



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:16 AM UTC

PDB ID : 2WSB / pdb_00002wsb
Title : Crystal structure of the short-chain dehydrogenase Galactitol- Dehydrogenase (GatDH) of Rhodobacter sphaeroides in complex with NAD
Authors : Carius, Y.; Christian, H.; Faust, A.; Kornberger, P.; Kohring, G.W.; Giffhorn, F.; Scheidig, A.J.
Deposited on : 2009-09-04
Resolution : 1.25 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

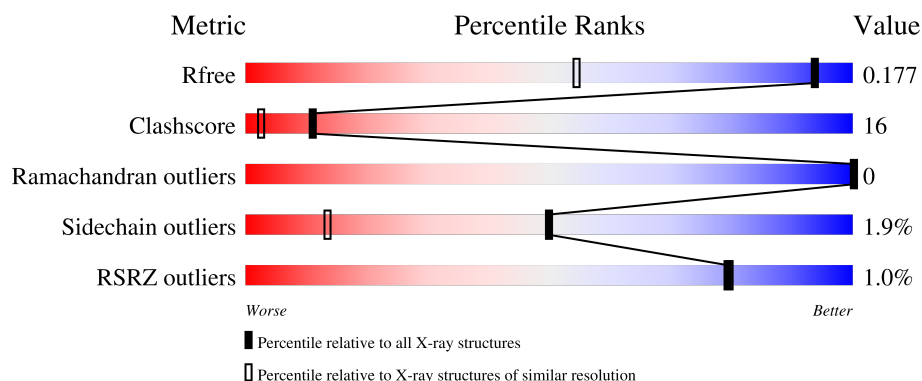
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	254	86% 13% .
1	B	254	3% 78% 17% ..
1	C	254	82% 17% .
1	D	254	% 82% 17% .

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	POL	A	1256	-	X	-	-
4	POL	B	1255[A]	-	-	X	-
4	POL	B	1255[B]	-	-	X	-
4	POL	C	1255	-	X	-	-
4	POL	D	1256	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9942 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 GALACTITOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	14	0
			1968	1227	354	371	16			
1	B	254	Total	C	N	O	S	0	19	0
			2010	1249	373	371	17			
1	C	254	Total	C	N	O	S	0	18	0
			2007	1249	367	372	19			
1	D	254	Total	C	N	O	S	0	14	0
			1978	1228	366	368	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

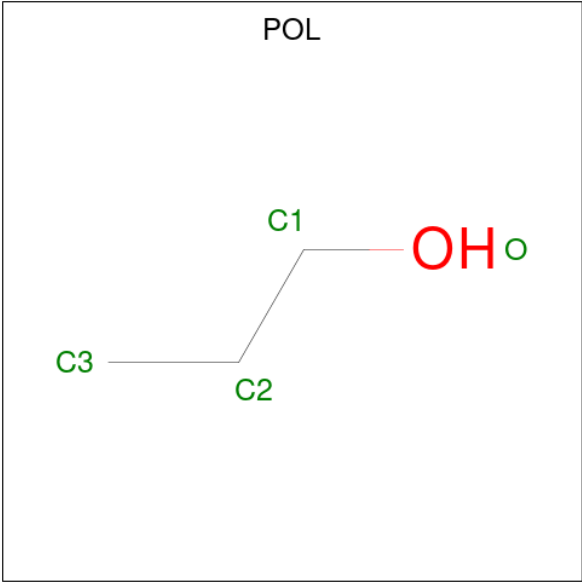
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 4 is N-PROPANOL (CCD ID: POL) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	B	1	Total C O 8 6 2	0	1
4	B	1	Total C O 4 3 1	0	0
4	C	1	Total C O 4 3 1	0	0
4	C	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0

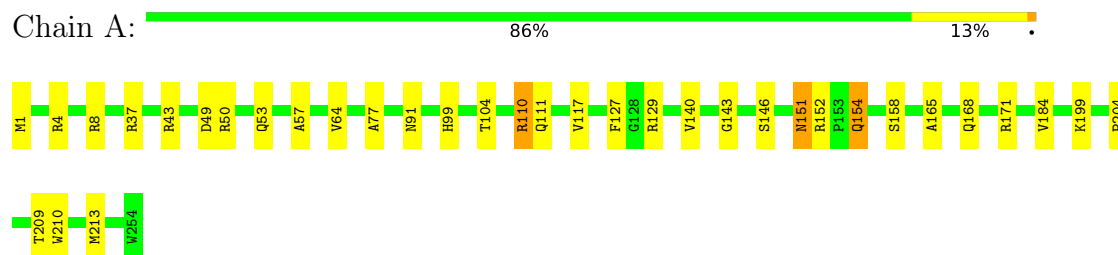
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	469	Total O 469 469	0	0
5	B	417	Total O 417 417	0	0
5	C	456	Total O 456 456	0	0
5	D	423	Total O 423 423	0	0

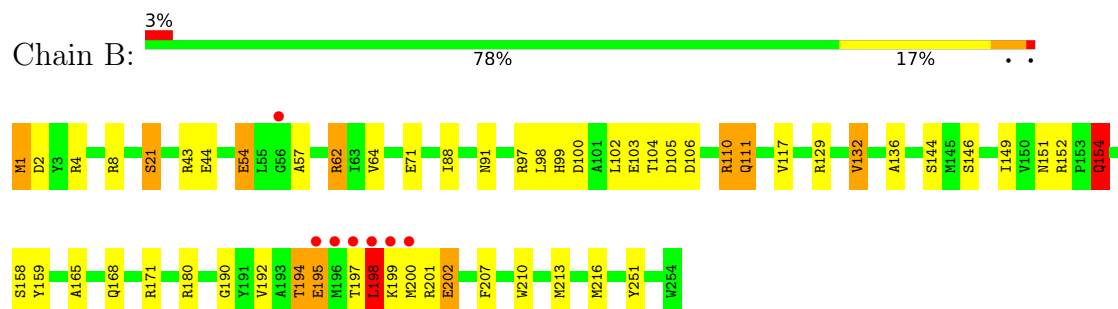
3 Residue-property plots

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.

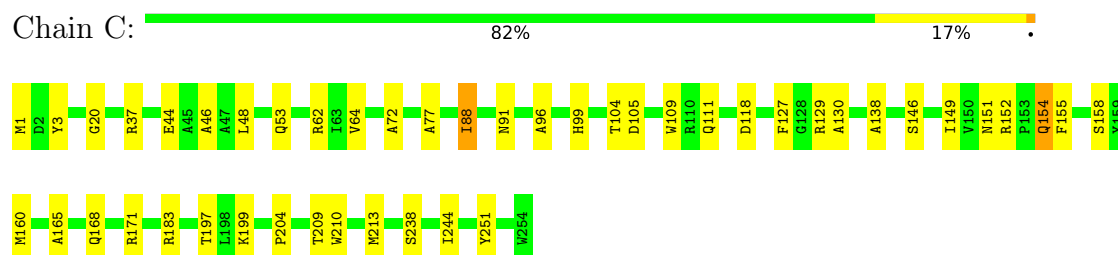
• Molecule 1: GALACTITOL DEHYDROGENASE



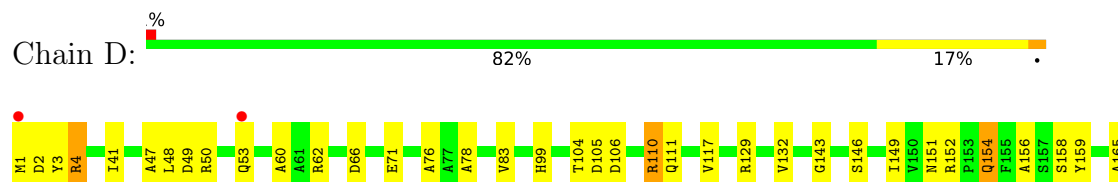
• Molecule 1: GALACTITOL DEHYDROGENASE

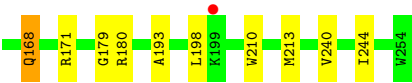


• Molecule 1: GALACTITOL DEHYDROGENASE



• Molecule 1: GALACTITOL DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.79Å 106.62Å 109.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.25 19.94 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.94-1.25) 99.8 (19.94-1.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.134 , 0.177 (Not available) , 0.177	Depositor DCC
R_{free} test set	15688 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9942	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.63	10/2004 (0.5%)	1.36	4/2716 (0.1%)
1	B	1.73	20/2052 (1.0%)	1.36	6/2777 (0.2%)
1	C	1.62	13/2043 (0.6%)	1.35	4/2766 (0.1%)
1	D	1.66	18/2011 (0.9%)	1.34	3/2725 (0.1%)
All	All	1.66	61/8110 (0.8%)	1.35	17/10984 (0.2%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	GLU	C-O	10.10	1.37	1.24
1	B	198	LEU	N-CA	9.37	1.57	1.46
1	D	117	VAL	CA-CB	8.51	1.62	1.55
1	B	117	VAL	CA-CB	7.83	1.62	1.55
1	B	216	MET	SD-CE	-7.81	1.60	1.79
1	A	110	ARG	CG-CD	7.65	1.75	1.52
1	D	41	ILE	C-O	7.53	1.31	1.24
1	B	21	SER	CA-CB	7.46	1.66	1.53
1	A	110	ARG	CZ-NH2	-7.35	1.23	1.33
1	B	111	GLN	CG-CD	7.33	1.70	1.52
1	C	62	ARG	CZ-NH1	7.07	1.42	1.32
1	A	1	MET	CB-CG	7.02	1.73	1.52
1	C	88	ILE	N-CA	6.85	1.54	1.46
1	C	197	THR	CA-CB	6.70	1.64	1.53
1	D	198	LEU	C-O	6.45	1.31	1.24
1	C	209	THR	CA-CB	6.36	1.63	1.53
1	B	91	ASN	CG-OD1	6.22	1.35	1.23
1	B	136	ALA	N-CA	6.18	1.53	1.46
1	D	168	GLN	CD-OE1	6.14	1.35	1.23
1	D	1	MET	SD-CE	6.12	1.94	1.79
1	D	244	ILE	CA-CB	6.08	1.61	1.53
1	B	64	VAL	C-O	6.01	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	ALA	CA-CB	5.95	1.62	1.53
1	B	154	GLN	CD-OE1	5.94	1.34	1.23
1	D	1	MET	CG-SD	5.88	1.95	1.80
1	C	160	MET	CA-C	5.83	1.60	1.52
1	B	88	ILE	N-CA	5.82	1.53	1.46
1	D	50	ARG	CB-CG	-5.78	1.35	1.52
1	D	193	ALA	CA-C	5.73	1.60	1.52
1	B	8	ARG	CG-CD	-5.71	1.35	1.52
1	D	48	LEU	CB-CG	-5.70	1.42	1.53
1	D	50	ARG	CZ-NH1	5.68	1.40	1.32
1	B	103	GLU	CA-C	-5.64	1.45	1.53
1	A	117	VAL	CA-CB	5.62	1.62	1.54
1	C	91	ASN	CG-OD1	5.57	1.34	1.23
1	B	202	GLU	CA-C	5.56	1.60	1.52
1	A	64	VAL	CA-CB	5.49	1.60	1.54
1	D	83	VAL	C-O	5.45	1.29	1.23
1	D	149	ILE	CA-C	-5.37	1.46	1.52
1	D	3	TYR	C-O	5.34	1.30	1.24
1	B	199	LYS	C-O	5.33	1.30	1.24
1	C	197	THR	CA-C	-5.29	1.45	1.52
1	B	98	LEU	CA-CB	5.26	1.61	1.53
1	A	140	VAL	C-O	5.24	1.30	1.24
1	B	103	GLU	C-O	-5.24	1.16	1.23
1	D	156	ALA	N-CA	5.22	1.52	1.46
1	D	78	ALA	CA-CB	-5.19	1.45	1.53
1	A	151	ASN	CG-ND2	-5.18	1.22	1.33
1	B	102	LEU	N-CA	5.16	1.53	1.46
1	C	20	GLY	C-O	5.16	1.30	1.24
1	C	183	ARG	N-CA	5.15	1.52	1.45
1	D	240	VAL	N-CA	5.12	1.52	1.46
1	C	130	ALA	CA-CB	-5.12	1.44	1.53
1	C	238	SER	C-N	5.12	1.40	1.33
1	A	110	ARG	NE-CZ	5.11	1.38	1.33
1	D	50	ARG	N-CA	-5.11	1.40	1.46
1	B	132	VAL	CA-C	5.10	1.59	1.52
1	A	91	ASN	CG-ND2	-5.06	1.22	1.33
1	A	50	ARG	CG-CD	5.05	1.67	1.52
1	C	244	ILE	CA-CB	5.02	1.60	1.53
1	B	192	VAL	CA-CB	-5.00	1.48	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ASP	CA-CB-CG	-7.01	105.59	112.60
1	B	194	THR	CB-CA-C	-6.83	97.43	111.22
1	A	49	ASP	N-CA-C	-6.78	103.81	111.07
1	A	110	ARG	NE-CZ-NH1	-6.70	114.80	121.50
1	D	47	ALA	N-CA-C	-6.21	104.59	111.36
1	C	46	ALA	N-CA-C	-6.08	104.76	111.82
1	B	54	GLU	O-C-N	-5.98	114.11	122.37
1	D	60	ALA	N-CA-C	-5.59	105.57	112.90
1	A	8	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	B	190	GLY	O-C-N	-5.35	118.05	122.92
1	C	118	ASP	CA-C-O	-5.29	115.26	120.82
1	D	76	ALA	N-CA-C	-5.21	105.60	111.28
1	B	91	ASN	O-C-N	5.20	129.19	122.43
1	C	155	PHE	CA-C-O	5.17	126.19	120.71
1	A	184	VAL	CA-C-O	5.09	125.29	120.25
1	B	198	LEU	CB-CG-CD1	5.09	125.96	110.70
1	C	109	TRP	CZ3-CH2-CZ2	5.08	128.11	121.50

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	1968	0	1954	45	0
1	B	2010	0	2013	127	0
1	C	2007	0	2004	55	0
1	D	1978	0	1967	57	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	7	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
4	A	8	0	16	1	0
4	B	12	0	23	20	0
4	C	8	0	16	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	16	7	0
5	A	469	0	0	12	2
5	B	417	0	0	21	1
5	C	456	0	0	15	2
5	D	423	0	0	14	1
All	All	9942	0	8113	268	3

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 16.

All (268) 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:A:110:ARG:CG	1:A:110:ARG:CD	1.75	1.55
1:B:198:LEU:CD2	1:B:198:LEU:H	1.29	1.38
1:B:195[B]:GLU:C	1:B:198:LEU:HD21	1.49	1.38
1:B:1[B]:MET:HE2	5:C:2432:HOH:O	1.24	1.32
1:B:198:LEU:N	1:B:198:LEU:HD22	1.36	1.28
1:A:4[A]:ARG:NH1	5:A:2015:HOH:O	1.69	1.26
1:B:197:THR:O	1:B:201[B]:ARG:HG3	1.17	1.26
5:B:2395:HOH:O	1:C:1[B]:MET:HE3	1.36	1.24
1:C:213[A]:MET:HE2	5:D:2419:HOH:O	1.18	1.22
3:B:500:NAD:C5N	4:B:1255[B]:POL:O	1.90	1.18
1:C:213[A]:MET:CE	5:D:2419:HOH:O	1.64	1.16
1:B:198:LEU:CA	1:B:201[B]:ARG:HD3	1.76	1.15
1:C:213[B]:MET:HE1	1:D:213[B]:MET:CE	1.78	1.11
1:A:110:ARG:NH1	5:A:2326:HOH:O	1.60	1.11
1:B:43:ARG:NH1	1:B:44[B]:GLU:OE2	1.84	1.10
1:C:152[A]:ARG:HD3	1:C:213[A]:MET:SD	1.94	1.08
1:B:110[A]:ARG:NH1	5:B:2276:HOH:O	1.71	1.07
1:B:21:SER:OG	1:B:195[A]:GLU:HG3	1.55	1.06
1:B:195[B]:GLU:CA	1:B:198:LEU:HD21	1.87	1.04
1:B:198:LEU:HA	1:B:201[B]:ARG:CD	1.85	1.04
1:B:198:LEU:HA	1:B:201[B]:ARG:HD3	1.04	1.04
1:D:152[A]:ARG:HD3	1:D:213[A]:MET:HE1	1.41	1.03
1:B:197:THR:O	1:B:201[B]:ARG:CG	2.08	1.01
1:D:111[B]:GLN:OE1	5:D:2291:HOH:O	1.76	1.00
1:B:198:LEU:H	1:B:198:LEU:HD23	1.25	1.00
1:D:71[A]:GLU:HG2	5:D:2201:HOH:O	1.59	0.99
1:B:195[B]:GLU:O	1:B:198:LEU:HD21	1.61	0.99
1:B:195[B]:GLU:O	1:B:198:LEU:CD2	2.12	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213[B]:MET:HE1	1:D:213[B]:MET:HE3	1.46	0.96
1:B:195[B]:GLU:N	1:B:198:LEU:HD11	1.81	0.95
1:B:198:LEU:H	1:B:198:LEU:HD22	0.91	0.94
1:B:195[A]:GLU:C	1:B:198:LEU:HD21	1.92	0.94
1:B:195[B]:GLU:C	1:B:198:LEU:CD2	2.41	0.94
1:B:195[B]:GLU:CA	1:B:198:LEU:HD11	1.97	0.94
1:D:49:ASP:OD1	1:D:62[A]:ARG:NE	2.01	0.94
1:A:152:ARG:HD3	1:A:213[B]:MET:SD	2.08	0.93
1:B:195[B]:GLU:HA	1:B:198:LEU:HD21	1.47	0.93
1:D:152[A]:ARG:HH11	1:D:213[A]:MET:HE1	1.33	0.92
1:B:159:TYR:OH	4:B:1255[B]:POL:H12	1.70	0.92
1:D:152[A]:ARG:HH11	1:D:213[A]:MET:CE	1.82	0.91
1:B:195[B]:GLU:HA	1:B:198:LEU:HD11	1.52	0.91
1:B:110[A]:ARG:NH1	5:B:2280:HOH:O	2.02	0.90
1:B:21:SER:HG	1:B:195[A]:GLU:HG3	1.34	0.90
1:C:213[B]:MET:CE	1:D:213[B]:MET:CE	2.50	0.90
1:C:204:PRO:HG3	5:C:2072:HOH:O	1.72	0.89
1:B:195[B]:GLU:HA	1:B:198:LEU:CD2	2.03	0.89
1:B:195[A]:GLU:OE2	5:B:2353:HOH:O	1.90	0.88
1:B:201[B]:ARG:HB2	5:B:2358:HOH:O	1.74	0.88
1:B:213[B]:MET:HA	1:B:213[B]:MET:HE2	1.56	0.88
1:B:198:LEU:CD2	1:B:198:LEU:N	2.00	0.87
1:B:110[A]:ARG:NE	5:B:2276:HOH:O	2.04	0.87
1:B:54:GLU:HG2	5:B:2166:HOH:O	1.76	0.86
1:B:195[B]:GLU:HA	1:B:198:LEU:CG	2.08	0.83
1:B:195[B]:GLU:HA	1:B:198:LEU:CD1	2.08	0.83
1:B:154:GLN:H	1:B:154:GLN:HE21	1.28	0.81
1:C:152[A]:ARG:HD3	1:C:213[A]:MET:CE	2.10	0.80
1:C:213[B]:MET:CE	1:D:213[B]:MET:HE1	2.11	0.80
1:C:105[B]:ASP:OD1	5:C:2293:HOH:O	1.99	0.79
1:A:37[A]:ARG:NH1	1:A:57:ALA:O	2.16	0.78
1:C:213[B]:MET:SD	1:D:213[B]:MET:HE1	2.23	0.77
1:B:159:TYR:CZ	4:B:1255[B]:POL:H12	2.21	0.76
1:D:105[A]:ASP:OD1	5:D:2273:HOH:O	2.04	0.76
1:C:111[B]:GLN:NE2	5:C:2312:HOH:O	2.18	0.76
1:C:152[B]:ARG:NH2	5:C:2346:HOH:O	2.18	0.76
1:D:154:GLN:H	1:D:154:GLN:HE21	1.33	0.75
3:B:500:NAD:C6N	4:B:1255[B]:POL:O	2.35	0.75
1:B:1[A]:MET:HE1	5:B:2112:HOH:O	1.87	0.74
1:B:194:THR:C	1:B:198:LEU:HD11	2.12	0.74
1:A:37[B]:ARG:HD3	5:A:2135:HOH:O	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLN:HE22	1:C:210:TRP:HE1	1.35	0.74
1:B:144:SER:OG	4:B:1255[B]:POL:H11	1.88	0.74
5:B:2395:HOH:O	1:C:1[B]:MET:CE	2.11	0.74
1:B:194:THR:O	1:B:198:LEU:CD1	2.36	0.74
1:A:199[B]:LYS:NZ	5:A:2401:HOH:O	2.22	0.73
3:B:500:NAD:C4N	4:B:1255[B]:POL:O	2.37	0.72
1:B:152[A]:ARG:NH2	5:B:2308:HOH:O	2.22	0.72
1:B:146:SER:OG	4:B:1255[B]:POL:H33	1.89	0.72
1:B:194:THR:C	1:B:198:LEU:CD1	2.63	0.72
1:B:195[A]:GLU:HA	1:B:198:LEU:HD11	1.71	0.72
1:C:154:GLN:HE21	1:C:154:GLN:H	1.38	0.71
1:B:195[B]:GLU:O	1:B:198:LEU:HD23	1.90	0.71
1:C:152[A]:ARG:CD	1:C:213[A]:MET:SD	2.78	0.70
1:B:159:TYR:CE2	4:B:1255[B]:POL:H12	2.25	0.70
1:A:154:GLN:H	1:A:154:GLN:HE21	1.38	0.70
4:B:1255[A]:POL:H22	4:B:1256:POL:H12	1.73	0.70
1:B:154:GLN:HE22	1:B:210:TRP:HE1	1.39	0.70
1:D:105[B]:ASP:OD1	5:D:2269:HOH:O	2.09	0.70
1:B:197:THR:HG22	4:B:1255[A]:POL:H32	1.75	0.69
1:C:213[B]:MET:CE	1:D:152[B]:ARG:NH1	2.55	0.69
1:A:43[A]:ARG:NH1	5:A:2146:HOH:O	2.27	0.68
1:B:146:SER:HG	4:B:1255[B]:POL:H33	1.59	0.68
1:C:99:HIS:HD2	1:C:104:THR:OG1	1.77	0.67
1:B:154:GLN:H	1:B:154:GLN:NE2	1.92	0.67
1:D:152[A]:ARG:NE	5:D:2317:HOH:O	2.27	0.67
1:A:37[A]:ARG:CZ	1:A:57:ALA:O	2.43	0.66
1:C:53[B]:GLN:NE2	5:C:2158:HOH:O	2.17	0.66
1:C:152[A]:ARG:HD3	1:C:213[A]:MET:HE1	1.76	0.66
1:D:154:GLN:HE22	1:D:210:TRP:HE1	1.42	0.66
1:A:53:GLN:NE2	5:A:2194:HOH:O	2.29	0.66
1:D:152[A]:ARG:HD3	1:D:213[A]:MET:CE	2.23	0.66
1:A:110:ARG:CG	1:A:110:ARG:NE	2.57	0.65
1:D:99:HIS:HD2	1:D:104:THR:OG1	1.78	0.65
1:D:152[A]:ARG:NH2	5:D:2316:HOH:O	2.28	0.64
1:C:213[B]:MET:HE3	1:D:152[B]:ARG:NH1	2.12	0.64
1:D:62[A]:ARG:NH1	5:D:2170:HOH:O	2.28	0.64
1:B:159:TYR:OH	4:B:1255[B]:POL:C1	2.46	0.64
1:B:180[B]:ARG:HD2	5:B:2330:HOH:O	1.96	0.64
1:C:44[B]:GLU:OE2	5:C:2137:HOH:O	2.15	0.63
1:C:146:SER:HG	4:C:1255:POL:H21	1.64	0.63
1:A:154:GLN:H	1:A:154:GLN:NE2	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97[B]:ARG:NH2	1:B:111:GLN:HG2	2.13	0.63
1:B:197:THR:HG22	4:B:1255[A]:POL:C3	2.29	0.63
1:B:197:THR:C	1:B:201[B]:ARG:HG3	2.15	0.62
1:D:154:GLN:H	1:D:154:GLN:NE2	1.97	0.62
1:B:201[A]:ARG:HG2	1:B:207:PHE:CE1	2.33	0.62
1:C:213[B]:MET:HE3	1:C:213[B]:MET:HA	1.81	0.62
1:D:159:TYR:OH	4:D:1256:POL:C1	2.47	0.62
1:B:105[B]:ASP:OD1	5:B:2269:HOH:O	2.16	0.61
1:B:194:THR:O	1:B:198:LEU:CD2	2.48	0.61
1:A:213[B]:MET:HE1	5:A:2356:HOH:O	2.00	0.61
1:C:154:GLN:H	1:C:154:GLN:NE2	1.98	0.61
1:D:152[A]:ARG:CD	1:D:213[A]:MET:HE1	2.26	0.61
1:B:1[A]:MET:CG	5:C:2432:HOH:O	2.48	0.60
1:D:159:TYR:CZ	4:D:1256:POL:H11	2.36	0.60
1:B:195[A]:GLU:N	1:B:198:LEU:HD11	2.17	0.60
1:A:152:ARG:NH1	1:B:213[B]:MET:CE	2.64	0.60
1:B:194:THR:O	1:B:198:LEU:HD13	2.02	0.59
1:D:49:ASP:OD1	1:D:62[A]:ARG:CZ	2.50	0.59
1:B:110[A]:ARG:CZ	5:B:2276:HOH:O	2.13	0.59
1:C:129[B]:ARG:NH1	5:C:2327:HOH:O	2.35	0.59
1:B:1[A]:MET:HG3	5:C:2432:HOH:O	2.02	0.58
1:A:213[B]:MET:CE	1:B:213[B]:MET:HE1	2.34	0.58
1:B:4[A]:ARG:NH2	5:B:2022:HOH:O	2.35	0.58
1:D:152[A]:ARG:NH1	1:D:213[A]:MET:CE	2.61	0.58
1:C:213[B]:MET:HE1	1:D:152[B]:ARG:NH1	2.17	0.58
1:B:99:HIS:HD2	1:B:104:THR:OG1	1.87	0.57
1:A:152:ARG:HH12	1:B:213[B]:MET:CE	2.17	0.57
1:B:57[A]:ALA:HB1	5:B:2168:HOH:O	2.04	0.57
1:B:197:THR:C	1:B:198:LEU:HD22	2.21	0.57
1:A:99:HIS:HD2	1:A:104:THR:OG1	1.88	0.57
1:D:129[B]:ARG:NH1	5:D:2299:HOH:O	2.30	0.57
1:D:152[A]:ARG:HG2	5:D:2317:HOH:O	2.04	0.57
1:A:37[A]:ARG:NH2	1:A:57:ALA:O	2.38	0.56
1:A:110:ARG:CD	1:A:110:ARG:CB	2.76	0.56
1:B:159:TYR:CE2	4:B:1255[B]:POL:C1	2.88	0.56
1:B:201[B]:ARG:HA	1:B:207:PHE:CD1	2.41	0.56
1:B:198:LEU:HD13	1:B:201[A]:ARG:NH2	2.21	0.56
1:B:195[A]:GLU:CA	1:B:198:LEU:HD11	2.33	0.55
1:B:195[A]:GLU:CG	3:B:500:NAD:O2A	2.55	0.55
1:B:151:ASN:H	1:B:151:ASN:HD22	1.55	0.55
1:B:195[A]:GLU:HG3	3:B:500:NAD:O2A	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:HE22	1:A:210:TRP:HE1	1.54	0.54
1:A:129:ARG:NH1	5:A:2339:HOH:O	2.06	0.54
1:D:159:TYR:CE2	4:D:1256:POL:H11	2.42	0.54
1:C:1[B]:MET:SD	1:C:3:TYR:CE1	3.00	0.54
1:A:151:ASN:HD22	1:A:151:ASN:H	1.54	0.53
1:D:151:ASN:HD22	1:D:151:ASN:H	1.56	0.53
1:A:152:ARG:CD	1:A:213[B]:MET:SD	2.90	0.53
3:B:500:NAD:O7N	4:B:1255[A]:POL:H33	2.08	0.53
1:D:2:ASP:OD1	1:D:4[A]:ARG:HB2	2.09	0.53
1:D:179:GLY:C	1:D:180[A]:ARG:HG3	2.32	0.53
1:D:146:SER:OG	4:D:1256:POL:H33	2.08	0.53
1:B:159:TYR:HE2	4:B:1255[B]:POL:C1	2.22	0.52
1:A:152:ARG:HH12	1:B:213[B]:MET:HE2	1.74	0.52
1:B:198:LEU:N	1:B:201[B]:ARG:HD3	2.24	0.52
1:C:213[B]:MET:CE	1:D:213[B]:MET:SD	2.98	0.52
1:D:152[A]:ARG:NH1	1:D:213[A]:MET:HE1	2.15	0.52
1:B:110[A]:ARG:CZ	1:B:110[A]:ARG:HA	2.40	0.51
1:B:195[A]:GLU:CA	1:B:198:LEU:HD21	2.34	0.51
1:C:37[A]:ARG:HG2	1:C:37[A]:ARG:HH21	1.75	0.51
1:C:213[B]:MET:CE	1:D:152[B]:ARG:HH12	2.24	0.51
1:A:110:ARG:HD3	5:A:2143:HOH:O	2.10	0.51
1:C:154:GLN:NE2	1:C:210:TRP:HE1	2.04	0.50
1:A:152:ARG:NH1	1:B:213[B]:MET:HE1	2.26	0.50
1:A:213[B]:MET:HE1	1:B:213[B]:MET:HE1	1.92	0.50
1:D:105[B]:ASP:O	1:D:106:ASP:C	2.51	0.50
1:B:201[A]:ARG:HA	1:B:207:PHE:CD1	2.46	0.50
1:C:99:HIS:HE1	1:C:158:SER:OG	1.95	0.50
1:B:54:GLU:CG	5:B:2166:HOH:O	2.45	0.49
1:C:48[A]:LEU:HD12	1:C:64:VAL:HG22	1.94	0.49
1:D:132:VAL:HG13	1:D:180[B]:ARG:HD2	1.94	0.49
1:C:168:GLN:HE22	1:C:171:ARG:HE	1.60	0.49
1:C:151:ASN:HD22	1:C:151:ASN:H	1.60	0.49
1:C:152[A]:ARG:CD	1:C:213[A]:MET:HE1	2.41	0.49
1:C:204:PRO:CG	5:C:2072:HOH:O	2.45	0.49
1:D:154:GLN:NE2	1:D:210:TRP:HE1	2.10	0.49
1:B:154:GLN:NE2	1:B:210:TRP:HE1	2.06	0.49
1:A:209:THR:O	1:A:213[B]:MET:HG3	2.12	0.48
1:C:213[A]:MET:HE3	5:D:2419:HOH:O	1.65	0.48
1:C:111[A]:GLN:OE1	5:C:2311:HOH:O	2.20	0.48
1:A:37[B]:ARG:CD	5:A:2135:HOH:O	2.54	0.48
1:B:99:HIS:HE1	1:B:158:SER:OG	1.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2280:HOH:O	1:D:110[A]:ARG:NH2	2.46	0.48
1:C:213[B]:MET:HE2	1:D:213[B]:MET:SD	2.53	0.48
1:B:99:HIS:CE1	1:B:158:SER:H	2.32	0.48
1:B:1[A]:MET:HG2	5:C:2432:HOH:O	2.12	0.48
1:A:154:GLN:NE2	1:A:210:TRP:HE1	2.11	0.47
1:B:144:SER:OG	4:B:1255[B]:POL:C1	2.61	0.47
1:B:201[A]:ARG:HG2	1:B:207:PHE:CD1	2.49	0.47
1:A:152:ARG:NH1	1:B:213[B]:MET:HE2	2.28	0.47
1:A:204:PRO:HG2	5:A:2093:HOH:O	2.13	0.47
1:B:198:LEU:HD13	1:B:201[B]:ARG:NH1	2.29	0.47
1:D:168:GLN:HE22	1:D:171:ARG:HE	1.63	0.47
1:A:168:GLN:HE22	1:A:171:ARG:HE	1.62	0.47
1:B:62[B]:ARG:O	1:B:62[B]:ARG:HG3	2.14	0.47
1:B:198:LEU:HD13	1:B:201[A]:ARG:HH22	1.79	0.47
1:C:99:HIS:CD2	1:C:104:THR:OG1	2.65	0.47
1:B:201[A]:ARG:CG	1:B:207:PHE:CE1	2.98	0.47
1:B:57[A]:ALA:CB	5:B:2168:HOH:O	2.60	0.46
1:B:213[B]:MET:HE2	1:B:213[B]:MET:CA	2.37	0.46
1:D:110[A]:ARG:NH2	5:D:2285:HOH:O	2.45	0.46
1:B:129[B]:ARG:NH1	5:B:2293:HOH:O	2.48	0.46
1:D:159:TYR:OH	4:D:1256:POL:H11	2.16	0.46
1:C:96:ALA:HB1	4:C:1256:POL:H31	1.98	0.46
1:C:1[B]:MET:CE	5:C:2439:HOH:O	2.64	0.46
1:B:197:THR:CG2	4:B:1255[A]:POL:C3	2.93	0.45
1:B:201[A]:ARG:HG2	1:B:207:PHE:HE1	1.77	0.45
1:B:71:GLU:HG3	5:B:2204:HOH:O	2.15	0.45
1:B:197:THR:C	1:B:201[B]:ARG:CG	2.83	0.45
1:B:97[B]:ARG:HH22	1:B:111:GLN:HG2	1.80	0.45
1:A:99:HIS:HE1	1:A:158:SER:OG	2.00	0.45
1:B:159:TYR:HE2	4:B:1255[B]:POL:H11	1.80	0.45
1:B:197:THR:C	1:B:201[B]:ARG:CD	2.89	0.45
1:B:202:GLU:HG3	5:B:2358:HOH:O	2.15	0.45
1:A:4[A]:ARG:NH2	5:A:2021:HOH:O	2.49	0.45
1:A:213[B]:MET:HE3	1:B:213[B]:MET:HE1	1.99	0.45
1:B:165:ALA:HB2	1:D:165:ALA:HB2	1.99	0.45
1:B:194:THR:C	1:B:198:LEU:HD13	2.38	0.45
1:C:99:HIS:CE1	1:C:158:SER:H	2.34	0.45
1:D:146:SER:OG	4:D:1256:POL:C3	2.65	0.45
1:D:4[B]:ARG:NE	5:D:2028:HOH:O	2.48	0.44
1:A:99:HIS:CE1	1:A:158:SER:H	2.36	0.44
1:D:99:HIS:CE1	1:D:158:SER:H	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:OG	4:A:1256:POL:C3	2.66	0.44
1:B:197:THR:OG1	1:B:201[B]:ARG:HD2	2.16	0.44
1:C:105[B]:ASP:CG	5:C:2293:HOH:O	2.57	0.43
1:D:146:SER:HG	4:D:1256:POL:H33	1.82	0.43
1:B:168:GLN:HE22	1:B:171:ARG:HE	1.65	0.43
1:C:99:HIS:CE1	1:C:158:SER:OG	2.71	0.43
1:B:99:HIS:HE1	1:B:158:SER:H	1.67	0.43
1:A:99:HIS:HE1	1:A:158:SER:H	1.65	0.43
1:C:77:ALA:HA	1:C:127:PHE:CE1	2.54	0.43
1:A:77:ALA:HA	1:A:127:PHE:CE1	2.54	0.43
1:B:198:LEU:HD13	1:B:201[B]:ARG:HH11	1.83	0.43
1:B:2:ASP:OD1	1:B:4[B]:ARG:HB2	2.20	0.42
1:C:213[B]:MET:HE1	1:D:213[B]:MET:HE1	1.69	0.42
1:D:99:HIS:HE1	1:D:158:SER:OG	2.02	0.42
1:D:143:GLY:O	3:D:500:NAD:H6N	2.20	0.42
1:A:165:ALA:HB2	1:C:165:ALA:HB2	2.01	0.42
1:B:21:SER:OG	1:B:195[A]:GLU:CG	2.46	0.42
1:D:99:HIS:CD2	1:D:104:THR:OG1	2.66	0.42
1:A:111[B]:GLN:HA	1:A:111[B]:GLN:HE21	1.85	0.42
1:B:1[B]:MET:HE3	1:B:1[B]:MET:HB3	1.78	0.41
1:B:99:HIS:CE1	1:B:158:SER:OG	2.72	0.41
1:A:99:HIS:CE1	1:A:158:SER:OG	2.73	0.41
1:C:213[B]:MET:HB2	1:C:251:TYR:CE1	2.56	0.41
3:B:500:NAD:C4N	4:B:1255[A]:POL:H11	2.50	0.41
1:D:66[B]:ASP:OD2	3:D:500:NAD:N6A	2.53	0.41
1:B:110[A]:ARG:HB2	1:B:110[A]:ARG:HH21	1.85	0.41
1:B:200:MET:HB3	1:B:210:TRP:CH2	2.55	0.41
1:B:213[B]:MET:HB3	1:B:251:TYR:CE1	2.55	0.41
1:B:132:VAL:HG13	1:B:180[A]:ARG:HD2	2.03	0.40
1:A:143:GLY:O	3:A:500:NAD:H6N	2.21	0.40
1:B:105[B]:ASP:O	1:B:106:ASP:C	2.63	0.40
1:C:149:ILE:C	1:C:149:ILE:HD12	2.46	0.40
1:B:149:ILE:HD12	1:B:149:ILE:C	2.46	0.40
1:C:88:ILE:HA	1:C:138:ALA:O	2.21	0.40
1:B:194:THR:O	1:B:198:LEU:CG	2.70	0.40

All (3) 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)
5:A:2208:HOH:O	5:C:2144:HOH:O[3_655]	1.99	0.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2089:HOH:O	5:B:2362:HOH:O[3_655]	2.04	0.16
5:C:2068:HOH:O	5:D:2215:HOH:O[2_674]	2.12	0.08

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	266/254 (105%)	262 (98%)	4 (2%)	0	100	100
1	B	270/254 (106%)	266 (98%)	4 (2%)	0	100	100
1	C	269/254 (106%)	264 (98%)	5 (2%)	0	100	100
1	D	266/254 (105%)	264 (99%)	2 (1%)	0	100	100
All	All	1071/1016 (105%)	1056 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	188/174 (108%)	187 (100%)	1 (0%)	81	56
1	B	191/174 (110%)	181 (95%)	10 (5%)	21	1
1	C	192/174 (110%)	190 (99%)	2 (1%)	68	34
1	D	188/174 (108%)	182 (97%)	6 (3%)	34	4
All	All	759/696 (109%)	740 (98%)	19 (2%)	50	8

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	B	1[A]	MET
1	B	1[B]	MET
1	B	62[A]	ARG
1	B	62[B]	ARG
1	B	110[A]	ARG
1	B	110[B]	ARG
1	B	154	GLN
1	B	195[A]	GLU
1	B	195[B]	GLU
1	B	198	LEU
1	C	154	GLN
1	C	199	LYS
1	D	4[A]	ARG
1	D	4[B]	ARG
1	D	53	GLN
1	D	110[A]	ARG
1	D	110[B]	ARG
1	D	154	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	91	ASN
1	A	99	HIS
1	A	154	GLN
1	A	168	GLN
1	B	99	HIS
1	B	151	ASN
1	B	154	GLN
1	B	168	GLN
1	C	91	ASN
1	C	99	HIS
1	C	154	GLN
1	C	168	GLN
1	D	53	GLN
1	D	91	ASN
1	D	99	HIS
1	D	154	GLN
1	D	168	GLN

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 ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POL	A	1256	-	3,3,3	1.48	1 (33%)	2,2,2	2.56	1 (50%)
4	POL	B	1255[A]	-	3,3,3	0.59	0	2,2,2	1.25	0
4	POL	C	1256	-	3,3,3	0.56	0	2,2,2	1.22	0
3	NAD	A	500	-	46,48,48	1.85	9 (19%)	64,73,73	2.10	13 (20%)
4	POL	D	1255	-	3,3,3	0.17	0	2,2,2	1.05	0
4	POL	A	1255	-	3,3,3	0.70	0	2,2,2	0.95	0
3	NAD	C	500	-	46,48,48	1.76	6 (13%)	64,73,73	1.58	8 (12%)
4	POL	C	1255	-	3,3,3	1.64	1 (33%)	2,2,2	2.28	1 (50%)
3	NAD	B	500	-	46,48,48	1.52	8 (17%)	64,73,73	2.05	10 (15%)
4	POL	D	1256	-	3,3,3	1.30	1 (33%)	2,2,2	2.92	2 (100%)
3	NAD	D	500	-	46,48,48	1.39	7 (15%)	64,73,73	1.37	10 (15%)
4	POL	B	1255[B]	-	3,3,3	1.63	1 (33%)	2,2,2	0.57	0
4	POL	B	1256	-	3,3,3	0.38	0	2,2,2	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POL	A	1256	-	-	1/1/1/1	-
4	POL	B	1255[A]	-	-	0/1/1/1	-
4	POL	C	1256	-	-	1/1/1/1	-
3	NAD	A	500	-	-	5/30/62/62	0/5/5/5
4	POL	D	1255	-	-	1/1/1/1	-
4	POL	A	1255	-	-	1/1/1/1	-
3	NAD	C	500	-	-	6/30/62/62	0/5/5/5
4	POL	C	1255	-	-	1/1/1/1	-
3	NAD	B	500	-	-	4/30/62/62	0/5/5/5
4	POL	D	1256	-	-	0/1/1/1	-
3	NAD	D	500	-	-	5/30/62/62	0/5/5/5
4	POL	B	1255[B]	-	-	1/1/1/1	-
4	POL	B	1256	-	-	0/1/1/1	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	O7N-C7N	6.83	1.36	1.24
3	C	500	NAD	O7N-C7N	6.73	1.36	1.24
3	B	500	NAD	C2N-N1N	5.29	1.40	1.35
3	D	500	NAD	O7N-C7N	4.55	1.32	1.24
3	C	500	NAD	C3N-C7N	-4.34	1.44	1.50
3	A	500	NAD	C6N-N1N	4.03	1.44	1.35
3	C	500	NAD	C6N-N1N	3.80	1.44	1.35
3	A	500	NAD	C2N-N1N	3.73	1.39	1.35
3	B	500	NAD	C8A-N9A	3.70	1.43	1.37
3	C	500	NAD	C4N-C3N	3.69	1.45	1.39
3	D	500	NAD	C4N-C3N	3.68	1.45	1.39
3	A	500	NAD	C8A-N7A	3.50	1.38	1.31
3	B	500	NAD	O7N-C7N	3.35	1.30	1.24
3	D	500	NAD	C8A-N7A	2.99	1.37	1.31
3	A	500	NAD	O4B-C4B	2.91	1.51	1.45
3	C	500	NAD	C2A-N3A	2.86	1.39	1.33
3	B	500	NAD	C8A-N7A	2.81	1.37	1.31
4	C	1255	POL	O-C1	2.71	1.55	1.42
4	B	1255[B]	POL	O-C1	-2.67	1.28	1.42
3	C	500	NAD	C8A-N7A	2.67	1.36	1.31
3	B	500	NAD	C5N-C4N	2.60	1.43	1.38
3	A	500	NAD	C2N-C3N	-2.52	1.35	1.39
3	B	500	NAD	C6N-N1N	2.39	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	NAD	PN-O3	2.38	1.62	1.59
4	A	1256	POL	O-C1	2.37	1.54	1.42
3	A	500	NAD	C3N-C7N	-2.36	1.47	1.50
3	A	500	NAD	C4A-N3A	2.30	1.38	1.34
3	A	500	NAD	O4B-C1B	2.28	1.47	1.42
4	D	1256	POL	C3-C2	2.24	1.66	1.50
3	D	500	NAD	PA-O3	2.22	1.61	1.59
3	B	500	NAD	C2A-N3A	2.18	1.37	1.33
3	D	500	NAD	C2A-N1A	2.17	1.37	1.33
3	D	500	NAD	C6N-N1N	2.11	1.40	1.35
3	B	500	NAD	C3N-C7N	-2.09	1.47	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	NAD	C3N-C7N-N7N	9.39	129.31	117.74
3	B	500	NAD	C3N-C7N-N7N	6.29	125.49	117.74
3	B	500	NAD	N9A-C8A-N7A	-6.17	105.18	113.94
3	A	500	NAD	O7N-C7N-C3N	-5.86	112.43	119.60
3	C	500	NAD	N3A-C2A-N1A	-5.28	120.58	128.58
3	B	500	NAD	C2N-C3N-C4N	5.17	124.27	118.26
3	A	500	NAD	C4A-N9A-C8A	5.15	111.15	105.74
3	B	500	NAD	N3A-C2A-N1A	-5.07	120.90	128.58
3	B	500	NAD	C2A-N1A-C6A	4.85	126.69	118.73
3	B	500	NAD	C4A-N9A-C8A	4.71	110.69	105.74
3	A	500	NAD	N9A-C8A-N7A	-4.67	107.31	113.94
3	C	500	NAD	C3N-C7N-N7N	4.56	123.36	117.74
3	C	500	NAD	C6N-N1N-C2N	-4.45	118.09	121.88
3	B	500	NAD	O7N-C7N-C3N	-4.36	114.27	119.60
3	D	500	NAD	C4A-N9A-C8A	4.09	110.03	105.74
3	D	500	NAD	N9A-C8A-N7A	-3.87	108.45	113.94
3	C	500	NAD	C5N-C4N-C3N	-3.74	116.69	120.36
3	A	500	NAD	C2N-C3N-C4N	3.68	122.54	118.26
4	A	1256	POL	C3-C2-C1	-3.59	73.26	113.89
4	D	1256	POL	O-C1-C2	-3.52	77.77	112.82
3	D	500	NAD	C6N-N1N-C2N	3.36	124.74	121.88
3	B	500	NAD	C5A-N7A-C8A	3.32	108.67	103.45
4	C	1255	POL	C3-C2-C1	-3.22	77.47	113.89
3	A	500	NAD	O7N-C7N-N7N	-3.08	118.16	122.62
3	A	500	NAD	C5A-C4A-N3A	-2.95	122.65	126.72
3	D	500	NAD	C3N-C7N-N7N	2.72	121.09	117.74
3	C	500	NAD	C2A-N1A-C6A	2.65	123.08	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	500	NAD	O7N-C7N-N7N	-2.62	118.83	122.62
3	A	500	NAD	C4A-C5A-N7A	-2.56	107.66	110.58
3	D	500	NAD	C6N-N1N-C1D	-2.50	114.82	119.73
3	D	500	NAD	O4B-C1B-C2B	-2.49	101.29	106.62
3	A	500	NAD	C6A-C5A-C4A	2.49	120.57	117.18
3	A	500	NAD	C6N-N1N-C2N	-2.48	119.77	121.88
3	D	500	NAD	O3D-C3D-C2D	-2.45	103.98	111.82
3	A	500	NAD	O4B-C4B-C5B	-2.29	101.98	109.33
3	A	500	NAD	C5A-N7A-C8A	2.20	106.90	103.45
3	C	500	NAD	C4N-C3N-C7N	-2.20	115.08	121.06
4	D	1256	POL	C3-C2-C1	2.15	138.27	113.89
3	D	500	NAD	C4A-N9A-C1B	-2.15	121.60	126.63
3	D	500	NAD	N3A-C4A-N9A	2.15	130.82	127.17
3	B	500	NAD	O4B-C4B-C5B	-2.12	102.56	109.33
3	C	500	NAD	O4B-C1B-C2B	-2.08	102.16	106.62
3	A	500	NAD	C3B-C2B-C1B	2.03	105.31	101.46
3	D	500	NAD	O2A-PA-O1A	2.02	121.84	112.44
3	B	500	NAD	C5N-C4N-C3N	-2.00	118.40	120.36

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	NAD	C5D-O5D-PN-O3
3	A	500	NAD	C5D-O5D-PN-O2N
3	A	500	NAD	O4D-C1D-N1N-C2N
3	A	500	NAD	O4D-C1D-N1N-C6N
3	B	500	NAD	C5D-O5D-PN-O2N
3	B	500	NAD	O4D-C1D-N1N-C2N
3	C	500	NAD	C5D-O5D-PN-O1N
3	C	500	NAD	O4D-C1D-N1N-C2N
3	C	500	NAD	O4D-C1D-N1N-C6N
3	D	500	NAD	C5D-O5D-PN-O3
3	D	500	NAD	C5D-O5D-PN-O2N
3	D	500	NAD	O4D-C1D-N1N-C2N
4	A	1255	POL	O-C1-C2-C3
3	A	500	NAD	C5D-O5D-PN-O1N
3	B	500	NAD	C5D-O5D-PN-O3
3	C	500	NAD	C5D-O5D-PN-O3
3	C	500	NAD	C5D-O5D-PN-O2N
3	D	500	NAD	C5D-O5D-PN-O1N
4	B	1255[B]	POL	O-C1-C2-C3

Continued on next page...

Continued from previous page...

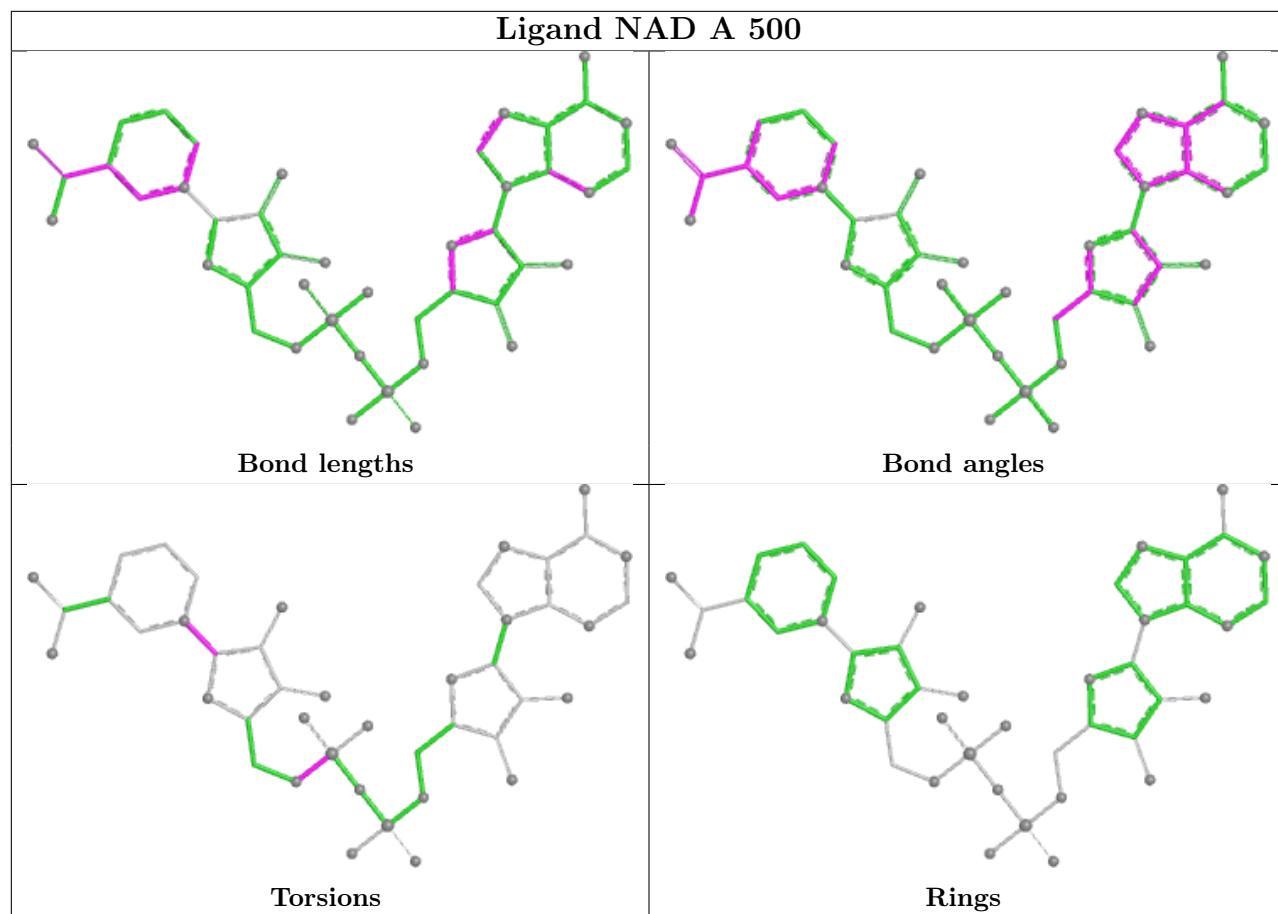
Mol	Chain	Res	Type	Atoms
3	C	500	NAD	C2D-C1D-N1N-C6N
3	B	500	NAD	O4D-C1D-N1N-C6N
3	D	500	NAD	O4D-C1D-N1N-C6N
4	C	1255	POL	O-C1-C2-C3
4	C	1256	POL	O-C1-C2-C3
4	D	1255	POL	O-C1-C2-C3
4	A	1256	POL	O-C1-C2-C3

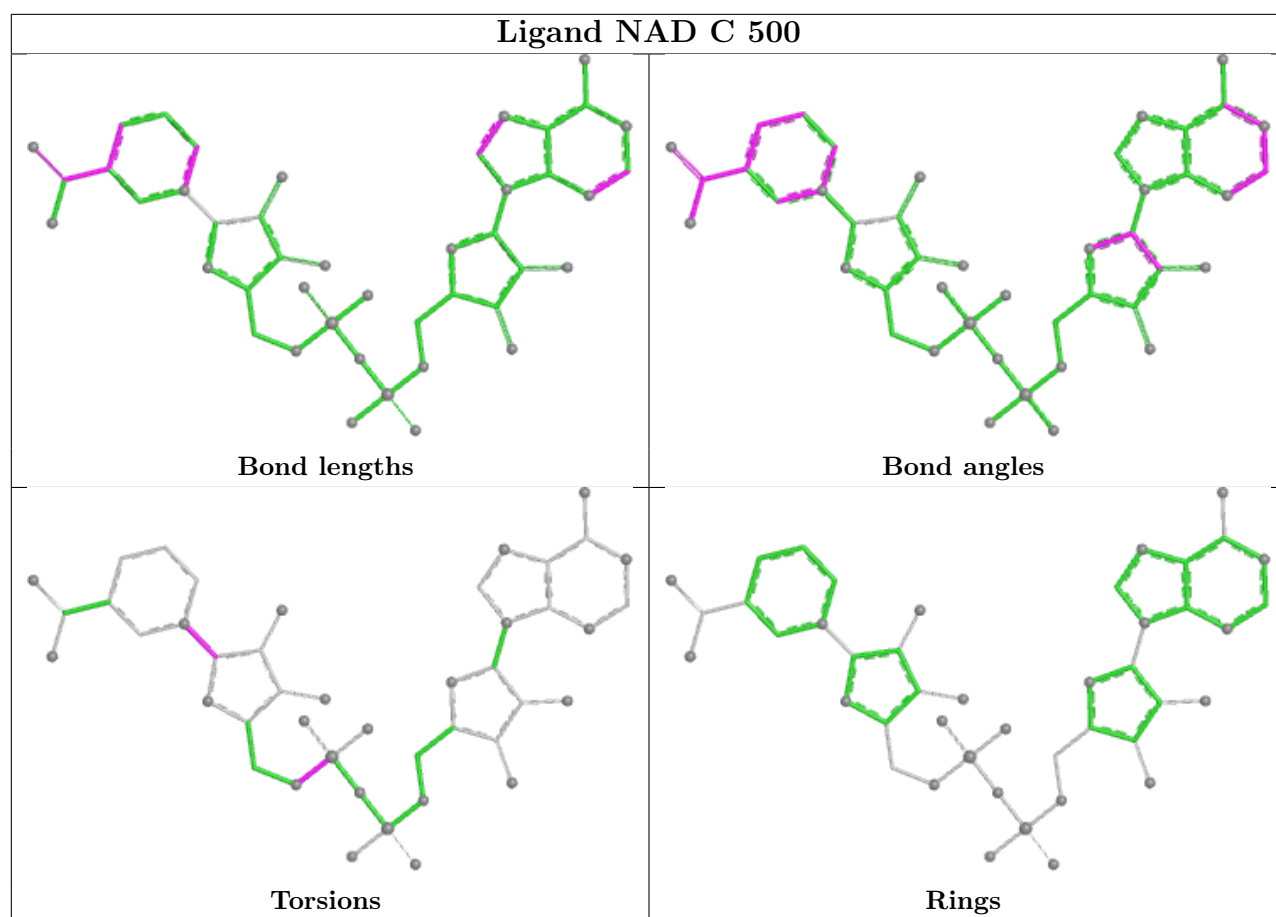
There are no ring outliers.

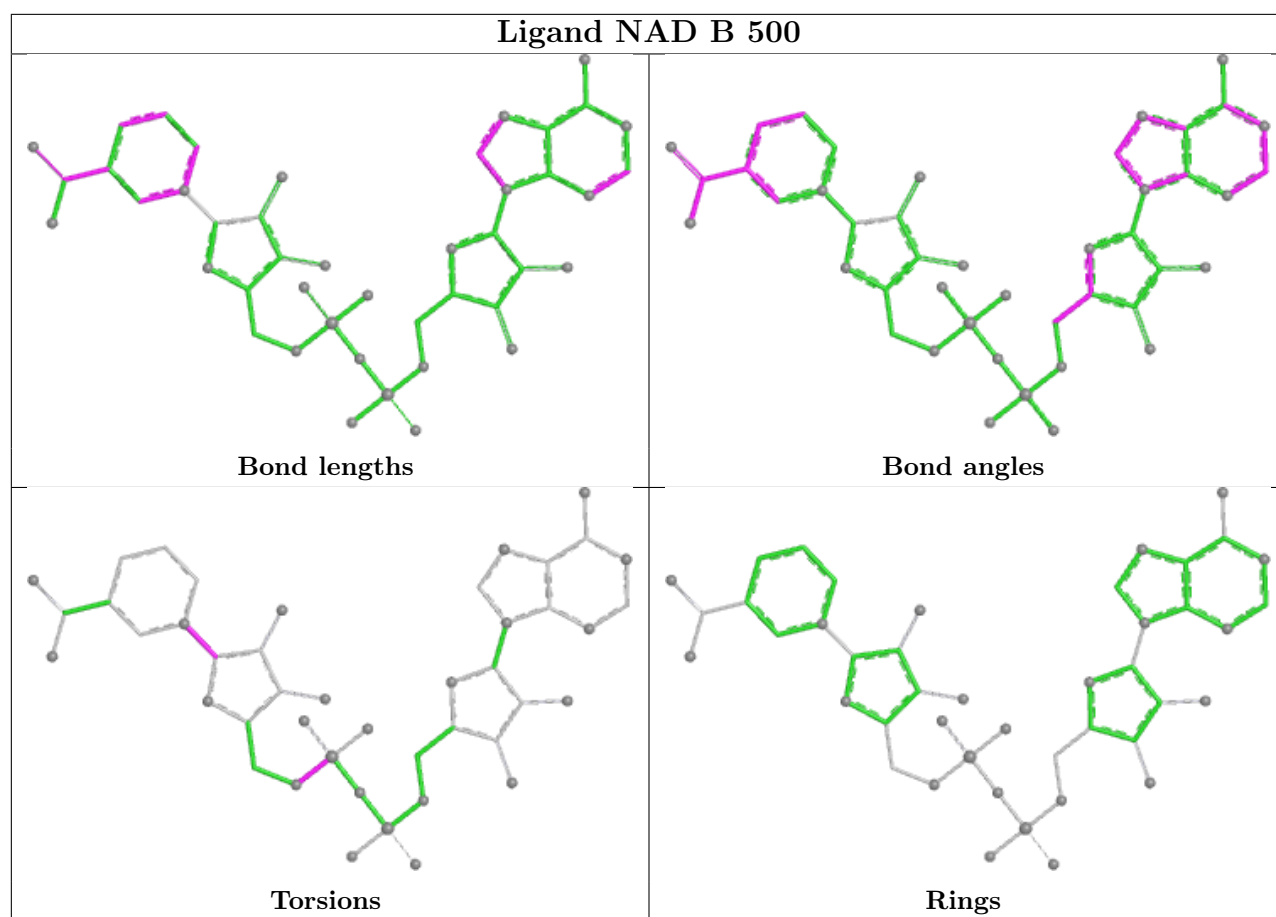
10 monomers are involved in 35 short contacts:

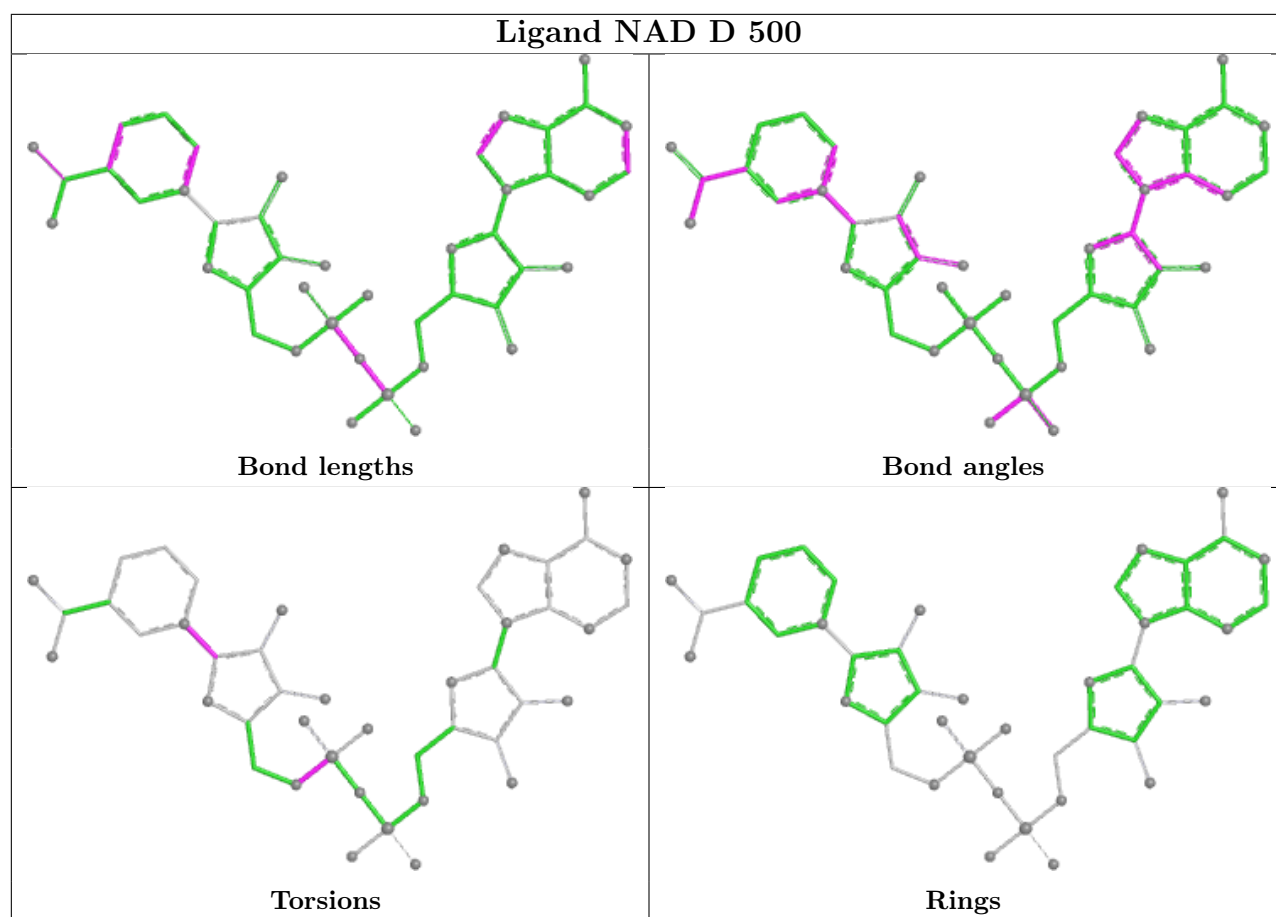
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1256	POL	1	0
4	B	1255[A]	POL	6	0
4	C	1256	POL	1	0
3	A	500	NAD	1	0
4	C	1255	POL	1	0
3	B	500	NAD	7	0
4	D	1256	POL	7	0
3	D	500	NAD	2	0
4	B	1255[B]	POL	14	0
4	B	1256	POL	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/254 (100%)	-0.45	0 100 100	6, 15, 25, 30	14 (5%)
1	B	254/254 (100%)	-0.41	7 (2%) 55 57	7, 15, 30, 51	19 (7%)
1	C	254/254 (100%)	-0.47	0 100 100	6, 15, 26, 36	18 (7%)
1	D	254/254 (100%)	-0.39	3 (1%) 76 77	9, 16, 30, 48	15 (5%)
All	All	1016/1016 (100%)	-0.43	10 (0%) 79 80	6, 15, 27, 51	66 (6%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	THR	3.5
1	B	198	LEU	3.4
1	B	56[A]	GLY	3.4
1	D	1	MET	2.8
1	B	196	MET	2.8
1	B	195[A]	GLU	2.7
1	B	199	LYS	2.5
1	D	53	GLN	2.5
1	D	199	LYS	2.4
1	B	200	MET	2.3

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

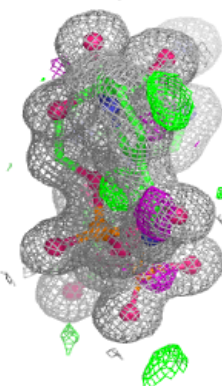
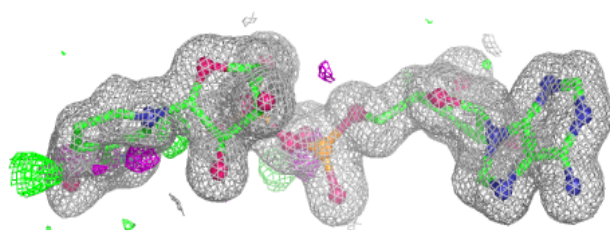
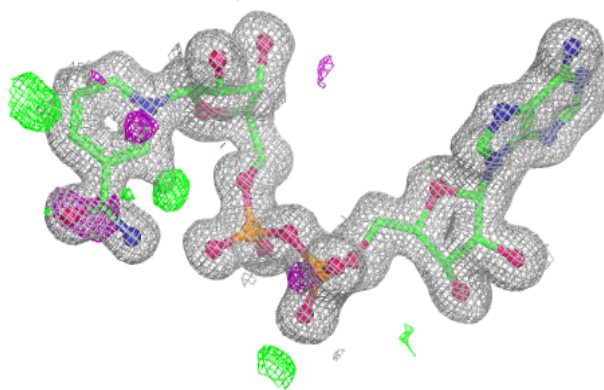
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	POL	B	1255[A]	4/4	0.72	0.23	26,26,26,28	4
4	POL	B	1255[B]	4/4	0.72	0.23	11,11,16,22	4
4	POL	A	1255	4/4	0.83	0.14	40,41,42,48	0
4	POL	A	1256	4/4	0.88	0.12	15,20,23,29	0
4	POL	B	1256	4/4	0.89	0.12	34,37,39,39	0
4	POL	D	1256	4/4	0.90	0.11	15,21,25,31	0
4	POL	C	1256	4/4	0.91	0.11	30,33,36,38	0
4	POL	C	1255	4/4	0.92	0.10	15,20,24,27	0
4	POL	D	1255	4/4	0.93	0.10	36,38,38,40	0
3	NAD	B	500	44/44	0.98	0.04	12,16,18,20	0
3	NAD	A	500	44/44	0.99	0.04	11,14,16,17	0
3	NAD	C	500	44/44	0.99	0.04	12,15,18,20	0
3	NAD	D	500	44/44	0.99	0.04	13,18,20,22	0
2	MG	C	256	1/1	1.00	0.01	12,12,12,12	0
2	MG	A	256	1/1	1.00	0.03	10,10,10,10	0

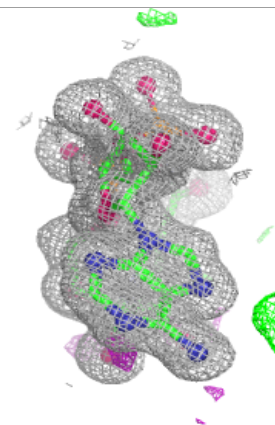
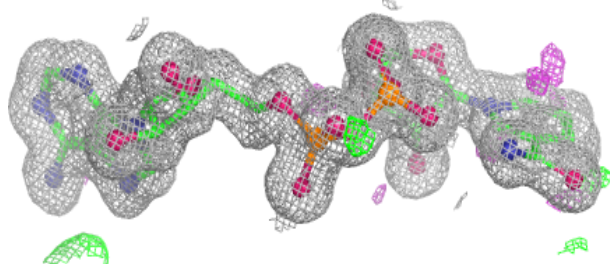
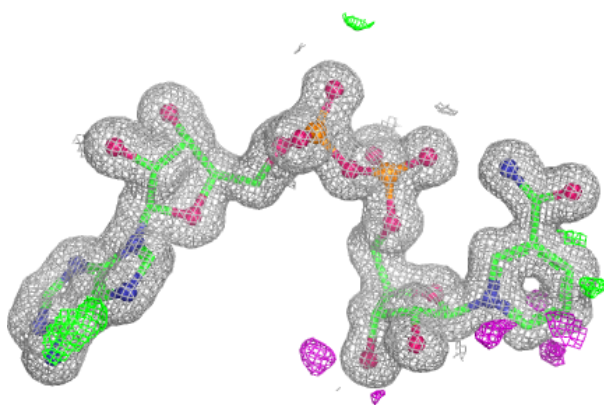
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 500:

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

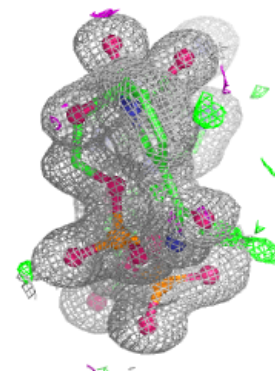
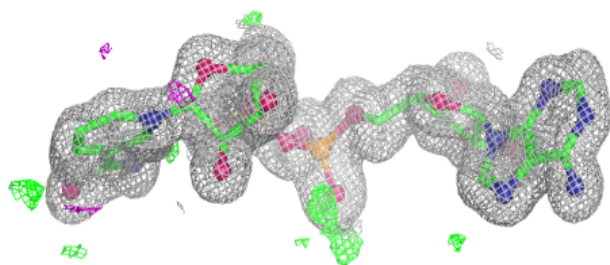
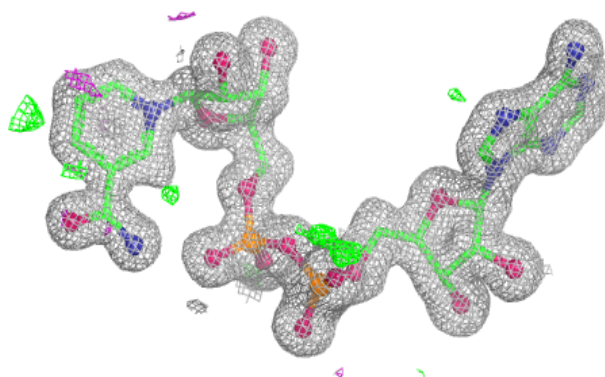
**Electron density around NAD A 500:**

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

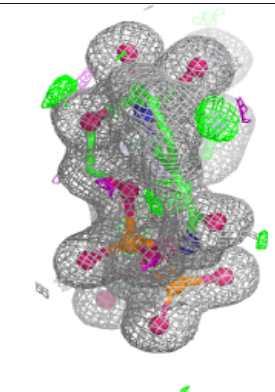
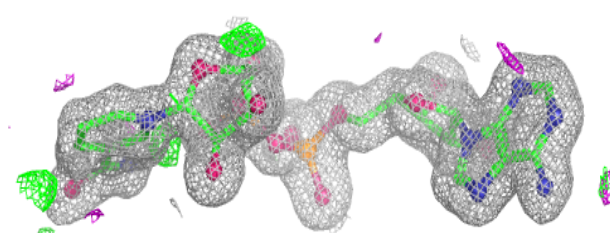
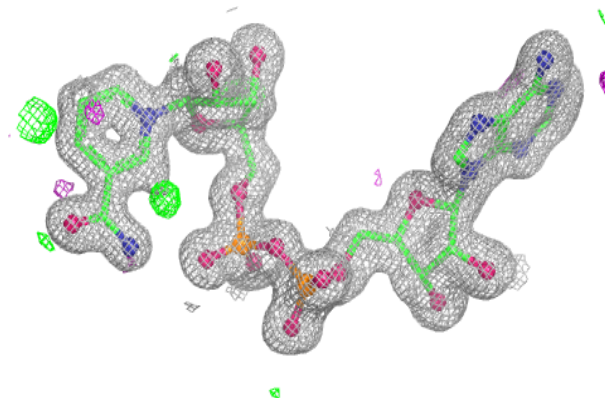


Electron density around NAD C 500:

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

**Electron density around NAD D 500:**

$2mF_o-DF_c$ (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.