



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:03 PM UTC

PDB ID : 9G8C / pdb_00009g8c
Title : Crystal structure of the photosensory core module (PCM) of a cyanophenylalanine mutant oCNF165 of the bathy phytochrome Agp2 from *Agrobacterium fabrum* in the Pfr state.
Authors : Sauthof, L.; Schmidt, A.; Scheerer, P.
Deposited on : 2024-07-23
Resolution : 1.90 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

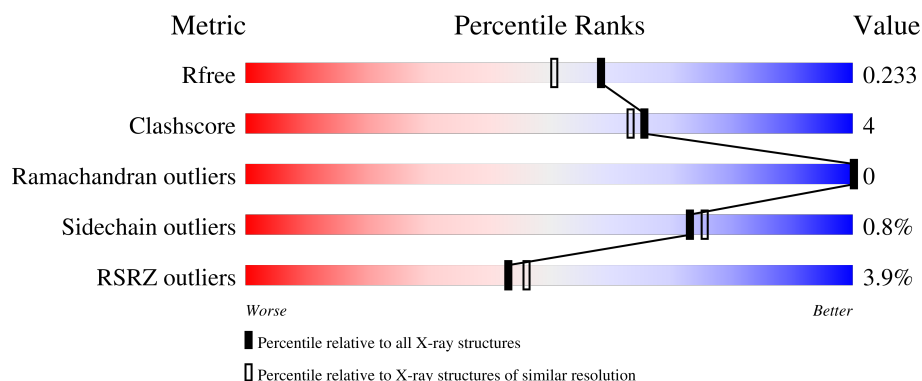
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	507	
2	B	507	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8767 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 histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	15	0
			3829	2440	678	690	21			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	9IJ	TYR	engineered mutation	UNP A9CI81
A	502	HIS	-	expression tag	UNP A9CI81
A	503	HIS	-	expression tag	UNP A9CI81
A	504	HIS	-	expression tag	UNP A9CI81
A	505	HIS	-	expression tag	UNP A9CI81
A	506	HIS	-	expression tag	UNP A9CI81
A	507	HIS	-	expression tag	UNP A9CI81

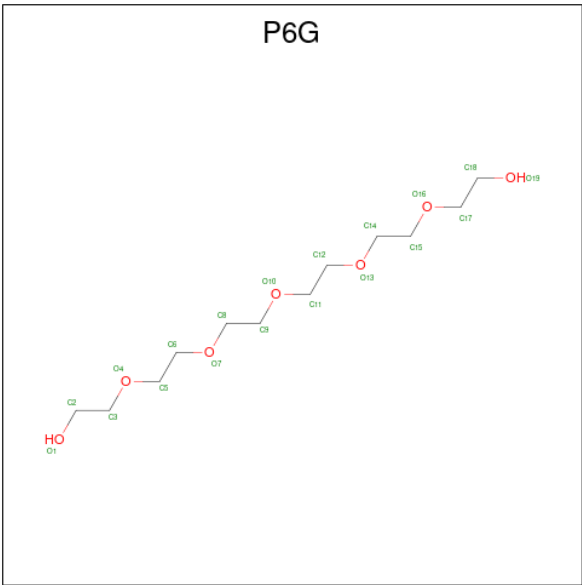
- Molecule 2 is a protein called histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	13	0
			3815	2425	674	694	22			

There are 7 discrepancies between the modelled and reference sequences:

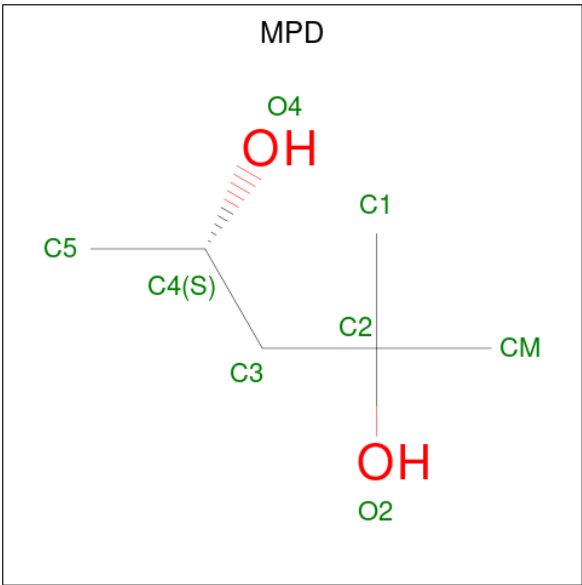
Chain	Residue	Modelled	Actual	Comment	Reference
B	165	9IJ	TYR	engineered mutation	UNP A9CI81
B	502	HIS	-	expression tag	UNP A9CI81
B	503	HIS	-	expression tag	UNP A9CI81
B	504	HIS	-	expression tag	UNP A9CI81
B	505	HIS	-	expression tag	UNP A9CI81
B	506	HIS	-	expression tag	UNP A9CI81
B	507	HIS	-	expression tag	UNP A9CI81

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



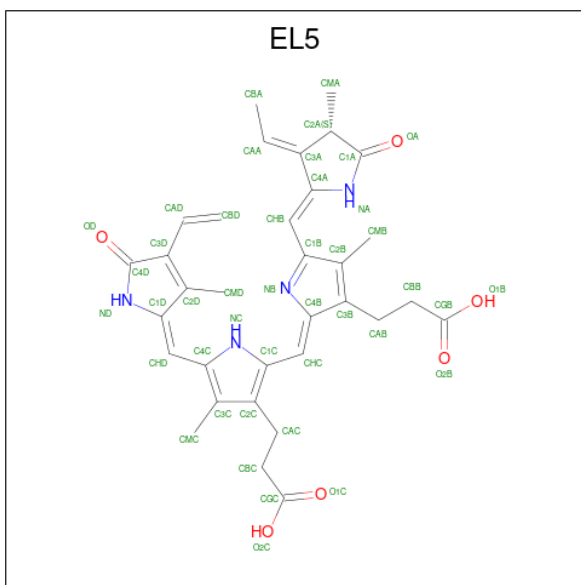
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- 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	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	1
			14	8	6		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 3-[(2Z)-2-({3-(2-carboxyethyl)-5-[(E)-(4-ethenyl-3-methyl-5-oxo-1,5-dihydro-2H-pyrrol-2-ylidene)methyl]-4-methyl-1H-pyrrol-2-yl}methylidene)-5-{(Z)-[(3E,4S)-3-ethylidene-4-methyl-5-oxopyrrolidin-2-ylidene]methyl}-4-methyl-2H-pyrrol-3-yl]propanoic acid (CCD ID: EL5) (formula: $C_{33}H_{36}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 43	C 33	N 4	O 6	0	0
6	B	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Cl 2 2	0	0

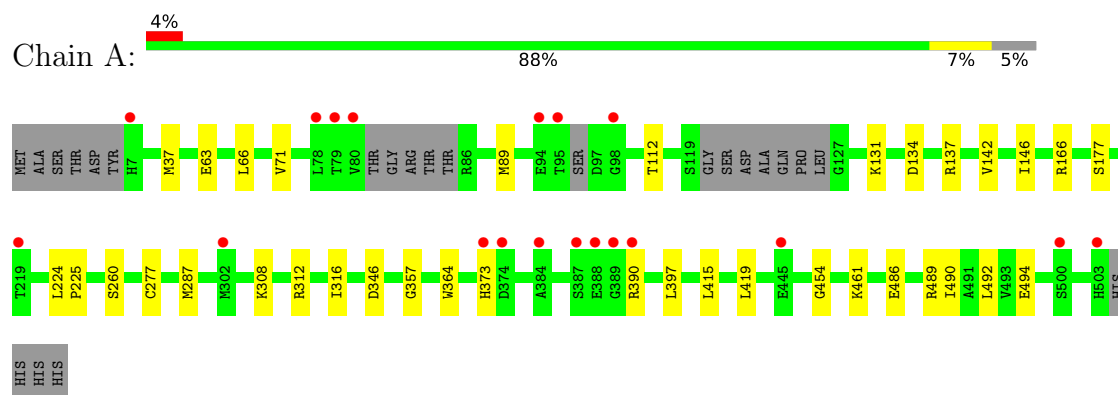
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	487	Total O 487 487	0	0
8	B	471	Total O 471 471	0	0

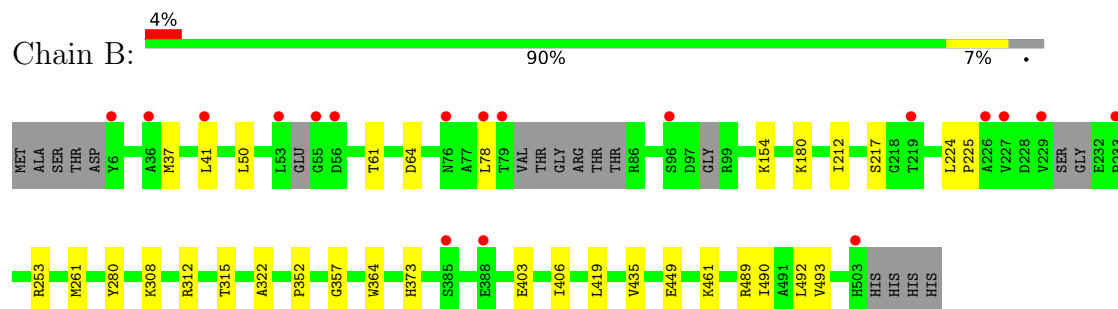
3 Residue-property plots

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: histidine kinase



- Molecule 2: histidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 93.76Å 174.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 1.90 45.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.95-1.90) 99.7 (45.95-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.223 0.196 , 0.233	Depositor DCC
R_{free} test set	4853 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8767	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: MPD, PEG, MLZ, 9IJ, CL, P6G, EL5

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	0/3802	1.26	2/5155 (0.0%)
2	B	1.05	0/3805	1.26	0/5165
All	All	1.03	0/7607	1.26	2/10320 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	GLY	CA-C-N	7.35	130.45	120.38
1	A	454	GLY	C-N-CA	7.35	130.45	120.38

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	3829	0	3799	32	0
2	B	3815	0	3748	29	0
3	A	10	0	13	4	0
3	B	9	0	11	1	0
4	A	8	0	14	3	0
4	B	8	0	14	2	0
5	A	7	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	35	0	50	4	0
6	A	43	0	0	0	0
6	B	43	0	0	0	0
7	B	2	0	0	1	0
8	A	487	0	0	2	0
8	B	471	0	0	2	0
All	All	8767	0	7659	59	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 4.

All (59) 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:419:LEU:HD22	1:A:492[B]:LEU:HD22	1.48	0.93
1:A:419:LEU:HD22	1:A:492[B]:LEU:CD2	2.02	0.88
2:B:449:GLU:HB2	5:B:606:PEG:H21	1.60	0.84
2:B:419:LEU:HA	2:B:492[B]:LEU:HD21	1.68	0.75
7:B:608:CL:CL	8:B:1134:HOH:O	2.43	0.73
2:B:419:LEU:HD22	2:B:492[B]:LEU:HD22	1.69	0.72
1:A:346:ASP:OD2	4:A:602:MPD:HM1	1.97	0.64
2:B:419:LEU:HA	2:B:492[B]:LEU:CD2	2.29	0.63
2:B:61[A]:THR:HG23	2:B:64:ASP:H	1.62	0.63
2:B:419:LEU:HD22	2:B:492[B]:LEU:CD2	2.31	0.61
1:A:142:VAL:HG11	3:A:601:P6G:H81	1.81	0.61
2:B:322:ALA:HB1	4:B:602:MPD:H51	1.82	0.61
1:A:490[B]:ILE:HG21	2:B:490:ILE:HG21	1.83	0.60
2:B:419:LEU:CD2	2:B:492[B]:LEU:HD22	2.31	0.60
1:A:419:LEU:CD2	1:A:492[B]:LEU:CD2	2.79	0.59
1:A:489:ARG:NH2	1:A:490[B]:ILE:HD11	2.17	0.59
1:A:419:LEU:HD22	1:A:492[A]:LEU:HD13	1.85	0.58
2:B:419:LEU:CD2	2:B:492[B]:LEU:CD2	2.82	0.57
1:A:166:ARG:NE	3:A:601:P6G:H61	2.20	0.57
2:B:280:TYR:HB2	3:B:601:P6G:H142	1.88	0.56
1:A:134:ASP:HA	1:A:137:ARG:HD2	1.87	0.56
2:B:357:GLY:HA3	2:B:364:TRP:CH2	2.42	0.55
4:A:602:MPD:O4	4:A:602:MPD:HM2	2.08	0.54
5:A:603:PEG:C1	8:A:750:HOH:O	2.55	0.54
1:A:37:MET:HG3	1:A:112:THR:HG21	1.88	0.54
2:B:403:GLU:O	2:B:406:ILE:HG22	2.10	0.52
1:A:419:LEU:HA	1:A:492[B]:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ILE:HG13	2:B:261:MET:HG3	1.92	0.51
1:A:490[B]:ILE:HG21	2:B:490:ILE:CG2	2.41	0.50
4:B:602:MPD:O2	4:B:602:MPD:H52	2.12	0.50
2:B:37:MET:HE2	2:B:78:LEU:HD11	1.94	0.50
1:A:66:LEU:HB2	1:A:71[B]:VAL:HG23	1.95	0.49
1:A:166:ARG:CD	3:A:601:P6G:H61	2.44	0.48
2:B:419:LEU:CA	2:B:492[B]:LEU:HD21	2.41	0.48
1:A:494:GLU:HG2	2:B:493:VAL:HG11	1.95	0.47
1:A:260:SER:HA	1:A:277:CYS:O	2.13	0.47
1:A:419:LEU:HA	1:A:492[B]:LEU:CD2	2.45	0.47
2:B:312:ARG:O	2:B:315[A]:THR:HG22	2.14	0.47
1:A:357:GLY:HA3	1:A:364:TRP:CH2	2.50	0.47
2:B:224:LEU:HA	2:B:225:PRO:HA	1.79	0.47
2:B:217:SER:OG	2:B:253:ARG:HD3	2.15	0.46
1:A:131:LYS:NZ	8:A:724:HOH:O	2.50	0.45
1:A:89:MET:HE3	1:A:287:MET:HE2	1.99	0.44
1:A:146[B]:ILE:HG22	1:A:177:SER:HB2	1.98	0.44
2:B:489:ARG:NH2	2:B:490:ILE:HD11	2.33	0.44
1:A:486:GLU:O	1:A:490[B]:ILE:HG12	2.18	0.43
1:A:494:GLU:OE1	2:B:490:ILE:CD1	2.66	0.43
2:B:352:PRO:HB2	5:B:605[B]:PEG:H21	2.01	0.43
1:A:490[B]:ILE:CG2	2:B:490:ILE:CG2	2.96	0.43
1:A:142:VAL:HG11	3:A:601:P6G:H51	2.01	0.43
1:A:415:LEU:HD23	1:A:415:LEU:C	2.44	0.42
1:A:490[A]:ILE:HG21	2:B:490:ILE:HG21	2.01	0.42
2:B:449:GLU:CB	5:B:606:PEG:H21	2.38	0.41
1:A:224:LEU:HA	1:A:225:PRO:HA	1.89	0.41
1:A:312:ARG:O	1:A:316:ILE:HG12	2.21	0.41
2:B:449:GLU:HA	5:B:606:PEG:H21	2.03	0.41
2:B:435[A]:VAL:CG1	8:B:796:HOH:O	2.69	0.41
1:A:63:GLU:HA	1:A:71[B]:VAL:HG21	2.03	0.40
1:A:346:ASP:CB	4:A:602:MPD:HM1	2.51	0.40

There are no symmetry-related clashes.

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	477/507 (94%)	470 (98%)	7 (2%)	0	100	100
2	B	479/507 (94%)	473 (99%)	6 (1%)	0	100	100
All	All	956/1014 (94%)	943 (99%)	13 (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	391/410 (95%)	387 (99%)	4 (1%)	68	70
2	B	389/411 (95%)	386 (99%)	3 (1%)	73	75
All	All	780/821 (95%)	773 (99%)	7 (1%)	73	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373[A]	HIS
1	A	373[B]	HIS
1	A	390	ARG
1	A	397	LEU
2	B	41	LEU
2	B	50	LEU
2	B	373	HIS

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	362	ASN
2	B	475	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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	MLZ	A	180[A]	-	8,9,10	0.41	0	4,9,11	0.60	0
2	MLZ	B	154[B]	-	8,9,10	0.40	0	4,9,11	0.35	0
1	MLZ	A	446	1	8,9,10	0.43	0	4,9,11	0.63	0
1	MLZ	A	154[B]	1	8,9,10	0.46	0	4,9,11	0.61	0
2	MLZ	B	174	2	8,9,10	0.44	0	4,9,11	0.73	0
1	MLZ	A	467	1	8,9,10	0.46	0	4,9,11	0.81	0
2	MLZ	B	154[A]	-	8,9,10	0.39	0	4,9,11	1.02	1 (25%)
2	MLZ	B	461	2	8,9,10	0.47	0	4,9,11	1.05	1 (25%)
2	MLZ	B	180[B]	-	8,9,10	0.42	0	4,9,11	0.58	0
1	MLZ	A	310	1	8,9,10	0.44	0	4,9,11	0.92	0
2	MLZ	B	432	2	8,9,10	0.50	0	4,9,11	0.71	0
1	MLZ	A	154[A]	1	8,9,10	0.46	0	4,9,11	1.02	0
1	MLZ	A	207[B]	-	8,9,10	0.39	0	4,9,11	0.79	0
1	MLZ	A	461	1	8,9,10	0.41	0	4,9,11	1.35	1 (25%)
2	MLZ	B	308	2	8,9,10	0.43	0	4,9,11	1.32	1 (25%)
1	MLZ	A	180[B]	-	8,9,10	0.41	0	4,9,11	1.00	0
1	MLZ	A	432	1	8,9,10	0.50	0	4,9,11	0.81	0
2	MLZ	B	207	2	8,9,10	0.42	0	4,9,11	0.92	0
2	MLZ	B	180[A]	-	8,9,10	0.42	0	4,9,11	1.08	1 (25%)
2	MLZ	B	467	2	8,9,10	0.40	0	4,9,11	0.72	0
1	MLZ	A	174	1	8,9,10	0.51	0	4,9,11	0.74	0
2	MLZ	B	446	2	8,9,10	0.42	0	4,9,11	0.45	0
1	MLZ	A	207[A]	-	8,9,10	0.39	0	4,9,11	0.80	0
1	MLZ	A	308	1	8,9,10	0.50	0	4,9,11	1.13	1 (25%)

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	MLZ	A	180[A]	-	-	0/7/8/10	-
2	MLZ	B	154[B]	-	-	1/7/8/10	-
1	MLZ	A	446	1	-	0/7/8/10	-
1	MLZ	A	154[B]	1	-	0/7/8/10	-
2	MLZ	B	174	2	-	1/7/8/10	-
1	MLZ	A	467	1	-	0/7/8/10	-
2	MLZ	B	154[A]	-	-	0/7/8/10	-
2	MLZ	B	461	2	-	0/7/8/10	-
2	MLZ	B	180[B]	-	-	0/7/8/10	-
1	MLZ	A	310	1	-	2/7/8/10	-
2	MLZ	B	432	2	-	0/7/8/10	-
1	MLZ	A	154[A]	1	-	0/7/8/10	-
1	MLZ	A	207[B]	-	-	1/7/8/10	-
1	MLZ	A	461	1	-	1/7/8/10	-
2	MLZ	B	308	2	-	1/7/8/10	-
1	MLZ	A	180[B]	-	-	1/7/8/10	-
1	MLZ	A	432	1	-	0/7/8/10	-
2	MLZ	B	207	2	-	1/7/8/10	-
2	MLZ	B	180[A]	-	-	0/7/8/10	-
2	MLZ	B	467	2	-	0/7/8/10	-
1	MLZ	A	174	1	-	1/7/8/10	-
2	MLZ	B	446	2	-	0/7/8/10	-
1	MLZ	A	207[A]	-	-	2/7/8/10	-
1	MLZ	A	308	1	-	1/7/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	MLZ	CM-NZ-CE	2.66	119.42	112.01
2	B	308	MLZ	CM-NZ-CE	2.50	118.97	112.01
1	A	308	MLZ	CM-NZ-CE	2.18	118.09	112.01
2	B	180[A]	MLZ	CM-NZ-CE	2.11	117.89	112.01
2	B	461	MLZ	CM-NZ-CE	2.03	117.67	112.01
2	B	154[A]	MLZ	CM-NZ-CE	2.01	117.61	112.01

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	180[B]	MLZ	CD-CE-NZ-CM
1	A	207[A]	MLZ	O-C-CA-CB
1	A	207[A]	MLZ	CD-CE-NZ-CM
1	A	207[B]	MLZ	O-C-CA-CB
1	A	308	MLZ	CD-CE-NZ-CM
1	A	310	MLZ	CD-CE-NZ-CM
1	A	461	MLZ	CD-CE-NZ-CM
2	B	174	MLZ	CD-CE-NZ-CM
2	B	207	MLZ	CD-CE-NZ-CM
2	B	308	MLZ	CD-CE-NZ-CM
1	A	310	MLZ	CG-CD-CE-NZ
1	A	174	MLZ	CD-CE-NZ-CM
2	B	154[B]	MLZ	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
5	PEG	B	605[A]	-	6,6,6	0.15	0	5,5,5	0.11	0
5	PEG	B	603	-	6,6,6	0.18	0	5,5,5	0.13	0
3	P6G	B	601	-	8,8,18	0.31	0	7,7,17	0.27	0
5	PEG	B	606	-	6,6,6	0.12	0	5,5,5	0.14	0
4	MPD	B	602	-	7,7,7	0.34	0	9,10,10	0.40	0
3	P6G	A	601	-	9,9,18	0.29	0	8,8,17	0.20	0
5	PEG	B	604	-	6,6,6	0.17	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EL5	B	607	2	46,46,46	2.69	9 (19%)	58,67,67	1.38	7 (12%)
5	PEG	A	603	-	6,6,6	0.16	0	5,5,5	0.14	0
4	MPD	A	602	-	7,7,7	0.31	0	9,10,10	0.56	0
6	EL5	A	604	1	46,46,46	2.56	9 (19%)	58,67,67	1.41	7 (12%)
5	PEG	B	605[B]	-	6,6,6	0.13	0	5,5,5	0.14	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
5	PEG	B	605[A]	-	-	3/4/4/4	-
5	PEG	B	603	-	-	2/4/4/4	-
3	P6G	B	601	-	-	4/6/6/16	-
5	PEG	B	606	-	-	2/4/4/4	-
4	MPD	B	602	-	-	0/5/5/5	-
3	P6G	A	601	-	-	5/7/7/16	-
5	PEG	B	604	-	-	2/4/4/4	-
6	EL5	B	607	2	-	7/26/74/74	0/4/4/4
5	PEG	A	603	-	-	2/4/4/4	-
4	MPD	A	602	-	-	3/5/5/5	-
6	EL5	A	604	1	-	6/26/74/74	0/4/4/4
5	PEG	B	605[B]	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	607	EL5	C2A-C1A	-11.68	1.38	1.52
6	A	604	EL5	C2A-C1A	-10.68	1.40	1.52
6	B	607	EL5	C2A-C3A	-9.52	1.39	1.51
6	A	604	EL5	C2A-C3A	-9.40	1.39	1.51
6	A	604	EL5	C4B-C3B	-4.13	1.39	1.45
6	B	607	EL5	CAA-C3A	3.94	1.43	1.33
6	B	607	EL5	C4B-C3B	-3.92	1.39	1.45
6	A	604	EL5	CAA-C3A	3.86	1.43	1.33
6	B	607	EL5	CBA-CAA	-3.55	1.36	1.49
6	A	604	EL5	CBA-CAA	-3.37	1.37	1.49
6	B	607	EL5	C1D-C2D	-3.23	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	604	EL5	C1D-C2D	-3.17	1.39	1.45
6	B	607	EL5	C1B-C2B	-2.97	1.39	1.45
6	A	604	EL5	C1B-C2B	-2.82	1.39	1.45
6	B	607	EL5	CAD-C3D	-2.81	1.39	1.47
6	A	604	EL5	C4A-C3A	-2.68	1.40	1.45
6	B	607	EL5	C4A-C3A	-2.65	1.40	1.45
6	A	604	EL5	CAD-C3D	-2.54	1.40	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	604	EL5	CHD-C1D-ND	-4.06	117.39	126.06
6	B	607	EL5	CHD-C4C-NC	3.94	134.20	125.29
6	B	607	EL5	CHD-C1D-C2D	3.90	134.75	126.97
6	B	607	EL5	CHD-C1D-ND	-3.84	117.86	126.06
6	A	604	EL5	CHD-C1D-C2D	3.76	134.47	126.97
6	A	604	EL5	CHD-C4C-C3C	-3.72	118.41	127.53
6	A	604	EL5	CHD-C4C-NC	3.71	133.68	125.29
6	B	607	EL5	CHD-C4C-C3C	-3.45	119.08	127.53
6	A	604	EL5	CMD-C2D-C1D	3.25	128.12	124.16
6	B	607	EL5	CMD-C2D-C1D	3.02	127.84	124.16
6	A	604	EL5	OA-C1A-C2A	2.72	129.62	126.74
6	A	604	EL5	C4C-CHD-C1D	2.08	136.82	130.82
6	B	607	EL5	C4C-CHD-C1D	2.07	136.77	130.82
6	B	607	EL5	CAA-C3A-C4A	2.02	128.80	126.36

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	604	EL5	NC-C4C-CHD-C1D
6	B	607	EL5	NC-C4C-CHD-C1D
6	A	604	EL5	C2D-C1D-CHD-C4C
6	B	607	EL5	C2D-C1D-CHD-C4C
6	A	604	EL5	C3C-C4C-CHD-C1D
6	B	607	EL5	C3C-C4C-CHD-C1D
3	A	601	P6G	C9-C8-O7-C6
5	B	604	PEG	O2-C3-C4-O4
3	A	601	P6G	O4-C5-C6-O7
3	B	601	P6G	O16-C17-C18-O19
5	A	603	PEG	O1-C1-C2-O2
5	B	605[A]	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	604	EL5	ND-C1D-CHD-C4C
6	B	607	EL5	ND-C1D-CHD-C4C
3	A	601	P6G	O1-C2-C3-O4
5	B	603	PEG	O2-C3-C4-O4
5	B	605[B]	PEG	O2-C3-C4-O4
5	B	606	PEG	C1-C2-O2-C3
3	A	601	P6G	C6-C5-O4-C3
3	A	601	P6G	C2-C3-O4-C5
5	B	604	PEG	C4-C3-O2-C2
5	B	603	PEG	C1-C2-O2-C3
3	B	601	P6G	C18-C17-O16-C15
5	B	605[B]	PEG	C1-C2-O2-C3
3	B	601	P6G	C15-C14-O13-C12
5	B	605[A]	PEG	C4-C3-O2-C2
4	A	602	MPD	C2-C3-C4-O4
5	B	605[A]	PEG	O2-C3-C4-O4
6	A	604	EL5	CAB-CBB-CGB-O1B
6	A	604	EL5	CAB-CBB-CGB-O2B
6	B	607	EL5	CAB-CBB-CGB-O2B
6	B	607	EL5	CAB-CBB-CGB-O1B
5	A	603	PEG	C1-C2-O2-C3
3	B	601	P6G	C11-C12-O13-C14
5	B	606	PEG	O1-C1-C2-O2
4	A	602	MPD	C1-C2-C3-C4
4	A	602	MPD	CM-C2-C3-C4
6	B	607	EL5	NB-C1B-CHB-C4A

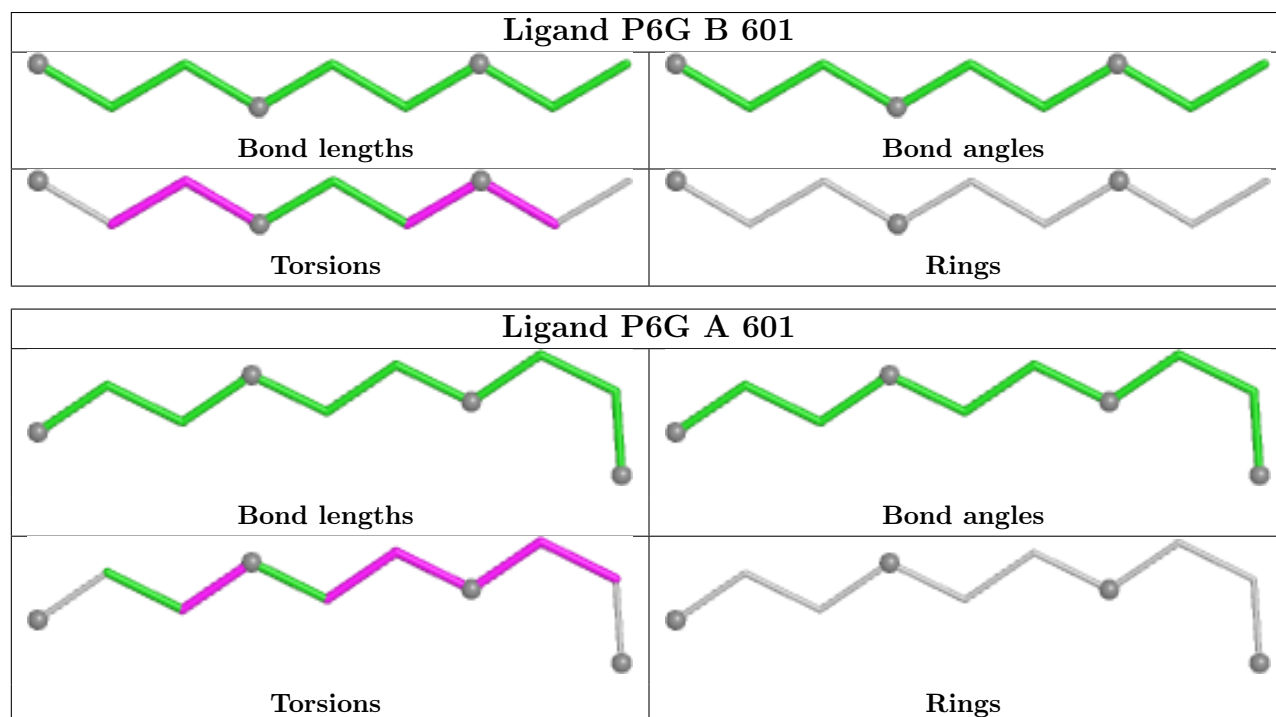
There are no ring outliers.

7 monomers are involved in 15 short contacts:

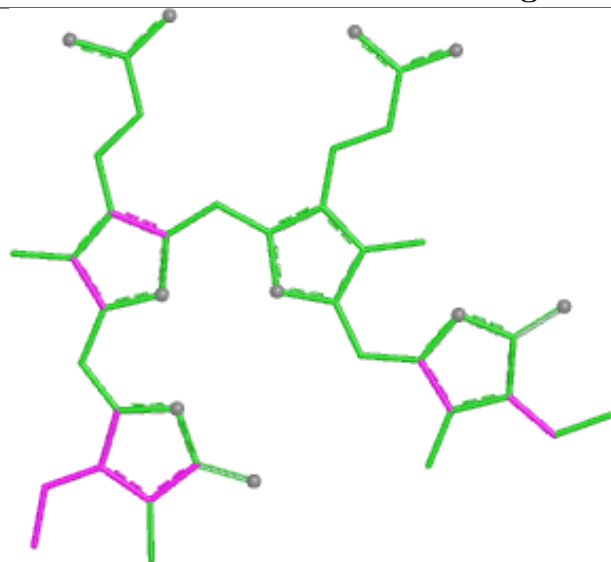
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	P6G	1	0
5	B	606	PEG	3	0
4	B	602	MPD	2	0
3	A	601	P6G	4	0
5	A	603	PEG	1	0
4	A	602	MPD	3	0
5	B	605[B]	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

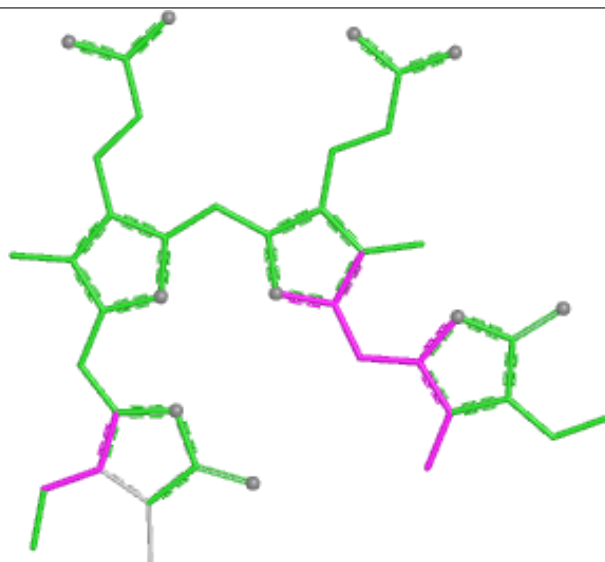
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



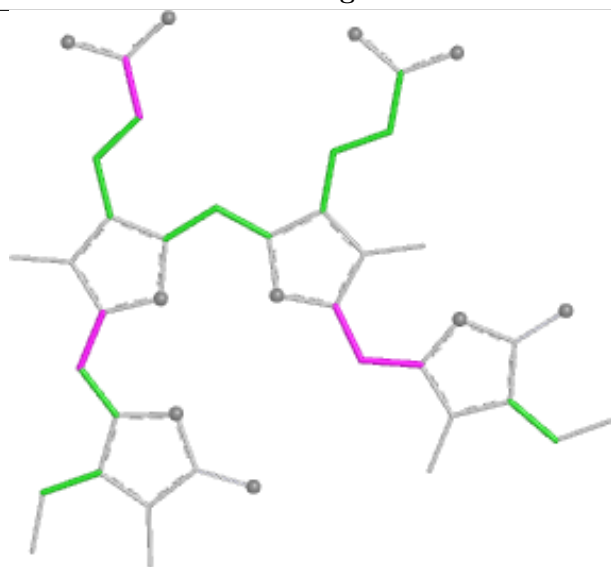
Ligand EL5 B 607



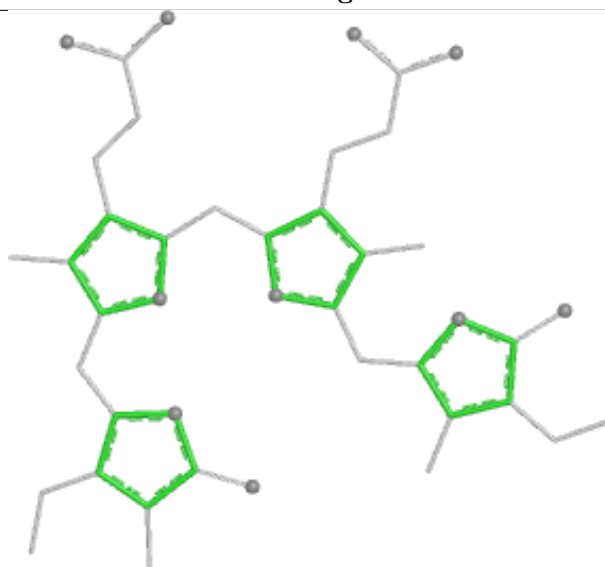
Bond lengths



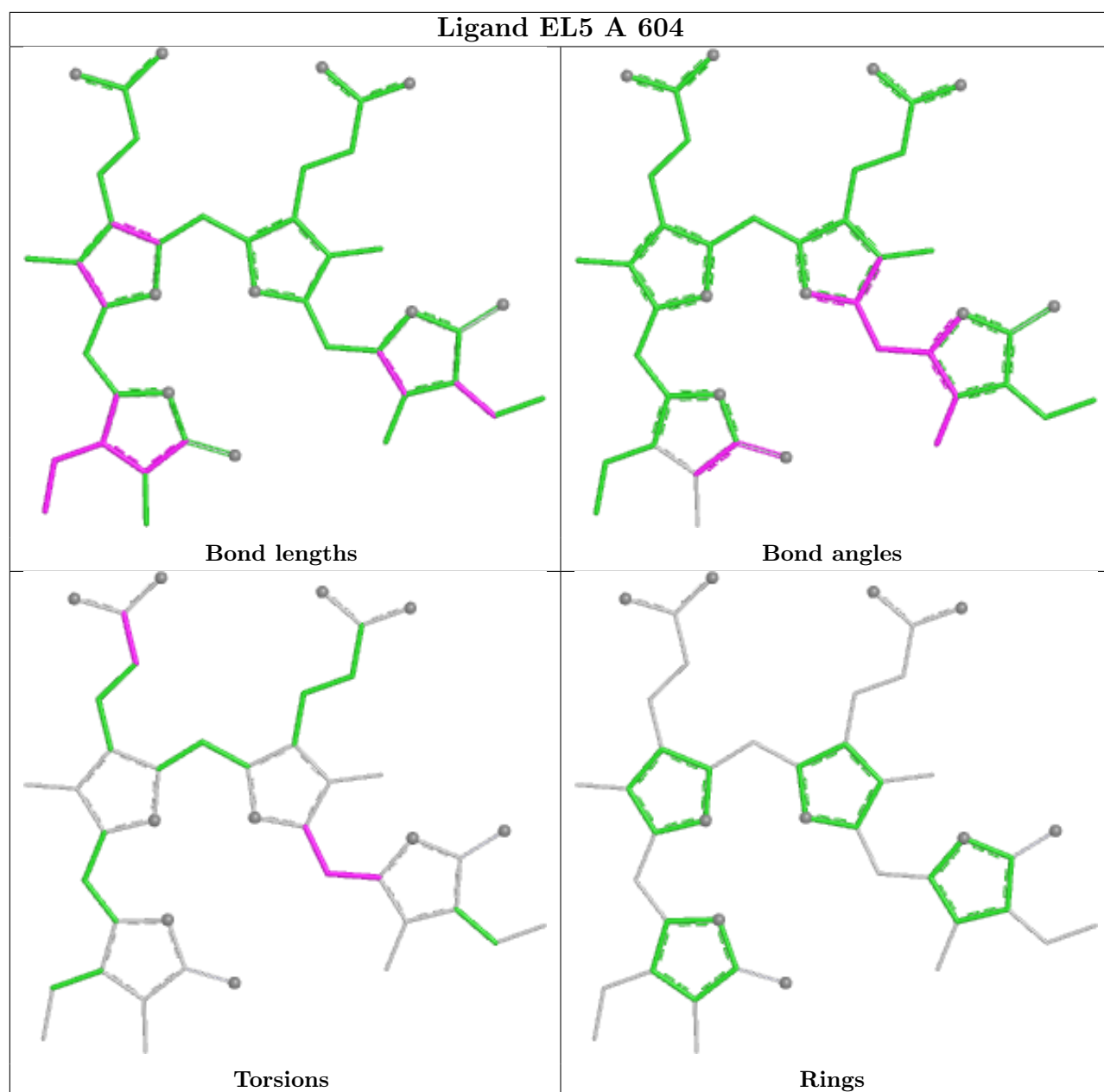
Bond angles



Torsions



Rings



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	473/507 (93%)	0.12	19 (4%)	42	45	12, 23, 42, 64	12 (2%)
2	B	478/507 (94%)	0.30	18 (3%)	44	47	12, 25, 46, 70	11 (2%)
All	All	951/1014 (93%)	0.21	37 (3%)	43	46	12, 24, 44, 70	23 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	55	GLY	5.0
2	B	229	VAL	4.1
2	B	6	TYR	4.0
2	B	79	THR	3.8
1	A	80	VAL	3.5
2	B	503	HIS	3.5
2	B	78	LEU	3.4
1	A	384	ALA	3.2
1	A	7	HIS	3.1
1	A	503	HIS	3.0
2	B	36	ALA	2.8
1	A	78	LEU	2.8
2	B	56	ASP	2.8
1	A	98	GLY	2.8
1	A	389	GLY	2.6
2	B	41	LEU	2.6
1	A	445	GLU	2.6
2	B	96	SER	2.5
2	B	227	VAL	2.5
1	A	95	THR	2.5
2	B	219	THR	2.5
2	B	53	LEU	2.4
1	A	387	SER	2.4
1	A	500	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	388	GLU	2.4
1	A	374	ASP	2.3
1	A	219	THR	2.3
2	B	226	ALA	2.3
1	A	302	MET	2.3
1	A	373[A]	HIS	2.2
2	B	233	PRO	2.2
2	B	76	ASN	2.2
2	B	385	SER	2.2
1	A	94	GLU	2.1
1	A	390	ARG	2.1
1	A	79	THR	2.1
2	B	388	GLU	2.0

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

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
2	MLZ	B	446	10/11	0.87	0.12	33,34,36,39	0
1	MLZ	A	154[B]	10/11	0.88	0.10	18,19,19,20	10
1	MLZ	A	154[A]	10/11	0.88	0.10	18,20,22,22	10
1	MLZ	A	446	10/11	0.92	0.09	33,35,37,40	0
2	MLZ	B	207	10/11	0.93	0.09	23,29,38,38	0
2	MLZ	B	308	10/11	0.93	0.09	20,23,30,30	0
1	MLZ	A	461	10/11	0.93	0.09	17,22,33,34	0
2	MLZ	B	461	10/11	0.93	0.10	21,25,39,40	0
2	MLZ	B	154[A]	10/11	0.94	0.10	16,17,18,19	7
2	MLZ	B	154[B]	10/11	0.94	0.10	16,17,19,19	7
2	MLZ	B	174	10/11	0.94	0.09	15,18,27,28	0
1	MLZ	A	207[B]	10/11	0.94	0.09	22,24,29,30	7
1	MLZ	A	308	10/11	0.94	0.08	18,21,25,26	0
2	MLZ	B	432	10/11	0.94	0.08	18,20,28,30	0
1	MLZ	A	174	10/11	0.94	0.09	14,15,25,25	0
1	MLZ	A	207[A]	10/11	0.94	0.09	22,24,29,30	7
1	MLZ	A	310	10/11	0.95	0.09	20,23,30,30	0
2	MLZ	B	467	10/11	0.95	0.07	19,21,27,27	0
1	MLZ	A	467	10/11	0.96	0.07	16,19,24,24	0
1	MLZ	A	432	10/11	0.96	0.07	16,19,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLZ	A	180[A]	10/11	0.96	0.08	18,19,19,20	7
1	MLZ	A	180[B]	10/11	0.96	0.08	18,18,19,19	7
2	MLZ	B	180[A]	10/11	0.96	0.07	14,15,16,16	7
2	MLZ	B	180[B]	10/11	0.96	0.07	14,15,16,16	7

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

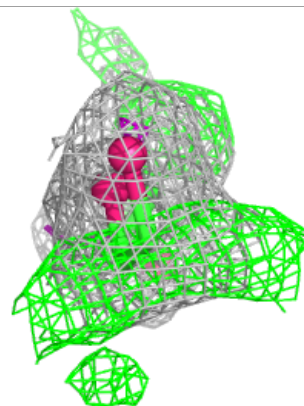
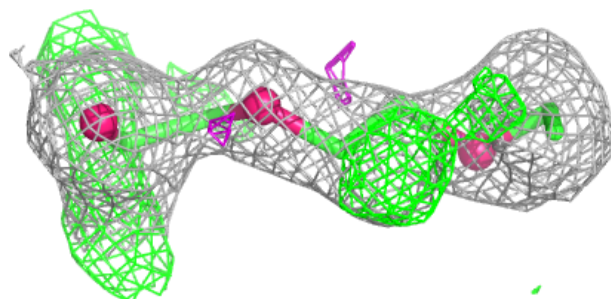
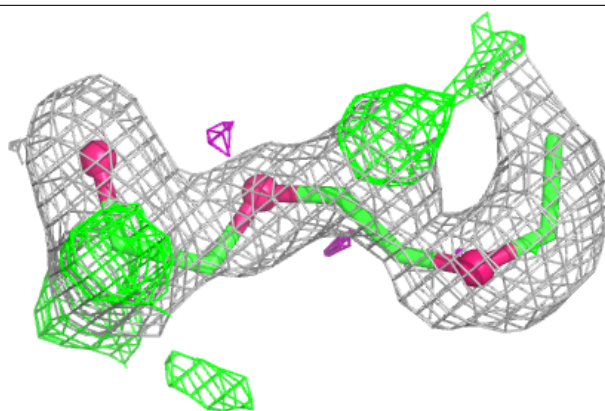
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	PEG	B	605[A]	7/7	0.58	0.29	49,56,60,61	7
5	PEG	B	605[B]	7/7	0.58	0.29	28,31,33,34	7
3	P6G	B	601	9/19	0.69	0.22	35,40,44,46	0
5	PEG	B	606	7/7	0.69	0.16	52,53,55,57	0
5	PEG	B	603	7/7	0.77	0.17	40,50,57,59	0
5	PEG	A	603	7/7	0.77	0.20	54,55,59,59	0
3	P6G	A	601	10/19	0.78	0.18	24,36,52,54	0
5	PEG	B	604	7/7	0.81	0.18	55,57,59,59	0
4	MPD	A	602	8/8	0.90	0.11	23,25,26,27	0
6	EL5	A	604	43/43	0.92	0.09	17,20,25,27	0
4	MPD	B	602	8/8	0.93	0.08	20,21,23,25	0
6	EL5	B	607	43/43	0.93	0.08	18,21,24,30	0
7	CL	B	609	1/1	0.94	0.19	64,64,64,64	0
7	CL	B	608	1/1	0.95	0.08	38,38,38,38	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.

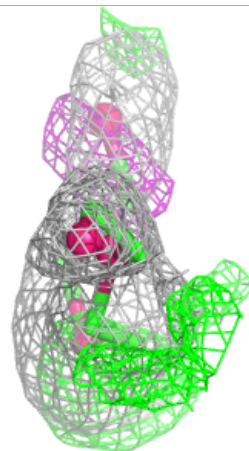
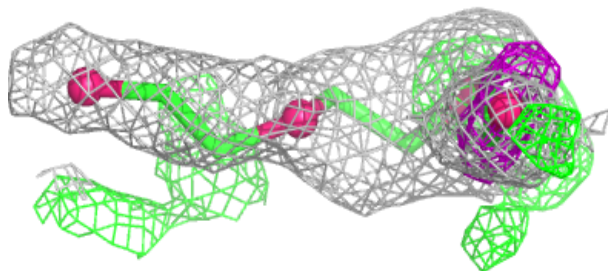
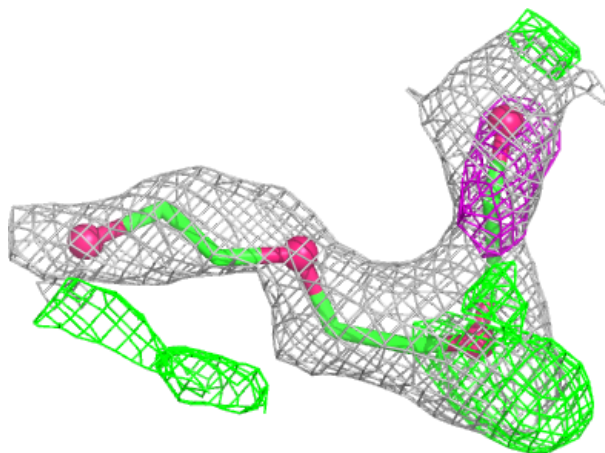
Electron density around P6G B 601:

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



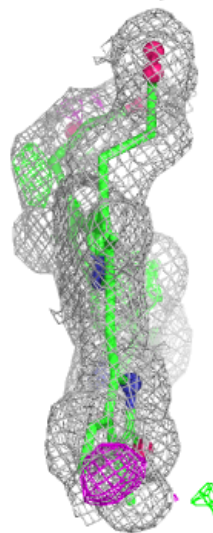
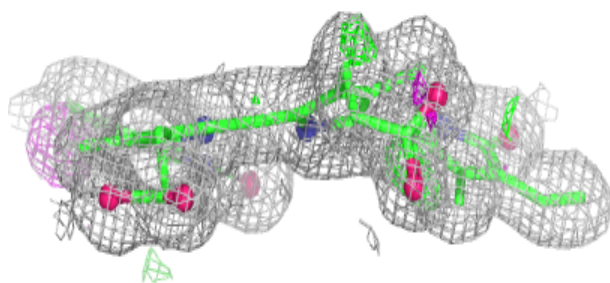
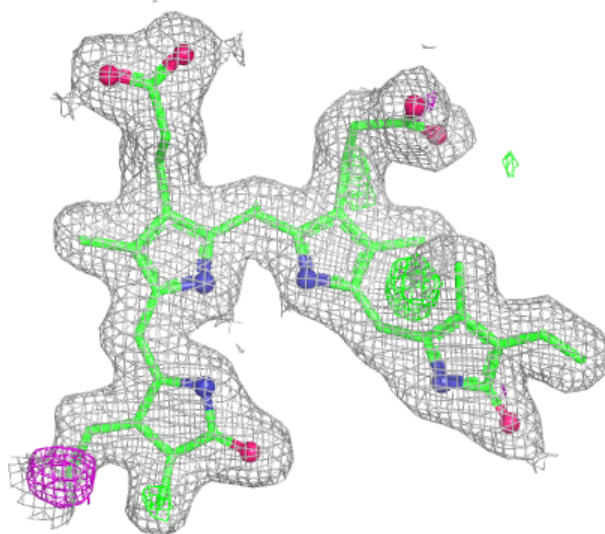
Electron density around P6G A 601:

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



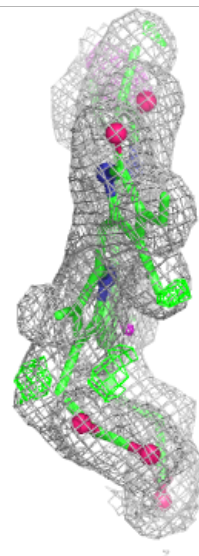
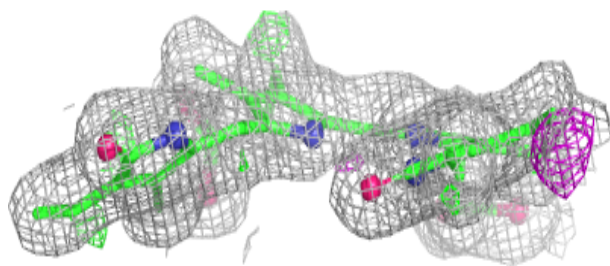
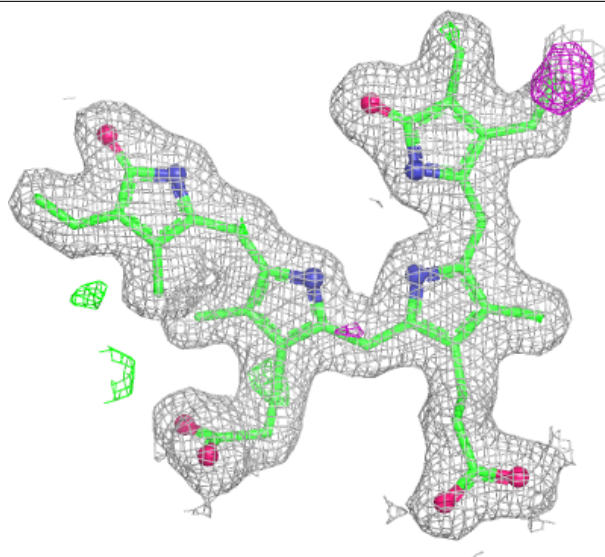
Electron density around EL5 A 604:

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



Electron density around EL5 B 607:

$2mF_o-DF_c$ (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.