



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:12 PM UTC

PDB ID : 4C4O / pdb_00004c4o
Title : Structure of carbonyl reductase CPCR2 from *Candida parapsilosis* in complex with NADH
Authors : Man, H.; Loderer, C.; Ansorge-Schumacher, M.; Grogan, G.
Deposited on : 2013-09-06
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

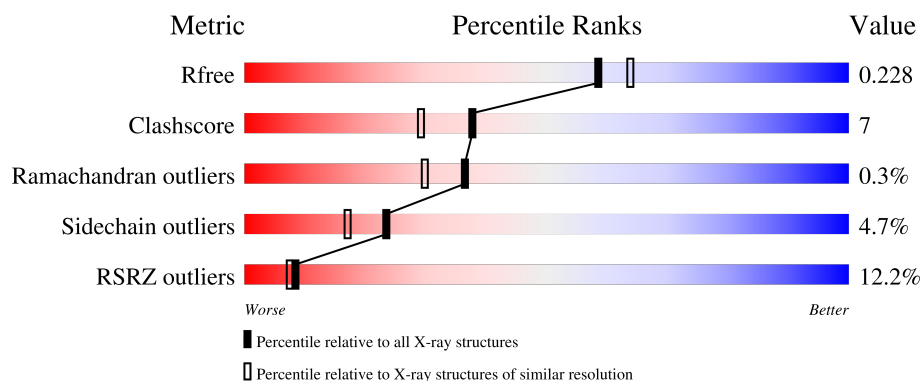
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	336	 10% 85% 10% . .
1	B	336	 % 85% 12% . .
1	C	336	 16% 77% 11% . . 10%
1	D	336	 17% 68% 10% . 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	1337	-	-	X	-
4	EDO	C	1337	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9234 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 CARBONYL REDUCTASE CPR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2318	1468	397	443	10			
1	B	335	Total	C	N	O	S	0	1	0
			2502	1590	424	476	12			
1	C	302	Total	C	N	O	S	0	0	0
			2111	1329	365	407	10			
1	D	270	Total	C	N	O	S	0	0	0
			1855	1165	320	361	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

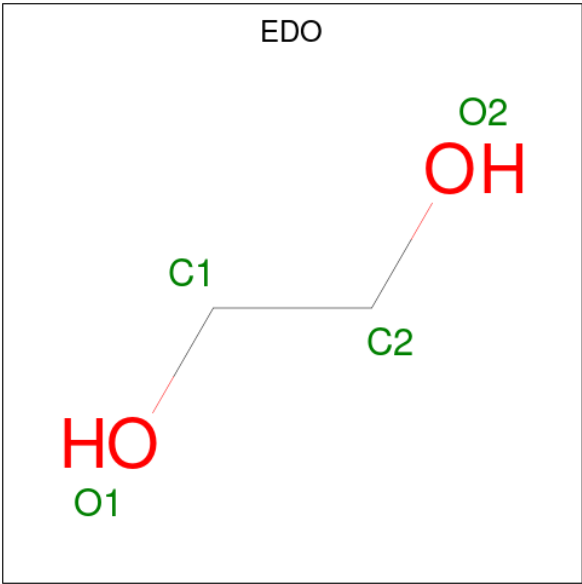
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	3	Total	Zn	0	0
			3	3		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	6	13	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

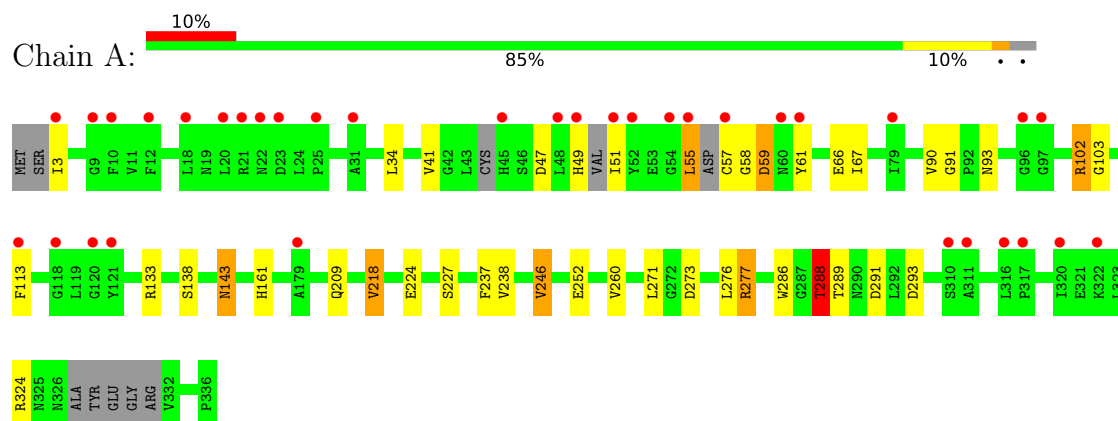
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	102	Total O 102 102	0	0
5	C	44	Total O 44 44	0	0
5	D	34	Total O 34 34	0	0

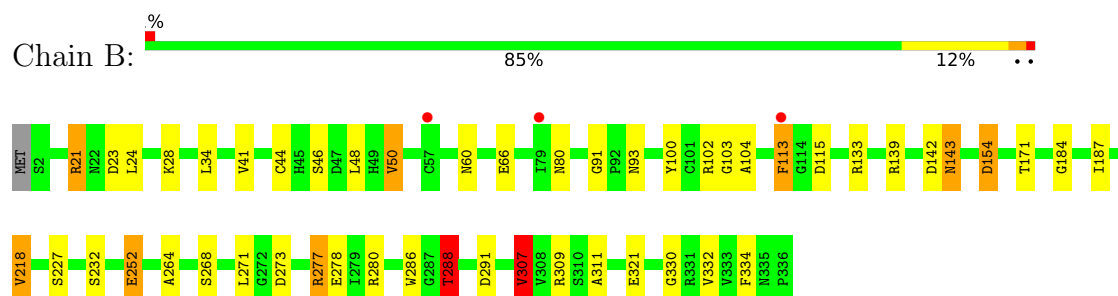
3 Residue-property plots [i](#)

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

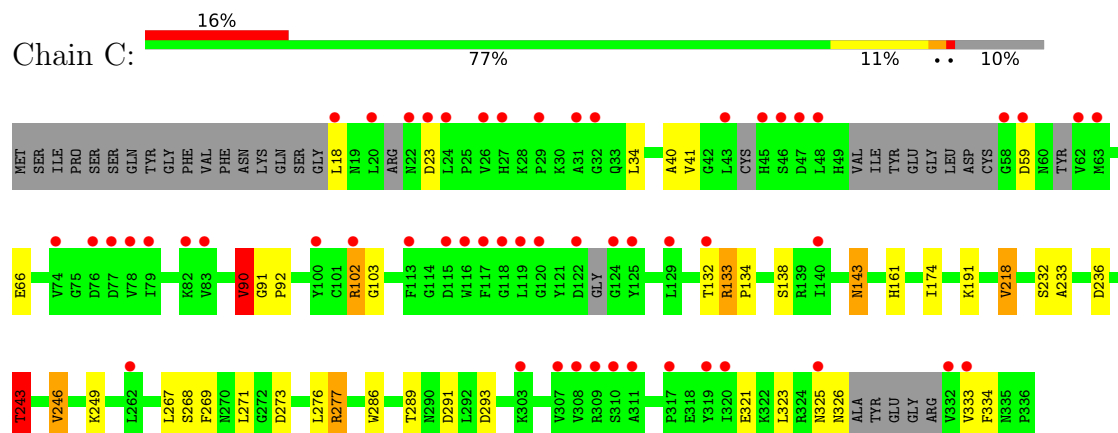
• Molecule 1: CARBONYL REDUCTASE CPR2



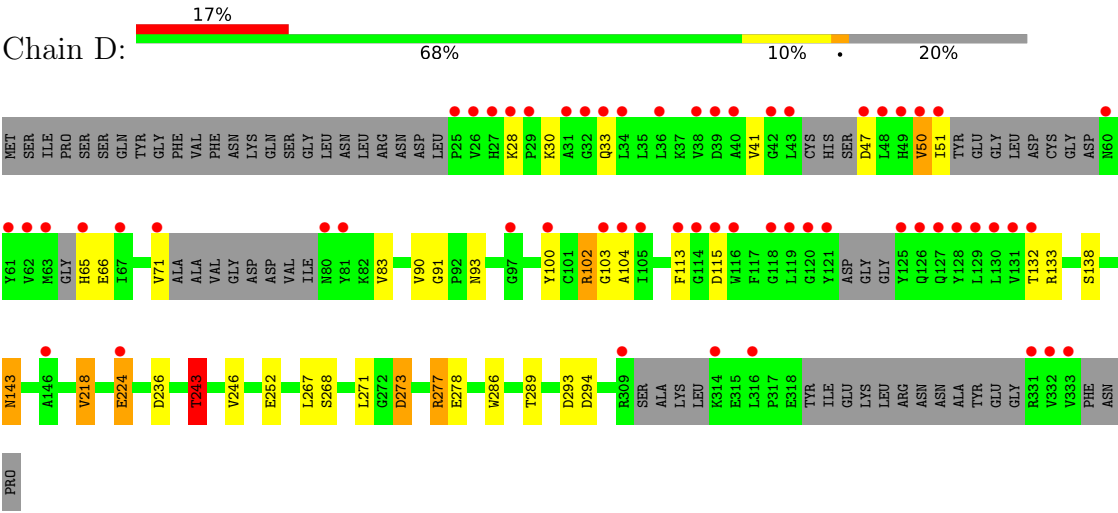
• Molecule 1: CARBONYL REDUCTASE CPR2



• Molecule 1: CARBONYL REDUCTASE CPR2



● Molecule 1: CARBONYL REDUCTASE CPR2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.72Å 88.84Å 118.20Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	58.13 – 2.05 58.13 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.13-2.05) 99.8 (58.13-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.205 , 0.241 (Not available) , 0.228	Depositor DCC
R_{free} test set	4253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9234	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: NAD, EDO, ZN

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	1.09	3/2359 (0.1%)	1.04	8/3211 (0.2%)
1	B	1.24	7/2553 (0.3%)	1.09	12/3467 (0.3%)
1	C	1.07	3/2145 (0.1%)	1.06	9/2922 (0.3%)
1	D	1.52	3/1880 (0.2%)	1.10	10/2559 (0.4%)
All	All	1.23	16/8937 (0.2%)	1.07	39/12159 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	VAL	C-N	-42.99	0.73	1.33
1	B	277	ARG	CD-NE	-7.99	1.35	1.46
1	B	44	CYS	CA-C	-7.96	1.43	1.52
1	A	227	SER	CA-C	6.47	1.60	1.53
1	B	187	ILE	CA-C	-5.98	1.45	1.52
1	B	227	SER	CA-C	5.94	1.59	1.52
1	C	267	LEU	CA-C	-5.60	1.45	1.52
1	A	252	GLU	CA-CB	5.47	1.60	1.53
1	C	191	LYS	C-O	-5.24	1.17	1.24
1	C	269	PHE	CA-C	-5.24	1.46	1.52
1	B	154	ASP	CG-OD2	5.19	1.35	1.25
1	B	280	ARG	CA-C	-5.17	1.46	1.52
1	D	267	LEU	CA-C	-5.11	1.46	1.52
1	A	277	ARG	CD-NE	-5.09	1.39	1.46
1	B	60	ASN	CG-ND2	-5.05	1.22	1.33
1	D	273	ASP	CA-C	5.01	1.59	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	VAL	O-C-N	11.96	134.15	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	THR	N-CA-C	-10.28	93.52	109.25
1	B	102	ARG	N-CA-C	9.96	125.58	113.23
1	D	243	THR	N-CA-CB	-8.66	97.34	110.16
1	B	277	ARG	NE-CZ-NH2	-8.57	111.49	119.20
1	D	102	ARG	N-CA-C	8.51	123.78	113.23
1	A	288	THR	N-CA-CB	-8.02	98.03	110.46
1	C	243	THR	N-CA-CB	-7.98	98.00	110.30
1	C	102	ARG	N-CA-C	7.79	122.88	113.23
1	B	288	THR	N-CA-CB	-7.75	98.47	110.56
1	A	102	ARG	N-CA-C	7.70	122.77	113.23
1	A	277	ARG	NE-CZ-NH2	-7.66	112.31	119.20
1	C	277	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	B	307	VAL	CB-CA-C	7.37	119.19	111.23
1	D	277	ARG	NE-CZ-NH2	-7.24	112.68	119.20
1	A	277	ARG	NE-CZ-NH1	7.13	128.63	121.50
1	C	277	ARG	NE-CZ-NH1	6.96	128.47	121.50
1	D	252	GLU	CB-CA-C	-6.83	96.88	109.51
1	B	277	ARG	NE-CZ-NH1	6.56	128.06	121.50
1	A	252	GLU	CB-CA-C	-6.50	96.92	110.31
1	D	277	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	D	243	THR	CB-CA-C	6.24	121.47	110.85
1	A	218	VAL	CB-CA-C	6.17	120.00	110.50
1	C	243	THR	CB-CA-C	6.00	122.62	110.38
1	D	132	THR	CB-CA-C	-5.99	99.18	110.67
1	B	50	VAL	CB-CA-C	-5.95	104.27	112.24
1	B	277	ARG	CD-NE-CZ	5.78	132.50	124.40
1	B	252	GLU	CB-CA-C	-5.71	98.96	109.51
1	B	44	CYS	CB-CA-C	-5.68	97.51	109.38
1	B	218	VAL	N-CA-C	5.56	116.29	108.17
1	D	277	ARG	CD-NE-CZ	5.46	132.05	124.40
1	C	90	VAL	N-CA-CB	5.18	117.68	111.31
1	C	218	VAL	CB-CA-C	5.16	118.45	110.50
1	A	246	VAL	N-CA-CB	5.13	117.52	110.54
1	D	218	VAL	CB-CA-C	5.10	118.36	110.50
1	B	28	LYS	N-CA-C	-5.10	103.35	109.72
1	B	307	VAL	N-CA-CB	5.06	117.26	111.39
1	C	246	VAL	N-CA-CB	5.05	117.42	110.54
1	A	67	ILE	N-CA-C	5.01	115.13	108.11

There are no chirality outliers.

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	2318	0	2156	27	0
1	B	2502	0	2459	35	1
1	C	2111	0	1944	36	1
1	D	1855	0	1664	32	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	36	0	20	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	4	0	6	0	0
4	B	12	0	18	9	0
4	C	8	0	12	8	0
5	A	67	0	0	1	0
5	B	102	0	0	2	0
5	C	44	0	0	0	0
5	D	34	0	0	1	0
All	All	9234	0	8357	122	1

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 7.

All (122) 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:D:50:VAL:CA	1:D:51:ILE:N	1.84	1.39
1:D:50:VAL:C	1:D:51:ILE:CA	1.92	1.39
1:D:47:ASP:O	1:D:51:ILE:HG12	1.34	1.22
1:C:323:LEU:O	1:C:326:ASN:HB2	1.39	1.20
1:D:50:VAL:O	1:D:51:ILE:N	1.81	1.11
1:A:55:LEU:C	1:A:57:CYS:N	2.14	1.04
1:A:58:GLY:HA3	1:A:61:TYR:HE2	1.28	0.97
1:A:58:GLY:HA3	1:A:61:TYR:CE2	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LEU:O	1:C:326:ASN:CB	2.24	0.85
1:B:113:PHE:CE2	1:B:113:PHE:CE1	2.60	0.83
1:D:50:VAL:C	1:D:51:ILE:N	0.73	0.82
1:A:288:THR:HG21	5:A:2019:HOH:O	1.81	0.81
1:A:276:LEU:HD21	1:B:113:PHE:CE1	2.16	0.79
1:D:115:ASP:OD2	1:D:133:ARG:NH2	2.16	0.78
1:B:115:ASP:OD2	1:B:133:ARG:NH2	2.17	0.78
1:C:321:GLU:O	1:C:325:ASN:ND2	2.16	0.78
1:D:224:GLU:H	1:D:224:GLU:CD	1.91	0.78
1:B:288:THR:HG22	1:B:291:ASP:H	1.51	0.75
1:B:104:ALA:HA	1:C:102:ARG:O	1.87	0.75
1:D:93:ASN:O	1:D:133:ARG:NH1	2.19	0.74
1:B:184:GLY:HA3	4:B:1337:EDO:H21	1.67	0.73
1:B:93:ASN:O	1:B:133:ARG:NH1	2.21	0.73
1:A:55:LEU:O	1:A:57:CYS:N	2.23	0.72
1:B:288:THR:HG21	5:B:2034:HOH:O	1.89	0.72
1:C:249:LYS:HB2	4:C:1337:EDO:H11	1.72	0.71
1:D:50:VAL:C	1:D:51:ILE:HA	2.13	0.71
1:D:50:VAL:O	1:D:51:ILE:CA	2.32	0.70
1:A:288:THR:HG22	1:A:291:ASP:H	1.56	0.70
1:D:71:VAL:HG12	1:D:83:VAL:HA	1.74	0.69
1:A:58:GLY:O	1:A:59:ASP:HB2	1.92	0.69
1:C:233:ALA:HB2	4:C:1338:EDO:H21	1.75	0.69
1:B:80:ASN:O	1:B:139:ARG:NH2	2.26	0.68
1:B:307:VAL:HG22	1:B:330:GLY:HA3	1.75	0.68
1:C:236:ASP:OD2	1:C:243:THR:HG23	1.95	0.67
1:C:90:VAL:HG11	1:C:289:THR:HA	1.77	0.66
1:D:50:VAL:N	1:D:51:ILE:N	2.44	0.66
1:C:161:HIS:HE1	1:D:278:GLU:OE2	1.78	0.65
1:D:236:ASP:OD2	1:D:243:THR:HG23	1.97	0.65
1:C:233:ALA:HB2	4:C:1338:EDO:C2	2.26	0.65
1:D:90:VAL:HG21	1:D:289:THR:HG22	1.79	0.64
1:C:90:VAL:HG23	1:C:92:PRO:HD2	1.79	0.64
1:A:58:GLY:CA	1:A:61:TYR:HE2	2.08	0.64
1:A:161:HIS:HE1	1:B:278:GLU:OE2	1.81	0.63
1:A:161:HIS:HD2	1:A:291:ASP:OD2	1.81	0.63
1:A:90:VAL:HG21	1:A:289:THR:HG22	1.81	0.62
1:D:50:VAL:CB	1:D:51:ILE:N	2.62	0.62
1:A:237:PHE:CE1	1:A:260:VAL:HG21	2.36	0.61
1:C:90:VAL:HG11	1:C:289:THR:HG22	1.83	0.60
1:C:236:ASP:OD2	1:C:243:THR:CG2	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ASP:OD2	1:D:243:THR:CG2	2.51	0.58
1:A:47:ASP:O	1:A:51:ILE:CB	2.52	0.58
1:A:161:HIS:CD2	1:A:291:ASP:OD2	2.58	0.57
1:A:102:ARG:O	1:D:104:ALA:HA	2.04	0.57
1:D:50:VAL:O	1:D:51:ILE:HA	2.02	0.57
1:B:113:PHE:CE1	4:B:1339:EDO:H11	2.40	0.56
1:C:161:HIS:CD2	1:C:291:ASP:OD2	2.59	0.56
1:C:249:LYS:HB2	4:C:1337:EDO:C1	2.35	0.56
1:B:113:PHE:CD1	4:B:1339:EDO:H11	2.41	0.56
1:C:236:ASP:CG	1:C:243:THR:HG23	2.30	0.55
1:C:161:HIS:HD2	1:C:291:ASP:OD2	1.90	0.55
1:D:138:SER:OG	1:D:293:ASP:OD1	2.25	0.55
1:C:40:ALA:HB1	1:C:333:VAL:HG21	1.90	0.54
1:B:21:ARG:NH1	1:B:23:ASP:OD1	2.40	0.54
1:D:236:ASP:CG	1:D:243:THR:HG23	2.33	0.53
1:B:309:ARG:CG	1:B:332:VAL:HG22	2.40	0.52
1:B:143:ASN:H	1:B:143:ASN:HD22	1.58	0.51
1:C:138:SER:OG	1:C:293:ASP:OD1	2.25	0.50
1:A:93:ASN:O	1:A:133:ARG:NH1	2.45	0.50
1:B:330:GLY:HA2	4:B:1337:EDO:C1	2.41	0.50
1:C:41:VAL:C	1:C:333:VAL:HG23	2.38	0.49
1:D:47:ASP:O	1:D:51:ILE:CG1	2.30	0.49
1:D:65:HIS:CE1	5:D:2003:HOH:O	2.66	0.48
1:C:249:LYS:CB	4:C:1337:EDO:H11	2.42	0.48
1:A:138:SER:OG	1:A:293:ASP:OD1	2.31	0.48
1:B:309:ARG:HG3	1:B:332:VAL:HG22	1.96	0.48
1:C:40:ALA:HB1	1:C:333:VAL:CG2	2.43	0.48
1:C:91:GLY:HA3	1:C:286:TRP:CZ2	2.49	0.47
1:D:91:GLY:HA3	1:D:286:TRP:CZ2	2.49	0.47
1:A:161:HIS:CE1	1:B:278:GLU:OE2	2.65	0.47
1:C:232:SER:OG	4:C:1338:EDO:H11	2.15	0.47
1:C:90:VAL:CG1	1:C:289:THR:HG22	2.45	0.46
1:B:91:GLY:HA3	1:B:286:TRP:CZ2	2.50	0.46
1:C:102:ARG:N	1:C:103:GLY:HA3	2.31	0.46
1:B:46:SER:O	1:B:50:VAL:HG23	2.15	0.46
1:A:143:ASN:HD22	1:A:143:ASN:H	1.63	0.45
1:A:91:GLY:HA3	1:A:286:TRP:CZ2	2.52	0.45
1:D:30:LYS:HA	1:D:33:GLN:HB2	1.98	0.45
1:B:330:GLY:HA2	4:B:1337:EDO:H11	1.97	0.45
1:C:161:HIS:CE1	1:D:278:GLU:OE2	2.65	0.45
1:A:49:HIS:HB3	1:A:55:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:C	1:A:34:LEU:HD12	2.42	0.44
1:D:41:VAL:HA	1:D:66:GLU:O	2.19	0.43
1:B:273:ASP:OD1	1:B:277:ARG:HD3	2.19	0.43
1:C:41:VAL:HA	1:C:66:GLU:O	2.19	0.43
1:D:143:ASN:HD22	1:D:143:ASN:H	1.64	0.43
1:B:171:THR:HG21	1:D:294:ASP:CG	2.43	0.43
1:C:273:ASP:OD1	1:C:277:ARG:HD3	2.19	0.43
1:D:273:ASP:OD1	1:D:277:ARG:HD3	2.18	0.42
1:B:100:TYR:O	1:B:103:GLY:HA3	2.19	0.42
1:B:288:THR:CG2	1:B:291:ASP:H	2.28	0.42
1:B:252:GLU:OE2	4:B:1338:EDO:C2	2.67	0.42
1:C:143:ASN:H	1:C:143:ASN:HD22	1.67	0.42
1:A:90:VAL:HG21	1:A:289:THR:HA	2.02	0.42
1:C:249:LYS:N	4:C:1337:EDO:H11	2.35	0.42
1:B:232:SER:HB3	4:B:1338:EDO:C2	2.49	0.41
1:D:100:TYR:O	1:D:103:GLY:HA3	2.20	0.41
1:B:34:LEU:HD12	1:B:34:LEU:C	2.46	0.41
1:B:252:GLU:OE2	4:B:1338:EDO:H22	2.20	0.41
1:B:264:ALA:HB2	5:B:2087:HOH:O	2.19	0.41
1:A:41:VAL:HA	1:A:66:GLU:O	2.20	0.41
1:B:66[A]:GLU:HG2	1:B:154:ASP:CB	2.51	0.41
1:A:273:ASP:OD1	1:A:277:ARG:HD3	2.21	0.41
1:C:249:LYS:CA	4:C:1337:EDO:H11	2.51	0.41
1:A:102:ARG:N	1:A:103:GLY:HA3	2.35	0.41
1:D:102:ARG:N	1:D:103:GLY:HA3	2.36	0.41
1:C:34:LEU:C	1:C:34:LEU:HD12	2.46	0.41
1:C:133:ARG:N	1:C:134:PRO:HD3	2.36	0.41
1:B:311:ALA:O	1:B:334:PHE:HA	2.21	0.41
1:B:307:VAL:HG13	4:B:1337:EDO:H22	2.02	0.40
1:C:174:ILE:HD13	1:C:174:ILE:HG21	1.81	0.40
1:C:40:ALA:HA	1:C:334:PHE:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:OD2	1:C:23:ASP:O[2_545]	2.15	0.05

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	316/336 (94%)	301 (95%)	14 (4%)	1 (0%)	36	30
1	B	334/336 (99%)	320 (96%)	14 (4%)	0	100	100
1	C	288/336 (86%)	274 (95%)	12 (4%)	2 (1%)	18	10
1	D	254/336 (76%)	239 (94%)	14 (6%)	1 (0%)	30	22
All	All	1192/1344 (89%)	1134 (95%)	54 (4%)	4 (0%)	36	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	C	59	ASP
1	D	28	LYS
1	C	133	ARG

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	222/270 (82%)	210 (95%)	12 (5%)	20	12
1	B	261/270 (97%)	250 (96%)	11 (4%)	26	20
1	C	200/270 (74%)	191 (96%)	9 (4%)	24	18
1	D	168/270 (62%)	160 (95%)	8 (5%)	23	16
All	All	851/1080 (79%)	811 (95%)	40 (5%)	23	17

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	55	LEU
1	A	113	PHE
1	A	143	ASN
1	A	209	GLN
1	A	218	VAL
1	A	224	GLU
1	A	238	VAL
1	A	246	VAL
1	A	271	LEU
1	A	288	THR
1	A	324	ARG
1	B	21	ARG
1	B	24	LEU
1	B	48	LEU
1	B	113	PHE
1	B	143	ASN
1	B	218	VAL
1	B	268	SER
1	B	271	LEU
1	B	288	THR
1	B	307	VAL
1	B	321	GLU
1	C	18	LEU
1	C	90	VAL
1	C	143	ASN
1	C	218	VAL
1	C	243	THR
1	C	246	VAL
1	C	268	SER
1	C	271	LEU
1	C	276	LEU
1	D	113	PHE
1	D	143	ASN
1	D	218	VAL
1	D	224	GLU
1	D	243	THR
1	D	246	VAL
1	D	268	SER
1	D	271	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	49	HIS
1	A	80	ASN
1	A	143	ASN
1	A	161	HIS
1	B	22	ASN
1	B	93	ASN
1	B	143	ASN
1	C	136	ASN
1	C	143	ASN
1	C	161	HIS
1	D	143	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 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	$\# Z > 2$
3	NAD	C	1000	-	46,48,48	1.54	7 (15%)	64,73,73	1.84	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	D	1000	-	46,48,48	1.58	8 (17%)	64,73,73	1.91	14 (21%)
3	NAD	A	1000	-	38,39,48	1.46	3 (7%)	55,60,73	2.11	13 (23%)
4	EDO	B	1337	-	3,3,3	0.62	0	2,2,2	0.38	0
4	EDO	B	1338	-	3,3,3	0.58	0	2,2,2	0.31	0
4	EDO	C	1337	-	3,3,3	0.30	0	2,2,2	0.74	0
4	EDO	A	1337	-	3,3,3	0.42	0	2,2,2	0.44	0
4	EDO	C	1338	-	3,3,3	0.47	0	2,2,2	0.39	0
3	NAD	B	1000	-	46,48,48	1.24	3 (6%)	64,73,73	2.00	14 (21%)
4	EDO	B	1339	-	3,3,3	1.46	1 (33%)	2,2,2	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	1000	-	-	5/30/62/62	0/5/5/5
3	NAD	D	1000	-	-	6/30/62/62	0/5/5/5
3	NAD	A	1000	-	-	3/22/54/62	0/4/4/5
4	EDO	B	1337	-	-	1/1/1/1	-
4	EDO	B	1338	-	-	1/1/1/1	-
4	EDO	C	1337	-	-	1/1/1/1	-
4	EDO	A	1337	-	-	1/1/1/1	-
4	EDO	C	1338	-	-	1/1/1/1	-
3	NAD	B	1000	-	-	7/30/62/62	0/5/5/5
4	EDO	B	1339	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	NAD	PA-O3	5.48	1.65	1.59
3	A	1000	NAD	C5A-C4A	5.13	1.48	1.39
3	D	1000	NAD	PA-O3	5.11	1.65	1.59
3	D	1000	NAD	C5A-C4A	5.09	1.48	1.39
3	C	1000	NAD	PN-O3	4.73	1.64	1.59
3	A	1000	NAD	PN-O3	4.68	1.64	1.59
3	C	1000	NAD	PA-O3	4.01	1.63	1.59
3	C	1000	NAD	C5A-C4A	3.96	1.46	1.39
3	C	1000	NAD	O4D-C1D	3.55	1.45	1.40
3	C	1000	NAD	C8A-N7A	2.94	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	NAD	C2A-N1A	2.71	1.38	1.33
3	D	1000	NAD	C3N-C7N	2.65	1.54	1.50
3	A	1000	NAD	PA-O3	2.61	1.62	1.59
3	D	1000	NAD	C8A-N7A	2.38	1.36	1.31
3	D	1000	NAD	C2N-N1N	2.37	1.37	1.35
3	C	1000	NAD	C5A-C6A	2.34	1.47	1.41
3	C	1000	NAD	C5A-N7A	-2.34	1.34	1.39
3	D	1000	NAD	C4A-N3A	2.22	1.38	1.34
3	B	1000	NAD	C5A-C4A	2.06	1.42	1.39
3	D	1000	NAD	C5A-N7A	-2.05	1.35	1.39
3	B	1000	NAD	C5A-C6A	2.01	1.46	1.41
4	B	1339	EDO	O2-C2	2.01	1.52	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	NAD	C5A-C4A-N3A	-7.51	116.37	126.72
3	A	1000	NAD	C5A-C4A-N3A	-6.60	117.62	126.72
3	D	1000	NAD	N3A-C4A-N9A	6.33	137.94	127.17
3	A	1000	NAD	N3A-C4A-N9A	6.33	137.93	127.17
3	B	1000	NAD	N3A-C4A-N9A	6.23	137.77	127.17
3	C	1000	NAD	C5A-C4A-N3A	-5.97	118.49	126.72
3	D	1000	NAD	C5A-C4A-N3A	-5.35	119.35	126.72
3	D	1000	NAD	C4A-N9A-C8A	4.77	110.75	105.74
3	C	1000	NAD	N3A-C4A-N9A	4.66	135.09	127.17
3	A	1000	NAD	C4A-N9A-C8A	4.63	110.60	105.74
3	B	1000	NAD	C2A-N3A-C4A	4.54	122.92	111.83
3	A	1000	NAD	C2A-N3A-C4A	4.45	122.70	111.83
3	B	1000	NAD	C4D-O4D-C1D	-4.42	105.88	109.92
3	C	1000	NAD	N3A-C2A-N1A	-4.21	122.20	128.58
3	A	1000	NAD	N3A-C2A-N1A	-4.20	122.23	128.58
3	D	1000	NAD	N3A-C2A-N1A	-4.17	122.26	128.58
3	C	1000	NAD	C2A-N3A-C4A	4.02	121.66	111.83
3	C	1000	NAD	C4A-C5A-N7A	-3.87	106.16	110.58
3	D	1000	NAD	C5A-C6A-N6A	-3.77	113.95	123.29
3	B	1000	NAD	N3A-C2A-N1A	-3.61	123.12	128.58
3	D	1000	NAD	N6A-C6A-N1A	3.55	126.28	118.38
3	D	1000	NAD	C2A-N3A-C4A	3.54	120.48	111.83
3	C	1000	NAD	C5A-N7A-C8A	3.51	108.96	103.45
3	B	1000	NAD	O3-PA-O1A	-3.49	100.19	110.70
3	C	1000	NAD	C4A-N9A-C8A	3.47	109.38	105.74
3	B	1000	NAD	C4A-N9A-C8A	3.46	109.37	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1000	NAD	N9A-C8A-N7A	-3.43	109.08	113.94
3	A	1000	NAD	C4A-C5A-N7A	-3.32	106.78	110.58
3	D	1000	NAD	O3-PN-O1N	3.26	120.52	110.70
3	A	1000	NAD	C5A-N7A-C8A	3.25	108.56	103.45
3	C	1000	NAD	C4D-O4D-C1D	-3.08	107.11	109.92
3	A	1000	NAD	N9A-C8A-N7A	-3.08	109.57	113.94
3	D	1000	NAD	C5A-C4A-N9A	-2.88	102.67	105.81
3	A	1000	NAD	C1B-N9A-C8A	-2.82	120.85	127.09
3	C	1000	NAD	O7N-C7N-C3N	2.81	123.03	119.60
3	B	1000	NAD	C4A-C5A-N7A	-2.70	107.50	110.58
3	C	1000	NAD	C6N-N1N-C2N	-2.65	119.63	121.88
3	B	1000	NAD	O2A-PA-O1A	2.58	124.45	112.44
3	D	1000	NAD	C6N-N1N-C2N	-2.58	119.69	121.88
3	A	1000	NAD	C3D-C2D-C1D	2.56	106.29	101.46
3	B	1000	NAD	C5A-C6A-N6A	-2.52	117.05	123.29
3	A	1000	NAD	O2A-PA-O1A	2.48	123.99	112.44
3	B	1000	NAD	N9A-C8A-N7A	-2.42	110.50	113.94
3	A	1000	NAD	C5A-C6A-N6A	-2.36	117.45	123.29
3	A	1000	NAD	O2N-PN-O3	2.34	113.60	107.27
3	D	1000	NAD	C1B-N9A-C8A	-2.27	122.06	127.09
3	B	1000	NAD	C5A-N7A-C8A	2.19	106.90	103.45
3	B	1000	NAD	O2A-PA-O3	2.15	113.08	107.27
3	D	1000	NAD	N9A-C8A-N7A	-2.14	110.90	113.94
3	D	1000	NAD	C3N-C7N-N7N	2.09	120.31	117.74
3	B	1000	NAD	N6A-C6A-N1A	2.08	123.01	118.38
3	C	1000	NAD	C6A-C5A-N7A	2.08	136.10	132.09
3	D	1000	NAD	O3D-C3D-C4D	-2.07	105.15	111.08
3	C	1000	NAD	O7N-C7N-N7N	-2.02	119.70	122.62

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1000	NAD	O4D-C1D-N1N-C2N
3	B	1000	NAD	O4D-C1D-N1N-C6N
3	B	1000	NAD	C2D-C1D-N1N-C2N
3	B	1000	NAD	C2D-C1D-N1N-C6N
3	C	1000	NAD	O4D-C1D-N1N-C2N
3	C	1000	NAD	O4D-C1D-N1N-C6N
3	C	1000	NAD	C2D-C1D-N1N-C2N
3	C	1000	NAD	C2D-C1D-N1N-C6N
3	D	1000	NAD	O4D-C1D-N1N-C2N

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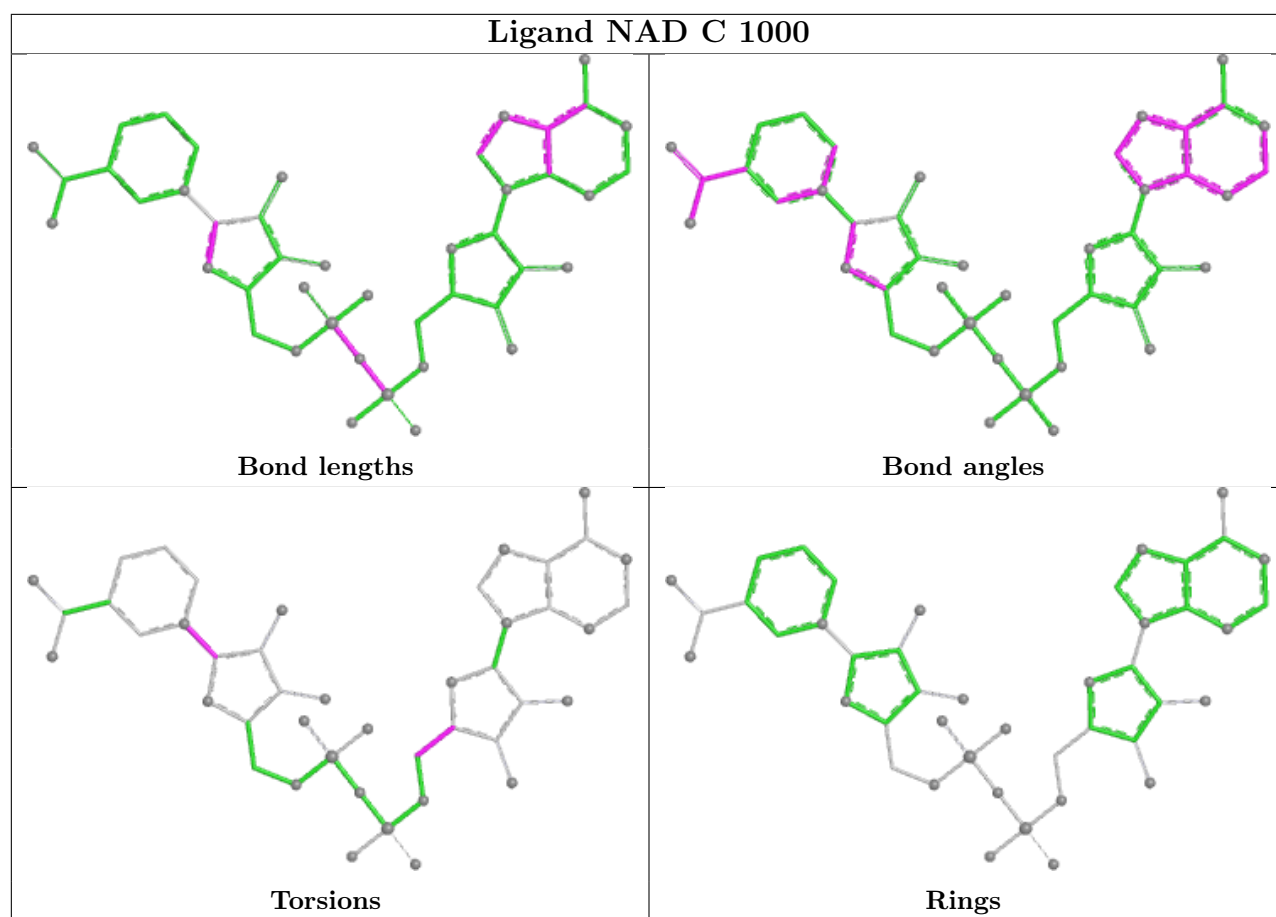
Mol	Chain	Res	Type	Atoms
3	D	1000	NAD	O4D-C1D-N1N-C6N
3	D	1000	NAD	C2D-C1D-N1N-C2N
3	D	1000	NAD	C2D-C1D-N1N-C6N
4	A	1337	EDO	O1-C1-C2-O2
4	B	1338	EDO	O1-C1-C2-O2
3	D	1000	NAD	PN-O3-PA-O1A
4	B	1337	EDO	O1-C1-C2-O2
4	C	1338	EDO	O1-C1-C2-O2
4	B	1339	EDO	O1-C1-C2-O2
3	A	1000	NAD	PN-O3-PA-O2A
3	D	1000	NAD	PN-O3-PA-O2A
3	A	1000	NAD	PN-O3-PA-O1A
3	B	1000	NAD	PN-O3-PA-O1A
3	B	1000	NAD	O4B-C4B-C5B-O5B
4	C	1337	EDO	O1-C1-C2-O2
3	C	1000	NAD	O4B-C4B-C5B-O5B
3	B	1000	NAD	PN-O3-PA-O2A
3	A	1000	NAD	O4B-C4B-C5B-O5B

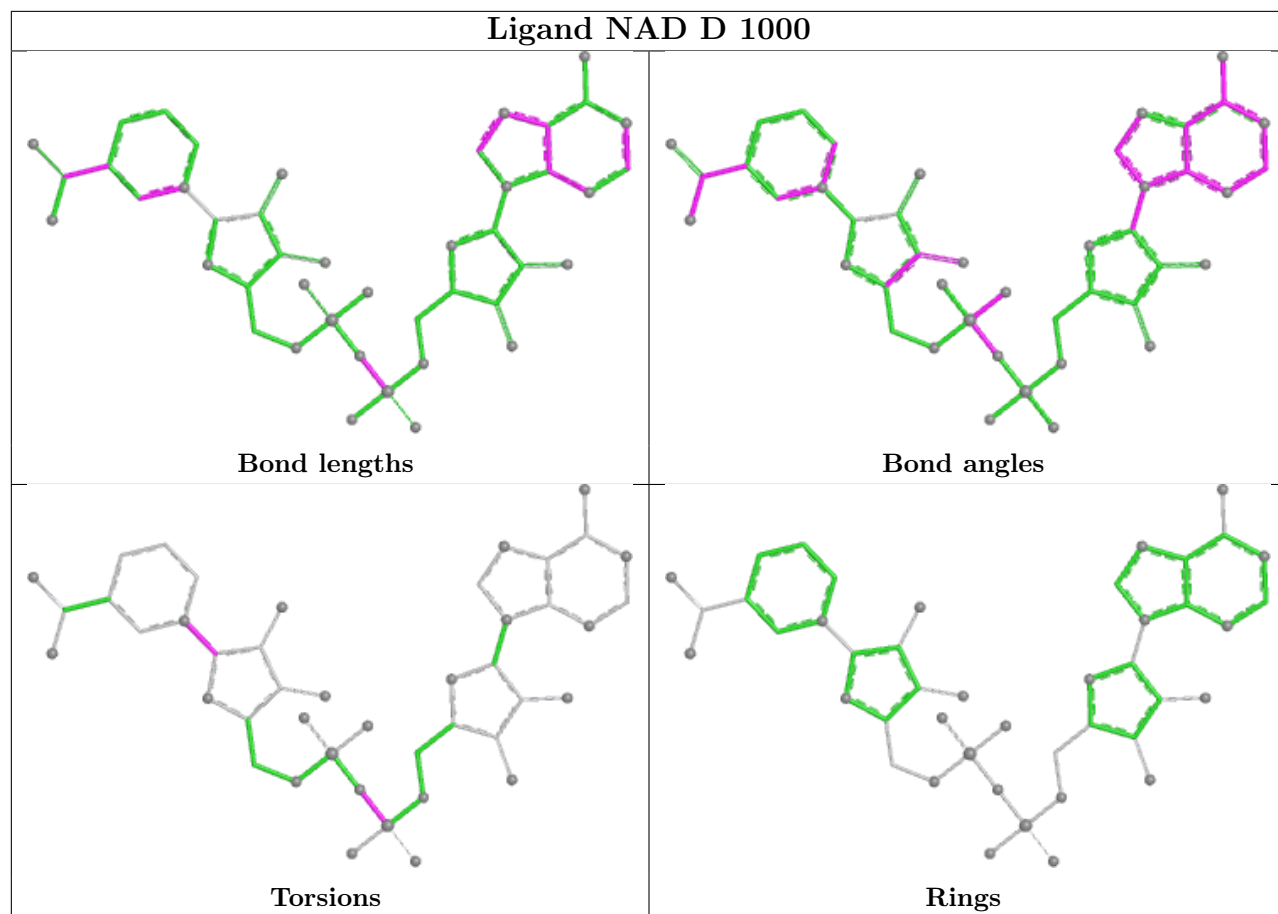
There are no ring outliers.

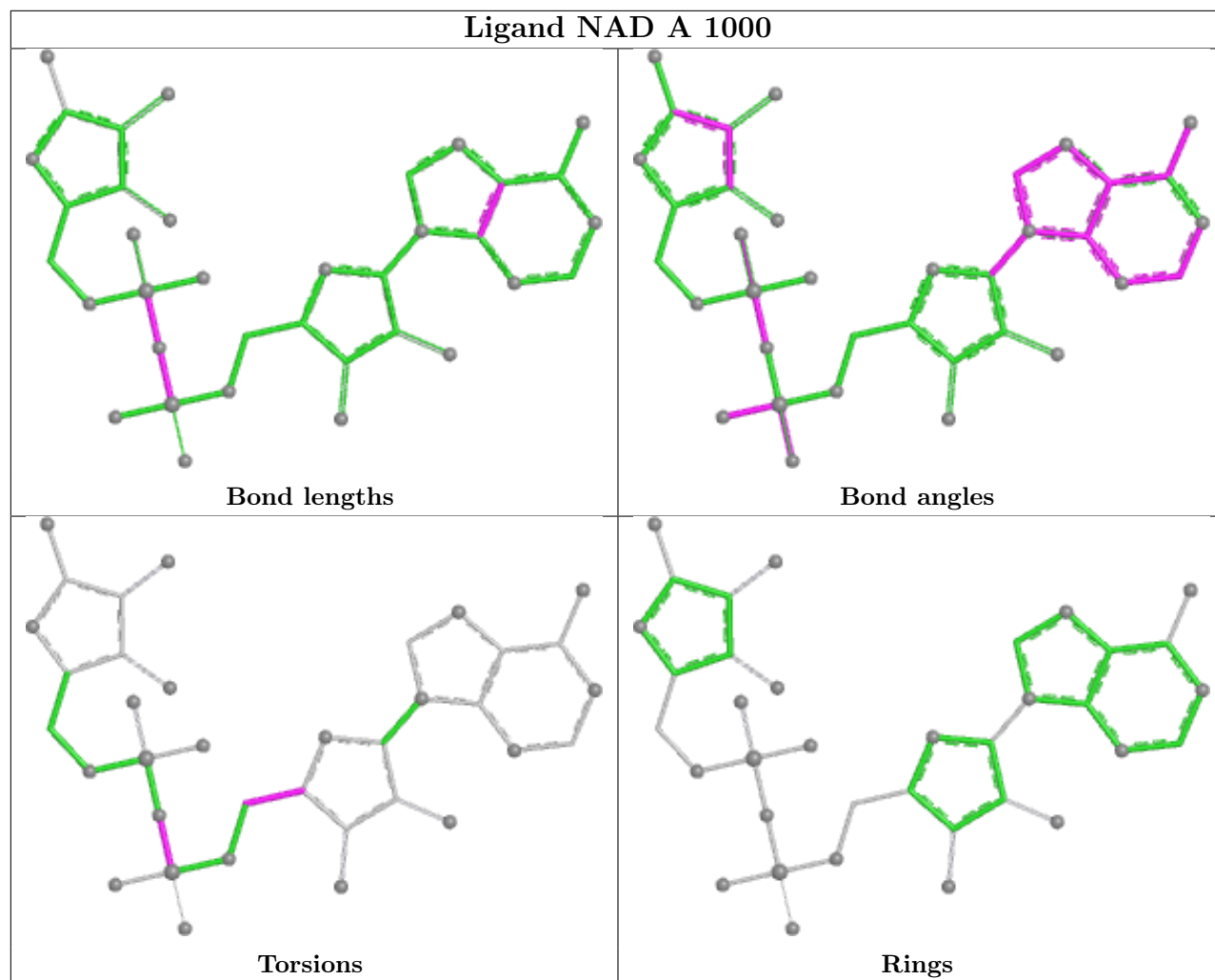
5 monomers are involved in 17 short contacts:

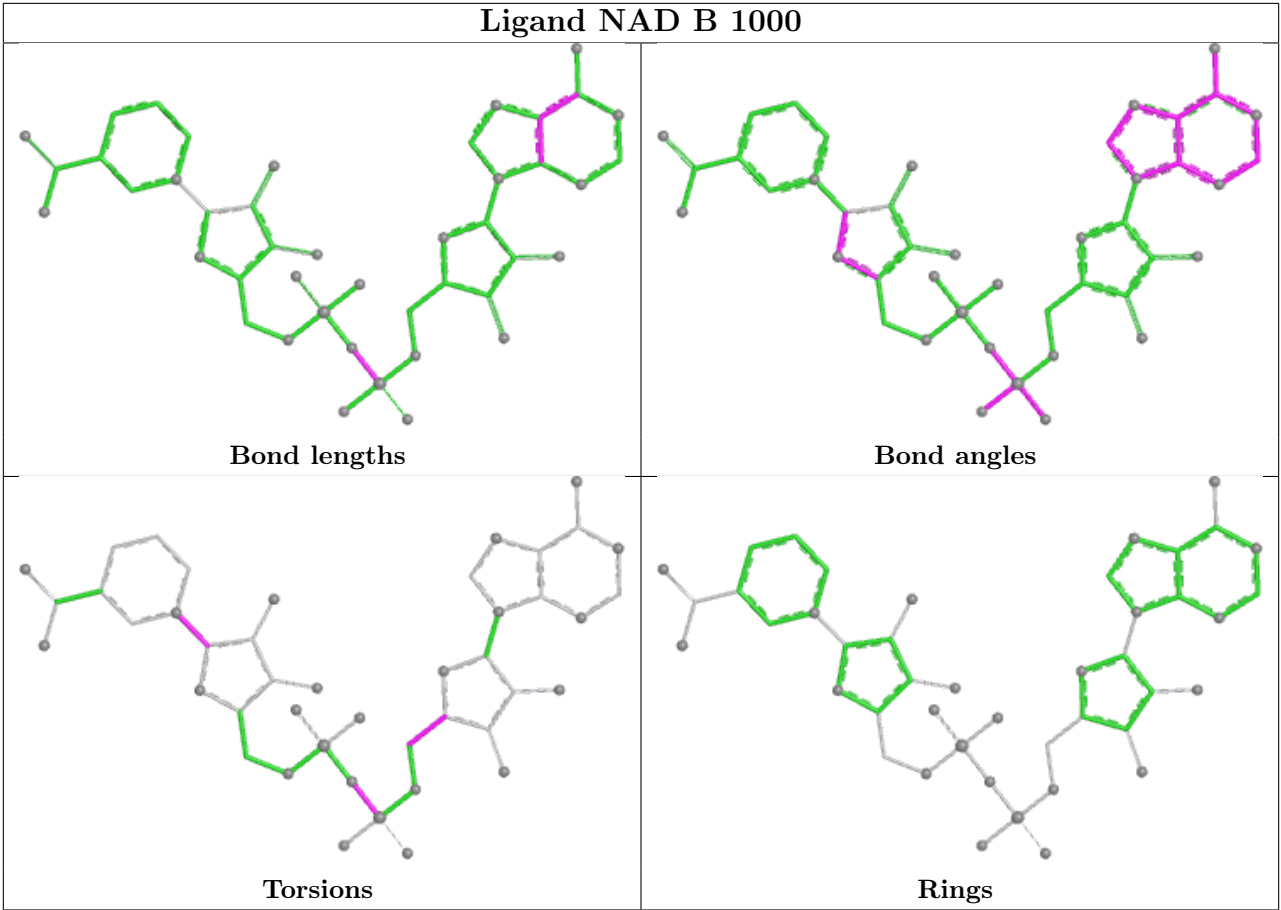
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1337	EDO	4	0
4	B	1338	EDO	3	0
4	C	1337	EDO	5	0
4	C	1338	EDO	3	0
4	B	1339	EDO	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	50:VAL	C	51:ILE	N	0.73

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	326/336 (97%)	0.70	35 (10%) 11 10	23, 46, 77, 96	0
1	B	335/336 (99%)	-0.04	3 (0%) 81 83	19, 33, 54, 73	1 (0%)
1	C	302/336 (89%)	1.00	54 (17%) 3 3	27, 49, 84, 108	0
1	D	270/336 (80%)	1.05	58 (21%) 2 1	25, 47, 93, 110	0
All	All	1233/1344 (91%)	0.65	150 (12%) 8 7	19, 43, 83, 110	1 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	CYS	7.6
1	D	48	LEU	5.3
1	D	131	VAL	5.3
1	A	55	LEU	5.2
1	D	80	ASN	5.1
1	D	125	TYR	5.1
1	D	62	VAL	5.1
1	C	119	LEU	5.0
1	D	36	LEU	5.0
1	C	20	LEU	4.9
1	C	18	LEU	4.8
1	C	113	PHE	4.7
1	D	63	MET	4.7
1	D	126	GLN	4.5
1	D	60	ASN	4.4
1	D	130	LEU	4.4
1	D	34	LEU	4.2
1	D	38	VAL	4.2
1	D	32	GLY	4.2
1	D	49	HIS	4.2
1	D	119	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	62	VAL	4.1
1	D	121	TYR	4.0
1	C	79	ILE	4.0
1	D	50	VAL	3.9
1	D	128	TYR	3.9
1	D	61	TYR	3.8
1	D	51	ILE	3.8
1	C	74	VAL	3.8
1	C	43	LEU	3.7
1	D	113	PHE	3.7
1	A	23	ASP	3.7
1	A	79	ILE	3.6
1	C	22	ASN	3.6
1	C	124	GLY	3.6
1	C	116	TRP	3.5
1	D	104	ALA	3.5
1	D	332	VAL	3.4
1	D	26	VAL	3.4
1	D	114	GLY	3.4
1	D	316	LEU	3.4
1	D	43	LEU	3.4
1	D	29	PRO	3.3
1	D	42	GLY	3.3
1	C	76	ASP	3.3
1	C	118	GLY	3.2
1	C	308	VAL	3.2
1	C	46	SER	3.1
1	C	325	ASN	3.1
1	A	20	LEU	3.1
1	C	45	HIS	3.1
1	A	21	ARG	3.1
1	A	113	PHE	3.0
1	D	333	VAL	3.0
1	D	309	ARG	3.0
1	C	100	TYR	3.0
1	D	100	TYR	3.0
1	C	58	GLY	2.9
1	D	33	GLN	2.9
1	D	129	LEU	2.9
1	A	9	GLY	2.9
1	C	122	ASP	2.9
1	C	132	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	18	LEU	2.8
1	D	65	HIS	2.8
1	D	67	ILE	2.8
1	A	22	ASN	2.8
1	C	59	ASP	2.8
1	C	31	ALA	2.8
1	C	120	GLY	2.8
1	D	27	HIS	2.7
1	C	48	LEU	2.7
1	C	332	VAL	2.7
1	A	54	GLY	2.7
1	A	45	HIS	2.7
1	D	105	ILE	2.7
1	C	262	LEU	2.6
1	C	47	ASP	2.6
1	C	24	LEU	2.6
1	D	118	GLY	2.6
1	C	27	HIS	2.6
1	D	40	ALA	2.6
1	A	317	PRO	2.6
1	B	113	PHE	2.5
1	D	120	GLY	2.5
1	A	60	ASN	2.5
1	D	224	GLU	2.5
1	A	48	LEU	2.5
1	C	117	PHE	2.5
1	C	32	GLY	2.5
1	D	103	GLY	2.5
1	D	47	ASP	2.5
1	C	29	PRO	2.5
1	C	309	ARG	2.5
1	A	320	ILE	2.5
1	C	125	TYR	2.4
1	D	132	THR	2.4
1	A	316	LEU	2.4
1	A	96	GLY	2.4
1	D	127	GLN	2.4
1	C	23	ASP	2.4
1	C	333	VAL	2.4
1	B	57	CYS	2.4
1	A	179	ALA	2.4
1	B	79	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	82	LYS	2.4
1	A	97	GLY	2.4
1	A	120	GLY	2.4
1	C	115	ASP	2.4
1	A	12	PHE	2.4
1	C	26	VAL	2.4
1	C	63	MET	2.4
1	D	146	ALA	2.3
1	C	307	VAL	2.3
1	D	331	ARG	2.3
1	C	140	ILE	2.3
1	C	83	VAL	2.3
1	D	81	TYR	2.3
1	D	314	LYS	2.3
1	A	10	PHE	2.3
1	C	317	PRO	2.3
1	D	28	LYS	2.3
1	C	310	SER	2.2
1	A	25	PRO	2.2
1	C	78	VAL	2.2
1	A	322	LYS	2.2
1	C	319	TYR	2.2
1	D	116	TRP	2.2
1	D	97	GLY	2.2
1	C	311	ALA	2.2
1	C	303	LYS	2.2
1	C	320	ILE	2.1
1	D	71	VAL	2.1
1	A	31	ALA	2.1
1	A	49	HIS	2.1
1	C	129	LEU	2.1
1	A	61	TYR	2.1
1	D	25	PRO	2.1
1	A	51	ILE	2.1
1	D	115	ASP	2.1
1	A	118	GLY	2.1
1	A	3	ILE	2.1
1	D	39	ASP	2.0
1	C	102	ARG	2.0
1	A	310	SER	2.0
1	A	311	ALA	2.0
1	D	31	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	77	ASP	2.0
1	A	52	TYR	2.0
1	A	121	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

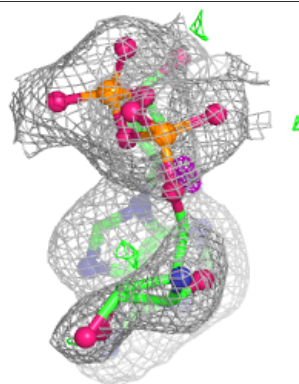
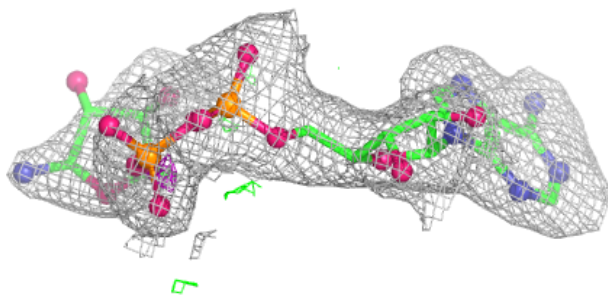
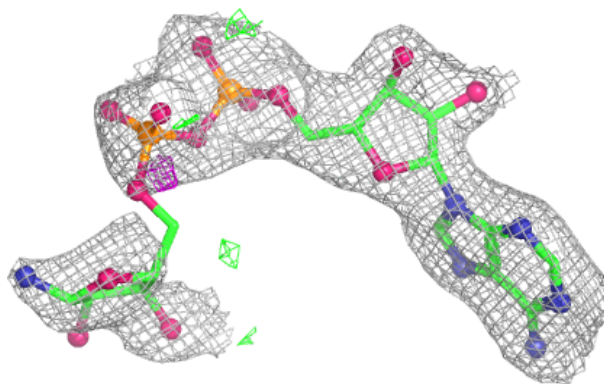
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	1339	4/4	0.81	0.18	46,48,48,56	0
3	NAD	A	1000	36/44	0.86	0.12	40,58,91,94	0
4	EDO	B	1338	4/4	0.88	0.22	40,41,43,46	0
4	EDO	C	1337	4/4	0.88	0.16	51,51,53,54	0
3	NAD	D	1000	44/44	0.89	0.11	43,51,58,67	0
3	NAD	C	1000	44/44	0.89	0.10	42,55,69,72	0
2	ZN	B	499	1/1	0.90	0.10	37,37,37,37	1
4	EDO	A	1337	4/4	0.91	0.17	46,53,59,62	0
4	EDO	B	1337	4/4	0.93	0.27	38,40,42,47	0
4	EDO	C	1338	4/4	0.93	0.20	41,43,45,48	0
2	ZN	D	500	1/1	0.94	0.13	92,92,92,92	0
2	ZN	B	500	1/1	0.97	0.06	28,28,28,28	1
2	ZN	C	500	1/1	0.98	0.08	60,60,60,60	1
3	NAD	B	1000	44/44	0.98	0.04	23,27,31,32	0
2	ZN	A	500	1/1	0.99	0.05	45,45,45,45	1
2	ZN	D	600	1/1	0.99	0.09	50,50,50,50	0
2	ZN	C	600	1/1	0.99	0.10	49,49,49,49	0
2	ZN	A	600	1/1	1.00	0.06	38,38,38,38	1
2	ZN	B	600	1/1	1.00	0.01	36,36,36,36	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.

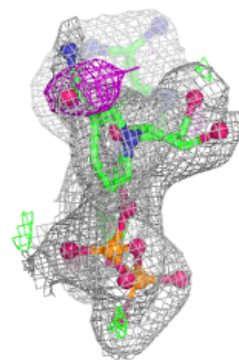
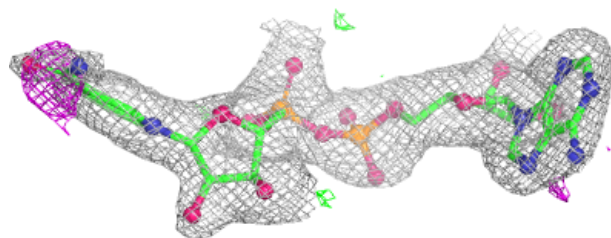
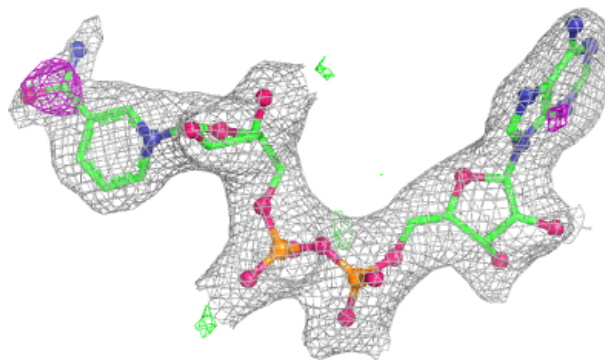
Electron density around NAD A 1000:

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

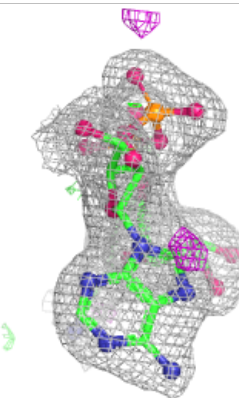
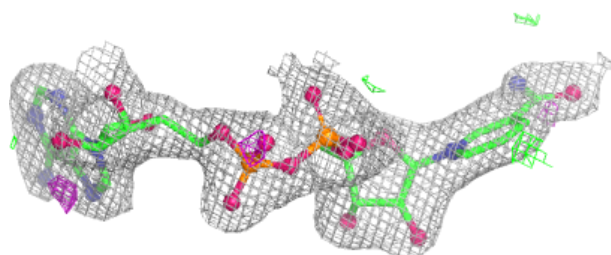
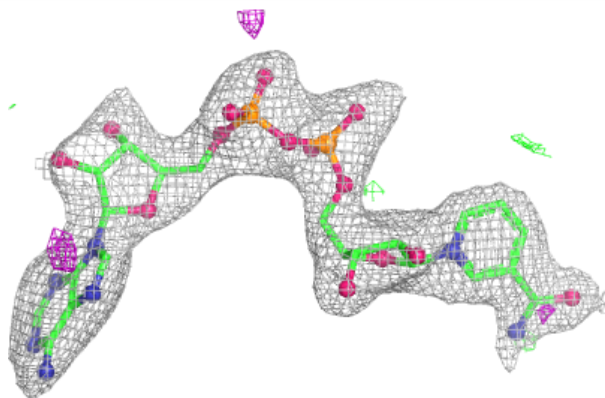


Electron density around NAD D 1000:

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

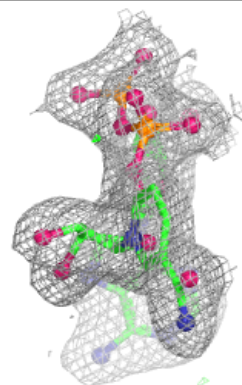
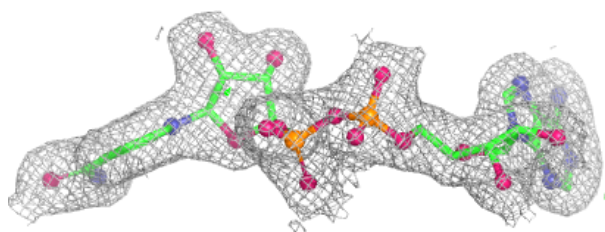
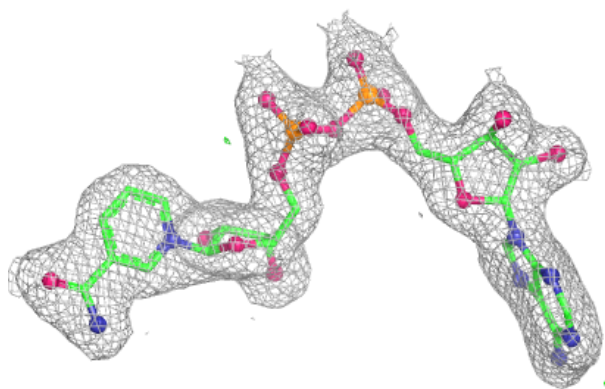
**Electron density around NAD C 1000:**

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



Electron density around NAD B 1000:

$2mF_o-DF_c$ (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.