



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:54 AM UTC

PDB ID : 4A0M / pdb_00004a0m
Title : CRYSTAL STRUCTURE OF BETAINE ALDEHYDE DEHYDROGENASE
FROM SPINACH IN COMPLEX WITH NAD
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R.A.
Deposited on : 2011-09-09
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

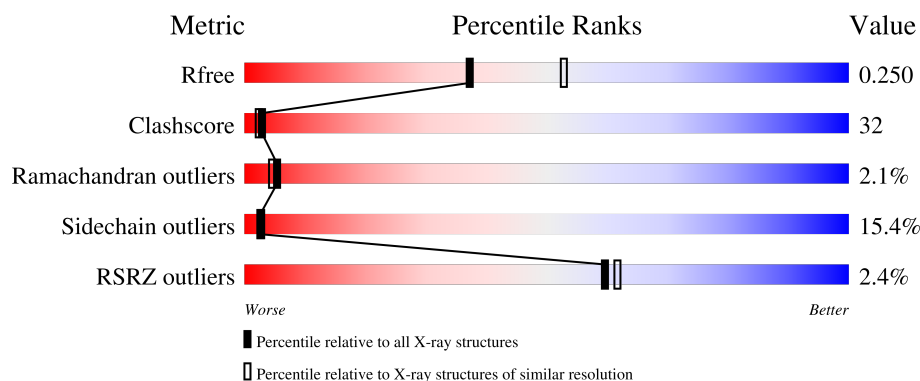
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	496	
1	B	496	
1	C	496	
1	D	496	

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
4	GOL	C	1499	-	-	X	-
4	GOL	D	1501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16124 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 BETAINE ALDEHYDE DEHYDROGENASE, CHLORO-PLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	5	0
			3838	2461	637	723	17			
1	B	494	Total	C	N	O	S	0	6	0
			3844	2462	639	726	17			
1	C	494	Total	C	N	O	S	0	7	0
			3854	2471	640	726	17			
1	D	494	Total	C	N	O	S	0	5	0
			3838	2461	637	723	17			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

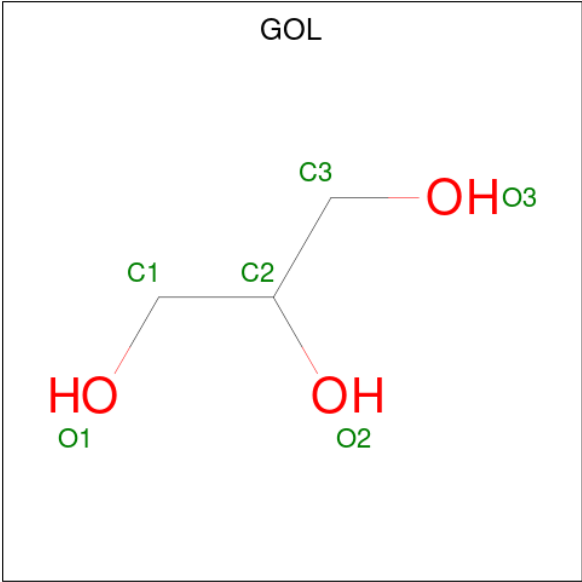
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	B	2	Total	K	0	0
			2	2		
2	C	3	Total	K	0	0
			3	3		
2	D	1	Total	K	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

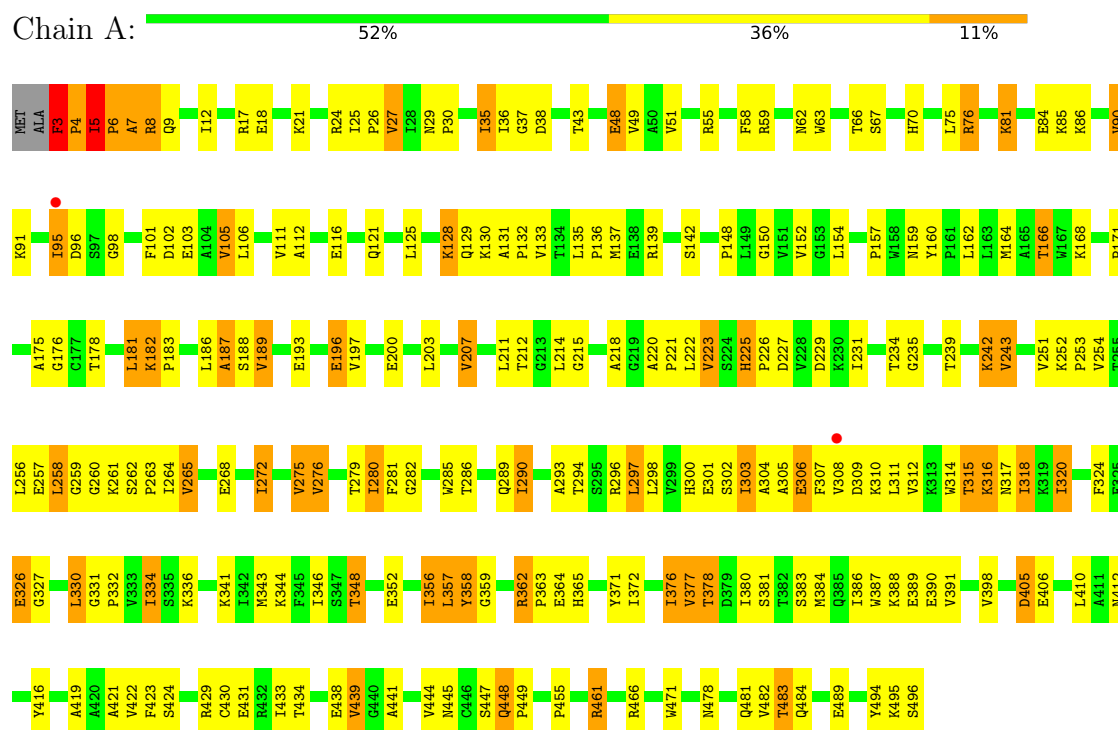
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	128	Total	O	0	0
			128	128		
5	C	129	Total	O	0	0
			129	129		
5	D	97	Total	O	0	0
			97	97		

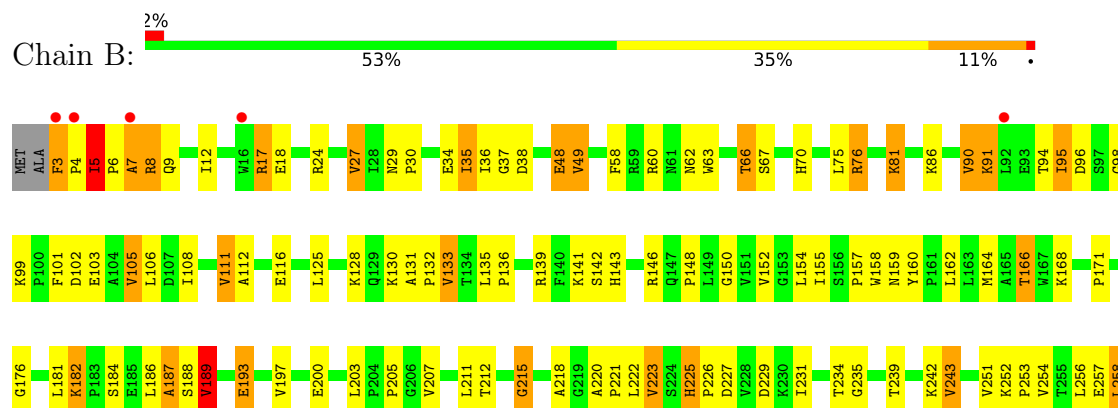
3 Residue-property plots

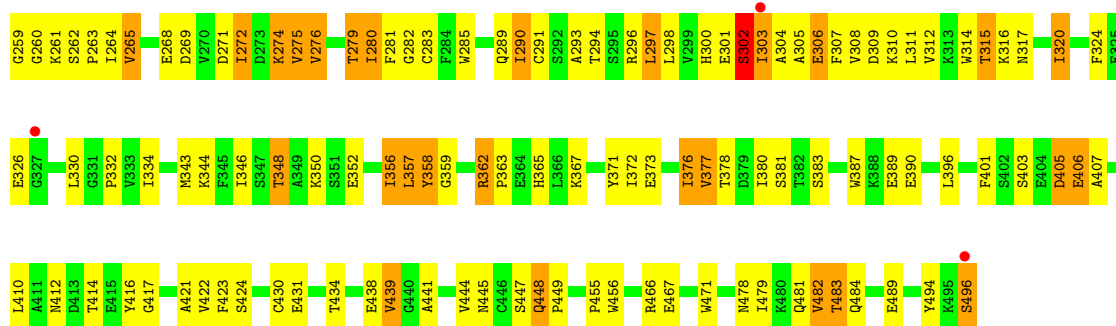
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

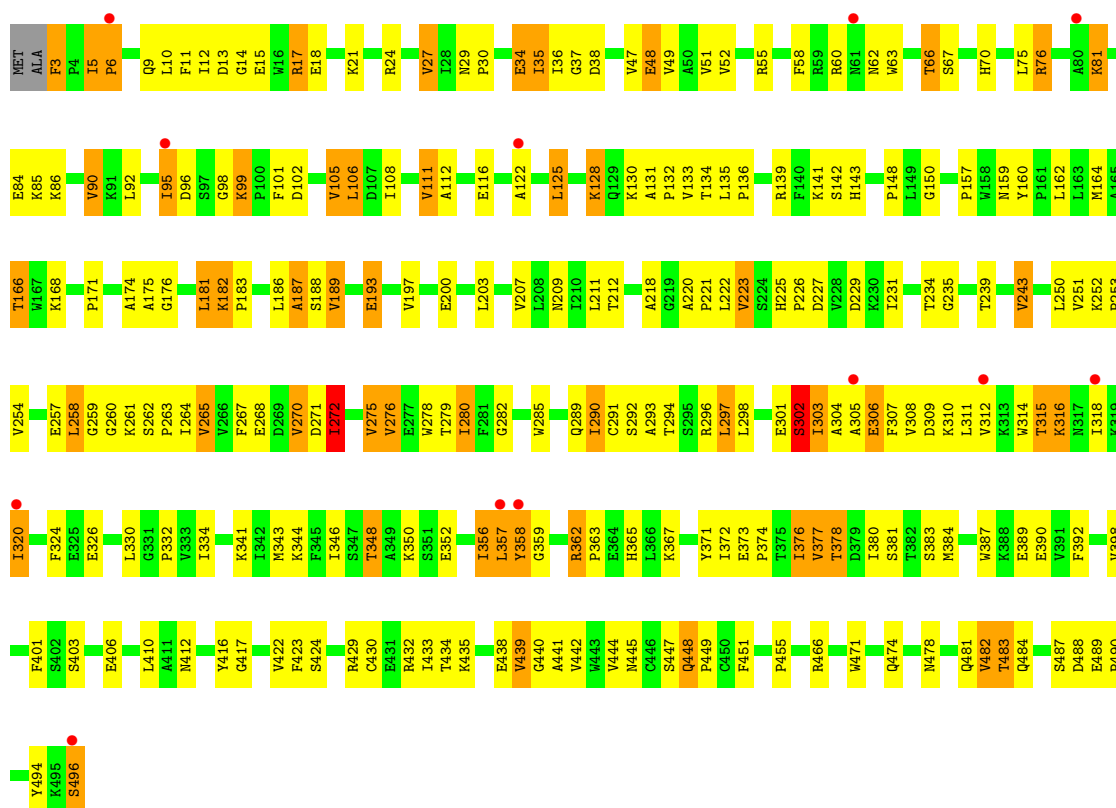


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

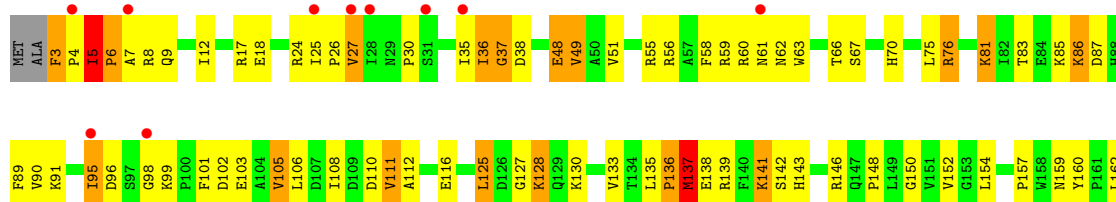


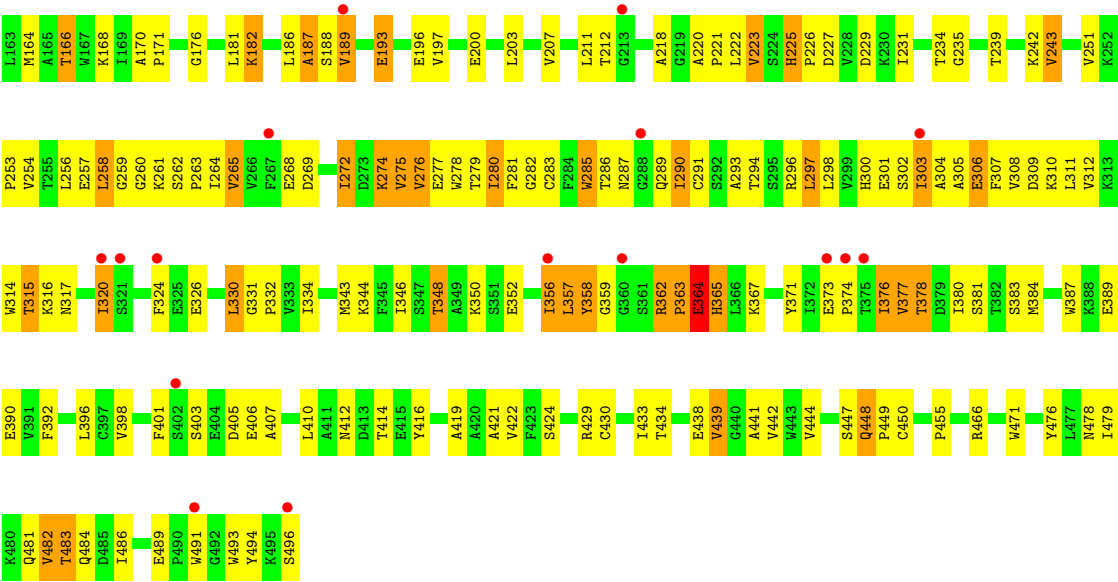


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC



• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.41Å 80.98Å 85.54Å 79.06° 84.94° 77.99°	Depositor
Resolution (Å)	29.08 – 2.30 29.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.08-2.30) 92.1 (29.08-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.247 0.228 , 0.250	Depositor DCC
R_{free} test set	3811 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16124	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, GOL, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	2/3932 (0.1%)	0.92	7/5349 (0.1%)
1	B	0.72	3/3938 (0.1%)	0.94	13/5356 (0.2%)
1	C	0.68	2/3948 (0.1%)	0.90	3/5371 (0.1%)
1	D	0.65	0/3932	0.91	7/5349 (0.1%)
All	All	0.69	7/15750 (0.0%)	0.92	30/21425 (0.1%)

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	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	ALA	C-N	-10.03	1.20	1.33
1	B	159	ASN	CG-OD1	5.42	1.33	1.23
1	A	159	ASN	CG-OD1	5.26	1.33	1.23
1	A	461	ARG	C-O	-5.25	1.17	1.24
1	B	7	ALA	CA-C	-5.21	1.46	1.52
1	C	159	ASN	CG-OD1	5.10	1.33	1.23
1	C	272	ILE	CA-CB	-5.04	1.47	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ALA	CA-C-N	-9.43	106.41	121.87
1	B	7	ALA	C-N-CA	-9.43	106.41	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ALA	O-C-N	8.57	133.96	123.16
1	C	128	LYS	N-CA-C	-8.48	102.71	113.23
1	D	7	ALA	N-CA-C	-8.17	98.19	110.28
1	D	138	GLU	N-CA-C	-8.11	103.59	113.97
1	B	128	LYS	N-CA-C	-7.87	103.47	113.23
1	A	128	LYS	N-CA-C	-7.51	103.92	113.23
1	D	128	LYS	N-CA-C	-6.95	104.27	112.89
1	B	7	ALA	N-CA-C	-5.86	100.64	109.95
1	A	225	HIS	CA-C-N	5.81	125.92	119.87
1	A	225	HIS	C-N-CA	5.81	125.92	119.87
1	B	258	LEU	N-CA-C	5.74	119.87	112.41
1	B	225	HIS	CA-C-N	5.72	125.82	119.87
1	B	225	HIS	C-N-CA	5.72	125.82	119.87
1	A	258	LEU	N-CA-C	5.64	119.75	112.41
1	B	5	ILE	CB-CA-C	-5.42	104.44	110.68
1	D	37	GLY	N-CA-C	5.39	118.34	110.63
1	C	258	LEU	N-CA-C	5.36	119.37	112.41
1	C	34	GLU	N-CA-C	5.34	117.43	108.73
1	D	225	HIS	CA-C-N	5.33	125.41	119.87
1	D	225	HIS	C-N-CA	5.33	125.41	119.87
1	B	406	GLU	N-CA-C	-5.31	106.64	113.23
1	B	189	VAL	N-CA-C	5.29	115.50	110.42
1	B	215	GLY	CA-C-N	5.22	125.02	119.28
1	B	215	GLY	C-N-CA	5.22	125.02	119.28
1	D	258	LEU	N-CA-C	5.19	119.16	112.41
1	A	334	ILE	N-CA-C	5.09	115.81	110.62
1	A	7	ALA	CA-C-N	-5.09	114.33	122.53
1	A	7	ALA	C-N-CA	-5.09	114.33	122.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3838	0	3831	245	0
1	B	3844	0	3829	251	0
1	C	3854	0	3846	275	0
1	D	3838	0	3831	287	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	5	0
3	B	44	0	26	9	0
3	C	44	0	26	8	0
3	D	44	0	26	6	0
4	A	12	0	16	1	0
4	C	6	0	8	8	0
4	D	24	0	32	9	0
5	A	170	0	0	13	0
5	B	128	0	0	14	0
5	C	129	0	0	11	0
5	D	97	0	0	10	0
All	All	16124	0	15497	1007	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1007) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:CB	1:B:62[B]:ASN:HD21	1.14	1.53
1:B:60:ARG:HB3	1:B:62[B]:ASN:ND2	1.17	1.46
1:A:6:PRO:HB2	1:A:7:ALA:CA	1.43	1.37
1:B:60:ARG:CB	1:B:62[B]:ASN:ND2	1.73	1.35
1:C:280:ILE:HG22	1:D:494:TYR:CE2	1.63	1.33
1:A:24:ARG:HD3	1:A:38:ASP:OD2	1.32	1.27
1:A:6:PRO:CB	1:A:7:ALA:HA	1.65	1.21
1:A:301:GLU:HB2	5:A:2094:HOH:O	1.38	1.18
1:C:55:ARG:HH12	4:C:1499:GOL:C3	1.57	1.17
1:D:450[B]:CYS:SG	4:D:1500:GOL:H2	1.87	1.14
1:A:5:ILE:HG22	1:A:6:PRO:N	1.64	1.11
1:C:270:VAL:HG21	1:C:275:VAL:HG11	1.29	1.11
1:C:270:VAL:CG2	1:C:275:VAL:HG11	1.84	1.06
1:C:280:ILE:CG2	1:D:494:TYR:CE2	2.38	1.06
1:B:5:ILE:HD11	1:B:95:ILE:HD11	1.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:PHE:CE2	1:D:95:ILE:HG21	1.95	1.01
1:B:271:ASP:CG	1:B:274:LYS:HD2	1.85	1.00
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.25	0.99
1:B:24:ARG:HD3	1:B:38:ASP:OD2	1.63	0.99
1:A:6:PRO:HB2	1:A:7:ALA:CB	1.94	0.98
1:C:76:ARG:HH11	1:C:76:ARG:HG3	1.26	0.98
1:C:225:HIS:HD2	1:C:227:ASP:H	1.12	0.97
1:A:315:THR:HA	1:A:318:ILE:HD12	1.43	0.97
1:C:5:ILE:HG23	1:C:6:PRO:N	1.78	0.97
1:B:76:ARG:HG3	1:B:76:ARG:HH11	1.29	0.97
1:D:225:HIS:HD2	1:D:227:ASP:H	1.11	0.97
1:D:297:LEU:HB2	5:D:2071:HOH:O	1.64	0.97
1:D:320:ILE:HG21	1:D:373:GLU:OE2	1.65	0.96
1:C:5:ILE:CG2	1:C:6:PRO:N	2.30	0.95
1:C:96:ASP:OD2	1:C:189:VAL:HG13	1.66	0.95
1:A:6:PRO:CB	1:A:7:ALA:CA	2.30	0.94
1:A:3:PHE:CD1	1:A:3:PHE:N	2.32	0.94
1:D:76:ARG:HG3	1:D:76:ARG:HH11	1.29	0.94
1:A:6:PRO:HB2	1:A:7:ALA:HA	0.94	0.93
1:D:110:ASP:OD2	4:D:1501:GOL:H2	1.65	0.93
1:B:60:ARG:HB2	1:B:62[B]:ASN:HD21	0.78	0.92
1:C:24:ARG:HD3	1:C:38:ASP:OD2	1.69	0.92
1:C:280:ILE:HG22	1:D:494:TYR:HE2	1.01	0.91
1:A:225:HIS:HD2	1:A:227:ASP:H	1.14	0.91
1:A:3:PHE:N	1:A:3:PHE:HD1	1.70	0.90
1:B:225:HIS:HD2	1:B:227:ASP:H	1.13	0.90
1:B:3:PHE:N	1:B:4:PRO:HD2	1.88	0.89
1:C:5:ILE:HG23	1:C:6:PRO:CD	2.01	0.89
1:C:55:ARG:NH1	4:C:1499:GOL:C3	2.36	0.87
1:C:316:LYS:HD2	1:C:358:TYR:HE2	1.39	0.87
1:D:95:ILE:HG22	1:D:324:PHE:CZ	2.09	0.86
1:D:363:PRO:O	1:D:364:GLU:HB2	1.73	0.86
1:D:5:ILE:HD13	1:D:5:ILE:H	1.41	0.85
1:A:242:LYS:HE2	1:D:127:GLY:CA	2.07	0.85
1:B:268:GLU:HA	1:B:303:ILE:HD11	1.57	0.85
1:B:60:ARG:HB3	1:B:62[B]:ASN:HD22	1.07	0.85
1:C:225:HIS:CD2	1:C:227:ASP:H	1.95	0.85
1:D:225:HIS:CD2	1:D:227:ASP:H	1.95	0.84
1:C:15:GLU:HG2	1:C:17:ARG:HH11	1.43	0.83
1:C:272:ILE:HG13	1:C:272:ILE:O	1.78	0.83
1:C:150:GLY:HA3	4:C:1499:GOL:O3	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:GLU:HA	1:D:303:ILE:HD11	1.58	0.83
1:B:3:PHE:HB2	1:B:91:LYS:HZ1	1.43	0.82
1:B:225:HIS:CD2	1:B:227:ASP:H	1.97	0.82
1:C:102:ASP:O	1:C:105:VAL:HG22	1.80	0.82
1:B:5:ILE:HD11	1:B:95:ILE:CD1	2.08	0.82
1:D:24:ARG:HD3	1:D:38:ASP:OD2	1.79	0.82
1:A:225:HIS:CD2	1:A:227:ASP:H	1.97	0.82
1:C:55:ARG:HH12	4:C:1499:GOL:H31	1.44	0.82
1:D:5:ILE:H	1:D:5:ILE:CD1	1.93	0.82
1:D:272:ILE:HD12	1:D:307:PHE:HA	1.60	0.82
1:A:5:ILE:CG2	1:A:6:PRO:N	2.39	0.81
1:A:481:GLN:HE21	1:A:483:THR:HG21	1.44	0.81
1:C:305:ALA:O	1:C:306:GLU:HB3	1.80	0.81
1:A:341:LYS:HE3	5:A:2110:HOH:O	1.79	0.81
1:C:268:GLU:HA	1:C:303:ILE:HD11	1.62	0.81
1:A:272:ILE:HD12	1:A:307:PHE:HA	1.61	0.81
1:D:95:ILE:HG22	1:D:324:PHE:HZ	1.46	0.81
1:A:481:GLN:HE21	1:A:483:THR:CG2	1.93	0.81
1:D:481:GLN:HE21	1:D:483:THR:HG21	1.46	0.81
1:B:272:ILE:HD12	1:B:307:PHE:HA	1.62	0.80
1:B:481:GLN:HE21	1:B:483:THR:CG2	1.94	0.80
1:D:3:PHE:CZ	1:D:95:ILE:HG21	2.16	0.80
1:C:101:PHE:O	1:C:105:VAL:HG13	1.82	0.79
1:C:481:GLN:HE21	1:C:483:THR:CG2	1.95	0.79
1:A:162:LEU:O	1:A:166:THR:HG23	1.83	0.79
1:D:157:PRO:HG3	1:D:234:THR:HG22	1.64	0.79
1:C:5:ILE:HG23	1:C:6:PRO:HD2	1.65	0.79
1:A:268:GLU:HA	1:A:303:ILE:HD11	1.66	0.78
1:B:95:ILE:HG22	1:B:324:PHE:CE2	2.17	0.78
1:A:24:ARG:CD	1:A:38:ASP:OD2	2.23	0.78
1:A:306:GLU:HG2	1:A:310:LYS:HZ3	1.48	0.78
1:C:5:ILE:HD11	1:C:95:ILE:HD11	1.63	0.78
1:D:481:GLN:HE21	1:D:483:THR:CG2	1.95	0.78
1:C:142:SER:OG	1:C:483:THR:HG22	1.84	0.78
1:A:95:ILE:HG22	1:A:324:PHE:CE2	2.17	0.77
1:C:481:GLN:HE21	1:C:483:THR:HG21	1.47	0.77
1:D:55:ARG:O	1:D:59:ARG:HG3	1.84	0.77
1:B:162:LEU:O	1:B:166:THR:HG23	1.84	0.77
1:A:5:ILE:H	1:A:6:PRO:HD3	1.50	0.77
1:C:9:GLN:OE1	1:C:18:GLU:HA	1.84	0.77
1:A:51:VAL:HG21	1:A:225:HIS:CE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:O	1:A:348:THR:HG23	1.86	0.76
1:C:162:LEU:O	1:C:166:THR:HG23	1.84	0.76
1:A:9:GLN:OE1	1:A:18:GLU:HA	1.85	0.76
1:A:242:LYS:HE2	1:D:127:GLY:HA2	1.65	0.76
1:D:320:ILE:HD11	1:D:371:TYR:CD1	2.21	0.76
1:A:362:ARG:HD3	1:A:363:PRO:HD2	1.66	0.76
1:D:51:VAL:HG21	1:D:225:HIS:CE1	2.21	0.76
1:B:9:GLN:OE1	1:B:18:GLU:HA	1.86	0.76
1:B:3:PHE:N	1:B:4:PRO:CD	2.49	0.76
1:B:95:ILE:HG22	1:B:324:PHE:CZ	2.21	0.75
1:B:261:LYS:HG3	1:B:296:ARG:HD2	1.68	0.75
1:D:365:HIS:H	1:D:365:HIS:CD2	2.03	0.75
1:A:455:PRO:HG3	1:A:471:TRP:CZ3	2.21	0.75
1:B:390[B]:GLU:OE2	5:B:2102:HOH:O	2.04	0.75
1:D:9:GLN:OE1	1:D:18:GLU:HA	1.87	0.75
1:B:320:ILE:HD11	1:B:371:TYR:CD1	2.22	0.75
1:D:260:GLY:HA2	1:D:416:TYR:CD1	2.22	0.75
1:D:278:TRP:O	1:D:281:PHE:N	2.20	0.75
1:C:5:ILE:HD11	1:C:95:ILE:CD1	2.17	0.75
1:C:362:ARG:HD3	1:C:363:PRO:HD2	1.68	0.75
1:C:429:ARG:HA	1:C:432:ARG:NH2	2.02	0.75
1:B:271:ASP:CG	1:B:274:LYS:CD	2.59	0.75
1:B:362:ARG:HD3	1:B:363:PRO:HD2	1.69	0.75
1:B:5:ILE:HG22	1:B:6:PRO:O	1.86	0.74
1:C:95:ILE:HG22	1:C:324:PHE:CE2	2.21	0.74
1:A:142:SER:OG	1:A:483:THR:HG22	1.87	0.74
1:D:320:ILE:HD11	1:D:371:TYR:HD1	1.51	0.74
1:B:275:VAL:O	1:B:279:THR:HG23	1.87	0.74
1:B:3:PHE:CB	1:B:91:LYS:HZ1	2.01	0.74
1:C:15:GLU:CG	1:C:17:ARG:HH11	2.01	0.74
1:C:267:PHE:O	1:C:270:VAL:CG1	2.35	0.74
1:D:162:LEU:O	1:D:166:THR:HG23	1.86	0.73
1:B:142:SER:OG	1:B:483:THR:HG22	1.88	0.73
1:C:455:PRO:HG3	1:C:471:TRP:CZ3	2.23	0.73
1:D:3:PHE:CG	1:D:91:LYS:NZ	2.56	0.73
1:B:320:ILE:HD11	1:B:371:TYR:HD1	1.53	0.73
1:C:270:VAL:CG2	1:C:275:VAL:CG1	2.66	0.73
1:C:316:LYS:HD2	1:C:358:TYR:CE2	2.23	0.73
1:D:297:LEU:N	5:D:2071:HOH:O	2.21	0.73
1:B:60:ARG:HB2	1:B:62[B]:ASN:ND2	1.64	0.73
1:C:261:LYS:HG3	1:C:296:ARG:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:CYS:O	1:C:434:THR:HG23	1.89	0.73
1:A:280:ILE:HG22	1:B:494:TYR:CE2	2.23	0.72
1:A:289:GLN:HE22	1:A:334:ILE:H	1.37	0.72
1:B:157:PRO:HG3	1:B:234:THR:HG22	1.69	0.72
1:A:96:ASP:OD2	1:A:189:VAL:HG13	1.89	0.72
1:A:130:LYS:NZ	1:B:431:GLU:OE1	2.22	0.72
1:A:157:PRO:HG3	1:A:234:THR:HG22	1.72	0.72
1:B:481:GLN:HE21	1:B:483:THR:HG21	1.53	0.72
1:D:3:PHE:HE2	1:D:95:ILE:HG21	1.50	0.72
1:D:430:CYS:O	1:D:434:THR:HG23	1.89	0.72
1:A:261:LYS:HG3	1:A:296:ARG:HD2	1.70	0.72
1:C:320:ILE:HD11	1:C:371:TYR:CD1	2.24	0.72
1:D:396:LEU:HD21	5:D:2071:HOH:O	1.88	0.72
1:A:95:ILE:HG22	1:A:324:PHE:CZ	2.25	0.72
1:D:274:LYS:O	1:D:277:GLU:N	2.23	0.72
1:C:341:LYS:NZ	5:C:2081:HOH:O	2.23	0.72
1:D:311:LEU:O	1:D:315:THR:HG22	1.90	0.71
1:C:135:LEU:HD21	1:C:142:SER:CB	2.21	0.71
1:D:289:GLN:HE22	1:D:334:ILE:H	1.39	0.71
1:B:300:HIS:ND1	1:B:302:SER:HB2	2.05	0.71
1:C:251[A]:VAL:HG11	1:D:258:LEU:HD11	1.72	0.71
1:B:430:CYS:O	1:B:434:THR:HG23	1.90	0.71
1:D:5:ILE:CD1	1:D:5:ILE:N	2.53	0.71
1:D:455:PRO:HG3	1:D:471:TRP:CZ3	2.25	0.71
1:B:455:PRO:HG3	1:B:471:TRP:CZ3	2.26	0.71
1:A:135:LEU:HD21	1:A:142:SER:CB	2.21	0.71
1:A:260:GLY:HA2	1:A:416:TYR:CD1	2.25	0.71
1:A:320:ILE:HD11	1:A:371:TYR:CD1	2.26	0.71
1:B:357:LEU:HD23	1:B:357:LEU:O	1.91	0.71
1:C:251[A]:VAL:HG12	1:C:251[A]:VAL:O	1.91	0.70
1:D:4:PRO:C	1:D:5:ILE:O	2.30	0.70
1:C:157:PRO:HG3	1:C:234:THR:HG22	1.73	0.70
1:D:344:LYS:O	1:D:348:THR:HG23	1.91	0.70
1:A:430:CYS:O	1:A:434:THR:HG23	1.91	0.70
1:B:260:GLY:HA2	1:B:416:TYR:CD1	2.26	0.70
1:C:320:ILE:HD11	1:C:371:TYR:HD1	1.56	0.70
1:D:414:THR:CG2	5:D:2070:HOH:O	2.40	0.70
1:C:272:ILE:O	1:C:272:ILE:CG1	2.39	0.70
1:D:5:ILE:HG12	1:D:36:ILE:HG13	1.74	0.70
1:B:135:LEU:HD21	1:B:142:SER:CB	2.22	0.70
1:B:261:LYS:HG3	1:B:296:ARG:CD	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LYS:O	1:C:348:THR:HG23	1.92	0.70
1:C:270:VAL:HG23	1:C:275:VAL:HG11	1.74	0.70
1:D:261:LYS:HG3	1:D:296:ARG:HD2	1.73	0.70
1:A:251:VAL:HG11	1:B:258:LEU:HD11	1.73	0.70
1:C:260:GLY:HA2	1:C:416:TYR:CD1	2.26	0.69
1:D:450[B]:CYS:SG	4:D:1500:GOL:C2	2.76	0.69
1:D:63:TRP:O	1:D:66:THR:HB	1.92	0.69
1:D:275:VAL:O	1:D:279:THR:HG23	1.92	0.69
1:D:261:LYS:HG3	1:D:296:ARG:CD	2.23	0.69
1:A:405:ASP:OD1	1:A:405:ASP:C	2.30	0.69
1:D:112:ALA:O	1:D:116:GLU:HG3	1.93	0.69
1:D:135:LEU:HD21	1:D:142:SER:CB	2.23	0.69
1:D:272:ILE:HA	1:D:275:VAL:HG13	1.75	0.69
1:B:63:TRP:O	1:B:66:THR:HB	1.91	0.69
1:D:142:SER:OG	1:D:483:THR:HG22	1.92	0.69
1:B:289:GLN:HE22	1:B:334:ILE:H	1.41	0.69
1:B:414:THR:HG22	5:B:2108:HOH:O	1.92	0.69
1:C:55:ARG:HH12	4:C:1499:GOL:H32	1.55	0.69
1:C:76:ARG:HG3	1:C:76:ARG:NH1	2.05	0.69
1:C:95:ILE:HG22	1:C:324:PHE:CZ	2.27	0.69
1:C:272:ILE:HA	1:C:275:VAL:HG13	1.75	0.69
1:C:289:GLN:HE22	1:C:334:ILE:H	1.38	0.69
1:C:482:VAL:HG21	5:C:2039:HOH:O	1.93	0.69
1:A:63:TRP:O	1:A:66:THR:HB	1.93	0.69
1:B:311:LEU:O	1:B:315:THR:HG22	1.92	0.69
1:C:311:LEU:O	1:C:315:THR:HG22	1.93	0.69
1:A:261:LYS:HG3	1:A:296:ARG:CD	2.22	0.69
1:A:357:LEU:O	1:A:357:LEU:HD23	1.93	0.69
1:D:274:LYS:O	1:D:275:VAL:C	2.35	0.69
1:A:275:VAL:O	1:A:279:THR:HG23	1.93	0.68
1:C:357:LEU:HD23	1:C:357:LEU:O	1.93	0.68
1:D:357:LEU:O	1:D:357:LEU:HD23	1.93	0.68
1:C:435:LYS:HE2	5:C:2103:HOH:O	1.93	0.68
1:D:3:PHE:HE2	1:D:95:ILE:HD12	1.59	0.68
1:B:3:PHE:HB2	1:B:91:LYS:NZ	2.09	0.68
1:C:76:ARG:HH11	1:C:76:ARG:CG	2.06	0.68
1:D:196:GLU:HG2	5:D:2002:HOH:O	1.93	0.68
1:D:3:PHE:HZ	1:D:324:PHE:CZ	2.12	0.68
1:D:182:LYS:HD2	1:D:218:ALA:HB3	1.76	0.68
1:B:96:ASP:OD2	1:B:189:VAL:HG13	1.94	0.67
1:B:272:ILE:HA	1:B:275:VAL:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:PHE:O	1:C:270:VAL:HG13	1.94	0.67
1:B:447:SER:C	1:B:449:PRO:HD3	2.20	0.67
1:C:96:ASP:OD2	1:C:189:VAL:CG1	2.40	0.67
1:C:258:LEU:HD11	1:D:251:VAL:HG11	1.75	0.67
1:C:275:VAL:O	1:C:279:THR:HG23	1.95	0.67
1:A:76:ARG:HH11	1:A:76:ARG:CG	2.03	0.67
1:C:270:VAL:HG23	1:C:275:VAL:CG1	2.25	0.67
1:A:215:GLY:HA3	3:A:1498:NAD:C8A	2.24	0.67
1:A:444:VAL:HB	1:B:484:GLN:CB	2.25	0.67
1:D:305:ALA:O	1:D:306:GLU:CB	2.43	0.67
1:B:5:ILE:CG2	1:B:6:PRO:O	2.43	0.67
1:A:251:VAL:O	1:A:251:VAL:HG12	1.95	0.67
1:C:3:PHE:CD1	1:C:3:PHE:C	2.67	0.67
1:A:258:LEU:HD11	1:B:251:VAL:HG11	1.76	0.66
1:C:305:ALA:O	1:C:306:GLU:CB	2.43	0.66
1:D:9:GLN:NE2	1:D:24:ARG:HH21	1.93	0.66
1:A:320:ILE:HD11	1:A:371:TYR:HD1	1.57	0.66
1:A:272:ILE:HA	1:A:275:VAL:HG13	1.77	0.66
1:A:431:GLU:HB2	5:A:2136:HOH:O	1.95	0.66
1:B:76:ARG:HH11	1:B:76:ARG:CG	2.06	0.66
1:C:447:SER:C	1:C:449:PRO:HD3	2.21	0.66
1:D:390[B]:GLU:O	1:D:390[B]:GLU:HG3	1.94	0.66
1:A:81:LYS:HD3	1:A:200:GLU:OE1	1.96	0.66
1:B:406:GLU:O	1:B:410:LEU:HB2	1.96	0.66
1:C:142:SER:HG	1:C:483:THR:HG22	1.61	0.66
1:A:259:GLY:HA3	3:A:1498:NAD:O2D	1.96	0.66
1:B:3:PHE:CB	1:B:91:LYS:NZ	2.59	0.66
1:D:135:LEU:HD21	1:D:142:SER:HB3	1.77	0.66
1:B:6:PRO:HG2	1:B:193:GLU:OE2	1.96	0.65
1:B:357:LEU:O	1:B:358:TYR:HB2	1.96	0.65
1:C:63:TRP:O	1:C:66:THR:HB	1.97	0.65
1:D:493:TRP:HD1	1:D:494:TYR:CE1	2.14	0.65
1:C:55:ARG:NH1	4:C:1499:GOL:H32	2.10	0.65
1:D:272:ILE:HD13	1:D:306:GLU:HG2	1.77	0.65
1:C:390[B]:GLU:HG3	1:C:390[B]:GLU:O	1.97	0.65
1:B:6:PRO:CG	1:B:193:GLU:OE2	2.45	0.65
1:B:251:VAL:HG12	1:B:251:VAL:O	1.96	0.65
1:C:261:LYS:HG3	1:C:296:ARG:CD	2.26	0.65
1:D:272:ILE:CD1	1:D:306:GLU:HG2	2.27	0.65
1:C:306:GLU:O	1:C:310:LYS:HG2	1.96	0.65
1:D:450[B]:CYS:HG	4:D:1501:GOL:HO3	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390[B]:GLU:O	1:B:390[B]:GLU:HG3	1.97	0.65
1:D:3:PHE:HZ	1:D:324:PHE:HZ	1.44	0.65
1:C:272:ILE:HD11	1:C:306:GLU:HG2	1.78	0.64
1:D:314:TRP:O	1:D:317:ASN:HB2	1.97	0.64
1:B:168:LYS:O	1:B:171:PRO:HD2	1.98	0.64
1:B:271:ASP:OD2	1:B:274:LYS:NZ	2.29	0.64
1:C:259:GLY:H	3:C:1498:NAD:H71N	1.45	0.64
1:C:365:HIS:CD2	1:C:365:HIS:H	2.13	0.64
1:D:27:VAL:HG13	1:D:37:GLY:C	2.23	0.64
1:A:66:THR:HG22	1:A:67:SER:O	1.98	0.64
1:D:3:PHE:CZ	1:D:95:ILE:CG2	2.80	0.64
1:D:259:GLY:HA3	3:D:1498:NAD:O2D	1.98	0.64
1:A:5:ILE:HG22	1:A:6:PRO:CA	2.28	0.64
1:D:76:ARG:HH11	1:D:76:ARG:CG	2.09	0.64
1:A:30:PRO:HB2	1:A:332:PRO:HG2	1.79	0.64
1:B:365:HIS:H	1:B:365:HIS:CD2	2.15	0.64
1:C:251[A]:VAL:HG11	1:D:258:LEU:CD1	2.28	0.64
1:C:34:GLU:O	1:C:36:ILE:HG23	1.98	0.63
5:A:2162:HOH:O	1:B:314:TRP:HE3	1.81	0.63
1:B:182:LYS:HD2	1:B:218:ALA:HB3	1.79	0.63
1:A:447:SER:C	1:A:449:PRO:HD3	2.24	0.63
1:A:251:VAL:HG11	1:B:258:LEU:CD1	2.29	0.63
1:C:66:THR:HG22	1:C:67:SER:O	1.99	0.63
1:A:390[B]:GLU:O	1:A:390[B]:GLU:HG3	1.97	0.63
1:B:308:VAL:O	1:B:312:VAL:HG13	1.99	0.63
1:C:182:LYS:HD2	1:C:218:ALA:HB3	1.80	0.63
1:A:76:ARG:HG3	1:A:76:ARG:NH1	2.04	0.62
1:C:6:PRO:HB3	1:C:193:GLU:OE2	1.98	0.62
1:D:396:LEU:CD2	5:D:2071:HOH:O	2.46	0.62
1:A:96:ASP:CG	1:A:189:VAL:HG13	2.24	0.62
1:C:455:PRO:HG3	1:C:471:TRP:CE3	2.34	0.62
1:D:373:GLU:O	1:D:374:PRO:C	2.40	0.62
1:B:96:ASP:CG	1:B:189:VAL:HG13	2.24	0.62
1:B:298:LEU:HD21	1:B:387:TRP:HH2	1.65	0.62
1:C:135:LEU:HD21	1:C:142:SER:HB2	1.81	0.62
1:C:377:VAL:CG2	1:C:380:ILE:HD11	2.29	0.62
1:D:291:CYS:HB3	3:D:1498:NAD:C6N	2.29	0.62
1:A:306:GLU:HG2	1:A:310:LYS:NZ	2.13	0.62
1:A:494:TYR:HB3	5:A:2162:HOH:O	2.00	0.62
1:B:103:GLU:OE2	1:B:285:TRP:CD1	2.53	0.62
1:B:412:ASN:HD21	1:B:438:GLU:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:HD11	1:C:211:LEU:HD21	1.81	0.61
1:C:259:GLY:HA3	3:C:1498:NAD:O2D	1.99	0.61
1:D:76:ARG:HG3	1:D:76:ARG:NH1	2.07	0.61
1:D:251:VAL:HG12	1:D:251:VAL:O	1.99	0.61
1:C:9:GLN:NE2	1:C:24:ARG:HH21	1.97	0.61
1:D:447:SER:C	1:D:449:PRO:HD3	2.24	0.61
1:D:312:VAL:O	1:D:316:LYS:HB2	2.01	0.61
1:A:305:ALA:O	1:A:306:GLU:CB	2.49	0.61
1:A:305:ALA:O	1:A:306:GLU:HB2	1.99	0.61
1:C:298:LEU:HD21	1:C:387:TRP:HH2	1.65	0.61
1:C:312:VAL:O	1:C:316:LYS:HB2	2.00	0.61
1:C:412:ASN:HD21	1:C:438:GLU:H	1.49	0.61
1:D:493:TRP:CD1	1:D:494:TYR:CE1	2.88	0.61
1:B:350:LYS:HE3	1:B:356:ILE:HD12	1.81	0.61
1:A:377:VAL:CG2	1:A:380:ILE:HD11	2.31	0.61
1:A:298:LEU:HD21	1:A:387:TRP:HH2	1.66	0.61
3:C:1498:NAD:H52A	3:C:1498:NAD:O2N	2.01	0.61
1:A:455:PRO:HG3	1:A:471:TRP:CE3	2.36	0.60
1:C:258:LEU:CD1	1:D:251:VAL:HG11	2.31	0.60
1:C:444:VAL:HB	1:D:484:GLN:CB	2.31	0.60
1:C:105:VAL:HG23	1:C:106:LEU:HD13	1.83	0.60
1:A:135:LEU:HD21	1:A:142:SER:HB3	1.82	0.60
1:B:17:ARG:HG2	5:B:2006:HOH:O	2.01	0.60
1:B:76:ARG:HG3	1:B:76:ARG:NH1	2.09	0.60
1:D:66:THR:CG2	1:D:70:HIS:HB3	2.31	0.60
1:B:3:PHE:HD1	1:B:3:PHE:C	2.10	0.60
1:A:494:TYR:CE2	1:B:280:ILE:HG22	2.36	0.60
1:C:66:THR:CG2	1:C:70:HIS:HB3	2.31	0.60
1:D:265:VAL:HG22	1:D:422:VAL:HG23	1.84	0.60
1:A:168:LYS:O	1:A:171:PRO:HD2	2.02	0.60
1:B:3:PHE:C	1:B:3:PHE:CD1	2.77	0.60
1:D:3:PHE:CE2	1:D:95:ILE:CG2	2.80	0.60
1:B:265:VAL:HG22	1:B:422:VAL:HG23	1.83	0.60
1:D:3:PHE:CB	1:D:91:LYS:NZ	2.64	0.60
1:C:150:GLY:CA	4:C:1499:GOL:O3	2.48	0.60
1:D:298:LEU:HD21	1:D:387:TRP:HH2	1.66	0.60
1:A:311:LEU:O	1:A:315:THR:HG22	2.02	0.59
1:C:377:VAL:HG22	1:C:380:ILE:HD11	1.84	0.59
1:C:81:LYS:HG2	1:C:197:VAL:HG13	1.84	0.59
1:D:412:ASN:HD21	1:D:438:GLU:H	1.49	0.59
1:A:316:LYS:HD2	1:A:358:TYR:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:TRP:HD1	1:B:184:SER:HG	1.50	0.59
1:B:377:VAL:CG2	1:B:380:ILE:HD11	2.33	0.59
1:A:6:PRO:HB2	1:A:7:ALA:HB2	1.82	0.59
1:B:66:THR:CG2	1:B:70:HIS:HB3	2.32	0.59
1:B:81:LYS:HG2	1:B:197:VAL:HG13	1.85	0.59
1:C:135:LEU:HD21	1:C:142:SER:HB3	1.85	0.59
1:C:315:THR:HG23	5:C:2074:HOH:O	2.01	0.59
1:D:377:VAL:CG2	1:D:380:ILE:HD11	2.32	0.59
1:A:135:LEU:HD21	1:A:142:SER:HB2	1.84	0.59
1:B:377:VAL:HG22	1:B:380:ILE:HD11	1.84	0.59
1:D:66:THR:HG22	1:D:67:SER:O	2.02	0.59
1:A:258:LEU:CD1	1:B:251:VAL:HG11	2.31	0.59
1:B:301:GLU:HA	1:B:304:ALA:HB2	1.85	0.59
1:C:357:LEU:O	1:C:358:TYR:HB2	2.02	0.59
1:D:264:ILE:CD1	1:D:279:THR:HG22	2.32	0.59
1:A:101:PHE:O	1:A:105:VAL:HG13	2.03	0.59
1:B:312:VAL:O	1:B:316:LYS:HB2	2.02	0.59
1:D:168:LYS:O	1:D:171:PRO:HD2	2.03	0.59
1:B:135:LEU:HD21	1:B:142:SER:HB2	1.83	0.58
1:D:81:LYS:HG2	1:D:197:VAL:HG13	1.85	0.58
1:A:66:THR:CG2	1:A:70:HIS:HB3	2.34	0.58
1:A:182:LYS:HD2	1:A:218:ALA:HB3	1.84	0.58
1:B:30:PRO:HB2	1:B:332:PRO:HG2	1.85	0.58
1:B:182:LYS:NZ	3:B:1498:NAD:O2B	2.37	0.58
1:C:51:VAL:HG21	1:C:225:HIS:CE1	2.38	0.58
1:C:55:ARG:NH1	4:C:1499:GOL:H31	2.12	0.58
1:C:81:LYS:HD3	1:C:200:GLU:OE1	2.03	0.58
1:D:56:ARG:HD2	1:D:60:ARG:HH12	1.66	0.58
1:D:412:ASN:ND2	1:D:438:GLU:H	2.02	0.58
1:C:3:PHE:CD1	1:C:3:PHE:O	2.56	0.58
1:A:365:HIS:H	1:A:365:HIS:CD2	2.21	0.58
1:B:135:LEU:HD21	1:B:142:SER:HB3	1.84	0.58
1:B:306:GLU:O	1:B:310:LYS:HG2	2.04	0.58
1:C:265:VAL:HG22	1:C:422:VAL:HG23	1.84	0.58
1:A:377:VAL:HG22	1:A:380:ILE:HD11	1.84	0.58
1:A:304:ALA:O	1:A:308:VAL:HG12	2.03	0.58
1:A:336:LYS:NZ	1:D:116:GLU:OE1	2.35	0.58
1:A:484:GLN:CB	1:B:444:VAL:HB	2.33	0.58
1:D:278:TRP:O	1:D:279:THR:C	2.46	0.58
1:A:311:LEU:O	1:A:315:THR:CG2	2.51	0.58
1:B:257[A]:GLU:HB3	3:B:1498:NAD:N7N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ALA:HB3	1:A:221:PRO:HD3	1.85	0.57
1:A:265:VAL:HG22	1:A:422:VAL:HG23	1.85	0.57
1:C:350:LYS:HE3	1:C:356:ILE:HD12	1.85	0.57
1:D:95:ILE:HG22	1:D:324:PHE:CE2	2.38	0.57
1:D:314:TRP:O	1:D:317:ASN:CB	2.52	0.57
1:A:25[B]:ILE:HG23	1:A:26:PRO:HD2	1.86	0.57
1:B:101:PHE:O	1:B:105:VAL:HG13	2.04	0.57
1:D:301:GLU:HA	1:D:304:ALA:HB2	1.85	0.57
1:C:105:VAL:CG2	1:C:106:LEU:HD13	2.34	0.57
1:D:30:PRO:HB2	1:D:332:PRO:HG2	1.86	0.57
1:D:101:PHE:O	1:D:105:VAL:HG13	2.04	0.57
1:B:242:LYS:NZ	5:B:2083:HOH:O	2.36	0.57
1:D:377:VAL:HG22	1:D:380:ILE:HD11	1.86	0.57
1:D:414:THR:HG23	5:D:2070:HOH:O	2.03	0.57
1:B:103:GLU:HG2	1:B:285:TRP:HE1	1.69	0.57
1:B:141:LYS:CD	5:B:2051:HOH:O	2.51	0.57
1:C:101:PHE:O	1:C:105:VAL:CG1	2.52	0.57
1:A:301:GLU:HA	1:A:304:ALA:HB2	1.87	0.57
1:A:306:GLU:O	1:A:310:LYS:HG2	2.05	0.57
1:B:95:ILE:HG22	1:B:324:PHE:HE2	1.69	0.57
1:C:308:VAL:O	1:C:311:LEU:HB3	2.03	0.57
1:D:5:ILE:HG22	1:D:6:PRO:N	2.19	0.57
1:D:304:ALA:O	1:D:308:VAL:HG12	2.04	0.57
1:D:308:VAL:O	1:D:312:VAL:HG13	2.04	0.57
1:D:396:LEU:HD11	5:D:2071:HOH:O	2.04	0.57
1:C:490:PRO:HA	1:D:274:LYS:HG2	1.87	0.57
1:B:35:ILE:HG13	1:B:35:ILE:O	2.05	0.57
1:B:242:LYS:NZ	5:B:2080:HOH:O	2.25	0.57
1:B:268:GLU:CA	1:B:303:ILE:HD11	2.33	0.57
1:B:48:GLU:HG3	5:B:2019:HOH:O	2.04	0.56
1:A:308:VAL:O	1:A:312:VAL:HG13	2.05	0.56
1:B:481:GLN:HE21	1:B:483:THR:HG23	1.67	0.56
1:C:412:ASN:ND2	1:C:438:GLU:H	2.03	0.56
1:D:188:SER:HB3	1:D:212:THR:HG21	1.88	0.56
1:C:280:ILE:HG21	1:D:494:TYR:CE2	2.38	0.56
1:D:4:PRO:O	1:D:5:ILE:C	2.49	0.56
1:D:96:ASP:OD2	1:D:189:VAL:CG1	2.53	0.56
1:A:95:ILE:HB	5:A:2011:HOH:O	2.04	0.56
1:B:81:LYS:HD3	1:B:200:GLU:OE1	2.05	0.56
1:D:406:GLU:O	1:D:410:LEU:HB2	2.05	0.56
1:A:66:THR:HG23	1:A:70:HIS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:HG23	1:B:70:HIS:HB3	1.88	0.56
1:B:141:LYS:HD3	5:B:2051:HOH:O	2.04	0.56
1:D:455:PRO:HG3	1:D:471:TRP:CE3	2.40	0.56
1:C:21:LYS:NZ	5:C:2002:HOH:O	2.37	0.56
1:D:220:ALA:HB3	1:D:221:PRO:HD3	1.86	0.56
1:D:102:ASP:O	1:D:105:VAL:HG22	2.06	0.56
1:D:268:GLU:CA	1:D:303:ILE:HD11	2.34	0.56
1:A:55:ARG:HD2	1:A:59:ARG:CZ	2.36	0.56
1:B:412:ASN:ND2	1:B:438:GLU:H	2.02	0.56
1:A:444:VAL:HB	1:B:484:GLN:HB3	1.87	0.55
1:A:357:LEU:O	1:A:358:TYR:HB2	2.05	0.55
1:A:381:SER:HB3	1:A:384:MET:HG2	1.89	0.55
1:B:188:SER:HB3	1:B:212:THR:HG21	1.88	0.55
1:C:188:SER:HB3	1:C:212:THR:HG21	1.87	0.55
1:C:301:GLU:HA	1:C:304:ALA:HB2	1.87	0.55
1:B:268:GLU:HA	1:B:303:ILE:CD1	2.34	0.55
1:C:168:LYS:O	1:C:171:PRO:HD2	2.06	0.55
1:D:272:ILE:HD11	1:D:310:LYS:HG3	1.87	0.55
1:D:357:LEU:O	1:D:358:TYR:HB2	2.06	0.55
1:C:30:PRO:HB2	1:C:332:PRO:HG2	1.88	0.55
1:C:225:HIS:HD2	1:C:227:ASP:N	1.94	0.55
1:D:25[B]:ILE:HG23	1:D:26:PRO:HD2	1.87	0.55
1:D:81:LYS:HD3	1:D:200:GLU:OE1	2.07	0.55
1:D:291:CYS:HB3	3:D:1498:NAD:C5N	2.36	0.55
1:C:66:THR:HG23	1:C:70:HIS:HB3	1.88	0.55
1:D:66:THR:HG23	1:D:70:HIS:HB3	1.89	0.55
1:A:264:ILE:CD1	1:A:279:THR:HG22	2.37	0.55
1:C:496:SER:HB3	1:D:314:TRP:CZ2	2.42	0.55
1:A:444:VAL:HB	1:B:484:GLN:HB2	1.88	0.55
1:B:308:VAL:O	1:B:311:LEU:HB3	2.07	0.55
1:B:344:LYS:O	1:B:348:THR:HG23	2.05	0.55
1:B:455:PRO:HG3	1:B:471:TRP:CE3	2.42	0.55
1:C:304:ALA:O	1:C:308:VAL:HG12	2.06	0.55
1:D:363:PRO:O	1:D:364:GLU:CB	2.48	0.55
1:B:48:GLU:HA	1:B:48:GLU:OE1	2.06	0.55
1:A:326:GLU:HG2	1:A:327:GLY:N	2.20	0.54
1:B:158:TRP:CD1	1:B:184:SER:HG	2.25	0.54
1:C:27:VAL:HG13	1:C:37:GLY:C	2.32	0.54
1:A:95:ILE:HG22	1:A:324:PHE:HE2	1.67	0.54
1:B:182:LYS:C	1:B:182:LYS:HE2	2.32	0.54
1:C:60:ARG:O	1:C:62:ASN:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ALA:HB3	1:C:221:PRO:HD3	1.89	0.54
1:B:220:ALA:HB3	1:B:221:PRO:HD3	1.89	0.54
1:B:223:VAL:HA	1:B:231:ILE:HD11	1.89	0.54
1:C:235:GLY:O	1:C:258:LEU:HA	2.07	0.54
1:B:272:ILE:HD11	1:B:310:LYS:HG3	1.87	0.54
1:C:95:ILE:HG22	1:C:324:PHE:HE2	1.70	0.54
1:B:242:LYS:HD3	1:D:486:ILE:HD12	1.90	0.54
1:A:268:GLU:H	1:A:268:GLU:CD	2.13	0.54
1:A:308:VAL:O	1:A:311:LEU:HB3	2.08	0.54
1:B:259:GLY:HA3	3:B:1498:NAD:O2D	2.08	0.54
1:B:260:GLY:HA2	1:B:416:TYR:CG	2.43	0.54
1:B:275:VAL:O	1:B:279:THR:CG2	2.55	0.54
1:B:304:ALA:O	1:B:308:VAL:HG12	2.07	0.54
1:C:308:VAL:O	1:C:312:VAL:HG13	2.08	0.54
1:D:308:VAL:O	1:D:311:LEU:HB3	2.07	0.54
1:C:15:GLU:CD	1:C:17:ARG:NH1	2.66	0.54
1:D:225:HIS:HD2	1:D:227:ASP:N	1.94	0.54
1:A:268:GLU:OE1	1:A:268:GLU:N	2.29	0.54
1:B:66:THR:HG22	1:B:67:SER:O	2.08	0.54
1:B:76:ARG:HD2	5:B:2012:HOH:O	2.06	0.54
1:C:86:LYS:HE3	5:C:2024:HOH:O	2.08	0.54
1:C:481:GLN:NE2	1:C:483:THR:HG21	2.20	0.54
1:A:214:LEU:CD1	1:D:70:HIS:HB2	2.37	0.53
1:B:481:GLN:NE2	1:B:483:THR:HG21	2.23	0.53
1:A:496:SER:O	1:B:317:ASN:ND2	2.41	0.53
1:B:66:THR:HG21	1:B:70:HIS:CD2	2.42	0.53
1:C:66:THR:CG2	1:C:67:SER:N	2.71	0.53
1:D:396:LEU:CD1	5:D:2071:HOH:O	2.57	0.53
1:A:272:ILE:HG21	1:A:303:ILE:HG21	1.91	0.53
1:A:406:GLU:O	1:A:410:LEU:HB2	2.08	0.53
1:B:155:ILE:HG22	3:B:1498:NAD:H4B	1.90	0.53
1:C:182:LYS:HE2	1:C:182:LYS:C	2.32	0.53
1:D:239:THR:HA	1:D:242:LYS:HE3	1.91	0.53
1:D:260:GLY:HA2	1:D:416:TYR:CG	2.44	0.53
1:B:8:ARG:O	1:B:24:ARG:NH2	2.35	0.53
1:C:264:ILE:CD1	1:C:279:THR:HG22	2.38	0.53
1:C:96:ASP:CG	1:C:189:VAL:HG13	2.31	0.53
1:A:242:LYS:HE2	1:D:127:GLY:HA3	1.88	0.53
1:D:358:TYR:CD1	1:D:359:GLY:N	2.77	0.53
1:A:272:ILE:HD11	1:A:310:LYS:HG3	1.90	0.53
1:B:257[B]:GLU:HG2	3:B:1498:NAD:H72N	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:O	1:B:358:TYR:CB	2.56	0.53
1:D:141:LYS:HG3	1:D:486:ILE:HD13	1.91	0.53
1:A:27:VAL:HG13	1:A:37:GLY:C	2.34	0.53
1:C:406:GLU:O	1:C:410:LEU:HB2	2.09	0.52
1:B:225:HIS:CD2	1:B:226:PRO:HD2	2.44	0.52
1:D:103:GLU:HG2	1:D:285:TRP:CZ3	2.45	0.52
1:C:223:VAL:HG22	5:C:2051:HOH:O	2.10	0.52
1:C:290:ILE:HB	1:C:293:ALA:HB2	1.91	0.52
1:C:494:TYR:CE2	1:D:280:ILE:HG22	2.44	0.52
1:A:21:LYS:NZ	1:D:61:ASN:HD22	2.07	0.52
1:A:182:LYS:C	1:A:182:LYS:HE2	2.35	0.52
1:C:148:PRO:HG3	1:C:175:ALA:O	2.09	0.52
1:D:56:ARG:HD2	1:D:60:ARG:NH1	2.25	0.52
1:A:412:ASN:ND2	1:A:438:GLU:H	2.07	0.52
1:B:133:VAL:HG11	5:B:2054:HOH:O	2.09	0.52
1:C:223:VAL:HA	1:C:231:ILE:HD11	1.92	0.52
1:A:48:GLU:OE1	1:A:48:GLU:HA	2.08	0.52
1:D:66:THR:HG21	1:D:70:HIS:CD2	2.44	0.52
1:B:272:ILE:HG21	1:B:303:ILE:HG21	1.92	0.52
1:B:305:ALA:O	1:B:306:GLU:CB	2.56	0.52
1:C:60:ARG:C	1:C:62:ASN:H	2.17	0.52
1:A:102:ASP:O	1:A:105:VAL:HG22	2.09	0.52
1:D:76:ARG:CG	1:D:76:ARG:NH1	2.71	0.52
1:D:348:THR:O	1:D:352:GLU:HG3	2.10	0.52
1:D:305:ALA:O	1:D:306:GLU:HB3	2.09	0.52
1:D:381:SER:HB3	1:D:384:MET:HG2	1.91	0.52
1:A:343:MET:HE2	1:A:372:ILE:HG12	1.91	0.51
1:B:271:ASP:OD1	1:B:274:LYS:HD2	2.09	0.51
1:D:5:ILE:N	1:D:5:ILE:HD12	2.26	0.51
1:A:188:SER:HB3	1:A:212:THR:HG21	1.93	0.51
1:A:412:ASN:HD21	1:A:438:GLU:H	1.58	0.51
1:A:439:VAL:HG13	1:A:441:ALA:H	1.76	0.51
1:B:142:SER:HG	1:B:483:THR:HG22	1.75	0.51
1:B:186:LEU:O	1:B:187:ALA:HB2	2.11	0.51
1:B:414:THR:CG2	5:B:2108:HOH:O	2.55	0.51
1:C:95:ILE:HA	5:C:2009:HOH:O	2.08	0.51
1:D:272:ILE:O	1:D:272:ILE:HG13	2.09	0.51
1:D:279:THR:HG21	1:D:307:PHE:HZ	1.75	0.51
1:C:5:ILE:HG22	1:C:6:PRO:N	2.24	0.51
1:D:160:TYR:CE1	4:D:1500:GOL:H32	2.46	0.51
1:D:447:SER:O	1:D:448:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG22	1:A:207:VAL:HG22	1.93	0.51
1:A:196:GLU:O	1:A:197:VAL:C	2.54	0.51
1:A:235:GLY:O	1:A:258:LEU:HA	2.10	0.51
1:C:260:GLY:HA2	1:C:416:TYR:CG	2.45	0.51
1:D:300:HIS:ND1	1:D:302:SER:HB2	2.26	0.51
1:A:300:HIS:ND1	1:A:302:SER:HB2	2.25	0.51
1:A:35:ILE:HG13	1:A:35:ILE:O	2.08	0.51
1:C:279:THR:HG21	1:C:307:PHE:HZ	1.76	0.51
1:D:96:ASP:O	1:D:96:ASP:OD1	2.29	0.51
1:C:29:ASN:HB2	1:C:36:ILE:HD13	1.93	0.51
1:D:272:ILE:HG21	1:D:303:ILE:HG21	1.92	0.51
1:A:481:GLN:NE2	1:A:483:THR:HG21	2.18	0.51
1:A:481:GLN:HE21	1:A:483:THR:HG23	1.74	0.51
1:C:257[B]:GLU:HB3	3:C:1498:NAD:C7N	2.41	0.50
1:C:444:VAL:HB	1:D:484:GLN:HB3	1.93	0.50
1:D:58:PHE:CE1	1:D:150:GLY:HA2	2.46	0.50
1:D:235:GLY:O	1:D:258:LEU:HA	2.11	0.50
1:C:66:THR:HG21	1:C:70:HIS:CD2	2.45	0.50
1:D:4:PRO:O	1:D:5:ILE:O	2.30	0.50
1:D:225:HIS:CD2	1:D:226:PRO:HD2	2.46	0.50
1:A:5:ILE:H	1:A:6:PRO:CD	2.20	0.50
1:A:5:ILE:O	1:A:6:PRO:O	2.29	0.50
1:A:348:THR:HG22	1:C:134:THR:OG1	2.12	0.50
1:A:481:GLN:NE2	5:A:2157:HOH:O	2.41	0.50
1:C:15:GLU:HG2	1:C:17:ARG:NH1	2.19	0.50
1:C:381:SER:HB3	1:C:384:MET:HG2	1.93	0.50
1:D:186:LEU:O	1:D:187:ALA:HB2	2.11	0.50
1:D:291:CYS:SG	3:D:1498:NAD:C4N	2.99	0.50
1:C:6:PRO:HG2	1:C:92:LEU:HD13	1.93	0.50
1:C:225:HIS:CD2	1:C:226:PRO:HD2	2.46	0.50
1:C:272:ILE:CD1	1:C:306:GLU:HG2	2.42	0.50
1:D:85:LYS:NZ	1:D:200:GLU:OE2	2.45	0.50
1:D:223:VAL:HA	1:D:231:ILE:HD11	1.94	0.50
1:D:264:ILE:HD11	1:D:279:THR:HG22	1.94	0.50
1:D:481:GLN:NE2	1:D:483:THR:HG21	2.21	0.50
1:A:5:ILE:N	1:A:6:PRO:CD	2.74	0.50
1:B:27:VAL:HG13	1:B:37:GLY:C	2.36	0.50
1:B:66:THR:HG21	1:B:70:HIS:HD2	1.76	0.50
1:C:186:LEU:O	1:C:187:ALA:HB2	2.11	0.50
1:C:474:GLN:NE2	5:C:2122:HOH:O	2.42	0.50
1:A:148:PRO:HG3	1:A:175:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:HG22	1:B:5:ILE:O	2.06	0.50
1:C:48:GLU:OE1	1:C:48:GLU:HA	2.12	0.50
1:D:358:TYR:CD1	1:D:358:TYR:C	2.90	0.50
1:C:478:ASN:ND2	1:D:466:ARG:HH21	2.09	0.50
1:B:343:MET:HE2	1:B:372:ILE:HG12	1.94	0.49
1:D:282:GLY:HA2	1:D:448:GLN:CG	2.42	0.49
1:D:290:ILE:HB	1:D:293:ALA:HB2	1.94	0.49
1:C:51:VAL:HG23	1:C:52:VAL:N	2.27	0.49
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.77	0.49
1:C:160:TYR:HB2	1:C:164:MET:HG2	1.94	0.49
1:A:282:GLY:HA2	1:A:448:GLN:CG	2.43	0.49
1:A:348:THR:O	1:A:352:GLU:HG3	2.12	0.49
1:C:10:LEU:HD13	1:C:211:LEU:HD22	1.94	0.49
1:C:315:THR:HG21	1:C:376:ILE:HD11	1.95	0.49
1:C:438:GLU:HG2	4:D:1502:GOL:H31	1.94	0.49
1:A:386:ILE:HB	5:A:2113:HOH:O	2.13	0.49
1:B:235:GLY:O	1:B:258:LEU:HA	2.12	0.49
1:D:3:PHE:CZ	1:D:324:PHE:CZ	2.98	0.49
1:A:484:GLN:HB3	1:B:444:VAL:HB	1.94	0.49
1:D:148:PRO:HG3	1:D:176:GLY:HA3	1.95	0.49
1:A:182:LYS:HG2	1:A:211:LEU:O	2.13	0.49
1:C:268:GLU:HA	1:C:303:ILE:CD1	2.38	0.49
1:C:348:THR:O	1:C:352:GLU:HG3	2.12	0.49
1:C:392:PHE:CE1	3:C:1498:NAD:H2D	2.48	0.49
1:B:141:LYS:HG2	5:B:2051:HOH:O	2.13	0.49
1:B:257[B]:GLU:HG2	3:B:1498:NAD:N7N	2.28	0.49
1:B:447:SER:O	1:B:448:GLN:HB2	2.13	0.49
1:C:62:ASN:OD1	1:C:62:ASN:O	2.31	0.49
1:A:223:VAL:HA	1:A:231:ILE:HD11	1.93	0.49
1:C:291:CYS:HB3	3:C:1498:NAD:C6N	2.42	0.49
1:A:290:ILE:HB	1:A:293:ALA:HB2	1.93	0.48
1:B:7:ALA:O	1:B:8:ARG:HD3	2.12	0.48
1:B:148:PRO:HG3	1:B:176:GLY:HA3	1.95	0.48
1:D:95:ILE:CG2	1:D:324:PHE:HZ	2.21	0.48
1:D:160:TYR:HB2	1:D:164:MET:HG2	1.94	0.48
1:D:261:LYS:HG3	1:D:296:ARG:HD3	1.95	0.48
1:A:98:GLY:O	1:A:332:PRO:HD2	2.13	0.48
1:A:314:TRP:CZ2	1:B:496:SER:HB3	2.48	0.48
1:C:257[B]:GLU:HG2	3:C:1498:NAD:O7N	2.12	0.48
1:C:439:VAL:HG13	1:C:441:ALA:H	1.77	0.48
1:A:264:ILE:HD13	1:A:279:THR:HG22	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:HB2	1:B:36:ILE:HD13	1.94	0.48
1:C:66:THR:HG21	1:C:70:HIS:HD2	1.78	0.48
1:A:260:GLY:HA2	1:A:416:TYR:CG	2.48	0.48
1:A:29:ASN:HB2	1:A:36:ILE:HD13	1.95	0.48
1:B:160:TYR:HB2	1:B:164:MET:HG2	1.95	0.48
1:D:239:THR:O	1:D:243:VAL:HG13	2.13	0.48
1:D:320:ILE:O	1:D:365:HIS:HE1	1.97	0.48
1:A:66:THR:CG2	1:A:67:SER:N	2.76	0.48
1:A:168:LYS:C	1:A:171:PRO:HD2	2.39	0.48
1:B:225:HIS:HD2	1:B:227:ASP:N	1.96	0.48
1:C:76:ARG:NH1	1:C:76:ARG:CG	2.69	0.48
1:C:148:PRO:HG3	1:C:176:GLY:HA3	1.95	0.48
1:C:11:PHE:CZ	1:C:14:GLY:HA2	2.49	0.48
1:D:110:ASP:CG	4:D:1501:GOL:H2	2.35	0.48
1:D:146:ARG:HG2	1:D:479:ILE:HD13	1.95	0.48
1:A:3:PHE:O	1:A:4:PRO:O	2.32	0.48
1:A:276:VAL:HG11	1:A:314:TRP:CD1	2.49	0.48
1:B:168:LYS:C	1:B:171:PRO:HD2	2.39	0.48
1:B:257[B]:GLU:OE2	1:B:456:TRP:O	2.31	0.48
1:B:242:LYS:HD3	1:D:486:ILE:CD1	2.44	0.48
1:C:60:ARG:HB3	1:C:62:ASN:HB3	1.95	0.48
1:B:86:LYS:O	1:B:90:VAL:HG12	2.14	0.48
1:C:448:GLN:N	1:C:449:PRO:CD	2.76	0.48
1:D:136:PRO:O	1:D:137:MET:C	2.55	0.48
1:D:315:THR:HG21	1:D:376:ILE:HD11	1.96	0.48
1:A:51:VAL:HG21	1:A:225:HIS:NE2	2.28	0.47
1:B:182:LYS:HG2	1:B:211:LEU:O	2.14	0.47
1:C:358:TYR:CD1	1:C:358:TYR:C	2.92	0.47
1:A:62:ASN:OD1	1:A:62:ASN:O	2.32	0.47
1:A:300:HIS:O	1:A:301:GLU:C	2.58	0.47
1:D:48:GLU:HA	1:D:48:GLU:OE1	2.13	0.47
1:D:159:ASN:HD21	3:D:1498:NAD:H5N	1.79	0.47
1:A:256:LEU:HB3	1:A:258:LEU:HD21	1.97	0.47
1:B:76:ARG:CG	1:B:76:ARG:NH1	2.71	0.47
1:C:106:LEU:HD12	1:C:106:LEU:HA	1.54	0.47
1:C:280:ILE:CG2	1:D:494:TYR:CD2	2.93	0.47
1:A:225:HIS:HD2	1:A:227:ASP:N	1.96	0.47
1:D:135:LEU:HD21	1:D:142:SER:HB2	1.93	0.47
1:A:279:THR:HG21	1:A:307:PHE:HZ	1.79	0.47
1:B:271:ASP:OD2	1:B:274:LYS:CD	2.62	0.47
1:B:282:GLY:HA2	1:B:448:GLN:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TYR:CD1	1:B:358:TYR:C	2.93	0.47
1:C:239:THR:O	1:C:243:VAL:HG13	2.15	0.47
1:D:3:PHE:HZ	1:D:95:ILE:CG2	2.27	0.47
1:A:86:LYS:O	1:A:90:VAL:HG12	2.14	0.47
1:A:466:ARG:HH21	1:B:478:ASN:ND2	2.12	0.47
1:C:15:GLU:CG	1:C:17:ARG:NH1	2.76	0.47
1:C:98:GLY:O	1:C:332:PRO:HD2	2.15	0.47
1:D:481:GLN:HE21	1:D:483:THR:HG23	1.75	0.47
1:A:58:PHE:CE1	1:A:150:GLY:HA2	2.50	0.47
1:A:358:TYR:CD1	1:A:359:GLY:N	2.83	0.47
1:B:279:THR:HG21	1:B:307:PHE:HZ	1.80	0.47
1:C:86:LYS:O	1:C:90:VAL:HG12	2.15	0.47
1:D:3:PHE:CB	1:D:4:PRO:CD	2.92	0.47
1:A:66:THR:HG21	1:A:70:HIS:CD2	2.50	0.47
1:A:225:HIS:HA	1:A:226:PRO:HD3	1.71	0.47
1:B:102:ASP:O	1:B:105:VAL:HG22	2.14	0.47
1:B:229:ASP:O	1:B:253:PRO:HD2	2.14	0.47
1:B:272:ILE:O	1:B:272:ILE:HG13	2.13	0.47
1:C:303:ILE:H	1:C:303:ILE:HG13	1.48	0.47
1:C:444:VAL:HB	1:D:484:GLN:HB2	1.96	0.47
1:D:362:ARG:HG3	1:D:362:ARG:HH11	1.79	0.47
1:A:25[B]:ILE:HD11	1:A:214:LEU:HD11	1.97	0.47
1:A:358:TYR:CD1	1:A:358:TYR:C	2.93	0.47
1:C:66:THR:HG22	1:C:67:SER:N	2.30	0.47
1:B:58:PHE:CE1	1:B:150:GLY:HA2	2.50	0.46
1:B:261:LYS:CG	1:B:296:ARG:HD2	2.44	0.46
1:C:48:GLU:OE1	1:C:48:GLU:CA	2.64	0.46
1:C:276:VAL:HG11	1:C:314:TRP:CD1	2.50	0.46
1:A:225:HIS:O	1:A:252:LYS:NZ	2.49	0.46
1:A:306:GLU:CG	1:A:310:LYS:NZ	2.78	0.46
1:B:3:PHE:HD1	1:B:4:PRO:HD3	1.78	0.46
1:B:12:ILE:HD11	1:B:211:LEU:HD21	1.96	0.46
1:B:448:GLN:N	1:B:449:PRO:CD	2.78	0.46
1:D:182:LYS:C	1:D:182:LYS:HE2	2.40	0.46
1:B:48:GLU:OE1	1:B:48:GLU:CA	2.63	0.46
1:B:95:ILE:HG22	1:B:324:PHE:HZ	1.78	0.46
1:B:281:PHE:O	1:B:285:TRP:HB3	2.15	0.46
1:A:182:LYS:NZ	3:A:1498:NAD:O2B	2.48	0.46
1:A:229:ASP:O	1:A:253:PRO:HD2	2.16	0.46
1:B:66:THR:CG2	1:B:67:SER:N	2.78	0.46
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:CYS:SG	1:D:396:LEU:HD23	2.56	0.46
1:D:306:GLU:O	1:D:307:PHE:C	2.57	0.46
1:A:76:ARG:CG	1:A:76:ARG:NH1	2.68	0.46
1:C:324:PHE:HD2	5:C:2077:HOH:O	1.97	0.46
1:C:358:TYR:CD1	1:C:359:GLY:N	2.83	0.46
1:D:51:VAL:HG21	1:D:225:HIS:NE2	2.31	0.46
1:D:256:LEU:HB3	1:D:258:LEU:HD21	1.97	0.46
1:B:315:THR:HG21	1:B:376:ILE:HD11	1.97	0.46
1:C:5:ILE:CG2	1:C:6:PRO:CD	2.81	0.46
1:C:466:ARG:HH21	1:D:478:ASN:ND2	2.13	0.46
1:D:12:ILE:HD11	1:D:211:LEU:HD21	1.98	0.46
1:B:91:LYS:O	1:B:95:ILE:HG23	2.16	0.46
1:B:348:THR:O	1:B:352:GLU:HG3	2.14	0.46
1:B:350:LYS:HE3	1:B:356:ILE:CD1	2.43	0.46
1:A:148:PRO:HG3	1:A:176:GLY:HA3	1.98	0.46
1:C:278:TRP:CH2	1:D:491:TRP:CD2	3.04	0.46
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.80	0.46
1:C:229:ASP:O	1:C:253:PRO:HD2	2.16	0.46
1:D:268:GLU:HA	1:D:303:ILE:CD1	2.36	0.46
1:A:181:LEU:HD13	1:A:183:PRO:HG3	1.97	0.45
1:A:447:SER:O	1:A:448:GLN:HB2	2.15	0.45
1:B:98:GLY:O	1:B:332:PRO:HD2	2.16	0.45
1:B:242:LYS:HG2	1:D:486:ILE:HD12	1.97	0.45
1:B:276:VAL:HG11	1:B:314:TRP:CD1	2.51	0.45
1:C:264:ILE:HD13	1:C:279:THR:HG22	1.98	0.45
1:C:357:LEU:O	1:C:358:TYR:CB	2.65	0.45
1:D:276:VAL:HG11	1:D:314:TRP:CD1	2.51	0.45
1:D:401:PHE:CD2	1:D:407:ALA:HB2	2.51	0.45
1:D:264:ILE:HG23	1:D:297:LEU:HA	1.99	0.45
1:D:414:THR:HB	1:D:416:TYR:H	1.82	0.45
1:A:8:ARG:O	1:A:24:ARG:NH2	2.30	0.45
1:A:262:SER:HA	1:A:263:PRO:HD3	1.87	0.45
1:A:320:ILE:O	1:A:365:HIS:HE1	1.99	0.45
1:B:215:GLY:HA3	3:B:1498:NAD:C8A	2.47	0.45
1:C:6:PRO:CB	1:C:193:GLU:OE2	2.62	0.45
1:C:51:VAL:CG2	1:C:52:VAL:N	2.79	0.45
1:C:250:LEU:C	1:C:251[B]:VAL:HG22	2.42	0.45
1:C:268:GLU:CA	1:C:303:ILE:HD11	2.38	0.45
1:C:282:GLY:HA2	1:C:448:GLN:CG	2.47	0.45
1:D:168:LYS:C	1:D:171:PRO:HD2	2.41	0.45
1:D:264:ILE:HD13	1:D:279:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:GLN:N	1:D:449:PRO:CD	2.79	0.45
1:A:280:ILE:HD11	1:A:311:LEU:HD12	1.98	0.45
1:B:108:ILE:HA	1:B:111:VAL:HG13	1.98	0.45
1:C:168:LYS:C	1:C:171:PRO:HD2	2.42	0.45
1:D:182:LYS:HG2	1:D:211:LEU:O	2.17	0.45
1:A:8:ARG:HG3	1:A:9:GLN:H	1.81	0.45
1:A:35:ILE:O	1:A:35:ILE:CG1	2.65	0.45
1:A:341:LYS:CE	5:A:2110:HOH:O	2.49	0.45
1:A:448:GLN:N	1:A:449:PRO:CD	2.79	0.45
1:B:103:GLU:OE2	1:B:285:TRP:HD1	2.00	0.45
1:B:146:ARG:HG2	1:B:479:ILE:HD13	1.99	0.45
1:B:264:ILE:HG21	5:B:2091:HOH:O	2.16	0.45
1:B:381:SER:C	1:B:383[A]:SER:H	2.25	0.45
1:C:343:MET:HE2	1:C:372:ILE:HG12	1.99	0.45
1:D:285:TRP:C	1:D:287:ASN:N	2.74	0.45
1:D:478:ASN:ND2	1:D:478:ASN:C	2.70	0.45
1:B:29:ASN:OD1	1:B:30:PRO:HD2	2.17	0.45
1:B:403:SER:OG	1:B:405:ASP:OD1	2.33	0.45
1:C:3:PHE:CD1	1:C:3:PHE:N	2.84	0.45
1:A:272:ILE:HG13	1:A:272:ILE:O	2.12	0.45
1:A:309:ASP:O	1:A:312:VAL:HG22	2.17	0.45
1:C:481:GLN:HE21	1:C:483:THR:HG23	1.74	0.45
1:D:346:ILE:HG23	1:D:356:ILE:HD11	1.99	0.45
1:A:5:ILE:N	1:A:6:PRO:HD3	2.17	0.44
1:A:48:GLU:OE1	1:A:48:GLU:CA	2.64	0.44
1:B:282:GLY:HA2	1:B:448:GLN:HG2	1.99	0.44
1:C:487:SER:O	1:C:488:ASP:CB	2.62	0.44
1:D:66:THR:CG2	1:D:67:SER:N	2.80	0.44
1:D:89:PHE:HB3	1:D:108:ILE:HD12	1.98	0.44
1:D:229:ASP:O	1:D:253:PRO:HD2	2.17	0.44
1:D:350:LYS:HE3	1:D:356:ILE:HD12	1.98	0.44
1:D:392:PHE:O	5:D:2069:HOH:O	2.21	0.44
1:A:160:TYR:HB2	1:A:164:MET:HG2	1.99	0.44
1:A:239:THR:O	1:A:243:VAL:HG13	2.17	0.44
1:A:257[B]:GLU:HB3	3:A:1498:NAD:C7N	2.47	0.44
1:A:362:ARG:HG3	1:A:362:ARG:NH1	2.32	0.44
1:D:3:PHE:HB3	1:D:91:LYS:NZ	2.32	0.44
1:D:282:GLY:HA2	1:D:448:GLN:HG2	1.98	0.44
1:A:261:LYS:HG3	1:A:296:ARG:HD3	1.98	0.44
1:C:451:PHE:CZ	1:D:137:MET:HG3	2.51	0.44
1:A:478:ASN:ND2	1:B:466:ARG:HH21	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:HB2	1:B:444:VAL:HB	1.99	0.44
1:B:218:ALA:C	1:B:221:PRO:HD2	2.43	0.44
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.82	0.44
1:D:261:LYS:CG	1:D:296:ARG:HD2	2.46	0.44
1:A:381:SER:C	1:A:383[A]:SER:H	2.25	0.44
1:C:5:ILE:HA	1:C:6:PRO:HD3	1.81	0.44
1:D:96:ASP:OD2	1:D:189:VAL:HG13	2.17	0.44
1:D:401:PHE:HD2	1:D:403:SER:O	2.01	0.44
1:D:439:VAL:HG13	1:D:441:ALA:H	1.82	0.44
1:D:450[A]:CYS:O	4:D:1501:GOL:H12	2.18	0.44
1:B:291:CYS:HB3	3:B:1498:NAD:C6N	2.48	0.44
1:C:112:ALA:O	1:C:116:GLU:HG3	2.18	0.44
1:C:429:ARG:HA	1:C:432:ARG:HH21	1.77	0.44
1:C:51:VAL:HG21	1:C:225:HIS:NE2	2.32	0.44
1:C:139:ARG:HH12	1:C:489:GLU:HB2	1.83	0.44
1:A:103:GLU:HG2	1:A:285:TRP:HE1	1.82	0.44
1:A:251:VAL:HG13	1:B:256:LEU:HD12	1.99	0.44
1:C:280:ILE:HG21	1:D:494:TYR:CD2	2.53	0.44
1:D:9:GLN:NE2	1:D:24:ARG:NH2	2.64	0.44
1:D:193:GLU:OE1	1:D:193:GLU:HA	2.18	0.44
1:A:152:VAL:HG23	1:A:154:LEU:HD21	1.99	0.44
1:B:112:ALA:O	1:B:116:GLU:HG3	2.18	0.44
1:B:256:LEU:HB3	1:B:258:LEU:HD21	1.99	0.44
1:B:261:LYS:HG3	1:B:296:ARG:HD3	1.97	0.44
1:D:170:ALA:HB3	1:D:171:PRO:HD3	2.00	0.44
1:D:429:ARG:O	1:D:433:ILE:HG12	2.18	0.44
1:A:21:LYS:HG3	1:A:43:THR:HG21	2.00	0.43
1:A:186:LEU:O	1:A:187:ALA:HB2	2.18	0.43
1:A:307:PHE:CD1	1:A:307:PHE:C	2.96	0.43
1:A:315:THR:C	1:A:317:ASN:N	2.76	0.43
1:A:381:SER:C	1:A:383[B]:SER:H	2.26	0.43
1:D:66:THR:HG21	1:D:70:HIS:HD2	1.80	0.43
1:D:108:ILE:HA	1:D:111:VAL:HG13	2.00	0.43
1:A:495:LYS:HG2	5:A:2163:HOH:O	2.18	0.43
1:B:264:ILE:HG23	1:B:297:LEU:HA	2.00	0.43
1:C:320:ILE:O	1:C:365:HIS:HE1	2.01	0.43
1:A:268:GLU:HA	1:A:303:ILE:CD1	2.44	0.43
1:B:401:PHE:CD2	1:B:407:ALA:HB2	2.53	0.43
1:C:99:LYS:HB3	1:C:99:LYS:HE2	1.76	0.43
1:D:152:VAL:HG23	1:D:154:LEU:HD21	2.01	0.43
1:D:309:ASP:O	1:D:312:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HH12	1:B:489:GLU:HB2	1.83	0.43
1:B:262:SER:HA	1:B:263:PRO:HD3	1.91	0.43
1:D:5:ILE:CG2	1:D:6:PRO:N	2.79	0.43
1:A:312:VAL:O	1:A:316:LYS:HB2	2.18	0.43
1:B:297:LEU:HB2	1:B:396:LEU:HD11	2.00	0.43
1:D:257[B]:GLU:HB3	3:D:1498:NAD:C7N	2.49	0.43
1:D:447:SER:O	1:D:448:GLN:CB	2.66	0.43
1:A:12:ILE:HD11	1:A:211:LEU:HD21	1.99	0.43
1:A:91:LYS:O	1:A:95:ILE:HG23	2.17	0.43
1:A:225:HIS:CD2	1:A:226:PRO:HD2	2.53	0.43
1:A:252:LYS:HE3	1:A:252:LYS:HB2	1.83	0.43
1:A:346:ILE:HG23	1:A:356:ILE:HD11	2.00	0.43
1:A:378:THR:HG22	1:A:398:VAL:HB	2.01	0.43
1:C:401:PHE:HD2	1:C:403:SER:O	2.02	0.43
1:A:137:MET:HB3	5:A:2044:HOH:O	2.19	0.43
1:B:94:THR:HG23	1:B:99:LYS:O	2.18	0.43
1:B:280:ILE:HD11	1:B:311:LEU:HD12	2.00	0.43
1:C:122:ALA:HB2	1:C:174:ALA:HB1	2.01	0.43
1:C:478:ASN:ND2	1:C:478:ASN:C	2.75	0.43
1:D:401:PHE:CE2	1:D:407:ALA:HB2	2.54	0.43
1:C:58:PHE:CE1	1:C:150:GLY:HA2	2.54	0.43
1:D:98:GLY:O	1:D:332:PRO:HD2	2.19	0.43
1:A:131:ALA:HA	1:A:132:PRO:HD3	1.86	0.43
1:A:262:SER:HB3	1:A:419:ALA:O	2.19	0.43
1:A:391:VAL:HB	5:A:2126:HOH:O	2.19	0.43
1:B:5:ILE:HG23	1:B:6:PRO:HD2	2.00	0.43
1:C:35:ILE:O	1:C:35:ILE:HG13	2.15	0.43
1:C:359:GLY:HA2	1:C:373:GLU:OE1	2.19	0.43
1:D:272:ILE:HD12	1:D:307:PHE:CA	2.41	0.43
1:C:30:PRO:HG2	1:C:98:GLY:HA3	2.00	0.43
1:C:272:ILE:HG21	1:C:303:ILE:HG21	2.00	0.43
1:C:381:SER:C	1:C:383[A]:SER:H	2.26	0.43
1:C:390[A]:GLU:HG3	5:C:2065:HOH:O	2.18	0.43
1:D:48:GLU:OE1	1:D:48:GLU:CA	2.67	0.43
1:D:303:ILE:H	1:D:303:ILE:HG13	1.53	0.43
1:A:280:ILE:HG21	1:A:318:ILE:HD11	2.00	0.42
1:A:282:GLY:HA2	1:A:448:GLN:HG2	2.00	0.42
1:A:348:THR:HG22	1:C:134:THR:CG2	2.49	0.42
1:B:252:LYS:HE3	1:B:252:LYS:HB2	1.75	0.42
1:B:439:VAL:HG13	1:B:441:ALA:H	1.84	0.42
1:C:9:GLN:HB3	1:C:17:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:MET:H	1:D:137:MET:HG2	1.54	0.42
1:D:478:ASN:C	1:D:478:ASN:HD22	2.27	0.42
1:D:482:VAL:O	1:D:482:VAL:HG22	2.19	0.42
1:B:62[A]:ASN:OD1	1:B:62[A]:ASN:O	2.37	0.42
1:C:193:GLU:HA	1:C:193:GLU:OE1	2.20	0.42
1:C:225:HIS:HA	1:C:226:PRO:HD3	1.76	0.42
1:C:301:GLU:O	1:C:302:SER:C	2.59	0.42
1:C:314:TRP:CZ2	1:D:496:SER:HB3	2.54	0.42
1:D:3:PHE:HB2	1:D:4:PRO:CD	2.49	0.42
1:D:278:TRP:O	1:D:280:ILE:N	2.52	0.42
1:D:307:PHE:C	1:D:307:PHE:CD1	2.96	0.42
1:A:357:LEU:O	1:A:358:TYR:CB	2.68	0.42
1:C:105:VAL:CG2	1:C:106:LEU:N	2.83	0.42
1:D:262:SER:HA	1:D:263:PRO:HD3	1.89	0.42
1:D:357:LEU:O	1:D:357:LEU:CD2	2.67	0.42
1:A:129:GLN:O	1:A:130:LYS:HB2	2.20	0.42
1:C:264:ILE:HD11	1:C:279:THR:HG22	2.01	0.42
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.34	0.42
3:C:1498:NAD:H8A	3:C:1498:NAD:H2B	1.80	0.42
1:D:139:ARG:HH12	1:D:489:GLU:HB2	1.85	0.42
1:D:493:TRP:HD1	1:D:494:TYR:CD1	2.37	0.42
1:A:84:GLU:C	1:A:86:LYS:H	2.27	0.42
1:B:35:ILE:O	1:B:35:ILE:CG1	2.65	0.42
1:C:60:ARG:C	1:C:62:ASN:N	2.72	0.42
1:C:108:ILE:HA	1:C:111:VAL:HG13	2.01	0.42
1:C:272:ILE:HG21	1:C:272:ILE:HD13	1.79	0.42
1:D:305:ALA:O	1:D:306:GLU:HB2	2.18	0.42
1:D:330:LEU:HD22	1:D:331:GLY:O	2.20	0.42
1:B:3:PHE:CD1	1:B:3:PHE:O	2.73	0.42
1:C:130:LYS:HA	1:C:143:HIS:CD2	2.54	0.42
1:C:264:ILE:HG23	1:C:297:LEU:HA	2.01	0.42
1:C:447:SER:O	1:C:448:GLN:HB2	2.19	0.42
1:D:125:LEU:O	1:D:128:LYS:HB2	2.20	0.42
1:D:381:SER:C	1:D:383[A]:SER:H	2.28	0.42
1:A:264:ILE:HG23	1:A:297:LEU:HA	2.02	0.42
1:A:315:THR:HG21	1:A:376:ILE:HD11	2.02	0.42
1:B:362:ARG:HG3	1:B:362:ARG:NH1	2.35	0.42
1:C:3:PHE:O	1:C:3:PHE:HD1	2.00	0.42
1:D:362:ARG:HG3	1:D:362:ARG:NH1	2.35	0.42
1:C:181:LEU:HD13	1:C:183:PRO:HG3	2.01	0.42
1:C:182:LYS:HG2	1:C:211:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:TRP:O	1:D:286:THR:C	2.60	0.42
1:A:30:PRO:HG2	1:A:98:GLY:HA3	2.02	0.42
1:A:121:GLN:NE2	5:A:2038:HOH:O	2.53	0.42
1:B:205:PRO:HD2	5:B:2022:HOH:O	2.19	0.42
1:B:264:ILE:HA	1:B:421:ALA:O	2.19	0.42
1:C:251[A]:VAL:HG13	1:D:256:LEU:HD12	2.02	0.42
1:C:307:PHE:CD1	1:C:307:PHE:C	2.97	0.42
1:C:350:LYS:HE3	1:C:356:ILE:CD1	2.49	0.42
1:D:12:ILE:HG21	1:D:49:VAL:HG23	2.02	0.42
1:D:62:ASN:OD1	1:D:62:ASN:O	2.37	0.42
1:D:356:ILE:C	1:D:358:TYR:H	2.28	0.42
1:A:256:LEU:HD12	1:B:251:VAL:HG13	2.02	0.41
1:A:261:LYS:CG	1:A:296:ARG:HD2	2.45	0.41
1:A:264:ILE:HA	1:A:421:ALA:O	2.20	0.41
1:A:423:PHE:CD2	1:A:445:ASN:HA	2.55	0.41
1:B:257[A]:GLU:OE2	1:B:467:GLU:HG3	2.20	0.41
1:B:257[B]:GLU:CG	3:B:1498:NAD:H72N	2.33	0.41
1:B:283:CYS:SG	1:B:396:LEU:HD23	2.60	0.41
1:B:359:GLY:HA2	1:B:373:GLU:OE1	2.20	0.41
1:B:478:ASN:ND2	1:B:478:ASN:C	2.78	0.41
1:C:3:PHE:N	1:C:3:PHE:HD1	2.18	0.41
1:D:381:SER:C	1:D:383[B]:SER:H	2.28	0.41
1:A:251:VAL:O	1:A:251:VAL:CG1	2.67	0.41
1:B:381:SER:C	1:B:383[B]:SER:H	2.26	0.41
1:C:252:LYS:HE3	1:C:252:LYS:HB2	1.82	0.41
1:C:303:ILE:O	1:C:304:ALA:C	2.63	0.41
1:D:268:GLU:HG2	1:D:269:ASP:N	2.34	0.41
1:A:139:ARG:HH12	1:A:489:GLU:HB2	1.85	0.41
1:B:143:HIS:CE1	1:B:482:VAL:HG22	2.55	0.41
1:B:357:LEU:O	1:B:357:LEU:CD2	2.66	0.41
1:C:125:LEU:O	1:C:128:LYS:HB2	2.19	0.41
1:D:262:SER:HB3	1:D:419:ALA:O	2.21	0.41
1:D:405:ASP:OD1	1:D:405:ASP:C	2.64	0.41
1:C:84:GLU:C	1:C:86:LYS:H	2.28	0.41
1:C:280:ILE:HD11	1:C:311:LEU:HD12	2.02	0.41
1:C:434:THR:HB	1:C:442:VAL:HG11	2.02	0.41
1:D:58:PHE:CZ	1:D:150:GLY:HA2	2.56	0.41
1:B:12:ILE:HG21	1:B:49:VAL:HG23	2.03	0.41
1:B:60:ARG:C	1:B:62[B]:ASN:ND2	2.77	0.41
1:D:86:LYS:O	1:D:87:ASP:C	2.62	0.41
1:D:182:LYS:HD2	1:D:218:ALA:CB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG23	1:B:154:LEU:HD21	2.03	0.41
1:C:47:VAL:O	1:C:51:VAL:HG13	2.21	0.41
1:D:30:PRO:HG2	1:D:98:GLY:HA3	2.03	0.41
1:A:264:ILE:HG23	1:A:264:ILE:O	2.20	0.41
1:A:285:TRP:O	1:A:286:THR:C	2.62	0.41
1:A:494:TYR:CZ	1:B:280:ILE:HG22	2.55	0.41
1:B:143:HIS:CE1	1:B:482:VAL:CG2	3.04	0.41
1:B:307:PHE:CD1	1:B:307:PHE:C	2.98	0.41
1:B:346:ILE:HG23	1:B:356:ILE:HD11	2.03	0.41
1:B:423:PHE:CD2	1:B:445:ASN:HA	2.56	0.41
1:C:373:GLU:O	1:C:374:PRO:C	2.62	0.41
1:D:357:LEU:O	1:D:358:TYR:CB	2.68	0.41
1:A:429:ARG:O	1:A:433:ILE:HG12	2.21	0.41
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.82	0.41
1:B:271:ASP:OD2	1:B:274:LYS:CE	2.68	0.41
1:C:182:LYS:CE	1:C:183:PRO:O	2.69	0.41
1:C:262:SER:HA	1:C:263:PRO:HD3	1.86	0.41
1:C:315:THR:HA	1:C:318:ILE:HD12	2.03	0.41
1:C:346:ILE:HG23	1:C:356:ILE:HD11	2.02	0.41
1:C:378:THR:HG22	1:C:398:VAL:HB	2.02	0.41
1:D:171:PRO:HB2	1:D:476:TYR:CE2	2.55	0.41
1:D:264:ILE:HA	1:D:421:ALA:O	2.20	0.41
1:A:447:SER:O	1:A:448:GLN:CB	2.69	0.41
1:B:239:THR:O	1:B:243:VAL:HG13	2.21	0.41
1:B:130:LYS:HA	1:B:143:HIS:CD2	2.56	0.40
1:B:268:GLU:HG2	1:B:269:ASP:N	2.37	0.40
1:C:423:PHE:CD2	1:C:445:ASN:HA	2.56	0.40
1:D:83:THR:O	1:D:86:LYS:HB2	2.21	0.40
1:D:306:GLU:O	1:D:309:ASP:N	2.54	0.40
1:A:112:ALA:O	1:A:116:GLU:HG3	2.21	0.40
1:A:281:PHE:O	1:A:285:TRP:HB3	2.21	0.40
1:A:330:LEU:HD22	1:A:331:GLY:O	2.22	0.40
1:C:131:ALA:HA	1:C:132:PRO:HD3	1.90	0.40
1:C:309:ASP:O	1:C:312:VAL:HG22	2.20	0.40
1:C:439:VAL:HG13	1:C:440:GLY:N	2.36	0.40
1:C:484:GLN:CB	1:D:444:VAL:HB	2.51	0.40
1:D:434:THR:HB	1:D:442:VAL:HG11	2.03	0.40
1:A:471:TRP:CZ2	4:A:1499:GOL:H12	2.57	0.40
1:B:401:PHE:CE2	1:B:407:ALA:HB2	2.56	0.40
1:C:438:GLU:HG2	4:D:1502:GOL:C3	2.52	0.40
1:D:378:THR:HG22	1:D:398:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1498:NAD:H8A	3:A:1498:NAD:H2B	1.97	0.40
1:B:131:ALA:HA	1:B:132:PRO:HD3	1.88	0.40
1:C:429:ARG:O	1:C:433:ILE:HG12	2.21	0.40
1:D:130:LYS:HA	1:D:143:HIS:CD2	2.56	0.40
1:D:280:ILE:HD11	1:D:311:LEU:HD12	2.03	0.40
1:B:60:ARG:C	1:B:62[B]:ASN:H	2.30	0.40
1:C:95:ILE:HG22	1:C:324:PHE:HZ	1.84	0.40
1:C:343:MET:O	1:C:346:ILE:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/496 (100%)	456 (92%)	31 (6%)	10 (2%)	6	5
1	B	498/496 (100%)	463 (93%)	26 (5%)	9 (2%)	6	6
1	C	499/496 (101%)	458 (92%)	30 (6%)	11 (2%)	5	4
1	D	497/496 (100%)	450 (90%)	35 (7%)	12 (2%)	4	4
All	All	1991/1984 (100%)	1827 (92%)	122 (6%)	42 (2%)	5	4

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	306	GLU
1	A	358	TYR
1	A	448	GLN
1	B	306	GLU
1	B	358	TYR
1	B	448	GLN

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Mol	Chain	Res	Type
1	C	306	GLU
1	C	358	TYR
1	C	448	GLN
1	D	306	GLU
1	D	358	TYR
1	D	364	GLU
1	D	448	GLN
1	B	187	ALA
1	B	302	SER
1	C	187	ALA
1	D	137	MET
1	D	187	ALA
1	A	4	PRO
1	A	5	ILE
1	A	187	ALA
1	B	357	LEU
1	D	357	LEU
1	B	424	SER
1	C	357	LEU
1	A	136	PRO
1	A	357	LEU
1	B	136	PRO
1	C	6	PRO
1	C	302	SER
1	C	424	SER
1	D	5	ILE
1	D	6	PRO
1	D	424	SER
1	A	424	SER
1	D	363	PRO
1	C	136	PRO
1	C	272	ILE
1	D	136	PRO
1	C	417	GLY
1	B	417	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/409 (101%)	351 (85%)	62 (15%)	3	3
1	B	414/409 (101%)	353 (85%)	61 (15%)	3	3
1	C	415/409 (102%)	350 (84%)	65 (16%)	2	2
1	D	413/409 (101%)	350 (85%)	63 (15%)	3	3
All	All	1655/1636 (101%)	1404 (85%)	251 (15%)	2	3

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	5	ILE
1	A	8	ARG
1	A	17	ARG
1	A	27	VAL
1	A	35	ILE
1	A	48	GLU
1	A	49	VAL
1	A	75	LEU
1	A	76	ARG
1	A	81	LYS
1	A	85	LYS
1	A	90	VAL
1	A	95	ILE
1	A	105	VAL
1	A	106	LEU
1	A	111	VAL
1	A	125	LEU
1	A	128	LYS
1	A	133	VAL
1	A	166	THR
1	A	181	LEU
1	A	182	LYS
1	A	189	VAL
1	A	193	GLU
1	A	196	GLU
1	A	203	LEU
1	A	207	VAL
1	A	222	LEU
1	A	223	VAL
1	A	242	LYS

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Mol	Chain	Res	Type
1	A	243	VAL
1	A	254	VAL
1	A	265	VAL
1	A	272	ILE
1	A	275	VAL
1	A	276	VAL
1	A	280	ILE
1	A	290	ILE
1	A	294	THR
1	A	297	LEU
1	A	303	ILE
1	A	315	THR
1	A	316	LYS
1	A	318	ILE
1	A	320	ILE
1	A	326	GLU
1	A	330	LEU
1	A	348	THR
1	A	356	ILE
1	A	362	ARG
1	A	364	GLU
1	A	376	ILE
1	A	377	VAL
1	A	378	THR
1	A	388	LYS
1	A	389	GLU
1	A	405	ASP
1	A	439	VAL
1	A	461	ARG
1	A	482	VAL
1	A	483	THR
1	B	3	PHE
1	B	5	ILE
1	B	8	ARG
1	B	17	ARG
1	B	27	VAL
1	B	34	GLU
1	B	35	ILE
1	B	48	GLU
1	B	49	VAL
1	B	66	THR
1	B	75	LEU

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Mol	Chain	Res	Type
1	B	76	ARG
1	B	81	LYS
1	B	90	VAL
1	B	91	LYS
1	B	95	ILE
1	B	105	VAL
1	B	106	LEU
1	B	111	VAL
1	B	125	LEU
1	B	133	VAL
1	B	166	THR
1	B	181	LEU
1	B	182	LYS
1	B	189	VAL
1	B	193	GLU
1	B	207	VAL
1	B	222	LEU
1	B	223	VAL
1	B	243	VAL
1	B	254	VAL
1	B	265	VAL
1	B	272	ILE
1	B	274	LYS
1	B	275	VAL
1	B	276	VAL
1	B	279	THR
1	B	280	ILE
1	B	290	ILE
1	B	294	THR
1	B	297	LEU
1	B	302	SER
1	B	303	ILE
1	B	309	ASP
1	B	315	THR
1	B	320	ILE
1	B	326	GLU
1	B	330	LEU
1	B	348	THR
1	B	356	ILE
1	B	362	ARG
1	B	367	LYS
1	B	376	ILE

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Mol	Chain	Res	Type
1	B	377	VAL
1	B	378	THR
1	B	389	GLU
1	B	405	ASP
1	B	439	VAL
1	B	482	VAL
1	B	483	THR
1	B	496	SER
1	C	3	PHE
1	C	5	ILE
1	C	13	ASP
1	C	17	ARG
1	C	27	VAL
1	C	35	ILE
1	C	48	GLU
1	C	49	VAL
1	C	66	THR
1	C	75	LEU
1	C	76	ARG
1	C	81	LYS
1	C	85	LYS
1	C	90	VAL
1	C	95	ILE
1	C	99	LYS
1	C	105	VAL
1	C	106	LEU
1	C	111	VAL
1	C	125	LEU
1	C	133	VAL
1	C	141	LYS
1	C	166	THR
1	C	181	LEU
1	C	182	LYS
1	C	189	VAL
1	C	193	GLU
1	C	203	LEU
1	C	207	VAL
1	C	209	ASN
1	C	222	LEU
1	C	223	VAL
1	C	243	VAL
1	C	254	VAL

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Mol	Chain	Res	Type
1	C	265	VAL
1	C	270	VAL
1	C	271	ASP
1	C	272	ILE
1	C	275	VAL
1	C	276	VAL
1	C	280	ILE
1	C	285	TRP
1	C	290	ILE
1	C	292	SER
1	C	294	THR
1	C	297	LEU
1	C	302	SER
1	C	303	ILE
1	C	315	THR
1	C	316	LYS
1	C	320	ILE
1	C	326	GLU
1	C	330	LEU
1	C	348	THR
1	C	356	ILE
1	C	362	ARG
1	C	367	LYS
1	C	376	ILE
1	C	377	VAL
1	C	378	THR
1	C	389	GLU
1	C	439	VAL
1	C	482	VAL
1	C	483	THR
1	C	496	SER
1	D	3	PHE
1	D	5	ILE
1	D	8	ARG
1	D	17	ARG
1	D	27	VAL
1	D	35	ILE
1	D	36	ILE
1	D	48	GLU
1	D	49	VAL
1	D	75	LEU
1	D	76	ARG

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Mol	Chain	Res	Type
1	D	81	LYS
1	D	86	LYS
1	D	90	VAL
1	D	95	ILE
1	D	99	LYS
1	D	105	VAL
1	D	106	LEU
1	D	111	VAL
1	D	125	LEU
1	D	133	VAL
1	D	137	MET
1	D	141	LYS
1	D	166	THR
1	D	181	LEU
1	D	182	LYS
1	D	189	VAL
1	D	193	GLU
1	D	203	LEU
1	D	207	VAL
1	D	222	LEU
1	D	223	VAL
1	D	243	VAL
1	D	254	VAL
1	D	265	VAL
1	D	272	ILE
1	D	274	LYS
1	D	275	VAL
1	D	276	VAL
1	D	280	ILE
1	D	285	TRP
1	D	290	ILE
1	D	294	THR
1	D	297	LEU
1	D	303	ILE
1	D	315	THR
1	D	320	ILE
1	D	326	GLU
1	D	330	LEU
1	D	343	MET
1	D	348	THR
1	D	356	ILE
1	D	362	ARG

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Mol	Chain	Res	Type
1	D	364	GLU
1	D	365	HIS
1	D	367	LYS
1	D	376	ILE
1	D	377	VAL
1	D	378	THR
1	D	389	GLU
1	D	439	VAL
1	D	482	VAL
1	D	483	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	143	HIS
1	A	225	HIS
1	A	289	GLN
1	A	365	HIS
1	A	412	ASN
1	A	425	ASN
1	A	478	ASN
1	A	481	GLN
1	A	484	GLN
1	B	70	HIS
1	B	143	HIS
1	B	225	HIS
1	B	249	GLN
1	B	289	GLN
1	B	338	GLN
1	B	365	HIS
1	B	412	ASN
1	B	425	ASN
1	B	478	ASN
1	B	481	GLN
1	B	484	GLN
1	C	70	HIS
1	C	143	HIS
1	C	225	HIS
1	C	289	GLN
1	C	365	HIS
1	C	412	ASN

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Mol	Chain	Res	Type
1	C	425	ASN
1	C	478	ASN
1	C	481	GLN
1	C	484	GLN
1	D	61	ASN
1	D	70	HIS
1	D	143	HIS
1	D	225	HIS
1	D	289	GLN
1	D	365	HIS
1	D	385	GLN
1	D	412	ASN
1	D	425	ASN
1	D	478	ASN
1	D	481	GLN
1	D	484	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](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	1501	-	5,5,5	0.43	0	5,5,5	0.80	0
3	NAD	B	1498	-	46,48,48	1.59	11 (23%)	64,73,73	1.91	13 (20%)
3	NAD	A	1498	-	46,48,48	1.44	5 (10%)	64,73,73	1.83	16 (25%)
4	GOL	A	1500	-	5,5,5	0.60	0	5,5,5	1.06	0
3	NAD	C	1498	-	46,48,48	1.53	9 (19%)	64,73,73	1.80	14 (21%)
4	GOL	D	1502	-	5,5,5	0.65	0	5,5,5	0.79	0
3	NAD	D	1498	-	46,48,48	1.42	6 (13%)	64,73,73	1.82	14 (21%)
4	GOL	D	1499	-	5,5,5	0.74	0	5,5,5	1.46	0
4	GOL	A	1499	-	5,5,5	0.95	0	5,5,5	1.04	0
4	GOL	D	1500	-	5,5,5	0.56	0	5,5,5	1.75	2 (40%)
4	GOL	C	1499	-	5,5,5	0.45	0	5,5,5	0.23	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
4	GOL	D	1501	-	-	2/4/4/4	-
3	NAD	B	1498	-	-	4/30/62/62	0/5/5/5
3	NAD	A	1498	-	-	6/30/62/62	0/5/5/5
4	GOL	A	1500	-	-	3/4/4/4	-
3	NAD	C	1498	-	-	6/30/62/62	0/5/5/5
4	GOL	D	1502	-	-	2/4/4/4	-
3	NAD	D	1498	-	-	7/30/62/62	0/5/5/5
4	GOL	D	1499	-	-	4/4/4/4	-
4	GOL	A	1499	-	-	3/4/4/4	-
4	GOL	D	1500	-	-	2/4/4/4	-
4	GOL	C	1499	-	-	2/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1498	NAD	C5A-N7A	-4.35	1.31	1.39
3	C	1498	NAD	C8A-N9A	-4.04	1.30	1.37
3	B	1498	NAD	C5A-N7A	-3.91	1.31	1.39
3	B	1498	NAD	C8A-N9A	-3.88	1.30	1.37
3	B	1498	NAD	C2N-N1N	-3.69	1.30	1.35
3	C	1498	NAD	C5A-N7A	-3.55	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1498	NAD	O7N-C7N	3.45	1.30	1.24
3	A	1498	NAD	C8A-N9A	-3.44	1.31	1.37
3	D	1498	NAD	C2N-N1N	-3.39	1.31	1.35
3	D	1498	NAD	C8A-N9A	-3.33	1.31	1.37
3	D	1498	NAD	C5A-N7A	-3.17	1.33	1.39
3	A	1498	NAD	O7N-C7N	3.14	1.30	1.24
3	C	1498	NAD	O7N-C7N	3.09	1.29	1.24
3	A	1498	NAD	C4A-N9A	-2.88	1.31	1.37
3	B	1498	NAD	C4A-N9A	-2.87	1.31	1.37
3	C	1498	NAD	C2A-N1A	-2.59	1.29	1.33
3	D	1498	NAD	C4A-N9A	-2.51	1.32	1.37
3	C	1498	NAD	C4A-N9A	-2.50	1.32	1.37
3	C	1498	NAD	C2N-N1N	-2.48	1.32	1.35
3	B	1498	NAD	C7N-N7N	-2.36	1.28	1.33
3	B	1498	NAD	PA-O2A	-2.35	1.44	1.55
3	D	1498	NAD	PA-O2A	-2.30	1.44	1.55
3	C	1498	NAD	C5A-C4A	-2.22	1.35	1.39
3	B	1498	NAD	O7N-C7N	2.22	1.28	1.24
3	A	1498	NAD	PA-O2A	-2.22	1.45	1.55
3	C	1498	NAD	C2A-N3A	-2.11	1.30	1.33
3	B	1498	NAD	C3N-C7N	-2.06	1.47	1.50
3	B	1498	NAD	O4B-C4B	-2.06	1.40	1.45
3	C	1498	NAD	C6A-N1A	-2.06	1.30	1.35
3	B	1498	NAD	C6N-N1N	-2.01	1.30	1.35
3	B	1498	NAD	C5A-C4A	-2.01	1.35	1.39

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1498	NAD	C5A-C4A-N3A	-6.45	117.83	126.72
3	A	1498	NAD	C5A-C4A-N3A	-6.28	118.08	126.72
3	C	1498	NAD	C5A-C4A-N3A	-6.27	118.08	126.72
3	D	1498	NAD	N3A-C2A-N1A	-5.56	120.17	128.58
3	D	1498	NAD	C5A-C4A-N3A	-5.27	119.46	126.72
3	B	1498	NAD	N3A-C2A-N1A	-5.11	120.85	128.58
3	C	1498	NAD	N3A-C2A-N1A	-4.81	121.31	128.58
3	B	1498	NAD	C2A-N3A-C4A	4.27	122.27	111.83
3	B	1498	NAD	N3A-C4A-N9A	4.22	134.34	127.17
3	C	1498	NAD	C4A-C5A-N7A	-4.17	105.81	110.58
3	A	1498	NAD	N3A-C2A-N1A	-4.04	122.47	128.58
3	B	1498	NAD	O7N-C7N-N7N	-4.03	116.79	122.62
3	A	1498	NAD	N3A-C4A-N9A	3.86	133.73	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1498	NAD	O4B-C1B-C2B	-3.82	98.44	106.62
3	B	1498	NAD	N9A-C8A-N7A	-3.73	108.65	113.94
3	C	1498	NAD	C2A-N3A-C4A	3.72	120.91	111.83
3	D	1498	NAD	C2A-N3A-C4A	3.61	120.66	111.83
3	A	1498	NAD	C2A-N3A-C4A	3.58	120.59	111.83
3	D	1498	NAD	N3A-C4A-N9A	3.51	133.14	127.17
3	C	1498	NAD	C5A-C4A-N9A	3.46	109.58	105.81
3	C	1498	NAD	N9A-C8A-N7A	-3.45	109.05	113.94
3	B	1498	NAD	C3N-C7N-N7N	3.37	121.89	117.74
3	D	1498	NAD	N9A-C8A-N7A	-3.32	109.23	113.94
3	A	1498	NAD	O7N-C7N-N7N	-3.24	117.93	122.62
3	A	1498	NAD	C5N-C4N-C3N	-3.18	117.24	120.36
3	D	1498	NAD	C4A-C5A-N7A	-3.17	106.95	110.58
3	C	1498	NAD	C5A-N7A-C8A	3.14	108.39	103.45
3	B	1498	NAD	C4A-C5A-N7A	-3.14	106.99	110.58
3	B	1498	NAD	C5N-C4N-C3N	-3.06	117.36	120.36
3	A	1498	NAD	O2B-C2B-C3B	-3.05	102.04	111.82
3	C	1498	NAD	N3A-C4A-N9A	3.04	132.34	127.17
3	D	1498	NAD	C3N-C7N-N7N	3.02	121.47	117.74
3	B	1498	NAD	C5A-N7A-C8A	2.98	108.14	103.45
3	A	1498	NAD	O2N-PN-O3	2.96	115.27	107.27
3	C	1498	NAD	O7N-C7N-N7N	-2.95	118.35	122.62
3	D	1498	NAD	C5A-N7A-C8A	2.88	107.98	103.45
3	B	1498	NAD	C5D-C4D-C3D	-2.78	105.21	115.21
3	A	1498	NAD	O2A-PA-O3	2.76	114.73	107.27
3	A	1498	NAD	O4B-C1B-C2B	-2.75	100.73	106.62
3	D	1498	NAD	C2A-N1A-C6A	2.71	123.18	118.73
3	D	1498	NAD	O2N-PN-O3	2.59	114.26	107.27
3	D	1498	NAD	C5N-C4N-C3N	-2.58	117.83	120.36
3	D	1498	NAD	C4A-N9A-C8A	2.56	108.43	105.74
3	C	1498	NAD	O2A-PA-O3	2.51	114.06	107.27
3	B	1498	NAD	C4A-N9A-C8A	2.50	108.36	105.74
3	A	1498	NAD	C6A-C5A-C4A	2.43	120.50	117.18
3	A	1498	NAD	C4A-C5A-N7A	-2.42	107.82	110.58
3	C	1498	NAD	C5N-C4N-C3N	-2.41	117.99	120.36
3	C	1498	NAD	O2B-C2B-C1B	2.41	118.40	110.10
3	A	1498	NAD	C6N-N1N-C2N	-2.38	119.85	121.88
4	D	1500	GOL	O1-C1-C2	2.27	120.58	110.38
3	C	1498	NAD	O3-PA-O1A	-2.24	103.96	110.70
3	A	1498	NAD	C4B-O4B-C1B	2.23	114.39	109.47
3	A	1498	NAD	C5A-C4A-N9A	2.19	108.19	105.81
3	C	1498	NAD	C3N-C7N-N7N	2.16	120.40	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1498	NAD	O4B-C1B-N9A	-2.14	103.97	108.09
3	A	1498	NAD	O7N-C7N-C3N	2.13	122.20	119.60
3	D	1498	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
4	D	1500	GOL	O2-C2-C1	2.02	117.55	109.18

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1498	NAD	C5B-O5B-PA-O1A
3	D	1498	NAD	C5B-O5B-PA-O2A
3	D	1498	NAD	C5B-O5B-PA-O3
4	A	1499	GOL	O1-C1-C2-C3
4	A	1500	GOL	O1-C1-C2-C3
4	D	1499	GOL	C1-C2-C3-O3
4	D	1500	GOL	O1-C1-C2-O2
4	D	1501	GOL	C1-C2-C3-O3
4	D	1502	GOL	C1-C2-C3-O3
4	A	1499	GOL	O1-C1-C2-O2
4	C	1499	GOL	O2-C2-C3-O3
4	C	1499	GOL	C1-C2-C3-O3
4	D	1499	GOL	O1-C1-C2-C3
4	D	1500	GOL	O1-C1-C2-C3
3	A	1498	NAD	C3D-C4D-C5D-O5D
3	A	1498	NAD	C2B-C1B-N9A-C8A
4	A	1500	GOL	O1-C1-C2-O2
4	D	1499	GOL	O2-C2-C3-O3
4	D	1502	GOL	O2-C2-C3-O3
4	A	1500	GOL	C1-C2-C3-O3
3	D	1498	NAD	O4B-C4B-C5B-O5B
3	A	1498	NAD	O4D-C4D-C5D-O5D
3	B	1498	NAD	PN-O3-PA-O5B
4	D	1501	GOL	O2-C2-C3-O3
3	A	1498	NAD	C2B-C1B-N9A-C4A
3	B	1498	NAD	C2B-C1B-N9A-C8A
3	C	1498	NAD	C2B-C1B-N9A-C8A
3	D	1498	NAD	C2B-C1B-N9A-C8A
3	C	1498	NAD	C5B-O5B-PA-O1A
3	C	1498	NAD	C5B-O5B-PA-O2A
3	C	1498	NAD	C5B-O5B-PA-O3
3	D	1498	NAD	C5B-O5B-PA-O1A
3	C	1498	NAD	C4D-C5D-O5D-PN

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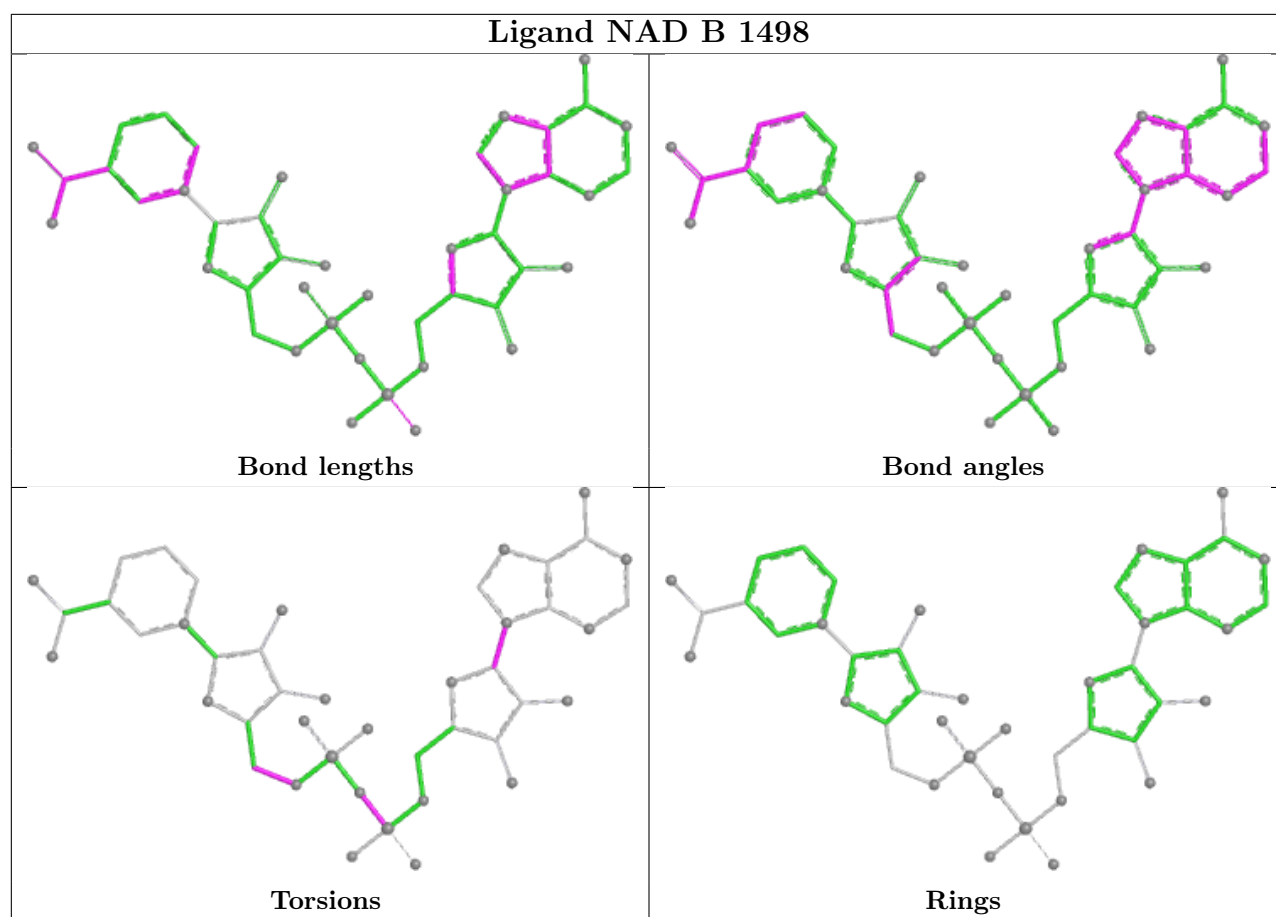
Mol	Chain	Res	Type	Atoms
3	B	1498	NAD	C4D-C5D-O5D-PN
4	D	1499	GOL	O1-C1-C2-O2
3	B	1498	NAD	C2B-C1B-N9A-C4A
3	D	1498	NAD	C4D-C5D-O5D-PN
3	A	1498	NAD	O4B-C1B-N9A-C8A
4	A	1499	GOL	O2-C2-C3-O3
3	D	1498	NAD	C2B-C1B-N9A-C4A
3	C	1498	NAD	O4B-C1B-N9A-C8A

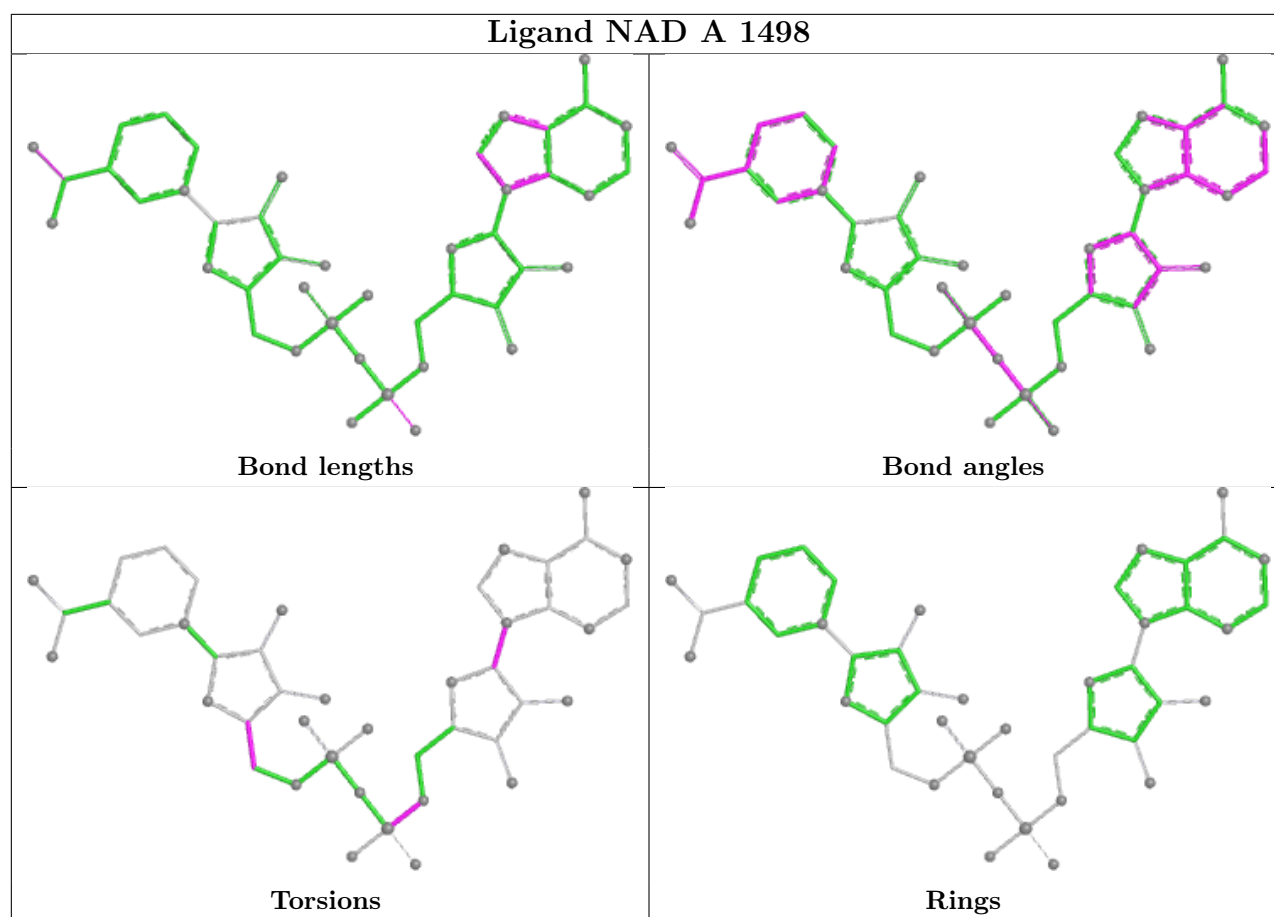
There are no ring outliers.

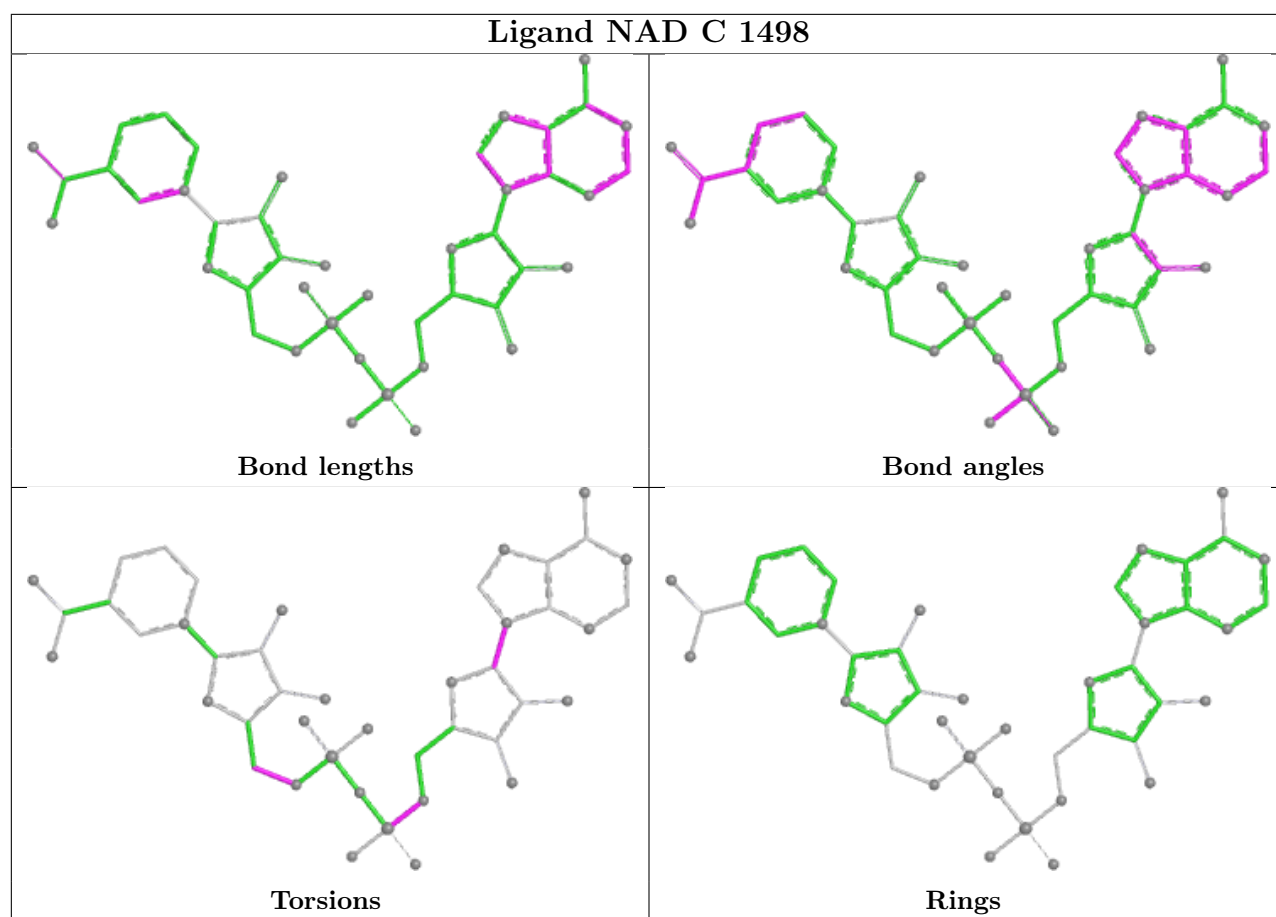
9 monomers are involved in 46 short contacts:

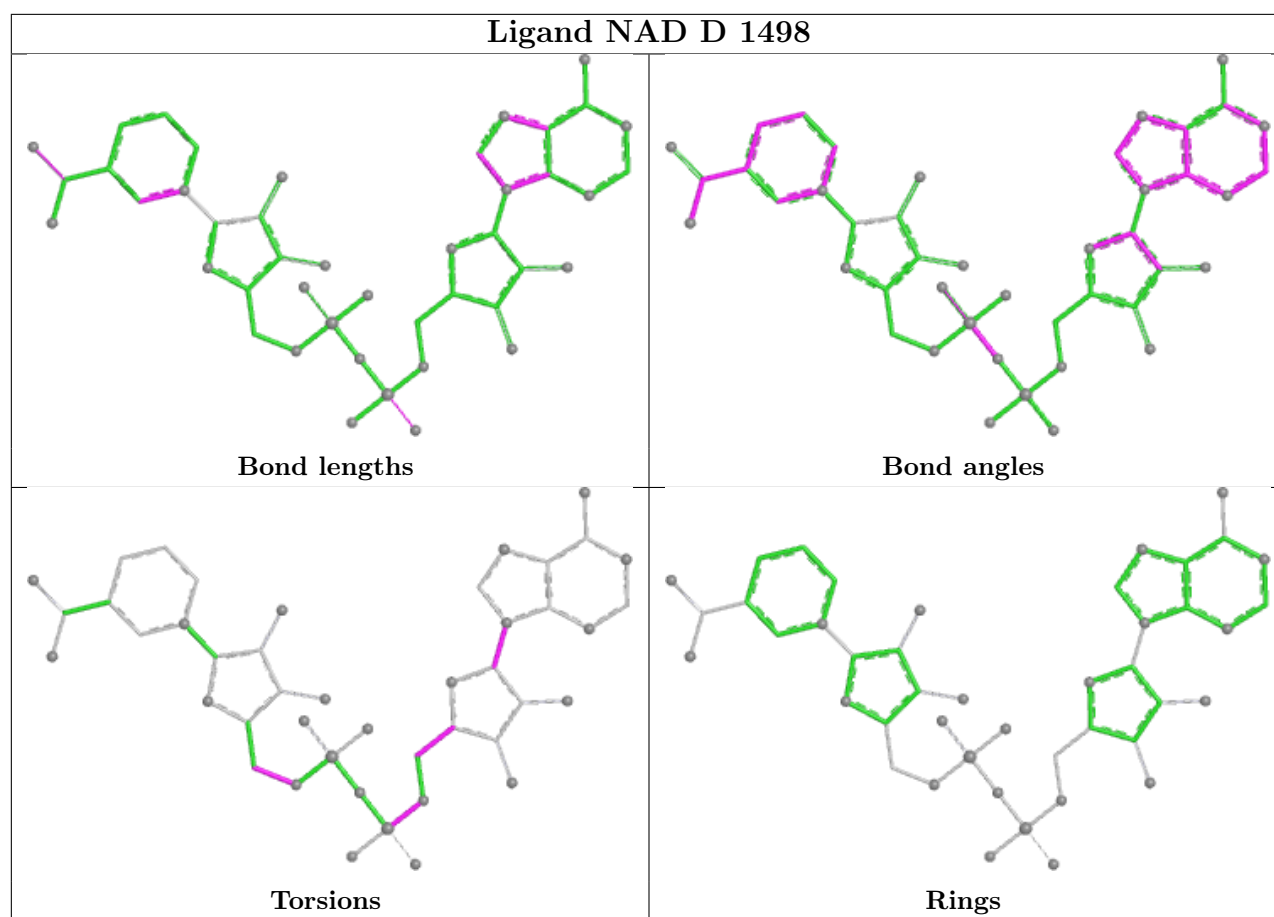
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1501	GOL	4	0
3	B	1498	NAD	9	0
3	A	1498	NAD	5	0
3	C	1498	NAD	8	0
4	D	1502	GOL	2	0
3	D	1498	NAD	6	0
4	A	1499	GOL	1	0
4	D	1500	GOL	3	0
4	C	1499	GOL	8	0

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	494/496 (99%)	0.22	2 (0%) 88 89	17, 52, 74, 103	5 (1%)
1	B	494/496 (99%)	0.37	8 (1%) 70 72	18, 52, 74, 111	6 (1%)
1	C	494/496 (99%)	0.49	12 (2%) 59 62	19, 57, 81, 93	7 (1%)
1	D	494/496 (99%)	0.59	26 (5%) 32 34	19, 58, 84, 95	5 (1%)
All	All	1976/1984 (99%)	0.42	48 (2%) 59 62	17, 54, 80, 111	23 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	496	SER	4.1
1	C	6	PRO	4.1
1	C	305	ALA	3.5
1	D	98	GLY	3.4
1	C	95	ILE	3.1
1	D	189	VAL	2.8
1	B	327	GLY	2.6
1	B	7	ALA	2.6
1	A	308	VAL	2.5
1	D	402	SER	2.5
1	D	373	GLU	2.5
1	B	3	PHE	2.5
1	D	25[A]	ILE	2.5
1	D	303	ILE	2.5
1	D	374	PRO	2.5
1	B	496	SER	2.4
1	C	496	SER	2.4
1	D	288	GLY	2.3
1	D	213	GLY	2.3
1	D	7	ALA	2.3
1	C	318	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	61	ASN	2.3
1	D	320	ILE	2.3
1	D	267	PHE	2.3
1	C	61	ASN	2.3
1	C	80	ALA	2.3
1	C	320	ILE	2.3
1	D	95	ILE	2.3
1	D	28	ILE	2.2
1	B	16	TRP	2.2
1	C	357	LEU	2.2
1	B	4	PRO	2.2
1	D	360	GLY	2.2
1	D	491	TRP	2.1
1	D	4	PRO	2.1
1	D	375	THR	2.1
1	A	95	ILE	2.1
1	C	358	TYR	2.1
1	C	312	VAL	2.1
1	D	31	SER	2.0
1	C	122	ALA	2.0
1	B	303	ILE	2.0
1	D	27	VAL	2.0
1	D	324	PHE	2.0
1	D	321	SER	2.0
1	B	92	LEU	2.0
1	D	35	ILE	2.0
1	D	356	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

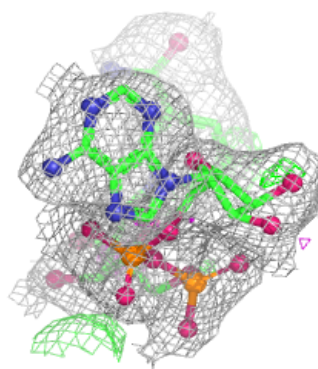
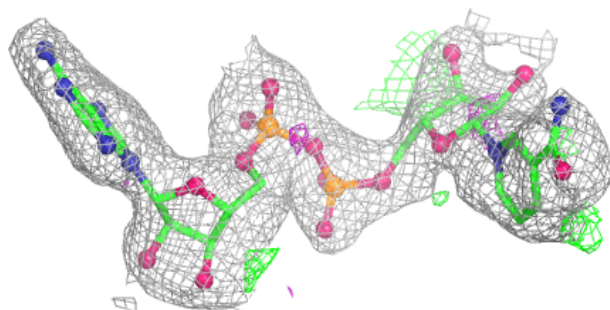
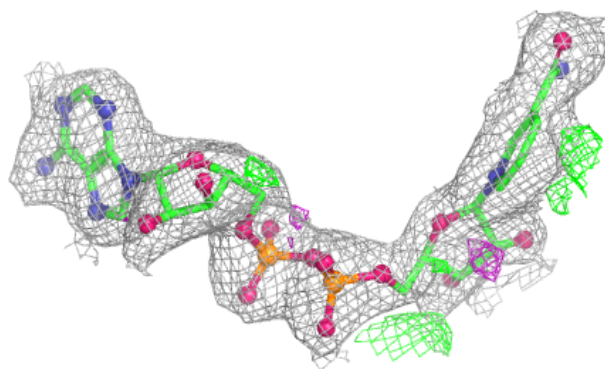
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	D	1497	1/1	0.61	0.18	94,94,94,94	0
4	GOL	D	1501	6/6	0.69	0.12	58,61,64,73	0
4	GOL	A	1500	6/6	0.82	0.13	51,59,65,65	0
2	K	C	1501	1/1	0.84	0.22	64,64,64,64	0
4	GOL	D	1499	6/6	0.84	0.14	45,50,54,58	0
2	K	A	1497	1/1	0.84	0.11	85,85,85,85	0
2	K	C	1497	1/1	0.85	0.10	85,85,85,85	0
4	GOL	D	1502	6/6	0.85	0.17	62,65,73,74	0
4	GOL	C	1499	6/6	0.86	0.19	54,62,64,73	0
2	K	A	1501	1/1	0.88	0.26	76,76,76,76	0
4	GOL	A	1499	6/6	0.89	0.08	56,61,69,70	0
3	NAD	A	1498	44/44	0.90	0.09	34,48,58,71	0
4	GOL	D	1500	6/6	0.90	0.12	41,51,52,65	0
3	NAD	D	1498	44/44	0.91	0.09	38,51,61,70	0
2	K	B	1499	1/1	0.92	0.26	69,69,69,69	0
3	NAD	C	1498	44/44	0.92	0.08	37,49,62,66	0
2	K	B	1497	1/1	0.93	0.06	63,63,63,63	0
2	K	C	1500	1/1	0.94	0.20	69,69,69,69	0
3	NAD	B	1498	44/44	0.96	0.06	31,43,51,55	0

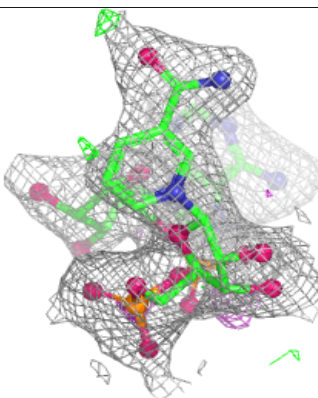
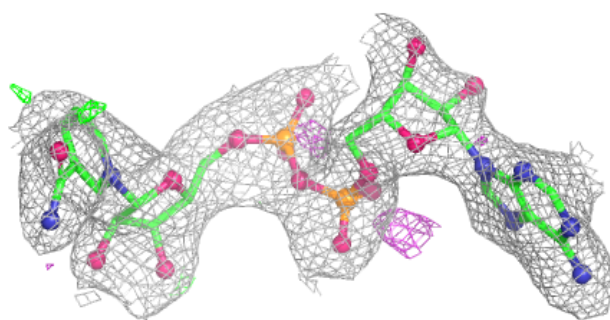
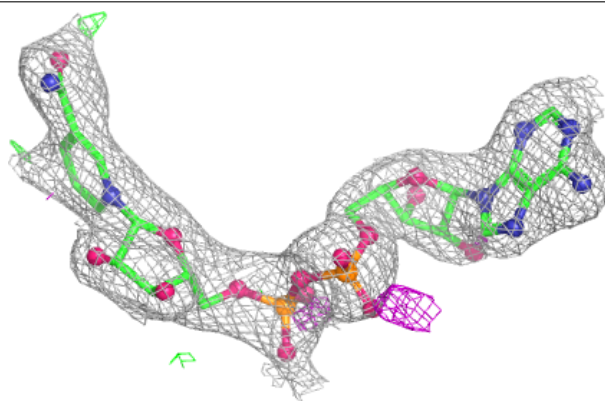
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 1498:

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

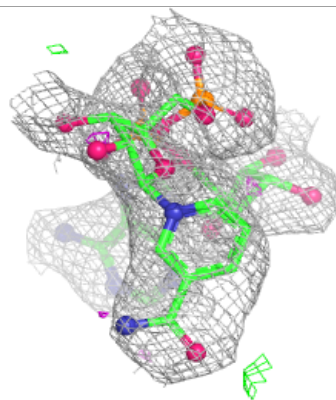
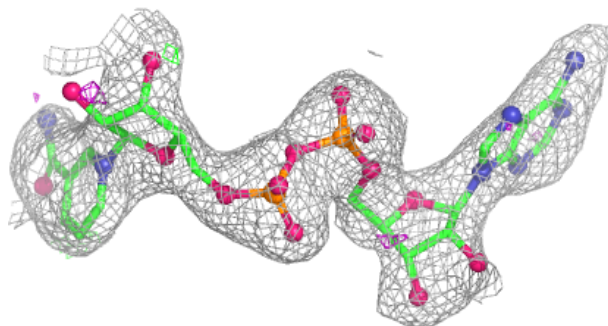
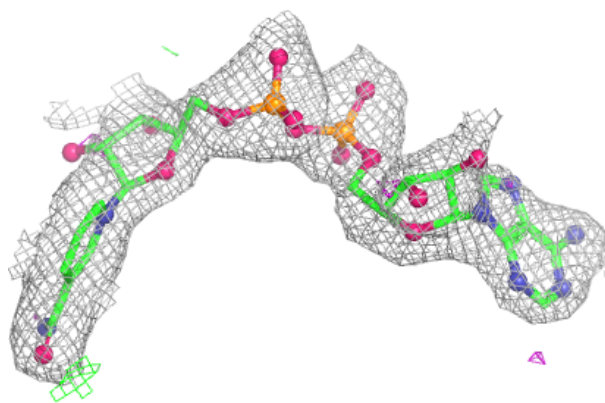
**Electron density around NAD D 1498:**

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

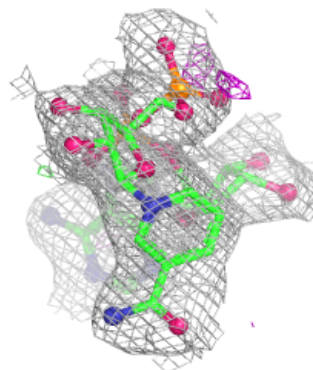
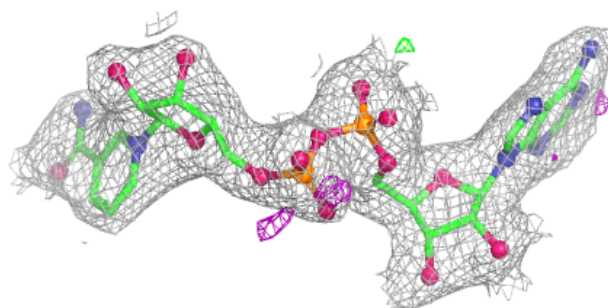
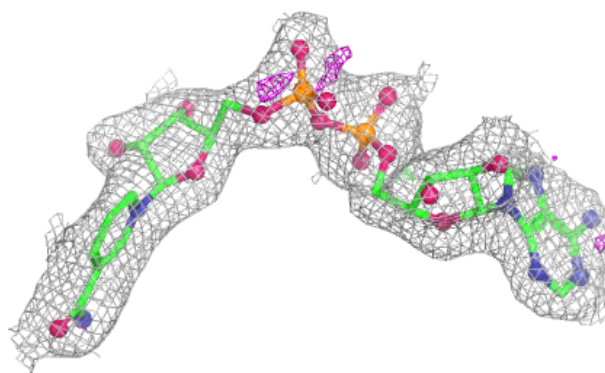


Electron density around NAD C 1498:

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

**Electron density around NAD B 1498:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.