



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 AM UTC

PDB ID : 1ORR / pdb_00001orr
Title : Crystal Structure of CDP-Tyvelose 2-Epimerase complexed with NAD and CDP
Authors : Koropatkin, N.M.; Liu, H.; Holden, H.M.
Deposited on : 2003-03-14
Resolution : 1.50 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

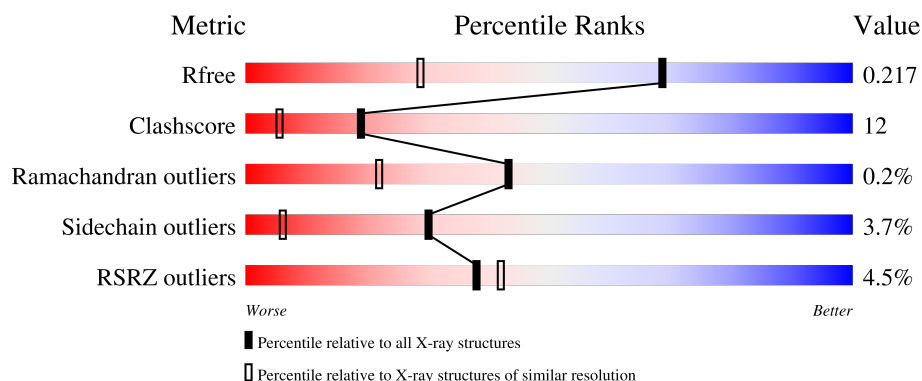
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	347	
1	B	347	
1	C	347	
1	D	347	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12059 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 CDP-tyvelose-2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	11	0
			2706	1712	458	520	16			
1	B	338	Total	C	N	O	S	0	4	0
			2676	1695	451	514	16			
1	C	335	Total	C	N	O	S	0	6	0
			2661	1686	448	511	16			
1	D	336	Total	C	N	O	S	0	5	0
			2661	1685	450	510	16			

There are 40 discrepancies between the modelled and reference sequences:

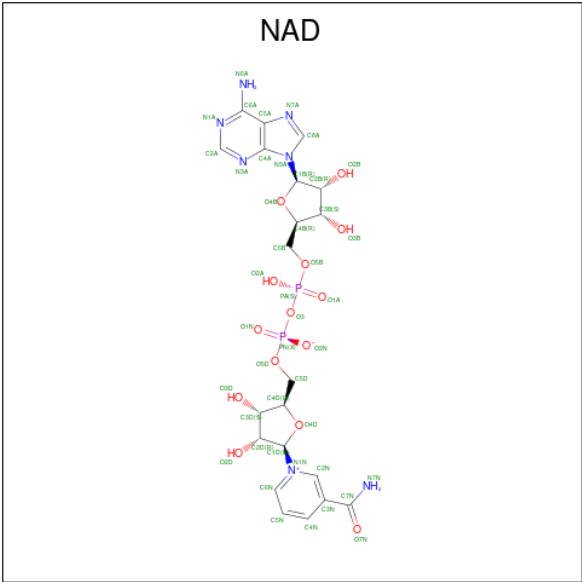
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P14169
A	2	ALA	-	cloning artifact	UNP P14169
A	340	LEU	-	expression tag	UNP P14169
A	341	GLU	-	expression tag	UNP P14169
A	342	HIS	-	expression tag	UNP P14169
A	343	HIS	-	expression tag	UNP P14169
A	344	HIS	-	expression tag	UNP P14169
A	345	HIS	-	expression tag	UNP P14169
A	346	HIS	-	expression tag	UNP P14169
A	347	HIS	-	expression tag	UNP P14169
B	1	MET	-	cloning artifact	UNP P14169
B	2	ALA	-	cloning artifact	UNP P14169
B	340	LEU	-	expression tag	UNP P14169
B	341	GLU	-	expression tag	UNP P14169
B	342	HIS	-	expression tag	UNP P14169
B	343	HIS	-	expression tag	UNP P14169
B	344	HIS	-	expression tag	UNP P14169
B	345	HIS	-	expression tag	UNP P14169
B	346	HIS	-	expression tag	UNP P14169
B	347	HIS	-	expression tag	UNP P14169
C	1	MET	-	cloning artifact	UNP P14169

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	cloning artifact	UNP P14169
C	340	LEU	-	expression tag	UNP P14169
C	341	GLU	-	expression tag	UNP P14169
C	342	HIS	-	expression tag	UNP P14169
C	343	HIS	-	expression tag	UNP P14169
C	344	HIS	-	expression tag	UNP P14169
C	345	HIS	-	expression tag	UNP P14169
C	346	HIS	-	expression tag	UNP P14169
C	347	HIS	-	expression tag	UNP P14169
D	1	MET	-	cloning artifact	UNP P14169
D	2	ALA	-	cloning artifact	UNP P14169
D	340	LEU	-	expression tag	UNP P14169
D	341	GLU	-	expression tag	UNP P14169
D	342	HIS	-	expression tag	UNP P14169
D	343	HIS	-	expression tag	UNP P14169
D	344	HIS	-	expression tag	UNP P14169
D	345	HIS	-	expression tag	UNP P14169
D	346	HIS	-	expression tag	UNP P14169
D	347	HIS	-	expression tag	UNP P14169

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



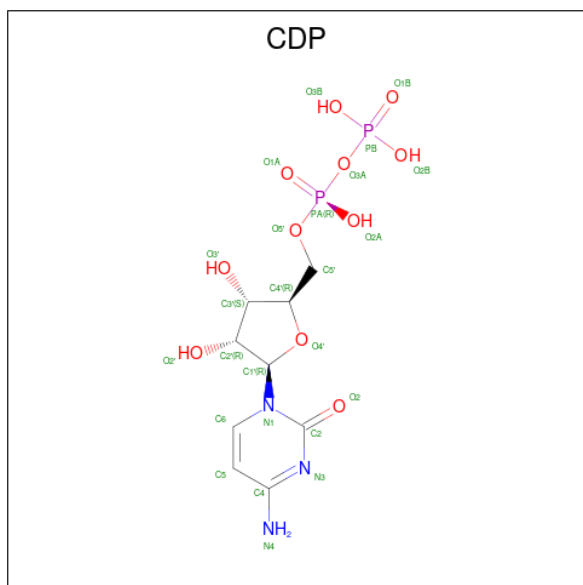
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			44	21	7	14	2	

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

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (CCD ID: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	310	Total O 310 310	0	0
4	B	277	Total O 277 277	0	0

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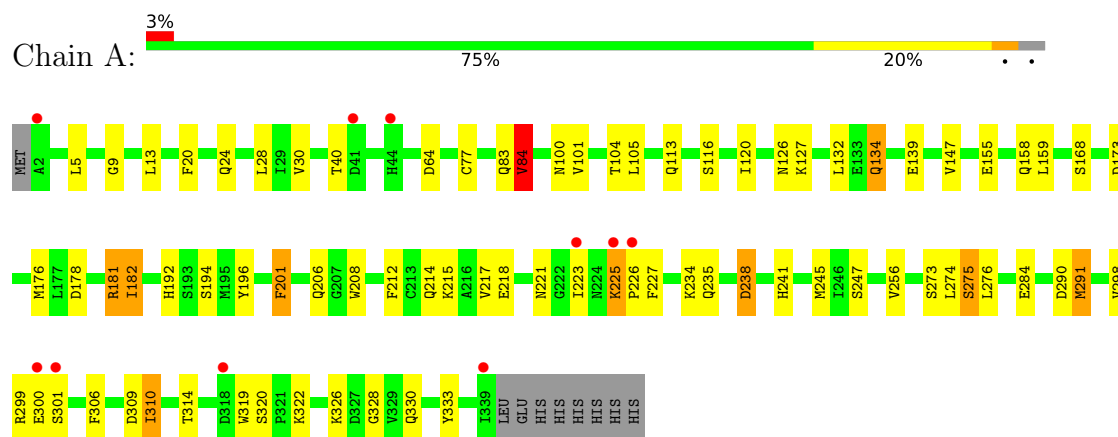
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	259	Total 259	O 259	0	0
4	D	233	Total 233	O 233	0	0

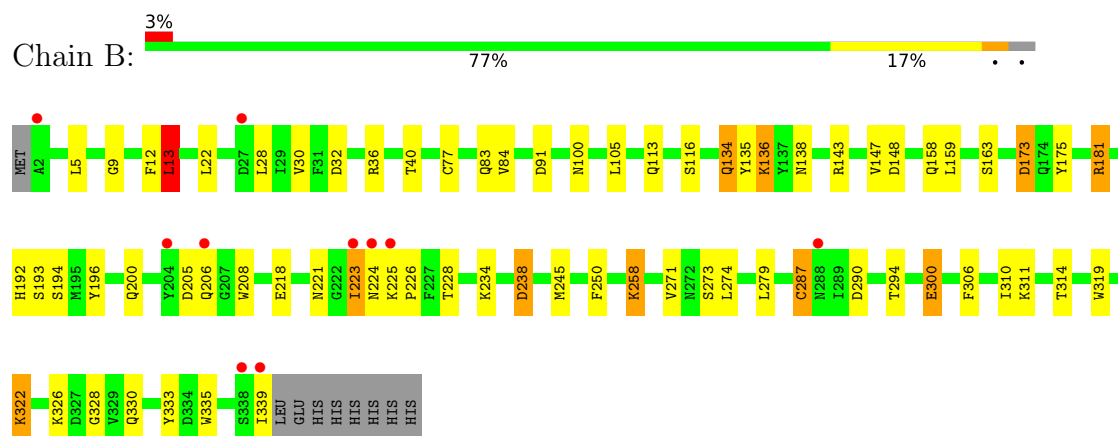
3 Residue-property plots

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.

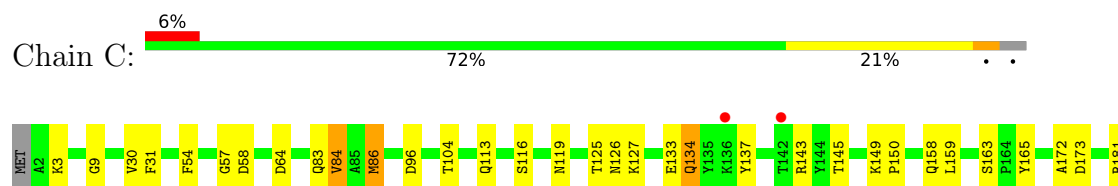
- Molecule 1: CDP-tyvelose-2-epimerase

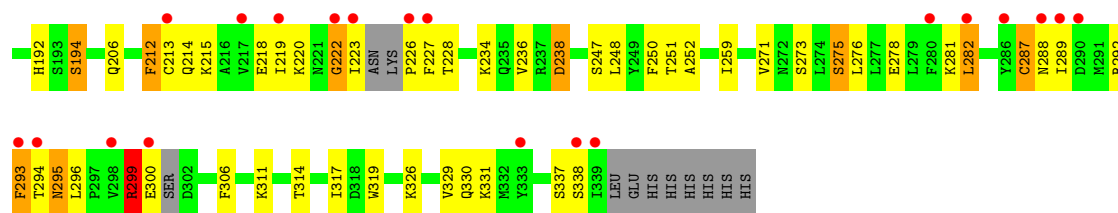


- Molecule 1: CDP-tyvelose-2-epimerase

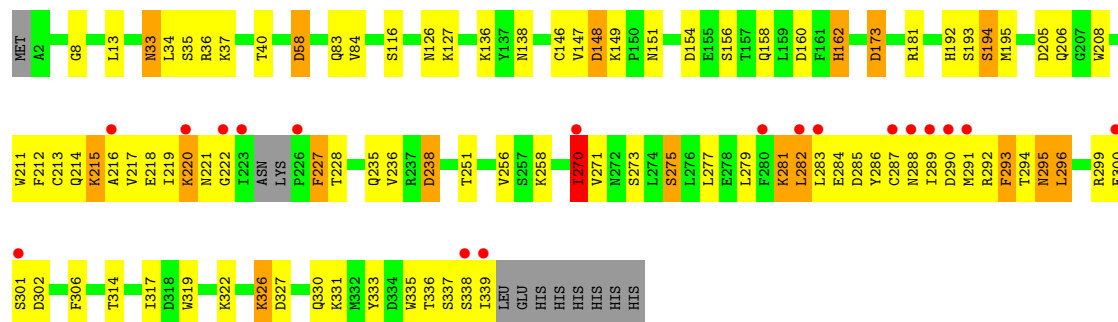


- Molecule 1: CDP-tyvelose-2-epimerase





● Molecule 1: CDP-tyvelose-2-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.00Å 168.10Å 89.60Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 30.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-1.50) 96.1 (30.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 1.46Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.178 , 0.229 (Not available) , 0.217	Depositor DCC
R_{free} test set	22493 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	0/2828	1.47	29/3830 (0.8%)
1	B	1.06	0/2761	1.48	31/3738 (0.8%)
1	C	1.04	2/2757 (0.1%)	1.50	25/3729 (0.7%)
1	D	1.08	1/2740 (0.0%)	1.50	29/3704 (0.8%)
All	All	1.06	3/11086 (0.0%)	1.49	114/15001 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	0
All	All	2	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	ASP	CG-OD2	5.50	1.35	1.25
1	D	58	ASP	CG-OD2	5.42	1.35	1.25
1	C	96	ASP	CG-OD2	5.02	1.34	1.25

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	PHE	N-CA-CB	8.92	124.81	110.90
1	D	293	PHE	CA-CB-CG	-8.64	105.16	113.80
1	D	116	SER	N-CA-C	8.51	123.09	112.87
1	C	306	PHE	N-CA-CB	8.37	123.96	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASP	CA-CB-CG	8.08	120.68	112.60
1	B	300	GLU	N-CA-CB	7.93	121.75	109.94
1	A	306	PHE	N-CA-CB	7.92	123.26	110.90
1	B	205	ASP	CA-CB-CG	7.92	120.52	112.60
1	B	287	CYS	CB-CA-C	-7.87	95.96	109.65
1	C	116	SER	N-CA-C	7.66	122.06	112.87
1	C	293	PHE	CA-CB-CG	-7.33	106.47	113.80
1	A	306	PHE	CA-CB-CG	-7.29	106.52	113.80
1	D	270	ILE	N-CA-C	7.25	117.97	110.36
1	D	306	PHE	N-CA-CB	7.20	123.40	110.95
1	C	306	PHE	CA-CB-CG	-7.19	106.61	113.80
1	C	194	SER	N-CA-C	7.16	120.33	110.24
1	D	173	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	83	GLN	N-CA-C	-7.11	97.14	108.73
1	C	181	ARG	CB-CA-C	-7.08	99.72	110.90
1	B	32	ASP	CA-CB-CG	6.91	119.51	112.60
1	D	275	SER	N-CA-C	-6.84	100.33	110.46
1	A	84[A]	VAL	N-CA-CB	-6.83	104.69	112.21
1	A	84[B]	VAL	N-CA-CB	-6.83	104.69	112.21
1	A	84[C]	VAL	N-CA-CB	-6.83	104.69	112.21
1	B	225	LYS	O-C-N	6.82	126.93	121.20
1	B	306	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	238	ASP	N-CA-C	-6.65	100.64	110.48
1	C	299	ARG	N-CA-CB	6.64	119.33	110.29
1	A	310	ILE	N-CA-C	6.61	117.80	111.91
1	A	147	VAL	N-CA-C	6.60	116.76	110.42
1	D	306	PHE	CA-CB-CG	-6.56	107.24	113.80
1	A	201	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	194	SER	N-CA-C	6.55	119.87	110.24
1	C	236	VAL	N-CA-C	6.54	118.02	108.53
1	C	299	ARG	N-CA-C	6.54	118.77	110.33
1	B	300	GLU	N-CA-C	6.53	118.94	111.11
1	D	327	ASP	CA-CB-CG	-6.47	106.12	112.60
1	B	238	ASP	N-CA-C	-6.45	100.94	110.48
1	A	116	SER	N-CA-C	6.38	120.17	112.38
1	A	227	PHE	N-CA-C	6.35	119.47	110.14
1	B	226	PRO	N-CA-CB	6.35	109.92	103.25
1	C	83	GLN	N-CA-C	-6.35	97.34	108.20
1	D	151	ASN	CA-CB-CG	6.35	118.95	112.60
1	D	333	TYR	CA-CB-CG	-6.34	102.49	113.90
1	D	8	GLY	N-CA-C	-6.30	105.19	114.90
1	D	83	GLN	N-CA-C	-6.25	97.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	VAL	N-CA-C	6.23	120.89	113.22
1	D	208	TRP	N-CA-C	6.22	117.73	111.07
1	D	238	ASP	N-CA-C	-6.22	101.28	110.48
1	D	194	SER	N-CA-C	6.17	118.93	110.24
1	D	192	HIS	CA-CB-CG	6.06	119.86	113.80
1	D	205	ASP	N-CA-C	6.02	120.35	112.89
1	A	173	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	119	ASN	CA-CB-CG	-5.96	106.64	112.60
1	B	13	LEU	CB-CA-C	-5.94	101.56	110.88
1	B	192	HIS	N-CA-C	5.79	119.68	109.96
1	C	275	SER	N-CA-C	-5.79	101.90	110.46
1	A	275	SER	N-CA-C	-5.78	102.22	110.59
1	B	113	GLN	N-CA-C	5.77	119.50	112.23
1	C	238	ASP	N-CA-C	-5.75	101.98	110.48
1	A	225	LYS	O-C-N	5.72	126.01	121.20
1	A	181	ARG	CB-CA-C	-5.71	101.88	110.90
1	A	192	HIS	N-CA-C	5.67	119.49	109.96
1	B	250	PHE	CA-CB-CG	-5.61	108.19	113.80
1	C	212	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	28	LEU	N-CA-C	5.57	118.48	109.40
1	B	181	ARG	CB-CA-C	-5.57	102.11	110.90
1	C	213	CYS	N-CA-C	-5.56	104.86	111.69
1	B	163	SER	N-CA-CB	5.53	120.22	110.37
1	A	212	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	259	ILE	N-CA-C	5.50	118.18	112.90
1	C	54	PHE	CA-CB-CG	-5.48	108.32	113.80
1	B	193	SER	N-CA-C	-5.44	101.95	110.17
1	C	329	VAL	N-CA-C	5.39	116.11	110.62
1	C	173	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	192	HIS	N-CA-C	5.36	118.67	110.20
1	D	193	SER	N-CA-C	-5.36	102.08	110.17
1	C	311	LYS	CB-CA-C	-5.35	102.24	110.81
1	C	250	PHE	CA-CB-CG	-5.35	108.45	113.80
1	B	274	LEU	CB-CA-C	-5.32	98.58	109.38
1	A	256	VAL	N-CA-C	5.32	116.68	110.62
1	C	86	MET	N-CA-CB	5.32	118.03	110.16
1	A	64	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	300	GLU	CB-CA-C	5.30	119.28	110.81
1	A	113	GLN	N-CA-C	5.28	118.88	112.23
1	D	146	CYS	N-CA-CB	5.28	118.21	110.35
1	D	295	ASN	CA-CB-CG	-5.27	107.33	112.60
1	B	194	SER	N-CA-C	5.27	117.98	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	HIS	CA-CB-CG	-5.25	108.56	113.80
1	B	224	ASN	CA-C-N	5.23	128.40	122.59
1	B	224	ASN	C-N-CA	5.23	128.40	122.59
1	B	100	ASN	N-CA-C	5.23	116.78	111.14
1	A	309	ASP	N-CA-C	-5.20	99.31	108.20
1	A	28	LEU	N-CA-C	5.20	118.03	109.72
1	B	290	ASP	N-CA-CB	5.19	118.75	110.65
1	D	227	PHE	N-CA-CB	5.18	118.75	110.46
1	D	258	LYS	CA-C-N	-5.17	115.53	122.72
1	D	258	LYS	C-N-CA	-5.17	115.53	122.72
1	B	83	GLN	N-CA-C	-5.16	99.37	108.20
1	A	290	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	116	SER	N-CA-C	5.14	119.04	112.87
1	A	182[A]	ILE	N-CA-C	5.14	115.80	110.82
1	A	182[B]	ILE	N-CA-C	5.14	115.80	110.82
1	D	236	VAL	N-CA-C	5.14	116.76	108.85
1	D	326	LYS	CA-C-O	5.11	125.96	120.55
1	D	327	ASP	N-CA-C	5.10	116.65	111.14
1	D	192	HIS	N-CA-C	5.09	118.25	110.20
1	C	192	HIS	CA-CB-CG	5.09	118.89	113.80
1	D	162	HIS	CA-CB-CG	-5.04	108.76	113.80
1	D	256	VAL	N-CA-C	5.04	116.36	110.62
1	B	91	ASP	CA-CB-CG	-5.03	107.57	112.60
1	B	138	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	274	LEU	CB-CA-C	-5.02	99.74	109.68
1	B	310	ILE	N-CA-C	5.00	119.75	109.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	300	GLU	CA
1	C	299	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2706	0	2639	72	0
1	B	2676	0	2612	52	0
1	C	2661	0	2592	71	0
1	D	2661	0	2584	70	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
2	C	44	0	26	3	0
2	D	44	0	26	1	0
3	A	25	0	12	0	0
3	B	25	0	12	0	0
3	C	25	0	12	1	0
3	D	25	0	12	1	0
4	A	310	0	0	12	0
4	B	277	0	0	5	0
4	C	259	0	0	4	0
4	D	233	0	0	6	0
All	All	12059	0	10579	254	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 12.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125[C]:THR:HG22	1:C:127:LYS:H	1.00	1.11
1:C:218:GLU:HA	1:C:223:ILE:HD12	1.34	1.05
1:C:218:GLU:HB3	1:C:223:ILE:HB	1.42	0.99
1:B:13:LEU:HD13	1:B:245:MET:HE2	1.46	0.95
1:B:134:GLN:HE21	1:B:134:GLN:H	1.14	0.94
1:C:125[C]:THR:HG22	1:C:127:LYS:N	1.85	0.90
1:C:134:GLN:H	1:C:134:GLN:HE21	1.13	0.90
1:A:134:GLN:H	1:A:134:GLN:HE21	1.18	0.89
1:C:218:GLU:CA	1:C:223:ILE:HD12	2.04	0.88
1:B:335:TRP:CZ2	1:B:339:ILE:HD11	2.09	0.86
1:C:295:ASN:N	1:C:295:ASN:HD22	1.77	0.83
1:D:314[A]:THR:HG22	1:D:319:TRP:O	1.82	0.80
1:D:326:LYS:O	1:D:330:GLN:HG3	1.82	0.79
1:C:125[C]:THR:CG2	1:C:127:LYS:H	1.92	0.78
1:A:310:ILE:O	1:A:314[C]:THR:HG22	1.83	0.78
1:B:13:LEU:CD1	1:B:245:MET:HE2	2.14	0.78
1:C:314[B]:THR:HG21	4:C:1644:HOH:O	1.84	0.78
1:C:314[B]:THR:HG22	1:C:319:TRP:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125[A]:THR:HG21	1:C:165:TYR:OH	1.86	0.76
1:C:214:GLN:O	1:C:218:GLU:HG3	1.87	0.75
1:D:314[A]:THR:HG21	4:D:1697:HOH:O	1.85	0.75
1:A:84[B]:VAL:HG13	4:A:1343:HOH:O	1.85	0.75
1:A:314[B]:THR:HG22	1:A:319:TRP:O	1.85	0.75
1:C:326:LYS:O	1:C:330:GLN:HG3	1.88	0.73
1:C:282:LEU:HD21	1:C:326:LYS:HA	1.70	0.73
1:C:134:GLN:HE21	1:C:134:GLN:N	1.86	0.72
1:A:238:ASP:HA	1:A:273:SER:HA	1.73	0.71
1:C:295:ASN:N	1:C:295:ASN:ND2	2.38	0.71
1:C:3[B]:LYS:HE3	4:C:1415:HOH:O	1.90	0.70
1:B:13:LEU:HD22	1:B:245:MET:CE	2.20	0.70
1:A:158[B]:GLN:HE21	1:A:159:LEU:H	1.40	0.70
1:A:314[C]:THR:HG23	4:A:1442:HOH:O	1.89	0.70
1:B:326:LYS:O	1:B:330:GLN:HG3	1.91	0.70
1:A:221:ASN:HB2	1:A:223:ILE:CD1	2.22	0.69
1:D:136:LYS:HD2	1:D:148:ASP:OD1	1.92	0.69
1:A:158[B]:GLN:HE22	1:C:159:LEU:H	1.40	0.69
1:A:218:GLU:HA	1:A:223:ILE:HD13	1.76	0.68
1:B:22:LEU:HD23	4:B:1391:HOH:O	1.94	0.68
1:C:134:GLN:H	1:C:134:GLN:NE2	1.90	0.67
1:C:226:PRO:HA	1:C:292:ARG:O	1.93	0.67
1:A:223:ILE:HG22	1:A:225:LYS:HG3	1.77	0.67
1:A:215:LYS:HE2	1:A:215:LYS:HA	1.77	0.66
1:B:314:THR:HG22	1:B:319:TRP:O	1.95	0.66
1:B:322:LYS:HD2	4:B:1572:HOH:O	1.95	0.66
1:A:226:PRO:HB3	4:A:1458:HOH:O	1.94	0.66
1:D:284:GLU:O	1:D:288:ASN:N	2.29	0.66
1:D:279:LEU:O	1:D:283:LEU:HD23	1.95	0.66
1:A:84[B]:VAL:HG22	2:A:1200:NAD:C2D	2.27	0.65
1:C:251[A]:THR:HG23	1:C:317:ILE:HD12	1.77	0.65
1:C:299:ARG:NH2	3:C:1401:CDP:O2A	2.29	0.65
1:D:289:ILE:HG22	1:D:290:ASP:N	2.12	0.65
1:B:36:ARG:NH2	1:B:206:GLN:HG3	2.11	0.64
1:A:320:SER:OG	1:A:322:LYS:NZ	2.30	0.64
1:C:143:ARG:HA	1:C:234:LYS:HB3	1.79	0.64
1:C:212:PHE:CE1	1:C:276[B]:LEU:HD21	2.33	0.64
1:B:12:PHE:CD1	1:B:200:GLN:HB2	2.33	0.64
1:B:221:ASN:HB2	1:B:223:ILE:CD1	2.28	0.64
1:C:125[A]:THR:HG22	2:C:1400:NAD:H5N	1.79	0.63
1:A:314[B]:THR:HG21	4:A:1446:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:CG	1:B:245:MET:HE2	2.28	0.63
1:B:13:LEU:HD22	1:B:245:MET:HE2	1.79	0.62
1:A:182[B]:ILE:CD1	1:C:163:SER:HA	2.29	0.62
1:D:219:ILE:O	1:D:222:GLY:N	2.32	0.62
1:A:182[B]:ILE:HD13	1:C:163:SER:HA	1.80	0.62
1:D:211:TRP:O	1:D:214:GLN:HB3	1.98	0.62
1:D:289:ILE:HG22	1:D:290:ASP:H	1.66	0.61
1:D:238:ASP:HA	1:D:273:SER:HA	1.82	0.61
1:D:214:GLN:HG2	4:D:1716:HOH:O	2.01	0.61
1:B:135:TYR:HB3	1:B:148:ASP:OD1	2.01	0.60
1:D:299:ARG:HD2	3:D:1501:CDP:O2'	2.01	0.60
1:D:213:CYS:O	1:D:216:ALA:HB3	2.01	0.60
1:D:36:ARG:HD3	2:D:1500:NAD:O1A	2.02	0.60
1:B:134:GLN:H	1:B:134:GLN:NE2	1.94	0.60
1:C:275:SER:OG	1:C:278:GLU:HG3	2.02	0.59
1:A:221:ASN:HB2	1:A:223:ILE:HD11	1.83	0.59
1:A:139:GLU:OE2	1:A:234:LYS:NZ	2.30	0.58
1:B:135:TYR:C	1:B:136:LYS:HE3	2.27	0.58
1:B:181:ARG:HD2	4:B:1521:HOH:O	2.03	0.58
1:B:238:ASP:HA	1:B:273:SER:HA	1.85	0.58
1:C:220:LYS:NZ	1:C:287:CYS:O	2.30	0.58
1:A:158[B]:GLN:NE2	1:C:158[B]:GLN:OE1	2.37	0.58
1:D:127:LYS:HE3	4:D:1663:HOH:O	2.04	0.58
1:D:287:CYS:O	1:D:289:ILE:HG13	2.04	0.58
1:D:162:HIS:HB2	4:D:1649:HOH:O	2.03	0.58
1:A:84[A]:VAL:HG22	4:A:1319:HOH:O	2.04	0.57
1:D:214:GLN:O	1:D:218:GLU:HG3	2.04	0.57
1:B:258:LYS:O	1:B:258:LYS:HG2	2.03	0.57
1:A:314[C]:THR:HG21	4:A:1446:HOH:O	2.03	0.57
1:C:228:THR:HG22	1:C:294:THR:OG1	2.04	0.56
1:C:84:VAL:HG23	1:C:206:GLN:HG3	1.88	0.56
1:B:134:GLN:HE21	1:B:134:GLN:N	1.96	0.56
1:C:125[A]:THR:HG22	2:C:1400:NAD:C5N	2.35	0.56
1:C:218:GLU:HB3	1:C:223:ILE:CB	2.27	0.56
1:C:113:GLN:NE2	4:C:1529:HOH:O	2.39	0.55
1:D:335:TRP:CH2	1:D:339:ILE:HD11	2.41	0.55
1:D:228:THR:HG22	1:D:294:THR:HG1	1.72	0.55
1:D:220:LYS:C	1:D:222:GLY:H	2.14	0.55
1:A:158[B]:GLN:HE21	1:A:159:LEU:N	2.05	0.54
1:C:247:SER:O	1:C:251[A]:THR:HG22	2.08	0.54
1:A:223:ILE:HG21	1:A:225:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASN:HB2	1:B:223:ILE:HD11	1.90	0.54
1:D:228:THR:HG22	1:D:294:THR:OG1	2.08	0.54
1:A:223:ILE:CG2	1:A:225:LYS:HD2	2.37	0.54
1:C:228:THR:HB	1:C:296:LEU:HG	1.89	0.54
1:B:13:LEU:CD2	1:B:245:MET:HE2	2.37	0.54
1:A:9:GLY:HA3	1:A:30:VAL:HG13	1.90	0.53
1:D:212:PHE:O	1:D:215:LYS:HB2	2.09	0.53
1:A:84[B]:VAL:HG22	2:A:1200:NAD:H2D	1.90	0.53
1:A:84[C]:VAL:HG13	4:A:1319:HOH:O	2.07	0.53
1:D:335:TRP:CZ2	1:D:339:ILE:HD11	2.44	0.53
1:D:219:ILE:HG22	1:D:220:LYS:N	2.24	0.53
1:A:182[A]:ILE:HG23	1:C:300:GLU:OE1	2.09	0.52
1:C:125[C]:THR:CG2	1:C:127:LYS:HG2	2.39	0.52
1:C:287:CYS:O	1:C:288:ASN:C	2.51	0.52
1:A:126[C]:ASN:HD21	1:A:127:LYS:NZ	2.07	0.52
1:B:12:PHE:CD2	1:B:13:LEU:HD23	2.44	0.52
1:A:214:GLN:HG2	4:A:1462:HOH:O	2.08	0.52
1:C:227:PHE:CE1	1:C:293:PHE:HB3	2.45	0.51
1:D:214:GLN:OE1	1:D:214:GLN:HA	2.09	0.51
1:B:218:GLU:O	1:B:223:ILE:HD12	2.10	0.51
1:D:37:LYS:HE3	4:D:1623:HOH:O	2.10	0.51
1:A:84[C]:VAL:HG23	4:A:1343:HOH:O	2.10	0.51
1:C:9:GLY:HA3	1:C:30:VAL:HG13	1.93	0.51
1:D:283:LEU:O	1:D:287:CYS:N	2.42	0.51
1:A:13:LEU:HG	1:A:245:MET:HE2	1.93	0.51
1:C:126:ASN:H	1:C:126:ASN:HD22	1.58	0.51
1:B:136:LYS:HE3	1:B:136:LYS:N	2.25	0.51
1:B:158:GLN:HA	1:D:158[A]:GLN:OE1	2.11	0.51
1:B:36:ARG:HH22	1:B:206:GLN:HG3	1.75	0.50
1:A:300:GLU:HG2	4:C:1609:HOH:O	2.11	0.50
1:A:134:GLN:H	1:A:134:GLN:NE2	1.97	0.50
1:A:298:VAL:HG22	1:A:299:ARG:N	2.27	0.50
1:C:295:ASN:C	1:C:296:LEU:HD23	2.36	0.50
1:B:158:GLN:OE1	1:D:158[B]:GLN:OE1	2.29	0.50
1:B:13:LEU:HD22	1:B:245:MET:HE3	1.93	0.49
1:C:222:GLY:C	1:C:223:ILE:HG13	2.37	0.49
1:A:100:ASN:HB2	1:A:168:SER:HB2	1.93	0.49
1:A:206:GLN:NE2	4:A:1318:HOH:O	2.45	0.49
1:D:217:VAL:HG21	1:D:336:THR:HG22	1.93	0.49
1:C:125[A]:THR:HG23	2:C:1400:NAD:H6N	1.95	0.49
1:A:134:GLN:HE21	1:A:134:GLN:N	1.98	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HE2	1:A:215:LYS:CA	2.43	0.49
1:A:235:GLN:O	1:A:275:SER:HA	2.13	0.49
1:B:143:ARG:HA	1:B:234:LYS:HB3	1.96	0.48
1:C:248:LEU:O	1:C:251[A]:THR:HG22	2.14	0.48
1:B:228:THR:HG22	1:B:294[C]:THR:CG2	2.44	0.48
1:D:289:ILE:CG2	1:D:290:ASP:H	2.27	0.48
1:A:20:PHE:CE2	1:A:24:GLN:HG3	2.49	0.48
1:C:86:MET:O	1:C:86:MET:HG2	2.09	0.48
1:D:289:ILE:CG2	1:D:290:ASP:N	2.77	0.48
1:C:58:ASP:OD2	1:D:58:ASP:OD2	2.32	0.47
1:C:251[A]:THR:HG23	1:C:252:ALA:N	2.30	0.47
1:A:84[B]:VAL:CG2	2:A:1200:NAD:H2D	2.44	0.47
1:A:20:PHE:CZ	1:A:24:GLN:HG3	2.49	0.47
1:D:138:ASN:ND2	1:D:147:VAL:HG22	2.29	0.47
1:A:104:THR:HG23	1:A:176:MET:HE2	1.95	0.47
1:A:178:ASP:OD2	1:A:182[B]:ILE:HD13	2.15	0.47
1:A:218:GLU:O	1:A:223:ILE:HD12	2.15	0.47
1:D:288:ASN:C	1:D:289:ILE:HG13	2.40	0.47
1:D:251:THR:HG22	1:D:317:ILE:HD12	1.96	0.46
1:B:13:LEU:CA	1:B:245:MET:HE1	2.46	0.46
1:B:84:VAL:HG12	1:B:84:VAL:O	2.14	0.46
1:B:105:LEU:HD21	1:B:175:TYR:CD1	2.51	0.46
1:B:221:ASN:CB	1:B:223:ILE:HD11	2.45	0.46
1:A:158[A]:GLN:HE22	1:C:159:LEU:H	1.62	0.46
1:D:215:LYS:CA	1:D:215:LYS:HE2	2.45	0.46
1:D:148:ASP:C	1:D:149:LYS:HG2	2.40	0.46
1:A:208:TRP:CZ3	1:A:276:LEU:CD2	2.99	0.46
1:D:84:VAL:HG23	1:D:206:GLN:HG3	1.97	0.46
1:A:84[A]:VAL:CG2	1:A:206:GLN:NE2	2.79	0.46
1:D:215:LYS:HE2	1:D:215:LYS:N	2.31	0.46
1:A:84[A]:VAL:HG21	1:A:206:GLN:CD	2.41	0.46
1:A:159:LEU:H	1:C:158[A]:GLN:HE22	1.63	0.45
1:B:287:CYS:SG	1:B:333:TYR:CE1	3.09	0.45
1:C:149:LYS:HA	1:C:150:PRO:HD2	1.68	0.45
1:C:218:GLU:CB	1:C:223:ILE:HB	2.30	0.45
1:B:13:LEU:HA	1:B:245:MET:HE1	1.99	0.45
1:D:13:LEU:HD21	1:D:195:MET:HE1	1.99	0.45
1:D:160:ASP:CG	1:D:162:HIS:HE2	2.25	0.45
1:D:270:ILE:O	1:D:270:ILE:HG13	2.17	0.45
1:D:284:GLU:OE2	1:D:291:MET:N	2.34	0.45
1:B:12:PHE:CG	1:B:200:GLN:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:THR:HG22	1:B:294[C]:THR:HG22	1.99	0.45
1:A:291:MET:HE3	1:A:291:MET:HB3	1.92	0.44
1:C:133:GLU:OE1	1:C:133:GLU:HA	2.16	0.44
1:C:212:PHE:CE1	1:C:276[B]:LEU:CD2	2.99	0.44
1:A:40:THR:HG23	4:A:1222:HOH:O	2.17	0.44
1:A:126[C]:ASN:HD21	1:A:127:LYS:HZ2	1.64	0.44
1:C:125[C]:THR:HG21	1:C:165:TYR:HE2	1.82	0.44
1:D:126:ASN:H	1:D:126:ASN:ND2	2.16	0.44
1:D:126:ASN:H	1:D:126:ASN:HD22	1.65	0.44
1:D:228:THR:HB	1:D:296:LEU:HD22	2.00	0.44
1:D:285:ASP:O	1:D:286:TYR:C	2.58	0.44
1:D:295:ASN:C	1:D:296:LEU:HD13	2.43	0.44
1:B:9:GLY:HA3	1:B:30:VAL:HG13	2.00	0.44
1:D:227:PHE:CE1	1:D:293:PHE:HB3	2.53	0.44
1:C:31:PHE:CE1	1:C:57:GLY:HA3	2.53	0.43
1:A:84[B]:VAL:HG22	2:A:1200:NAD:O2D	2.18	0.43
1:A:217:VAL:CG2	1:A:333:TYR:CE1	3.01	0.43
1:D:138:ASN:ND2	1:D:147:VAL:CG2	2.81	0.43
1:D:283:LEU:N	1:D:283:LEU:HD22	2.33	0.43
1:D:300:GLU:C	1:D:302:ASP:H	2.26	0.43
1:D:235:GLN:O	1:D:275:SER:HA	2.18	0.43
1:D:33:ASN:ND2	1:D:35:SER:H	2.16	0.43
1:B:13:LEU:HA	1:B:245:MET:CE	2.48	0.43
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.83	0.43
1:B:40:THR:HG23	4:B:1317:HOH:O	2.19	0.42
1:A:201:PHE:HD1	4:A:1306:HOH:O	2.02	0.42
1:C:215:LYS:HE2	1:C:215:LYS:HA	2.02	0.42
1:C:215:LYS:HE2	1:C:215:LYS:N	2.34	0.42
1:A:225:LYS:N	1:A:226:PRO:HD3	2.35	0.42
1:C:215:LYS:HE2	1:C:215:LYS:CA	2.50	0.42
1:D:281:LYS:O	1:D:282:LEU:C	2.62	0.42
1:A:5:LEU:O	1:A:77:CYS:HA	2.20	0.42
1:D:154:ASP:OD1	1:D:156:SER:OG	2.37	0.42
1:B:208:TRP:CZ3	1:B:279:LEU:HD22	2.54	0.42
1:B:221:ASN:CB	1:B:223:ILE:CD1	2.98	0.42
1:A:326:LYS:O	1:A:330:GLN:HG3	2.19	0.42
1:C:137:TYR:HA	1:C:145:THR:O	2.20	0.42
1:D:220:LYS:C	1:D:222:GLY:N	2.77	0.41
1:D:295:ASN:OD1	1:D:295:ASN:N	2.53	0.41
1:A:217:VAL:HG22	1:A:333:TYR:CE1	2.56	0.41
1:D:34:LEU:HD13	1:D:40:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ILE:O	1:D:220:LYS:C	2.63	0.41
1:D:335:TRP:CZ3	1:D:339:ILE:HD11	2.55	0.41
1:A:284:GLU:HG3	1:A:291:MET:HG3	2.03	0.41
1:B:221:ASN:HB2	1:B:223:ILE:HD12	1.99	0.41
1:A:120:ILE:HD13	1:A:120:ILE:HG21	1.85	0.41
1:B:196:TYR:OH	1:B:328:GLY:HA3	2.20	0.41
1:A:101:VAL:O	1:A:105:LEU:HD23	2.21	0.41
1:B:13:LEU:CB	1:B:245:MET:HE2	2.50	0.41
1:C:219:ILE:HG21	1:C:289:ILE:HD12	2.03	0.41
1:D:277:LEU:HD23	1:D:277:LEU:HA	1.75	0.41
1:D:282:LEU:HD12	1:D:282:LEU:HA	1.86	0.41
1:C:293:PHE:CD1	1:C:293:PHE:C	2.99	0.41
1:A:155:GLU:H	1:A:155:GLU:CD	2.29	0.40
1:C:104:THR:HG21	1:C:172:ALA:HB1	2.03	0.40
1:D:13:LEU:HD11	1:D:195:MET:HE3	2.03	0.40
1:D:219:ILE:C	1:D:221:ASN:N	2.79	0.40
1:D:292:ARG:HA	4:D:1694:HOH:O	2.21	0.40
1:A:182[B]:ILE:HD11	1:C:163:SER:HA	2.02	0.40
1:C:126:ASN:H	1:C:126:ASN:ND2	2.19	0.40
1:C:247:SER:O	1:C:251[C]:THR:HG23	2.21	0.40
1:A:196:TYR:OH	1:A:328:GLY:HA3	2.21	0.40
1:C:238:ASP:HA	1:C:273:SER:HA	2.03	0.40
1:A:105:LEU:HD13	1:A:105:LEU:HA	1.88	0.40
1:B:311:LYS:NZ	4:B:1378:HOH:O	2.51	0.40
1:A:132:LEU:HA	1:A:134:GLN:NE2	2.36	0.40
1:B:5:LEU:O	1:B:77:CYS:HA	2.21	0.40
1:B:13:LEU:CB	1:B:245:MET:CE	2.99	0.40
1:C:294:THR:C	1:C:295:ASN:ND2	2.80	0.40
1:D:283:LEU:O	1:D:287:CYS:SG	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/347 (101%)	339 (97%)	11 (3%)	0	100	100
1	B	342/347 (99%)	332 (97%)	10 (3%)	0	100	100
1	C	337/347 (97%)	325 (96%)	11 (3%)	1 (0%)	36	17
1	D	337/347 (97%)	319 (95%)	17 (5%)	1 (0%)	36	17
All	All	1366/1388 (98%)	1315 (96%)	49 (4%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	GLY
1	D	301	SER

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	306/301 (102%)	297 (97%)	9 (3%)	37	10
1	B	298/301 (99%)	286 (96%)	12 (4%)	28	5
1	C	297/301 (99%)	286 (96%)	11 (4%)	30	6
1	D	294/301 (98%)	277 (94%)	17 (6%)	18	2
All	All	1195/1204 (99%)	1146 (96%)	49 (4%)	30	5

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84[A]	VAL
1	A	84[B]	VAL
1	A	84[C]	VAL
1	A	134	GLN
1	A	181	ARG
1	A	247[A]	SER
1	A	247[B]	SER
1	A	291	MET
1	A	301	SER

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Mol	Chain	Res	Type
1	B	13	LEU
1	B	134	GLN
1	B	136	LYS
1	B	147	VAL
1	B	173	ASP
1	B	223	ILE
1	B	258	LYS
1	B	271[A]	VAL
1	B	271[B]	VAL
1	B	271[C]	VAL
1	B	300	GLU
1	B	322	LYS
1	C	134	GLN
1	C	194	SER
1	C	271	VAL
1	C	281	LYS
1	C	282	LEU
1	C	287	CYS
1	C	295	ASN
1	C	299	ARG
1	C	331	LYS
1	C	337	SER
1	C	338	SER
1	D	33	ASN
1	D	148	ASP
1	D	173	ASP
1	D	181	ARG
1	D	194	SER
1	D	215	LYS
1	D	220	LYS
1	D	270	ILE
1	D	271	VAL
1	D	281	LYS
1	D	282	LEU
1	D	296	LEU
1	D	322[A]	LYS
1	D	322[B]	LYS
1	D	331	LYS
1	D	337	SER
1	D	338	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	113	GLN
1	A	134	GLN
1	A	200	GLN
1	A	206	GLN
1	A	214	GLN
1	A	330	GLN
1	B	63	ASN
1	B	113	GLN
1	B	134	GLN
1	B	138	ASN
1	B	200	GLN
1	B	206	GLN
1	B	330	GLN
1	C	44	HIS
1	C	63	ASN
1	C	113	GLN
1	C	126	ASN
1	C	134	GLN
1	C	295	ASN
1	D	33	ASN
1	D	63	ASN
1	D	113	GLN
1	D	126	ASN
1	D	138	ASN
1	D	255	ASN
1	D	265	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	1400	-	46,48,48	2.20	9 (19%)	64,73,73	1.44	5 (7%)
2	NAD	B	1300	-	46,48,48	2.08	9 (19%)	64,73,73	1.64	6 (9%)
2	NAD	A	1200	-	46,48,48	1.97	10 (21%)	64,73,73	1.79	5 (7%)
3	CDP	A	1201	-	25,26,26	2.04	4 (16%)	38,40,40	1.35	6 (15%)
3	CDP	C	1401	-	25,26,26	1.86	4 (16%)	38,40,40	1.27	5 (13%)
3	CDP	D	1501	-	25,26,26	2.13	4 (16%)	38,40,40	1.35	5 (13%)
3	CDP	B	1301	-	25,26,26	1.55	4 (16%)	38,40,40	1.35	5 (13%)
2	NAD	D	1500	-	46,48,48	2.13	8 (17%)	64,73,73	1.41	5 (7%)

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	C	1400	-	-	3/30/62/62	0/5/5/5
2	NAD	B	1300	-	-	5/30/62/62	0/5/5/5
2	NAD	A	1200	-	-	3/30/62/62	0/5/5/5
3	CDP	A	1201	-	-	0/16/32/32	0/2/2/2
3	CDP	C	1401	-	-	1/16/32/32	0/2/2/2
3	CDP	D	1501	-	-	0/16/32/32	0/2/2/2
3	CDP	B	1301	-	-	0/16/32/32	0/2/2/2
2	NAD	D	1500	-	-	0/30/62/62	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1501	CDP	PA-O3A	8.21	1.68	1.59
2	C	1400	NAD	C4N-C3N	7.77	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	CDP	PA-O3A	7.71	1.67	1.59
2	D	1500	NAD	C4N-C3N	7.51	1.50	1.39
2	D	1500	NAD	C5N-C4N	6.81	1.50	1.38
2	C	1400	NAD	C5N-C4N	6.69	1.50	1.38
2	B	1300	NAD	C5N-C4N	6.55	1.50	1.38
3	C	1401	CDP	PA-O3A	6.30	1.66	1.59
2	C	1400	NAD	C2N-C3N	6.19	1.48	1.39
2	A	1200	NAD	C4N-C3N	6.10	1.48	1.39
2	A	1200	NAD	C5N-C4N	6.06	1.49	1.38
2	B	1300	NAD	C4N-C3N	5.88	1.48	1.39
2	D	1500	NAD	PN-O3	5.10	1.65	1.59
2	A	1200	NAD	C2N-C3N	5.00	1.46	1.39
2	D	1500	NAD	C2N-C3N	4.90	1.46	1.39
2	B	1300	NAD	C2N-C3N	4.90	1.46	1.39
2	B	1300	NAD	PA-O3	-4.72	1.54	1.59
3	B	1301	CDP	PA-O3A	4.45	1.64	1.59
2	B	1300	NAD	C3N-C7N	-4.34	1.44	1.50
2	C	1400	NAD	PN-O3	4.25	1.64	1.59
3	A	1201	CDP	C4-N4	3.62	1.42	1.33
3	A	1201	CDP	PB-O1B	3.62	1.61	1.50
3	D	1501	CDP	PB-O1B	3.59	1.61	1.50
3	C	1401	CDP	C4-N4	3.59	1.42	1.33
2	A	1200	NAD	PN-O3	3.57	1.63	1.59
3	D	1501	CDP	C4-N4	3.55	1.42	1.33
3	B	1301	CDP	C4-N4	3.40	1.42	1.33
2	A	1200	NAD	C2N-N1N	3.40	1.38	1.35
2	A	1200	NAD	C3N-C7N	-3.34	1.45	1.50
2	C	1400	NAD	C6N-N1N	3.29	1.42	1.35
3	B	1301	CDP	PB-O1B	3.24	1.60	1.50
3	C	1401	CDP	PB-O1B	3.20	1.60	1.50
2	D	1500	NAD	C6N-C5N	-3.08	1.32	1.38
2	D	1500	NAD	C6N-N1N	3.03	1.42	1.35
2	C	1400	NAD	C6N-C5N	-2.83	1.32	1.38
2	B	1300	NAD	C6N-C5N	-2.77	1.32	1.38
2	A	1200	NAD	C8A-N7A	2.66	1.36	1.31
2	B	1300	NAD	C6N-N1N	2.65	1.41	1.35
2	A	1200	NAD	C6N-C5N	-2.65	1.33	1.38
2	D	1500	NAD	C2N-N1N	2.58	1.37	1.35
2	D	1500	NAD	PA-O3	-2.54	1.56	1.59
2	C	1400	NAD	C2A-N1A	2.51	1.38	1.33
3	A	1201	CDP	C4-N3	2.45	1.39	1.34
3	C	1401	CDP	C4-N3	2.45	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1300	NAD	C2N-N1N	2.42	1.37	1.35
2	C	1400	NAD	PA-O3	-2.37	1.56	1.59
2	B	1300	NAD	C8A-N7A	2.34	1.36	1.31
2	A	1200	NAD	C6N-N1N	2.27	1.40	1.35
3	B	1301	CDP	C4-N3	2.20	1.39	1.34
2	C	1400	NAD	C3N-C7N	-2.20	1.47	1.50
3	D	1501	CDP	C4-N3	2.13	1.38	1.34
2	A	1200	NAD	O4B-C1B	-2.10	1.37	1.42

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1200	NAD	C5N-C4N-C3N	-10.54	110.01	120.36
2	B	1300	NAD	C5N-C4N-C3N	-8.33	112.18	120.36
2	C	1400	NAD	C5N-C4N-C3N	-8.05	112.45	120.36
2	D	1500	NAD	C3N-C7N-N7N	6.13	125.29	117.74
2	D	1500	NAD	C5N-C4N-C3N	-5.97	114.50	120.36
2	A	1200	NAD	C6N-N1N-C2N	-5.97	116.80	121.88
2	B	1300	NAD	C6N-N1N-C2N	-4.74	117.84	121.88
2	D	1500	NAD	O7N-C7N-C3N	-4.13	114.54	119.60
2	B	1300	NAD	O7N-C7N-C3N	-3.99	114.72	119.60
2	B	1300	NAD	C3N-C7N-N7N	3.93	122.58	117.74
2	B	1300	NAD	C6N-C5N-C4N	3.79	124.91	119.45
2	C	1400	NAD	C6N-N1N-C2N	-3.77	118.67	121.88
3	A	1201	CDP	O2B-PB-O3A	3.50	116.37	104.64
3	B	1301	CDP	O2B-PB-O3A	3.43	116.14	104.64
2	A	1200	NAD	C6N-C5N-C4N	3.38	124.31	119.45
2	C	1400	NAD	C3N-C7N-N7N	3.30	121.81	117.74
3	B	1301	CDP	O3A-PB-O1B	-3.06	94.95	111.04
2	A	1200	NAD	C3N-C7N-N7N	3.01	121.44	117.74
3	C	1401	CDP	O3B-PB-O3A	2.73	113.79	104.64
3	A	1201	CDP	O3B-PB-O3A	2.71	113.72	104.64
3	A	1201	CDP	C5-C4-N3	-2.69	116.80	121.32
3	C	1401	CDP	C4-N3-C2	2.66	124.45	120.26
3	B	1301	CDP	C4-N3-C2	2.65	124.43	120.26
3	B	1301	CDP	O3B-PB-O3A	2.65	113.51	104.64
3	D	1501	CDP	O4'-C1'-C2'	-2.61	101.03	106.62
3	B	1301	CDP	C5-C4-N3	-2.53	117.05	121.32
3	C	1401	CDP	C5-C4-N3	-2.52	117.07	121.32
2	A	1200	NAD	O7N-C7N-C3N	-2.48	116.56	119.60
3	D	1501	CDP	C4-N3-C2	2.44	124.10	120.26
2	C	1400	NAD	C6N-C5N-C4N	2.44	122.96	119.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	CDP	O2-C2-N1	2.42	123.64	118.90
3	D	1501	CDP	O2B-PB-O3A	2.42	112.75	104.64
3	D	1501	CDP	C5-C4-N3	-2.41	117.26	121.32
3	C	1401	CDP	O2B-PB-O3A	2.38	112.60	104.64
2	D	1500	NAD	C6N-C5N-C4N	2.29	122.75	119.45
3	D	1501	CDP	C2'-C3'-C4'	-2.25	98.25	102.61
2	B	1300	NAD	C2D-C3D-C4D	-2.14	98.47	102.61
3	C	1401	CDP	N4-C4-N3	2.09	121.64	117.91
3	A	1201	CDP	C4-N3-C2	2.06	123.50	120.26
2	D	1500	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
2	C	1400	NAD	C5N-C6N-N1N	2.02	123.14	120.38
3	A	1201	CDP	O2-C2-N3	-2.00	119.17	122.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1200	NAD	C5B-O5B-PA-O1A
2	A	1200	NAD	C5D-O5D-PN-O2N
2	B	1300	NAD	C5D-O5D-PN-O3
2	B	1300	NAD	C5D-O5D-PN-O2N
2	A	1200	NAD	C5B-O5B-PA-O2A
2	B	1300	NAD	C5D-O5D-PN-O1N
2	B	1300	NAD	PA-O3-PN-O2N
2	C	1400	NAD	PA-O3-PN-O2N
3	C	1401	CDP	C4'-C5'-O5'-PA
2	C	1400	NAD	O4B-C4B-C5B-O5B
2	C	1400	NAD	PA-O3-PN-O1N
2	B	1300	NAD	O4B-C4B-C5B-O5B

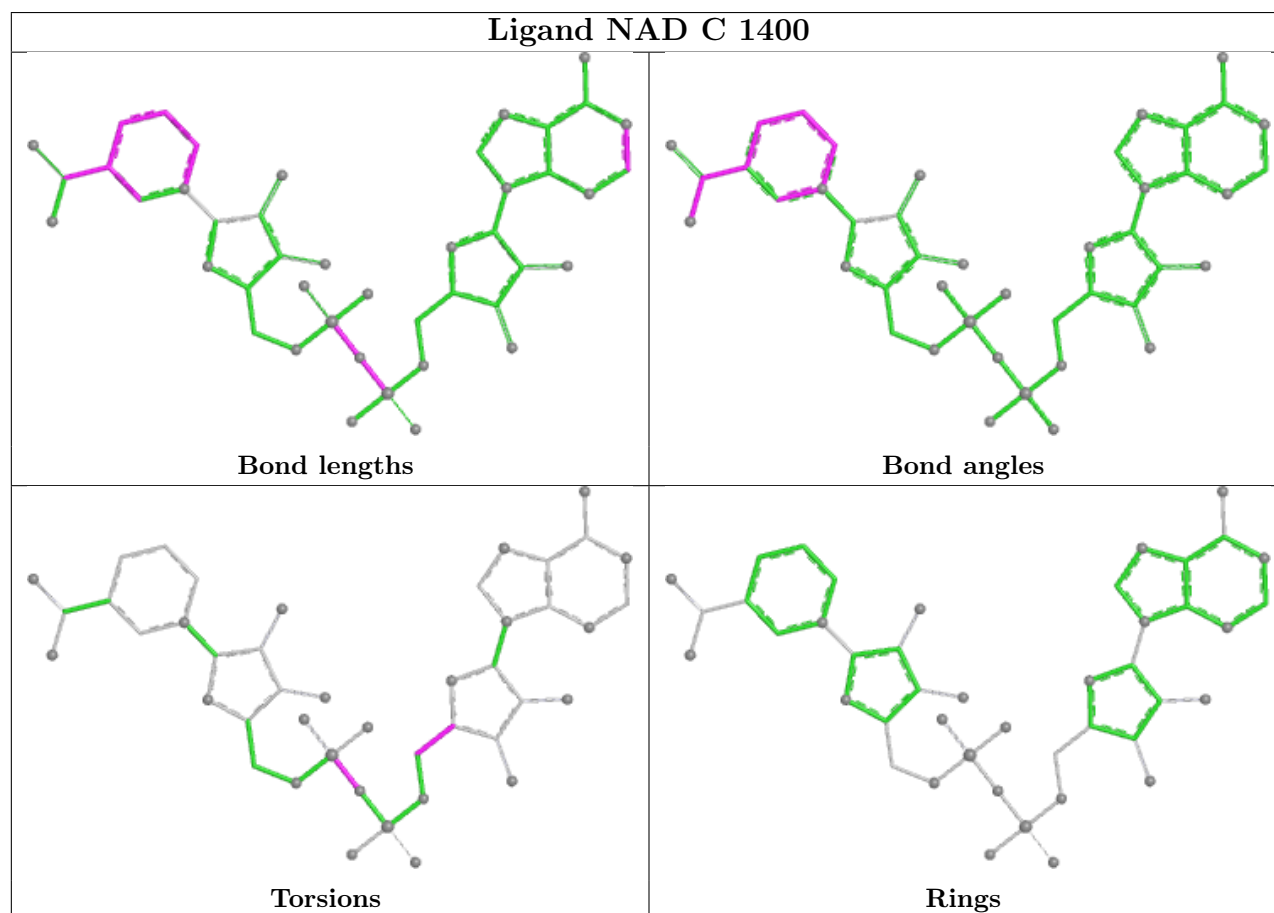
There are no ring outliers.

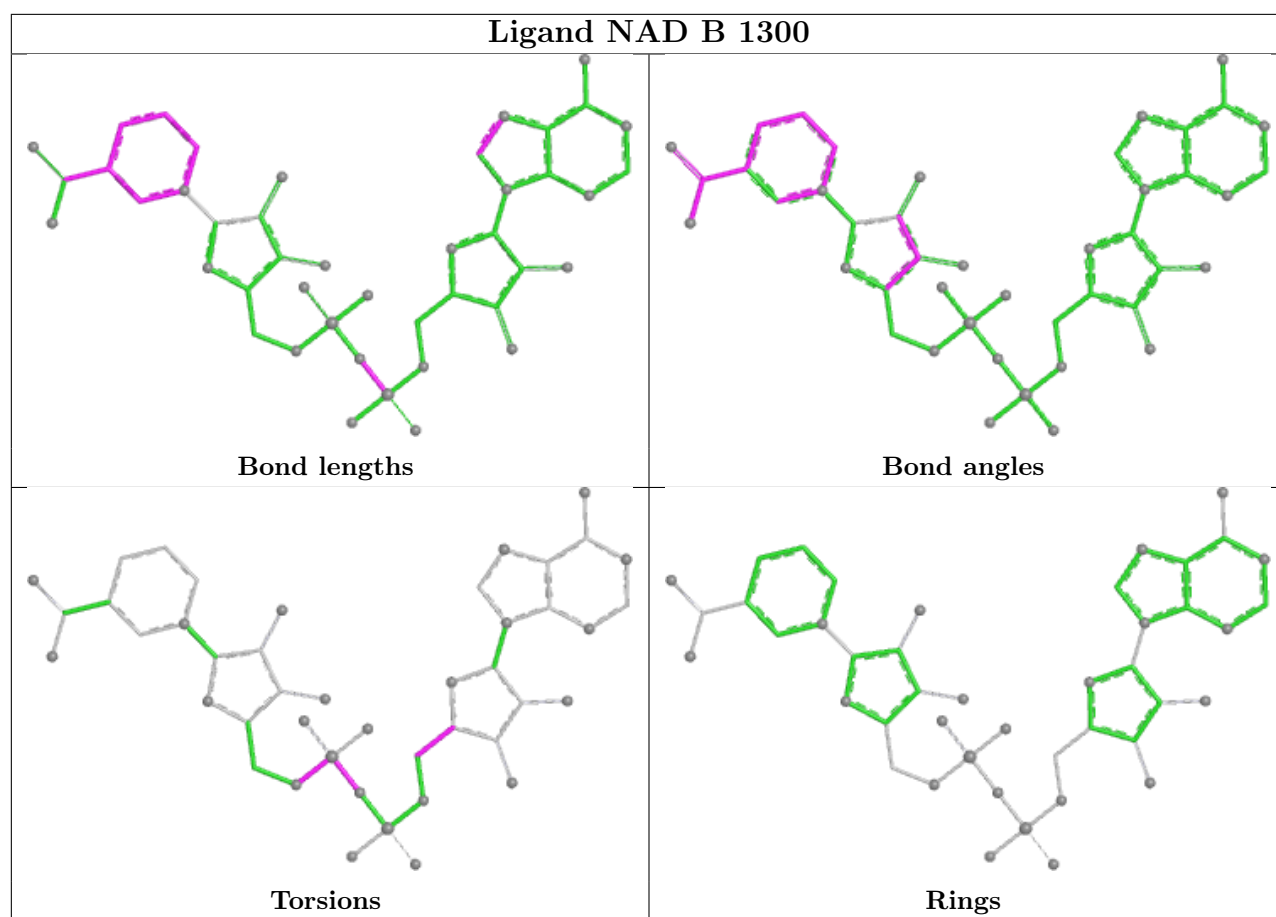
5 monomers are involved in 10 short contacts:

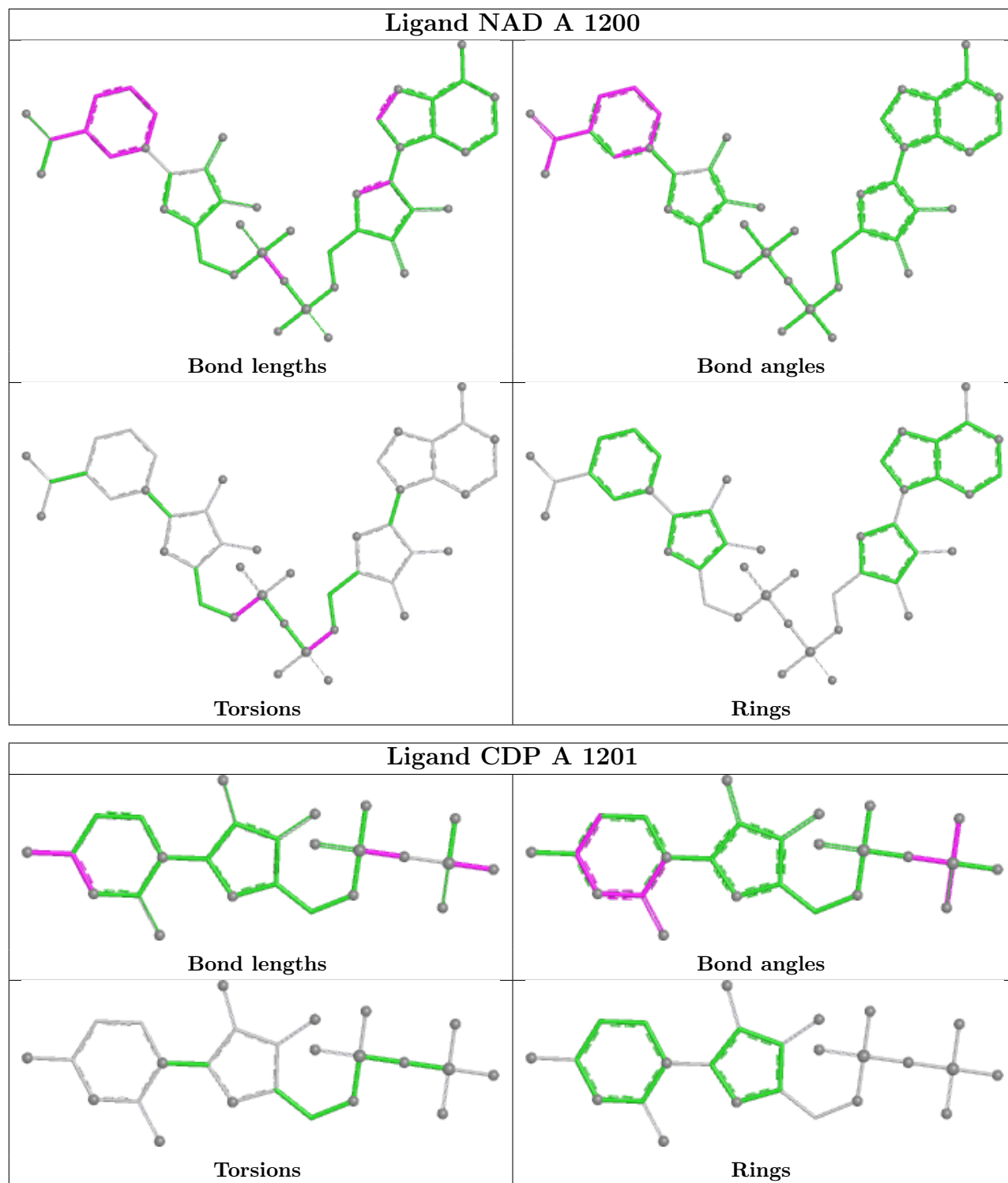
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1400	NAD	3	0
2	A	1200	NAD	4	0
3	C	1401	CDP	1	0
3	D	1501	CDP	1	0
2	D	1500	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

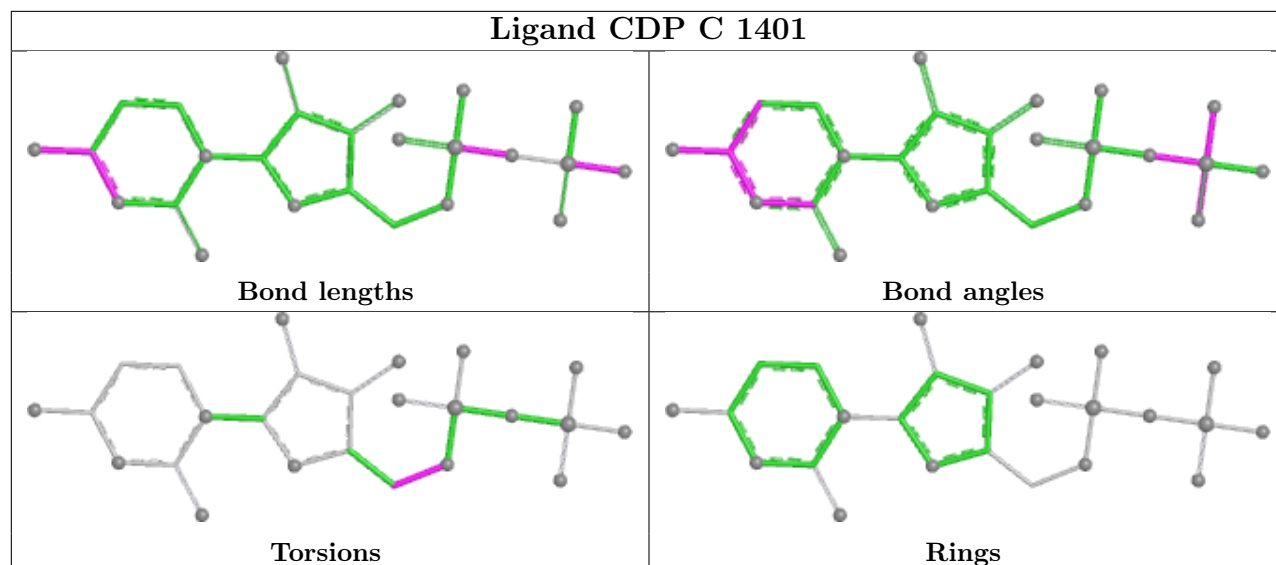
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



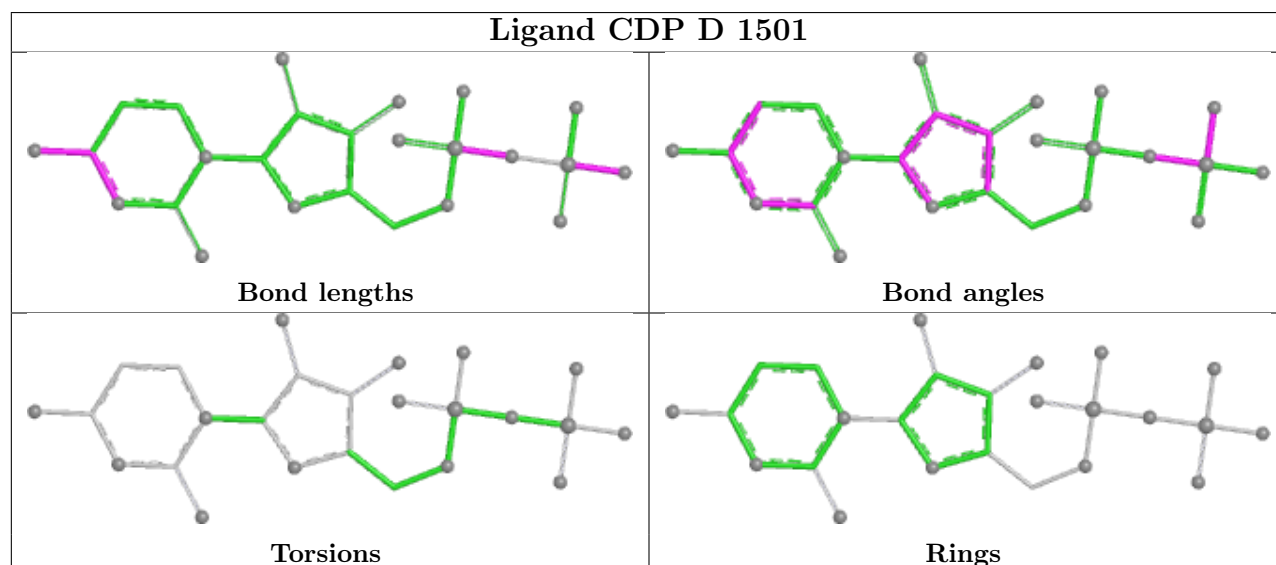




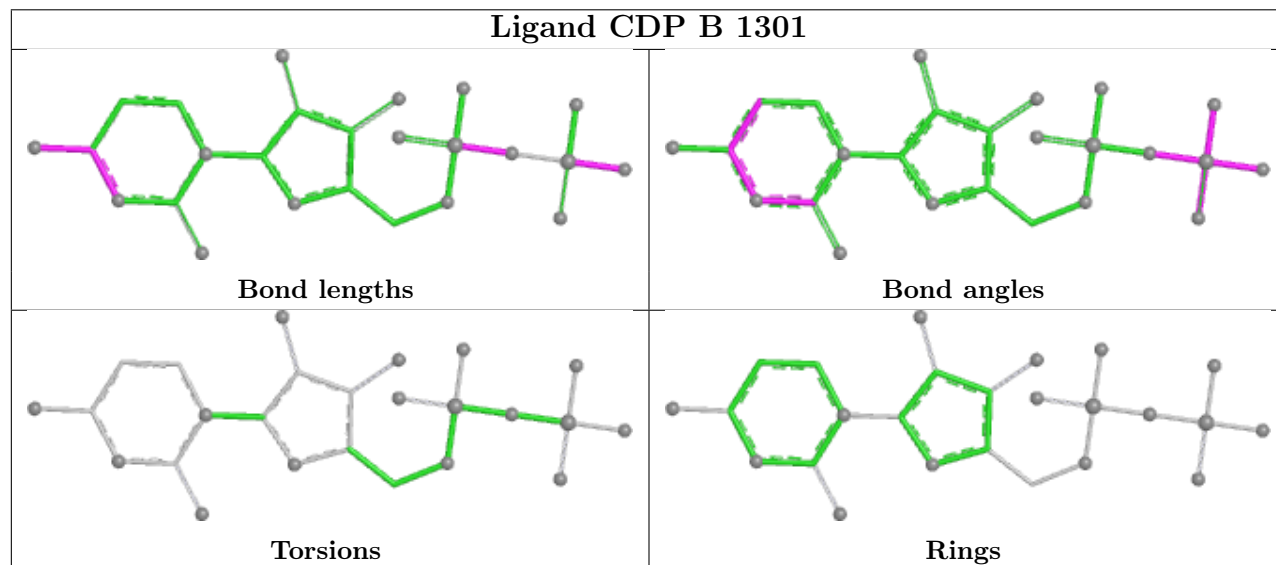
Ligand CDP C 1401

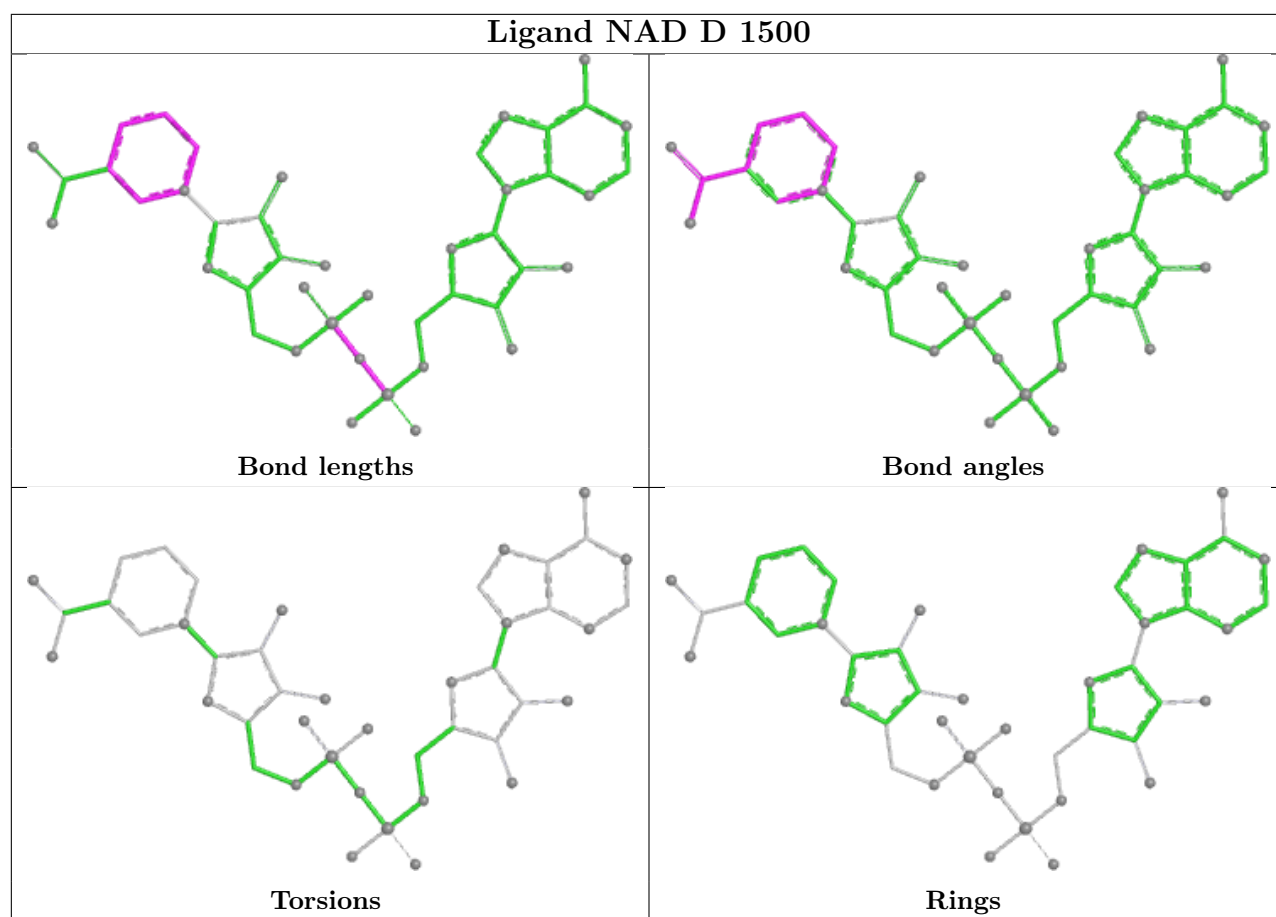


Ligand CDP D 1501



Ligand CDP B 1301





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	338/347 (97%)	-0.27	10 (2%) 52 56	9, 18, 47, 75	11 (3%)
1	B	338/347 (97%)	-0.15	10 (2%) 52 56	10, 19, 50, 95	4 (1%)
1	C	335/347 (96%)	0.15	22 (6%) 24 26	10, 21, 57, 95	6 (1%)
1	D	336/347 (96%)	0.11	18 (5%) 31 34	11, 20, 58, 90	5 (1%)
All	All	1347/1388 (97%)	-0.04	60 (4%) 38 42	9, 19, 55, 95	26 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	289	ILE	6.1
1	C	223	ILE	5.0
1	D	226	PRO	4.6
1	D	339	ILE	4.6
1	D	223	ILE	4.5
1	C	300	GLU	4.0
1	C	282	LEU	3.9
1	C	339	ILE	3.9
1	C	227	PHE	3.6
1	C	226	PRO	3.5
1	C	298	VAL	3.5
1	B	223	ILE	3.4
1	C	333	TYR	3.3
1	A	44[A]	HIS	3.3
1	B	204	TYR	3.3
1	B	339	ILE	3.1
1	B	2	ALA	3.1
1	B	206	GLN	3.0
1	D	301	SER	2.9
1	A	2	ALA	2.9
1	D	291	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	220	LYS	2.8
1	A	223	ILE	2.8
1	C	222	GLY	2.8
1	D	290	ASP	2.8
1	C	219	ILE	2.8
1	D	282	LEU	2.7
1	C	290	ASP	2.7
1	A	301	SER	2.7
1	D	270	ILE	2.6
1	C	136	LYS	2.6
1	B	224	ASN	2.6
1	D	300	GLU	2.6
1	C	142	THR	2.5
1	C	294	THR	2.5
1	D	287	CYS	2.5
1	A	300	GLU	2.5
1	D	338	SER	2.5
1	C	280	PHE	2.5
1	C	338	SER	2.4
1	A	339	ILE	2.4
1	A	318	ASP	2.4
1	C	293	PHE	2.4
1	C	288	ASN	2.4
1	B	338	SER	2.3
1	B	225	LYS	2.3
1	C	286	TYR	2.3
1	D	288	ASN	2.3
1	D	283	LEU	2.2
1	C	289	ILE	2.2
1	D	216	ALA	2.2
1	D	222	GLY	2.2
1	A	226	PRO	2.2
1	B	27	ASP	2.2
1	C	217	VAL	2.1
1	B	288	ASN	2.1
1	A	41	ASP	2.1
1	C	213	CYS	2.1
1	A	225	LYS	2.1
1	D	280	PHE	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](#)

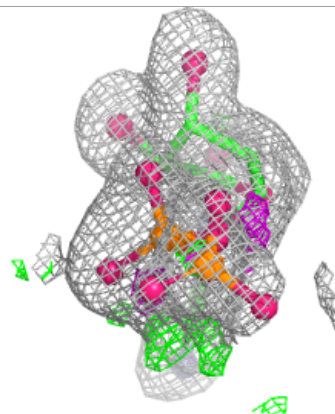
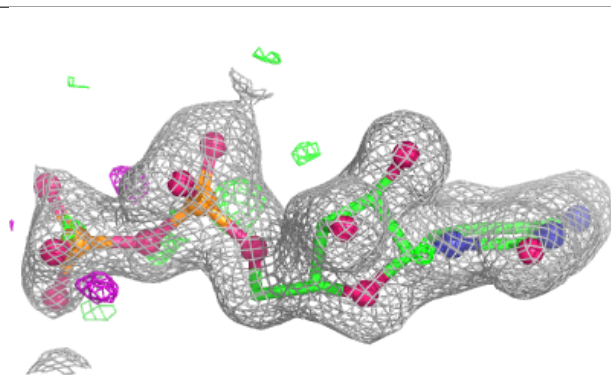
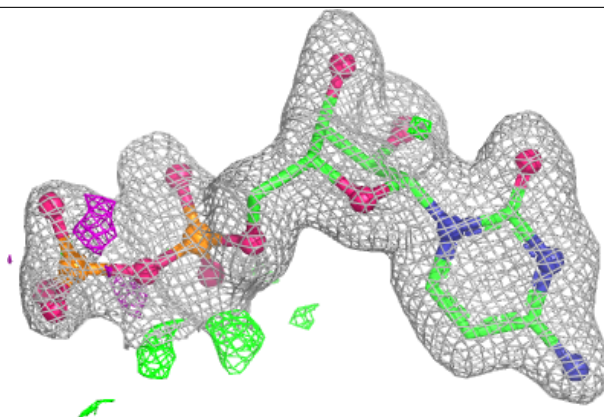
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	CDP	C	1401	25/25	0.96	0.09	19,25,100,100	0
3	CDP	D	1501	25/25	0.96	0.09	15,22,62,100	0
3	CDP	A	1201	25/25	0.97	0.07	14,21,45,100	0
3	CDP	B	1301	25/25	0.97	0.07	15,23,32,100	0
2	NAD	A	1200	44/44	0.99	0.04	11,15,24,37	0
2	NAD	B	1300	44/44	0.99	0.05	12,15,28,95	0
2	NAD	C	1400	44/44	0.99	0.05	11,16,26,100	0
2	NAD	D	1500	44/44	0.99	0.04	11,15,18,23	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.

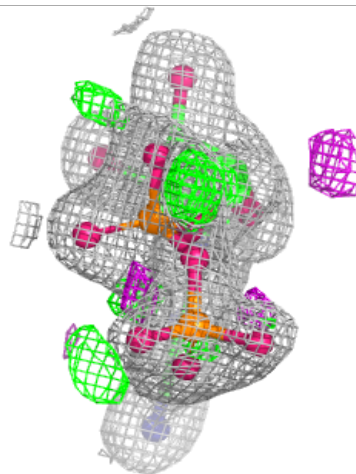
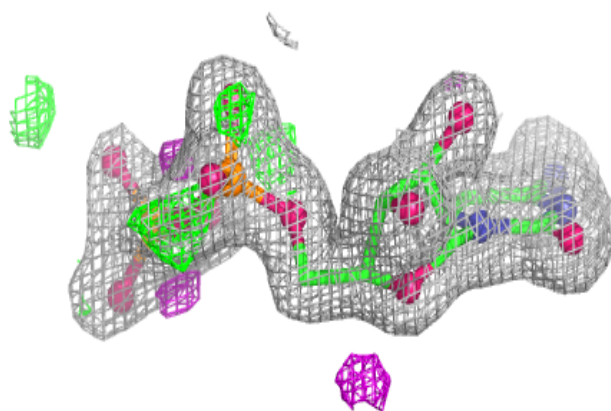
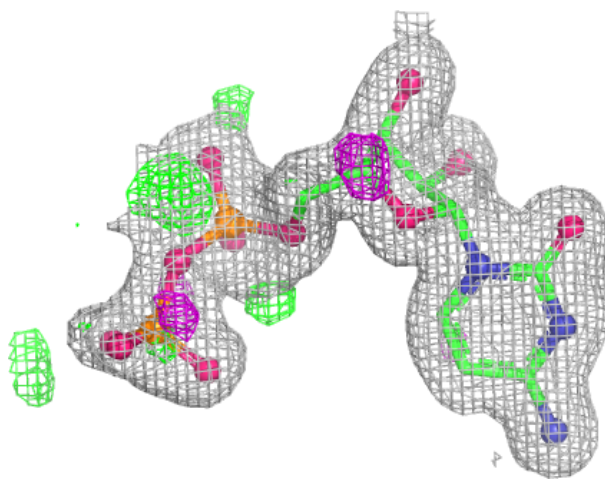
Electron density around CDP C 1401:

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



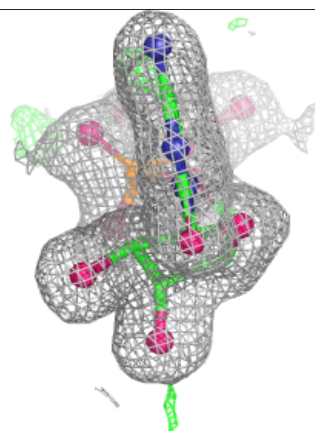
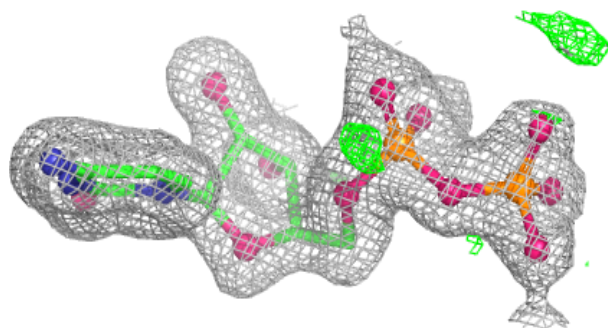
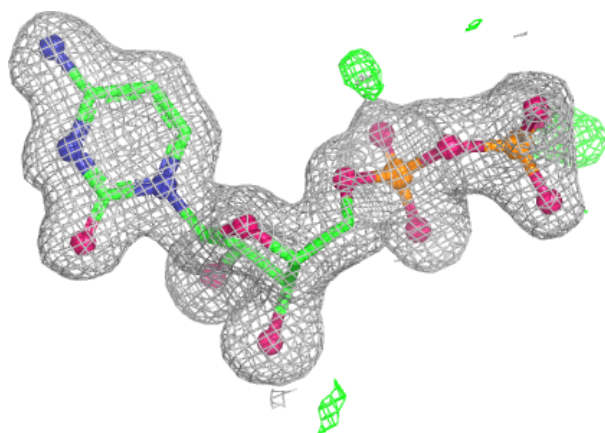
Electron density around CDP D 1501:

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

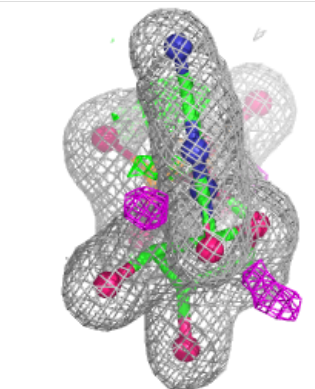
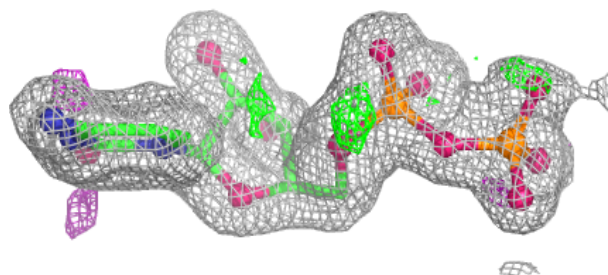
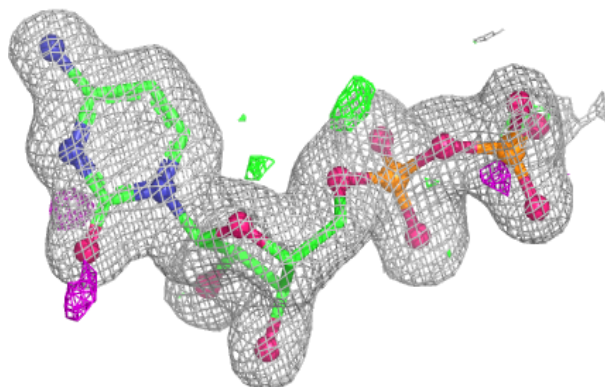


Electron density around CDP A 1201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

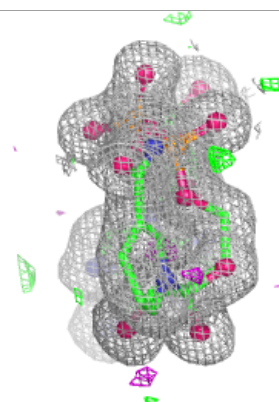
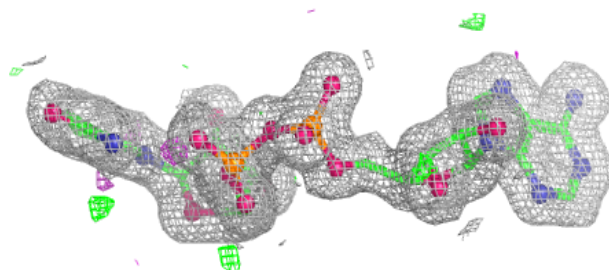
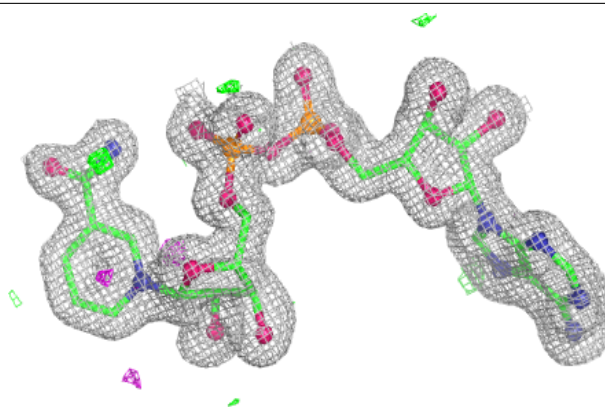
**Electron density around CDP B 1301:**

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and green (positive)

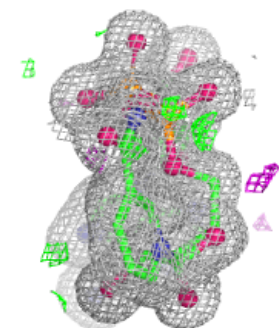
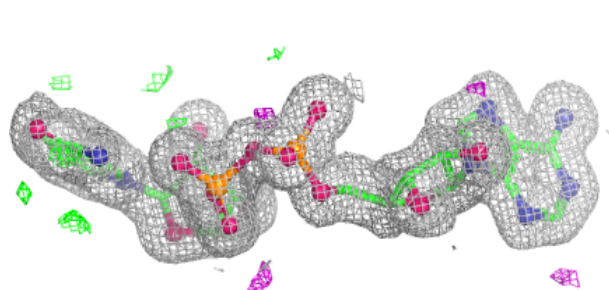
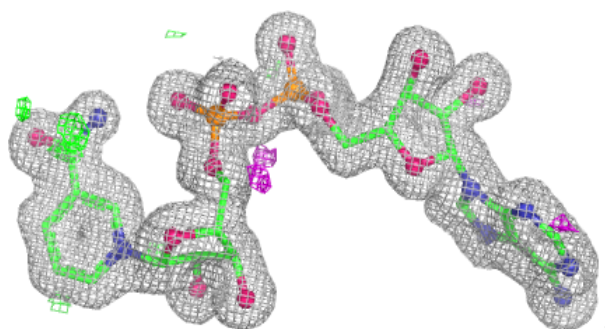


Electron density around NAD A 1200:

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

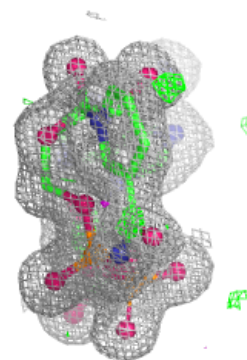
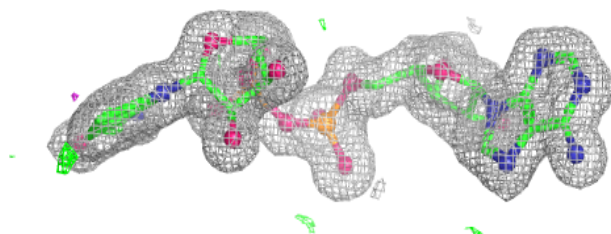
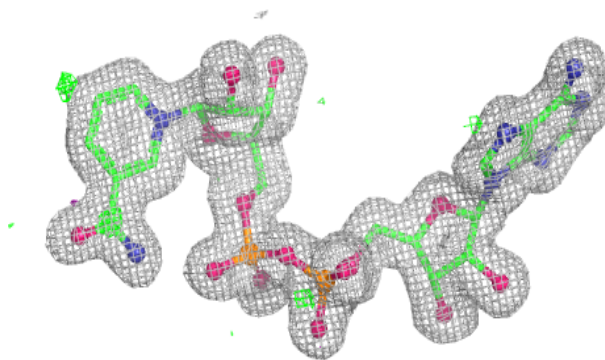
**Electron density around NAD B 1300:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

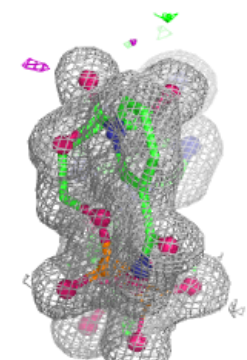
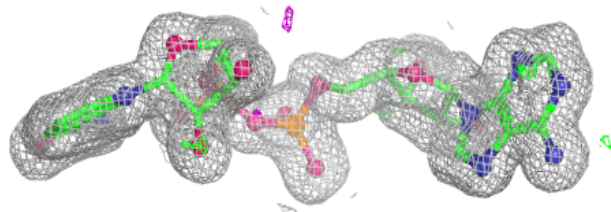
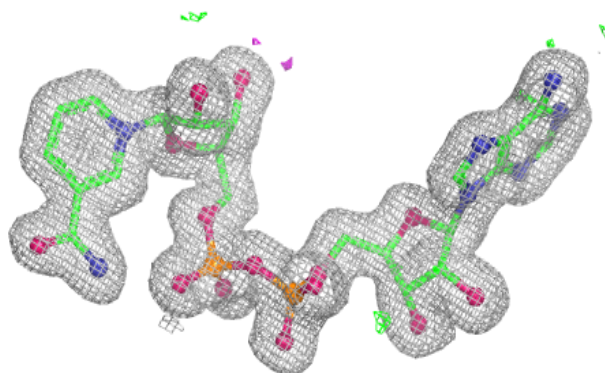


Electron density around NAD C 1400:

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

**Electron density around NAD D 1500:**

$2mF_o-DF_c$ (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.