Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 10:09 pm BST

PDB ID	:	8RJU / pdb_00008rju
Title	:	Serial femtosecond X-ray structure of a fluorescence optimized bathy phytochrome PAiRFP2 derived from wild-type Agp2 in I7 intermediate state.
Authors	:	Sauthof, L.; Schmidt, A.; Szczepek, M.; Brewster, A.S.; Kern, J.F.; Scheerer, P.
Deposited on	:	2023-12-21
Resolution	:	2.80 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:

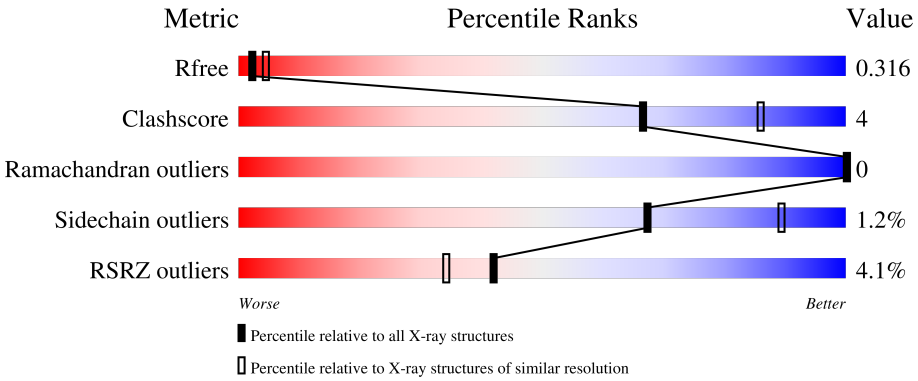
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 <=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	515	4% 87% 8% 5%
1	B	515	4% 85% 9% 6%

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
2	EL5	A	601	X	-	-	-
2	EL5	B	601	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7866 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	488	Total	C	N	O	S	0	2	0
			3697	2339	658	681	19			
1	B	485	Total	C	N	O	S	0	2	0
			3676	2328	648	680	20			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	ARG	LYS	engineered mutation	UNP A9CI81
A	83	LYS	ARG	engineered mutation	UNP A9CI81
A	120	ASP	GLY	engineered mutation	UNP A9CI81
A	123	THR	ALA	engineered mutation	UNP A9CI81
A	163	LEU	MET	engineered mutation	UNP A9CI81
A	168	GLU	GLN	engineered mutation	UNP A9CI81
A	220	PRO	ARG	engineered mutation	UNP A9CI81
A	243	ASN	SER	engineered mutation	UNP A9CI81
A	244	PHE	VAL	engineered mutation	UNP A9CI81
A	269	ASP	GLY	engineered mutation	UNP A9CI81
A	276	VAL	ALA	engineered mutation	UNP A9CI81
A	280	CYS	TYR	engineered mutation	UNP A9CI81
A	294	ALA	GLU	engineered mutation	UNP A9CI81
A	303	PHE	HIS	engineered mutation	UNP A9CI81
A	333	ARG	HIS	engineered mutation	UNP A9CI81
A	336	LEU	ILE	engineered mutation	UNP A9CI81
A	349	ARG	ASP	engineered mutation	UNP A9CI81
A	351	ILE	MET	engineered mutation	UNP A9CI81
A	386	VAL	ALA	engineered mutation	UNP A9CI81
A	409	ASP	GLY	engineered mutation	UNP A9CI81
A	419	ILE	LEU	engineered mutation	UNP A9CI81
A	469	SER	THR	engineered mutation	UNP A9CI81
A	487	THR	ALA	engineered mutation	UNP A9CI81
A	494	GLY	GLU	engineered mutation	UNP A9CI81
A	503	MET	-	insertion	UNP A9CI81

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Chain	Residue	Modelled	Actual	Comment	Reference
A	504	ALA	-	insertion	UNP A9CI81
A	505	GLY	-	insertion	UNP A9CI81
A	506	LEU	-	insertion	UNP A9CI81
A	507	GLU	-	insertion	UNP A9CI81
A	508	TYR	-	insertion	UNP A9CI81
A	509	LYS	-	insertion	UNP A9CI81
A	510	HIS	-	expression tag	UNP A9CI81
A	511	HIS	-	expression tag	UNP A9CI81
A	512	HIS	-	expression tag	UNP A9CI81
A	513	HIS	-	expression tag	UNP A9CI81
A	514	HIS	-	expression tag	UNP A9CI81
A	515	HIS	-	expression tag	UNP A9CI81
B	69	ARG	LYS	engineered mutation	UNP A9CI81
B	83	LYS	ARG	engineered mutation	UNP A9CI81
B	120	ASP	GLY	engineered mutation	UNP A9CI81
B	123	THR	ALA	engineered mutation	UNP A9CI81
B	163	LEU	MET	engineered mutation	UNP A9CI81
B	168	GLU	GLN	engineered mutation	UNP A9CI81
B	220	PRO	ARG	engineered mutation	UNP A9CI81
B	243	ASN	SER	engineered mutation	UNP A9CI81
B	244	PHE	VAL	engineered mutation	UNP A9CI81
B	269	ASP	GLY	engineered mutation	UNP A9CI81
B	276	VAL	ALA	engineered mutation	UNP A9CI81
B	280	CYS	TYR	engineered mutation	UNP A9CI81
B	294	ALA	GLU	engineered mutation	UNP A9CI81
B	303	PHE	HIS	engineered mutation	UNP A9CI81
B	333	ARG	HIS	engineered mutation	UNP A9CI81
B	336	LEU	ILE	engineered mutation	UNP A9CI81
B	349	ARG	ASP	engineered mutation	UNP A9CI81
B	351	ILE	MET	engineered mutation	UNP A9CI81
B	386	VAL	ALA	engineered mutation	UNP A9CI81
B	409	ASP	GLY	engineered mutation	UNP A9CI81
B	419	ILE	LEU	engineered mutation	UNP A9CI81
B	469	SER	THR	engineered mutation	UNP A9CI81
B	487	THR	ALA	engineered mutation	UNP A9CI81
B	494	GLY	GLU	engineered mutation	UNP A9CI81
B	503	MET	-	insertion	UNP A9CI81
B	504	ALA	-	insertion	UNP A9CI81
B	505	GLY	-	insertion	UNP A9CI81
B	506	LEU	-	insertion	UNP A9CI81
B	507	GLU	-	insertion	UNP A9CI81
B	508	TYR	-	insertion	UNP A9CI81

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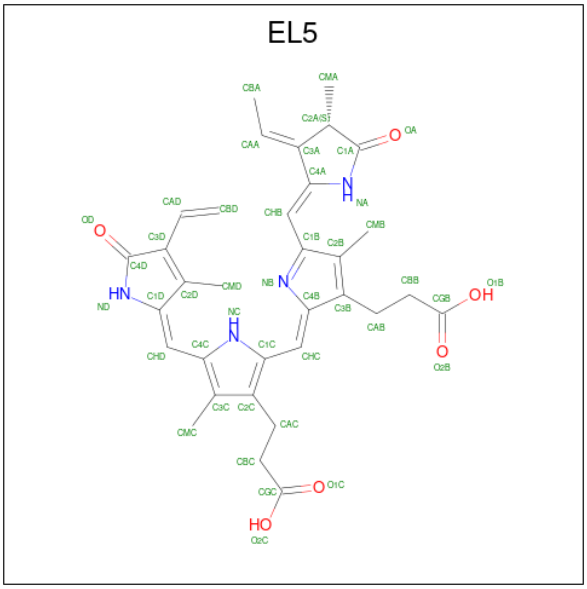
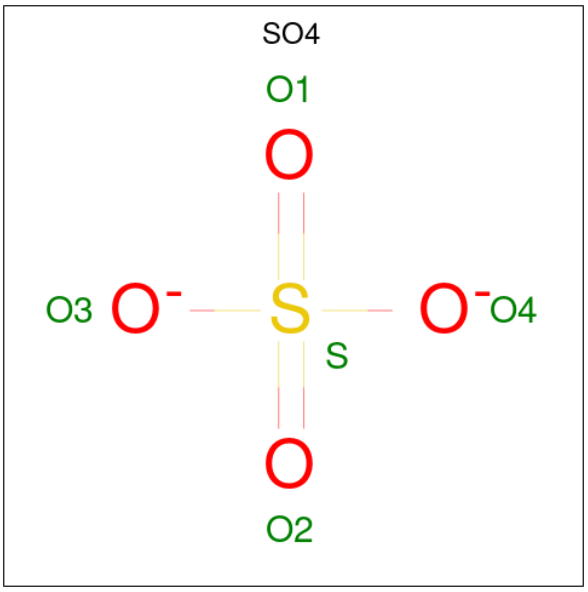
Chain	Residue	Modelled	Actual	Comment	Reference
B	509	LYS	-	insertion	UNP A9CI81
B	510	HIS	-	expression tag	UNP A9CI81
B	511	HIS	-	expression tag	UNP A9CI81
B	512	HIS	-	expression tag	UNP A9CI81
B	513	HIS	-	expression tag	UNP A9CI81
B	514	HIS	-	expression tag	UNP A9CI81
B	515	HIS	-	expression tag	UNP A9CI81

- Molecule 2 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).



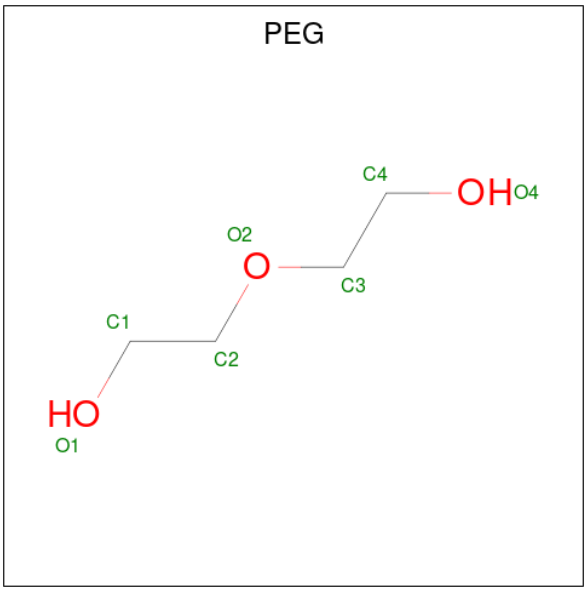
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 43 33 4 6	0	0
2	B	1	Total C N O 43 33 4 6	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

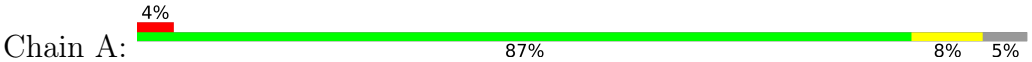
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	179	Total O 179 179	0	0
5	B	157	Total O 157 157	0	0

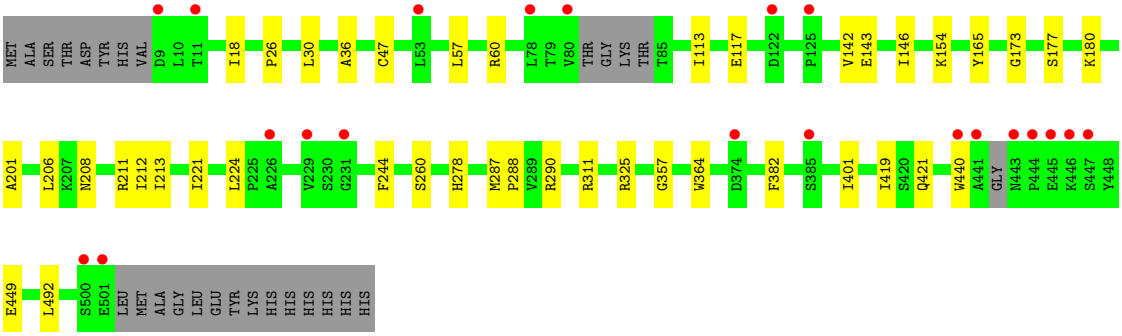
3 Residue-property plots (i)

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: histidine kinase

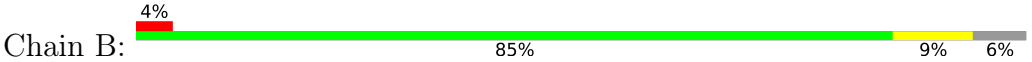
Chain A:

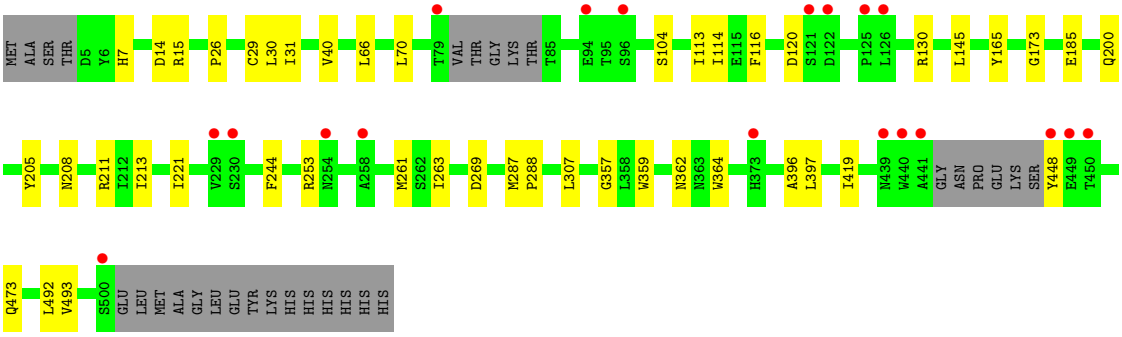




• Molecule 1: histidine kinase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	182.90Å 182.90Å 180.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.77 – 2.80 45.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.77-2.80) 97.8 (45.77-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.276 , 0.320 0.273 , 0.316	Depositor DCC
R_{free} test set	42409 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7866	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EL5, SO4, PEG

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	1.04	0/3788	1.42	0/5161
1	B	1.04	0/3766	1.42	2/5133 (0.0%)
All	All	1.04	0/7554	1.42	2/10294 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	493	VAL	CA-C-N	5.41	125.84	119.94
1	B	493	VAL	C-N-CA	5.41	125.84	119.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3697	0	3536	24	0
1	B	3676	0	3518	29	0
2	A	43	0	0	3	0
2	B	43	0	0	0	0
3	A	20	0	0	0	0
3	B	30	0	0	0	0
4	A	14	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	10	0	0
5	A	179	0	0	1	0
5	B	157	0	0	5	0
All	All	7866	0	7084	53	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 (53) 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:B:213:ILE:HD11	1:B:244:PHE:CD2	2.26	0.71
1:A:357:GLY:HA3	1:A:364:TRP:CH2	2.30	0.66
1:B:357:GLY:HA3	1:B:364:TRP:CH2	2.34	0.63
1:B:30:LEU:CD1	1:B:113:ILE:HG23	2.31	0.59
1:A:278:HIS:CE1	2:A:601:EL5:OD	2.56	0.59
1:B:208:ASN:O	1:B:211:ARG:NH1	2.38	0.56
1:A:165:TYR:CE1	1:A:173:GLY:HA3	2.41	0.56
1:A:26:PRO:HA	1:A:221:ILE:HD12	1.90	0.54
1:B:253:ARG:HD2	5:B:784:HOH:O	2.06	0.53
1:B:66:LEU:HB3	1:B:70:LEU:HD23	1.91	0.53
1:B:165:TYR:CE1	1:B:173:GLY:HA3	2.44	0.52
1:A:117:GLU:OE2	1:A:290:ARG:NH2	2.42	0.52
1:B:29:CYS:SG	1:B:116:PHE:HB2	2.50	0.52
1:A:212:ILE:HG13	1:A:290:ARG:HD3	1.92	0.51
1:A:36:ALA:HB2	1:B:15:ARG:NH1	2.26	0.51
1:B:30:LEU:HD13	1:B:113:ILE:HG23	1.93	0.50
1:B:145:LEU:HD22	1:B:307:LEU:HD12	1.94	0.50
1:A:30:LEU:CD1	1:A:113:ILE:HG23	2.41	0.50
1:A:421:GLN:NE2	5:A:705:HOH:O	2.42	0.49
2:A:601:EL5:CMC	2:A:601:EL5:ND	2.76	0.48
1:A:143:GLU:OE2	1:A:311:ARG:NH2	2.46	0.48
1:A:278:HIS:NE2	2:A:601:EL5:OD	2.47	0.47
1:B:26:PRO:HA	1:B:221:ILE:HD12	1.95	0.47
1:B:396:ALA:HB2	1:B:473:GLN:HG2	1.97	0.47
1:B:261:MET:HE3	1:B:263:ILE:HG13	1.96	0.46
1:A:165:TYR:CZ	1:A:173:GLY:HA3	2.50	0.46
1:A:419:ILE:HG22	1:A:492:LEU:HD13	1.98	0.46
1:A:382:PHE:CD2	1:A:401:ILE:HD11	2.51	0.46
1:B:185[B]:GLU:CD	1:B:448:TYR:OH	2.59	0.45
1:B:359:TRP:CZ2	1:B:362:ASN:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD11	1:A:244:PHE:CD2	2.51	0.45
1:B:419:ILE:HG22	1:B:492:LEU:HD13	1.99	0.45
4:A:607:PEG:H31	1:B:15:ARG:HH12	1.82	0.45
1:B:185[B]:GLU:CD	1:B:448:TYR:HH	2.24	0.45
1:A:57:LEU:HA	1:A:60:ARG:HD3	1.99	0.44
1:A:154:LYS:HE3	1:A:180:LYS:C	2.42	0.44
1:B:31:ILE:HG23	1:B:40:VAL:HG13	1.99	0.44
1:A:208:ASN:O	1:A:211:ARG:NH1	2.50	0.44
1:A:382:PHE:CG	1:A:401:ILE:HD11	2.54	0.43
1:A:18:ILE:HD11	1:A:201:ALA:HA	2.00	0.43
1:B:120:ASP:HA	5:B:761:HOH:O	2.18	0.43
1:B:7:HIS:HB3	5:B:779:HOH:O	2.19	0.43
1:B:31:ILE:O	1:B:114[B]:ILE:HG22	2.19	0.43
1:A:30:LEU:HD11	1:A:113:ILE:HG23	2.01	0.42
1:B:269:ASP:N	5:B:702:HOH:O	2.43	0.42
1:B:130:ARG:NH1	5:B:708:HOH:O	2.54	0.41
1:A:142:VAL:HG12	1:A:146:ILE:HD12	2.02	0.41
1:A:146:ILE:CG2	1:A:177:SER:HB2	2.51	0.41
1:A:287:MET:HB3	1:A:288:PRO:HD3	2.03	0.41
1:B:14:ASP:C	1:B:200:GLN:HE22	2.29	0.41
1:B:205:TYR:CE1	1:B:211:ARG:CD	3.04	0.41
1:B:30:LEU:HD11	1:B:113:ILE:HG23	2.02	0.41
1:B:287:MET:N	1:B:288:PRO:CD	2.84	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	484/515 (94%)	471 (97%)	13 (3%)	0	100	100
1	B	481/515 (93%)	458 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	965/1030 (94%)	929 (96%)	36 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	374/432 (87%)	367 (98%)	7 (2%)	52 82
1	B	374/432 (87%)	372 (100%)	2 (0%)	86 95
All	All	748/864 (87%)	739 (99%)	9 (1%)	67 89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	CYS
1	A	206	LEU
1	A	224	LEU
1	A	260	SER
1	A	325	ARG
1	A	440	TRP
1	A	449	GLU
1	B	104	SER
1	B	397	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	443	ASN
1	B	58	ASN
1	B	248	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

15 ligands 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	$\#\|Z\| > 2$
4	PEG	A	606	-	6,6,6	0.17	0	5,5,5	0.10	0
2	EL5	A	601	1	42,46,46	2.94	12 (28%)	47,67,67	1.26	4 (8%)
3	SO4	A	603	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	A	602	-	4,4,4	0.37	0	6,6,6	0.06	0
3	SO4	A	604	-	4,4,4	0.38	0	6,6,6	0.05	0
3	SO4	B	603	-	4,4,4	0.39	0	6,6,6	0.05	0
2	EL5	B	601	1	42,46,46	2.93	12 (28%)	47,67,67	1.36	5 (10%)
3	SO4	B	607	-	4,4,4	0.39	0	6,6,6	0.05	0
4	PEG	B	608	-	6,6,6	0.17	0	5,5,5	0.11	0
4	PEG	A	607	-	6,6,6	0.16	0	5,5,5	0.19	0
3	SO4	B	606	-	4,4,4	0.38	0	6,6,6	0.05	0
3	SO4	B	605	-	4,4,4	0.40	0	6,6,6	0.05	0
3	SO4	A	605	-	4,4,4	0.38	0	6,6,6	0.05	0
3	SO4	B	604	-	4,4,4	0.41	0	6,6,6	0.05	0
3	SO4	B	602	-	4,4,4	0.38	0	6,6,6	0.04	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
2	EL5	A	601	1	1/1/14/21	8/26/74/74	0/4/4/4
2	EL5	B	601	1	1/1/14/21	9/26/74/74	0/4/4/4
4	PEG	B	608	-	-	2/4/4/4	-
4	PEG	A	607	-	-	3/4/4/4	-
4	PEG	A	606	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	EL5	C2A-C1A	-11.20	1.38	1.51
2	B	601	EL5	C2A-C1A	-11.04	1.38	1.51
2	B	601	EL5	C2A-C3A	-9.83	1.38	1.51
2	A	601	EL5	C2A-C3A	-9.81	1.38	1.51
2	A	601	EL5	CHC-C4B	5.57	1.39	1.35
2	B	601	EL5	CHC-C4B	4.97	1.39	1.35
2	B	601	EL5	CBA-CAA	-4.46	1.32	1.49
2	A	601	EL5	CBA-CAA	-4.31	1.33	1.49
2	A	601	EL5	C4B-C3B	-3.91	1.39	1.45
2	B	601	EL5	C4B-C3B	-3.90	1.39	1.45
2	B	601	EL5	CAA-C3A	3.58	1.43	1.33
2	B	601	EL5	C1D-C2D	-3.23	1.39	1.45
2	B	601	EL5	C1B-C2B	-3.21	1.38	1.45
2	B	601	EL5	C4A-C3A	-3.15	1.39	1.45
2	A	601	EL5	C1D-C2D	-3.04	1.39	1.45
2	A	601	EL5	C1B-C2B	-3.02	1.39	1.45
2	A	601	EL5	C3D-C4D	-3.01	1.38	1.47
2	A	601	EL5	CAA-C3A	3.01	1.41	1.33
2	A	601	EL5	C4A-C3A	-3.00	1.39	1.45
2	B	601	EL5	C3D-C4D	-2.81	1.39	1.47
2	B	601	EL5	CHD-C1D	2.52	1.39	1.34
2	A	601	EL5	CHD-C1D	2.52	1.39	1.34
2	B	601	EL5	CAD-C3D	-2.45	1.40	1.47
2	A	601	EL5	CAD-C3D	-2.05	1.41	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	EL5	C2A-C3A-C4A	-4.93	102.41	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	EL5	C2A-C3A-C4A	-4.27	103.13	107.81
2	B	601	EL5	CHC-C4B-NB	-3.35	124.17	128.83
2	B	601	EL5	CBB-CAB-C3B	3.20	121.52	112.63
2	A	601	EL5	C1C-CHC-C4B	3.07	132.47	128.81
2	A	601	EL5	OA-C1A-C2A	2.87	129.05	126.28
2	B	601	EL5	OA-C1A-C2A	2.49	128.68	126.28
2	B	601	EL5	CHB-C4A-C3A	-2.30	122.96	127.12
2	A	601	EL5	CHC-C4B-NB	-2.01	126.04	128.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	EL5	C2A
2	B	601	EL5	C2A

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	EL5	C2A-C3A-CAA-CBA
2	A	601	EL5	C4A-C3A-CAA-CBA
2	B	601	EL5	C1C-C2C-CAC-CBC
2	B	601	EL5	C3C-C2C-CAC-CBC
2	B	601	EL5	C2A-C3A-CAA-CBA
2	B	601	EL5	C2C-CAC-CBC-CGC
4	A	606	PEG	O1-C1-C2-O2
4	A	607	PEG	O1-C1-C2-O2
4	A	607	PEG	O2-C3-C4-O4
2	B	601	EL5	NB-C1B-CHB-C4A
4	B	608	PEG	C4-C3-O2-C2
2	A	601	EL5	C2C-CAC-CBC-CGC
4	A	606	PEG	O2-C3-C4-O4
4	A	607	PEG	C1-C2-O2-C3
4	B	608	PEG	O1-C1-C2-O2
2	A	601	EL5	CAB-CBB-CGB-O1B
2	A	601	EL5	CAC-CBC-CGC-O1C
2	A	601	EL5	CAB-CBB-CGB-O2B
2	B	601	EL5	CAC-CBC-CGC-O1C
2	A	601	EL5	CAC-CBC-CGC-O2C
2	A	601	EL5	C3B-CAB-CBB-CGB
2	B	601	EL5	CAB-CBB-CGB-O1B
2	B	601	EL5	CAC-CBC-CGC-O2C
2	B	601	EL5	CAB-CBB-CGB-O2B

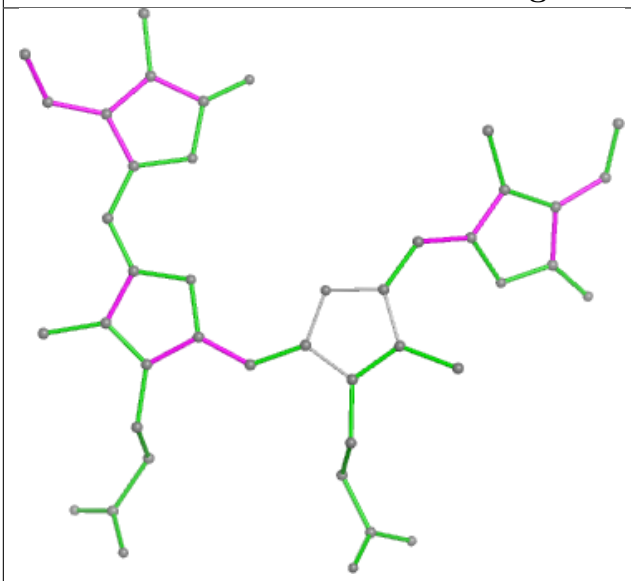
There are no ring outliers.

2 monomers are involved in 4 short contacts:

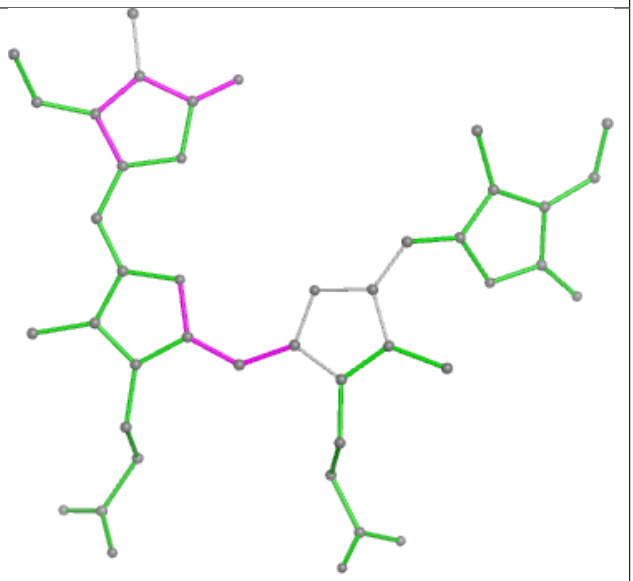
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EL5	3	0
4	A	607	PEG	1	0

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 then 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.

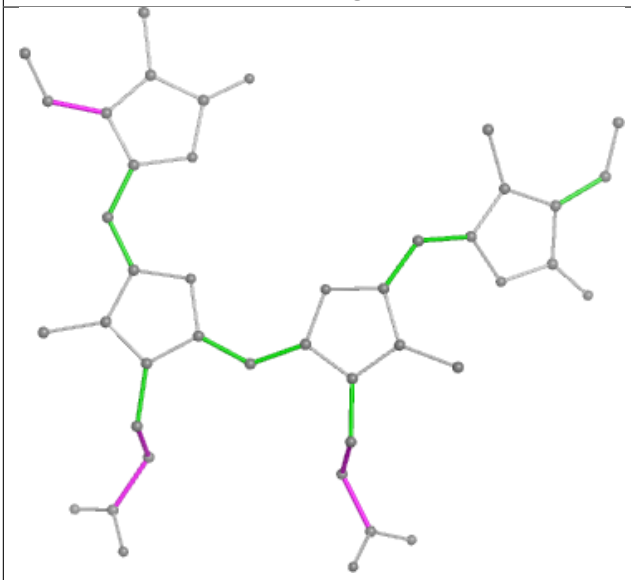
Ligand EL5 A 601



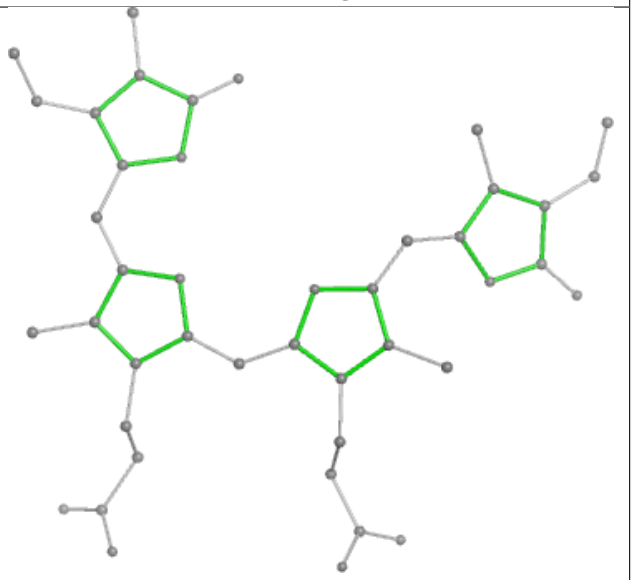
Bond lengths



Bond angles

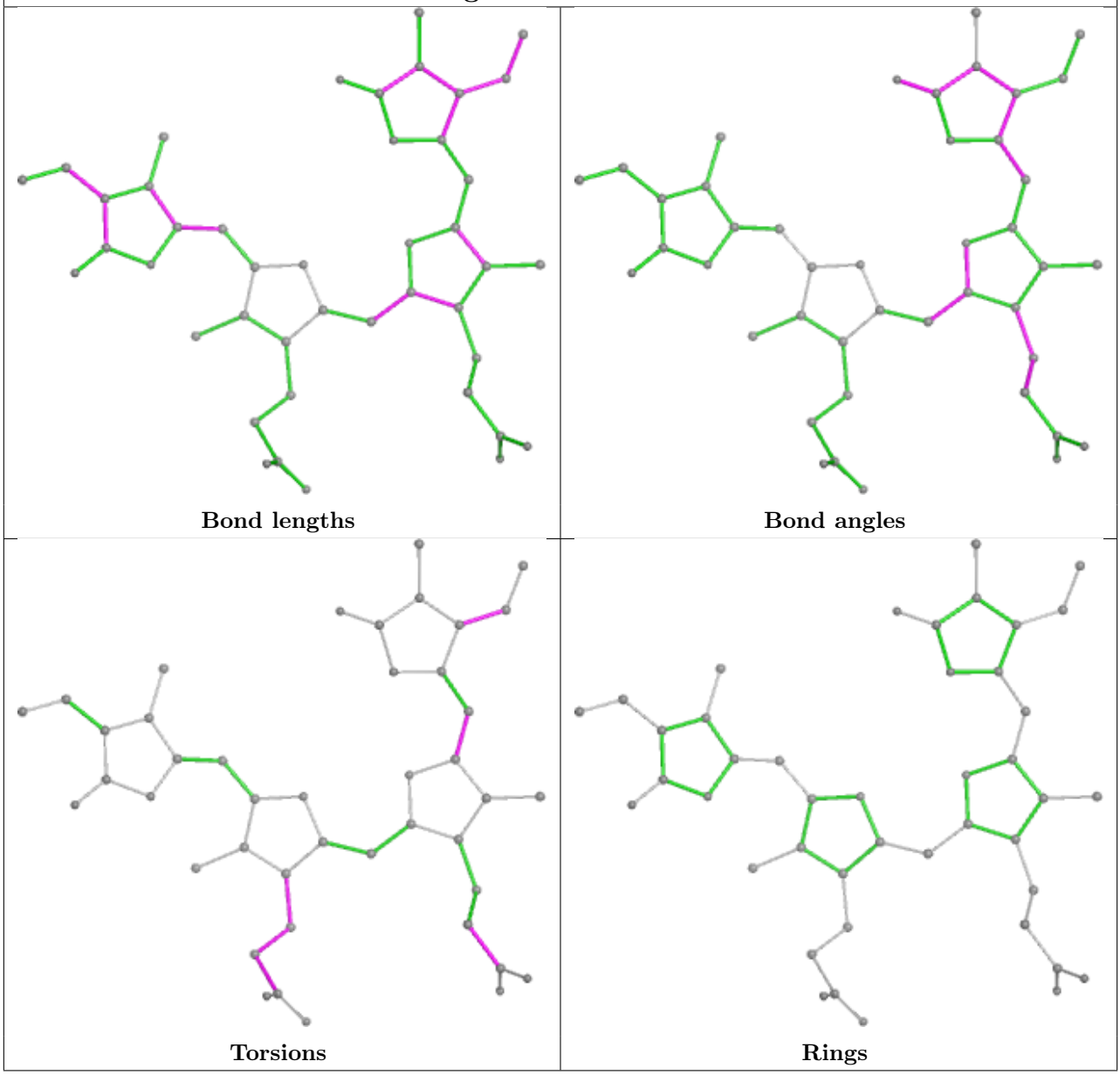


Torsions



Rings

Ligand EL5 B 601



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, 95^{th} 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	488/515 (94%)	0.19	21 (4%)	40	32	26, 56, 101, 144	3 (0%)
1	B	485/515 (94%)	0.22	19 (3%)	44	36	31, 60, 95, 131	2 (0%)
All	All	973/1030 (94%)	0.21	40 (4%)	42	34	26, 58, 99, 144	5 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	GLU	5.1
1	A	125	PRO	5.0
1	A	441	ALA	4.7
1	A	444	PRO	4.7
1	A	122	ASP	4.3
1	A	447	SER	3.9
1	A	440	TRP	3.7
1	B	126	LEU	3.7
1	A	11	THR	3.4
1	A	500	SER	3.3
1	B	258	ALA	3.3
1	A	385	SER	3.3
1	B	440	TRP	3.2
1	A	446	LYS	3.1
1	B	122	ASP	3.1
1	B	441	ALA	3.1
1	B	439	ASN	3.0
1	B	96	SER	2.8
1	B	450	THR	2.8
1	B	94	GLU	2.8
1	A	229	VAL	2.7
1	A	53	LEU	2.7
1	B	121	SER	2.7
1	A	80	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	374	ASP	2.6
1	B	254	ASN	2.5
1	B	229	VAL	2.5
1	A	443	ASN	2.5
1	B	448	TYR	2.4
1	A	501	GLU	2.3
1	A	445	GLU	2.3
1	A	9	ASP	2.3
1	A	231	GLY	2.2
1	B	125	PRO	2.2
1	B	500	SER	2.2
1	B	230	SER	2.1
1	B	373	HIS	2.1
1	A	78	LEU	2.1
1	B	79	THR	2.1
1	A	226	ALA	2.1

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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	607	5/5	0.59	0.14	157,159,160,163	0
4	PEG	A	606	7/7	0.67	0.28	103,107,110,111	0
4	PEG	A	607	7/7	0.68	0.14	96,100,102,105	0
4	PEG	B	608	7/7	0.75	0.15	92,95,97,98	0
3	SO4	A	605	5/5	0.77	0.12	124,127,128,130	0
3	SO4	B	605	5/5	0.78	0.14	146,148,152,155	0
3	SO4	B	603	5/5	0.79	0.10	117,117,117,118	5

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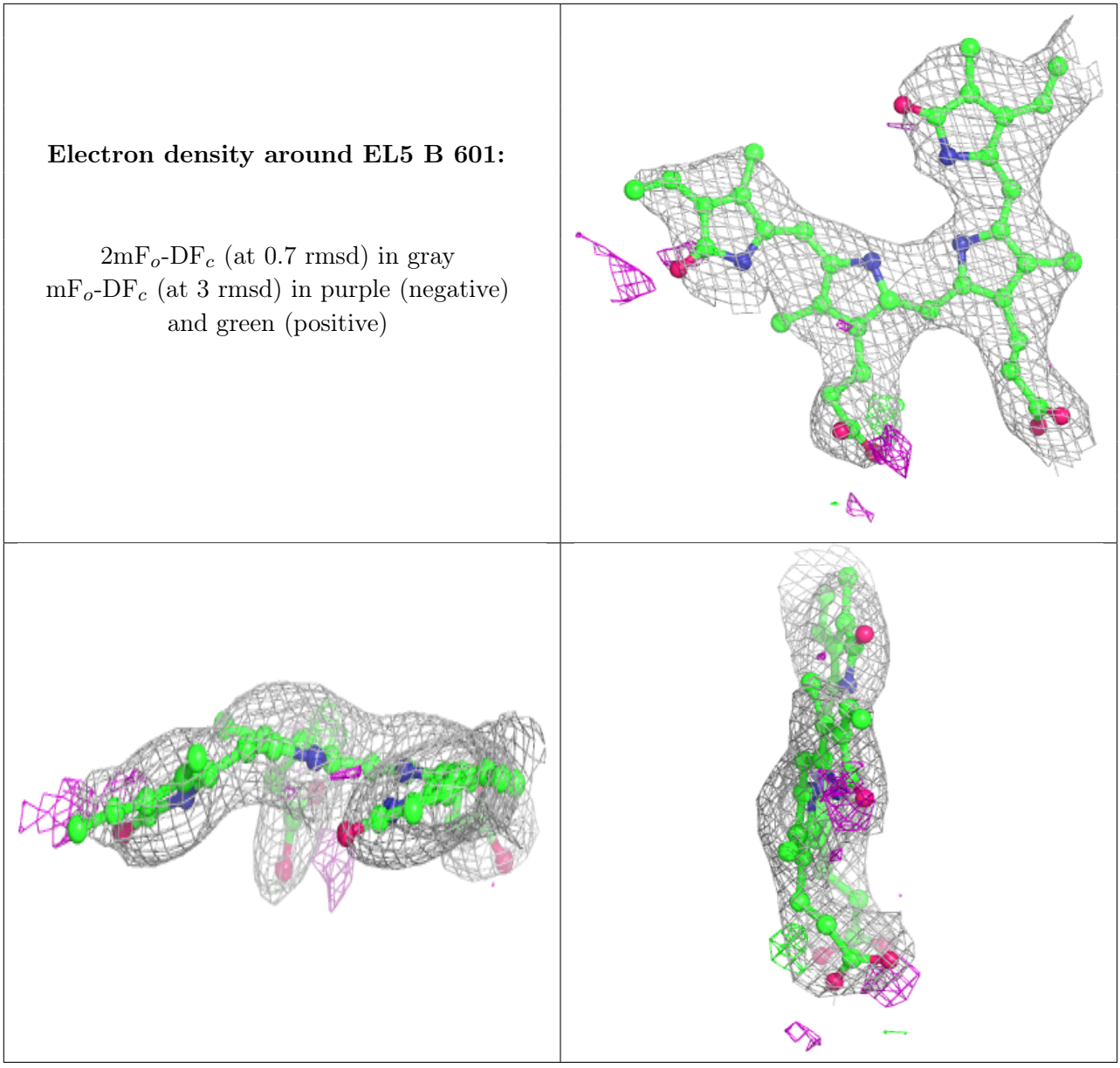
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	602	5/5	0.80	0.13	96,98,102,103	0
3	SO4	B	602	5/5	0.80	0.11	120,121,125,128	0
3	SO4	B	606	5/5	0.82	0.17	150,150,153,153	0
3	SO4	A	603	5/5	0.88	0.14	127,131,135,139	0
2	EL5	B	601	43/43	0.90	0.14	57,60,65,68	0
2	EL5	A	601	43/43	0.90	0.13	49,52,61,65	0
3	SO4	B	604	5/5	0.90	0.10	138,140,144,146	0
3	SO4	A	604	5/5	0.94	0.05	127,127,128,128	5

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.

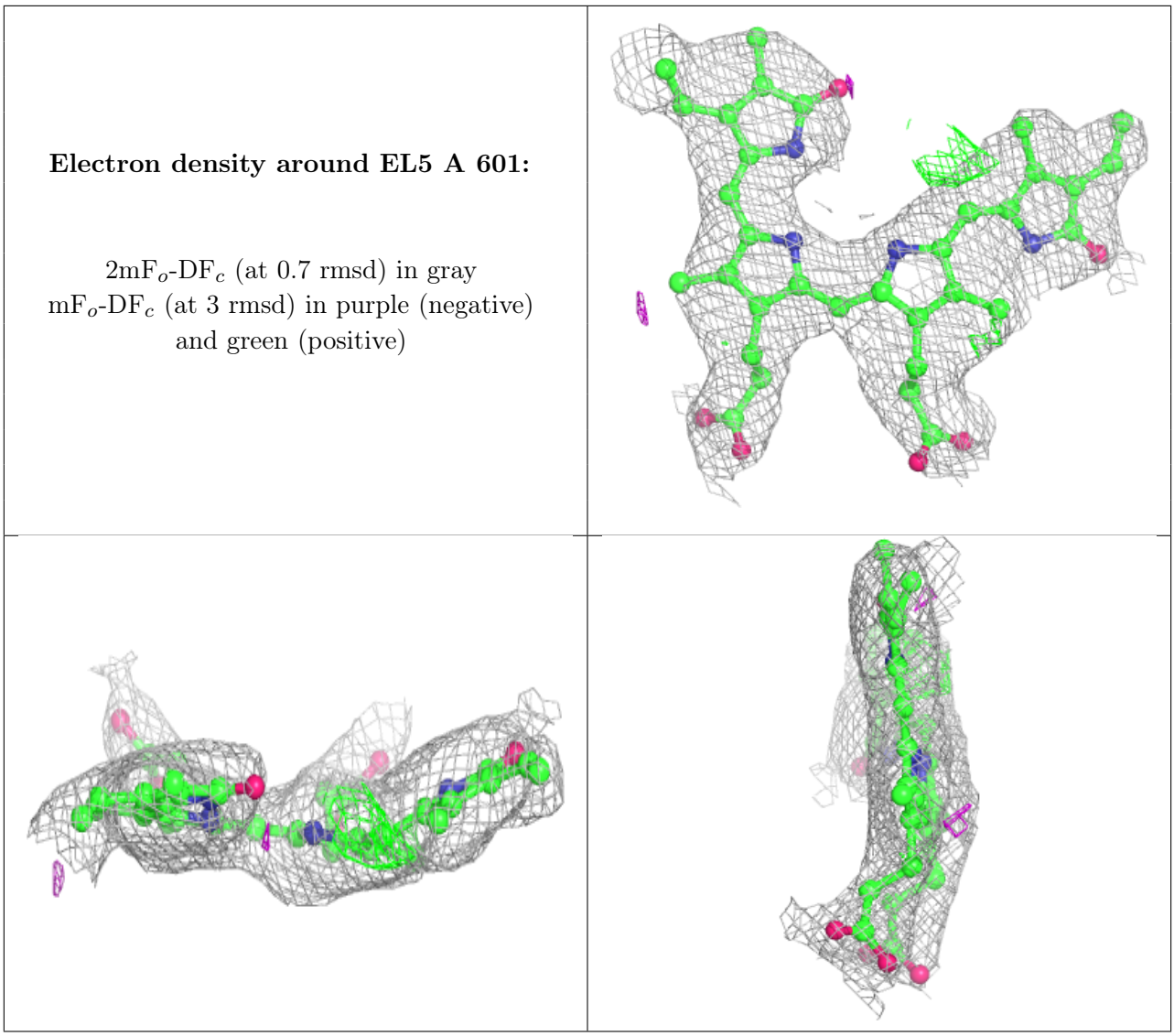
Electron density around EL5 B 601:

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



Electron density around EL5 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)



6.5 Other polymers

There are no such residues in this entry.