



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:18 PM UTC

PDB ID : 3JZD / pdb_00003jzd
Title : Crystal structure of Putative alcohol dehydrogenase (YP_298327.1) from RALSTONIA EUTROPHA JMP134 at 2.10 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-09-23
Resolution : 2.10 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

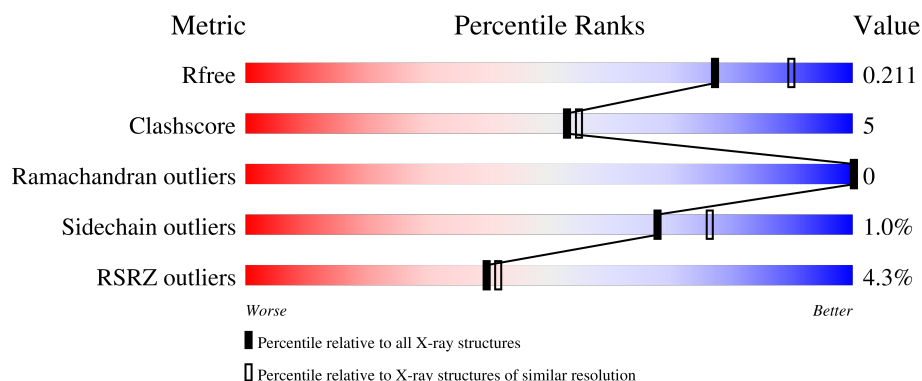
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

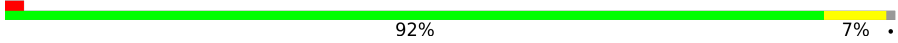
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	358	
1	B	358	
1	C	358	
1	D	358	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11566 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 Iron-containing alcohol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	Se	0	6	0
			2618	1639	475	489	5	10			
1	B	354	Total	C	N	O	S	Se	0	6	0
			2613	1634	478	488	5	8			
1	C	354	Total	C	N	O	S	Se	0	3	0
			2580	1615	471	482	5	7			
1	D	354	Total	C	N	O	S	Se	0	2	0
			2575	1610	467	485	5	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q46TQ1
B	0	GLY	-	expression tag	UNP Q46TQ1
C	0	GLY	-	expression tag	UNP Q46TQ1
D	0	GLY	-	expression tag	UNP Q46TQ1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	1
			3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

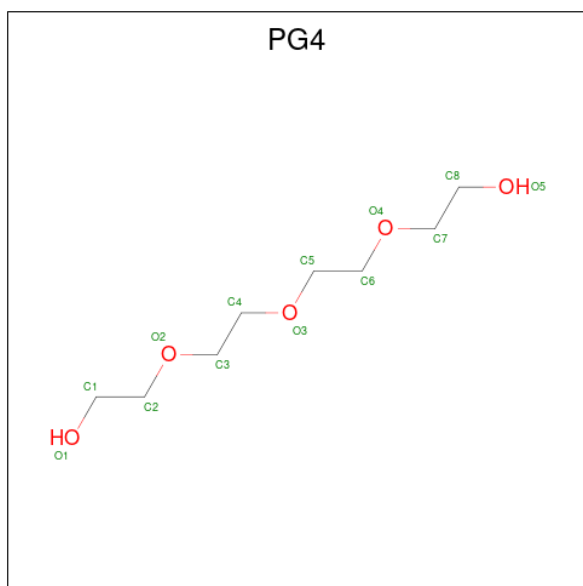
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



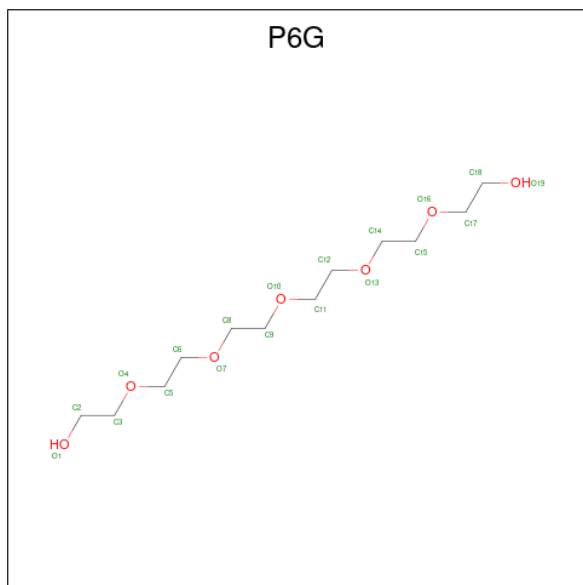
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



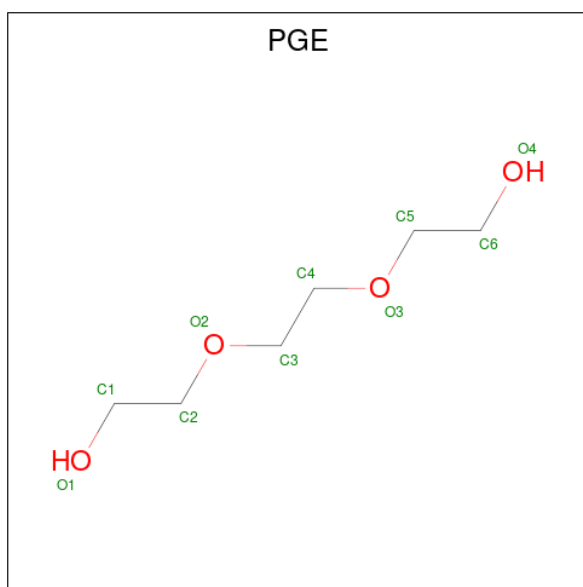
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			19	12	7		
7	D	1	Total	C	O	0	0
			19	12	7		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	272	Total 275	O 275	0	3
10	B	261	Total 264	O 264	0	3
10	C	147	Total 147	O 147	0	0
10	D	198	Total 198	O 198	0	0

3 Residue-property plots

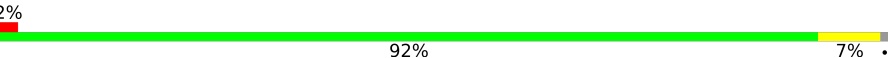
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

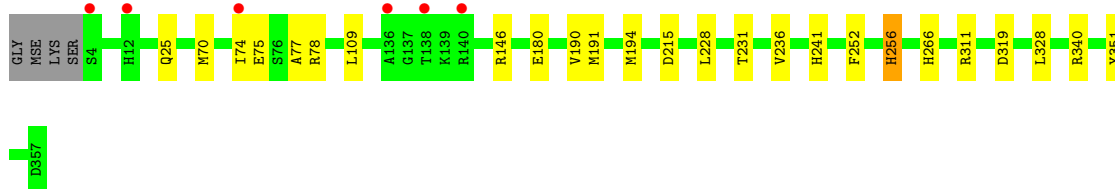
- Molecule 1: Iron-containing alcohol dehydrogenase

Chain A: 



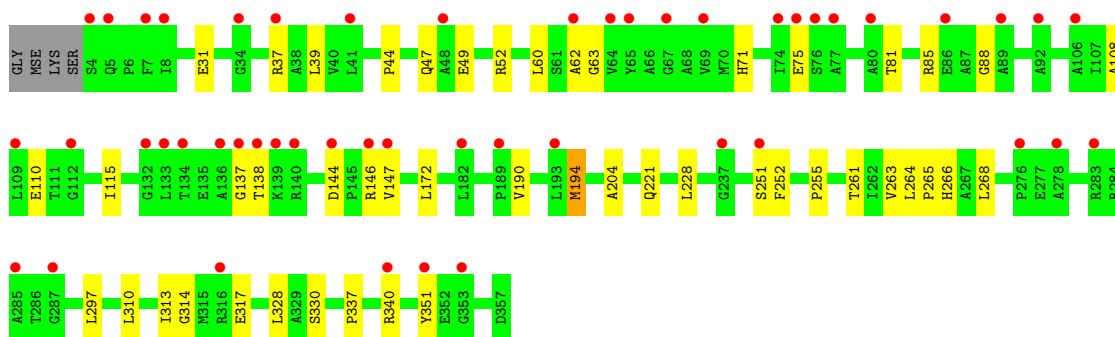
- Molecule 1: Iron-containing alcohol dehydrogenase

Chain B: 

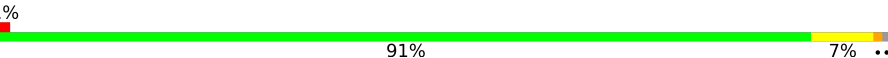


- Molecule 1: Iron-containing alcohol dehydrogenase

Chain C: 



- Molecule 1: Iron-containing alcohol dehydrogenase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.84Å 143.84Å 169.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.10 29.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.71-2.10) 99.8 (29.71-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0053, PHENIX	Depositor
R, R_{free}	0.174 , 0.210 0.177 , 0.211	Depositor DCC
R_{free} test set	5902 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11566	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: P6G, PEG, CL, NAD, GOL, PGE, PG4, CA

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	1.02	0/2683	1.01	3/3645 (0.1%)
1	B	0.98	0/2675	0.99	1/3634 (0.0%)
1	C	0.83	0/2633	0.98	4/3582 (0.1%)
1	D	0.90	0/2625	0.98	1/3572 (0.0%)
All	All	0.94	0/10616	0.99	9/14433 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	HIS	N-CA-C	7.04	118.65	110.97
1	A	329	ALA	N-CA-C	7.00	118.98	111.36
1	C	194	MSE	CG-SE-CE	-6.44	84.75	98.92
1	C	71	HIS	N-CA-C	5.63	119.45	112.24
1	C	314	GLY	N-CA-C	5.51	123.48	115.32
1	A	240	LEU	N-CA-C	5.42	117.61	111.11
1	A	115	ILE	CB-CA-C	-5.37	102.83	110.83
1	D	162	LEU	N-CA-C	-5.18	101.89	109.50
1	C	62	ALA	N-CA-C	-5.03	106.39	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2618	0	2630	32	0
1	B	2613	0	2621	24	0
1	C	2580	0	2574	35	0
1	D	2575	0	2553	18	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	14	0	20	1	0
5	B	7	0	10	0	0
6	A	13	0	18	1	0
6	B	13	0	18	4	0
7	C	19	0	26	0	0
7	D	19	0	26	0	0
8	C	12	0	16	0	0
8	D	6	0	8	1	0
9	D	10	0	14	2	0
10	A	275	0	0	5	0
10	B	264	0	0	1	0
10	C	147	0	0	1	0
10	D	198	0	0	2	0
All	All	11566	0	10638	106	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 5.

All (106) 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:74:ILE:HD12	1:D:78:ARG:CZ	2.08	0.83
1:A:70[C]:MSE:HE3	10:A:579:HOH:O	1.82	0.78
1:C:137:GLY:O	1:C:138:THR:HG23	1.85	0.77
1:B:194[A]:MSE:HE3	1:B:228:LEU:HD22	1.68	0.75
1:C:194:MSE:HE2	1:C:228:LEU:HD22	1.69	0.75
1:C:328[A]:LEU:HD21	1:C:340:ARG:HB2	1.70	0.71
1:A:194[A]:MSE:HE2	1:A:228:LEU:HD22	1.72	0.71
1:A:6:PRO:HB2	6:B:360:PG4:C4	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328[A]:LEU:CD2	1:C:340:ARG:HB2	2.21	0.70
1:A:194[B]:MSE:HE1	1:B:190:VAL:HG13	1.75	0.69
1:B:70:MSE:HE1	1:B:256:HIS:H	1.57	0.69
1:A:194[B]:MSE:HE1	1:B:190:VAL:CG1	2.25	0.67
1:A:211:ASN:ND2	10:A:628:HOH:O	2.28	0.65
1:A:6:PRO:HB2	6:B:360:PG4:H42	1.79	0.65
1:C:81:THR:O	1:C:85:ARG:HG3	1.96	0.65
1:C:37:ARG:HD3	1:C:88:GLY:O	1.98	0.64
1:A:70[A]:MSE:SE	10:A:579:HOH:O	2.64	0.64
1:B:194[A]:MSE:HE3	1:B:228:LEU:CD2	2.28	0.63
1:D:87:ALA:HB2	10:D:683:HOH:O	1.97	0.63
1:C:255:PRO:HD2	1:C:313:ILE:HD13	1.80	0.62
1:A:194[A]:MSE:CE	1:A:228:LEU:HD22	2.29	0.62
1:C:328[A]:LEU:HD21	1:C:340:ARG:CB	2.30	0.60
1:A:164:ARG:NH1	1:A:210:PHE:O	2.34	0.60
1:D:357:ASP:OD2	8:D:361:GOL:H2	2.01	0.60
1:C:81:THR:HG22	1:C:85:ARG:HD2	1.83	0.60
1:C:37:ARG:CD	1:C:88:GLY:O	2.50	0.60
1:A:144:ASP:OD1	1:A:146:ARG:HB2	2.03	0.59
1:C:328[A]:LEU:HD21	1:C:340:ARG:N	2.19	0.57
1:D:194[A]:MSE:HE2	1:D:228:LEU:HD22	1.87	0.57
1:C:328[A]:LEU:HD21	1:C:340:ARG:CA	2.35	0.56
1:B:194[A]:MSE:HE1	1:B:231:THR:HG21	1.88	0.55
1:C:144:ASP:O	1:C:147:VAL:HG22	2.07	0.54
1:B:328:LEU:HD21	1:B:340:ARG:N	2.23	0.54
1:C:108:ALA:HB2	1:C:115:ILE:HD11	1.88	0.54
1:A:194[A]:MSE:HE2	1:A:228:LEU:CD2	2.36	0.54
1:C:268:LEU:CD1	1:C:297:LEU:HD12	2.39	0.53
1:A:194[A]:MSE:CE	1:A:228:LEU:CD2	2.87	0.53
1:D:31:GLU:HG3	1:D:60:LEU:HD11	1.91	0.53
1:B:266:HIS:HE1	10:B:428:HOH:O	1.92	0.52
1:B:311[B]:ARG:HB3	1:B:351:TYR:CE1	2.45	0.52
1:A:328[A]:LEU:HD21	1:A:340[A]:ARG:HA	1.93	0.51
1:B:25:GLN:HE21	6:B:360:PG4:H21	1.75	0.51
1:B:109:LEU:O	1:B:146[B]:ARG:NH2	2.41	0.51
1:B:328:LEU:HD21	1:B:340:ARG:CA	2.41	0.51
1:A:144:ASP:O	1:A:147:VAL:HG22	2.10	0.51
1:C:328[A]:LEU:CD2	1:C:340:ARG:CB	2.90	0.50
1:D:25:GLN:NE2	9:D:359:PGE:H5	2.27	0.50
1:A:346:LEU:C	1:A:346:LEU:HD23	2.37	0.49
1:A:194[B]:MSE:SE	1:A:228:LEU:HD22	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HG2	10:A:578:HOH:O	2.13	0.49
1:A:25:GLN:NE2	6:A:363:PG4:H72	2.29	0.48
1:C:266:HIS:HD2	10:C:494:HOH:O	1.97	0.48
1:A:150:ARG:HD2	10:A:467:HOH:O	2.14	0.47
1:C:310:LEU:HB2	1:C:351:TYR:HA	1.95	0.47
1:A:70[A]:MSE:HE1	1:A:71:HIS:HE2	1.79	0.47
1:D:74:ILE:HD12	1:D:78:ARG:NH1	2.29	0.47
1:A:328[A]:LEU:HD21	1:A:340[A]:ARG:CA	2.43	0.47
1:B:74:ILE:O	1:B:78:ARG:HG3	2.14	0.47
1:D:25:GLN:HE21	9:D:359:PGE:H5	1.80	0.47
1:C:172:LEU:HD13	1:C:261:THR:HG23	1.96	0.47
1:C:328[A]:LEU:HD11	1:C:340:ARG:HA	1.97	0.47
1:D:204:ALA:HB3	1:D:221:GLN:OE1	2.15	0.47
1:A:310:LEU:HB2	1:A:351:TYR:HA	1.97	0.47
1:A:324:ALA:O	1:A:328[A]:LEU:HD13	2.14	0.47
1:D:172:LEU:HD13	1:D:261:THR:HG23	1.97	0.47
1:B:194[B]:MSE:CE	1:B:228:LEU:HD22	2.45	0.46
1:D:311:ARG:HB3	1:D:351:TYR:CE1	2.50	0.46
1:B:215:ASP:C	1:B:215:ASP:OD1	2.59	0.46
1:A:6:PRO:HB2	6:B:360:PG4:H41	1.97	0.46
1:D:144:ASP:OD1	1:D:146:ARG:HG2	2.17	0.45
1:C:204:ALA:HB3	1:C:221:GLN:OE1	2.17	0.45
1:A:253[B]:ASN:HD22	5:A:361:PEG:H11	1.82	0.45
1:D:194[A]:MSE:HE2	1:D:228:LEU:CD2	2.47	0.45
1:B:75:GLU:H	1:B:75:GLU:CD	2.25	0.45
1:C:268:LEU:HD12	1:C:297:LEU:HD12	1.98	0.45
1:B:328:LEU:HD22	1:B:340:ARG:HG3	1.99	0.44
1:C:31:GLU:HG3	1:C:60:LEU:HD11	1.99	0.44
1:C:317:GLU:HB2	1:C:351:TYR:CZ	2.52	0.44
1:C:44:PRO:HA	1:C:47:GLN:HE21	1.82	0.44
1:C:313:ILE:O	1:C:313:ILE:HD12	2.18	0.44
1:C:49:GLU:HA	1:C:52[B]:ARG:HD2	2.00	0.44
1:C:264:LEU:HB3	1:C:265:PRO:HD3	1.98	0.44
1:B:74:ILE:O	1:B:77:ALA:HB3	2.18	0.44
1:C:81:THR:HG21	1:C:110:GLU:HG2	2.00	0.44
1:B:252:PHE:CE1	1:B:319:ASP:HB3	2.53	0.43
1:C:190:VAL:O	1:C:194:MSE:HG3	2.18	0.43
1:A:70[C]:MSE:HE1	1:A:255:PRO:HA	1.99	0.43
1:B:194[B]:MSE:HE3	1:B:228:LEU:HD22	1.99	0.43
1:D:310:LEU:HB2	1:D:351:TYR:HA	2.01	0.43
1:A:194[B]:MSE:HE1	1:B:190:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328[A]:LEU:HD21	1:A:340[A]:ARG:CB	2.49	0.42
1:C:39:LEU:HD12	1:C:63:GLY:O	2.20	0.42
1:A:70[A]:MSE:HE1	1:A:71:HIS:NE2	2.34	0.42
1:B:328:LEU:HD21	1:B:340:ARG:HA	2.02	0.42
1:C:263:VAL:O	1:C:264:LEU:C	2.63	0.42
1:B:180:GLU:CD	1:B:241:HIS:HB3	2.45	0.41
1:C:31:GLU:CG	1:C:60:LEU:HD11	2.51	0.41
1:C:108:ALA:CB	1:C:115:ILE:HD11	2.51	0.41
1:D:5:GLN:HB2	1:D:6:PRO:HD2	2.03	0.41
1:B:191:MSE:HG3	1:B:236:VAL:HG13	2.03	0.41
1:D:122:TYR:HB3	1:D:226:ALA:HB2	2.03	0.41
1:D:346:LEU:C	1:D:346:LEU:HD23	2.47	0.40
1:A:176:ALA:HB1	1:A:241:HIS:CD2	2.57	0.40
1:A:68:ALA:HA	1:A:103:LEU:HD22	2.04	0.40
1:C:251:SER:HB2	1:C:252:PHE:CE2	2.57	0.40
1:D:341:GLU:HG2	10:D:720:HOH:O	2.21	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	359/358 (100%)	351 (98%)	8 (2%)	0	100	100
1	B	358/358 (100%)	351 (98%)	7 (2%)	0	100	100
1	C	355/358 (99%)	346 (98%)	9 (2%)	0	100	100
1	D	354/358 (99%)	346 (98%)	8 (2%)	0	100	100
All	All	1426/1432 (100%)	1394 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	258/248 (104%)	255 (99%)	3 (1%)	63	72
1	B	256/248 (103%)	256 (100%)	0	100	100
1	C	250/248 (101%)	246 (98%)	4 (2%)	55	64
1	D	249/248 (100%)	244 (98%)	5 (2%)	48	56
All	All	1013/992 (102%)	1001 (99%)	12 (1%)	68	72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70[A]	MSE
1	A	70[B]	MSE
1	A	70[C]	MSE
1	C	75	GLU
1	C	146	ARG
1	C	330	SER
1	C	337	PRO
1	D	70	MSE
1	D	74	ILE
1	D	95	VAL
1	D	185	ARG
1	D	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	173	ASN
1	A	211	ASN
1	A	266	HIS
1	B	173	ASN
1	B	266	HIS
1	C	46	GLN

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Mol	Chain	Res	Type
1	C	47	GLN
1	C	173	ASN
1	C	266	HIS
1	D	173	ASN
1	D	291	GLN
1	D	302	GLN

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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	$\# Z > 2$
6	PG4	A	363	-	12,12,12	0.72	0	11,11,11	1.05	0
5	PEG	A	361	-	6,6,6	0.35	0	5,5,5	0.54	0
7	P6G	C	359	-	18,18,18	0.56	0	17,17,17	0.49	0
9	PGE	D	359	-	9,9,9	0.62	0	8,8,8	0.83	0
5	PEG	A	362	-	6,6,6	0.36	0	5,5,5	0.56	0
2	NAD	A	400	-	46,48,48	1.71	6 (13%)	64,73,73	1.72	13 (20%)
8	GOL	C	360	-	5,5,5	0.34	0	5,5,5	0.13	0
5	PEG	B	359	-	6,6,6	0.41	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	P6G	D	360	-	18,18,18	0.55	0	17,17,17	0.55	0
2	NAD	B	400	-	46,48,48	1.94	10 (21%)	64,73,73	1.72	13 (20%)
8	GOL	C	361	-	5,5,5	0.22	0	5,5,5	0.34	0
8	GOL	D	361	-	5,5,5	0.29	0	5,5,5	1.12	0
2	NAD	D	400	-	46,48,48	1.71	5 (10%)	64,73,73	1.61	13 (20%)
2	NAD	C	400	-	46,48,48	1.99	8 (17%)	64,73,73	1.66	13 (20%)
6	PG4	B	360	-	12,12,12	0.61	0	11,11,11	0.60	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
6	PG4	A	363	-	-	9/10/10/10	-
5	PEG	A	361	-	-	2/4/4/4	-
7	P6G	C	359	-	-	2/16/16/16	-
9	PGE	D	359	-	-	3/7/7/7	-
5	PEG	A	362	-	-	1/4/4/4	-
2	NAD	A	400	-	-	3/30/62/62	0/5/5/5
8	GOL	C	360	-	-	2/4/4/4	-
5	PEG	B	359	-	-	2/4/4/4	-
7	P6G	D	360	-	-	7/16/16/16	-
2	NAD	B	400	-	-	3/30/62/62	0/5/5/5
8	GOL	C	361	-	-	2/4/4/4	-
8	GOL	D	361	-	-	4/4/4/4	-
2	NAD	D	400	-	-	3/30/62/62	0/5/5/5
2	NAD	C	400	-	-	3/30/62/62	0/5/5/5
6	PG4	B	360	-	-	8/10/10/10	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAD	O7N-C7N	8.98	1.40	1.24
2	C	400	NAD	O7N-C7N	8.90	1.40	1.24
2	A	400	NAD	O7N-C7N	8.52	1.40	1.24
2	B	400	NAD	O7N-C7N	7.55	1.38	1.24
2	B	400	NAD	PN-O3	5.48	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	NAD	PN-O3	4.88	1.64	1.59
2	C	400	NAD	PA-O3	4.41	1.64	1.59
2	B	400	NAD	C2N-N1N	3.67	1.39	1.35
2	B	400	NAD	PA-O3	3.50	1.63	1.59
2	B	400	NAD	C2A-N1A	3.29	1.39	1.33
2	C	400	NAD	C2N-N1N	3.14	1.38	1.35
2	B	400	NAD	C2A-N3A	3.09	1.39	1.33
2	D	400	NAD	O4D-C1D	2.75	1.44	1.40
2	A	400	NAD	C2A-N3A	2.72	1.38	1.33
2	C	400	NAD	C2A-N3A	2.67	1.38	1.33
2	D	400	NAD	C2A-N3A	2.61	1.38	1.33
2	C	400	NAD	C2A-N1A	2.57	1.38	1.33
2	B	400	NAD	C6N-C5N	2.56	1.43	1.38
2	A	400	NAD	C5A-N7A	-2.53	1.34	1.39
2	D	400	NAD	C2A-N1A	2.52	1.38	1.33
2	B	400	NAD	C4N-C3N	2.45	1.43	1.39
2	C	400	NAD	C8A-N7A	2.42	1.36	1.31
2	A	400	NAD	C2N-N1N	2.35	1.37	1.35
2	B	400	NAD	C2N-C3N	2.33	1.42	1.39
2	A	400	NAD	C2A-N1A	2.24	1.37	1.33
2	D	400	NAD	PN-O3	2.13	1.61	1.59
2	C	400	NAD	C5A-N7A	-2.08	1.35	1.39
2	A	400	NAD	PA-O3	2.04	1.61	1.59
2	B	400	NAD	C8A-N7A	2.02	1.35	1.31

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAD	N3A-C2A-N1A	-5.80	119.80	128.58
2	C	400	NAD	N3A-C2A-N1A	-5.23	120.66	128.58
2	A	400	NAD	N3A-C2A-N1A	-5.11	120.84	128.58
2	D	400	NAD	N3A-C2A-N1A	-4.89	121.18	128.58
2	C	400	NAD	C5A-C4A-N3A	-4.83	120.06	126.72
2	A	400	NAD	C5A-C4A-N3A	-4.73	120.21	126.72
2	D	400	NAD	C5A-C4A-N3A	-4.50	120.52	126.72
2	A	400	NAD	N9A-C8A-N7A	-4.28	107.87	113.94
2	A	400	NAD	C5A-N7A-C8A	4.10	109.90	103.45
2	D	400	NAD	N9A-C8A-N7A	-3.99	108.27	113.94
2	B	400	NAD	N9A-C8A-N7A	-3.99	108.27	113.94
2	C	400	NAD	C5A-N7A-C8A	3.81	109.44	103.45
2	C	400	NAD	N9A-C8A-N7A	-3.78	108.58	113.94
2	D	400	NAD	C5A-N7A-C8A	3.70	109.27	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAD	C5A-C4A-N3A	-3.69	121.64	126.72
2	A	400	NAD	C3N-C7N-N7N	3.66	122.24	117.74
2	B	400	NAD	C5N-C4N-C3N	-3.46	116.96	120.36
2	C	400	NAD	C2A-N3A-C4A	3.45	120.25	111.83
2	B	400	NAD	C2N-C3N-C4N	3.42	122.24	118.26
2	A	400	NAD	C4A-C5A-N7A	-3.30	106.81	110.58
2	B	400	NAD	C5A-N7A-C8A	3.29	108.62	103.45
2	A	400	NAD	O7N-C7N-N7N	-3.25	117.92	122.62
2	D	400	NAD	C2A-N3A-C4A	3.21	119.66	111.83
2	C	400	NAD	C4A-C5A-N7A	-3.20	106.93	110.58
2	B	400	NAD	C2A-N3A-C4A	3.15	119.53	111.83
2	D	400	NAD	C4A-C5A-N7A	-3.15	106.98	110.58
2	A	400	NAD	C2A-N3A-C4A	3.13	119.48	111.83
2	D	400	NAD	N3A-C4A-N9A	3.02	132.30	127.17
2	A	400	NAD	N3A-C4A-N9A	2.95	132.19	127.17
2	B	400	NAD	C3N-C7N-N7N	2.84	121.23	117.74
2	B	400	NAD	O2N-PN-O1N	2.79	125.42	112.44
2	B	400	NAD	C4A-N9A-C8A	2.75	108.63	105.74
2	A	400	NAD	O3-PN-O1N	-2.69	102.60	110.70
2	B	400	NAD	N3A-C4A-N9A	2.67	131.71	127.17
2	D	400	NAD	O3-PN-O1N	-2.67	102.68	110.70
2	B	400	NAD	O3-PN-O1N	-2.65	102.73	110.70
2	C	400	NAD	O3-PN-O1N	-2.62	102.81	110.70
2	C	400	NAD	N3A-C4A-N9A	2.55	131.51	127.17
2	D	400	NAD	C6N-N1N-C2N	-2.47	119.77	121.88
2	D	400	NAD	C4A-N9A-C8A	2.44	108.30	105.74
2	B	400	NAD	C4A-C5A-N7A	-2.41	107.83	110.58
2	C	400	NAD	C5A-C4A-N9A	2.40	108.42	105.81
2	C	400	NAD	O7N-C7N-N7N	-2.37	119.20	122.62
2	A	400	NAD	O2A-PA-O5B	2.33	118.14	107.57
2	C	400	NAD	C6N-N1N-C2N	-2.30	119.92	121.88
2	A	400	NAD	C6A-C5A-C4A	2.22	120.21	117.18
2	D	400	NAD	C6A-C5A-C4A	2.21	120.19	117.18
2	A	400	NAD	O2N-PN-O1N	2.20	122.67	112.44
2	D	400	NAD	O2N-PN-O1N	2.15	122.45	112.44
2	C	400	NAD	C6A-C5A-C4A	2.10	120.05	117.18
2	D	400	NAD	C5N-C4N-C3N	-2.05	118.35	120.36
2	C	400	NAD	O4B-C1B-N9A	2.02	111.97	108.09

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NAD	PA-O3-PN-O5D
2	A	400	NAD	C5D-O5D-PN-O1N
2	B	400	NAD	PA-O3-PN-O5D
2	C	400	NAD	PA-O3-PN-O5D
2	C	400	NAD	O4D-C1D-N1N-C6N
2	D	400	NAD	PA-O3-PN-O5D
2	D	400	NAD	O4D-C1D-N1N-C6N
8	C	361	GOL	C1-C2-C3-O3
8	D	361	GOL	O1-C1-C2-C3
7	D	360	P6G	C8-C9-O10-C11
6	A	363	PG4	O2-C3-C4-O3
6	B	360	PG4	O3-C5-C6-O4
6	B	360	PG4	O2-C3-C4-O3
8	D	361	GOL	O2-C2-C3-O3
7	D	360	P6G	O10-C11-C12-O13
7	C	359	P6G	O1-C2-C3-O4
6	A	363	PG4	O3-C5-C6-O4
6	A	363	PG4	O4-C7-C8-O5
7	D	360	P6G	O16-C17-C18-O19
8	C	360	GOL	O1-C1-C2-C3
8	D	361	GOL	C1-C2-C3-O3
6	A	363	PG4	O1-C1-C2-O2
7	D	360	P6G	O1-C2-C3-O4
9	D	359	PGE	O3-C5-C6-O4
8	C	361	GOL	O2-C2-C3-O3
6	B	360	PG4	O4-C7-C8-O5
2	B	400	NAD	C3D-C4D-C5D-O5D
5	A	361	PEG	O1-C1-C2-O2
6	B	360	PG4	O1-C1-C2-O2
8	C	360	GOL	O1-C1-C2-O2
8	D	361	GOL	O1-C1-C2-O2
2	B	400	NAD	O4D-C4D-C5D-O5D
9	D	359	PGE	O1-C1-C2-O2
7	C	359	P6G	C6-C5-O4-C3
7	D	360	P6G	C9-C8-O7-C6
5	B	359	PEG	O2-C3-C4-O4
7	D	360	P6G	C14-C15-O16-C17
6	A	363	PG4	C3-C4-O3-C5
6	A	363	PG4	C5-C6-O4-C7
6	B	360	PG4	C5-C6-O4-C7
6	B	360	PG4	C4-C3-O2-C2
9	D	359	PGE	C4-C3-O2-C2
2	A	400	NAD	O4D-C1D-N1N-C2N

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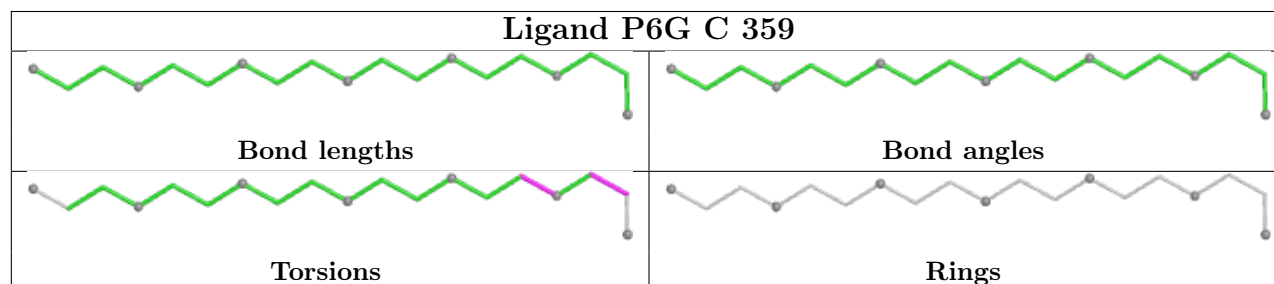
Mol	Chain	Res	Type	Atoms
2	C	400	NAD	O4D-C1D-N1N-C2N
2	D	400	NAD	O4D-C1D-N1N-C2N
7	D	360	P6G	C5-C6-O7-C8
5	A	362	PEG	O1-C1-C2-O2
5	A	361	PEG	C4-C3-O2-C2
5	B	359	PEG	C1-C2-O2-C3
6	B	360	PG4	C1-C2-O2-C3
6	B	360	PG4	C3-C4-O3-C5
6	A	363	PG4	C4-C3-O2-C2
6	A	363	PG4	C6-C5-O3-C4
6	A	363	PG4	C8-C7-O4-C6

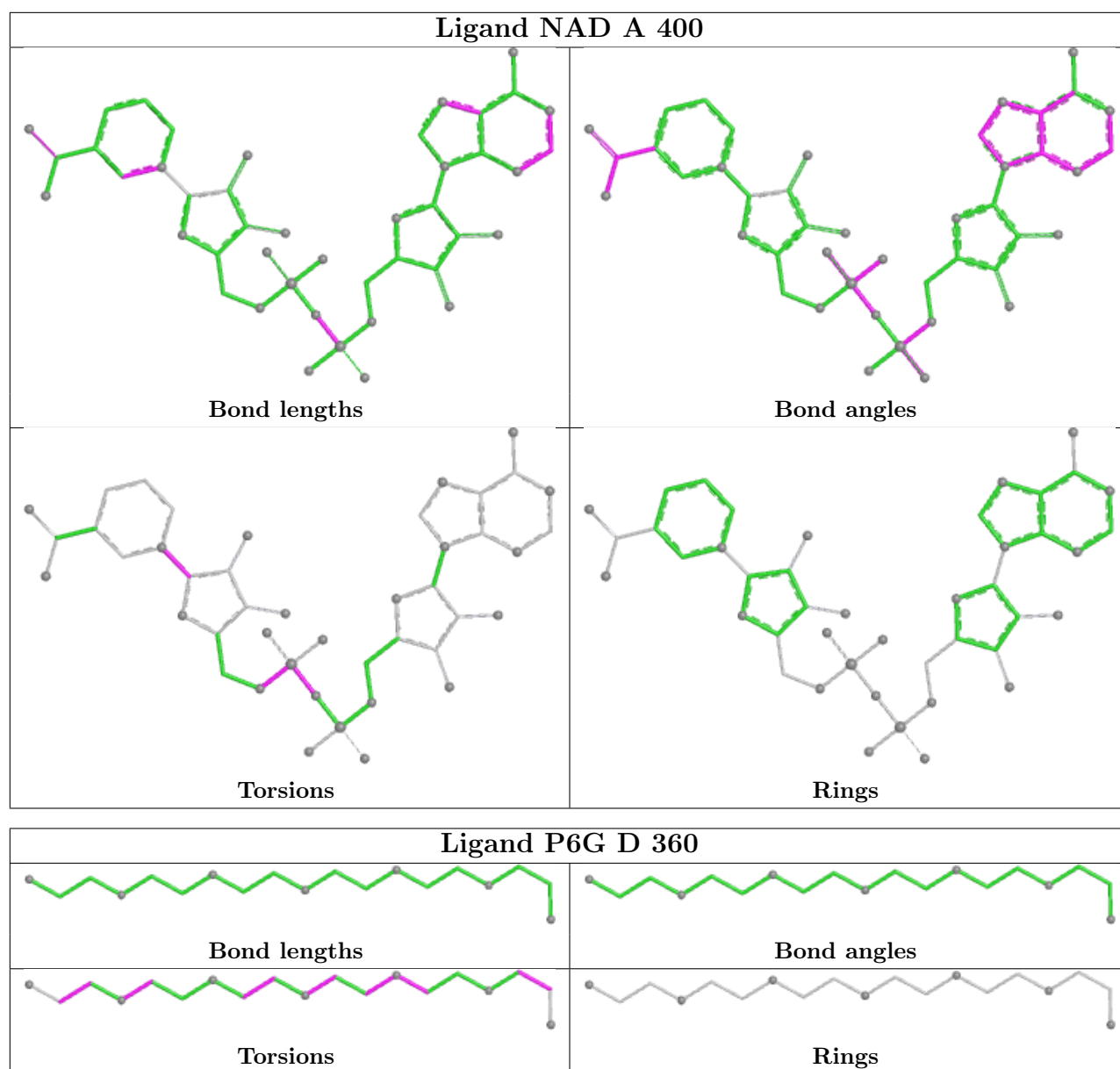
There are no ring outliers.

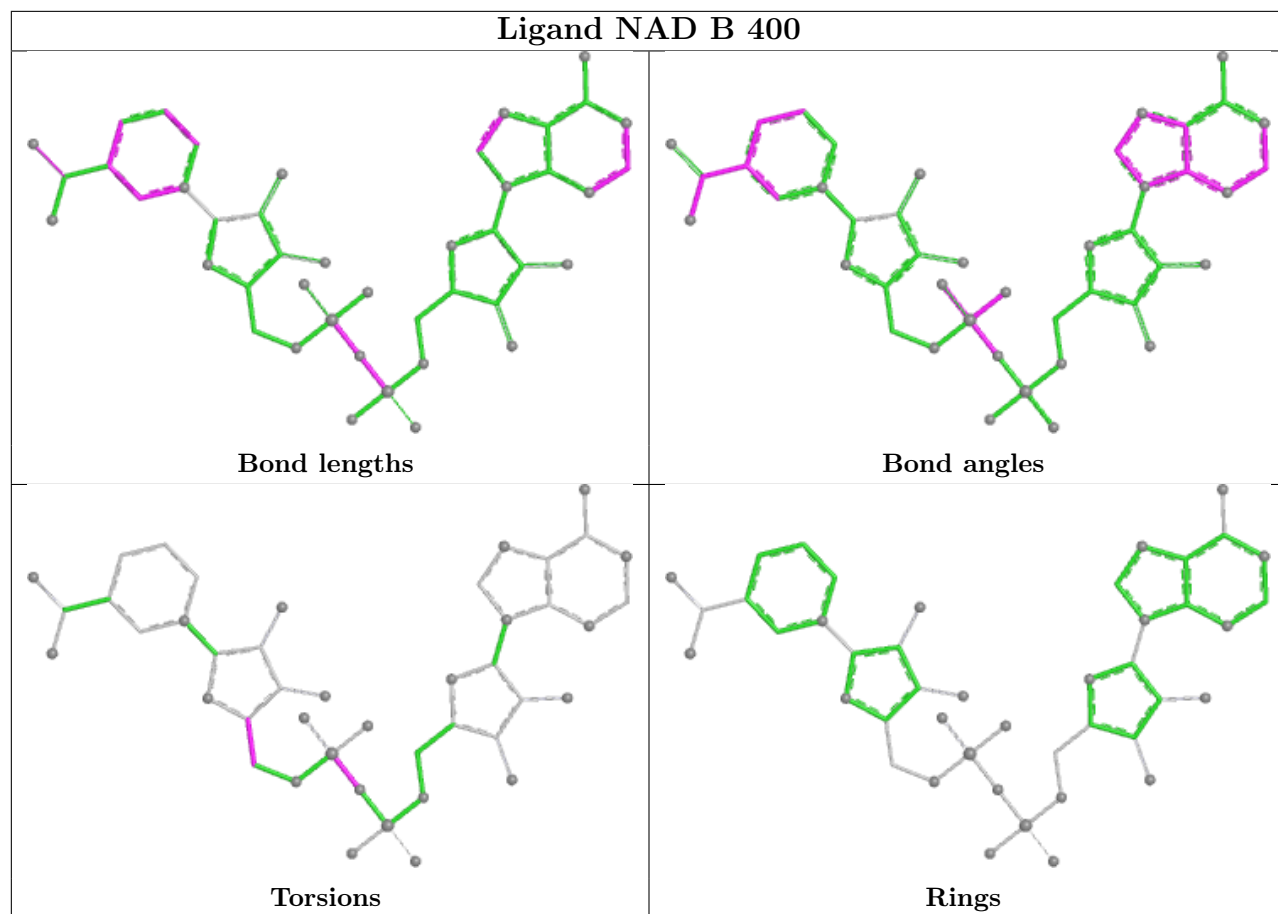
5 monomers are involved in 9 short contacts:

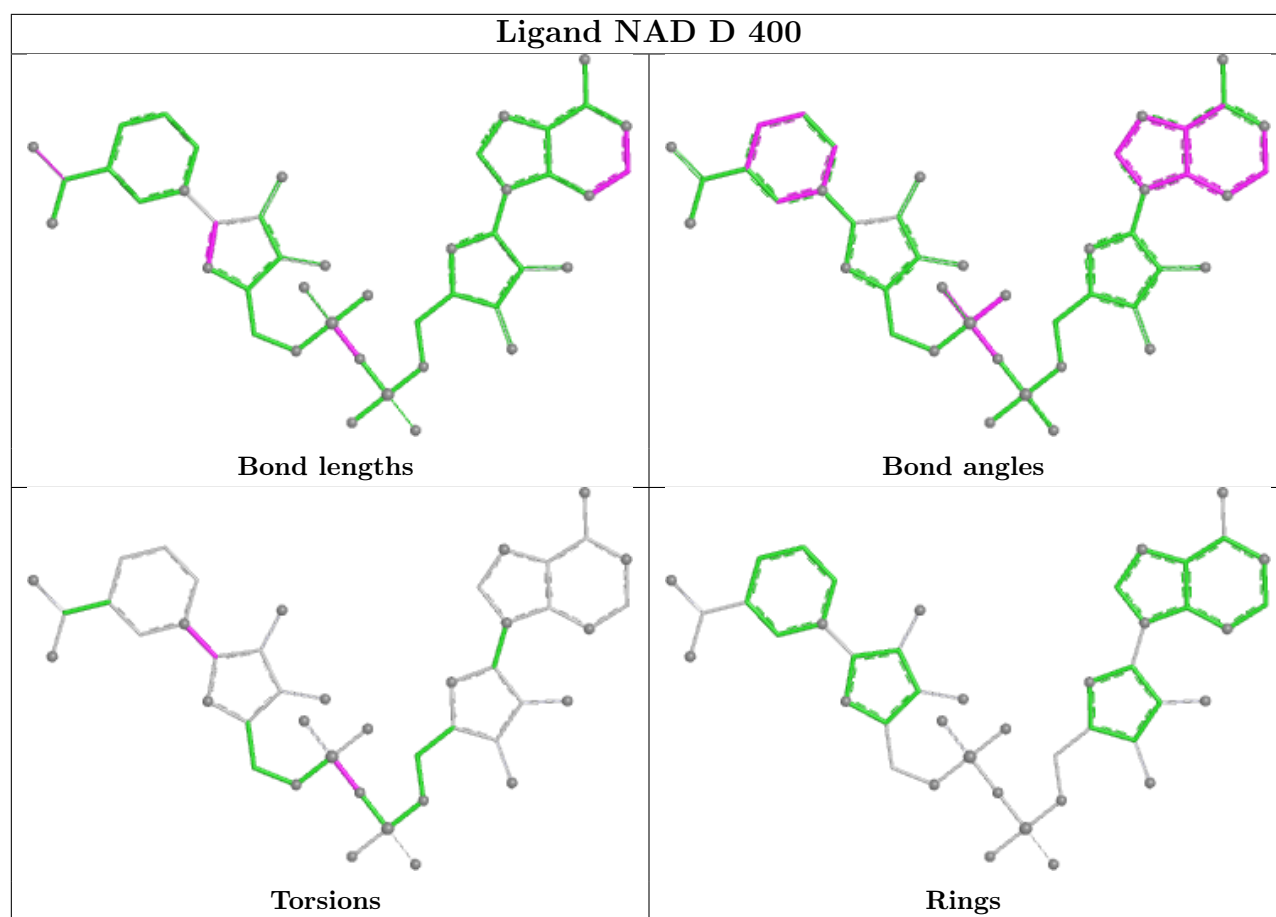
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	363	PG4	1	0
5	A	361	PEG	1	0
9	D	359	PGE	2	0
8	D	361	GOL	1	0
6	B	360	PG4	4	0

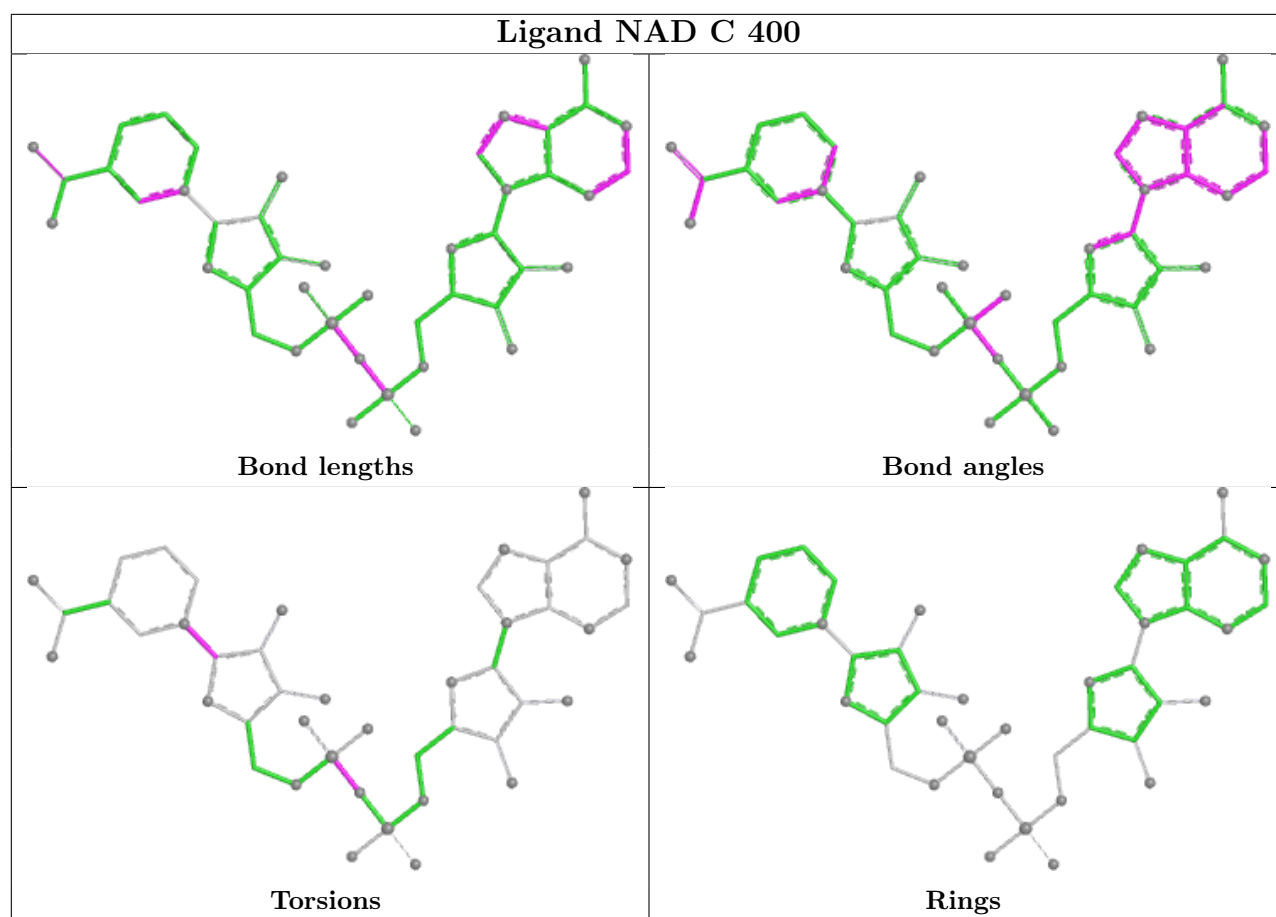
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	347/358 (96%)	-0.54	1 (0%) 90 91	10, 18, 35, 49	4 (1%)
1	B	347/358 (96%)	-0.31	6 (1%) 69 71	9, 19, 41, 50	5 (1%)
1	C	347/358 (96%)	1.03	49 (14%) 6 6	13, 24, 42, 50	3 (0%)
1	D	347/358 (96%)	-0.14	4 (1%) 76 78	14, 22, 41, 54	1 (0%)
All	All	1388/1432 (96%)	0.01	60 (4%) 40 41	9, 21, 41, 54	13 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	THR	4.1
1	C	136	ALA	3.8
1	C	109	LEU	3.6
1	C	89	ALA	3.4
1	C	140	ARG	3.4
1	C	64	VAL	3.4
1	C	4	SER	3.3
1	C	37	ARG	3.3
1	C	133	LEU	3.2
1	B	12	HIS	3.2
1	C	75	GLU	3.1
1	C	146	ARG	3.0
1	C	7	PHE	3.0
1	B	4	SER	2.9
1	C	132	GLY	2.9
1	C	80	ALA	2.8
1	A	4	SER	2.7
1	C	106	ALA	2.7
1	C	76	SER	2.7
1	C	147	VAL	2.7
1	B	136	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	4	SER	2.6
1	C	69	VAL	2.6
1	C	67	GLY	2.6
1	C	74	ILE	2.5
1	C	92	ALA	2.5
1	C	137	GLY	2.5
1	C	65	TYR	2.5
1	C	34	GLY	2.5
1	C	351	TYR	2.4
1	C	276	PRO	2.4
1	C	285	ALA	2.4
1	C	134	THR	2.4
1	D	138	THR	2.4
1	C	193	LEU	2.3
1	C	112	GLY	2.3
1	C	139	LYS	2.3
1	C	283	ARG	2.3
1	C	316	ARG	2.3
1	C	189	PRO	2.3
1	C	144	ASP	2.3
1	C	278	ALA	2.2
1	C	251	SER	2.2
1	C	8	ILE	2.2
1	C	287	GLY	2.2
1	B	140	ARG	2.2
1	B	74	ILE	2.2
1	C	353	GLY	2.2
1	B	138	THR	2.2
1	C	86	GLU	2.1
1	D	71	HIS	2.1
1	C	41	LEU	2.1
1	C	62	ALA	2.1
1	C	340	ARG	2.1
1	C	48	ALA	2.1
1	C	182	LEU	2.1
1	D	75	GLU	2.1
1	C	5	GLN	2.1
1	C	237	GLY	2.1
1	C	77	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

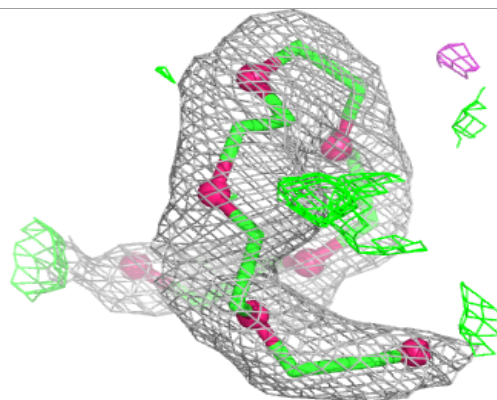
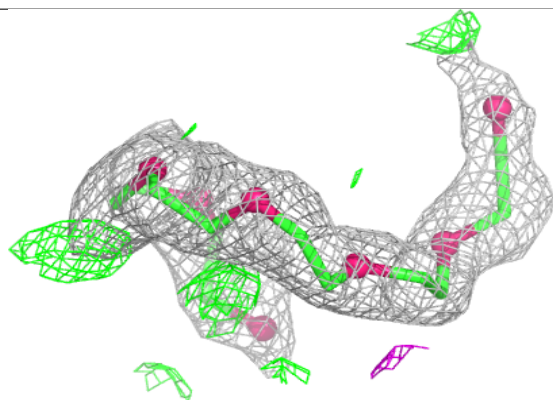
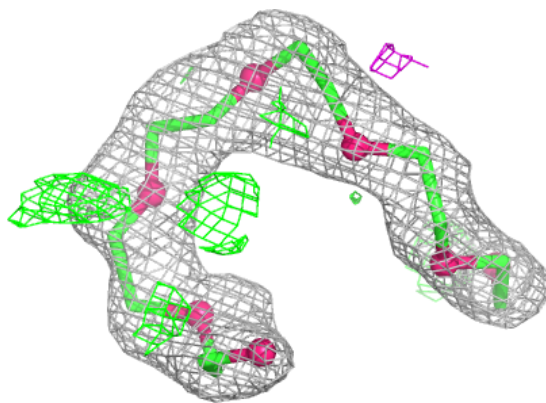
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	D	361	6/6	0.53	0.23	61,67,69,71	0
8	GOL	C	361	6/6	0.56	0.22	64,65,66,66	0
8	GOL	C	360	6/6	0.61	0.21	77,80,80,82	0
5	PEG	B	359	7/7	0.82	0.16	58,60,62,63	0
7	P6G	D	360	19/19	0.84	0.14	48,54,57,57	0
6	PG4	A	363	13/13	0.85	0.14	27,44,48,49	0
6	PG4	B	360	13/13	0.86	0.14	31,44,56,60	0
5	PEG	A	362	7/7	0.88	0.13	49,52,58,59	0
5	PEG	A	361	7/7	0.89	0.13	41,44,49,49	0
9	PGE	D	359	10/10	0.90	0.11	28,39,49,52	0
2	NAD	C	400	44/44	0.91	0.10	41,47,56,57	0
7	P6G	C	359	19/19	0.92	0.11	28,39,55,56	0
3	CA	A	359[B]	1/1	0.93	0.05	43,43,43,43	1
3	CA	A	359[A]	1/1	0.93	0.05	25,25,25,25	1
2	NAD	D	400	44/44	0.94	0.08	27,39,44,49	0
2	NAD	B	400	44/44	0.94	0.09	28,39,43,47	0
4	CL	C	358	1/1	0.97	0.05	39,39,39,39	0
4	CL	D	358	1/1	0.98	0.03	29,29,29,29	0
3	CA	A	358	1/1	0.98	0.08	27,27,27,27	0
4	CL	B	358	1/1	0.98	0.03	29,29,29,29	0
2	NAD	A	400	44/44	0.98	0.06	17,25,30,32	0
4	CL	A	360	1/1	0.99	0.03	30,30,30,30	0

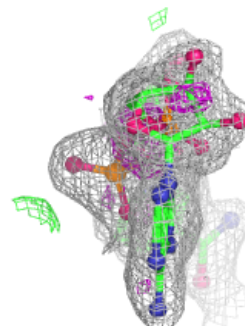
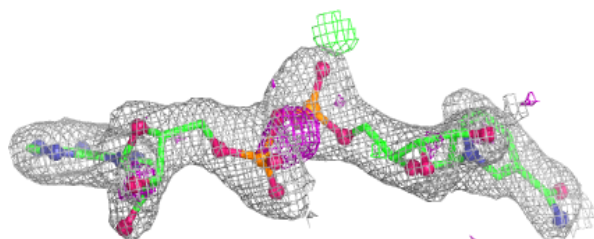
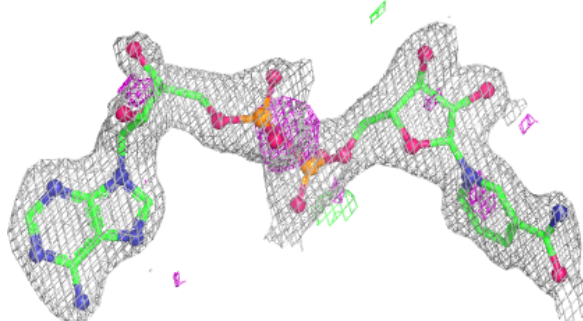
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G D 360:

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

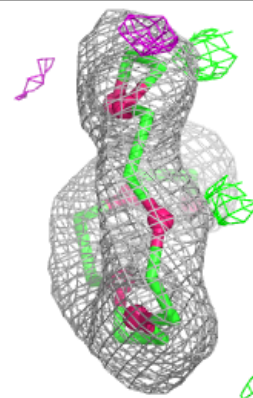
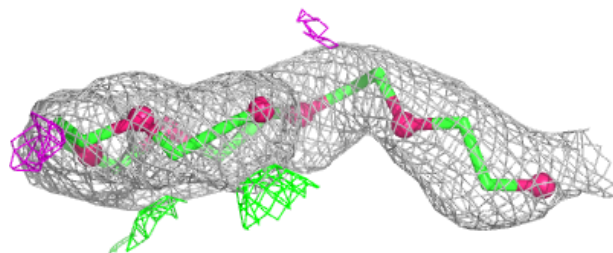
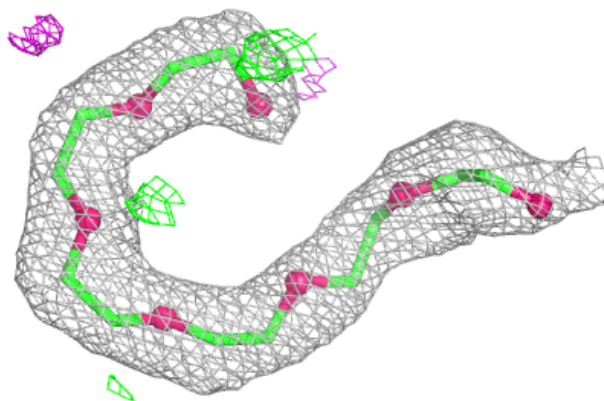
**Electron density around NAD C 400:**

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

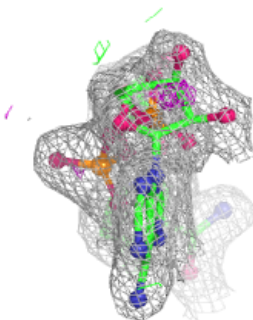
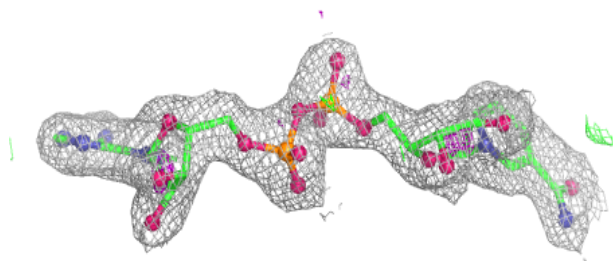
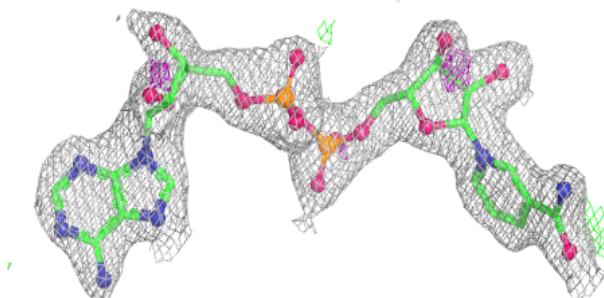


Electron density around P6G C 359:

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

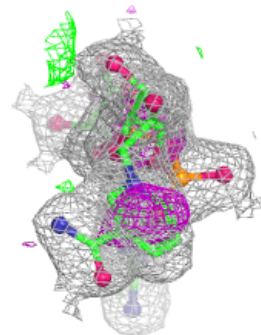
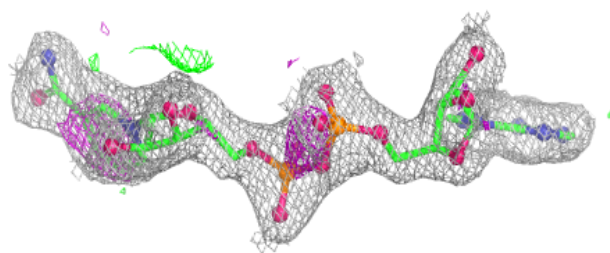
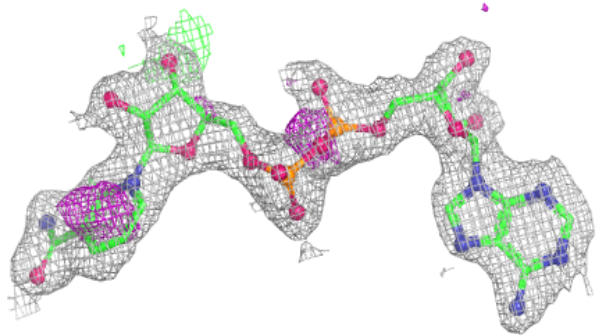
**Electron density around NAD D 400:**

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

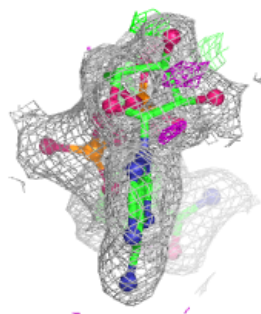
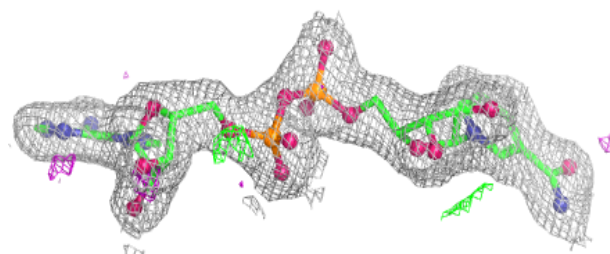
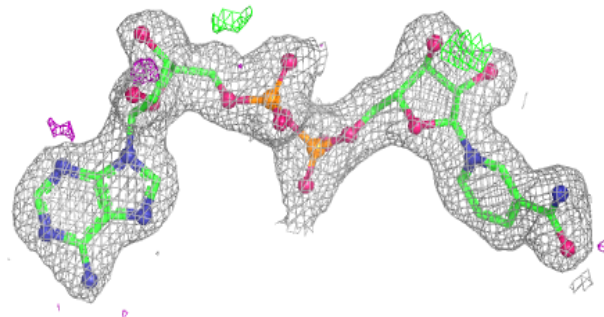


Electron density around NAD B 400:

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

**Electron density around NAD A 400:**

$2mF_o-DF_c$ (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.