



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:56 AM EDT

PDB ID : 1S7G / pdb_00001s7g
Title : Structural Basis for the Mechanism and Regulation of Sir2 Enzymes
Authors : Avalos, J.L.; Boeke, J.D.; Wolberger, C.
Deposited on : 2004-01-29
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

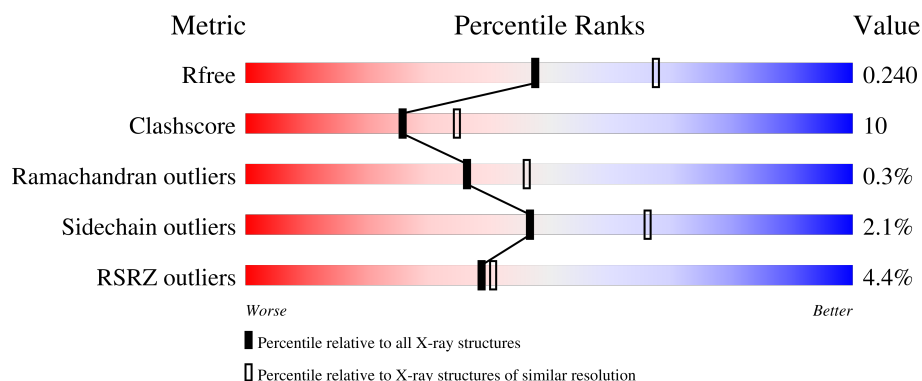
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	4% 74% 25% .
1	B	253	% 84% 15% .
1	C	253	2% 80% 19% .
1	D	253	3% 77% 16% 5% .
1	E	253	12% 72% 24% .

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
10	APR	E	704	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10187 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.

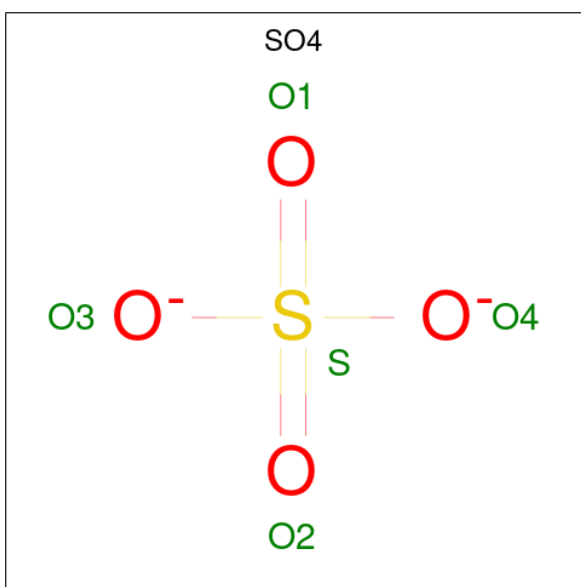
- Molecule 1 is a protein called NAD-dependent deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1930	1233	328	355	14			
1	B	252	Total	C	N	O	S	0	0	0
			1975	1262	339	360	14			
1	C	252	Total	C	N	O	S	0	0	0
			1947	1248	333	352	14			
1	D	240	Total	C	N	O	S	0	0	0
			1854	1188	318	336	12			
1	E	248	Total	C	N	O	S	0	0	0
			1830	1174	306	336	14			

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

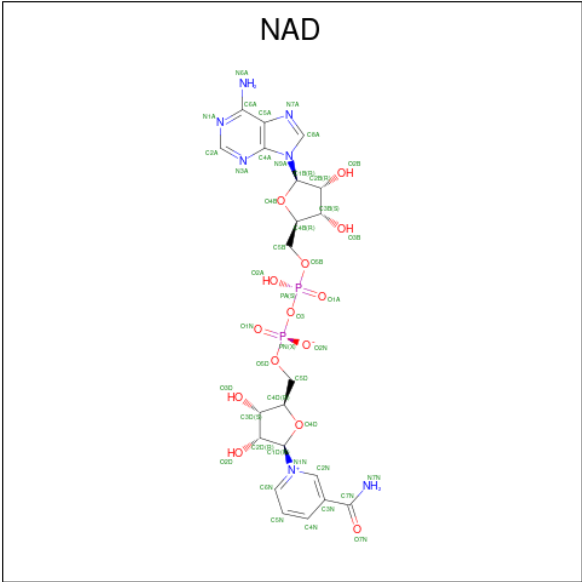
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



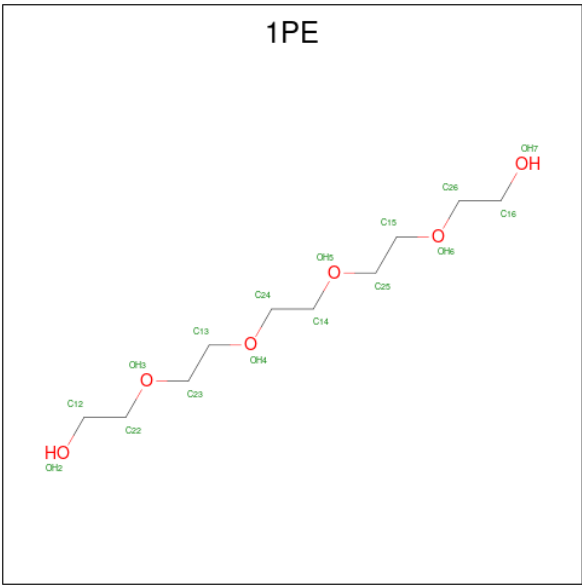
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



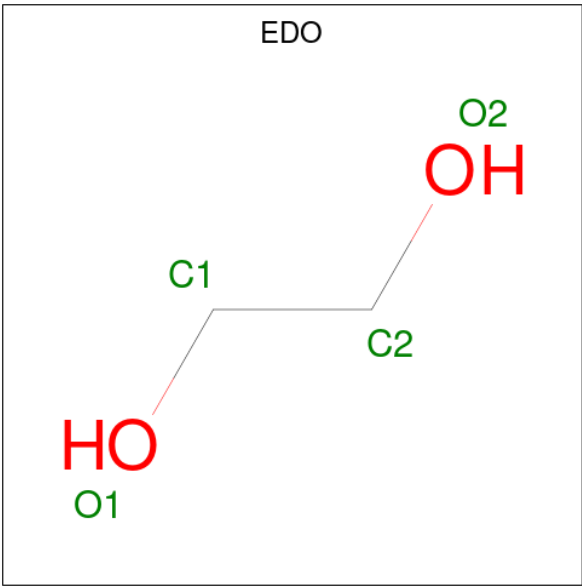
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



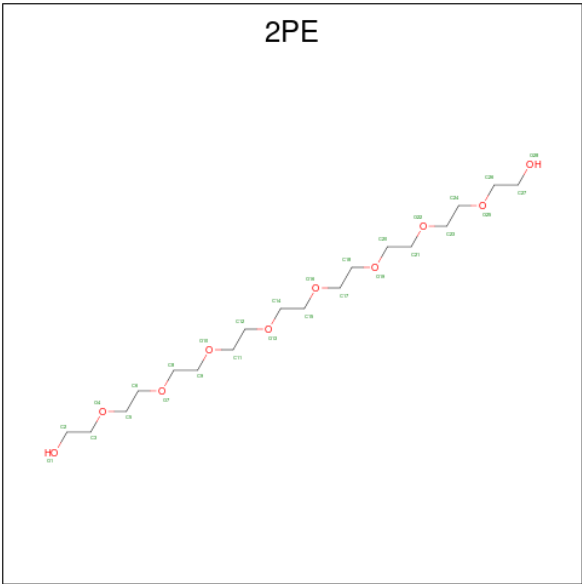
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



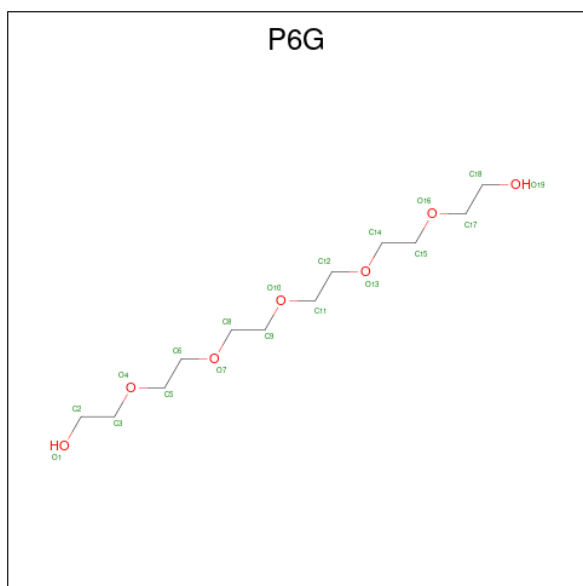
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



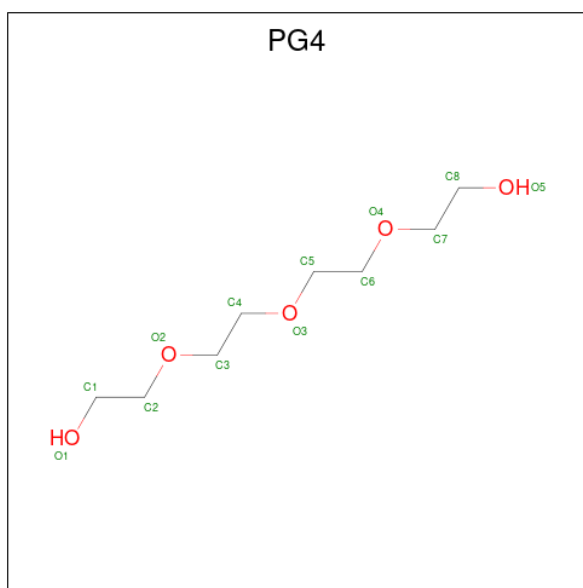
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			28	18	10		

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



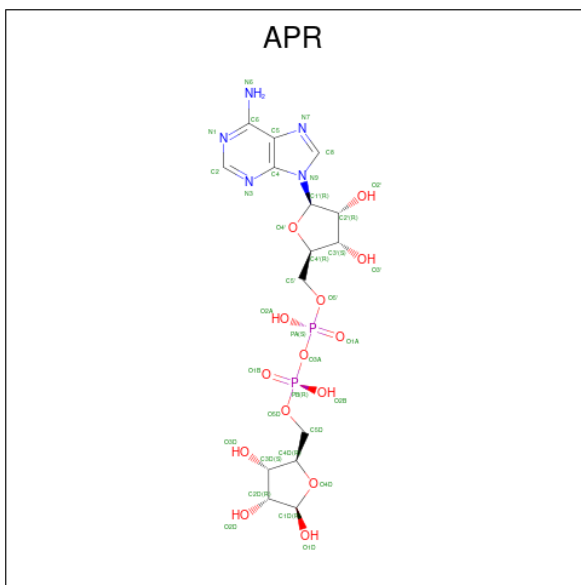
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			13	8	5		
9	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	E	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

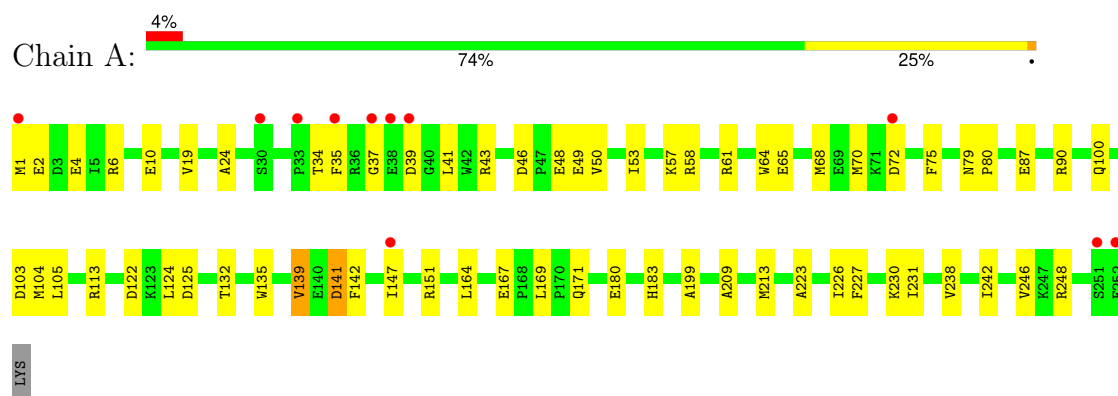
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	67	Total	O	0	0
			67	67		
11	B	96	Total	O	0	0
			96	96		
11	C	50	Total	O	0	0
			50	50		
11	D	77	Total	O	0	0
			77	77		
11	E	23	Total	O	0	0
			23	23		

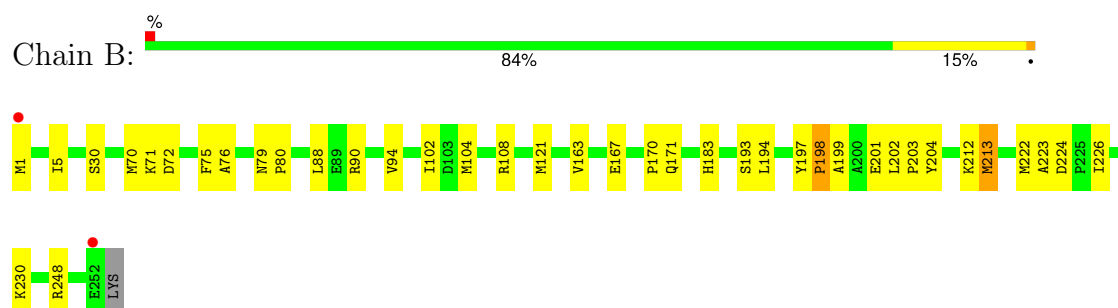
3 Residue-property plots [i](#)

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.

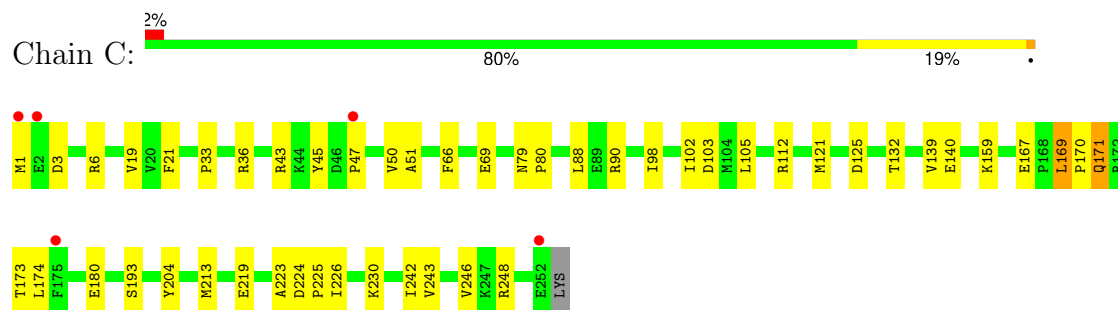
• Molecule 1: NAD-dependent deacetylase 2



• Molecule 1: NAD-dependent deacetylase 2

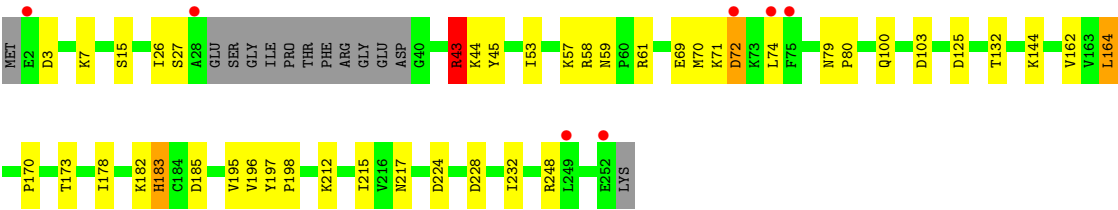


• Molecule 1: NAD-dependent deacetylase 2

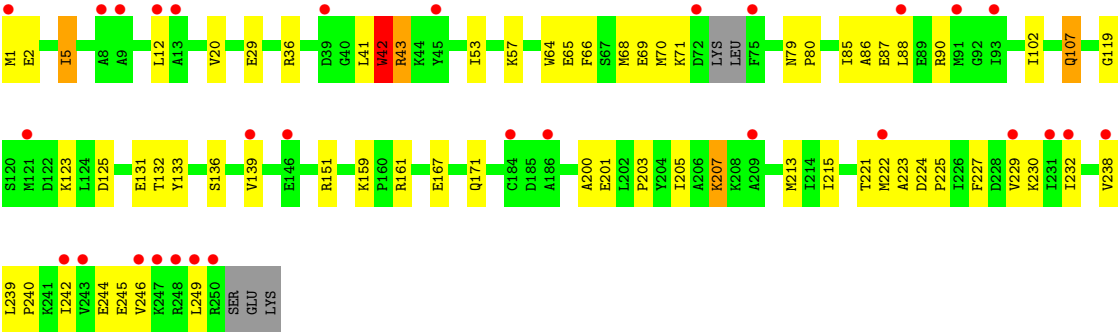


• Molecule 1: NAD-dependent deacetylase 2





● Molecule 1: NAD-dependent deacetylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.85Å 181.57Å 78.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.30 29.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.78-2.30) 99.6 (29.78-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.249 0.199 , 0.240	Depositor DCC
R_{free} test set	3420 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10187	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: PG4, ZN, EDO, 1PE, P6G, SO4, APR, 2PE, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/1973	0.87	3/2672 (0.1%)
1	B	0.41	0/2019	0.88	4/2724 (0.1%)
1	C	0.38	0/1991	0.87	1/2690 (0.0%)
1	D	0.39	0/1895	0.88	4/2563 (0.2%)
1	E	0.35	0/1872	0.84	3/2546 (0.1%)
All	All	0.39	0/9750	0.87	15/13195 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	N-CA-C	-6.46	105.52	113.41
1	E	43	ARG	N-CA-C	-6.17	106.73	114.56
1	C	213	MET	N-CA-C	6.13	119.39	109.40
1	E	171	GLN	N-CA-C	5.72	117.98	111.11
1	D	103	ASP	N-CA-C	5.69	119.20	112.72
1	A	171	GLN	N-CA-C	5.61	117.08	111.07
1	D	43	ARG	N-CA-C	-5.50	106.70	113.41
1	B	213	MET	N-CA-C	5.35	117.68	109.07
1	E	66	PHE	N-CA-C	-5.29	105.59	111.36
1	B	212	LYS	N-CA-C	-5.27	101.87	110.20
1	A	238	VAL	N-CA-C	5.24	115.45	110.53
1	D	100	GLN	N-CA-C	-5.24	106.57	113.17
1	B	171	GLN	N-CA-C	5.22	117.05	111.36
1	B	30	SER	N-CA-C	-5.21	106.92	113.28
1	D	144	LYS	N-CA-C	-5.02	106.93	113.16

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	1930	0	1879	48	0
1	B	1975	0	1970	27	0
1	C	1947	0	1932	34	0
1	D	1854	0	1824	26	0
1	E	1830	0	1724	53	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	25	2	0
4	C	44	0	26	2	0
5	A	16	0	22	0	0
6	A	4	0	6	0	0
6	B	8	0	12	2	0
7	B	28	0	38	0	0
8	C	19	0	26	1	0
9	C	13	0	18	0	0
9	D	13	0	18	0	0
10	E	36	0	21	1	0
11	A	67	0	0	3	0
11	B	96	0	0	1	0
11	C	50	0	0	1	0
11	D	77	0	0	1	0
11	E	23	0	0	0	0
All	All	10187	0	9567	185	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 10.

All (185) 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:E:107:GLN:H	1:E:107:GLN:HE21	1.03	1.02
1:A:151:ARG:HG3	1:A:151:ARG:HH11	1.41	0.86
1:E:65:GLU:HA	1:E:68:MET:HE3	1.59	0.84
1:E:5:ILE:HD13	1:E:242:ILE:HG12	1.60	0.83
1:E:107:GLN:H	1:E:107:GLN:NE2	1.76	0.82
1:E:79:ASN:HB2	1:E:80:PRO:HD2	1.63	0.81
1:A:169:LEU:HD11	1:B:222:MET:HE1	1.65	0.79
1:C:1:MET:HG3	1:C:3:ASP:H	1.47	0.78
1:A:6:ARG:O	1:A:10:GLU:HG3	1.82	0.78
1:A:19:VAL:HG21	1:A:180:GLU:HG3	1.64	0.77
1:A:34:THR:HG22	1:A:35:PHE:H	1.48	0.77
1:E:107:GLN:HE21	1:E:107:GLN:N	1.83	0.77
1:A:46:ASP:HB3	1:A:49:GLU:HG2	1.69	0.74
1:E:159:LYS:HE3	1:E:167:GLU:OE2	1.86	0.74
1:D:79:ASN:HB2	1:D:80:PRO:HD2	1.70	0.72
1:B:1:MET:HE3	1:B:1:MET:HA	1.72	0.72
1:E:5:ILE:CD1	1:E:242:ILE:HG12	2.19	0.71
1:C:66:PHE:O	1:C:69:GLU:HG2	1.91	0.70
1:D:195:VAL:HG23	1:D:196:VAL:HG23	1.75	0.68
1:E:133:TYR:HE2	1:E:151:ARG:HD2	1.61	0.66
1:B:104:MET:HE2	1:B:121:MET:HB2	1.78	0.65
1:B:163:VAL:HG22	6:B:508:EDO:H12	1.78	0.65
1:C:79:ASN:HB2	1:C:80:PRO:HD2	1.79	0.65
1:A:125:ASP:OD1	1:A:132:THR:HG22	1.97	0.64
1:E:159:LYS:HE3	1:E:167:GLU:CD	2.23	0.64
1:E:200:ALA:O	1:E:203:PRO:HD2	1.98	0.64
1:E:242:ILE:O	1:E:246:VAL:HG23	1.98	0.64
1:E:136:SER:O	1:E:139:VAL:HG12	1.98	0.64
1:E:213:MET:HB2	1:E:227:PHE:HA	1.79	0.63
1:E:245:GLU:O	1:E:249:LEU:HD23	1.98	0.62
1:A:151:ARG:HG3	1:A:151:ARG:NH1	2.09	0.62
1:A:164:LEU:O	1:A:167:GLU:HG2	1.99	0.62
1:A:65:GLU:HA	1:A:68:MET:HE3	1.82	0.62
1:E:36:ARG:HH22	10:E:704:APR:H5R2	1.65	0.61
1:E:238:VAL:O	1:E:242:ILE:HG13	2.02	0.60
1:B:70:MET:HE1	1:B:76:ALA:HB2	1.84	0.60
1:B:193:SER:HB3	4:B:701:NAD:O3B	2.01	0.60
1:C:223:ALA:O	1:C:226:ILE:HG12	2.02	0.59
1:E:131:GLU:HG2	1:E:151:ARG:NH1	2.18	0.59
1:C:45:TYR:CD1	1:C:50:VAL:HG11	2.39	0.58
1:B:70:MET:HE2	1:B:75:PHE:C	2.28	0.58
1:C:6:ARG:HH11	1:C:6:ARG:HG2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:SER:HB2	1:D:185:ASP:OD1	2.03	0.58
1:D:248:ARG:O	1:D:248:ARG:HD2	2.04	0.58
1:E:239:LEU:N	1:E:240:PRO:HD2	2.19	0.57
1:A:41:LEU:HD13	1:A:70:MET:HE2	1.87	0.57
1:D:248:ARG:HG3	1:D:248:ARG:HH11	1.69	0.56
1:C:47:PRO:O	1:C:51:ALA:HB3	2.05	0.56
1:E:68:MET:O	1:E:71:LYS:HG3	2.06	0.56
1:C:90:ARG:HH11	1:C:90:ARG:HG2	1.70	0.56
1:D:71:LYS:O	1:D:72:ASP:HB2	2.05	0.55
1:C:19:VAL:HG21	1:C:180:GLU:HG3	1.89	0.55
1:A:87:GLU:OE2	1:A:90:ARG:NH2	2.40	0.55
1:D:212:LYS:HE2	1:D:228:ASP:OD1	2.07	0.54
1:C:102:ILE:H	4:C:702:NAD:H71N	1.55	0.54
1:E:87:GLU:HA	1:E:90:ARG:NH1	2.23	0.54
1:A:79:ASN:HB2	1:A:80:PRO:CD	2.38	0.54
1:A:242:ILE:O	1:A:246:VAL:HG23	2.08	0.53
1:A:34:THR:HG22	1:A:35:PHE:N	2.21	0.53
1:E:107:GLN:NE2	1:E:107:GLN:N	2.50	0.53
1:E:5:ILE:O	1:E:5:ILE:HD12	2.08	0.53
1:B:204:TYR:CE1	1:B:226:ILE:HD13	2.43	0.53
1:E:86:ALA:O	1:E:90:ARG:HG3	2.08	0.53
1:A:135:TRP:NE1	1:A:139:VAL:HG13	2.25	0.52
1:E:53:ILE:HD11	1:E:57:LYS:HZ2	1.74	0.52
1:A:4:GLU:HB3	1:A:231:ILE:HG12	1.91	0.52
1:A:209:ALA:HA	1:E:151:ARG:NH2	2.24	0.52
1:C:1:MET:HG3	1:C:3:ASP:N	2.22	0.52
1:C:204:TYR:CE1	1:C:226:ILE:HD13	2.45	0.52
1:B:71:LYS:O	1:B:72:ASP:HB2	2.10	0.52
1:B:102:ILE:H	4:B:701:NAD:H71N	1.55	0.51
1:A:24:ALA:HB3	1:A:34:THR:HG23	1.91	0.51
1:A:53:ILE:HD11	1:A:57:LYS:HE3	1.92	0.51
1:E:41:LEU:C	1:E:43:ARG:H	2.19	0.51
1:D:44:LYS:HE3	1:D:45:TYR:CE1	2.46	0.51
1:A:41:LEU:CD1	1:A:70:MET:HE2	2.41	0.51
1:C:102:ILE:HD11	8:C:502:P6G:H81	1.92	0.51
1:E:20:VAL:HG11	1:E:85:ILE:HD12	1.92	0.50
1:D:215:ILE:HD11	1:D:217:ASN:HD22	1.76	0.50
1:A:79:ASN:HB2	1:A:80:PRO:HD2	1.92	0.50
1:C:125:ASP:OD1	1:C:132:THR:HG22	2.11	0.50
1:C:159:LYS:HE3	1:C:167:GLU:OE2	2.12	0.50
1:C:224:ASP:HB2	1:C:225:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PRO:HB2	1:D:173:THR:HB	1.94	0.49
1:E:133:TYR:CE2	1:E:151:ARG:HD2	2.45	0.49
1:D:178:ILE:HG22	1:D:182:LYS:HE2	1.94	0.49
1:B:167:GLU:HB3	6:B:508:EDO:H22	1.94	0.49
1:B:197:TYR:HA	11:B:767:HOH:O	2.13	0.49
1:D:183:HIS:CD2	1:D:183:HIS:C	2.91	0.49
1:E:244:GLU:HG3	1:E:245:GLU:N	2.28	0.49
1:A:248:ARG:HH11	1:A:248:ARG:HG2	1.77	0.48
1:E:125:ASP:OD1	1:E:132:THR:HG22	2.14	0.48
1:A:49:GLU:HG3	1:A:50:VAL:HG13	1.95	0.48
1:C:242:ILE:O	1:C:246:VAL:HG23	2.13	0.48
1:E:42:TRP:CE3	1:E:42:TRP:HA	2.48	0.48
1:B:88:LEU:HB3	1:B:94:VAL:HG23	1.96	0.47
1:C:169:LEU:HD22	1:C:169:LEU:N	2.28	0.47
1:D:26:ILE:HG23	1:D:27:SER:N	2.27	0.47
1:D:197:TYR:CG	1:D:198:PRO:HA	2.49	0.47
1:B:1:MET:HE1	1:B:5:ILE:HG21	1.96	0.47
1:C:36:ARG:HD3	11:C:735:HOH:O	2.15	0.47
1:A:100:GLN:OE1	1:A:199:ALA:HB2	2.14	0.47
1:D:3:ASP:OD1	1:D:7:LYS:HE3	2.14	0.47
1:E:42:TRP:HA	1:E:42:TRP:HE3	1.80	0.47
1:A:68:MET:HG2	1:A:142:PHE:CE2	2.50	0.47
1:B:224:ASP:O	1:B:230:LYS:HD3	2.15	0.47
1:C:230:LYS:N	1:C:230:LYS:HD3	2.30	0.47
1:E:5:ILE:HD11	1:E:242:ILE:HA	1.96	0.47
1:E:221:THR:C	1:E:223:ALA:H	2.23	0.47
1:D:248:ARG:HG3	1:D:248:ARG:NH1	2.31	0.46
1:D:69:GLU:O	1:D:70:MET:HE2	2.15	0.46
1:A:1:MET:SD	1:A:2:GLU:N	2.87	0.46
1:A:151:ARG:NH1	1:A:151:ARG:CG	2.79	0.46
1:A:61:ARG:NH1	1:A:147:ILE:HD12	2.31	0.46
1:A:65:GLU:HA	1:A:68:MET:CE	2.44	0.46
1:E:232:ILE:HG23	1:E:232:ILE:O	2.15	0.46
1:C:90:ARG:HG2	1:C:90:ARG:NH1	2.30	0.46
1:A:75:PHE:HE2	1:D:74:LEU:HD22	1.81	0.46
1:B:76:ALA:O	1:B:108:ARG:NH2	2.44	0.46
1:E:1:MET:O	1:E:5:ILE:HG22	2.15	0.45
1:A:213:MET:HB2	1:A:227:PHE:HA	1.98	0.45
1:C:112:ARG:HG2	1:C:112:ARG:HH11	1.80	0.45
1:E:64:TRP:O	1:E:68:MET:HG3	2.17	0.45
1:E:215:ILE:HB	1:E:227:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ARG:HD3	11:D:637:HOH:O	2.16	0.45
1:B:194:LEU:HD22	1:B:199:ALA:O	2.16	0.45
1:C:204:TYR:CZ	1:C:226:ILE:HD13	2.51	0.45
1:D:43:ARG:HH21	1:D:43:ARG:HG3	1.82	0.45
1:C:171:GLN:HE21	1:C:171:GLN:N	2.15	0.44
1:E:2:GLU:HA	1:E:5:ILE:HG23	1.99	0.44
1:A:6:ARG:HH21	1:A:6:ARG:HG3	1.83	0.44
1:E:102:ILE:HG22	1:E:119:GLY:O	2.18	0.44
1:E:207:LYS:HD3	1:E:207:LYS:C	2.42	0.44
1:A:223:ALA:O	1:A:226:ILE:HG12	2.17	0.44
1:A:248:ARG:HG2	1:A:248:ARG:NH1	2.33	0.44
1:B:163:VAL:HG21	1:B:170:PRO:HD3	1.99	0.44
1:B:183:HIS:CD2	1:B:183:HIS:C	2.96	0.44
1:C:33:PRO:HG2	1:C:43:ARG:NH2	2.32	0.44
1:E:131:GLU:HA	1:E:131:GLU:OE2	2.18	0.44
1:B:1:MET:HE2	1:B:5:ILE:HB	2.00	0.43
1:B:204:TYR:CE1	1:B:226:ILE:HG21	2.53	0.43
1:A:141:ASP:HB2	11:A:734:HOH:O	2.18	0.43
1:C:45:TYR:CD2	1:C:45:TYR:N	2.84	0.43
1:A:19:VAL:CG2	1:A:180:GLU:HG3	2.42	0.43
1:C:171:GLN:HE21	1:C:171:GLN:CA	2.31	0.43
1:E:215:ILE:O	1:E:215:ILE:HG23	2.18	0.43
1:A:103:ASP:CG	1:A:105:LEU:HG	2.44	0.43
1:D:26:ILE:CG2	1:D:27:SER:N	2.82	0.43
1:D:125:ASP:OD1	1:D:132:THR:HG22	2.18	0.43
1:D:162:VAL:HG23	1:D:164:LEU:HD13	2.01	0.43
1:B:197:TYR:CE1	1:B:198:PRO:HB3	2.54	0.43
1:C:248:ARG:HG2	1:C:248:ARG:HH11	1.84	0.43
1:E:69:GLU:C	1:E:70:MET:HE2	2.44	0.43
1:A:230:LYS:HD2	11:A:726:HOH:O	2.19	0.43
1:E:213:MET:HB3	1:E:227:PHE:CD2	2.54	0.43
1:A:104:MET:SD	1:A:122:ASP:HB3	2.59	0.42
1:A:124:LEU:N	1:A:124:LEU:HD12	2.33	0.42
1:B:223:ALA:O	1:B:226:ILE:HG12	2.19	0.42
1:E:201:GLU:O	1:E:205:ILE:HG13	2.18	0.42
1:E:224:ASP:N	1:E:225:PRO:CD	2.83	0.42
1:A:113:ARG:HG3	1:A:113:ARG:HH21	1.83	0.42
1:E:207:LYS:HD3	1:E:207:LYS:O	2.19	0.42
1:B:90:ARG:HG2	1:B:90:ARG:HH21	1.84	0.42
1:E:12:LEU:HD13	1:E:88:LEU:HD21	2.01	0.42
1:C:21:PHE:HA	1:C:98:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:HG2	4:C:702:NAD:O2B	2.20	0.42
1:A:135:TRP:O	1:A:139:VAL:HG22	2.20	0.42
1:C:170:PRO:HB2	1:C:173:THR:HB	2.02	0.42
1:B:248:ARG:HH21	1:B:248:ARG:HG2	1.84	0.41
1:B:203:PRO:O	1:B:213:MET:HE1	2.20	0.41
1:A:37:GLY:C	1:A:39:ASP:H	2.29	0.41
1:A:64:TRP:O	1:A:68:MET:HG3	2.20	0.41
1:D:53:ILE:O	1:D:57:LYS:HG3	2.21	0.41
1:C:88:LEU:HD21	1:C:243:VAL:HG22	2.03	0.41
1:C:139:VAL:HG13	1:C:140:GLU:N	2.36	0.41
1:A:48:GLU:OE1	1:A:58:ARG:NH2	2.52	0.41
1:D:217:ASN:O	1:D:232:ILE:HA	2.20	0.41
1:E:224:ASP:HB2	1:E:225:PRO:HD3	2.03	0.41
1:E:229:VAL:HG13	1:E:229:VAL:O	2.20	0.41
1:A:139:VAL:HG23	11:A:719:HOH:O	2.20	0.41
1:A:183:HIS:CD2	1:A:183:HIS:C	2.98	0.40
1:C:103:ASP:CG	1:C:105:LEU:HG	2.47	0.40
1:B:79:ASN:HB2	1:B:80:PRO:CD	2.51	0.40
1:D:59:ASN:HD21	1:D:61:ARG:HB2	1.87	0.40
1:E:123:LYS:HB3	1:E:161:ARG:NH2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/253 (99%)	236 (94%)	13 (5%)	1 (0%)	30	38
1	B	250/253 (99%)	245 (98%)	5 (2%)	0	100	100
1	C	250/253 (99%)	244 (98%)	6 (2%)	0	100	100
1	D	236/253 (93%)	226 (96%)	9 (4%)	1 (0%)	30	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	244/253 (96%)	232 (95%)	10 (4%)	2 (1%)	16	20
All	All	1230/1265 (97%)	1183 (96%)	43 (4%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	D	72	ASP
1	E	42	TRP
1	E	222	MET

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	196/212 (92%)	194 (99%)	2 (1%)	68	82
1	B	207/212 (98%)	204 (99%)	3 (1%)	59	76
1	C	201/212 (95%)	196 (98%)	5 (2%)	42	60
1	D	190/212 (90%)	186 (98%)	4 (2%)	47	66
1	E	177/212 (84%)	171 (97%)	6 (3%)	32	49
All	All	971/1060 (92%)	951 (98%)	20 (2%)	47	66

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	141	ASP
1	B	198	PRO
1	B	201	GLU
1	B	202	LEU
1	C	121	MET
1	C	169	LEU
1	C	171	GLN

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Mol	Chain	Res	Type
1	C	174	LEU
1	C	193	SER
1	D	43	ARG
1	D	164	LEU
1	D	183	HIS
1	D	224	ASP
1	E	5	ILE
1	E	29	GLU
1	E	42	TRP
1	E	107	GLN
1	E	207	LYS
1	E	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	143	ASN
1	B	100	GLN
1	B	101	ASN
1	C	100	GLN
1	C	101	ASN
1	C	171	GLN
1	D	59	ASN
1	D	171	GLN
1	D	217	ASN
1	E	100	GLN
1	E	107	GLN
1	E	143	ASN
1	E	171	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 9 are monoatomic - leaving 24 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	SO4	A	412	-	4,4,4	0.38	0	6,6,6	0.11	0
3	SO4	C	411	-	4,4,4	0.39	0	6,6,6	0.07	0
6	EDO	B	507	-	3,3,3	0.69	0	2,2,2	0.30	0
3	SO4	D	408	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	D	403	-	4,4,4	0.38	0	6,6,6	0.10	0
3	SO4	A	407	-	4,4,4	0.37	0	6,6,6	0.09	0
9	PG4	D	503	-	12,12,12	0.74	0	11,11,11	0.40	0
4	NAD	B	701	-	46,48,48	3.86	24 (52%)	64,73,73	2.09	15 (23%)
3	SO4	C	406	-	4,4,4	0.37	0	6,6,6	0.12	0
3	SO4	A	401	-	4,4,4	0.41	0	6,6,6	0.20	0
10	APR	E	704	-	39,39,39	2.65	13 (33%)	56,60,60	1.88	8 (14%)
3	SO4	B	404	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	B	409	-	4,4,4	0.39	0	6,6,6	0.10	0
7	2PE	B	501	-	27,27,27	0.71	0	26,26,26	0.45	0
6	EDO	A	505	-	3,3,3	0.68	0	2,2,2	0.31	0
3	SO4	B	402	-	4,4,4	0.38	0	6,6,6	0.11	0
3	SO4	B	410	-	4,4,4	0.39	0	6,6,6	0.08	0
5	1PE	A	504	-	15,15,15	0.65	0	14,14,14	0.43	0
6	EDO	B	508	-	3,3,3	0.70	0	2,2,2	0.20	0
4	NAD	A	703	-	46,48,48	4.74	28 (60%)	64,73,73	1.84	14 (21%)
8	P6G	C	502	-	18,18,18	0.78	0	17,17,17	0.74	0
3	SO4	A	405	-	4,4,4	0.38	0	6,6,6	0.08	0
4	NAD	C	702	-	46,48,48	3.81	18 (39%)	64,73,73	1.97	16 (25%)
9	PG4	C	506	-	12,12,12	0.68	0	11,11,11	0.44	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
7	2PE	B	501	-	-	13/25/25/25	-
9	PG4	D	503	-	-	7/10/10/10	-
4	NAD	B	701	-	-	2/30/62/62	0/5/5/5
6	EDO	B	507	-	-	0/1/1/1	-
6	EDO	A	505	-	-	1/1/1/1	-
4	NAD	A	703	-	-	5/30/62/62	0/5/5/5
8	P6G	C	502	-	-	12/16/16/16	-
10	APR	E	704	-	1/1/10/10	5/22/54/54	0/4/4/4
5	1PE	A	504	-	-	7/13/13/13	-
9	PG4	C	506	-	-	3/10/10/10	-
4	NAD	C	702	-	-	4/30/62/62	0/5/5/5
6	EDO	B	508	-	-	1/1/1/1	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	NAD	C2N-N1N	15.64	1.52	1.35
4	A	703	NAD	C4N-C3N	13.83	1.60	1.39
4	B	701	NAD	C2N-N1N	13.30	1.49	1.35
4	C	702	NAD	C4N-C3N	11.62	1.57	1.39
4	B	701	NAD	C4N-C3N	10.25	1.54	1.39
4	C	702	NAD	C2N-N1N	10.24	1.46	1.35
4	C	702	NAD	C5N-C4N	9.56	1.55	1.38
4	A	703	NAD	C5N-C4N	9.51	1.55	1.38
4	C	702	NAD	C6N-N1N	8.49	1.54	1.35
4	A	703	NAD	C6N-N1N	7.98	1.53	1.35
4	B	701	NAD	C5N-C4N	7.64	1.52	1.38
4	A	703	NAD	C4A-N3A	7.56	1.48	1.34
4	C	702	NAD	C2A-N3A	7.54	1.47	1.33
4	A	703	NAD	C2A-N3A	7.53	1.47	1.33
4	A	703	NAD	O4D-C1D	7.50	1.50	1.40
10	E	704	APR	C2-N3	7.26	1.46	1.33
4	B	701	NAD	O3B-C3B	6.36	1.58	1.43
4	B	701	NAD	C2A-N3A	6.04	1.44	1.33
10	E	704	APR	PB-O3A	6.02	1.66	1.59
4	B	701	NAD	C6N-N1N	5.97	1.49	1.35
10	E	704	APR	C4-N3	5.94	1.45	1.34
4	A	703	NAD	C5A-C6A	5.62	1.56	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	NAD	C6N-C5N	5.52	1.50	1.38
4	A	703	NAD	C6N-C5N	5.43	1.49	1.38
4	B	701	NAD	O7N-C7N	5.08	1.33	1.24
10	E	704	APR	C1D-C2D	5.01	1.58	1.52
4	A	703	NAD	C2A-N1A	4.79	1.42	1.33
4	A	703	NAD	PN-O3	-4.76	1.54	1.59
4	C	702	NAD	O7N-C7N	4.68	1.32	1.24
4	A	703	NAD	PA-O3	-4.66	1.54	1.59
4	B	701	NAD	C5A-C6A	4.66	1.54	1.41
10	E	704	APR	C5-C6	4.53	1.53	1.41
4	B	701	NAD	C5A-N7A	-4.41	1.31	1.39
4	C	702	NAD	C4A-N3A	4.40	1.42	1.34
4	C	702	NAD	C5A-C6A	4.26	1.52	1.41
4	B	701	NAD	C3B-C4B	4.21	1.63	1.53
4	C	702	NAD	C5A-N7A	-4.06	1.31	1.39
4	C	702	NAD	C8A-N9A	4.03	1.44	1.37
10	E	704	APR	C6-N1	3.99	1.46	1.35
4	C	702	NAD	C2N-C3N	3.94	1.45	1.39
10	E	704	APR	C5-C4	3.85	1.46	1.39
4	B	701	NAD	PA-O1A	-3.81	1.37	1.50
4	B	701	NAD	O4D-C1D	3.79	1.45	1.40
4	A	703	NAD	O7N-C7N	3.78	1.31	1.24
4	B	701	NAD	O5B-C5B	-3.75	1.30	1.44
4	B	701	NAD	C4A-N3A	3.68	1.41	1.34
4	A	703	NAD	C5A-C4A	3.48	1.45	1.39
4	A	703	NAD	C2N-C3N	3.34	1.44	1.39
10	E	704	APR	C5-N7	-3.30	1.33	1.39
4	A	703	NAD	C2D-C3D	3.20	1.62	1.53
4	B	701	NAD	O4B-C1B	-3.08	1.34	1.42
4	A	703	NAD	C6A-N6A	-2.99	1.26	1.34
4	A	703	NAD	C3B-C4B	2.90	1.60	1.53
4	C	702	NAD	C6A-N1A	2.88	1.43	1.35
4	A	703	NAD	O4D-C4D	2.81	1.51	1.45
4	A	703	NAD	C6A-N1A	2.77	1.43	1.35
4	C	702	NAD	C5A-C4A	2.77	1.44	1.39
4	B	701	NAD	C6A-N1A	2.73	1.43	1.35
4	B	701	NAD	C6N-C5N	2.68	1.44	1.38
10	E	704	APR	C2-N1	2.64	1.38	1.33
4	A	703	NAD	PA-O1A	-2.64	1.41	1.50
4	C	702	NAD	O5B-C5B	-2.62	1.34	1.44
4	C	702	NAD	C2A-N1A	2.61	1.38	1.33
4	B	701	NAD	C8A-N9A	2.61	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	NAD	C5A-C4A	2.59	1.43	1.39
10	E	704	APR	C8-N9	2.54	1.41	1.37
4	B	701	NAD	O2B-C2B	-2.53	1.36	1.43
4	A	703	NAD	C7N-N7N	2.51	1.37	1.33
4	A	703	NAD	PN-O1N	-2.50	1.42	1.50
10	E	704	APR	C5D-C4D	-2.50	1.44	1.51
10	E	704	APR	PA-O2A	-2.41	1.44	1.55
4	C	702	NAD	O4B-C1B	-2.39	1.36	1.42
4	B	701	NAD	PN-O1N	-2.34	1.42	1.50
4	A	703	NAD	PN-O5D	2.31	1.68	1.59
4	B	701	NAD	C2A-N1A	2.27	1.38	1.33
4	A	703	NAD	PA-O2A	-2.23	1.45	1.55
4	B	701	NAD	C6A-N6A	-2.23	1.28	1.34
4	C	702	NAD	O3B-C3B	2.23	1.48	1.43
4	A	703	NAD	C3N-C7N	2.21	1.53	1.50
4	B	701	NAD	PA-O2A	-2.15	1.45	1.55
4	A	703	NAD	O3D-C3D	2.09	1.48	1.43
4	A	703	NAD	C5A-N7A	-2.07	1.35	1.39
10	E	704	APR	O4D-C1D	2.06	1.45	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NAD	N3A-C2A-N1A	-7.59	117.09	128.58
4	C	702	NAD	N3A-C2A-N1A	-7.12	117.81	128.58
4	A	703	NAD	N3A-C2A-N1A	-7.01	117.97	128.58
10	E	704	APR	N3-C2-N1	-6.90	118.14	128.58
10	E	704	APR	C2-N1-C6	4.86	126.71	118.73
4	B	701	NAD	O4B-C4B-C5B	-4.75	94.12	109.33
4	B	701	NAD	C2A-N1A-C6A	4.71	126.47	118.73
4	C	702	NAD	C4D-O4D-C1D	4.33	113.89	109.92
4	A	703	NAD	C2A-N1A-C6A	4.31	125.82	118.73
4	C	702	NAD	C2A-N1A-C6A	4.12	125.50	118.73
4	B	701	NAD	O4B-C1B-N9A	-3.98	100.44	108.09
10	E	704	APR	C1'-N9-C8	3.97	135.91	127.09
4	B	701	NAD	C5B-C4B-C3B	3.94	129.40	115.21
4	B	701	NAD	C4A-N9A-C8A	-3.81	101.73	105.74
4	A	703	NAD	C1B-N9A-C8A	3.80	135.53	127.09
10	E	704	APR	O5D-C5D-C4D	3.78	121.85	108.99
10	E	704	APR	C4-N9-C8	-3.77	101.78	105.74
4	B	701	NAD	C2A-N3A-C4A	3.64	120.72	111.83
4	C	702	NAD	O4B-C1B-N9A	-3.61	101.16	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NAD	C1B-N9A-C8A	3.55	134.97	127.09
4	A	703	NAD	C5A-N7A-C8A	3.47	108.91	103.45
4	C	702	NAD	C5A-N7A-C8A	3.46	108.89	103.45
4	A	703	NAD	C4A-C5A-N7A	-3.39	106.71	110.58
10	E	704	APR	O1D-C1D-O4D	-3.28	106.94	111.12
4	B	701	NAD	C2N-N1N-C1D	-3.22	112.02	119.13
4	B	701	NAD	C5A-N7A-C8A	3.18	108.45	103.45
4	C	702	NAD	O4B-C4B-C5B	-3.17	99.18	109.33
4	C	702	NAD	C2N-N1N-C1D	-3.12	112.24	119.13
4	C	702	NAD	C2A-N3A-C4A	3.11	119.43	111.83
4	C	702	NAD	C1B-N9A-C8A	3.04	133.84	127.09
4	A	703	NAD	C2A-N3A-C4A	2.98	119.12	111.83
4	C	702	NAD	C5B-C4B-C3B	2.95	125.83	115.21
4	C	702	NAD	C4A-N9A-C8A	-2.93	102.66	105.74
4	A	703	NAD	C6A-C5A-N7A	2.92	137.73	132.09
10	E	704	APR	C2-N3-C4	2.87	118.84	111.83
4	B	701	NAD	PA-O5B-C5B	2.84	137.62	121.35
4	A	703	NAD	C2B-C3B-C4B	2.68	107.79	102.61
4	A	703	NAD	O2B-C2B-C3B	2.57	120.05	111.82
4	A	703	NAD	C4D-O4D-C1D	2.54	112.25	109.92
4	A	703	NAD	C4A-N9A-C1B	-2.49	120.82	126.63
4	C	702	NAD	C4B-O4B-C1B	2.47	114.91	109.47
4	C	702	NAD	O2B-C2B-C3B	2.39	119.48	111.82
4	A	703	NAD	O5D-C5D-C4D	2.38	117.09	108.99
4	B	701	NAD	O5B-C5B-C4B	2.32	116.90	108.99
4	C	702	NAD	O5B-C5B-C4B	2.25	116.66	108.99
4	A	703	NAD	O3B-C3B-C4B	-2.22	104.70	111.08
4	B	701	NAD	C6N-N1N-C1D	2.21	124.06	119.73
4	A	703	NAD	C5A-C4A-N3A	-2.20	123.68	126.72
4	B	701	NAD	C5A-C4A-N3A	-2.12	123.80	126.72
4	C	702	NAD	O4B-C4B-C3B	-2.06	101.06	105.15
10	E	704	APR	C5-N7-C8	2.05	106.67	103.45
4	B	701	NAD	C6A-C5A-N7A	2.04	136.02	132.09
4	C	702	NAD	C5A-C4A-N3A	-2.03	123.92	126.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	E	704	APR	C1D

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	NAD	PN-O3-PA-O5B
4	C	702	NAD	PN-O3-PA-O5B
10	E	704	APR	O4D-C4D-C5D-O5D
10	E	704	APR	C3D-C4D-C5D-O5D
8	C	502	P6G	O4-C5-C6-O7
7	B	501	2PE	O7-C8-C9-O10
7	B	501	2PE	O19-C20-C21-O22
8	C	502	P6G	O16-C17-C18-O19
9	D	503	PG4	O2-C3-C4-O3
5	A	504	1PE	OH2-C12-C22-OH3
9	D	503	PG4	O3-C5-C6-O4
7	B	501	2PE	O25-C26-C27-O28
7	B	501	2PE	O1-C2-C3-O4
8	C	502	P6G	O1-C2-C3-O4
7	B	501	2PE	O10-C11-C12-O13
9	C	506	PG4	O4-C7-C8-O5
7	B	501	2PE	O13-C14-C15-O16
9	D	503	PG4	O1-C1-C2-O2
5	A	504	1PE	OH5-C14-C24-OH4
6	A	505	EDO	O1-C1-C2-O2
7	B	501	2PE	O22-C23-C24-O25
4	B	701	NAD	C4B-C5B-O5B-PA
4	C	702	NAD	C4B-C5B-O5B-PA
4	A	703	NAD	O4D-C4D-C5D-O5D
7	B	501	2PE	O16-C17-C18-O19
10	E	704	APR	C2'-C1'-N9-C8
7	B	501	2PE	C9-C8-O7-C6
5	A	504	1PE	C14-C24-OH4-C13
4	A	703	NAD	C3D-C4D-C5D-O5D
7	B	501	2PE	C8-C9-O10-C11
9	D	503	PG4	C3-C4-O3-C5
9	D	503	PG4	C6-C5-O3-C4
9	D	503	PG4	C8-C7-O4-C6
8	C	502	P6G	C9-C8-O7-C6
8	C	502	P6G	C12-C11-O10-C9
8	C	502	P6G	C18-C17-O16-C15
7	B	501	2PE	C18-C17-O16-C15
8	C	502	P6G	C8-C9-O10-C11
4	A	703	NAD	C2B-C1B-N9A-C8A
8	C	502	P6G	C2-C3-O4-C5
5	A	504	1PE	C15-C25-OH5-C14
9	C	506	PG4	C5-C6-O4-C7
9	D	503	PG4	C1-C2-O2-C3

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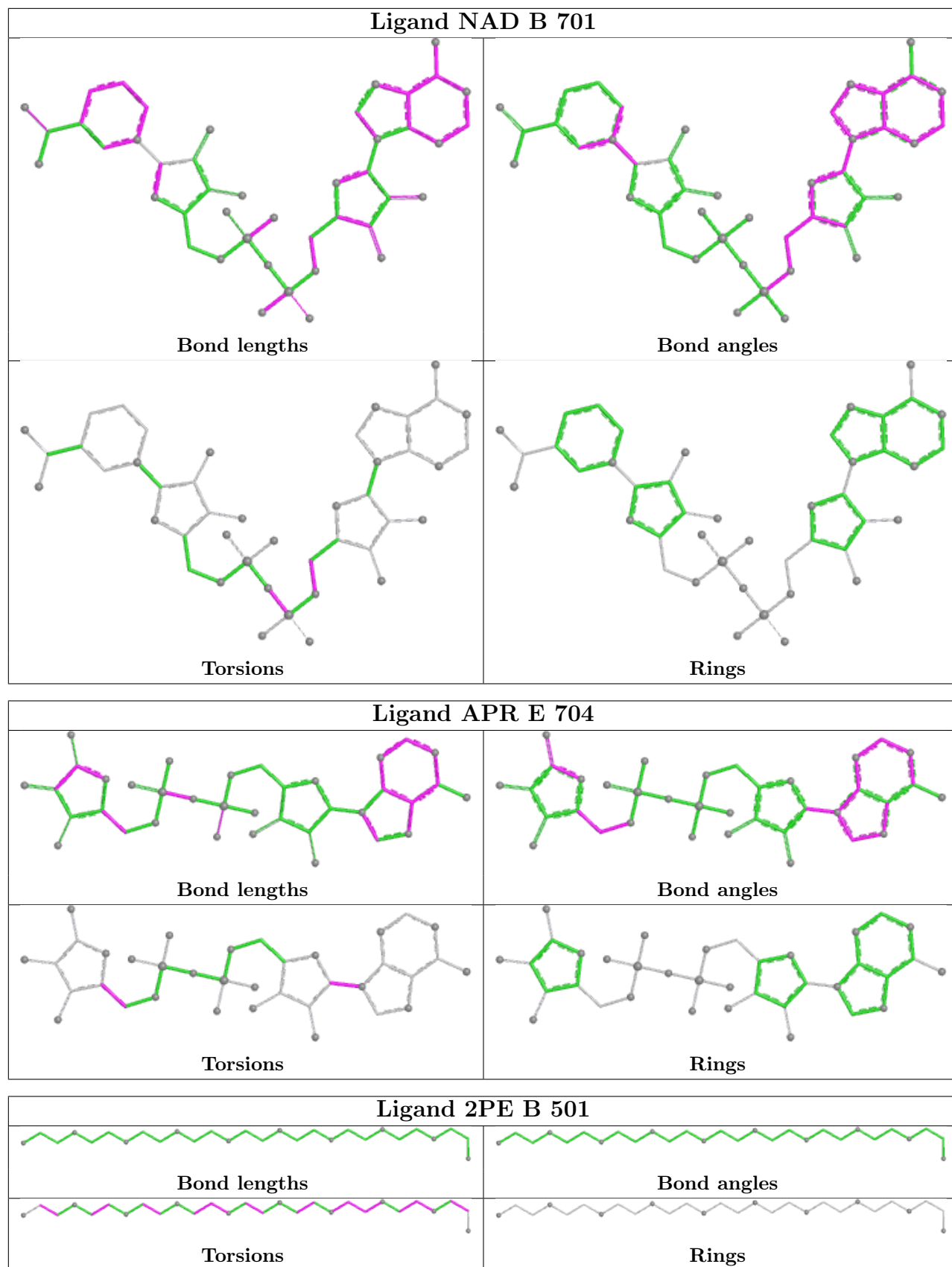
Mol	Chain	Res	Type	Atoms
8	C	502	P6G	C14-C15-O16-C17
8	C	502	P6G	C15-C14-O13-C12
5	A	504	1PE	C25-C15-OH6-C26
10	E	704	APR	C2'-C1'-N9-C4
6	B	508	EDO	O1-C1-C2-O2
7	B	501	2PE	C6-C5-O4-C3
5	A	504	1PE	C16-C26-OH6-C15
7	B	501	2PE	O4-C5-C6-O7
8	C	502	P6G	C11-C12-O13-C14
9	C	506	PG4	C3-C4-O3-C5
10	E	704	APR	O4'-C1'-N9-C8
4	A	703	NAD	O4B-C1B-N9A-C8A
4	C	702	NAD	C2B-C1B-N9A-C8A
5	A	504	1PE	OH7-C16-C26-OH6
4	A	703	NAD	O4B-C4B-C5B-O5B
8	C	502	P6G	C5-C6-O7-C8
4	C	702	NAD	O4B-C4B-C5B-O5B

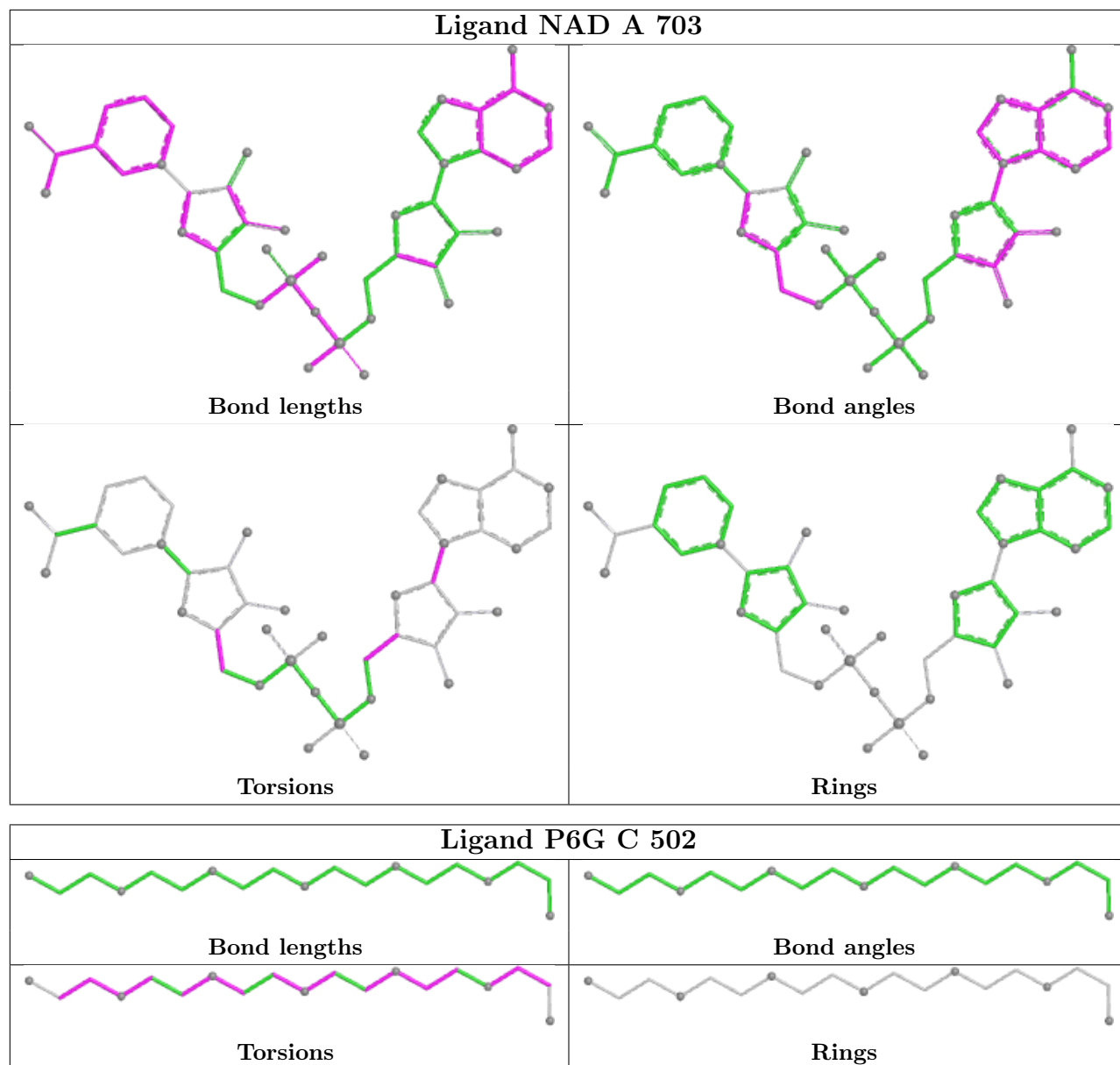
There are no ring outliers.

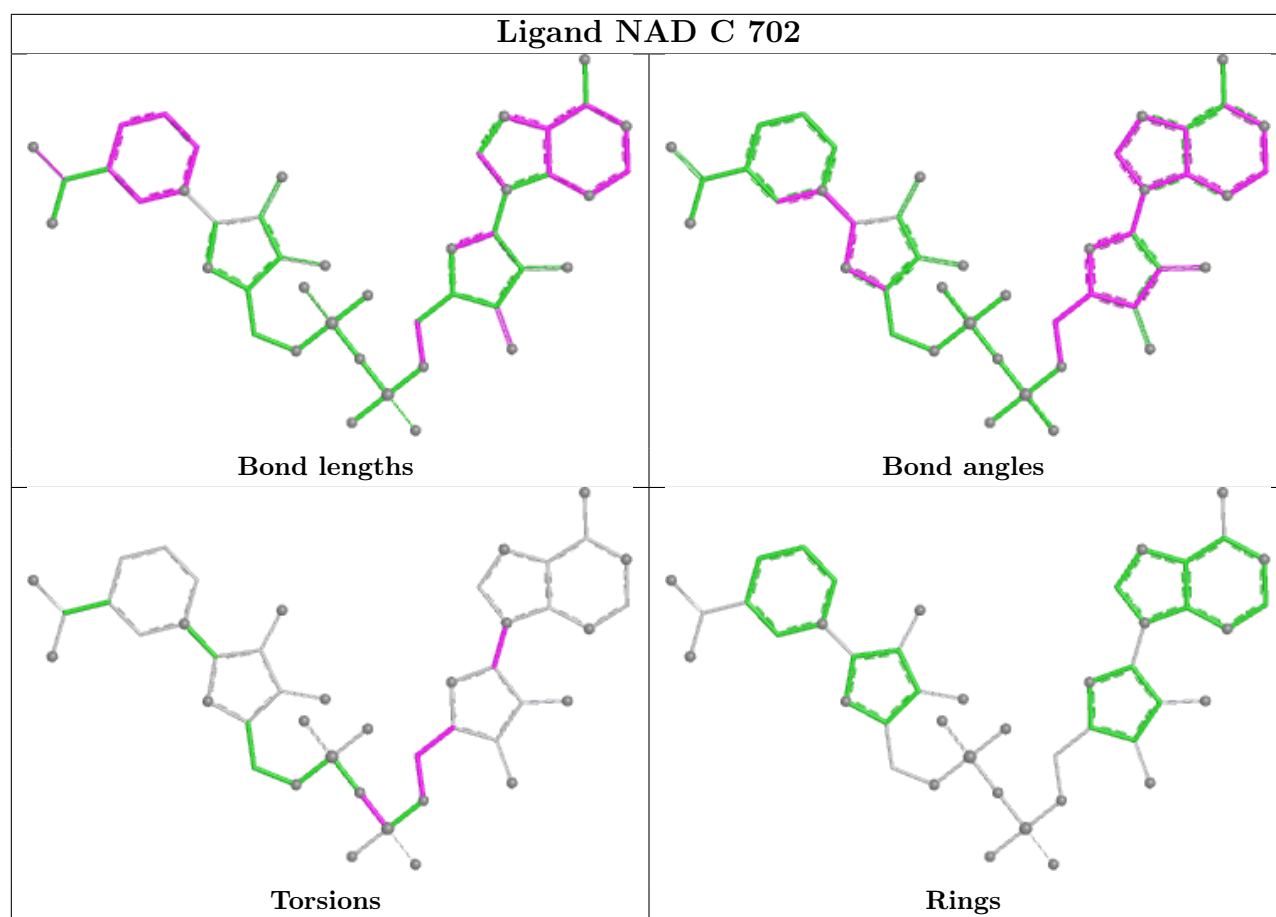
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	NAD	2	0
10	E	704	APR	1	0
6	B	508	EDO	2	0
8	C	502	P6G	1	0
4	C	702	NAD	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 [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	252/253 (99%)	0.10	11 (4%) 39 41	21, 34, 63, 84	0
1	B	252/253 (99%)	-0.13	2 (0%) 82 83	17, 30, 47, 77	0
1	C	252/253 (99%)	0.24	5 (1%) 65 66	23, 39, 60, 90	0
1	D	240/253 (94%)	-0.00	7 (2%) 53 56	18, 34, 60, 85	0
1	E	248/253 (98%)	0.92	30 (12%) 8 9	31, 54, 82, 98	0
All	All	1244/1265 (98%)	0.22	55 (4%) 39 41	17, 37, 73, 98	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	72	ASP	4.2
1	E	250	ARG	4.2
1	E	75	PHE	4.0
1	E	242	ILE	3.9
1	E	248	ARG	3.8
1	C	252	GLU	3.7
1	C	1	MET	3.6
1	A	35	PHE	3.5
1	A	38	GLU	3.4
1	A	1	MET	3.4
1	D	28	ALA	3.4
1	E	91	MET	3.3
1	D	72	ASP	3.2
1	E	243	VAL	3.2
1	D	249	LEU	3.0
1	E	246	VAL	3.0
1	A	251	SER	3.0
1	E	1	MET	3.0
1	A	252	GLU	2.9
1	E	249	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	252	GLU	2.8
1	E	45	TYR	2.8
1	E	88	LEU	2.8
1	E	13	ALA	2.7
1	E	184	CYS	2.7
1	A	37	GLY	2.6
1	E	186	ALA	2.5
1	E	238	VAL	2.5
1	E	8	ALA	2.5
1	E	12	LEU	2.5
1	C	2	GLU	2.4
1	A	39	ASP	2.4
1	E	209	ALA	2.4
1	E	231	ILE	2.4
1	E	232	ILE	2.4
1	E	93	ILE	2.3
1	D	75	PHE	2.3
1	A	33	PRO	2.3
1	B	252	GLU	2.3
1	D	2	GLU	2.3
1	D	74	LEU	2.2
1	C	175	PHE	2.2
1	E	121	MET	2.2
1	A	72	ASP	2.1
1	B	1	MET	2.1
1	E	247	LYS	2.1
1	C	47	PRO	2.1
1	E	146	GLU	2.1
1	E	139	VAL	2.1
1	A	30	SER	2.0
1	E	222	MET	2.0
1	E	229	VAL	2.0
1	E	9	ALA	2.0
1	E	39	ASP	2.0
1	A	147	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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
3	SO4	B	410	5/5	0.39	0.14	104,104,105,106	0
3	SO4	A	412	5/5	0.53	0.15	104,104,104,105	0
3	SO4	B	409	5/5	0.64	0.12	104,104,104,105	0
3	SO4	C	411	5/5	0.64	0.12	103,103,104,104	0
3	SO4	C	406	5/5	0.73	0.17	99,100,100,101	0
3	SO4	A	405	5/5	0.76	0.14	102,102,103,103	0
6	EDO	B	508	4/4	0.78	0.21	44,45,45,46	0
6	EDO	A	505	4/4	0.79	0.24	59,60,60,61	0
6	EDO	B	507	4/4	0.84	0.21	54,54,55,55	0
9	PG4	C	506	13/13	0.84	0.17	78,81,83,83	0
3	SO4	A	407	5/5	0.86	0.12	78,79,79,81	0
3	SO4	D	403	5/5	0.86	0.12	86,87,88,88	0
7	2PE	B	501	28/28	0.87	0.15	39,56,67,69	0
5	1PE	A	504	16/16	0.87	0.16	61,68,69,69	0
9	PG4	D	503	13/13	0.88	0.14	57,59,64,66	0
8	P6G	C	502	19/19	0.90	0.15	50,57,68,69	0
3	SO4	A	401	5/5	0.91	0.11	38,44,45,46	0
3	SO4	D	408	5/5	0.91	0.09	64,65,66,66	0
3	SO4	B	404	5/5	0.92	0.09	87,87,88,89	0
4	NAD	A	703	44/44	0.93	0.10	37,49,68,69	0
10	APR	E	704	36/36	0.94	0.09	46,51,55,56	0
4	NAD	C	702	44/44	0.96	0.07	24,30,34,38	0
4	NAD	B	701	44/44	0.96	0.07	18,23,26,31	0
3	SO4	B	402	5/5	0.99	0.05	33,33,33,34	0
2	ZN	B	603	1/1	0.99	0.03	32,32,32,32	0
2	ZN	C	606	1/1	0.99	0.03	33,33,33,33	0
2	ZN	D	608	1/1	0.99	0.06	31,31,31,31	0
2	ZN	E	609	1/1	0.99	0.02	31,31,31,31	0
2	ZN	B	604	1/1	1.00	0.04	28,28,28,28	0
2	ZN	C	605	1/1	1.00	0.02	32,32,32,32	0
2	ZN	A	602	1/1	1.00	0.05	32,32,32,32	0
2	ZN	D	607	1/1	1.00	0.05	27,27,27,27	0

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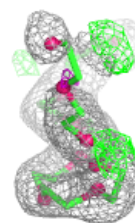
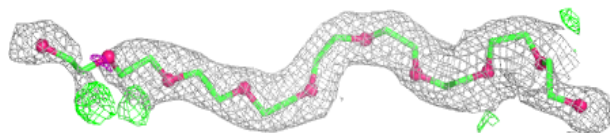
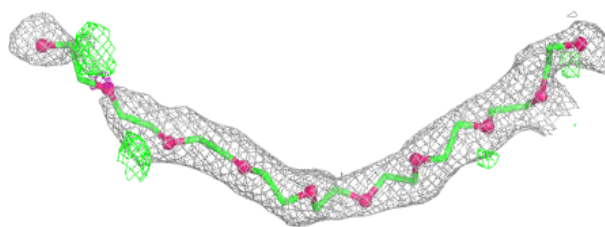
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	601	1/1	1.00	0.01	32,32,32,32	0

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.

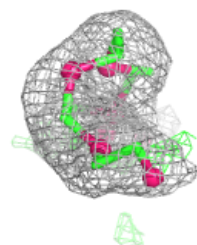
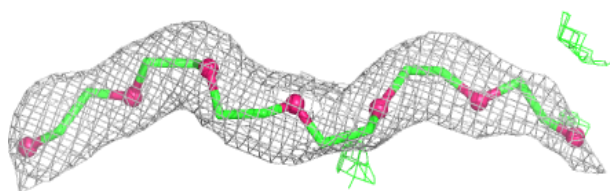
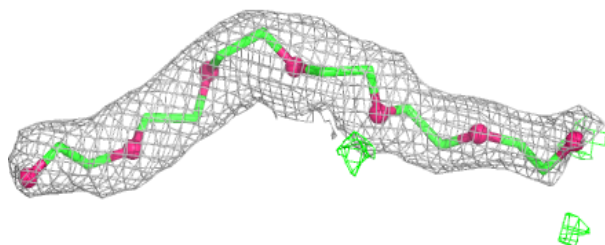
Electron density around 2PE B 501:

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

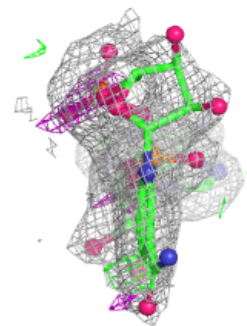
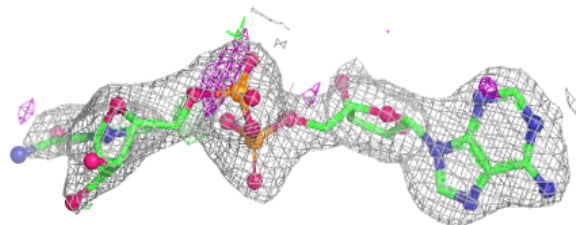
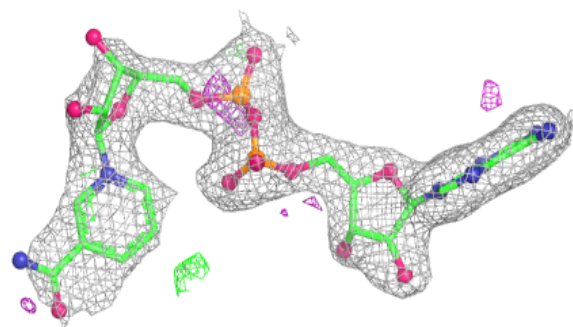


Electron density around P6G C 502:

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

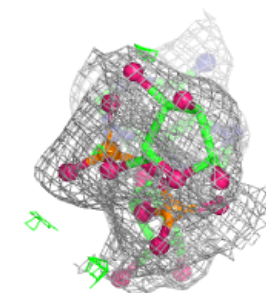
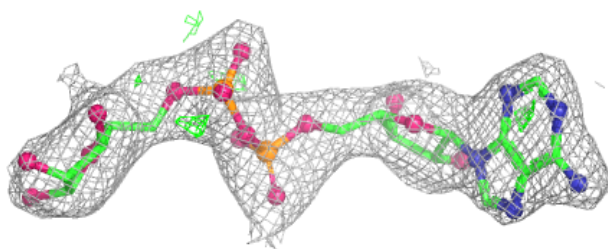
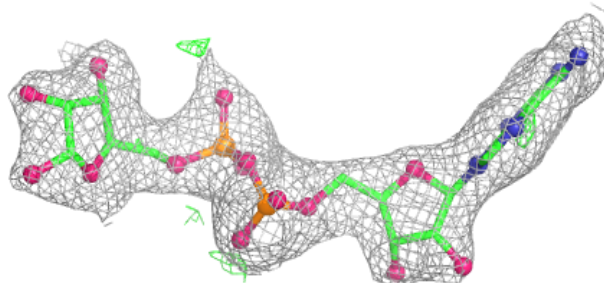
**Electron density around NAD A 703:**

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

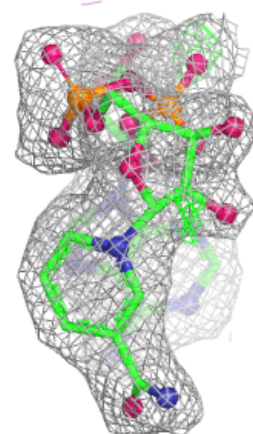
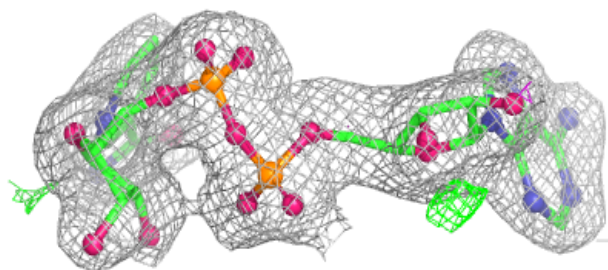
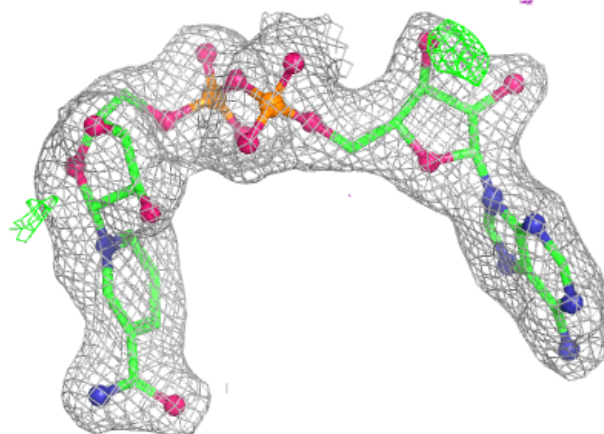


Electron density around APR E 704:

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

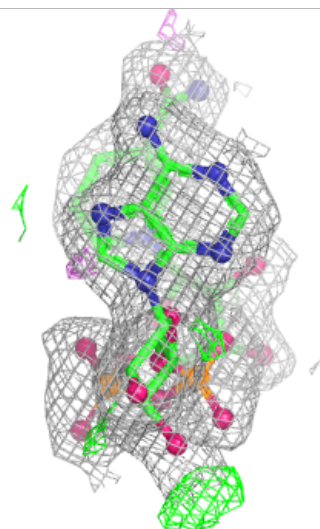
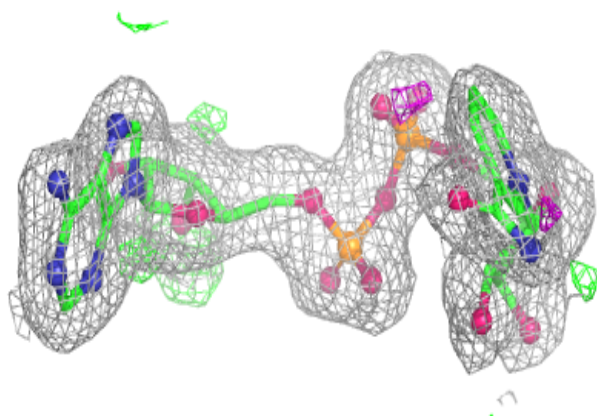
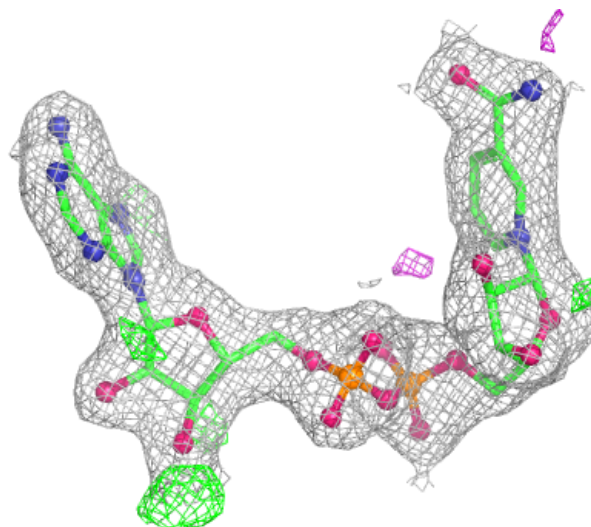
**Electron density around NAD C 702:**

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



Electron density around NAD B 701:

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.