



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 9F23 / pdb_00009f23
Title : DARPin eGFP complex DP2 (2G156)
Authors : Mittl, P.R.; Hansen, S.
Deposited on : 2024-04-22
Resolution : 1.59 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

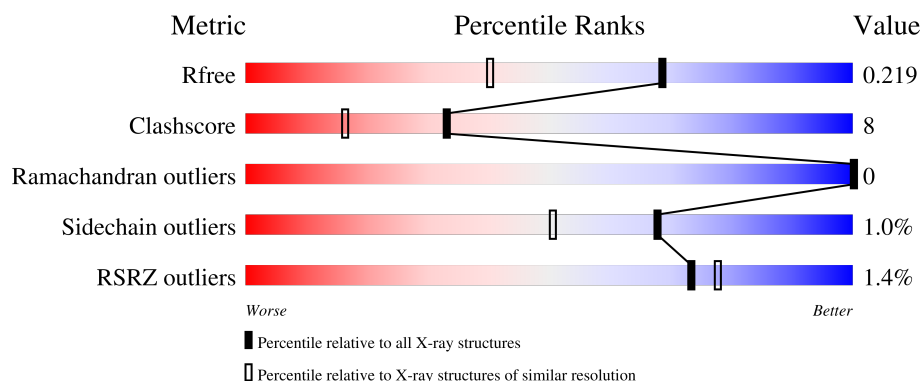
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	243	83% 10% 7%
1	C	243	87% 6% 6%
2	B	128	4% 85% 9% ...
2	D	128	2% 83% 14% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	203	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6867 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	18	0
			1964	1246	330	382	6			
1	C	228	Total	C	N	O	S	0	22	0
			2009	1272	336	395	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P42212
A	-3	PRO	-	expression tag	UNP P42212
A	-2	GLY	-	expression tag	UNP P42212
A	-1	SER	-	expression tag	UNP P42212
A	0	MET	-	expression tag	UNP P42212
A	1	VAL	-	expression tag	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	231	LEU	HIS	engineered mutation	UNP P42212
A	239	GLN	-	expression tag	UNP P42212
A	240	ALA	-	expression tag	UNP P42212
C	-4	GLY	-	expression tag	UNP P42212
C	-3	PRO	-	expression tag	UNP P42212
C	-2	GLY	-	expression tag	UNP P42212
C	-1	SER	-	expression tag	UNP P42212
C	0	MET	-	expression tag	UNP P42212
C	1	VAL	-	expression tag	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212
C	66	CRO	GLY	chromophore	UNP P42212
C	231	LEU	HIS	engineered mutation	UNP P42212
C	239	GLN	-	expression tag	UNP P42212

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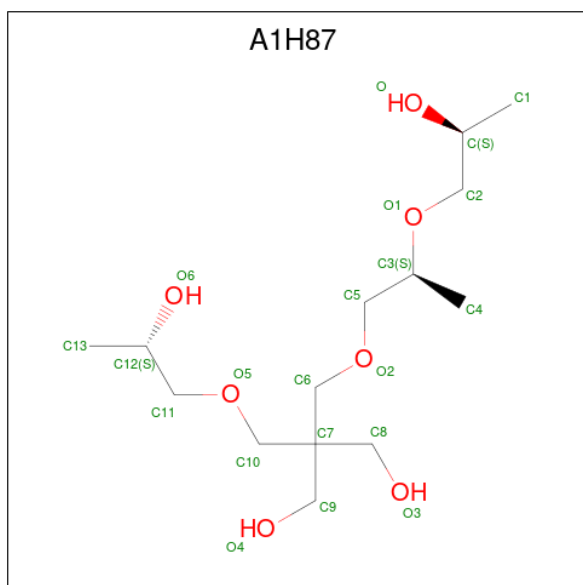
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Chain	Residue	Modelled	Actual	Comment	Reference
C	240	ALA	-	expression tag	UNP P42212

- Molecule 2 is a protein called DARPin DP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	7	0
			990	622	169	195	4			
2	D	124	Total	C	N	O	S	0	7	0
			983	618	169	192	4			

- Molecule 3 is 2-[[[(2S)-2-oxidanylpropoxy]methyl]-2-[[[(2S)-2-[(2S)-2-oxidanylpropoxy]propoxy]methyl]propane-1,3-diol (CCD ID: A1H87) (formula: C₁₄H₃₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	14	7		
3	C	1	Total	C	O	0	0
			21	14	7		

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



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

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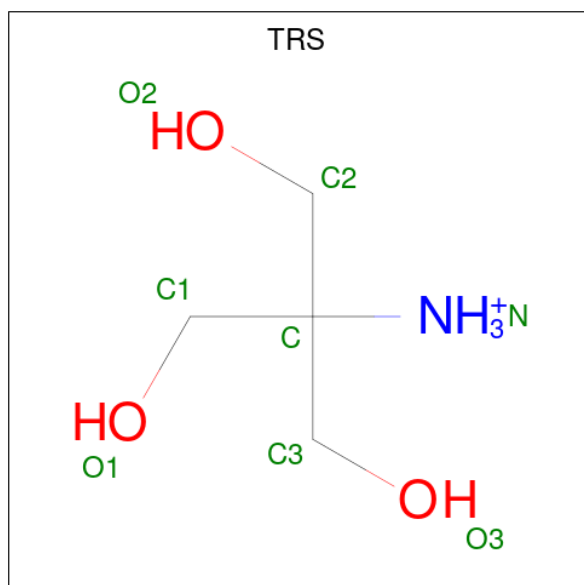
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

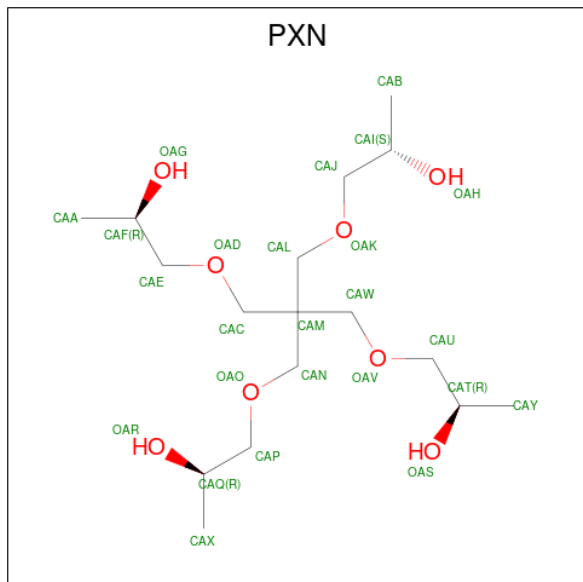
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 7 is (2S)-1-[3-{{[(2R)-2-hydroxypropyl]oxy}}-2,2-bis({[(2R)-2-hydroxypropyl]oxy}methyl)propoxy]propan-2-ol (CCD ID: PXN) (formula: C₁₇H₃₆O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			25	17	8		

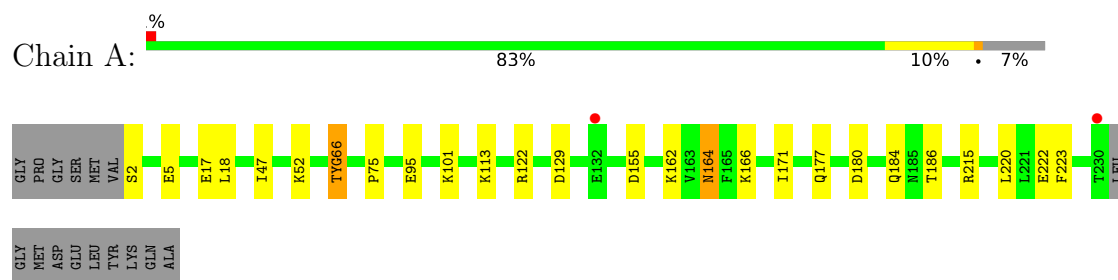
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	216	Total	O	0	0
			216	216		
8	B	143	Total	O	0	0
			143	143		
8	C	264	Total	O	0	0
			264	264		
8	D	121	Total	O	0	0
			121	121		

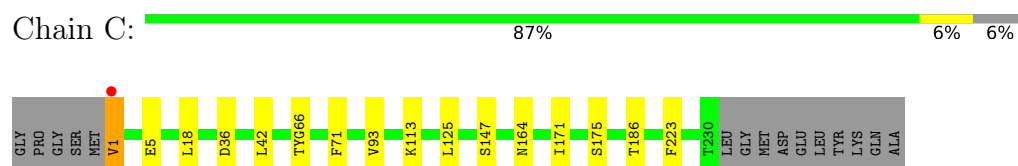
3 Residue-property plots

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.

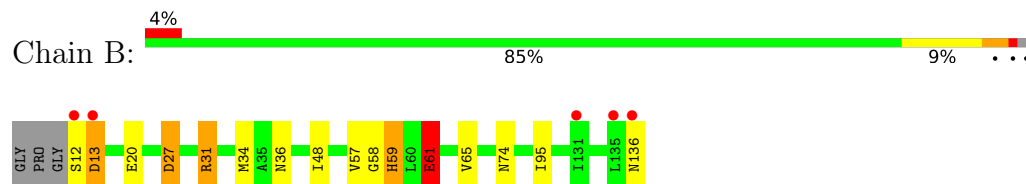
- Molecule 1: Green fluorescent protein



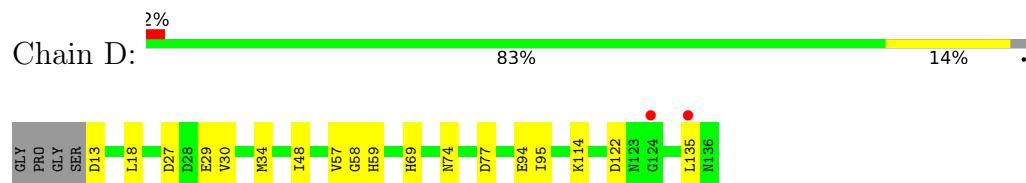
- Molecule 1: Green fluorescent protein



- Molecule 2: DARPin DP2



- Molecule 2: DARPin DP2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.87Å 95.16Å 69.47Å 90.00° 115.76° 90.00°	Depositor
Resolution (Å)	48.08 – 1.59 48.08 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.08-1.59) 98.7 (48.08-1.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.174 , 0.212 0.186 , 0.219	Depositor DCC
R_{free} test set	4677 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1873e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CRO, EDO, PXN, NA, A1H87, TRS

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	0.59	0/1982	0.88	1/2677 (0.0%)
1	C	0.60	0/2027	0.92	1/2736 (0.0%)
2	B	0.63	0/1001	1.01	6/1355 (0.4%)
2	D	0.64	0/994	0.94	1/1346 (0.1%)
All	All	0.61	0/6004	0.93	9/8114 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	ASP	CA-CB-CG	7.18	119.78	112.60
2	B	13	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	36	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	129	ASP	CA-CB-CG	5.63	118.23	112.60
2	B	59	HIS	CA-CB-CG	5.44	119.24	113.80
2	B	27	ASP	N-CA-CB	5.20	117.86	110.16
2	B	61[A]	GLU	CB-CG-CD	5.03	121.16	112.60
2	B	61[B]	GLU	CB-CG-CD	5.03	121.16	112.60
2	D	94	GLU	CB-CG-CD	5.03	121.14	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	31	ARG	Sidechain

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	1964	0	1899	26	0
1	C	2009	0	1937	19	0
2	B	990	0	987	22	0
2	D	983	0	982	23	0
3	A	21	0	0	0	0
3	C	21	0	0	0	0
4	A	12	0	18	0	0
4	B	16	0	24	5	0
4	C	20	0	30	1	0
4	D	12	0	18	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	24	0	36	0	0
6	D	24	0	36	2	0
7	C	25	0	36	0	0
8	A	216	0	0	13	0
8	B	143	0	0	11	1
8	C	264	0	0	11	1
8	D	121	0	0	7	2
All	All	6867	0	6003	95	2

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 8.

All (95) 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:C:113[A]:LYS:NZ	8:C:401:HOH:O	1.59	1.28
2:B:57[A]:VAL:HG21	2:B:59:HIS:CD2	1.92	1.04
1:C:223:PHE:CE1	8:D:301:HOH:O	2.20	0.95
2:B:57[A]:VAL:CG2	2:B:59:HIS:CD2	2.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113[A]:LYS:NZ	8:A:401:HOH:O	1.75	0.86
2:B:34[A]:MET:HE1	2:B:65:VAL:CG1	2.09	0.83
2:D:77:ASP:OD2	8:D:301:HOH:O	1.99	0.79
2:B:20[B]:GLU:OE1	8:B:301:HOH:O	1.98	0.79
2:D:34[A]:MET:HE2	2:D:69:HIS:CD2	2.18	0.78
2:D:57[B]:VAL:HG21	2:D:59:HIS:CE1	2.20	0.77
1:C:1:VAL:N	1:C:5[A]:GLU:OE1	2.19	0.75
1:C:5[B]:GLU:CG	8:C:435:HOH:O	2.33	0.75
1:A:180[B]:ASP:OD1	8:A:402:HOH:O	2.05	0.73
1:A:220[B]:LEU:C	1:A:220[B]:LEU:HD23	2.15	0.72
2:D:34[A]:MET:HE2	2:D:69:HIS:CG	2.27	0.69
2:D:34[A]:MET:CE	2:D:69:HIS:CG	2.75	0.69
2:D:74[A]:ASN:ND2	8:D:303:HOH:O	2.25	0.69
2:B:31:ARG:HA	2:B:34[A]:MET:HE2	1.75	0.68
2:B:59:HIS:HB3	4:B:203:EDO:O1	1.92	0.67
1:C:147:SER:OG	8:C:402:HOH:O	2.12	0.67
1:C:5[B]:GLU:HG3	8:C:435:HOH:O	1.91	0.67
2:D:48[B]:ILE:CD1	8:D:339:HOH:O	2.43	0.67
2:B:36:ASN:ND2	8:B:303:HOH:O	2.28	0.66
2:D:114:LYS:NZ	2:D:122:ASP:OD2	2.28	0.66
1:A:186[A]:THR:HG22	8:A:419:HOH:O	1.96	0.65
2:D:34[B]:MET:HA	2:D:34[B]:MET:HE2	1.76	0.65
2:D:48[B]:ILE:HD11	8:D:339:HOH:O	1.97	0.65
1:A:18[A]:LEU:C	1:A:18[A]:LEU:HD23	2.24	0.63
1:C:171[B]:ILE:CD1	8:C:529:HOH:O	2.45	0.63
2:B:31:ARG:HH22	2:B:61[B]:GLU:CD	2.06	0.63
1:A:223:PHE:HB3	8:A:585:HOH:O	1.98	0.62
1:C:171[B]:ILE:HD12	1:C:175:SER:OG	1.99	0.62
4:C:305:EDO:H21	8:C:479:HOH:O	1.98	0.62
2:D:57[B]:VAL:CG2	2:D:59:HIS:CE1	2.82	0.62
4:B:204:EDO:H21	8:B:371:HOH:O	2.00	0.61
2:B:57[A]:VAL:HG21	2:B:59:HIS:NE2	2.14	0.61
2:B:34[A]:MET:HE1	2:B:65:VAL:HG11	1.83	0.60
2:D:57[B]:VAL:CG2	2:D:59:HIS:ND1	2.64	0.60
1:C:186[B]:THR:HG22	8:C:498:HOH:O	2.00	0.60
1:C:18[B]:LEU:C	1:C:18[B]:LEU:HD23	2.26	0.59
1:A:52[B]:LYS:HE2	8:A:404:HOH:O	2.03	0.59
1:A:2:SER:O	1:A:5:GLU:HG2	2.03	0.59
1:A:52[B]:LYS:CE	8:A:404:HOH:O	2.52	0.58
2:D:58:GLY:HA2	2:D:95:ILE:CD1	2.33	0.58
2:B:34[A]:MET:HE1	2:B:65:VAL:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52[B]:LYS:NZ	8:A:404:HOH:O	2.28	0.57
2:B:36:ASN:CG	8:B:303:HOH:O	2.47	0.57
1:A:166:LYS:HE3	1:A:180[B]:ASP:OD2	2.05	0.57
1:A:171[A]:ILE:CD1	8:A:495:HOH:O	2.54	0.56
2:B:74:ASN:ND2	8:B:302:HOH:O	2.15	0.56
4:B:203:EDO:H21	8:B:351:HOH:O	2.05	0.56
1:A:164[B]:ASN:HB2	8:A:478:HOH:O	2.04	0.55
2:B:59:HIS:HB3	4:B:203:EDO:HO1	1.69	0.54
2:B:57[A]:VAL:HG23	2:B:59:HIS:CD2	2.40	0.54
2:D:57[B]:VAL:HG21	2:D:59:HIS:ND1	2.22	0.54
1:A:95[B]:GLU:OE1	1:A:184[B]:GLN:NE2	2.39	0.54
1:A:47[A]:ILE:HD13	1:A:215:ARG:CZ	2.39	0.53
2:B:31:ARG:NH2	2:B:61[B]:GLU:CD	2.68	0.52
1:C:42[A]:LEU:HD21	1:C:71:PHE:CB	2.39	0.51
1:A:75:PRO:HG2	8:B:320:HOH:O	2.10	0.51
1:A:162:LYS:HG2	1:A:184[A]:GLN:NE2	2.26	0.51
2:B:20[A]:GLU:HG2	8:B:306:HOH:O	2.12	0.50
1:A:162:LYS:HG2	1:A:184[A]:GLN:HE22	1.75	0.50
1:C:164[A]:ASN:HB2	8:C:513:HOH:O	2.11	0.50
2:B:58:GLY:HA2	2:B:95:ILE:HD12	1.93	0.49
1:A:164[A]:ASN:OD1	8:A:403:HOH:O	2.20	0.49
2:B:136:ASN:HB2	8:B:315:HOH:O	2.12	0.49
2:D:29:GLU:CD	6:D:205:TRS:HO1	2.21	0.48
1:A:220[B]:LEU:C	1:A:220[B]:LEU:CD2	2.87	0.48
2:D:58:GLY:HA2	2:D:95:ILE:HD12	1.96	0.47
1:A:101:LYS:NZ	8:A:411:HOH:O	2.48	0.47
1:C:42[A]:LEU:HD21	1:C:71:PHE:CG	2.49	0.46
1:A:171[A]:ILE:HD13	8:A:495:HOH:O	2.15	0.46
1:A:171[A]:ILE:HD11	1:A:177:GLN:HB2	1.97	0.46
1:A:17[B]:GLU:OE1	1:A:122:ARG:NH1	2.49	0.45
2:D:27:ASP:OD2	8:D:302:HOH:O	2.21	0.45
2:D:57[B]:VAL:HG23	2:D:59:HIS:ND1	2.31	0.45
4:B:203:EDO:H11	8:B:342:HOH:O	2.17	0.44
1:C:93:VAL:HB	1:C:186[B]:THR:CG2	2.48	0.44
2:B:12:SER:N	8:B:310:HOH:O	2.51	0.44
1:C:125:LEU:C	1:C:125:LEU:HD23	2.44	0.43
8:A:556:HOH:O	2:B:48[B]:ILE:HD12	2.19	0.42
1:C:93:VAL:HB	1:C:186[B]:THR:HG23	2.02	0.42
1:C:42[A]:LEU:HD21	1:C:71:PHE:HB2	2.01	0.42
2:D:30:VAL:O	2:D:34[B]:MET:HG2	2.19	0.42
2:D:18:LEU:HD22	2:D:34[B]:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34[B]:MET:HA	2:D:34[B]:MET:CE	2.46	0.41
6:D:205:TRS:O1	6:D:205:TRS:O3	2.32	0.41
8:C:602:HOH:O	2:D:48[B]:ILE:HD12	2.20	0.41
1:A:66:CRO:OG1	1:A:222[A]:GLU:OE2	2.30	0.41
1:A:155:ASP:OD2	1:A:162:LYS:HE2	2.20	0.41
2:B:57[A]:VAL:HG23	2:B:59:HIS:CG	2.56	0.41
1:C:171[B]:ILE:HD13	8:C:529:HOH:O	2.15	0.41
2:D:13:ASP:HA	8:D:384:HOH:O	2.19	0.40
1:C:5[B]:GLU:HG2	8:C:435:HOH:O	2.09	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:594:HOH:O	8:D:321:HOH:O[2_245]	2.18	0.02
8:B:321:HOH:O	8:D:363:HOH:O[1_656]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/243 (99%)	236 (98%)	4 (2%)	0	100	100
1	C	245/243 (101%)	241 (98%)	4 (2%)	0	100	100
2	B	130/128 (102%)	129 (99%)	1 (1%)	0	100	100
2	D	129/128 (101%)	128 (99%)	1 (1%)	0	100	100
All	All	744/742 (100%)	734 (99%)	10 (1%)	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	216/210 (103%)	214 (99%)	2 (1%)	70	55
1	C	221/210 (105%)	220 (100%)	1 (0%)	81	70
2	B	105/99 (106%)	101 (96%)	4 (4%)	29	9
2	D	104/99 (105%)	103 (99%)	1 (1%)	68	50
All	All	646/618 (104%)	638 (99%)	8 (1%)	68	43

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164[A]	ASN
1	A	164[B]	ASN
2	B	13	ASP
2	B	27	ASP
2	B	61[A]	GLU
2	B	61[B]	GLU
1	C	1	VAL
2	D	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
2	D	36	ASN
2	D	59	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CRO	C	66	1	22,23,24	0.83	1 (4%)	30,32,34	0.86	1 (3%)
1	CRO	A	66	1	22,23,24	1.08	1 (4%)	30,32,34	0.95	1 (3%)

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
1	CRO	C	66	1	-	2/12/31/32	0/2/2/2
1	CRO	A	66	1	-	1/12/31/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	C1-N2	4.08	1.38	1.32
1	C	66	CRO	C1-N2	2.81	1.36	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	C2-N3-C1	2.46	109.21	108.07
1	C	66	CRO	CA1-C1-N3	-2.00	122.31	124.69

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	N3-C1-CA1-CB1

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Mol	Chain	Res	Type	Atoms
1	C	66	CRO	N2-C1-CA1-CB1
1	C	66	CRO	N3-C1-CA1-CB1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 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	$\# Z > 2$
6	TRS	B	206	-	7,7,7	0.22	0	9,9,9	0.40	0
4	EDO	C	303	-	3,3,3	0.22	0	2,2,2	0.70	0
4	EDO	A	302	-	3,3,3	0.24	0	2,2,2	0.08	0
4	EDO	D	203	-	3,3,3	0.05	0	2,2,2	0.17	0
6	TRS	D	204	-	7,7,7	0.47	0	9,9,9	0.55	0
3	A1H87	A	301	-	20,20,20	0.42	0	25,25,25	1.03	1 (4%)
4	EDO	B	202	-	3,3,3	0.32	0	2,2,2	0.92	0
4	EDO	C	306	-	3,3,3	0.22	0	2,2,2	0.32	0
4	EDO	A	304	-	3,3,3	0.14	0	2,2,2	0.07	0
6	TRS	D	206	-	7,7,7	0.23	0	9,9,9	0.43	0
4	EDO	C	305	-	3,3,3	0.27	0	2,2,2	0.26	0
7	PXN	C	302	-	24,24,24	0.24	0	30,30,30	0.42	0
3	A1H87	C	301	-	20,20,20	0.40	0	25,25,25	0.98	1 (4%)
4	EDO	D	202	-	3,3,3	0.08	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	203	-	3,3,3	0.50	0	2,2,2	0.09	0
4	EDO	B	204	-	3,3,3	0.30	0	2,2,2	0.53	0
6	TRS	B	207	-	7,7,7	0.26	0	9,9,9	0.31	0
4	EDO	D	201	-	3,3,3	0.72	0	2,2,2	0.31	0
6	TRS	B	205	-	7,7,7	0.43	0	9,9,9	0.73	0
4	EDO	A	303	-	3,3,3	0.32	0	2,2,2	0.20	0
6	TRS	D	205	-	7,7,7	0.36	0	9,9,9	0.64	0
4	EDO	C	307	-	3,3,3	0.19	0	2,2,2	0.14	0
4	EDO	B	201	-	3,3,3	0.11	0	2,2,2	0.31	0
4	EDO	C	304	-	3,3,3	0.38	0	2,2,2	0.05	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	TRS	B	206	-	-	3/9/9/9	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	D	203	-	-	1/1/1/1	-
6	TRS	D	204	-	-	1/9/9/9	-
3	A1H87	A	301	-	-	8/25/25/25	-
4	EDO	B	202	-	-	1/1/1/1	-
4	EDO	C	306	-	-	0/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
6	TRS	D	206	-	-	0/9/9/9	-
4	EDO	C	305	-	-	1/1/1/1	-
7	PXN	C	302	-	-	14/28/28/28	-
3	A1H87	C	301	-	-	9/25/25/25	-
4	EDO	D	202	-	-	0/1/1/1	-
4	EDO	B	203	-	-	1/1/1/1	-
4	EDO	B	204	-	-	1/1/1/1	-
6	TRS	B	207	-	-	3/9/9/9	-
4	EDO	D	201	-	-	0/1/1/1	-
6	TRS	B	205	-	-	0/9/9/9	-
4	EDO	A	303	-	-	1/1/1/1	-
6	TRS	D	205	-	-	4/9/9/9	-
4	EDO	C	307	-	-	1/1/1/1	-
4	EDO	B	201	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	A1H87	O1-C2-C	3.54	115.84	108.94
3	A	301	A1H87	O1-C2-C	3.39	115.55	108.94

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	A1H87	C6-C7-C8-O3
3	C	301	A1H87	C10-C7-C8-O3
3	C	301	A1H87	O-C-C2-O1
6	D	205	TRS	C2-C-C1-O1
6	D	205	TRS	C3-C-C1-O1
6	D	205	TRS	N-C-C1-O1
7	C	302	PXN	CAB-CAI-CAJ-OAK
7	C	302	PXN	OAH-CAI-CAJ-OAK
7	C	302	PXN	OAS-CAT-CAU-OAV
7	C	302	PXN	CAY-CAT-CAU-OAV
7	C	302	PXN	CAC-CAM-CAW-OAV
3	A	301	A1H87	C8-C7-C9-O4
3	C	301	A1H87	C8-C7-C9-O4
3	C	301	A1H87	C6-C7-C9-O4
3	C	301	A1H87	C6-C7-C8-O3
7	C	302	PXN	CAL-CAM-CAW-OAV
7	C	302	PXN	CAN-CAM-CAW-OAV
3	A	301	A1H87	C10-C7-C9-O4
3	A	301	A1H87	C6-C7-C9-O4
3	A	301	A1H87	C9-C7-C8-O3
3	C	301	A1H87	C10-C7-C9-O4
3	C	301	A1H87	C9-C7-C8-O3
4	A	304	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2
4	C	305	EDO	O1-C1-C2-O2
3	A	301	A1H87	C12-C11-O5-C10
3	C	301	A1H87	C1-C-C2-O1
4	A	302	EDO	O1-C1-C2-O2
4	B	202	EDO	O1-C1-C2-O2
4	C	307	EDO	O1-C1-C2-O2
4	D	203	EDO	O1-C1-C2-O2
7	C	302	PXN	CAM-CAN-OAO-CAP
7	C	302	PXN	CAT-CAU-OAV-CAW

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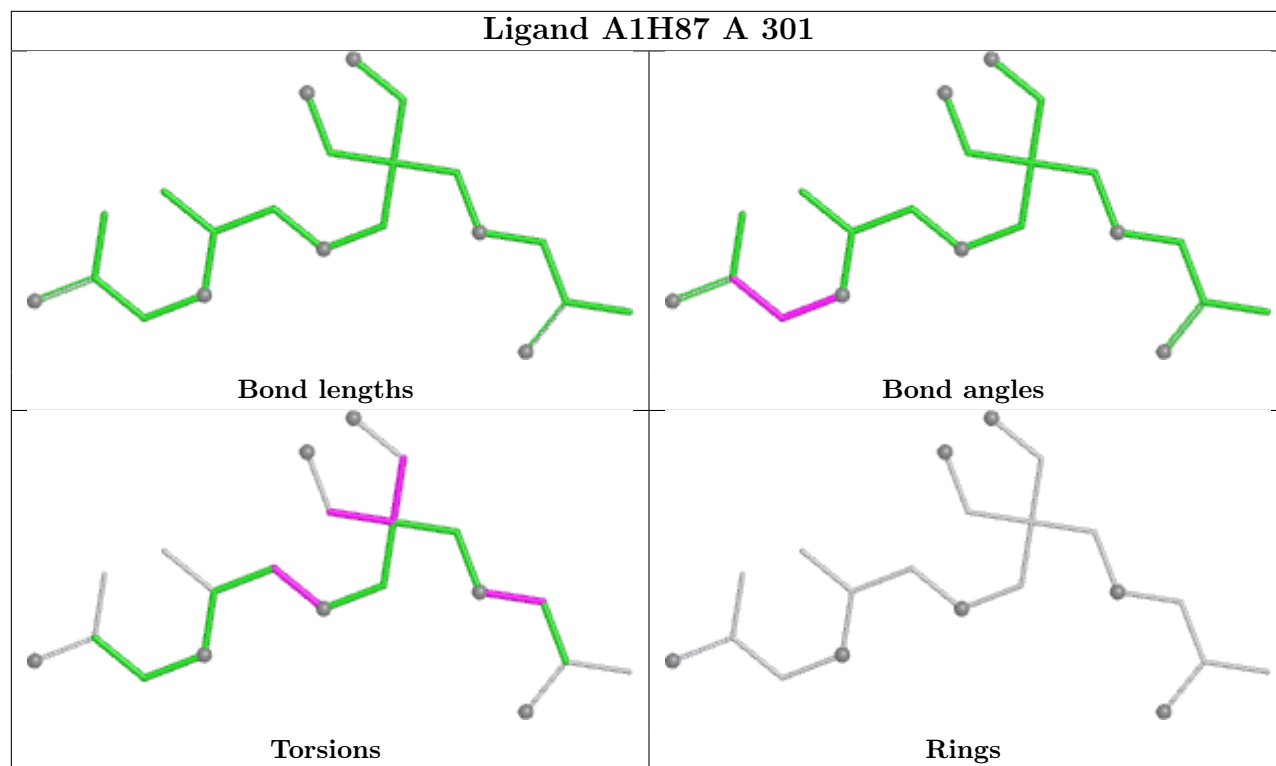
Mol	Chain	Res	Type	Atoms
6	B	206	TRS	N-C-C1-O1
6	B	207	TRS	N-C-C3-O3
4	B	204	EDO	O1-C1-C2-O2
3	C	301	A1H87	C3-C5-O2-C6
3	A	301	A1H87	C10-C7-C8-O3
6	B	206	TRS	C2-C-C1-O1
6	B	206	TRS	C3-C-C1-O1
6	B	207	TRS	C1-C-C3-O3
6	B	207	TRS	C2-C-C3-O3
7	C	302	PXN	CAI-CAJ-OAK-CAL
4	A	303	EDO	O1-C1-C2-O2
4	B	203	EDO	O1-C1-C2-O2
4	B	201	EDO	O1-C1-C2-O2
7	C	302	PXN	OAD-CAC-CAM-CAW
6	D	204	TRS	C1-C-C3-O3
7	C	302	PXN	OAO-CAP-CAQ-CAX
7	C	302	PXN	CAF-CAE-OAD-CAC
6	D	205	TRS	N-C-C2-O2
3	A	301	A1H87	C3-C5-O2-C6
7	C	302	PXN	OAD-CAC-CAM-CAL

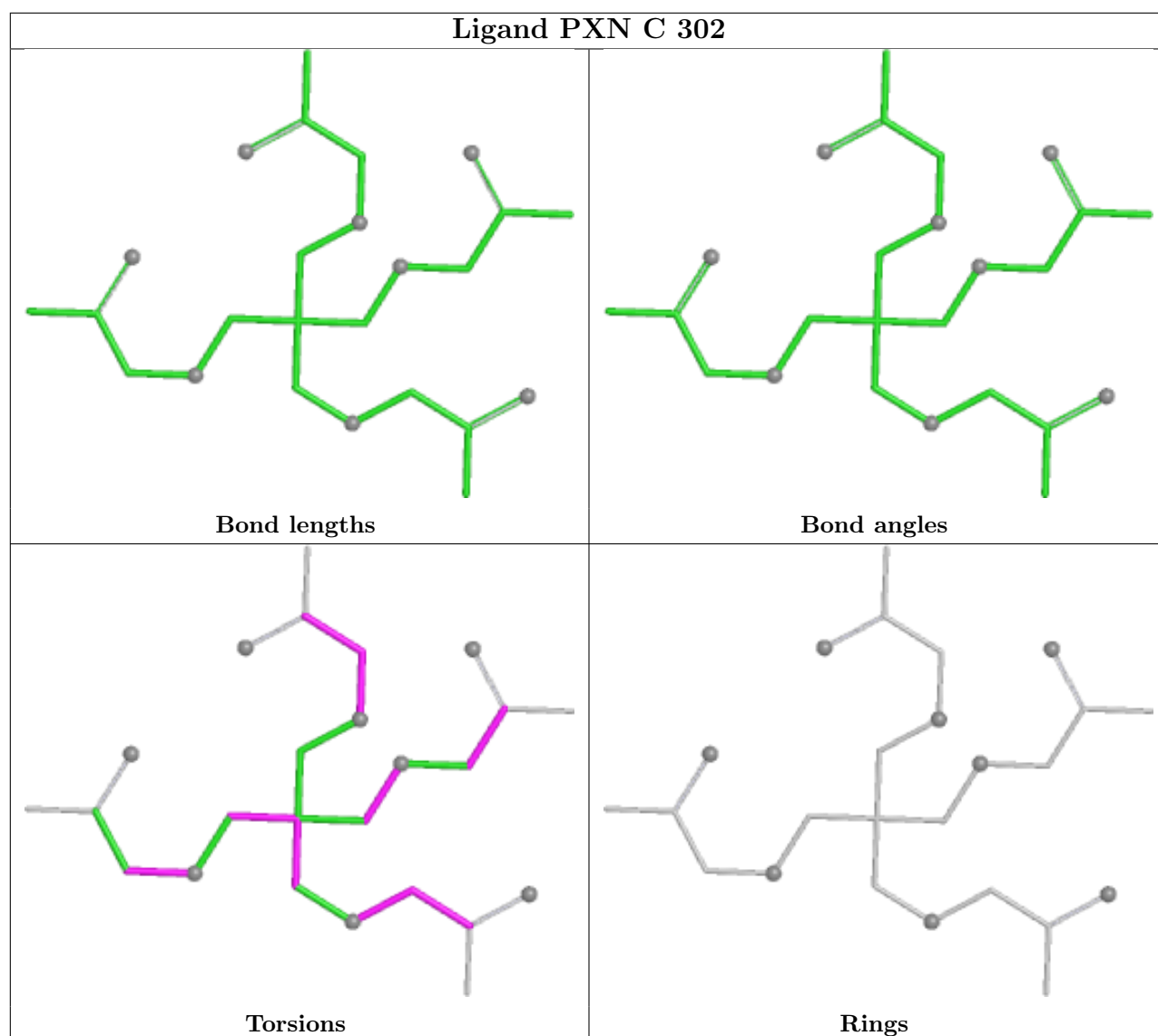
There are no ring outliers.

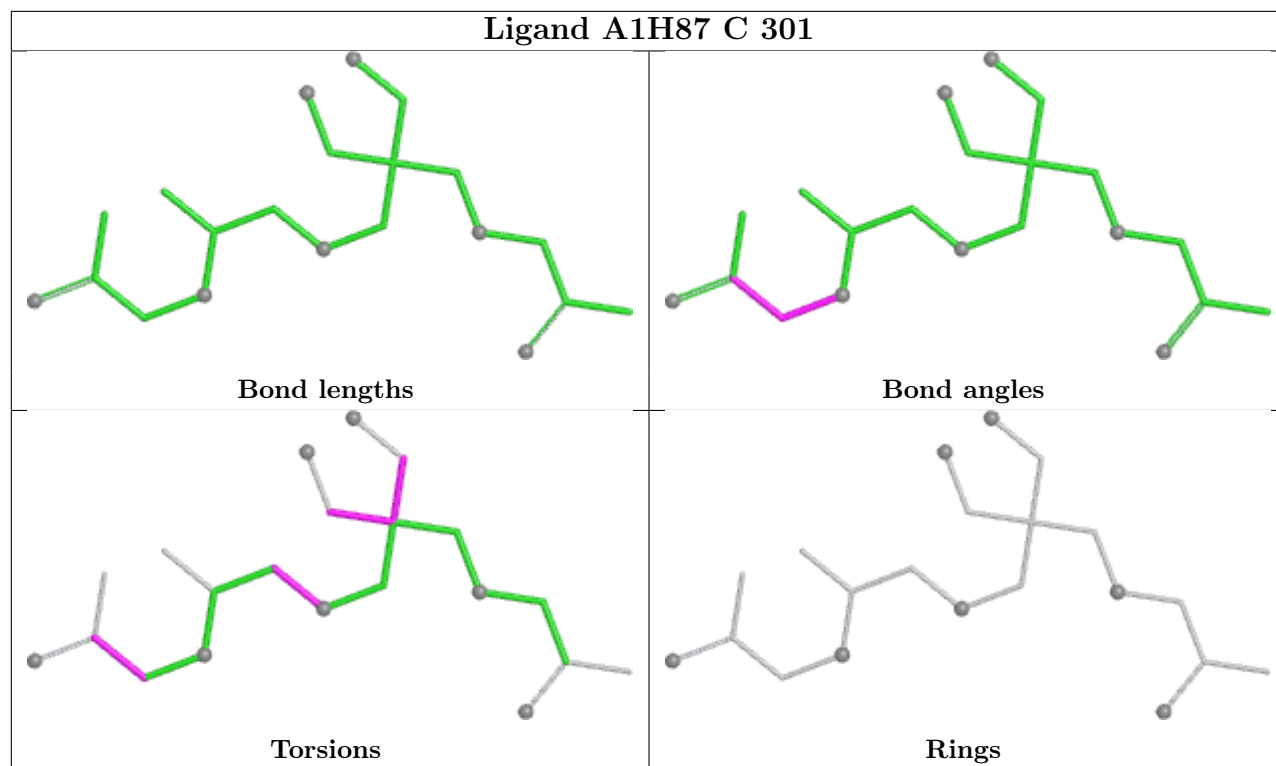
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	305	EDO	1	0
4	B	203	EDO	4	0
4	B	204	EDO	1	0
6	D	205	TRS	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	226/243 (93%)	-0.03	2 (0%) 81 84	6, 17, 33, 48	18 (7%)
1	C	227/243 (93%)	-0.23	1 (0%) 88 91	5, 14, 28, 45	22 (9%)
2	B	125/128 (97%)	0.17	5 (4%) 42 44	6, 18, 45, 54	7 (5%)
2	D	124/128 (96%)	0.16	2 (1%) 70 74	6, 19, 36, 52	7 (5%)
All	All	702/742 (94%)	-0.03	10 (1%) 73 78	5, 16, 34, 54	54 (7%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	VAL	5.3
2	B	12	SER	3.0
2	B	135	LEU	2.7
1	A	230	THR	2.3
2	B	13	ASP	2.2
2	D	135	LEU	2.2
1	A	132	GLU	2.2
2	B	131	ILE	2.1
2	D	124	GLY	2.1
2	B	136	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRO	A	66	22/23	0.97	0.05	11,12,13,15	0
1	CRO	C	66	22/23	0.97	0.05	9,9,10,12	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

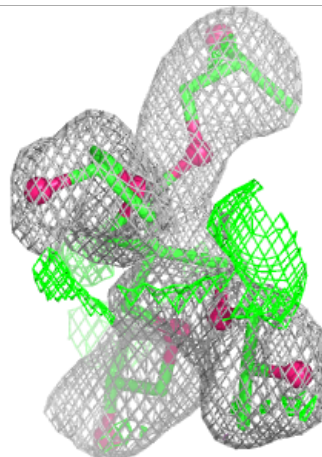
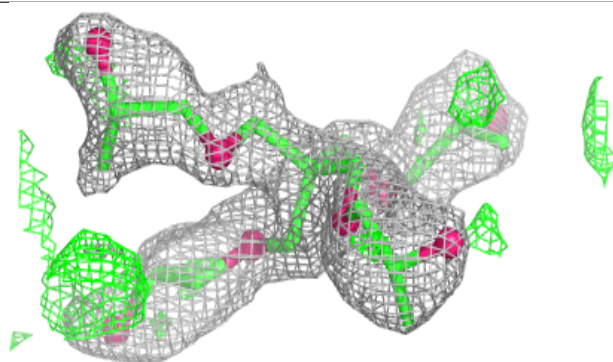
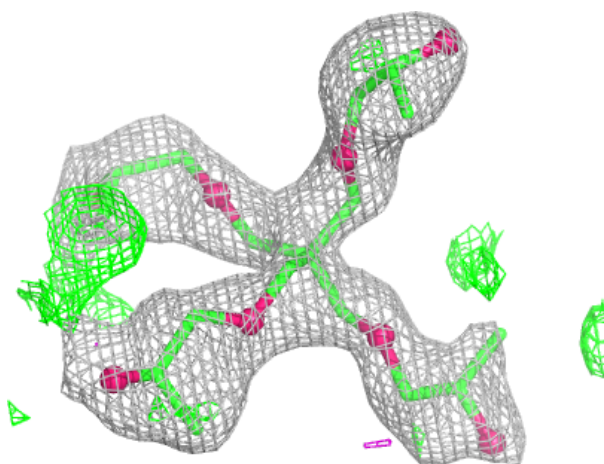
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	304	4/4	0.73	0.18	46,49,52,54	0
4	EDO	D	203	4/4	0.76	0.19	50,52,52,59	0
6	TRS	D	205	8/8	0.77	0.14	38,41,42,43	0
4	EDO	B	204	4/4	0.79	0.15	31,32,33,34	0
4	EDO	C	304	4/4	0.80	0.22	30,43,44,58	0
7	PXN	C	302	25/25	0.83	0.17	46,53,59,60	0
4	EDO	C	307	4/4	0.84	0.14	31,43,45,53	0
4	EDO	A	303	4/4	0.84	0.13	30,34,35,40	0
4	EDO	B	202	4/4	0.85	0.14	30,31,31,35	0
4	EDO	C	305	4/4	0.86	0.15	32,36,36,43	0
4	EDO	C	303	4/4	0.87	0.11	22,22,25,32	0
6	TRS	B	206	8/8	0.87	0.11	30,33,35,36	0
3	A1H87	C	301	21/21	0.88	0.12	22,32,39,40	0
4	EDO	D	201	4/4	0.88	0.13	27,30,30,33	0
4	EDO	C	306	4/4	0.89	0.11	32,33,37,39	0
4	EDO	D	202	4/4	0.89	0.12	45,46,46,50	0
6	TRS	D	206	8/8	0.89	0.10	23,26,27,28	0
3	A1H87	A	301	21/21	0.89	0.12	23,33,46,51	0
6	TRS	D	204	8/8	0.90	0.11	20,26,28,30	0
6	TRS	B	207	8/8	0.90	0.11	24,29,29,32	0
4	EDO	B	203	4/4	0.92	0.10	29,33,33,42	0
6	TRS	B	205	8/8	0.92	0.10	19,24,28,28	0
4	EDO	A	302	4/4	0.94	0.09	35,36,37,37	0
4	EDO	B	201	4/4	0.95	0.09	31,31,32,32	0
5	NA	C	308	1/1	0.98	0.06	13,13,13,13	0
5	NA	A	305	1/1	0.99	0.05	17,17,17,17	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.

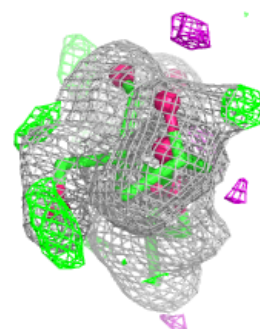
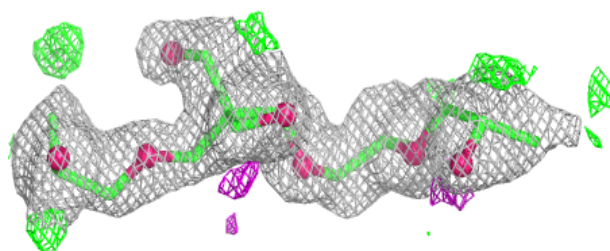
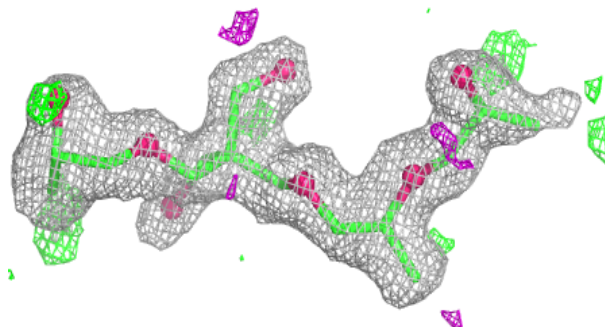
Electron density around PXN C 302:

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

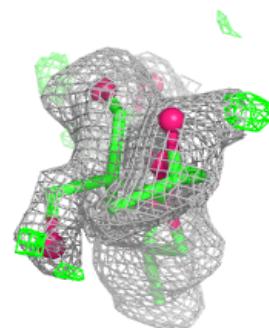
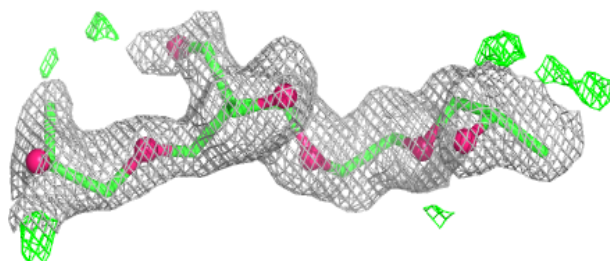
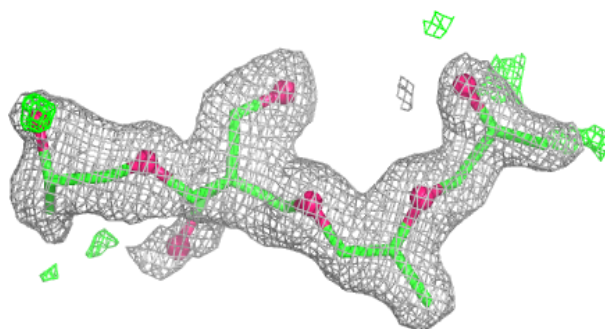


Electron density around A1H87 C 301:

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

**Electron density around A1H87 A 301:**

$2mF_o-DF_c$ (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.