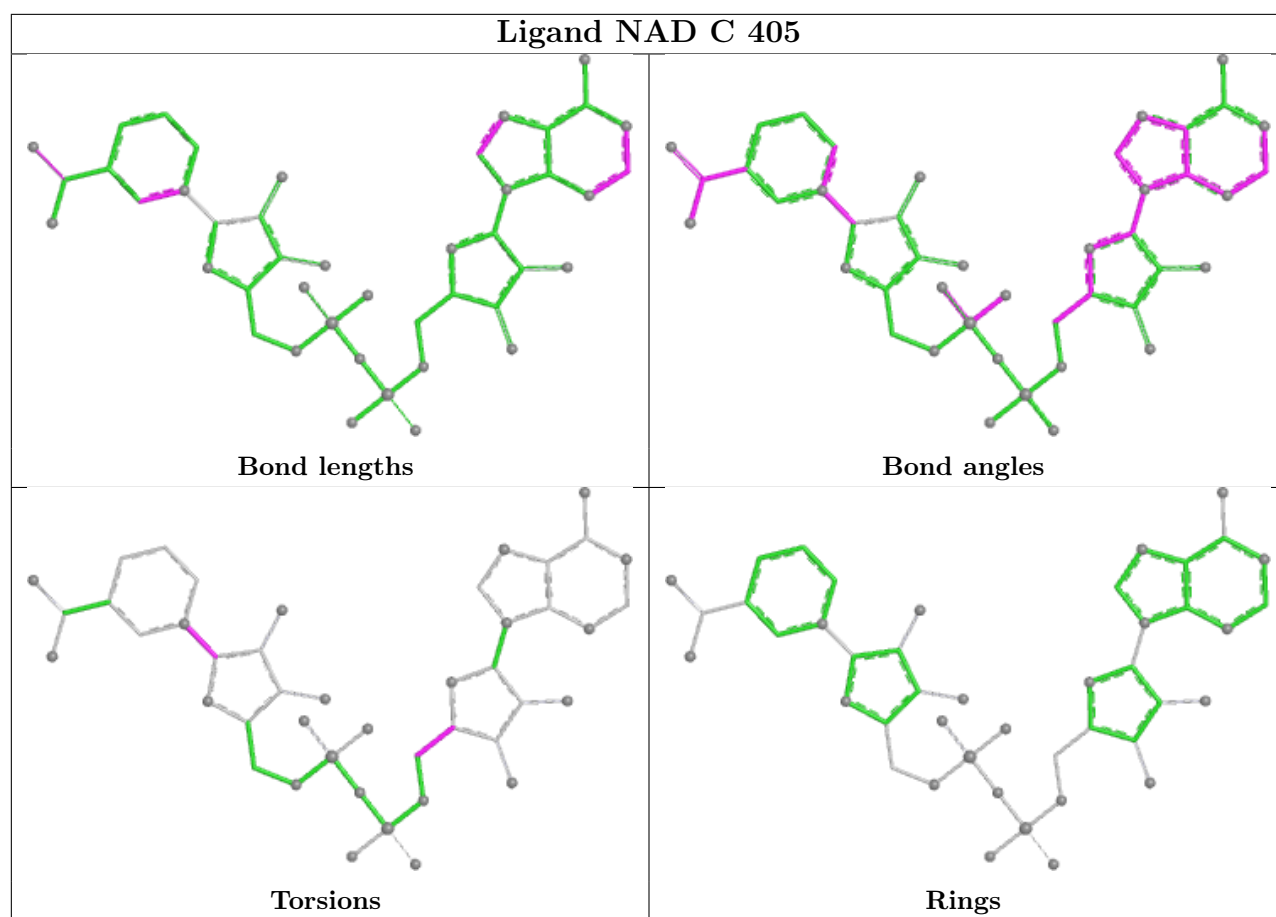
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	OXQ	1	0
2	A	401	NAD	1	0
2	B	403	NAD	4	0
3	C	406	OXQ	3	0
3	D	408	OXQ	2	0
3	A	402	OXQ	1	0
2	D	407	NAD	4	0
2	C	405	NAD	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.28	0 100 100	20, 50, 79, 93	11 (3%)
1	B	332/333 (99%)	0.01	2 (0%) 85 69	27, 60, 85, 90	15 (4%)
1	C	332/333 (99%)	-0.18	3 (0%) 81 61	20, 53, 82, 92	14 (4%)
1	D	332/333 (99%)	-0.19	0 100 100	26, 52, 82, 93	18 (5%)
All	All	1328/1332 (99%)	-0.16	5 (0%) 88 76	20, 53, 83, 93	58 (4%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	ASN	2.9
1	B	208	GLY	2.5
1	C	2	THR	2.1
1	B	107	LEU	2.0
1	C	219	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

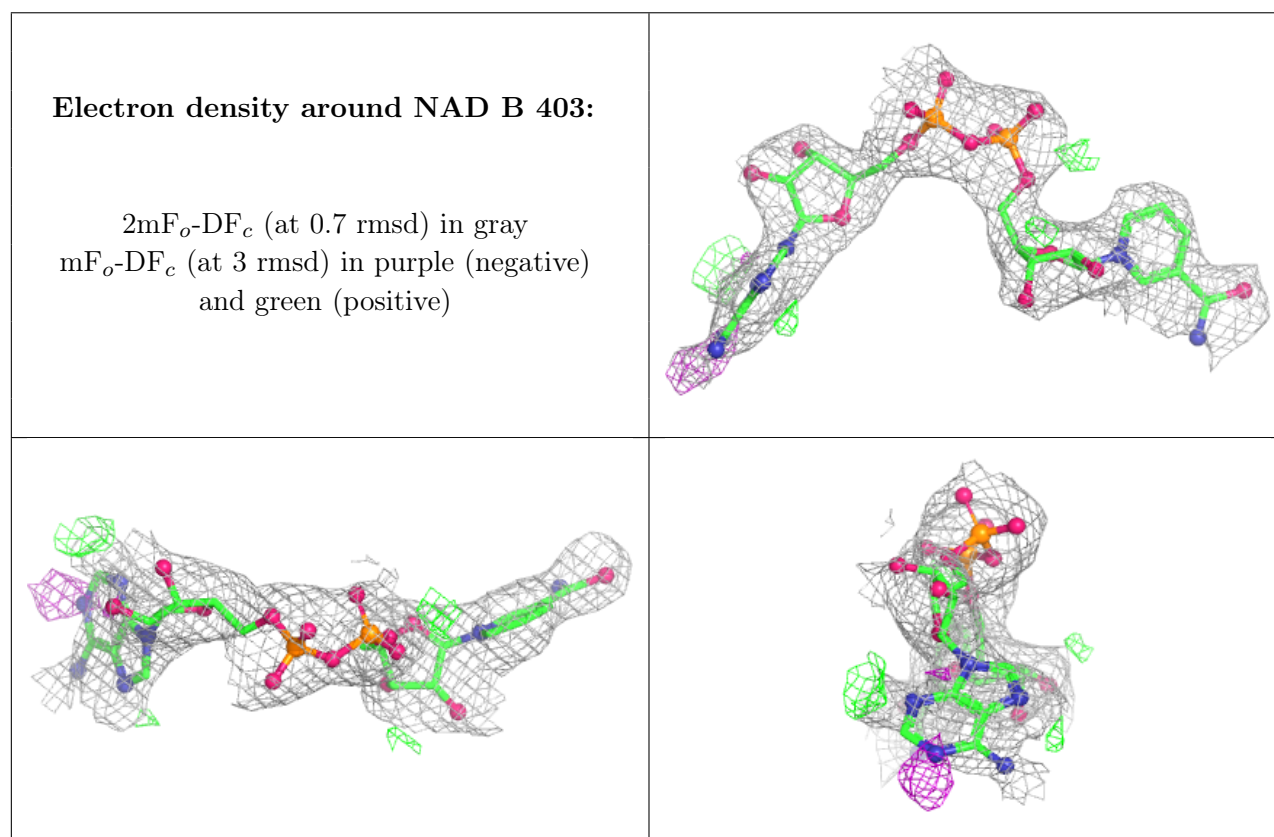
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

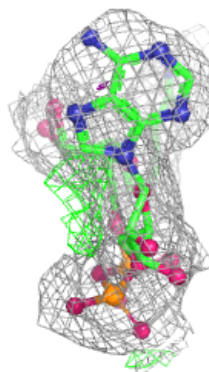
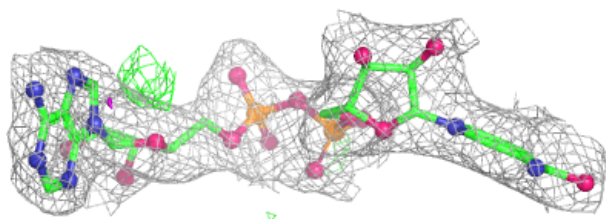
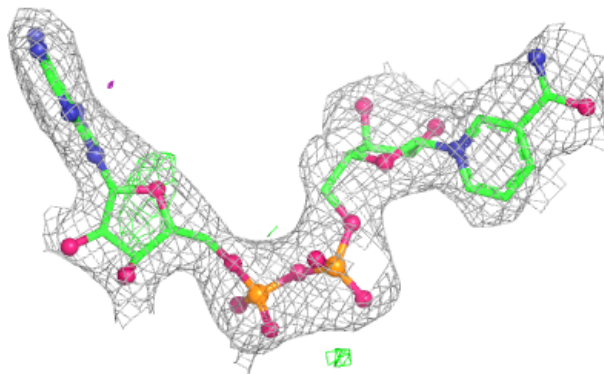
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OXQ	C	406	9/9	0.90	0.09	56,58,59,59	0
3	OXQ	B	404	9/9	0.92	0.13	53,56,60,62	0
2	NAD	B	403	44/44	0.93	0.10	46,61,84,87	0
2	NAD	A	401	44/44	0.95	0.08	29,40,50,51	0
2	NAD	C	405	44/44	0.95	0.08	33,43,52,57	0
2	NAD	D	407	44/44	0.96	0.07	33,42,47,49	0
3	OXQ	D	408	9/9	0.96	0.08	63,65,67,68	0
3	OXQ	A	402	9/9	0.97	0.07	63,64,65,65	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.

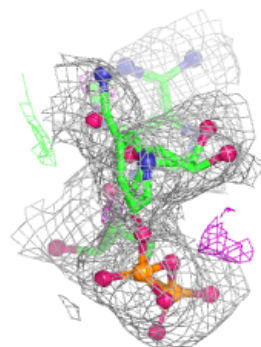
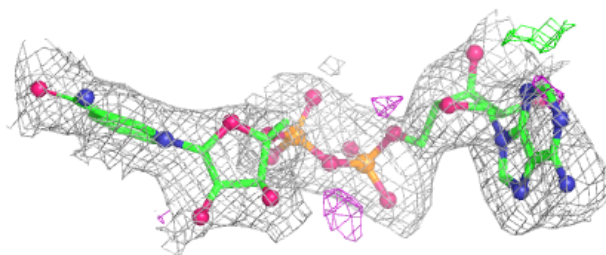
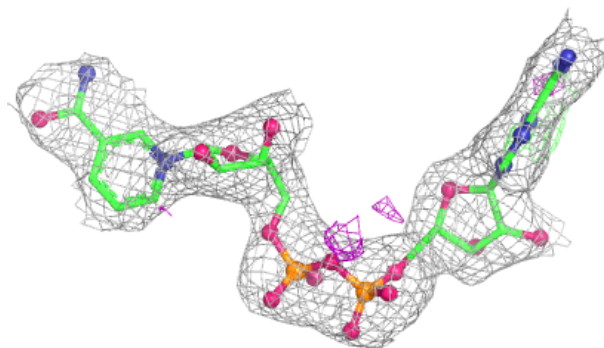


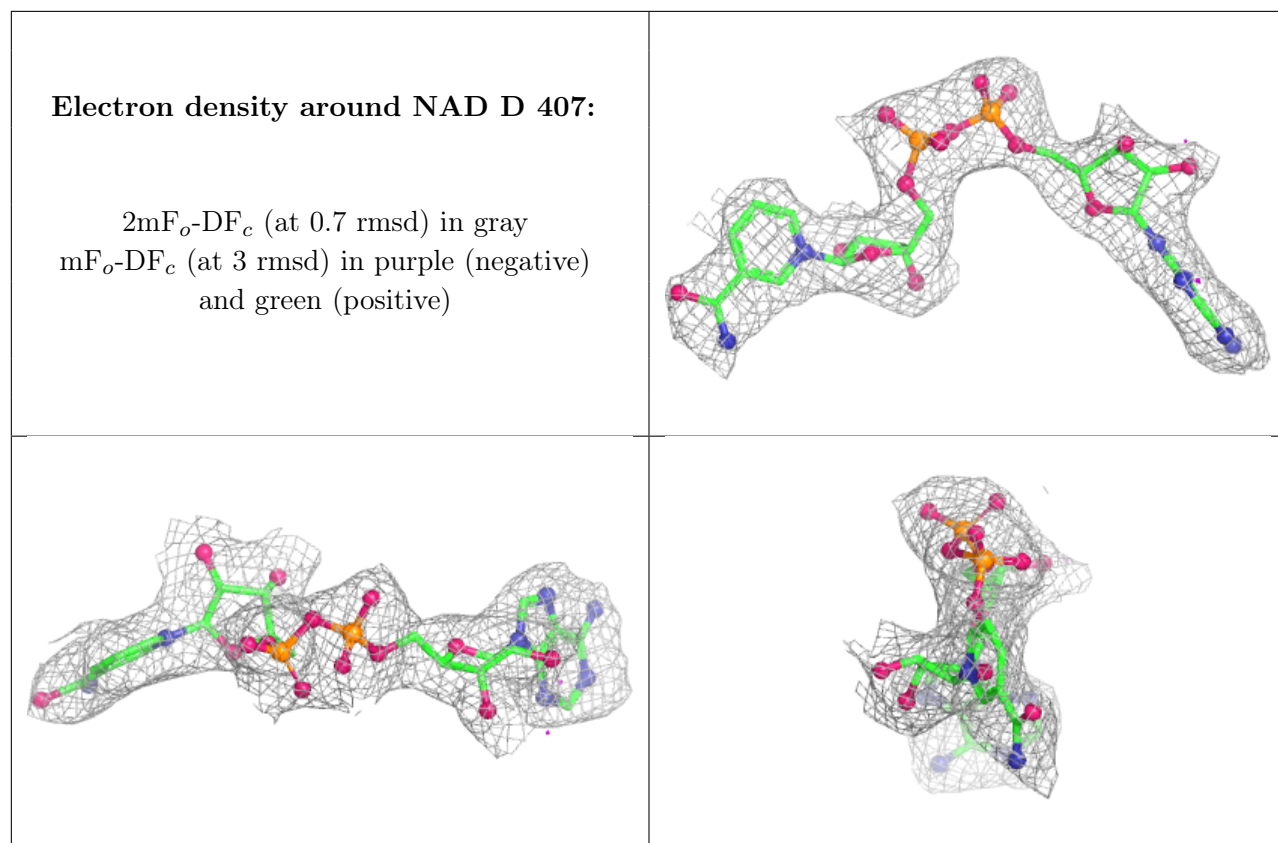
Electron density around NAD A 401:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.