



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:53 AM UTC

PDB ID : 9E5W / pdb_00009e5w
Title : Proline utilization A (PutA) from Sinorhizobium meliloti inactivated by N-propargylglycine
Authors : Tanner, J.J.
Deposited on : 2024-10-28
Resolution : 1.52 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

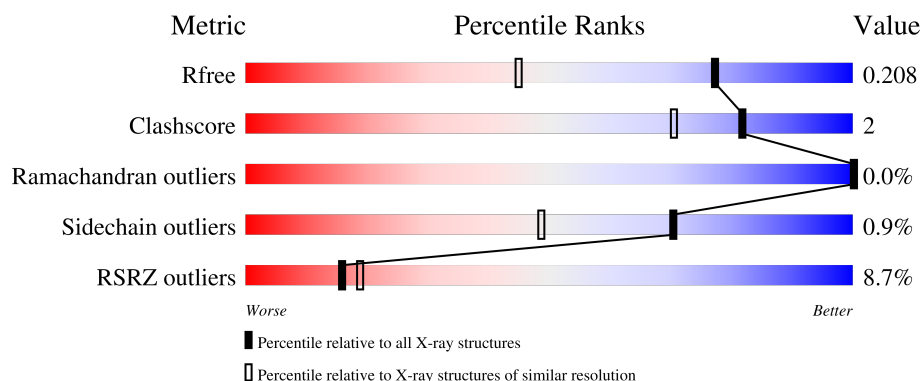
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	1235	6% 93% 5%
1	B	1235	10% 90% 8%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 19524 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.

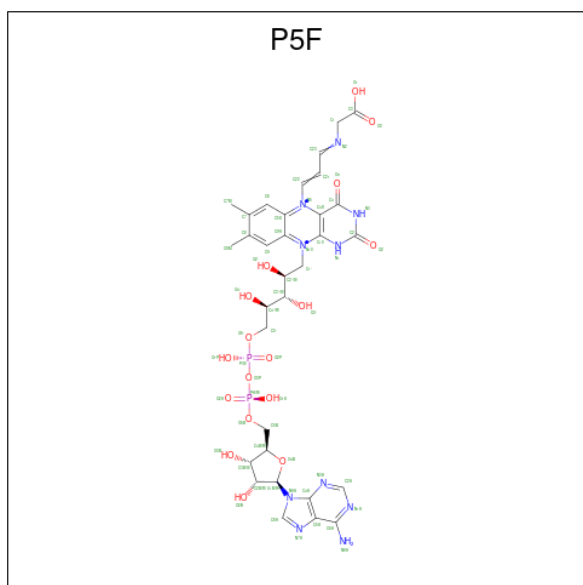
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1212	Total	C	N	O	S	0	17	0
			8954	5638	1596	1687	33			
1	B	1202	Total	C	N	O	S	0	6	0
			8839	5566	1582	1659	32			

There are 4 discrepancies between the modelled and reference sequences:

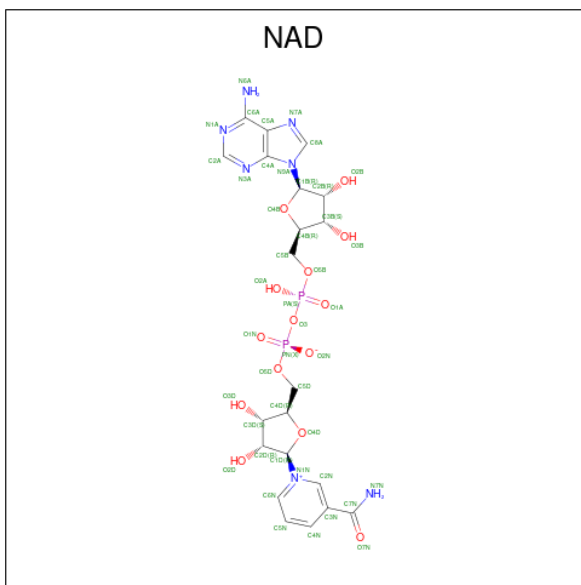
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q92SD7
A	0	MET	-	expression tag	UNP Q92SD7
B	-1	SER	-	expression tag	UNP Q92SD7
B	0	MET	-	expression tag	UNP Q92SD7

- Molecule 2 is N-propargylglycine-modified flavin adenine dinucleotide (CCD ID: P5F) (formula: $C_{32}H_{40}N_{10}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 56	C 30	N 9	O 15	P 2	0	0
2	B	1	Total 56	C 30	N 9	O 15	P 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

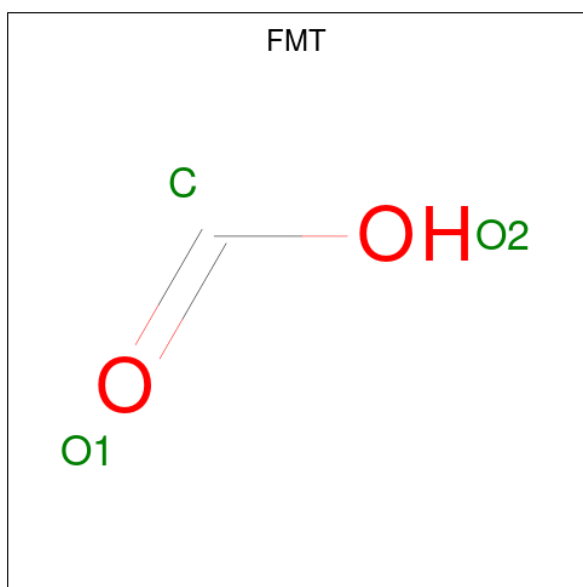


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

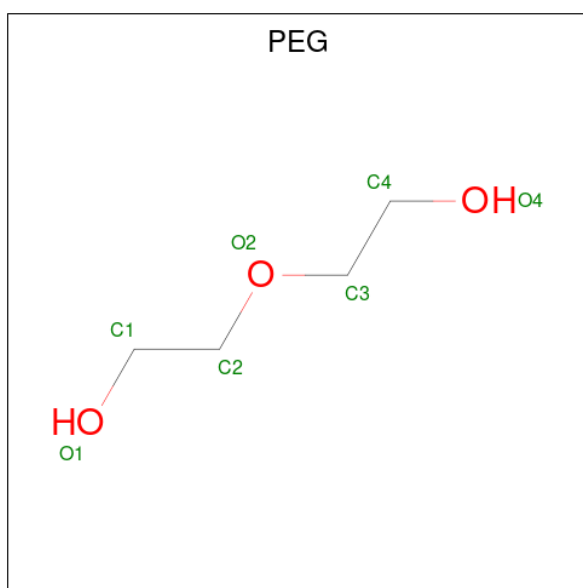
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



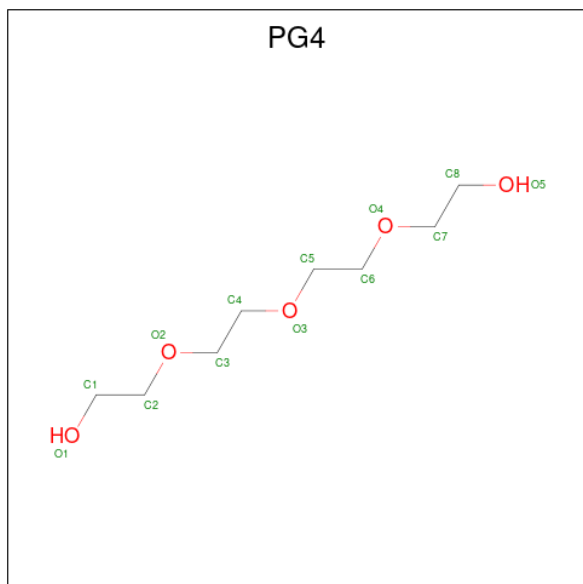
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		

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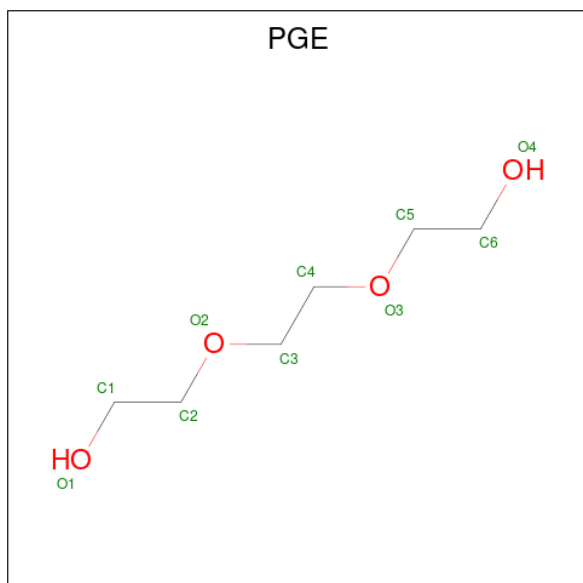
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

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



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

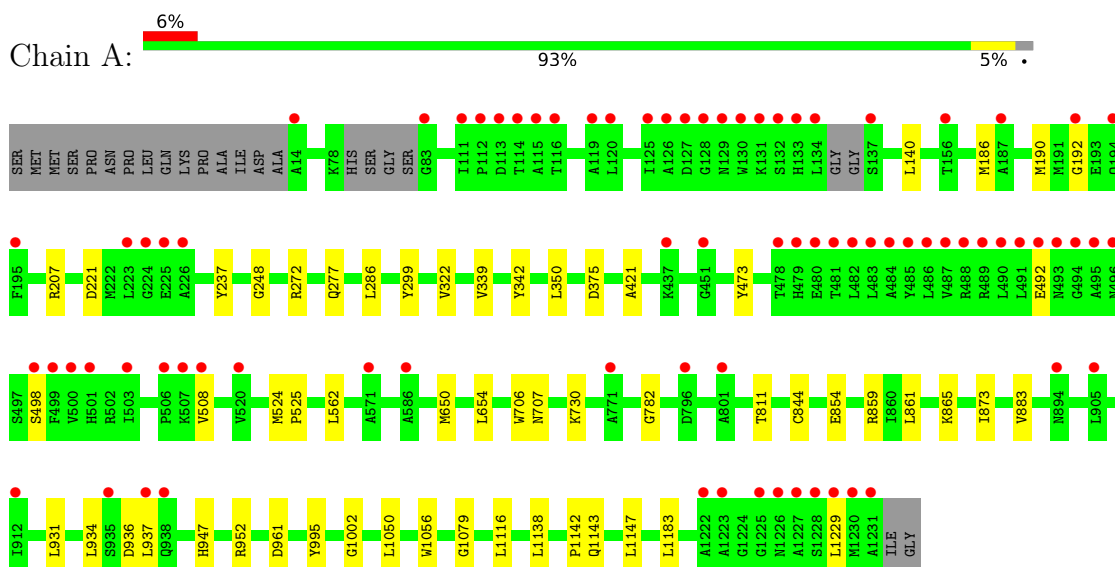
- Molecule 10 is water.

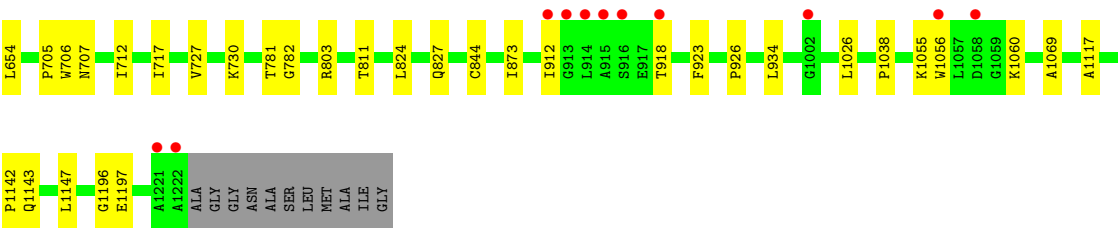
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	719	Total	O	0	0
			719	719		
10	B	725	Total	O	0	0
			725	725		

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: Bifunctional protein PutA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.85Å 101.97Å 126.57Å 90.00° 106.50° 90.00°	Depositor
Resolution (Å)	47.00 – 1.52 47.00 – 1.52	Depositor EDS
% Data completeness (in resolution range)	92.3 (47.00-1.52) 98.0 (47.00-1.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.191 , 0.211 0.188 , 0.208	Depositor DCC
R_{free} test set	18263 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.9	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	0.96	EDS
Total number of atoms	19524	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: PEG, FMT, PG4, PGE, MG, SO4, P5F, 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	0.24	0/9143	0.44	0/12460
1	B	0.25	0/9012	0.46	0/12278
All	All	0.24	0/18155	0.45	0/24738

There are no bond length outliers.

There are no bond angle outliers.

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	8954	0	8883	33	0
1	B	8839	0	8787	56	0
2	A	56	0	35	3	0
2	B	56	0	35	2	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
4	A	25	0	0	0	0
4	B	10	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	3	0	1	0	0
7	A	14	0	20	2	0
7	B	7	0	10	1	0
8	B	13	0	18	0	0
9	B	10	0	14	0	0
10	A	719	0	0	1	0
10	B	725	0	0	2	0
All	All	19524	0	17856	89	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 2.

All (89) 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:1079:GLY:HA2	7:A:1310:PEG:H41	1.48	0.94
1:B:55:THR:HG22	1:B:522:ARG:HH22	1.35	0.91
1:B:1196:GLY:HA3	7:B:1307:PEG:H12	1.64	0.78
1:B:844:CYS:SG	3:B:1302:NAD:C4N	2.79	0.70
1:B:539:GLU:OE1	10:B:1401:HOH:O	2.10	0.67
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.77	0.66
1:A:844:CYS:SG	3:A:1302:NAD:C4N	2.83	0.65
1:A:1183:LEU:O	10:A:1401:HOH:O	2.13	0.65
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.80	0.64
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.30	0.63
1:B:56:GLN:O	1:B:61:ARG:NH1	2.33	0.60
1:A:854:GLU:HG2	1:A:952:ARG:HE	1.66	0.60
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.85	0.59
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.85	0.59
1:B:51:VAL:O	1:B:55:THR:HG23	2.03	0.59
1:B:502:ARG:HB3	1:B:513:LEU:HD21	1.83	0.58
1:A:473:TYR:HB2	2:A:1301:P5F:H17	1.86	0.57
1:B:192:GLY:O	1:B:207:ARG:NH1	2.37	0.57
1:B:650:MET:O	1:B:654:LEU:HG	2.04	0.57
1:B:195:PHE:HB3	1:B:482:LEU:HD11	1.87	0.55
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.89	0.55
1:A:524[A]:MET:HE3	1:A:525:PRO:HD2	1.90	0.54
1:B:396:ILE:HD11	1:B:517:PRO:HA	1.91	0.53
1:B:459:GLU:OE1	1:B:465:LYS:NZ	2.39	0.52
1:B:473:TYR:HB2	2:B:1301:P5F:H17	1.91	0.52
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:LEU:HD23	1:B:827:GLN:HG3	1.92	0.51
1:B:494:GLY:HA2	1:B:501:HIS:HB2	1.93	0.51
1:A:995:TYR:OH	1:A:1002[A]:GLY:O	2.20	0.51
1:B:90:GLU:OE1	1:B:182:ARG:NH2	2.41	0.50
1:A:421:ALA:HB1	2:A:1301:P5F:H21	1.94	0.49
1:A:562:LEU:HD11	1:A:654:LEU:HD12	1.94	0.49
1:B:803:ARG:NH2	1:B:1197:GLU:OE1	2.28	0.49
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.49	0.47
1:B:65:ALA:HB1	1:B:514:ILE:HD12	1.95	0.47
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.50	0.47
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.50	0.47
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.97	0.47
1:B:181:ARG:NH1	1:B:185:ASP:OD1	2.46	0.47
2:A:1301:P5F:C4	2:A:1301:P5F:H35	2.45	0.47
1:B:270:HIS:HB2	1:B:285:LEU:HG	1.96	0.46
1:A:221:ASP:HB2	1:A:473:TYR:CZ	2.51	0.46
1:B:288:ARG:HD3	10:B:1707:HOH:O	2.16	0.46
1:B:197:THR:O	1:B:207:ARG:HD2	2.15	0.46
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.51	0.46
1:B:1056:TRP:CZ2	1:B:1060:LYS:HD2	2.50	0.46
1:A:844:CYS:SG	3:A:1302:NAD:C3N	3.04	0.46
1:A:931:LEU:HD13	1:A:936:ASP:HB2	1.98	0.45
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.97	0.45
1:A:650:MET:O	1:A:654:LEU:HG	2.17	0.45
1:B:118:ASP:OD1	1:B:181:ARG:NH2	2.49	0.45
1:A:782:GLY:O	1:A:811:THR:HA	2.17	0.45
7:A:1310:PEG:H42	7:A:1310:PEG:H21	1.71	0.45
1:B:128:GLY:O	1:B:130:TRP:N	2.46	0.45
1:A:1147:LEU:HD22	1:B:1147:LEU:HD13	1.99	0.45
1:B:782:GLY:O	1:B:811:THR:HA	2.17	0.44
1:B:448:CYS:HB2	1:B:453:GLY:HA3	2.00	0.44
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.18	0.44
1:A:192:GLY:O	1:A:207:ARG:NH1	2.46	0.43
1:B:424:ASN:HB2	2:B:1301:P5F:H1	1.82	0.43
1:B:1060:LYS:HB3	1:B:1060:LYS:HE3	1.72	0.43
1:B:844:CYS:SG	3:B:1302:NAD:C3N	3.06	0.43
1:A:1143:GLN:O	1:A:1147:LEU:HG	2.19	0.43
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.54	0.42
1:A:375[A]:ASP:OD1	1:A:1229:LEU:HB3	2.19	0.42
1:B:221:ASP:HB2	1:B:473:TYR:CZ	2.54	0.42
1:B:578:PRO:O	1:B:584:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:NH2	1:B:505:ASP:O	2.52	0.42
1:B:193:GLU:O	1:B:450:HIS:NE2	2.43	0.42
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.55	0.42
1:A:937:LEU:HD21	1:A:947:HIS:CD2	2.54	0.41
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.02	0.41
1:A:186:MET:O	1:A:190:MET:HG3	2.20	0.41
1:B:396:ILE:HG12	1:B:521:VAL:HG23	2.01	0.41
1:B:482:LEU:C	1:B:484:ALA:H	2.28	0.41
1:A:861:LEU:HG	1:A:865:LYS:HE3	2.01	0.41
1:B:918:THR:HB	1:B:923:PHE:CD1	2.55	0.41
1:B:461:VAL:HG12	1:B:468:ARG:O	2.21	0.41
1:B:712:ILE:HD13	1:B:781:THR:HG21	2.03	0.41
1:B:1069:ALA:HA	1:B:1117:ALA:HB1	2.02	0.41
1:B:338:VAL:HG22	1:B:367:ARG:HB3	2.01	0.41
1:B:396:ILE:HD11	1:B:520:VAL:HB	2.03	0.41
1:B:912:ILE:HD11	1:B:926:PRO:HD2	2.02	0.41
1:A:492:GLU:O	1:A:498:SER:OG	2.24	0.41
1:B:705:PRO:HD3	1:B:781:THR:HB	2.03	0.40
1:A:237:TYR:CD1	1:A:237:TYR:C	2.99	0.40
1:B:873:ILE:HD11	1:B:912:ILE:HD11	2.02	0.40
1:B:57:SER:O	1:B:61:ARG:HG3	2.20	0.40
1:A:1050:LEU:HD13	1:A:1050:LEU:C	2.45	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	1223/1235 (99%)	1204 (98%)	19 (2%)	0	100	100
1	B	1202/1235 (97%)	1174 (98%)	27 (2%)	1 (0%)	48	25
All	All	2425/2470 (98%)	2378 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	484	ALA

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	886/951 (93%)	880 (99%)	6 (1%)	76	57
1	B	875/951 (92%)	864 (99%)	11 (1%)	61	34
All	All	1761/1902 (93%)	1744 (99%)	17 (1%)	70	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	342	TYR
1	A	508	VAL
1	A	730	LYS
1	A	859	ARG
1	A	934	LEU
1	B	137	SER
1	B	139	SER
1	B	140[A]	LEU
1	B	140[B]	LEU
1	B	202	ARG
1	B	342	TYR
1	B	461	VAL
1	B	482	LEU
1	B	526	VAL
1	B	730	LYS
1	B	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	685	GLN
1	A	872	HIS

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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$
2	P5F	B	1301	1	56,61,66	2.79	18 (32%)	74,93,99	2.17	22 (29%)
7	PEG	B	1307	-	6,6,6	0.24	0	5,5,5	0.40	0
4	SO4	A	1306	-	4,4,4	0.67	0	6,6,6	0.14	0
4	SO4	A	1307	-	4,4,4	0.66	0	6,6,6	0.19	0
7	PEG	A	1310	-	6,6,6	0.25	0	5,5,5	0.15	0
8	PG4	B	1308	-	12,12,12	0.30	0	11,11,11	0.25	0
4	SO4	B	1303	-	4,4,4	0.62	0	6,6,6	0.21	0
4	SO4	A	1303	-	4,4,4	0.59	0	6,6,6	0.32	0
4	SO4	A	1305	-	4,4,4	0.66	0	6,6,6	0.28	0
2	P5F	A	1301	1	56,61,66	2.70	17 (30%)	74,93,99	2.14	22 (29%)
3	NAD	B	1302	5	46,48,48	3.50	18 (39%)	64,73,73	2.05	12 (18%)
6	FMT	B	1306	-	2,2,2	0.82	0	1,1,1	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	A	1311	-	6,6,6	0.24	0	5,5,5	0.11	0
6	FMT	A	1309	-	2,2,2	0.54	0	1,1,1	0.31	0
4	SO4	A	1304	-	4,4,4	0.62	0	6,6,6	0.29	0
4	SO4	B	1304	-	4,4,4	0.67	0	6,6,6	0.11	0
9	PGE	B	1309	-	9,9,9	0.30	0	8,8,8	0.54	0
3	NAD	A	1302	5	46,48,48	3.65	19 (41%)	64,73,73	2.09	12 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P5F	B	1301	1	-	1/34/53/58	0/6/6/6
7	PEG	B	1307	-	-	1/4/4/4	-
7	PEG	A	1310	-	-	2/4/4/4	-
8	PG4	B	1308	-	-	1/10/10/10	-
2	P5F	A	1301	1	-	3/34/53/58	0/6/6/6
3	NAD	B	1302	5	-	4/30/62/62	0/5/5/5
7	PEG	A	1311	-	-	0/4/4/4	-
9	PGE	B	1309	-	-	2/7/7/7	-
3	NAD	A	1302	5	-	5/30/62/62	0/5/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	P5F	PA-O3P	-9.54	1.49	1.59
3	B	1302	NAD	O4D-C1D	-9.52	1.28	1.40
3	A	1302	NAD	O4D-C1D	-9.03	1.29	1.40
2	A	1301	P5F	PA-O3P	-8.47	1.50	1.59
3	A	1302	NAD	PN-O3	8.36	1.68	1.59
3	B	1302	NAD	C3B-C4B	-8.32	1.31	1.53
3	A	1302	NAD	C3B-C4B	-8.31	1.31	1.53
3	B	1302	NAD	C7N-N7N	8.21	1.48	1.33
3	A	1302	NAD	C7N-N7N	7.91	1.47	1.33
3	A	1302	NAD	C3D-C4D	-7.55	1.33	1.53
3	A	1302	NAD	O4B-C4B	7.26	1.61	1.45
3	B	1302	NAD	C3D-C4D	-7.18	1.34	1.53
2	B	1301	P5F	C6-C5X	7.14	1.49	1.40
2	A	1301	P5F	C6-C5X	7.13	1.49	1.40
2	B	1301	P5F	O4-C4	6.93	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	NAD	PN-O3	6.82	1.66	1.59
3	A	1302	NAD	O4D-C4D	6.79	1.60	1.45
3	B	1302	NAD	O4B-C4B	6.70	1.59	1.45
3	B	1302	NAD	O4D-C4D	6.54	1.59	1.45
2	A	1301	P5F	O4-C4	6.41	1.35	1.23
2	B	1301	P5F	C9-C9A	6.21	1.48	1.40
3	B	1302	NAD	C6A-N6A	6.17	1.50	1.34
2	A	1301	P5F	P-O3P	6.16	1.66	1.59
2	B	1301	P5F	O2-C2	5.93	1.36	1.23
2	A	1301	P5F	C9-C9A	5.75	1.47	1.40
3	A	1302	NAD	C6A-N6A	5.63	1.48	1.34
2	A	1301	P5F	O2-C2	5.27	1.34	1.23
2	B	1301	P5F	C10-N1	4.86	1.44	1.36
2	B	1301	P5F	C2-N1	4.26	1.44	1.37
3	A	1302	NAD	PA-O3	4.16	1.64	1.59
2	A	1301	P5F	C10-N1	4.06	1.43	1.36
3	B	1302	NAD	C3N-C7N	4.03	1.56	1.50
3	B	1302	NAD	O3D-C3D	4.01	1.52	1.43
2	A	1301	P5F	C6A-N6A	3.92	1.44	1.34
3	A	1302	NAD	C3N-C7N	3.91	1.56	1.50
2	B	1301	P5F	C6A-N6A	3.84	1.44	1.34
2	B	1301	P5F	C9A-N10	3.83	1.45	1.37
3	A	1302	NAD	O3D-C3D	3.80	1.52	1.43
2	B	1301	P5F	P-O3P	3.57	1.63	1.59
2	A	1301	P5F	C2-N1	3.52	1.43	1.37
3	A	1302	NAD	O4B-C1B	-3.48	1.34	1.42
3	B	1302	NAD	O4B-C1B	-3.43	1.34	1.42
2	A	1301	P5F	C9A-N10	3.38	1.44	1.37
3	B	1302	NAD	C2N-N1N	3.10	1.38	1.35
3	A	1302	NAD	O3B-C3B	3.09	1.50	1.43
3	A	1302	NAD	C2N-N1N	2.99	1.38	1.35
3	A	1302	NAD	C5A-C4A	-2.93	1.33	1.39
2	A	1301	P5F	PA-O5B	-2.87	1.48	1.59
3	B	1302	NAD	O3B-C3B	2.86	1.50	1.43
2	A	1301	P5F	C5X-C9A	-2.82	1.36	1.42
2	B	1301	P5F	C5X-C9A	-2.82	1.36	1.42
3	A	1302	NAD	C8A-N9A	-2.72	1.32	1.37
3	A	1302	NAD	C2A-N1A	2.70	1.38	1.33
3	B	1302	NAD	C2A-N1A	2.63	1.38	1.33
2	A	1301	P5F	O2'-C2'	-2.61	1.37	1.43
3	A	1302	NAD	O7N-C7N	-2.55	1.19	1.24
2	B	1301	P5F	C23-C21	-2.53	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	P5F	C23-C21	-2.39	1.39	1.49
2	A	1301	P5F	C5A-C4A	2.37	1.43	1.39
2	B	1301	P5F	C4X-C4	2.32	1.49	1.43
3	A	1302	NAD	C5A-N7A	-2.27	1.34	1.39
3	B	1302	NAD	C8A-N7A	2.19	1.35	1.31
2	B	1301	P5F	PA-O2A	-2.19	1.43	1.50
2	B	1301	P5F	C5A-C4A	2.18	1.43	1.39
3	B	1302	NAD	C5A-C4A	-2.15	1.35	1.39
2	A	1301	P5F	C4X-C4	2.14	1.49	1.43
3	B	1302	NAD	C8A-N9A	-2.12	1.33	1.37
2	A	1301	P5F	C2B-C3B	-2.10	1.47	1.53
2	B	1301	P5F	O3B-C3B	-2.02	1.38	1.43
2	B	1301	P5F	C2B-C3B	-2.02	1.47	1.53
3	B	1302	NAD	O7N-C7N	-2.01	1.20	1.24
2	B	1301	P5F	O2'-C2'	-2.00	1.39	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	NAD	C4A-N9A-C1B	-6.09	112.40	126.63
3	A	1302	NAD	N3A-C2A-N1A	-5.94	119.59	128.58
2	B	1301	P5F	O3P-PA-O2A	-5.75	93.41	110.70
3	B	1302	NAD	N3A-C2A-N1A	-5.71	119.94	128.58
2	A	1301	P5F	C4-N3-C2	-5.65	118.59	126.37
3	B	1302	NAD	C5A-C4A-N3A	-5.62	118.98	126.72
2	B	1301	P5F	N3A-C2A-N1A	-5.48	120.29	128.58
2	A	1301	P5F	N3A-C2A-N1A	-5.41	120.39	128.58
2	B	1301	P5F	O1A-PA-O3P	5.35	121.72	107.27
3	B	1302	NAD	N9A-C8A-N7A	-5.29	106.44	113.94
3	A	1302	NAD	N9A-C8A-N7A	-5.24	106.51	113.94
3	A	1302	NAD	C4D-O4D-C1D	-5.15	105.20	109.92
2	A	1301	P5F	C5A-C4A-N3A	-4.98	119.85	126.72
3	B	1302	NAD	C4A-N9A-C1B	-4.85	115.28	126.63
3	A	1302	NAD	C1B-N9A-C8A	4.73	137.59	127.09
2	B	1301	P5F	C4-N3-C2	-4.65	119.97	126.37
3	A	1302	NAD	C5A-C4A-N3A	-4.63	120.35	126.72
2	B	1301	P5F	C5A-C4A-N3A	-4.44	120.60	126.72
3	B	1302	NAD	N3A-C4A-N9A	4.39	134.64	127.17
2	A	1301	P5F	N3A-C4A-N9A	4.31	134.50	127.17
3	B	1302	NAD	C4A-N9A-C8A	4.21	110.16	105.74
2	A	1301	P5F	C4X-C4-N3	4.18	120.48	111.84
2	B	1301	P5F	N3-C2-N1	4.11	122.21	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	NAD	C4A-N9A-C8A	4.04	109.98	105.74
2	A	1301	P5F	N3-C2-N1	4.04	122.09	115.74
2	A	1301	P5F	C5A-N7A-C8A	4.03	109.79	103.45
2	A	1301	P5F	O3P-PA-O2A	-3.98	98.72	110.70
3	B	1302	NAD	C2A-N3A-C4A	3.91	121.38	111.83
2	B	1301	P5F	N3A-C4A-N9A	3.81	133.65	127.17
3	A	1302	NAD	N3A-C4A-N9A	3.72	133.49	127.17
2	A	1301	P5F	N9A-C8A-N7A	-3.71	108.67	113.94
2	B	1301	P5F	O1P-P-O3P	3.65	117.15	107.27
2	A	1301	P5F	O1A-PA-O3P	3.62	117.05	107.27
2	A	1301	P5F	O1P-P-O3P	3.56	116.89	107.27
3	B	1302	NAD	C4D-O4D-C1D	-3.55	106.67	109.92
2	B	1301	P5F	C5A-N7A-C8A	3.54	109.01	103.45
2	A	1301	P5F	C2A-N3A-C4A	3.49	120.36	111.83
3	B	1302	NAD	C5A-N7A-C8A	3.42	108.83	103.45
3	A	1302	NAD	C5A-N7A-C8A	3.40	108.79	103.45
2	B	1301	P5F	C1'-N10-C9A	3.38	123.88	119.02
2	B	1301	P5F	C4X-C4-N3	3.38	118.83	111.84
3	B	1302	NAD	C1B-N9A-C8A	3.35	134.54	127.09
2	A	1301	P5F	O4-C4-C4X	-3.30	120.64	128.01
3	A	1302	NAD	C2A-N3A-C4A	3.24	119.73	111.83
2	B	1301	P5F	C2A-N3A-C4A	3.23	119.71	111.83
2	B	1301	P5F	C10-N10-C9A	-3.12	114.88	120.93
2	A	1301	P5F	C4A-C5A-N7A	-3.07	107.08	110.58
2	B	1301	P5F	O4-C4-C4X	-2.99	121.35	128.01
2	B	1301	P5F	N9A-C8A-N7A	-2.94	109.76	113.94
2	A	1301	P5F	C4A-N9A-C8A	2.93	108.81	105.74
2	B	1301	P5F	C4'-C3'-C2'	2.86	118.33	113.57
2	A	1301	P5F	C10-N10-C9A	-2.76	115.58	120.93
2	B	1301	P5F	C4A-C5A-N7A	-2.74	107.44	110.58
2	A	1301	P5F	C1'-N10-C9A	2.73	122.94	119.02
3	B	1302	NAD	C2B-C1B-N9A	-2.69	106.61	113.30
2	B	1301	P5F	O5B-PA-O2A	-2.61	98.57	108.94
2	A	1301	P5F	O3P-P-O2P	-2.38	103.54	110.70
2	B	1301	P5F	O5'-P-O2P	-2.35	99.62	108.94
3	A	1302	NAD	C2D-C3D-C4D	2.30	107.06	102.61
2	A	1301	P5F	O5'-C5'-C4'	2.28	115.43	109.36
2	B	1301	P5F	C7-C6-C5X	-2.19	118.30	121.30
2	B	1301	P5F	C4A-N9A-C8A	2.18	108.03	105.74
2	B	1301	P5F	C2A-N1A-C6A	2.10	122.18	118.73
3	B	1302	NAD	C4A-C5A-N7A	-2.10	108.19	110.58
2	A	1301	P5F	C7-C6-C5X	-2.09	118.44	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	P5F	O5'-P-O2P	-2.03	100.88	108.94
3	A	1302	NAD	C2N-C3N-C4N	2.02	120.61	118.26
2	A	1301	P5F	O5B-PA-O2A	-2.01	100.97	108.94

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1307	PEG	O2-C3-C4-O4
2	A	1301	P5F	C2'-C3'-C4'-O4'
3	B	1302	NAD	C4D-C5D-O5D-PN
7	A	1310	PEG	C4-C3-O2-C2
3	A	1302	NAD	C2B-C1B-N9A-C8A
3	B	1302	NAD	C2B-C1B-N9A-C8A
8	B	1308	PG4	O4-C7-C8-O5
3	A	1302	NAD	C5B-O5B-PA-O1A
3	B	1302	NAD	C5B-O5B-PA-O1A
3	A	1302	NAD	C4D-C5D-O5D-PN
9	B	1309	PGE	O3-C5-C6-O4
9	B	1309	PGE	C4-C3-O2-C2
3	A	1302	NAD	C3D-C4D-C5D-O5D
2	A	1301	P5F	PA-O3P-P-O1P
2	B	1301	P5F	PA-O3P-P-O1P
3	A	1302	NAD	C2B-C1B-N9A-C4A
3	B	1302	NAD	C2B-C1B-N9A-C4A
2	A	1301	P5F	C4'-C5'-O5'-P
7	A	1310	PEG	C1-C2-O2-C3

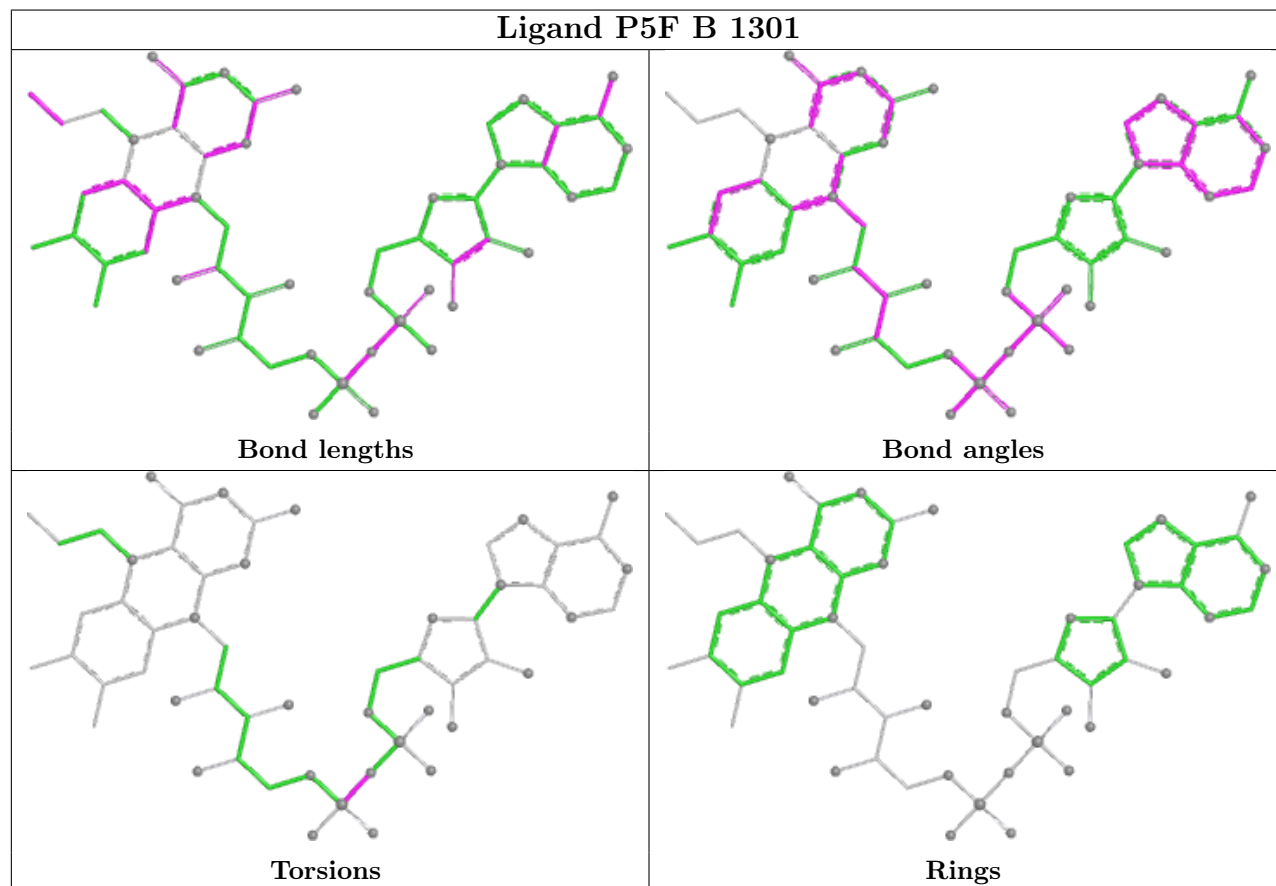
There are no ring outliers.

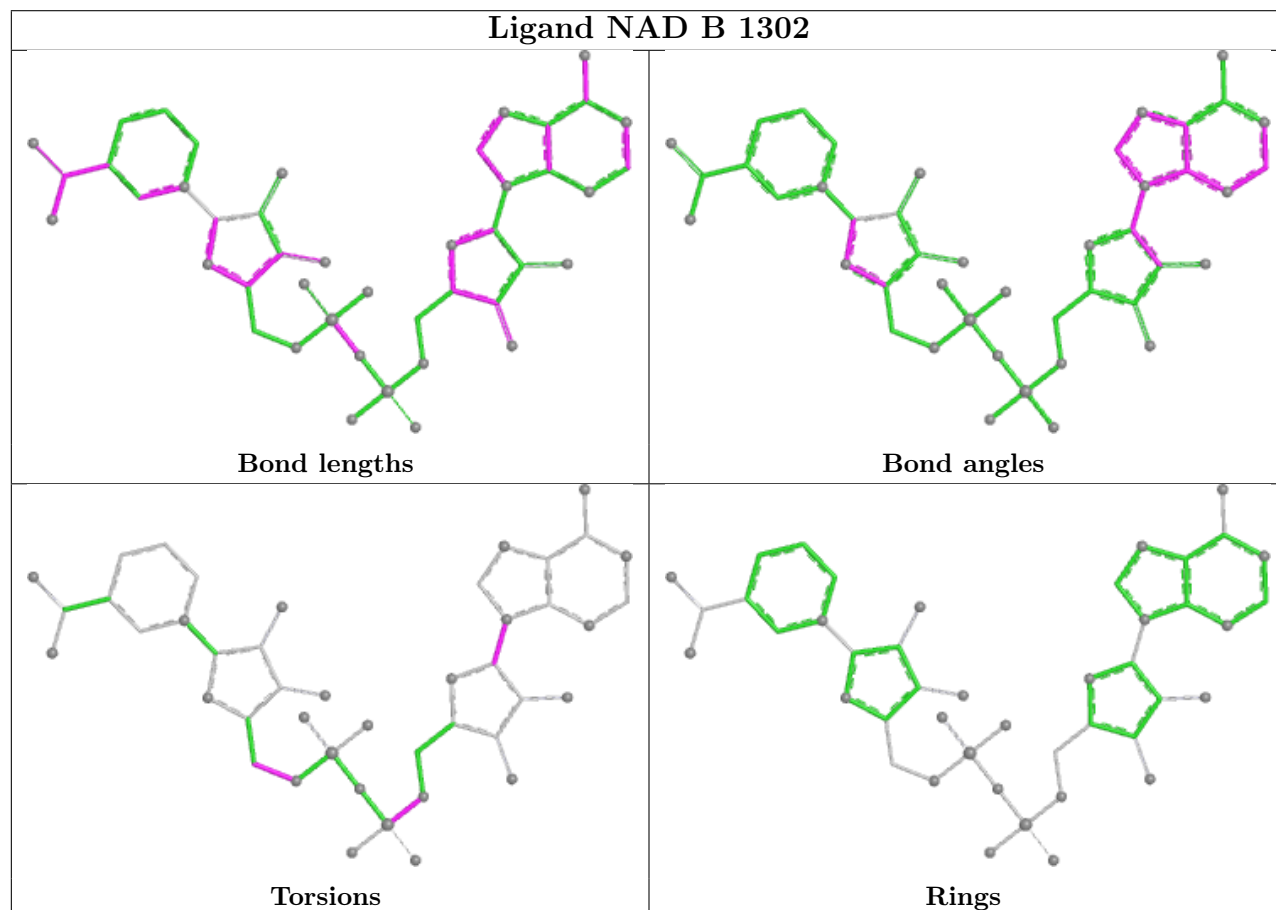
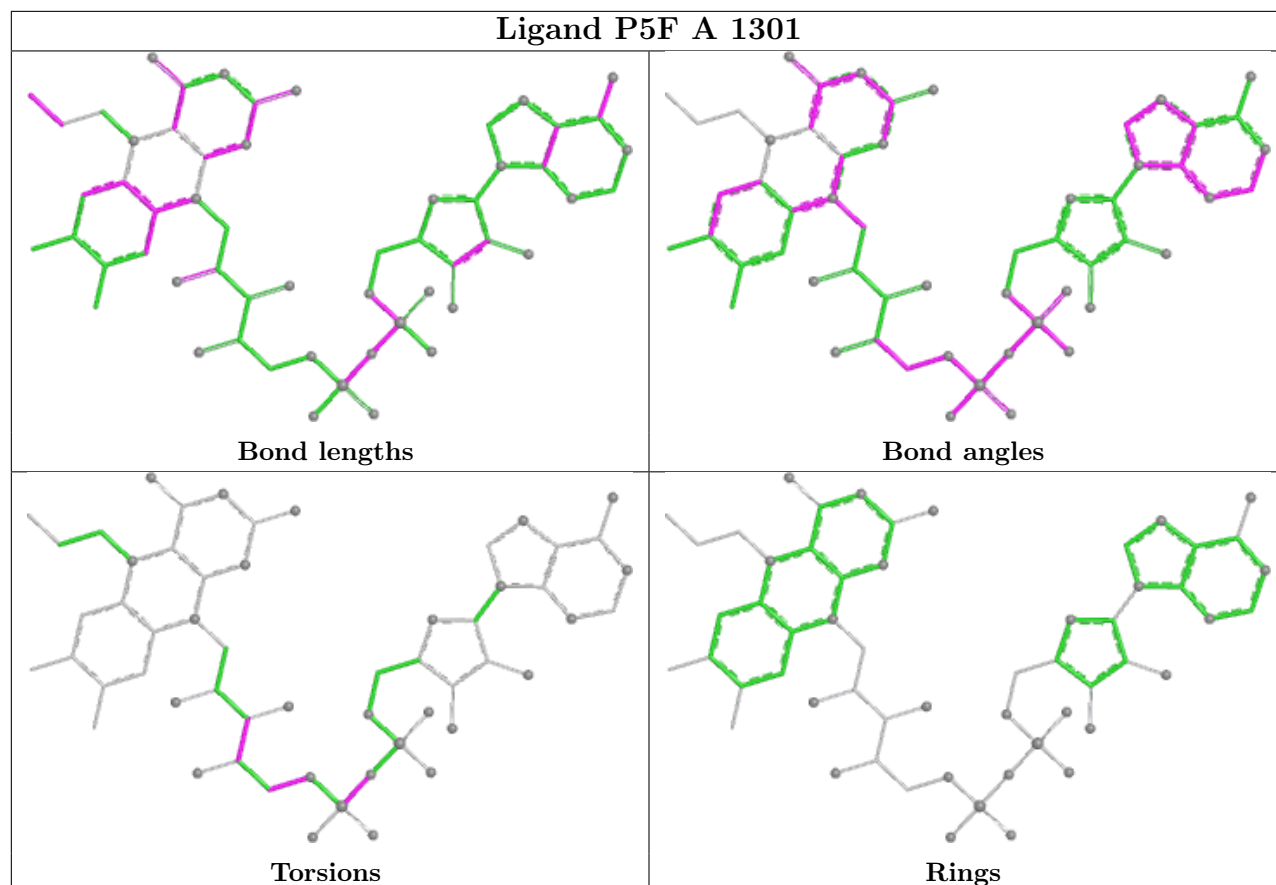
6 monomers are involved in 12 short contacts:

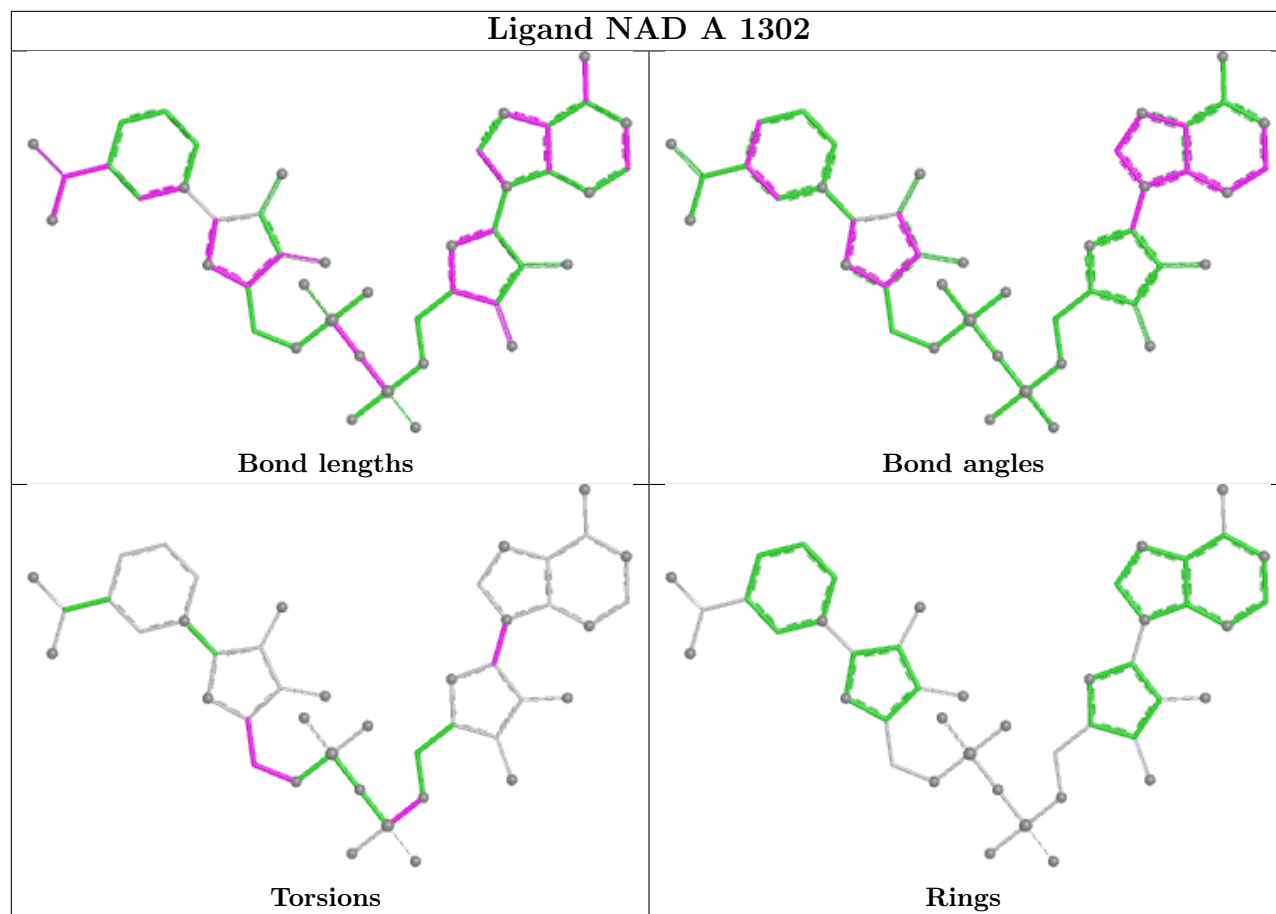
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	P5F	2	0
7	B	1307	PEG	1	0
7	A	1310	PEG	2	0
2	A	1301	P5F	3	0
3	B	1302	NAD	2	0
3	A	1302	NAD	2	0

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 [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	1212/1235 (98%)	0.28	80 (6%)	24 29	8, 23, 45, 90	17 (1%)
1	B	1202/1235 (97%)	0.42	129 (10%)	11 13	10, 22, 48, 83	6 (0%)
All	All	2414/2470 (97%)	0.35	209 (8%)	16 19	8, 22, 47, 90	23 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	TYR	9.2
1	B	491	LEU	8.7
1	B	487	VAL	8.2
1	B	486	LEU	7.9
1	A	483	LEU	7.1
1	A	490	LEU	7.0
1	B	490	LEU	7.0
1	B	488	ARG	6.9
1	B	484	ALA	6.6
1	A	485	TYR	6.5
1	B	494	GLY	6.5
1	A	486	LEU	6.3
1	B	495	ALA	6.2
1	B	500	VAL	6.2
1	A	487	VAL	6.1
1	A	484	ALA	6.0
1	B	508	VAL	5.9
1	B	483	LEU	5.8
1	A	491	LEU	5.7
1	B	493	ASN	5.6
1	B	192	GLY	5.6
1	B	1222	ALA	5.3
1	A	503	ILE	5.3
1	A	1231	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	503	ILE	5.1
1	B	912	ILE	5.1
1	B	14	ALA	5.1
1	B	496	ASN	4.8
1	A	127	ASP	4.6
1	A	482	LEU	4.6
1	B	915	ALA	4.6
1	A	496	ASN	4.5
1	B	129	ASN	4.5
1	A	493	ASN	4.4
1	B	224	GLY	4.4
1	B	489	ARG	4.4
1	A	195	PHE	4.3
1	A	134	LEU	4.3
1	B	497	SER	4.2
1	B	75	LEU	4.2
1	B	74	ALA	4.2
1	B	913	GLY	4.2
1	B	510	ILE	4.1
1	B	138	ARG	4.1
1	A	488	ARG	4.0
1	B	513	LEU	4.0
1	B	66	SER	3.9
1	B	499	PHE	3.9
1	A	132	SER	3.8
1	B	65	ALA	3.8
1	A	130	TRP	3.7
1	A	129	ASN	3.7
1	A	14	ALA	3.7
1	B	482	LEU	3.6
1	B	415	VAL	3.6
1	B	439	PHE	3.6
1	A	489	ARG	3.6
1	B	479	HIS	3.6
1	B	132	SER	3.6
1	A	796	ASP	3.6
1	B	71	LEU	3.6
1	B	456	LEU	3.6
1	A	115	ALA	3.6
1	B	137	SER	3.5
1	A	223	LEU	3.5
1	A	508	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	506	PRO	3.5
1	B	506	PRO	3.5
1	B	194	GLN	3.5
1	B	72	ILE	3.5
1	A	500	VAL	3.5
1	B	504	ASN	3.4
1	A	114	THR	3.4
1	B	515	ALA	3.4
1	A	494	GLY	3.4
1	B	498	SER	3.4
1	B	492	GLU	3.4
1	B	461	VAL	3.3
1	A	495	ALA	3.3
1	A	192	GLY	3.3
1	B	191	MET	3.2
1	B	120	LEU	3.2
1	B	918	THR	3.2
1	B	225	GLU	3.2
1	A	119	ALA	3.2
1	B	64	ALA	3.2
1	B	128	GLY	3.2
1	B	193	GLU	3.2
1	A	1222	ALA	3.2
1	A	481	THR	3.1
1	B	133	HIS	3.1
1	B	60	ILE	3.1
1	A	137	SER	3.1
1	B	460	VAL	3.1
1	B	501	HIS	3.1
1	B	223	LEU	3.1
1	A	938	GLN	3.1
1	B	68	ALA	3.1
1	B	481	THR	3.0
1	A	120	LEU	3.0
1	B	70	LYS	3.0
1	A	499	PHE	3.0
1	B	1221	ALA	3.0
1	A	905	LEU	3.0
1	B	466	LEU	3.0
1	B	55	THR	3.0
1	A	1226	ASN	2.9
1	B	464	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	514	ILE	2.9
1	B	509	SER	2.9
1	B	73	GLU	2.9
1	A	501	HIS	2.9
1	A	437	LYS	2.9
1	A	116	THR	2.9
1	B	77	GLY	2.8
1	B	914	LEU	2.8
1	A	1230	MET	2.8
1	B	69	ARG	2.8
1	B	412	ALA	2.7
1	A	451	GLY	2.7
1	A	226	ALA	2.7
1	B	134	LEU	2.7
1	A	1228	SER	2.7
1	B	83	GLY	2.6
1	A	1229	LEU	2.6
1	B	139	SER	2.6
1	A	912	ILE	2.6
1	A	1223	ALA	2.6
1	B	116	THR	2.6
1	B	155	LEU	2.6
1	B	478	THR	2.6
1	B	202	ARG	2.6
1	A	133	HIS	2.6
1	B	430	ALA	2.6
1	B	502	ARG	2.6
1	B	57	SER	2.6
1	B	236	TYR	2.6
1	B	432	TYR	2.6
1	B	462	GLY	2.6
1	A	894	ASN	2.5
1	B	115	ALA	2.5
1	B	429	ALA	2.5
1	A	125	ILE	2.5
1	B	410	LEU	2.5
1	A	801	ALA	2.5
1	B	63	ALA	2.5
1	B	125	ILE	2.5
1	B	84	VAL	2.5
1	B	126	ALA	2.4
1	B	136	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	126	ALA	2.4
1	A	498	SER	2.4
1	A	586	ALA	2.4
1	A	83	GLY	2.4
1	A	224	GLY	2.4
1	B	189	ARG	2.4
1	B	463	ARG	2.4
1	A	128	GLY	2.4
1	B	121	ILE	2.4
1	A	935	SER	2.4
1	A	479	HIS	2.3
1	B	87	LEU	2.3
1	B	149	LEU	2.3
1	B	195	PHE	2.3
1	A	478	THR	2.3
1	A	571	ALA	2.3
1	A	1227	ALA	2.3
1	B	480	GLU	2.3
1	B	135	GLY	2.3
1	B	451	GLY	2.3
1	B	1002	GLY	2.3
1	A	225	GLU	2.3
1	B	59	GLU	2.3
1	B	396	ILE	2.3
1	B	62	ASP	2.2
1	A	111	ILE	2.2
1	A	480	GLU	2.2
1	B	441	VAL	2.2
1	A	187	ALA	2.2
1	A	771	ALA	2.2
1	B	58	LYS	2.2
1	B	916	SER	2.2
1	B	511	ASP	2.2
1	A	520	VAL	2.2
1	B	124	LYS	2.2
1	A	937	LEU	2.1
1	B	226	ALA	2.1
1	A	156	THR	2.1
1	B	127	ASP	2.1
1	B	458	GLU	2.1
1	A	507	LYS	2.1
1	A	112	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	111	ILE	2.1
1	B	1056	TRP	2.1
1	B	525	PRO	2.1
1	A	131	LYS	2.1
1	B	131	LYS	2.1
1	B	130	TRP	2.1
1	B	1058	ASP	2.1
1	B	156	THR	2.0
1	A	194	GLN	2.0
1	A	492	GLU	2.0
1	A	1225	GLY	2.0
1	B	507	LYS	2.0
1	B	413	THR	2.0
1	B	440	HIS	2.0
1	B	512	GLU	2.0
1	B	411	ALA	2.0
1	A	113	ASP	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.

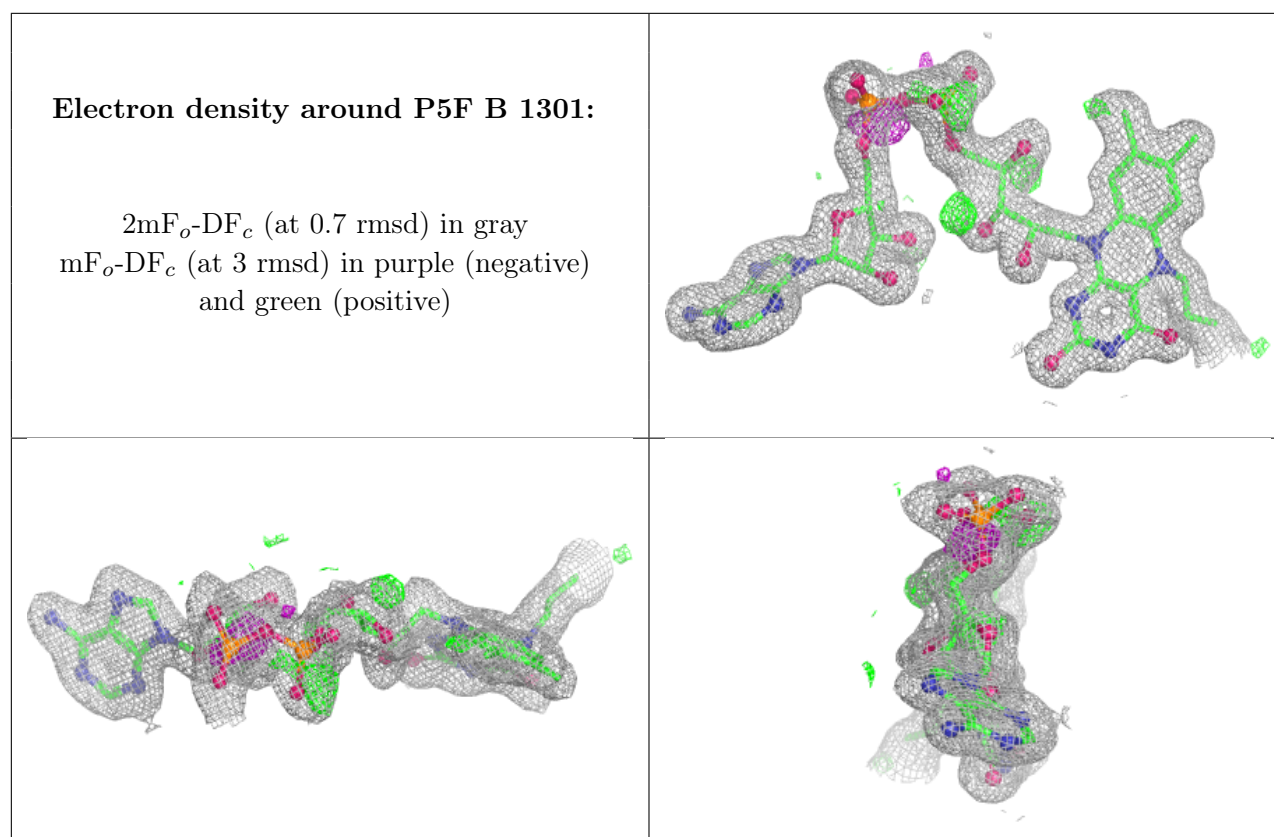
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	B	1307	7/7	0.75	0.18	34,38,44,46	0
4	SO4	A	1306	5/5	0.82	0.15	41,42,44,53	5
7	PEG	A	1311	7/7	0.86	0.12	30,30,36,38	0
8	PG4	B	1308	13/13	0.87	0.12	29,36,43,49	0
4	SO4	B	1304	5/5	0.89	0.12	44,44,45,45	5
4	SO4	A	1307	5/5	0.89	0.13	25,27,31,38	5

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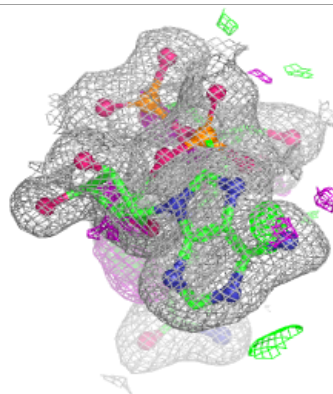
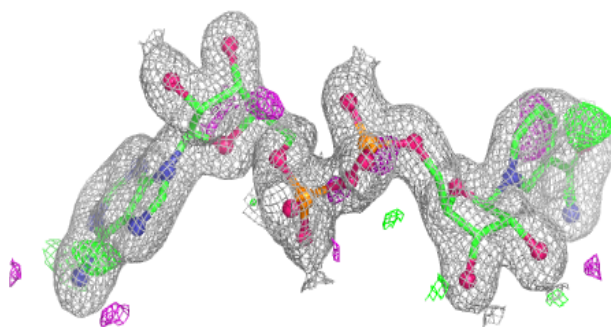
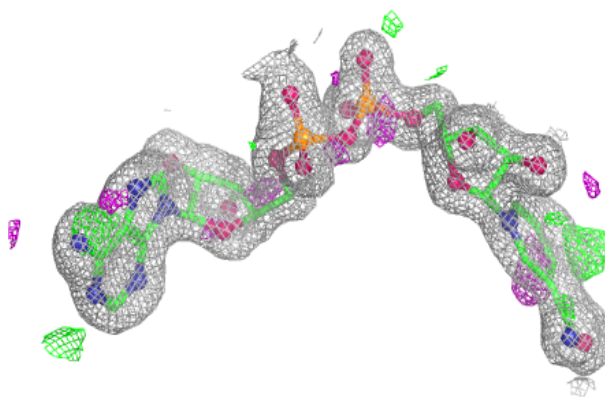
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1305	5/5	0.90	0.11	31,34,37,41	5
7	PEG	A	1310	7/7	0.91	0.10	21,32,35,44	0
9	PGE	B	1309	10/10	0.92	0.10	30,32,36,38	0
6	FMT	B	1306	3/3	0.94	0.09	15,15,28,31	0
2	P5F	B	1301	56/61	0.94	0.08	19,23,30,33	0
6	FMT	A	1309	3/3	0.94	0.09	25,25,30,32	0
4	SO4	A	1304	5/5	0.95	0.09	27,31,36,36	5
3	NAD	A	1302	44/44	0.95	0.08	17,23,25,27	0
2	P5F	A	1301	56/61	0.97	0.06	15,19,25,30	0
5	MG	B	1305	1/1	0.97	0.12	27,27,27,27	0
3	NAD	B	1302	44/44	0.97	0.06	14,16,18,23	0
5	MG	A	1308	1/1	0.99	0.09	26,26,26,26	0
4	SO4	B	1303	5/5	0.99	0.04	17,19,20,22	0
4	SO4	A	1303	5/5	0.99	0.05	19,20,22,23	0

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

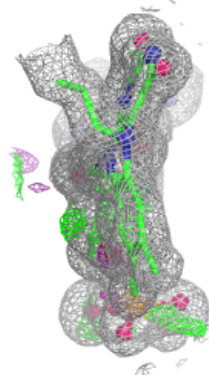
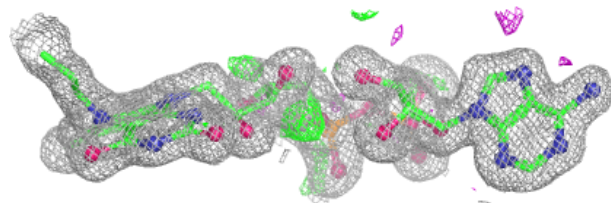
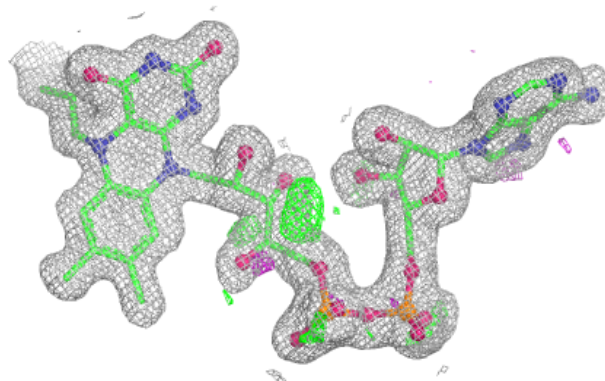


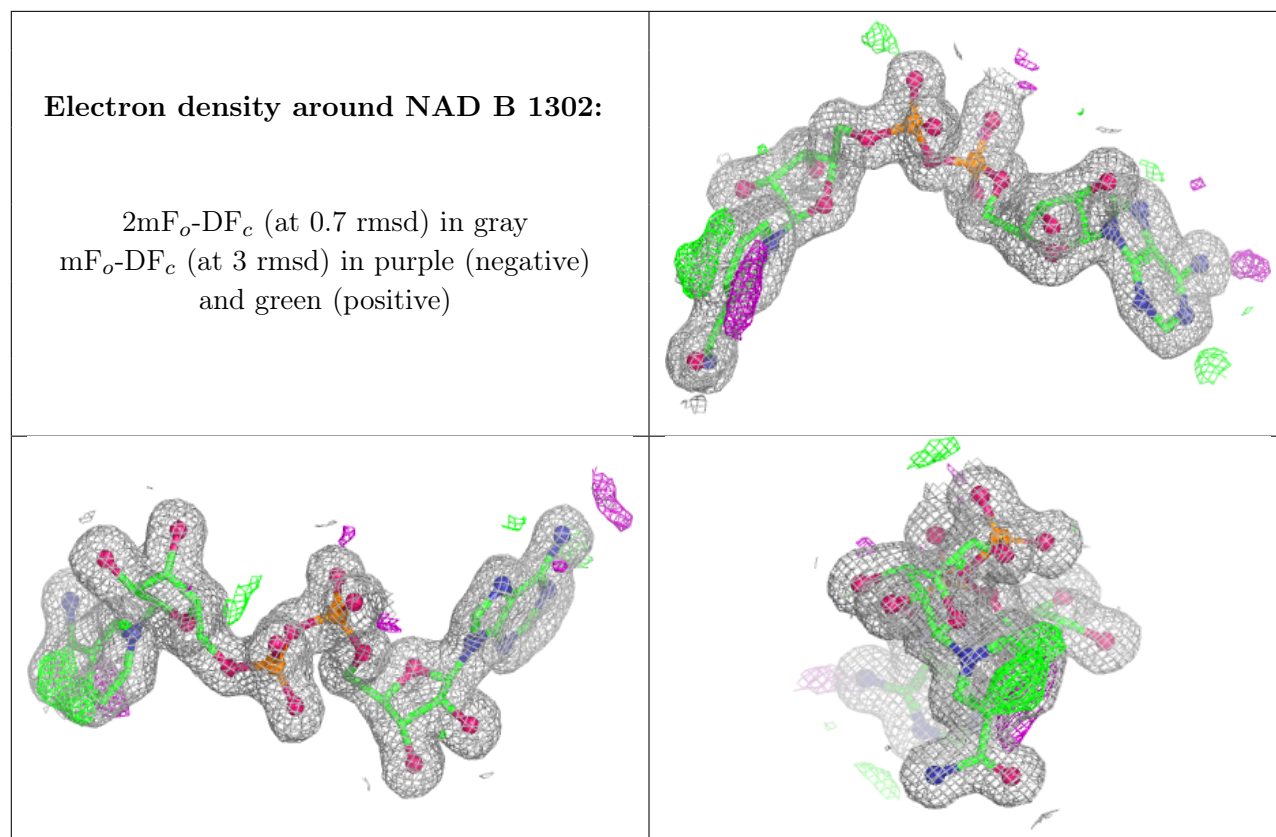
Electron density around NAD A 1302:

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

**Electron density around P5F A 1301:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.