



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 PM UTC

PDB ID : 2HAE / pdb_00002hae
Title : Crystal structure of a putative malic enzyme (malate oxidoreductase)
Authors : Seetharaman, J.; Swaminathan, S.; Burley, S.K.; New York SGX Research
Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-06-12
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

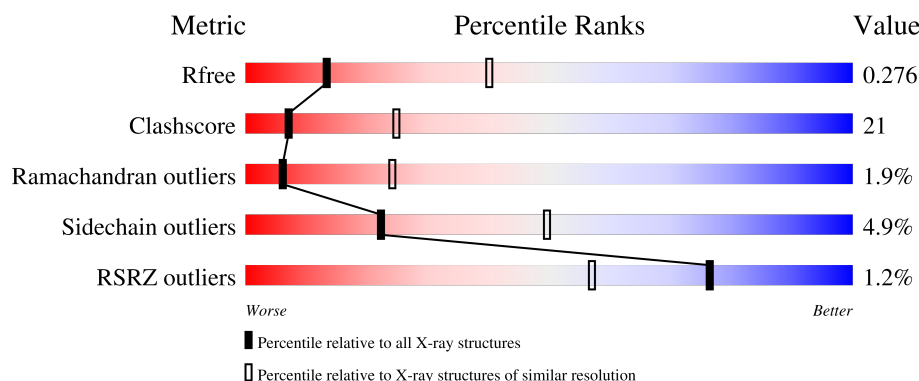
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	386	2% 63% 29% • •
1	B	386	% 63% 32% • •
1	C	386	% 58% 35% • •
1	D	386	% 53% 40% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Malate oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2860	1826	483	540	11			
1	B	373	Total	C	N	O	S	0	0	0
			2860	1826	483	540	11			
1	C	373	Total	C	N	O	S	0	0	0
			2860	1826	483	540	11			
1	D	373	Total	C	N	O	S	0	0	0
			2860	1826	483	540	11			

There are 48 discrepancies between the modelled and reference sequences:

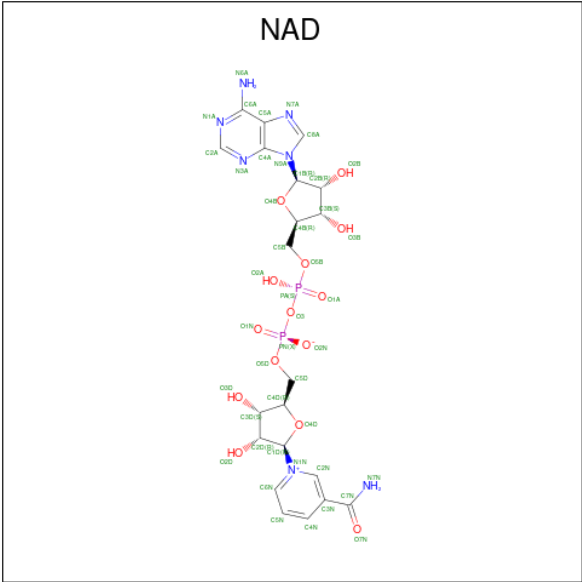
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q9WZ12
A	0	SER	-	cloning artifact	UNP Q9WZ12
A	1	LEU	-	cloning artifact	UNP Q9WZ12
A	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
A	377	GLU	-	cloning artifact	UNP Q9WZ12
A	378	GLY	-	cloning artifact	UNP Q9WZ12
A	379	HIS	-	cloning artifact	UNP Q9WZ12
A	380	HIS	-	cloning artifact	UNP Q9WZ12
A	381	HIS	-	cloning artifact	UNP Q9WZ12
A	382	HIS	-	cloning artifact	UNP Q9WZ12
A	383	HIS	-	cloning artifact	UNP Q9WZ12
A	384	HIS	-	cloning artifact	UNP Q9WZ12
B	-1	MET	-	cloning artifact	UNP Q9WZ12
B	0	SER	-	cloning artifact	UNP Q9WZ12
B	1	LEU	-	cloning artifact	UNP Q9WZ12
B	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
B	377	GLU	-	cloning artifact	UNP Q9WZ12
B	378	GLY	-	cloning artifact	UNP Q9WZ12
B	379	HIS	-	cloning artifact	UNP Q9WZ12
B	380	HIS	-	cloning artifact	UNP Q9WZ12
B	381	HIS	-	cloning artifact	UNP Q9WZ12

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Chain	Residue	Modelled	Actual	Comment	Reference
B	382	HIS	-	cloning artifact	UNP Q9WZ12
B	383	HIS	-	cloning artifact	UNP Q9WZ12
B	384	HIS	-	cloning artifact	UNP Q9WZ12
C	-1	MET	-	cloning artifact	UNP Q9WZ12
C	0	SER	-	cloning artifact	UNP Q9WZ12
C	1	LEU	-	cloning artifact	UNP Q9WZ12
C	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
C	377	GLU	-	cloning artifact	UNP Q9WZ12
C	378	GLY	-	cloning artifact	UNP Q9WZ12
C	379	HIS	-	cloning artifact	UNP Q9WZ12
C	380	HIS	-	cloning artifact	UNP Q9WZ12
C	381	HIS	-	cloning artifact	UNP Q9WZ12
C	382	HIS	-	cloning artifact	UNP Q9WZ12
C	383	HIS	-	cloning artifact	UNP Q9WZ12
C	384	HIS	-	cloning artifact	UNP Q9WZ12
D	-1	MET	-	cloning artifact	UNP Q9WZ12
D	0	SER	-	cloning artifact	UNP Q9WZ12
D	1	LEU	-	cloning artifact	UNP Q9WZ12
D	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
D	377	GLU	-	cloning artifact	UNP Q9WZ12
D	378	GLY	-	cloning artifact	UNP Q9WZ12
D	379	HIS	-	cloning artifact	UNP Q9WZ12
D	380	HIS	-	cloning artifact	UNP Q9WZ12
D	381	HIS	-	cloning artifact	UNP Q9WZ12
D	382	HIS	-	cloning artifact	UNP Q9WZ12
D	383	HIS	-	cloning artifact	UNP Q9WZ12
D	384	HIS	-	cloning artifact	UNP Q9WZ12

- 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		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

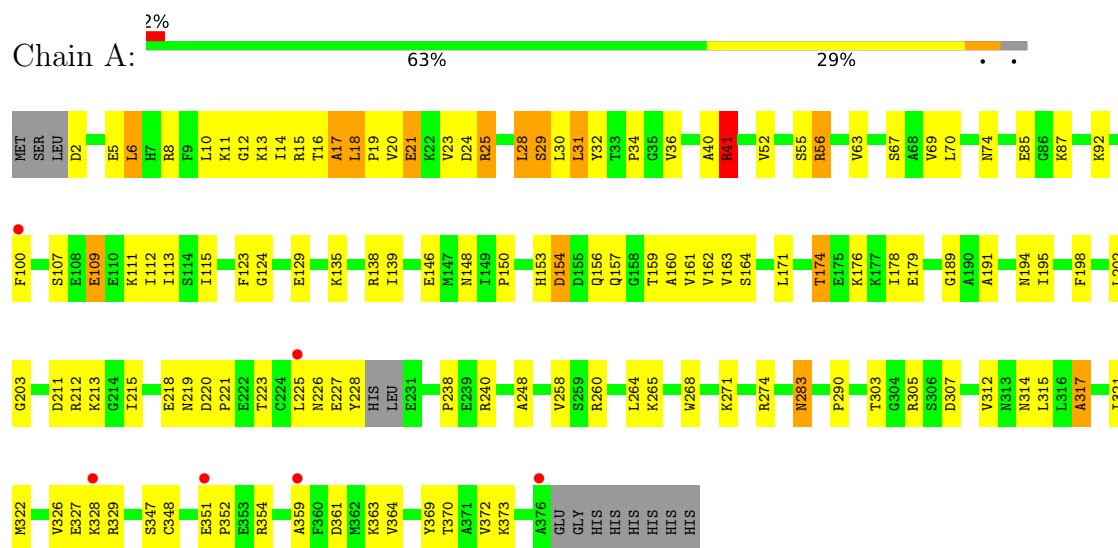
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	41	Total	O	0	0
			41	41		
4	C	46	Total	O	0	0
			46	46		
4	D	52	Total	O	0	0
			52	52		

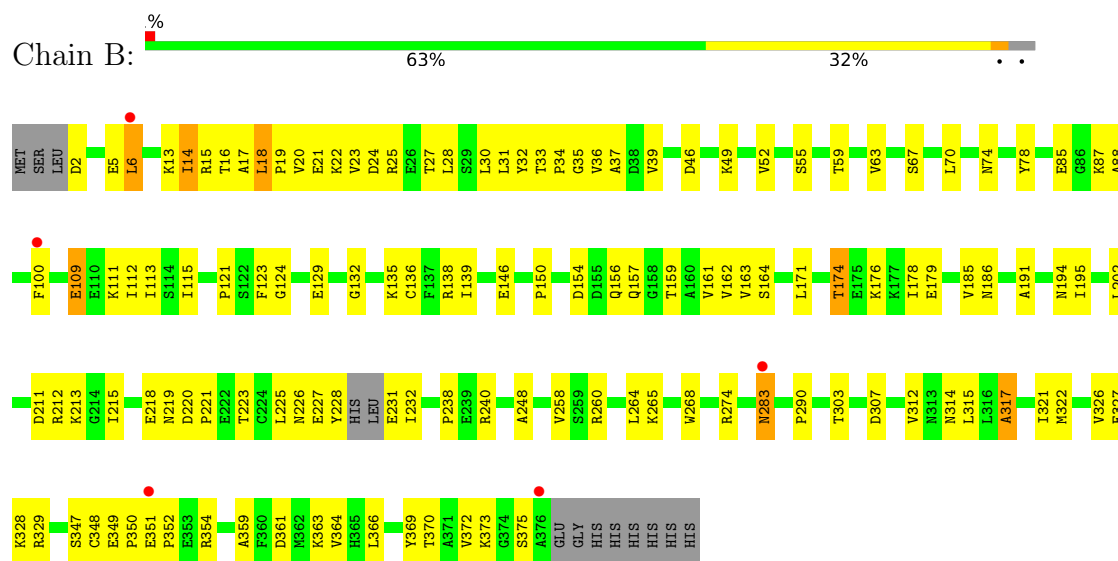
3 Residue-property plots

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

• Molecule 1: Malate oxidoreductase

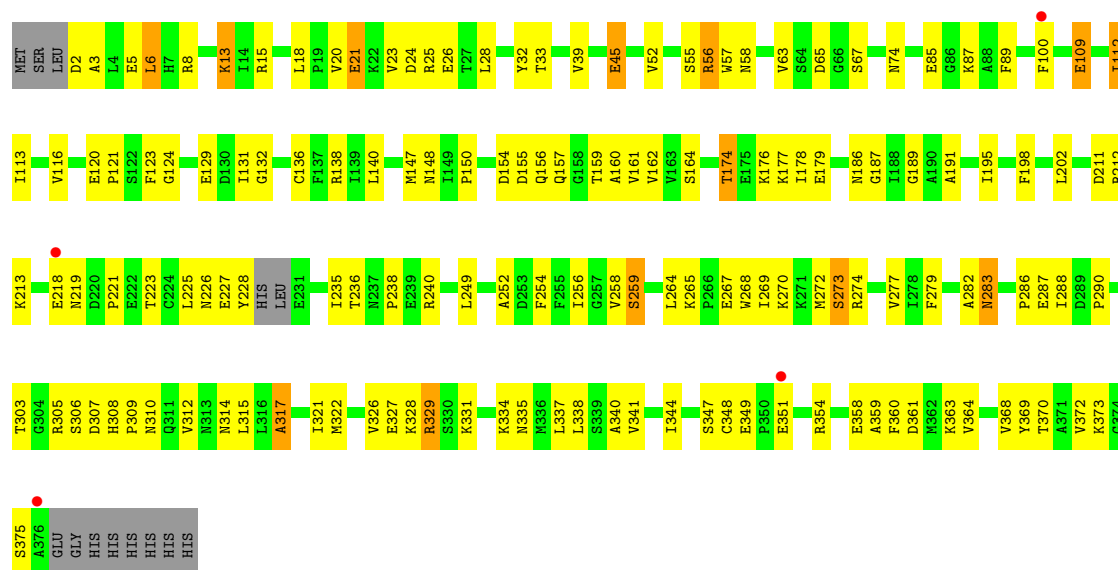


• Molecule 1: Malate oxidoreductase

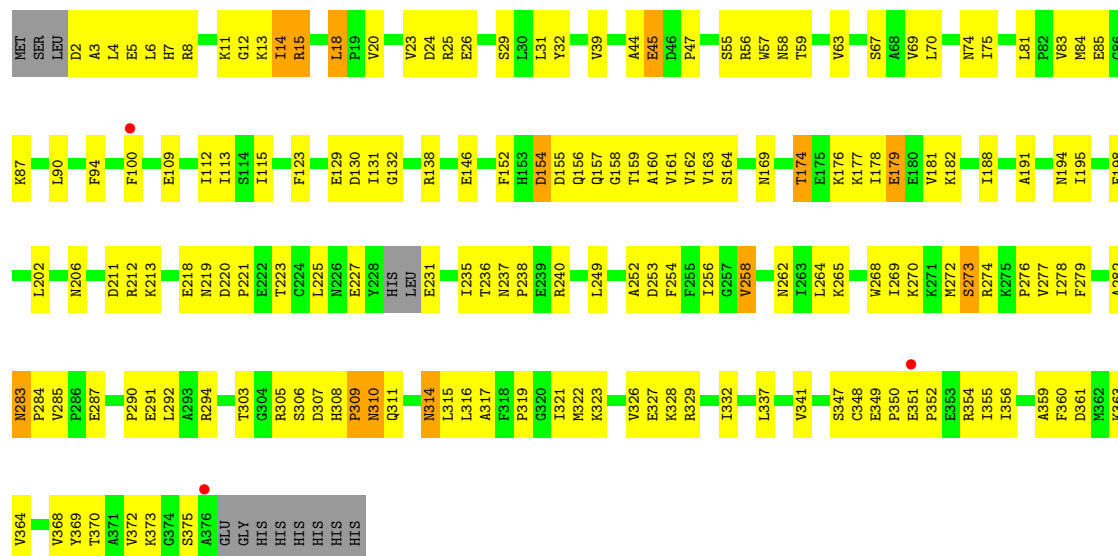


• Molecule 1: Malate oxidoreductase





• Molecule 1: Malate oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	145.80Å 145.80Å 159.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.13 50.00 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.13) 94.9 (50.00-3.13)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.282 0.243 , 0.276	Depositor DCC
R_{free} test set	2425 reflections (7.22%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11756	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: ZN, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/2910	0.97	8/3942 (0.2%)
1	B	0.61	0/2910	0.95	11/3942 (0.3%)
1	C	0.56	0/2910	1.03	12/3942 (0.3%)
1	D	0.57	0/2910	0.97	10/3942 (0.3%)
All	All	0.59	0/11640	0.98	41/15768 (0.3%)

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	D	0	1

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ILE	N-CA-C	-8.21	102.82	110.53
1	D	44	ALA	N-CA-C	-8.10	101.52	111.40
1	B	112	ILE	N-CA-C	-7.06	103.64	110.42
1	C	306	SER	N-CA-C	-6.61	104.85	113.17
1	B	85	GLU	N-CA-C	-6.34	104.47	111.82
1	C	109	GLU	N-CA-C	6.30	118.67	111.11
1	B	63	VAL	N-CA-C	6.27	117.61	108.58
1	A	63	VAL	N-CA-C	5.93	117.12	108.58
1	D	39	VAL	N-CA-C	-5.91	104.02	112.35
1	A	85	GLU	N-CA-C	-5.91	104.97	111.82
1	C	13	LYS	N-CA-C	-5.91	104.73	112.41
1	B	109	GLU	N-CA-C	5.89	118.46	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	THR	N-CA-C	5.78	117.10	109.93
1	D	94	PHE	N-CA-C	5.75	120.45	113.38
1	D	63	VAL	N-CA-C	5.67	116.75	108.58
1	D	85	GLU	N-CA-C	-5.60	105.18	112.23
1	D	146	GLU	N-CA-C	5.58	119.93	113.18
1	D	3	ALA	N-CA-C	5.55	117.01	111.07
1	A	41	ARG	N-CA-C	-5.51	104.50	111.11
1	A	317	ALA	N-CA-C	5.50	120.36	113.43
1	C	3	ALA	N-CA-C	5.50	117.70	111.11
1	D	112	ILE	N-CA-C	-5.49	105.15	110.42
1	B	349	GLU	CA-C-N	5.46	125.39	119.76
1	B	349	GLU	C-N-CA	5.46	125.39	119.76
1	D	278	ILE	N-CA-C	5.45	115.95	107.28
1	A	109	GLU	N-CA-C	5.44	117.91	111.33
1	C	112	ILE	N-CA-C	-5.41	105.10	110.62
1	C	259	SER	N-CA-C	5.30	116.57	108.30
1	A	146	GLU	N-CA-C	5.27	119.56	113.18
1	B	70	LEU	CB-CA-C	-5.24	110.52	116.54
1	C	317	ALA	N-CA-C	5.23	119.89	112.93
1	A	55	SER	N-CA-C	-5.19	106.95	113.28
1	C	132	GLY	N-CA-C	5.14	119.13	112.25
1	C	63	VAL	N-CA-C	5.13	115.97	108.58
1	C	349	GLU	CA-C-N	5.11	125.02	119.76
1	C	349	GLU	C-N-CA	5.11	125.02	119.76
1	B	146	GLU	N-CA-C	5.11	119.36	113.18
1	D	132	GLY	N-CA-C	5.11	117.95	112.33
1	C	85	GLU	N-CA-C	-5.04	105.97	111.82
1	B	317	ALA	N-CA-C	5.04	119.78	113.43
1	B	350	PRO	N-CA-C	5.01	118.95	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	316	LEU	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	2860	0	2920	118	0
1	B	2860	0	2920	123	0
1	C	2860	0	2920	130	0
1	D	2860	0	2920	160	0
2	A	44	0	26	10	0
2	B	44	0	26	13	0
2	C	44	0	26	12	0
3	D	1	0	0	0	0
4	A	44	0	0	11	0
4	B	41	0	0	16	0
4	C	46	0	0	19	0
4	D	52	0	0	22	0
All	All	11756	0	11758	487	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 21.

All (487) 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)
2:A:501:NAD:H6N	1:B:283:ASN:HD22	1.13	1.11
1:B:32:TYR:OH	1:D:87:LYS:HE3	1.58	1.01
1:D:15:ARG:HG2	1:D:15:ARG:HH11	1.28	0.94
1:A:159:THR:CG2	2:B:501:NAD:H72N	1.79	0.94
2:A:501:NAD:C6N	1:B:283:ASN:HD22	1.82	0.92
1:B:185:VAL:HG12	4:B:523:HOH:O	1.70	0.92
1:A:30:LEU:HD13	1:C:6:LEU:HG	1.51	0.91
2:A:501:NAD:H6N	1:B:283:ASN:ND2	1.87	0.89
1:C:249:LEU:HD22	1:C:272:MET:SD	2.14	0.88
1:A:13:LYS:HE2	4:C:532:HOH:O	1.75	0.86
1:A:283:ASN:HD22	2:B:501:NAD:H6N	1.38	0.85
1:C:177:LYS:HG3	4:C:521:HOH:O	1.74	0.85
1:C:358:GLU:HB2	4:C:519:HOH:O	1.76	0.85
1:D:69:VAL:HA	1:D:130:ASP:OD2	1.76	0.85
1:B:328:LYS:HE3	1:B:375:SER:O	1.76	0.84
1:C:2:ASP:O	1:C:6:LEU:HD23	1.75	0.84
1:D:67:SER:HA	1:D:74:ASN:OD1	1.78	0.83
1:A:159:THR:HG23	2:B:501:NAD:H72N	1.43	0.83
1:C:283:ASN:HB3	2:C:501:NAD:H6N	1.60	0.82
1:C:360:PHE:HB2	4:C:519:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:PRO:HG3	4:D:834:HOH:O	1.81	0.81
1:B:231:GLU:HB3	4:B:510:HOH:O	1.81	0.80
1:C:267:GLU:HA	4:C:540:HOH:O	1.82	0.80
1:B:32:TYR:OH	1:D:87:LYS:CE	2.29	0.80
1:A:67:SER:HA	1:A:74:ASN:OD1	1.83	0.79
1:D:15:ARG:HG2	1:D:15:ARG:NH1	1.90	0.79
1:A:321:ILE:HA	1:A:372:VAL:HG21	1.65	0.77
1:A:32:TYR:OH	1:C:87:LYS:HE2	1.84	0.77
1:D:291:GLU:HB2	4:D:804:HOH:O	1.84	0.77
1:C:140:LEU:HB2	4:C:533:HOH:O	1.84	0.77
1:D:292:LEU:HA	4:D:851:HOH:O	1.83	0.77
1:D:284:PRO:HA	4:D:821:HOH:O	1.84	0.77
1:B:232:ILE:HG12	4:B:510:HOH:O	1.85	0.77
1:B:67:SER:HA	1:B:74:ASN:OD1	1.85	0.76
1:A:363:LYS:HE3	1:B:363:LYS:HE3	1.69	0.75
1:B:55:SER:O	1:B:59:THR:HG23	1.87	0.75
1:C:328:LYS:HE3	1:C:375:SER:O	1.86	0.75
1:B:23:VAL:HG12	1:D:360:PHE:HE1	1.50	0.75
1:B:20:VAL:HG12	1:B:21:GLU:N	2.02	0.74
1:B:87:LYS:HE2	1:D:32:TYR:OH	1.87	0.73
1:A:203:GLY:HA3	4:A:524:HOH:O	1.87	0.73
1:C:67:SER:HA	1:C:74:ASN:OD1	1.88	0.72
1:D:328:LYS:HE3	1:D:375:SER:O	1.90	0.72
1:A:18:LEU:HD12	1:A:18:LEU:H	1.55	0.72
1:A:87:LYS:HE2	1:C:32:TYR:OH	1.89	0.72
2:A:501:NAD:H72N	1:B:159:THR:CG2	2.02	0.72
1:B:321:ILE:HA	1:B:372:VAL:HG21	1.70	0.71
1:D:2:ASP:HB3	1:D:5:GLU:OE1	1.89	0.71
1:C:351:GLU:HG3	1:C:354:ARG:HB3	1.72	0.71
1:C:269:ILE:HG21	4:C:511:HOH:O	1.89	0.71
1:D:18:LEU:HD13	1:D:20:VAL:O	1.91	0.71
1:D:290:PRO:HA	4:D:835:HOH:O	1.90	0.71
2:A:501:NAD:H61A	1:B:260:ARG:HH21	1.37	0.71
1:A:21:GLU:HB2	1:B:15:ARG:NH1	2.05	0.70
1:D:211:ASP:HB3	4:D:816:HOH:O	1.90	0.70
1:D:174:THR:HG23	1:D:176:LYS:HG3	1.73	0.70
1:D:2:ASP:HB3	1:D:5:GLU:CD	2.16	0.70
1:A:219:ASN:O	1:A:221:PRO:HD3	1.92	0.69
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.57	0.69
1:A:159:THR:CG2	2:B:501:NAD:N7N	2.54	0.69
1:B:32:TYR:C	1:B:36:VAL:HG12	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:O	1:B:221:PRO:HD3	1.93	0.69
1:C:282:ALA:HA	2:C:501:NAD:H1D	1.75	0.69
1:C:159:THR:CG2	2:C:501:NAD:H72N	2.04	0.69
1:C:321:ILE:HA	1:C:372:VAL:HG21	1.74	0.69
1:B:30:LEU:HD13	1:D:6:LEU:HD12	1.75	0.69
1:D:87:LYS:NZ	1:D:129:GLU:OE2	2.24	0.69
1:D:321:ILE:HA	1:D:372:VAL:HG21	1.74	0.68
1:D:237:ASN:HB3	4:D:829:HOH:O	1.93	0.68
1:A:283:ASN:HD22	2:B:501:NAD:C6N	2.06	0.68
1:C:23:VAL:HG11	1:C:28:LEU:HD21	1.75	0.68
1:C:174:THR:HG23	1:C:176:LYS:HG3	1.76	0.68
1:D:23:VAL:HG12	1:D:24:ASP:N	2.08	0.68
1:A:19:PRO:HG2	1:A:20:VAL:H	1.57	0.68
1:B:18:LEU:HD12	1:B:18:LEU:H	1.58	0.68
1:D:156:GLN:HB3	1:D:194:ASN:ND2	2.07	0.67
1:B:351:GLU:HG3	1:B:354:ARG:HB3	1.77	0.67
1:D:70:LEU:N	1:D:130:ASP:OD2	2.27	0.66
1:A:174:THR:HG23	1:A:176:LYS:HG3	1.78	0.66
1:C:57:TRP:CE3	1:C:58:ASN:HB2	2.31	0.65
1:D:219:ASN:O	1:D:221:PRO:HD3	1.95	0.65
1:B:174:THR:HG23	1:B:176:LYS:HG3	1.79	0.65
1:D:109:GLU:OE2	1:D:138:ARG:HD2	1.96	0.65
1:B:20:VAL:HG12	1:B:21:GLU:H	1.61	0.65
1:A:290:PRO:HG3	1:A:303:THR:HG21	1.77	0.65
1:C:191:ALA:O	1:C:195:ILE:HG13	1.97	0.65
1:C:24:ASP:OD2	1:C:26:GLU:HB3	1.98	0.64
1:A:328:LYS:O	1:A:328:LYS:HG2	1.97	0.64
1:C:322:MET:O	1:C:326:VAL:HG23	1.98	0.64
1:B:290:PRO:HG3	1:B:303:THR:HG21	1.80	0.63
1:C:159:THR:HG23	2:C:501:NAD:H72N	1.63	0.63
1:C:249:LEU:O	1:C:272:MET:HG2	1.99	0.63
1:A:219:ASN:CB	4:A:540:HOH:O	2.46	0.62
1:D:69:VAL:HG11	1:D:75:ILE:HD11	1.80	0.62
1:C:351:GLU:CG	1:C:354:ARG:HB3	2.28	0.62
1:D:258:VAL:HG13	1:D:258:VAL:O	1.99	0.62
2:A:501:NAD:H72N	1:B:159:THR:HG23	1.64	0.62
1:A:283:ASN:ND2	2:B:501:NAD:H6N	2.13	0.62
1:A:351:GLU:HG3	1:A:354:ARG:HB3	1.80	0.62
1:B:13:LYS:HE2	4:D:825:HOH:O	1.98	0.62
1:B:32:TYR:CZ	1:D:87:LYS:HE3	2.35	0.62
1:D:314:ASN:O	1:D:317:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LYS:HB2	4:A:512:HOH:O	1.99	0.61
1:C:189:GLY:HA3	2:C:501:NAD:O5B	1.99	0.61
1:D:351:GLU:HG3	1:D:354:ARG:HB3	1.83	0.61
1:C:219:ASN:O	1:C:221:PRO:HD3	1.99	0.61
1:C:6:LEU:HD23	1:C:6:LEU:H	1.65	0.61
4:B:511:HOH:O	1:D:14:ILE:HG12	2.01	0.61
1:A:258:VAL:O	1:A:258:VAL:HG13	2.01	0.61
1:D:283:ASN:HB2	4:D:821:HOH:O	2.01	0.60
1:B:156:GLN:HB3	1:B:194:ASN:ND2	2.15	0.60
1:A:87:LYS:HE3	1:A:129:GLU:CD	2.27	0.60
1:B:157:GLN:O	1:B:161:VAL:HG23	2.01	0.60
1:B:258:VAL:O	1:B:258:VAL:HG13	2.02	0.60
1:C:327:GLU:C	1:C:329:ARG:H	2.10	0.60
1:C:287:GLU:HG2	4:C:535:HOH:O	2.01	0.60
1:C:87:LYS:HE3	1:C:129:GLU:CD	2.27	0.60
1:B:109:GLU:O	1:B:113:ILE:HG13	2.01	0.59
1:A:157:GLN:O	1:A:161:VAL:HG23	2.03	0.59
1:A:159:THR:HG23	2:B:501:NAD:N7N	2.17	0.59
1:A:219:ASN:HB2	4:A:540:HOH:O	2.02	0.59
1:B:123:PHE:CE1	1:D:100:PHE:HE2	2.20	0.59
1:B:23:VAL:HG12	1:D:360:PHE:CE1	2.34	0.59
1:C:272:MET:O	1:C:273:SER:O	2.21	0.59
1:C:235:ILE:HG13	1:C:236:THR:HG23	1.84	0.59
1:C:6:LEU:N	1:C:6:LEU:CD2	2.66	0.59
1:C:65:ASP:HB2	4:C:514:HOH:O	2.02	0.58
1:D:270:LYS:HG3	4:D:802:HOH:O	2.03	0.58
1:B:13:LYS:HG2	1:D:31:LEU:HD22	1.83	0.58
1:D:90:LEU:HD13	1:D:315:LEU:HD13	1.86	0.58
1:A:56:ARG:HG2	1:A:56:ARG:HH11	1.69	0.58
1:B:15:ARG:HH11	1:B:15:ARG:HG2	1.68	0.58
1:D:231:GLU:N	4:D:803:HOH:O	2.36	0.58
1:A:138:ARG:HD3	4:A:522:HOH:O	2.01	0.58
1:D:2:ASP:OD2	1:D:5:GLU:HG3	2.03	0.58
1:D:177:LYS:O	1:D:181:VAL:HG13	2.03	0.58
1:A:156:GLN:HB3	1:A:194:ASN:ND2	2.19	0.58
1:B:366:LEU:HD12	4:B:535:HOH:O	2.03	0.58
1:B:46:ASP:HB3	1:B:49:LYS:HG2	1.85	0.58
1:A:2:ASP:N	4:A:504:HOH:O	2.37	0.58
1:D:253:ASP:HA	4:D:811:HOH:O	2.04	0.58
1:C:15:ARG:HG2	1:C:15:ARG:NH1	2.19	0.58
1:D:182:LYS:HG3	1:D:206:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:SER:OG	1:D:12:GLY:HA3	2.05	0.57
4:B:511:HOH:O	1:D:14:ILE:HA	2.03	0.57
1:D:294:ARG:CB	4:D:809:HOH:O	2.52	0.57
1:D:314:ASN:O	1:D:317:ALA:HB3	2.03	0.57
1:C:45:GLU:HB3	4:C:536:HOH:O	2.03	0.57
1:D:249:LEU:HD22	1:D:272:MET:SD	2.44	0.57
1:D:290:PRO:HG3	1:D:303:THR:HG21	1.85	0.57
1:A:6:LEU:N	1:A:6:LEU:CD2	2.67	0.56
1:C:155:ASP:HB3	4:C:503:HOH:O	2.05	0.56
1:C:258:VAL:HG13	1:C:258:VAL:O	2.04	0.56
1:C:273:SER:HB2	4:C:534:HOH:O	2.05	0.56
1:D:157:GLN:O	1:D:161:VAL:HG23	2.05	0.56
1:A:8:ARG:HH11	1:C:52:VAL:HG13	1.71	0.56
1:C:290:PRO:HG3	1:C:303:THR:HG21	1.88	0.56
1:B:30:LEU:HD13	1:D:6:LEU:CD1	2.36	0.56
1:A:10:LEU:O	1:A:11:LYS:HB2	2.05	0.56
1:C:307:ASP:HB3	1:C:308:HIS:CD2	2.40	0.56
1:D:18:LEU:HD12	1:D:18:LEU:H	1.70	0.56
1:B:20:VAL:CG1	1:B:21:GLU:N	2.69	0.56
1:B:31:LEU:HD22	1:D:13:LYS:HD3	1.88	0.56
1:B:327:GLU:C	1:B:329:ARG:H	2.13	0.56
1:C:354:ARG:NH2	4:C:543:HOH:O	2.39	0.56
1:D:327:GLU:C	1:D:329:ARG:H	2.12	0.56
1:C:348:CYS:HB2	1:C:354:ARG:HH21	1.71	0.56
1:D:57:TRP:CE3	1:D:58:ASN:HB2	2.41	0.56
1:D:169:ASN:HA	4:D:834:HOH:O	2.06	0.55
1:D:314:ASN:OD1	1:D:314:ASN:N	2.32	0.55
1:A:18:LEU:HD12	1:A:18:LEU:N	2.21	0.55
1:D:23:VAL:CG1	1:D:24:ASP:N	2.69	0.55
1:B:14:ILE:C	1:B:15:ARG:HG3	2.31	0.55
1:B:87:LYS:HE3	1:B:129:GLU:CD	2.32	0.55
1:D:138:ARG:HD3	4:D:820:HOH:O	2.07	0.55
1:C:211:ASP:CG	1:C:212:ARG:H	2.15	0.55
1:A:14:ILE:C	1:A:15:ARG:HG3	2.33	0.54
1:C:186:ASN:HB3	4:C:535:HOH:O	2.06	0.54
1:D:282:ALA:HB2	1:D:287:GLU:OE2	2.06	0.54
1:B:34:PRO:HG3	1:D:305:ARG:HH22	1.72	0.54
1:D:55:SER:O	1:D:56:ARG:C	2.50	0.54
1:C:315:LEU:HD23	1:C:359:ALA:CB	2.36	0.54
1:C:57:TRP:CZ3	1:C:58:ASN:HB2	2.42	0.54
1:D:211:ASP:CG	1:D:212:ARG:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ASP:OD1	1:D:363:LYS:HB2	2.08	0.54
1:C:23:VAL:CG1	1:C:28:LEU:HD21	2.37	0.54
1:C:87:LYS:HE3	1:C:129:GLU:OE1	2.07	0.54
1:D:15:ARG:HH11	1:D:15:ARG:CG	2.10	0.54
1:D:138:ARG:NH1	1:D:138:ARG:HB2	2.23	0.54
1:C:112:ILE:O	1:C:116:VAL:HG23	2.07	0.54
1:B:238:PRO:C	1:B:240:ARG:H	2.16	0.54
1:D:23:VAL:HG12	1:D:24:ASP:H	1.72	0.54
1:A:6:LEU:N	1:A:6:LEU:HD23	2.21	0.54
1:A:21:GLU:HB2	1:B:15:ARG:HH11	1.73	0.54
1:A:327:GLU:C	1:A:329:ARG:H	2.15	0.54
1:B:20:VAL:CG1	1:B:21:GLU:H	2.21	0.53
1:A:32:TYR:C	1:A:36:VAL:HG12	2.34	0.53
1:D:238:PRO:C	1:D:240:ARG:H	2.17	0.53
1:D:138:ARG:HB2	1:D:138:ARG:CZ	2.39	0.53
1:D:174:THR:HG23	1:D:176:LYS:H	1.73	0.53
1:B:231:GLU:N	4:B:517:HOH:O	2.41	0.53
1:D:191:ALA:O	1:D:195:ILE:HG13	2.09	0.53
1:A:238:PRO:C	1:A:240:ARG:H	2.17	0.52
1:C:315:LEU:HD23	1:C:359:ALA:HB1	1.91	0.52
1:A:2:ASP:OD2	1:A:5:GLU:HG3	2.09	0.52
1:C:2:ASP:HB3	1:C:5:GLU:OE1	2.10	0.52
1:C:109:GLU:O	1:C:113:ILE:HG13	2.08	0.52
1:A:271:LYS:HE3	4:A:512:HOH:O	2.09	0.52
1:C:6:LEU:HD23	1:C:6:LEU:N	2.24	0.52
1:A:14:ILE:O	1:A:15:ARG:HG3	2.10	0.52
1:B:13:LYS:HD3	1:D:31:LEU:HD22	1.92	0.52
1:A:159:THR:CB	2:B:501:NAD:H72N	2.22	0.52
1:A:6:LEU:HD23	1:A:6:LEU:H	1.75	0.52
1:B:363:LYS:HA	4:B:535:HOH:O	2.09	0.52
1:A:109:GLU:O	1:A:113:ILE:HG13	2.10	0.51
1:A:159:THR:O	1:A:163:VAL:HG23	2.10	0.51
1:D:87:LYS:HZ3	1:D:129:GLU:CD	2.16	0.51
1:C:238:PRO:C	1:C:240:ARG:H	2.17	0.51
1:D:178:ILE:HG23	1:D:179:GLU:N	2.26	0.51
1:A:159:THR:OG1	2:B:501:NAD:N7N	2.43	0.51
1:A:219:ASN:HB3	4:A:540:HOH:O	2.06	0.51
1:B:211:ASP:CG	1:B:212:ARG:H	2.17	0.51
1:B:228:TYR:HA	4:B:510:HOH:O	2.10	0.51
1:A:283:ASN:C	1:A:283:ASN:OD1	2.53	0.51
1:B:185:VAL:C	4:B:523:HOH:O	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ILE:HG13	1:D:236:THR:HG23	1.92	0.51
1:D:109:GLU:O	1:D:113:ILE:HG13	2.11	0.51
1:A:138:ARG:HB2	1:A:138:ARG:CZ	2.41	0.51
1:A:322:MET:O	1:A:326:VAL:HG23	2.10	0.51
1:D:23:VAL:CG1	1:D:24:ASP:H	2.23	0.51
1:A:32:TYR:HH	1:C:87:LYS:HE2	1.75	0.50
1:A:164:SER:HB3	1:A:202:LEU:HD11	1.93	0.50
1:B:52:VAL:HG13	1:D:8:ARG:HH11	1.76	0.50
1:A:211:ASP:CG	1:A:212:ARG:H	2.18	0.50
2:A:501:NAD:H6N	1:B:283:ASN:HB3	1.93	0.50
1:C:109:GLU:OE2	1:C:138:ARG:HD2	2.12	0.50
1:D:162:VAL:HG22	1:D:317:ALA:HB2	1.93	0.50
1:D:272:MET:O	1:D:273:SER:O	2.29	0.50
1:A:260:ARG:HH21	2:B:501:NAD:H61A	1.58	0.50
1:B:6:LEU:N	1:B:6:LEU:HD23	2.27	0.50
1:B:19:PRO:HG2	1:B:20:VAL:H	1.75	0.50
1:B:164:SER:HB3	1:B:202:LEU:HD11	1.94	0.50
1:D:294:ARG:HB3	4:D:809:HOH:O	2.10	0.50
1:D:351:GLU:CG	1:D:354:ARG:HB3	2.41	0.50
1:D:156:GLN:HB3	1:D:194:ASN:HD21	1.77	0.50
1:D:174:THR:CG2	1:D:176:LYS:H	2.25	0.50
1:D:315:LEU:C	1:D:317:ALA:H	2.20	0.50
1:A:171:LEU:O	1:A:174:THR:HG22	2.11	0.50
1:A:138:ARG:HB2	1:A:138:ARG:NH1	2.27	0.49
1:A:226:ASN:C	1:A:228:TYR:H	2.20	0.49
1:C:264:LEU:HD23	1:C:264:LEU:C	2.36	0.49
1:A:111:LYS:O	1:A:115:ILE:HG13	2.13	0.49
1:C:187:GLY:HA2	2:C:501:NAD:N3A	2.28	0.49
1:B:159:THR:O	1:B:163:VAL:HG23	2.12	0.49
1:B:78:TYR:CG	1:D:47:PRO:HB3	2.47	0.49
1:B:213:LYS:O	1:B:223:THR:HG22	2.13	0.49
1:A:18:LEU:H	1:A:18:LEU:CD1	2.18	0.49
1:C:265:LYS:HB2	1:C:268:TRP:CE2	2.47	0.49
2:A:501:NAD:N7N	1:B:159:THR:CG2	2.75	0.49
1:B:171:LEU:O	1:B:174:THR:HG22	2.13	0.49
1:C:212:ARG:HD3	2:C:501:NAD:C8A	2.43	0.49
1:A:20:VAL:HG12	1:A:21:GLU:N	2.28	0.48
1:C:328:LYS:HD2	1:C:373:LYS:O	2.13	0.48
1:B:111:LYS:O	1:B:115:ILE:HG13	2.13	0.48
1:D:57:TRP:CZ3	1:D:58:ASN:HB2	2.48	0.48
1:C:334:LYS:O	1:C:338:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLY:HA3	2:B:501:NAD:O5B	2.14	0.48
1:B:231:GLU:N	4:B:509:HOH:O	2.46	0.48
1:D:154:ASP:O	1:D:158:GLY:N	2.46	0.48
1:D:308:HIS:CD2	1:D:308:HIS:H	2.30	0.48
1:B:186:ASN:C	4:B:523:HOH:O	2.56	0.48
1:C:283:ASN:HB3	2:C:501:NAD:C6N	2.39	0.48
1:A:315:LEU:HD23	1:A:359:ALA:CB	2.43	0.48
1:D:174:THR:HG23	1:D:176:LYS:CG	2.41	0.48
1:A:18:LEU:HB3	1:C:89:PHE:CD2	2.49	0.48
1:A:361:ASP:OD1	1:A:363:LYS:HB2	2.13	0.48
1:C:174:THR:HG23	1:C:176:LYS:CG	2.42	0.48
1:A:12:GLY:O	1:A:15:ARG:NH2	2.47	0.48
1:B:13:LYS:CD	1:D:31:LEU:HD22	2.44	0.47
1:B:121:PRO:O	1:D:81:LEU:HD22	2.14	0.47
1:B:135:LYS:O	1:B:139:ILE:HG13	2.14	0.47
1:B:322:MET:O	1:B:326:VAL:HG23	2.14	0.47
1:C:138:ARG:HB2	1:C:138:ARG:NH1	2.29	0.47
1:C:286:PRO:O	1:C:287:GLU:C	2.56	0.47
1:A:153:HIS:HD2	4:A:516:HOH:O	1.96	0.47
1:A:154:ASP:HB2	4:A:516:HOH:O	2.14	0.47
1:B:28:LEU:HD21	1:D:90:LEU:HD21	1.96	0.47
1:C:55:SER:O	1:C:56:ARG:C	2.56	0.47
1:D:328:LYS:HD2	1:D:373:LYS:O	2.14	0.47
1:D:310:ASN:N	4:D:852:HOH:O	2.47	0.47
2:A:501:NAD:N7N	1:B:159:THR:OG1	2.48	0.47
1:B:138:ARG:HB2	1:B:138:ARG:CZ	2.44	0.47
1:B:226:ASN:C	1:B:228:TYR:H	2.22	0.47
1:C:156:GLN:NE2	4:C:533:HOH:O	2.47	0.47
1:A:361:ASP:HB3	1:A:364:VAL:HG23	1.96	0.47
1:C:213:LYS:HB2	1:C:223:THR:HA	1.97	0.47
1:C:361:ASP:HB3	1:C:364:VAL:HG23	1.96	0.47
1:D:188:ILE:HG22	1:D:188:ILE:O	2.13	0.47
1:D:254:PHE:CD2	1:D:277:VAL:HB	2.50	0.47
1:B:24:ASP:OD1	1:B:24:ASP:N	2.48	0.47
1:B:32:TYR:O	1:B:36:VAL:HG12	2.13	0.47
1:C:287:GLU:CG	4:C:535:HOH:O	2.61	0.47
1:C:347:SER:O	1:C:348:CYS:HB3	2.15	0.47
1:D:265:LYS:HB2	1:D:268:TRP:CE2	2.49	0.47
1:B:28:LEU:CD2	1:D:90:LEU:HD21	2.45	0.46
1:B:351:GLU:CG	1:B:354:ARG:HB3	2.42	0.46
1:D:219:ASN:O	1:D:221:PRO:CD	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:MET:HE3	1:D:326:VAL:HG23	1.97	0.46
1:D:270:LYS:N	4:D:802:HOH:O	2.48	0.46
1:A:109:GLU:OE2	1:A:138:ARG:HD2	2.16	0.46
1:B:283:ASN:OD1	1:B:283:ASN:C	2.58	0.46
1:C:340:ALA:O	1:C:344:ILE:HG13	2.15	0.46
1:C:259:SER:O	2:C:501:NAD:O3D	2.28	0.46
1:C:369:TYR:O	1:C:373:LYS:HB2	2.15	0.46
1:D:309:PRO:O	1:D:310:ASN:C	2.58	0.46
1:B:369:TYR:O	1:B:373:LYS:HB2	2.16	0.46
1:A:52:VAL:HG12	1:A:52:VAL:O	2.15	0.46
1:A:159:THR:HG21	2:B:501:NAD:N7N	2.31	0.46
1:A:213:LYS:O	1:A:223:THR:HG22	2.16	0.46
1:D:311:GLN:O	1:D:356:ILE:HD11	2.15	0.46
1:B:178:ILE:HG23	1:B:179:GLU:N	2.31	0.46
1:D:159:THR:O	1:D:163:VAL:HG23	2.16	0.46
1:D:240:ARG:NH2	4:D:806:HOH:O	2.48	0.46
1:D:314:ASN:O	1:D:317:ALA:CB	2.64	0.46
1:D:369:TYR:O	1:D:373:LYS:HB2	2.15	0.46
1:A:347:SER:O	1:A:348:CYS:HB3	2.15	0.46
1:D:154:ASP:OD2	1:D:314:ASN:HB3	2.16	0.46
1:D:314:ASN:O	1:D:315:LEU:C	2.58	0.46
1:B:174:THR:CG2	1:B:176:LYS:H	2.28	0.46
1:D:294:ARG:HB2	4:D:809:HOH:O	2.13	0.46
1:A:92:LYS:HB3	1:C:18:LEU:HD21	1.98	0.45
1:D:361:ASP:HB3	1:D:364:VAL:HG23	1.98	0.45
1:B:231:GLU:N	4:B:506:HOH:O	2.49	0.45
1:C:138:ARG:HB2	1:C:138:ARG:CZ	2.46	0.45
1:C:178:ILE:HG23	1:C:179:GLU:N	2.32	0.45
1:C:212:ARG:C	1:C:213:LYS:HD2	2.41	0.45
1:D:211:ASP:OD1	1:D:212:ARG:HG2	2.16	0.45
1:D:152:PHE:HB2	1:D:332:ILE:CD1	2.47	0.45
1:D:262:ASN:ND2	1:D:285:VAL:HG11	2.31	0.45
1:A:16:THR:O	1:A:17:ALA:HB2	2.17	0.45
1:A:87:LYS:HE3	1:A:129:GLU:OE1	2.15	0.45
1:B:109:GLU:OE2	1:B:138:ARG:HD2	2.15	0.45
1:B:232:ILE:N	4:B:510:HOH:O	2.46	0.45
1:D:354:ARG:HG3	1:D:354:ARG:HH11	1.81	0.45
1:B:14:ILE:HG23	1:B:15:ARG:N	2.30	0.45
1:B:138:ARG:HB2	1:B:138:ARG:NH1	2.31	0.45
1:B:347:SER:O	1:B:348:CYS:HB3	2.16	0.45
1:D:83:VAL:HB	1:D:84:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:OD2	1:B:5:GLU:HG3	2.16	0.45
1:C:164:SER:HB3	1:C:202:LEU:HD11	1.99	0.45
1:D:129:GLU:O	1:D:130:ASP:C	2.58	0.45
1:A:265:LYS:HB2	1:A:268:TRP:CE2	2.51	0.45
1:A:317:ALA:O	1:A:321:ILE:HG13	2.16	0.45
1:B:13:LYS:CG	1:D:31:LEU:HD22	2.47	0.45
1:B:361:ASP:OD1	1:B:363:LYS:HB2	2.16	0.45
1:D:56:ARG:HG2	1:D:56:ARG:HH11	1.81	0.45
1:D:69:VAL:CA	1:D:130:ASP:OD2	2.57	0.45
1:D:249:LEU:O	1:D:272:MET:HG2	2.17	0.45
1:D:322:MET:O	1:D:326:VAL:HG23	2.17	0.45
1:B:265:LYS:HB2	1:B:268:TRP:CE2	2.52	0.45
1:D:25:ARG:HG3	1:D:25:ARG:HH11	1.81	0.45
1:D:269:ILE:HB	4:D:802:HOH:O	2.16	0.45
1:D:327:GLU:C	1:D:329:ARG:N	2.75	0.45
1:C:283:ASN:HD22	2:C:501:NAD:C6N	2.30	0.45
1:D:290:PRO:HG2	1:D:308:HIS:CD2	2.51	0.45
1:B:35:GLY:O	1:B:36:VAL:C	2.58	0.44
1:B:315:LEU:HD23	1:B:359:ALA:CB	2.46	0.44
1:C:162:VAL:HG12	1:C:312:VAL:HG13	1.99	0.44
1:A:123:PHE:CE1	1:C:100:PHE:HE2	2.35	0.44
1:A:162:VAL:HG12	1:A:312:VAL:HG13	1.98	0.44
1:B:328:LYS:HG2	1:B:328:LYS:O	2.17	0.44
1:C:269:ILE:HD13	4:C:511:HOH:O	2.16	0.44
1:C:270:LYS:HG3	4:C:540:HOH:O	2.18	0.44
1:D:138:ARG:NH1	1:D:138:ARG:CB	2.80	0.44
1:C:32:TYR:O	1:C:33:THR:C	2.60	0.44
1:C:264:LEU:HB3	1:C:288:ILE:HB	1.99	0.44
1:A:178:ILE:HG23	1:A:179:GLU:N	2.32	0.44
1:A:174:THR:CG2	1:A:176:LYS:H	2.30	0.44
1:C:56:ARG:HH11	1:C:56:ARG:HG2	1.81	0.44
1:A:219:ASN:O	1:A:221:PRO:CD	2.65	0.44
1:C:174:THR:CG2	1:C:176:LYS:H	2.31	0.44
1:A:18:LEU:HB3	1:C:89:PHE:CE2	2.53	0.44
1:A:29:SER:HA	1:A:34:PRO:HD2	1.99	0.44
1:A:56:ARG:HG2	1:A:56:ARG:NH1	2.31	0.44
1:B:290:PRO:HG3	1:B:303:THR:CG2	2.48	0.44
1:D:347:SER:O	1:D:348:CYS:HB3	2.18	0.44
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.74	0.43
1:B:123:PHE:HE1	1:D:100:PHE:CE2	2.36	0.43
1:C:213:LYS:O	1:C:223:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ASN:CB	2:C:501:NAD:H6N	2.39	0.43
1:C:337:LEU:O	1:C:341:VAL:HG23	2.18	0.43
1:D:213:LYS:O	1:D:223:THR:HG22	2.18	0.43
1:C:327:GLU:C	1:C:329:ARG:N	2.76	0.43
1:A:315:LEU:HD23	1:A:359:ALA:HB1	2.01	0.43
1:B:191:ALA:O	1:B:195:ILE:HG13	2.18	0.43
1:C:252:ALA:O	1:C:272:MET:HB3	2.18	0.43
1:A:28:LEU:O	1:A:30:LEU:N	2.52	0.43
1:A:290:PRO:CG	1:A:303:THR:HG21	2.47	0.43
1:A:215:ILE:HD11	1:A:248:ALA:HB2	2.00	0.43
1:C:124:GLY:O	1:C:150:PRO:HD2	2.19	0.43
1:A:135:LYS:O	1:A:139:ILE:HG13	2.19	0.43
1:B:16:THR:O	1:B:17:ALA:HB2	2.19	0.43
1:B:361:ASP:HB3	1:B:364:VAL:HG23	2.00	0.43
1:D:160:ALA:HB1	1:D:198:PHE:CD1	2.53	0.43
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.83	0.43
1:D:169:ASN:ND2	1:D:355:ILE:O	2.52	0.43
1:A:290:PRO:HG3	1:A:303:THR:CG2	2.46	0.42
1:A:351:GLU:CG	1:A:354:ARG:HB3	2.45	0.42
1:B:132:GLY:O	1:B:136:CYS:HB3	2.19	0.42
1:C:147:MET:O	1:C:331:LYS:NZ	2.52	0.42
1:A:8:ARG:HG3	1:C:52:VAL:HG13	2.01	0.42
1:C:361:ASP:OD1	1:C:363:LYS:HB2	2.18	0.42
1:B:219:ASN:O	1:B:221:PRO:CD	2.65	0.42
4:B:526:HOH:O	1:D:306:SER:HB3	2.19	0.42
1:C:228:TYR:C	4:C:523:HOH:O	2.62	0.42
1:D:315:LEU:HD23	1:D:359:ALA:CB	2.49	0.42
1:C:56:ARG:HG2	1:C:56:ARG:NH1	2.35	0.42
1:D:337:LEU:O	1:D:341:VAL:HG23	2.20	0.42
1:A:24:ASP:OD1	1:A:24:ASP:N	2.52	0.42
1:A:87:LYS:HE2	1:C:32:TYR:HH	1.79	0.42
1:A:160:ALA:HB1	1:A:198:PHE:CD1	2.55	0.42
1:B:22:LYS:HB2	1:C:57:TRP:CH2	2.55	0.42
1:C:120:GLU:HB3	1:C:121:PRO:HD3	2.01	0.42
1:D:164:SER:HB3	1:D:202:LEU:HD11	2.02	0.42
1:D:276:PRO:HA	4:D:811:HOH:O	2.19	0.42
1:A:31:LEU:HD13	1:C:13:LYS:HG2	2.02	0.42
1:A:124:GLY:O	1:A:150:PRO:HD2	2.19	0.42
1:A:264:LEU:HD23	1:A:264:LEU:C	2.45	0.42
1:C:364:VAL:O	1:C:368:VAL:HG23	2.20	0.42
1:A:369:TYR:O	1:A:373:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.63	0.42
1:C:157:GLN:O	1:C:161:VAL:HG23	2.19	0.42
1:C:315:LEU:CD2	1:C:359:ALA:HB1	2.50	0.42
2:A:501:NAD:O2D	1:B:283:ASN:ND2	2.53	0.41
1:B:39:VAL:CG2	1:D:4:LEU:HD23	2.50	0.41
1:C:174:THR:HG22	1:C:176:LYS:H	1.85	0.41
1:D:129:GLU:O	1:D:131:ILE:HG13	2.20	0.41
1:A:40:ALA:O	1:A:41:ARG:C	2.63	0.41
1:A:283:ASN:HB3	2:B:501:NAD:H6N	2.02	0.41
1:D:317:ALA:O	1:D:321:ILE:HG13	2.20	0.41
1:D:364:VAL:O	1:D:368:VAL:HG23	2.19	0.41
1:B:124:GLY:O	1:B:150:PRO:HD2	2.20	0.41
1:A:327:GLU:C	1:A:329:ARG:N	2.78	0.41
1:C:226:ASN:OD1	1:C:228:TYR:HD2	2.03	0.41
1:D:69:VAL:O	1:D:70:LEU:C	2.62	0.41
1:D:252:ALA:O	1:D:272:MET:HB3	2.21	0.41
1:D:323:LYS:HG2	1:D:369:TYR:CE1	2.55	0.41
1:B:36:VAL:HG13	1:B:37:ALA:N	2.35	0.41
1:B:39:VAL:HG22	1:D:4:LEU:HD23	2.03	0.41
1:B:290:PRO:CG	1:B:303:THR:HG21	2.50	0.41
1:C:305:ARG:HB3	1:C:307:ASP:HB2	2.02	0.41
1:D:349:GLU:HA	1:D:350:PRO:HD2	1.93	0.41
1:A:305:ARG:NH2	4:A:517:HOH:O	2.45	0.41
1:C:160:ALA:HB1	1:C:198:PHE:CD1	2.56	0.41
1:C:226:ASN:C	1:C:228:TYR:H	2.28	0.41
1:A:19:PRO:CG	1:A:20:VAL:H	2.32	0.41
1:B:15:ARG:HH11	1:B:15:ARG:CG	2.33	0.41
1:B:115:ILE:HG23	1:D:115:ILE:HG23	2.03	0.41
1:B:162:VAL:HG12	1:B:312:VAL:HG13	2.02	0.41
1:B:215:ILE:HD11	1:B:248:ALA:HB2	2.01	0.41
1:B:228:TYR:C	4:B:510:HOH:O	2.64	0.41
1:C:57:TRP:CD2	1:C:58:ASN:HB2	2.55	0.41
1:C:131:ILE:HG22	1:C:136:CYS:HB3	2.02	0.41
1:C:256:ILE:HA	1:C:279:PHE:HB2	2.02	0.41
1:D:26:GLU:O	1:D:29:SER:OG	2.37	0.41
1:D:169:ASN:HB3	1:D:350:PRO:HB3	2.03	0.41
1:D:57:TRP:CD2	1:D:58:ASN:HB2	2.55	0.41
1:A:191:ALA:O	1:A:195:ILE:HG13	2.21	0.40
1:A:69:VAL:O	1:A:70:LEU:C	2.63	0.40
1:C:20:VAL:HG12	1:C:21:GLU:N	2.35	0.40
1:D:55:SER:HB3	1:D:59:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LEU:O	1:D:319:PRO:HD2	2.20	0.40
1:A:100:PHE:HE2	1:C:123:PHE:CE1	2.39	0.40
1:C:55:SER:O	1:C:57:TRP:N	2.54	0.40
1:C:159:THR:CG2	2:C:501:NAD:N7N	2.78	0.40
1:C:219:ASN:O	1:C:221:PRO:CD	2.66	0.40
1:C:254:PHE:CD2	1:C:277:VAL:HB	2.57	0.40
1:A:174:THR:HG23	1:A:176:LYS:CG	2.48	0.40
1:B:14:ILE:CD1	1:B:88:ALA:HB1	2.51	0.40
1:B:100:PHE:HE2	1:D:123:PHE:CE1	2.40	0.40
1:B:264:LEU:HD23	1:B:264:LEU:C	2.46	0.40
1:B:317:ALA:O	1:B:321:ILE:HG13	2.21	0.40
1:C:317:ALA:O	1:C:321:ILE:HG13	2.22	0.40
1:D:256:ILE:HA	1:D:279:PHE:HB2	2.02	0.40
1:D:294:ARG:HH22	1:D:309:PRO:HD2	1.87	0.40
1:B:30:LEU:O	1:D:7:HIS:HE1	2.03	0.40
1:D:264:LEU:HD23	1:D:264:LEU:C	2.46	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	369/386 (96%)	319 (86%)	43 (12%)	7 (2%)	6	24
1	B	369/386 (96%)	318 (86%)	47 (13%)	4 (1%)	11	36
1	C	369/386 (96%)	322 (87%)	39 (11%)	8 (2%)	5	21
1	D	369/386 (96%)	314 (85%)	46 (12%)	9 (2%)	4	19
All	All	1476/1544 (96%)	1273 (86%)	175 (12%)	28 (2%)	6	24

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	LEU
1	B	225	LEU
1	C	225	LEU
1	C	273	SER
1	D	225	LEU
1	D	273	SER
1	A	17	ALA
1	A	29	SER
1	A	227	GLU
1	B	227	GLU
1	C	227	GLU
1	C	309	PRO
1	D	227	GLU
1	D	310	ASN
1	A	56	ARG
1	C	310	ASN
1	C	329	ARG
1	D	45	GLU
1	D	307	ASP
1	C	21	GLU
1	D	309	PRO
1	A	25	ARG
1	B	25	ARG
1	C	56	ARG
1	B	220	ASP
1	A	220	ASP
1	D	258	VAL
1	D	220	ASP

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	309/321 (96%)	291 (94%)	18 (6%)	18	44
1	B	309/321 (96%)	296 (96%)	13 (4%)	26	54
1	C	309/321 (96%)	295 (96%)	14 (4%)	24	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	309/321 (96%)	294 (95%)	15 (5%)	22	49
All	All	1236/1284 (96%)	1176 (95%)	60 (5%)	22	49

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	18	LEU
1	A	21	GLU
1	A	23	VAL
1	A	25	ARG
1	A	28	LEU
1	A	31	LEU
1	A	41	ARG
1	A	107	SER
1	A	154	ASP
1	A	174	THR
1	A	218	GLU
1	A	274	ARG
1	A	283	ASN
1	A	307	ASP
1	A	314	ASN
1	A	352	PRO
1	A	370	THR
1	B	6	LEU
1	B	14	ILE
1	B	18	LEU
1	B	27	THR
1	B	154	ASP
1	B	174	THR
1	B	218	GLU
1	B	274	ARG
1	B	283	ASN
1	B	307	ASP
1	B	314	ASN
1	B	352	PRO
1	B	370	THR
1	C	6	LEU
1	C	8	ARG
1	C	25	ARG
1	C	39	VAL
1	C	45	GLU

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Mol	Chain	Res	Type
1	C	148	ASN
1	C	154	ASP
1	C	174	THR
1	C	218	GLU
1	C	274	ARG
1	C	283	ASN
1	C	314	ASN
1	C	335	ASN
1	C	370	THR
1	D	11	LYS
1	D	14	ILE
1	D	15	ARG
1	D	18	LEU
1	D	45	GLU
1	D	154	ASP
1	D	155	ASP
1	D	174	THR
1	D	179	GLU
1	D	218	GLU
1	D	274	ARG
1	D	283	ASN
1	D	314	ASN
1	D	352	PRO
1	D	370	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	148	ASN
1	A	186	ASN
1	A	194	ASN
1	A	262	ASN
1	A	283	ASN
1	A	335	ASN
1	B	127	ASN
1	B	148	ASN
1	B	186	ASN
1	B	194	ASN
1	B	262	ASN
1	B	283	ASN
1	B	335	ASN

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Mol	Chain	Res	Type
1	C	127	ASN
1	C	148	ASN
1	C	186	ASN
1	C	194	ASN
1	C	262	ASN
1	C	283	ASN
1	C	308	HIS
1	C	335	ASN
1	D	7	HIS
1	D	127	ASN
1	D	148	ASN
1	D	186	ASN
1	D	194	ASN
1	D	262	ASN
1	D	311	GLN
1	D	335	ASN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
2	NAD	A	501	-	46,48,48	2.07	8 (17%)	64,73,73	1.99	16 (25%)
2	NAD	C	501	-	46,48,48	2.08	11 (23%)	64,73,73	1.99	16 (25%)
2	NAD	B	501	-	46,48,48	1.99	10 (21%)	64,73,73	1.94	17 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	501	-	-	5/30/62/62	0/5/5/5
2	NAD	C	501	-	-	3/30/62/62	0/5/5/5
2	NAD	B	501	-	-	5/30/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O7N-C7N	8.76	1.40	1.24
2	A	501	NAD	O7N-C7N	8.73	1.40	1.24
2	C	501	NAD	O7N-C7N	8.67	1.40	1.24
2	A	501	NAD	C2N-N1N	4.60	1.40	1.35
2	C	501	NAD	C2A-N1A	4.44	1.41	1.33
2	C	501	NAD	C2N-N1N	4.34	1.39	1.35
2	B	501	NAD	C2N-N1N	4.10	1.39	1.35
2	B	501	NAD	C2A-N3A	3.73	1.40	1.33
2	A	501	NAD	C2A-N1A	3.68	1.40	1.33
2	B	501	NAD	C2A-N1A	3.59	1.40	1.33
2	A	501	NAD	C4N-C3N	3.09	1.44	1.39
2	A	501	NAD	C2A-N3A	3.08	1.39	1.33
2	C	501	NAD	C6N-N1N	2.92	1.42	1.35
2	A	501	NAD	PN-O3	2.90	1.62	1.59
2	C	501	NAD	C4N-C3N	2.74	1.43	1.39
2	B	501	NAD	C6N-N1N	2.61	1.41	1.35
2	C	501	NAD	C8A-N7A	2.56	1.36	1.31
2	C	501	NAD	C2A-N3A	2.53	1.38	1.33
2	C	501	NAD	C4A-N3A	2.53	1.39	1.34
2	B	501	NAD	C4N-C3N	2.53	1.43	1.39
2	A	501	NAD	C6N-N1N	2.52	1.41	1.35
2	C	501	NAD	C2N-C3N	2.45	1.42	1.39
2	A	501	NAD	C3N-C7N	-2.39	1.47	1.50
2	B	501	NAD	C3N-C7N	-2.30	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C5A-N7A	-2.28	1.34	1.39
2	C	501	NAD	C5A-C4A	2.24	1.43	1.39
2	B	501	NAD	C8A-N7A	2.04	1.35	1.31
2	B	501	NAD	O4B-C4B	-2.03	1.40	1.45
2	C	501	NAD	PA-O3	2.02	1.61	1.59

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	O2N-PN-O5D	-5.83	81.14	107.57
2	B	501	NAD	O2N-PN-O5D	-5.67	81.88	107.57
2	A	501	NAD	O2N-PN-O5D	-5.62	82.08	107.57
2	C	501	NAD	O5D-PN-O1N	-5.22	88.27	108.94
2	A	501	NAD	N3A-C2A-N1A	-5.16	120.78	128.58
2	B	501	NAD	N3A-C2A-N1A	-5.12	120.83	128.58
2	B	501	NAD	O5D-PN-O1N	-5.11	88.67	108.94
2	C	501	NAD	N3A-C2A-N1A	-5.09	120.88	128.58
2	A	501	NAD	O5D-PN-O1N	-5.03	89.00	108.94
2	A	501	NAD	N9A-C8A-N7A	-3.99	108.28	113.94
2	A	501	NAD	C5A-N7A-C8A	3.96	109.67	103.45
2	B	501	NAD	C5A-N7A-C8A	3.96	109.67	103.45
2	C	501	NAD	N9A-C8A-N7A	-3.96	108.32	113.94
2	B	501	NAD	N9A-C8A-N7A	-3.82	108.52	113.94
2	A	501	NAD	C5A-C4A-N3A	-3.78	121.50	126.72
2	C	501	NAD	C4A-C5A-N7A	-3.77	106.27	110.58
2	C	501	NAD	C5A-N7A-C8A	3.77	109.38	103.45
2	A	501	NAD	C4A-C5A-N7A	-3.66	106.39	110.58
2	C	501	NAD	C3N-C7N-N7N	3.63	122.21	117.74
2	A	501	NAD	O3-PN-O1N	3.60	121.52	110.70
2	C	501	NAD	C5A-C4A-N3A	-3.48	121.92	126.72
2	B	501	NAD	C5A-C4A-N3A	-3.40	122.04	126.72
2	C	501	NAD	O3-PN-O1N	3.20	120.33	110.70
2	B	501	NAD	O3-PN-O1N	3.18	120.27	110.70
2	B	501	NAD	C4A-C5A-N7A	-3.18	106.95	110.58
2	A	501	NAD	C2A-N3A-C4A	3.14	119.49	111.83
2	A	501	NAD	C3N-C7N-N7N	3.07	121.52	117.74
2	C	501	NAD	C2A-N3A-C4A	3.02	119.20	111.83
2	B	501	NAD	C4D-O4D-C1D	-2.95	107.22	109.92
2	B	501	NAD	C2A-N3A-C4A	2.91	118.93	111.83
2	B	501	NAD	C3N-C7N-N7N	2.78	121.16	117.74
2	B	501	NAD	O2N-PN-O3	2.73	114.64	107.27
2	A	501	NAD	C4D-O4D-C1D	-2.71	107.44	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C4B-O4B-C1B	-2.67	103.58	109.47
2	B	501	NAD	C2B-C1B-N9A	2.62	119.80	113.30
2	A	501	NAD	C2B-C1B-N9A	2.59	119.73	113.30
2	A	501	NAD	C4A-N9A-C8A	2.39	108.25	105.74
2	C	501	NAD	O2N-PN-O1N	2.37	123.46	112.44
2	A	501	NAD	N3A-C4A-N9A	2.30	131.08	127.17
2	A	501	NAD	O2N-PN-O3	2.23	113.29	107.27
2	A	501	NAD	C2N-C3N-C4N	2.18	120.80	118.26
2	C	501	NAD	C4A-N9A-C8A	2.13	107.98	105.74
2	C	501	NAD	C4A-N9A-C1B	-2.11	121.69	126.63
2	B	501	NAD	C2N-C3N-C4N	2.06	120.66	118.26
2	C	501	NAD	C5A-C4A-N9A	2.05	108.04	105.81
2	B	501	NAD	O4B-C1B-C2B	-2.05	102.24	106.62
2	C	501	NAD	O2N-PN-O3	2.03	112.76	107.27
2	B	501	NAD	N3A-C4A-N9A	2.03	130.61	127.17
2	B	501	NAD	C4B-O4B-C1B	-2.01	105.02	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	A	501	NAD	PN-O3-PA-O1A
2	B	501	NAD	PN-O3-PA-O1A
2	C	501	NAD	C3D-C4D-C5D-O5D
2	C	501	NAD	PA-O3-PN-O1N
2	A	501	NAD	PA-O3-PN-O1N
2	B	501	NAD	PA-O3-PN-O1N
2	C	501	NAD	C2B-C1B-N9A-C8A
2	A	501	NAD	PN-O3-PA-O2A
2	B	501	NAD	PN-O3-PA-O2A

There are no ring outliers.

3 monomers are involved in 35 short contacts:

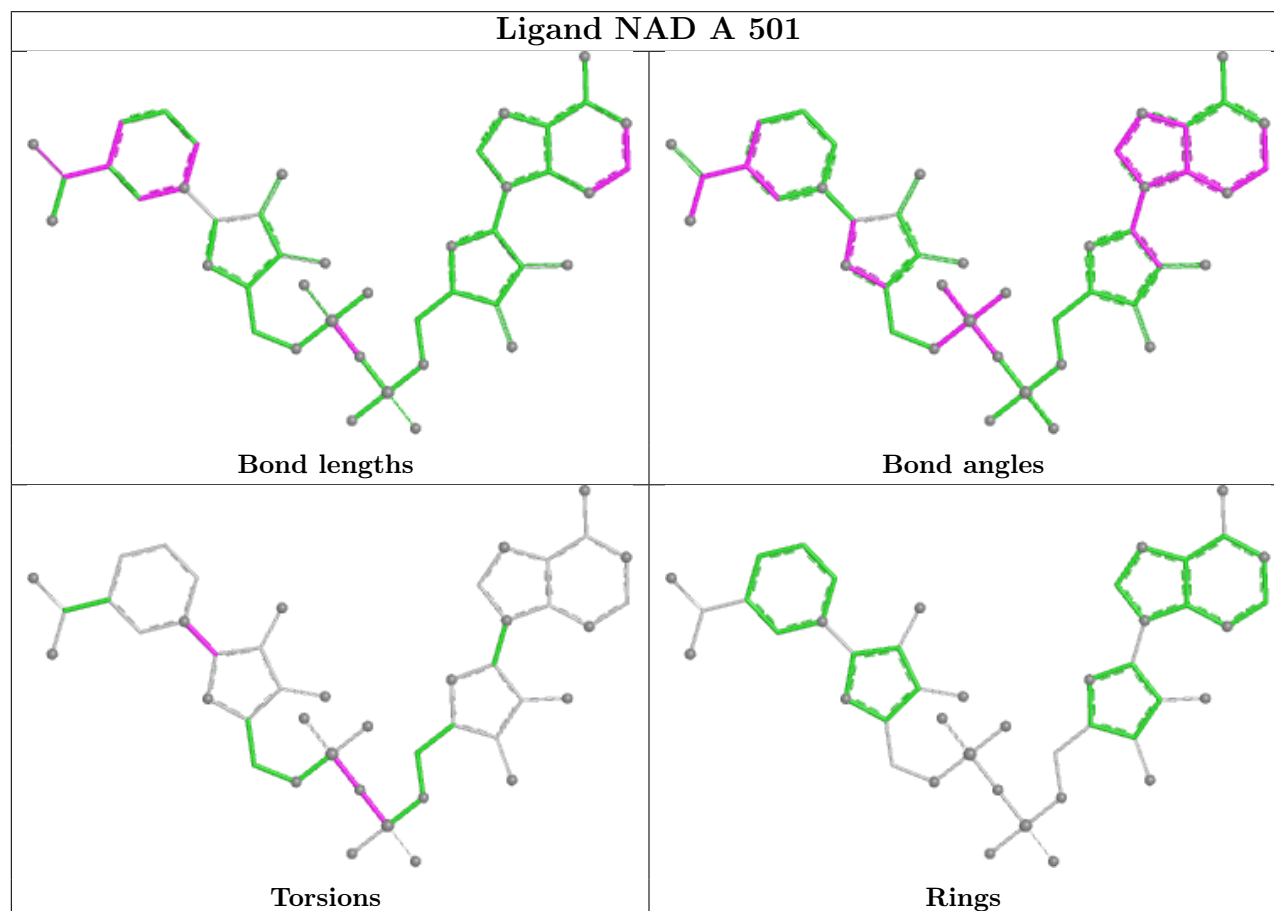
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	10	0
2	C	501	NAD	12	0

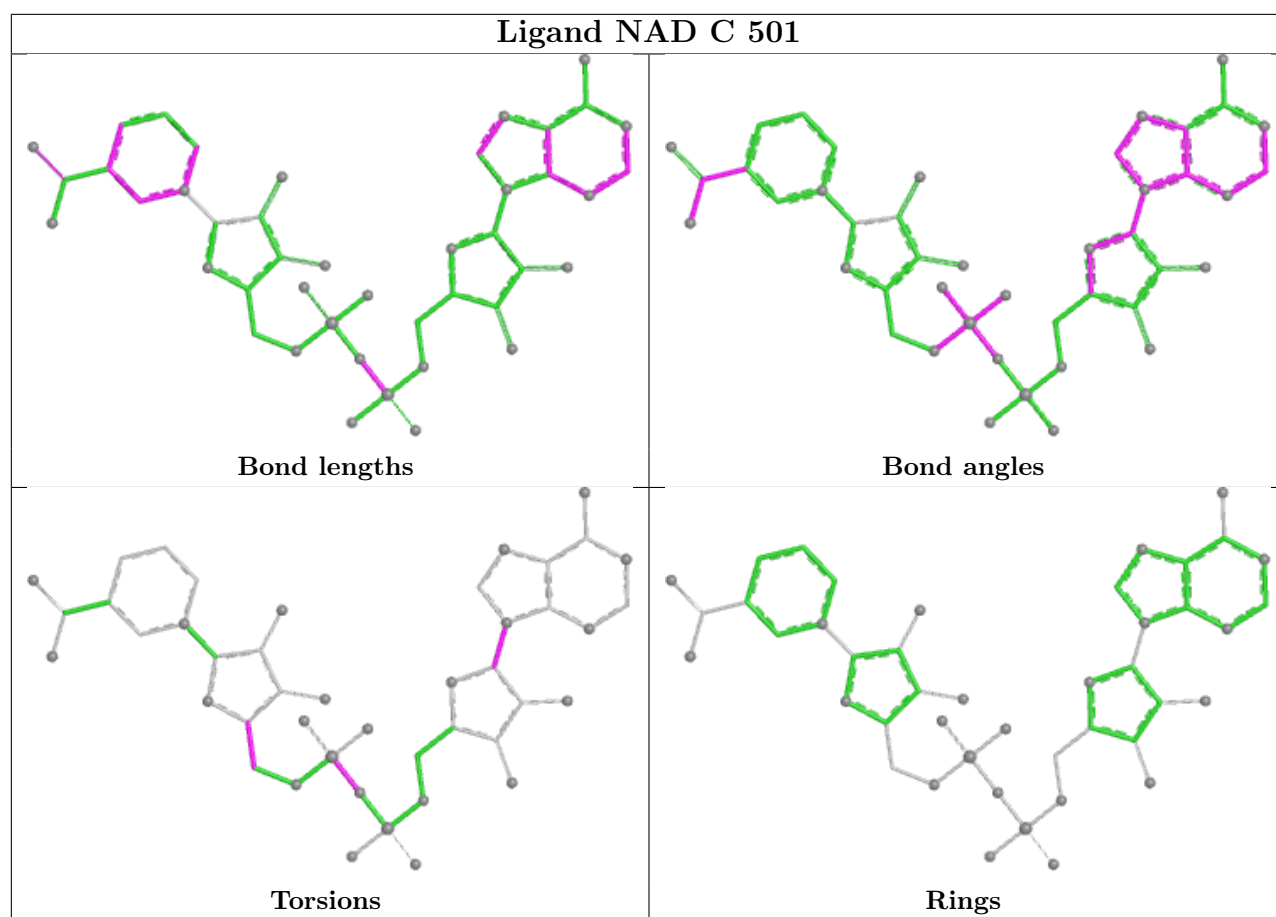
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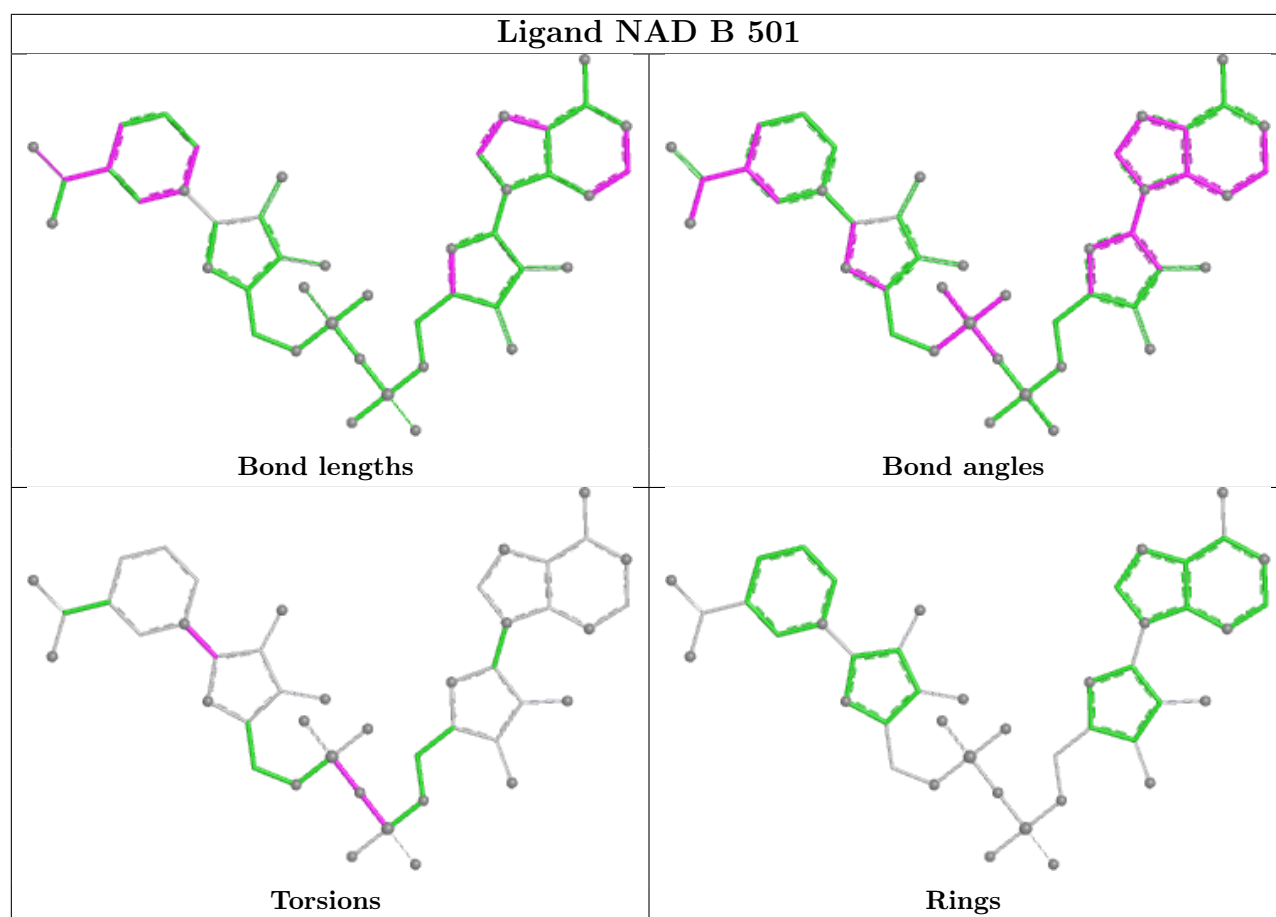
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAD	13	0

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	373/386 (96%)	0.05	6 (1%)	70 49	20, 51, 66, 75	2 (0%)
1	B	373/386 (96%)	0.02	5 (1%)	75 55	20, 52, 66, 75	2 (0%)
1	C	373/386 (96%)	0.07	4 (1%)	78 59	20, 54, 67, 77	2 (0%)
1	D	373/386 (96%)	0.10	3 (0%)	82 65	20, 54, 67, 76	2 (0%)
All	All	1492/1544 (96%)	0.06	18 (1%)	76 57	20, 53, 67, 77	8 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	PHE	12.0
1	C	100	PHE	11.6
1	A	100	PHE	10.0
1	B	100	PHE	9.9
1	B	351	GLU	4.8
1	C	351	GLU	4.5
1	A	351	GLU	4.3
1	A	376	ALA	4.2
1	C	376	ALA	4.1
1	B	376	ALA	3.9
1	D	351	GLU	3.9
1	D	376	ALA	3.1
1	A	225	LEU	2.7
1	A	328	LYS	2.5
1	B	6	LEU	2.5
1	C	218	GLU	2.3
1	A	359	ALA	2.2
1	B	283	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

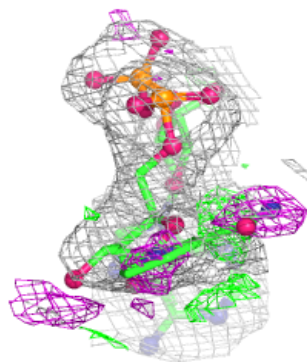
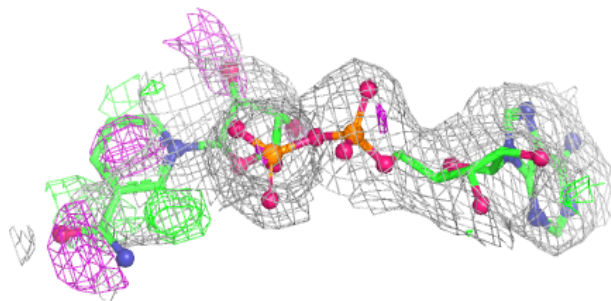
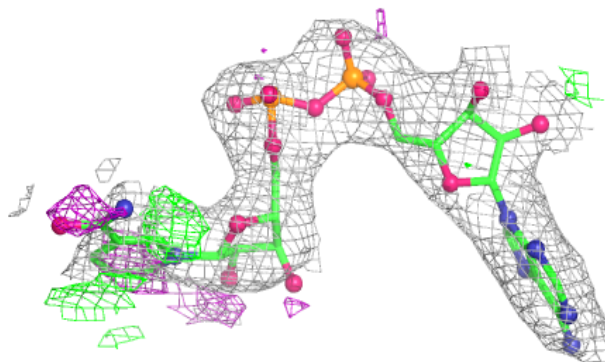
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	501	44/44	0.83	0.12	53,55,64,67	0
2	NAD	C	501	44/44	0.83	0.11	54,56,65,66	0
2	NAD	B	501	44/44	0.84	0.12	52,56,64,68	0
3	ZN	D	800	1/1	0.92	0.14	20,20,20,20	0

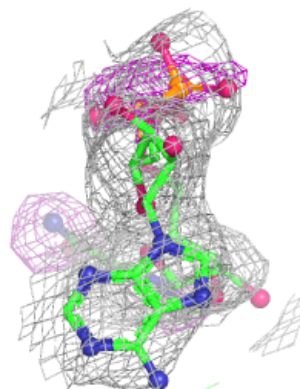
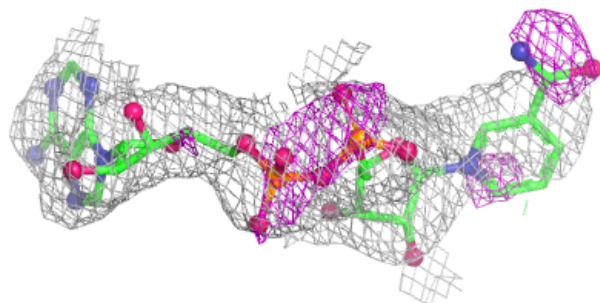
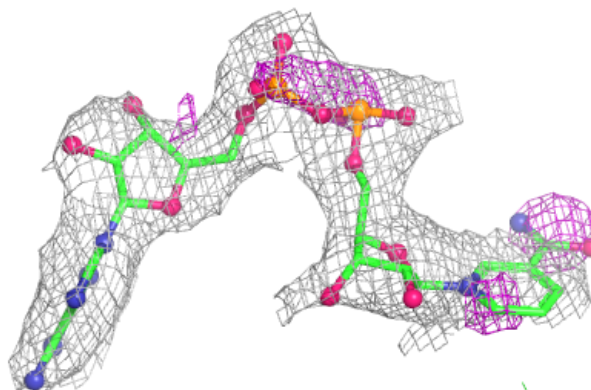
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 501:

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

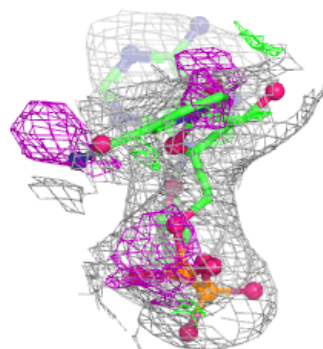
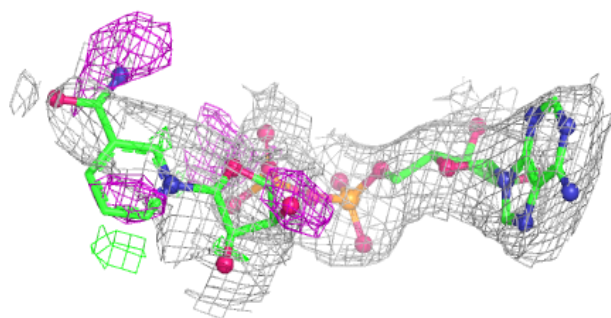
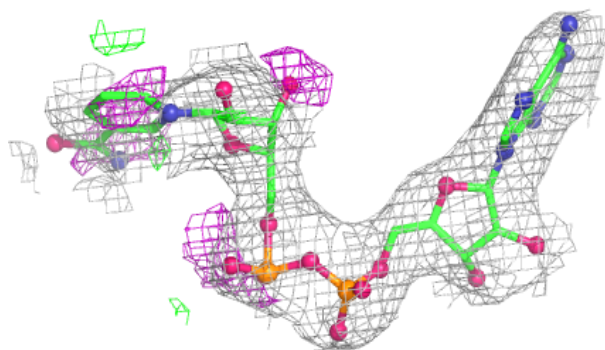
**Electron density around NAD C 501:**

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



Electron density around NAD B 501:

$2mF_o - DF_c$ (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.