



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:09 PM UTC

PDB ID : 6PU2 / pdb_00006pu2
Title : Dark, Mutant H275T , 100K, PCM Myxobacterial Phytochrome, P2
Authors : Pandey, S.; Schmidt, M.; Stojkovic, E.A.
Deposited on : 2019-07-16
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

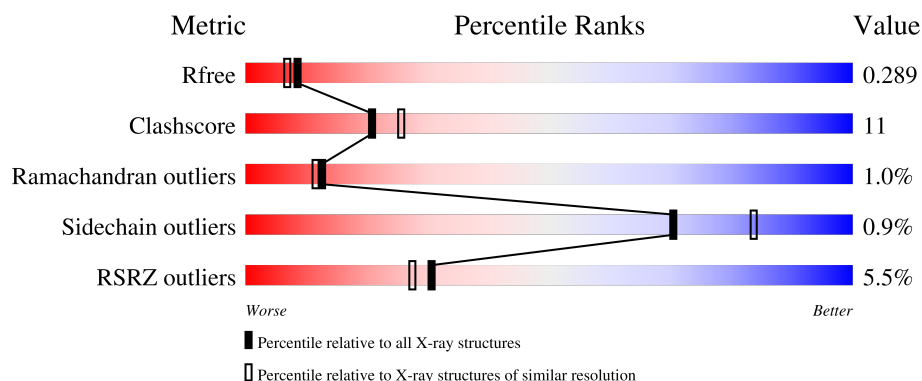
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	481	5% 79% 20%
1	B	481	6% 80% 19%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7692 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.

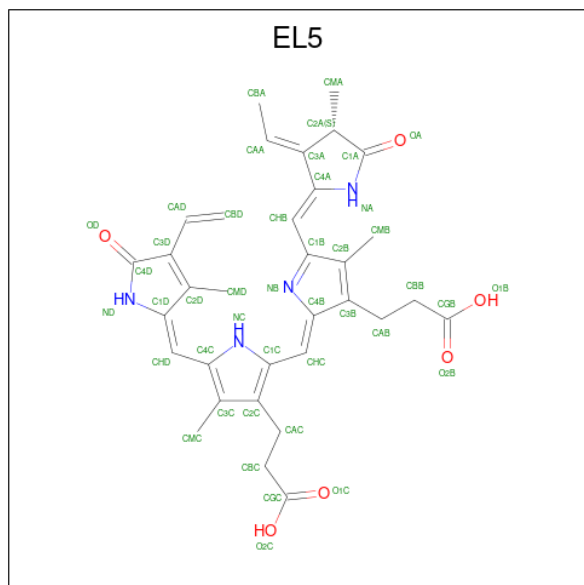
- Molecule 1 is a protein called Photoreceptor-histidine kinase BphP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3651	2312	663	666	10			
1	B	481	Total	C	N	O	S	0	0	0
			3651	2312	663	666	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	THR	HIS	engineered mutation	UNP Q09E27
B	275	THR	HIS	engineered mutation	UNP Q09E27

- 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: C₃₃H₃₆N₄O₆).



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

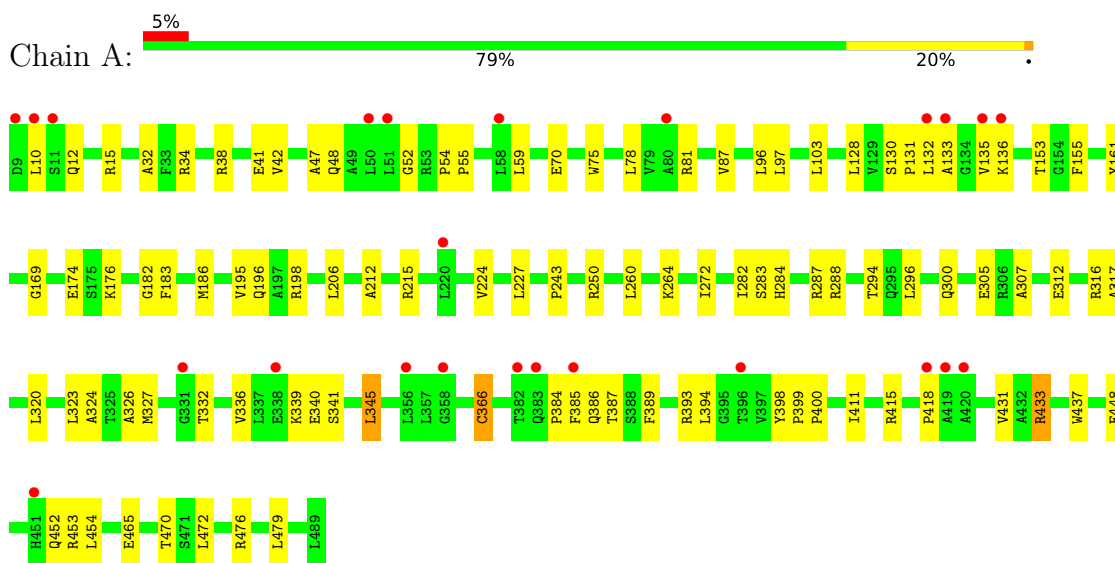
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total 151	O 151	0	0
3	B	153	Total 153	O 153	0	0

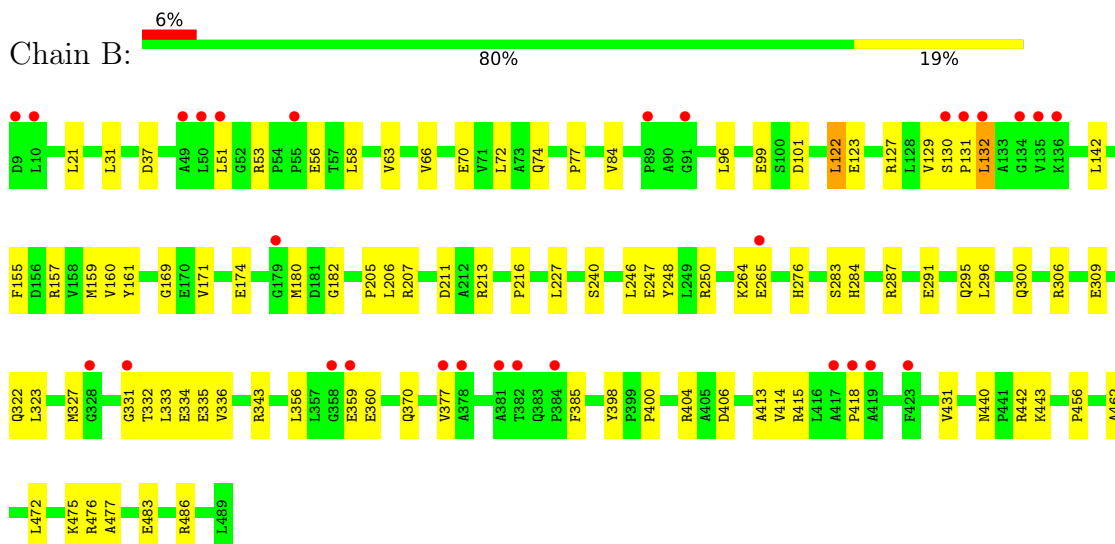
3 Residue-property plots

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: Photoreceptor-histidine kinase BphP



• Molecule 1: Photoreceptor-histidine kinase BphP



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.41Å 81.79Å 83.49Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	42.24 – 2.20 42.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	82.7 (42.24-2.20) 82.6 (42.24-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.290 0.217 , 0.289	Depositor DCC
R_{free} test set	2189 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7692	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/3731	0.61	0/5089
1	B	0.39	0/3731	0.59	0/5089
All	All	0.40	0/7462	0.60	0/10178

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3651	0	3694	82	0
1	B	3651	0	3694	85	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
3	A	151	0	0	24	0
3	B	153	0	0	11	0
All	All	7692	0	7388	164	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 11.

All (164) 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:332:THR:HG21	1:B:335:GLU:CD	1.68	1.18
1:B:440:ASN:HB3	1:B:443:LYS:HE3	1.44	0.98
1:B:74:GLN:HG3	1:B:84:VAL:HG21	1.46	0.97
1:A:320:LEU:N	3:A:601:HOH:O	1.98	0.96
1:B:123:GLU:OE2	1:B:127:ARG:NH2	2.06	0.88
1:B:332:THR:HG22	1:B:335:GLU:HB2	1.62	0.82
1:B:360:GLU:OE1	1:B:370:GLN:NE2	2.14	0.81
1:B:247:GLU:HA	1:B:250:ARG:HD2	1.62	0.80
1:B:332:THR:HG21	1:B:335:GLU:CG	2.14	0.77
1:B:356:LEU:HD11	1:B:377:VAL:HG21	1.66	0.76
1:B:332:THR:CG2	1:B:335:GLU:CD	2.56	0.75
1:B:476:ARG:HD3	1:B:476:ARG:H	1.51	0.75
1:B:99:GLU:OE1	3:B:601:HOH:O	2.04	0.74
1:A:243:PRO:O	3:A:602:HOH:O	2.06	0.72
1:A:324:ALA:HA	1:A:327:MET:HE2	1.71	0.72
1:A:264:LYS:NZ	1:A:305:GLU:OE1	2.21	0.71
1:B:332:THR:CG2	1:B:335:GLU:CG	2.70	0.70
1:A:312:GLU:OE1	3:A:603:HOH:O	2.10	0.69
1:B:127:ARG:NH1	3:B:609:HOH:O	2.23	0.69
1:B:157:ARG:HE	1:B:159:MET:HE2	1.58	0.69
1:A:52:GLY:N	3:A:605:HOH:O	2.24	0.69
1:B:332:THR:HG22	1:B:335:GLU:CB	2.22	0.69
1:A:48:GLN:O	3:A:605:HOH:O	2.11	0.68
1:A:215:ARG:NH2	3:A:611:HOH:O	2.27	0.68
1:A:212:ALA:O	3:A:604:HOH:O	2.11	0.68
1:B:476:ARG:NH1	1:B:477:ALA:H	1.91	0.67
1:B:332:THR:HG21	1:B:335:GLU:OE1	1.93	0.67
1:A:316:ARG:O	3:A:601:HOH:O	2.13	0.66
1:B:53:ARG:NH1	3:B:614:HOH:O	2.28	0.66
1:B:130:SER:O	1:B:132:LEU:N	2.28	0.66
1:A:288:ARG:NH2	1:B:123:GLU:OE1	2.27	0.66
1:A:176:LYS:NZ	3:A:613:HOH:O	2.28	0.66
1:A:431:VAL:HB	1:A:433:ARG:NH1	2.12	0.65
1:A:47:ALA:HB3	1:A:55:PRO:HB3	1.78	0.64
1:B:475:LYS:NZ	3:B:615:HOH:O	2.30	0.64
1:A:96:LEU:HD21	1:A:284:HIS:CE1	2.33	0.64
1:A:32:ALA:HB3	1:A:42:VAL:HB	1.80	0.63
1:B:37:ASP:OD1	3:B:603:HOH:O	2.15	0.63
1:B:96:LEU:HD21	1:B:284:HIS:CE1	2.33	0.62
1:B:21:LEU:O	3:B:604:HOH:O	2.16	0.62
1:B:332:THR:CG2	1:B:335:GLU:HB2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:CD2	1:A:97:LEU:HG	2.31	0.61
1:A:317:ALA:O	3:A:601:HOH:O	2.17	0.60
1:B:247:GLU:HA	1:B:250:ARG:CD	2.31	0.59
1:A:437:TRP:NE1	1:A:465:GLU:OE1	2.31	0.59
1:A:283:SER:O	1:A:287:ARG:HG3	2.02	0.58
1:A:323:LEU:O	1:A:327:MET:HG3	2.03	0.58
1:A:317:ALA:C	3:A:601:HOH:O	2.46	0.58
1:A:366:CYS:SG	3:A:627:HOH:O	2.49	0.58
1:B:211:ASP:OD1	1:B:213:ARG:HG3	2.04	0.57
1:A:282:ILE:O	1:A:287:ARG:NH1	2.38	0.56
1:A:183:PHE:CD1	1:A:186:MET:HE3	2.41	0.56
1:B:322:GLN:OE1	1:B:343:ARG:NE	2.32	0.56
1:B:63:VAL:HG22	1:B:72:LEU:HD21	1.86	0.56
1:A:195:VAL:HG22	1:A:198:ARG:NH2	2.20	0.55
1:A:38:ARG:NH1	3:A:624:HOH:O	2.37	0.55
1:B:476:ARG:HH11	1:B:477:ALA:H	1.52	0.55
1:B:385:PHE:O	1:B:415:ARG:NH1	2.39	0.55
1:A:183:PHE:HD1	1:A:186:MET:HE3	1.71	0.55
1:B:142:LEU:HD22	1:B:160:VAL:HG11	1.89	0.54
1:B:159:MET:SD	3:B:747:HOH:O	2.58	0.54
1:A:12:GLN:HA	1:A:15:ARG:HD3	1.89	0.53
1:B:31:LEU:HD21	1:B:51:LEU:HD11	1.89	0.53
1:B:443:LYS:O	1:B:443:LYS:HD2	2.09	0.53
1:A:250:ARG:HG3	3:A:604:HOH:O	2.09	0.53
1:A:399:PRO:N	1:A:400:PRO:HD2	2.24	0.53
1:A:284:HIS:NE2	1:A:288:ARG:HD2	2.24	0.53
1:B:414:VAL:HB	1:B:486:ARG:HD2	1.91	0.52
1:A:161:TYR:CZ	1:A:169:GLY:HA3	2.45	0.52
1:A:131:PRO:HD3	1:B:295:GLN:NE2	2.24	0.52
1:B:74:GLN:HB2	1:B:77:PRO:HG2	1.91	0.51
1:B:58:LEU:HD13	1:B:66:VAL:HA	1.92	0.51
1:B:283:SER:O	1:B:287:ARG:HG3	2.09	0.51
1:A:398:TYR:CE2	1:A:400:PRO:HG2	2.45	0.51
1:A:431:VAL:HG21	1:A:472:LEU:HG	1.91	0.51
1:A:339:LYS:O	1:A:339:LYS:HD2	2.11	0.50
1:A:195:VAL:HG22	1:A:198:ARG:HH22	1.75	0.50
1:A:132:LEU:HB3	1:A:135:VAL:HG21	1.92	0.50
1:B:161:TYR:CZ	1:B:169:GLY:HA3	2.47	0.50
1:B:475:LYS:HB3	1:B:476:ARG:NH1	2.26	0.50
1:B:264:LYS:O	1:B:265:GLU:HG3	2.12	0.50
1:A:34:ARG:HE	1:A:103:LEU:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HD11	1:B:291:GLU:HB2	1.95	0.49
1:B:483:GLU:OE1	1:B:486:ARG:HD3	2.12	0.49
1:B:157:ARG:NE	1:B:159:MET:HE2	2.27	0.48
1:A:398:TYR:CZ	1:A:400:PRO:HG2	2.48	0.48
1:B:404:ARG:HH21	1:B:406:ASP:CG	2.20	0.48
1:A:250:ARG:NH2	3:A:602:HOH:O	2.46	0.48
1:A:385:PHE:CG	1:A:389:PHE:HB2	2.48	0.48
1:A:174:GLU:OE2	1:A:182:GLY:HA3	2.13	0.48
1:B:129:VAL:HB	1:B:296:LEU:HD21	1.94	0.48
1:A:42:VAL:HG21	1:A:224:VAL:HG12	1.96	0.48
1:B:440:ASN:CB	1:B:443:LYS:HE3	2.31	0.48
1:B:440:ASN:ND2	3:B:605:HOH:O	2.40	0.47
1:B:431:VAL:HG21	1:B:472:LEU:HG	1.96	0.47
1:A:272:ILE:HD12	1:A:294:THR:HG22	1.96	0.47
1:B:332:THR:CG2	1:B:335:GLU:CB	2.90	0.47
1:B:333:LEU:C	1:B:333:LEU:HD13	2.39	0.47
1:B:413:ALA:O	3:B:606:HOH:O	2.20	0.47
1:A:433:ARG:NH2	1:A:470:THR:HG23	2.30	0.47
1:A:307:ALA:HB2	1:B:306:ARG:HD3	1.97	0.47
1:A:433:ARG:HH22	1:A:470:THR:HG23	1.79	0.47
1:B:334:GLU:H	1:B:334:GLU:CD	2.23	0.47
1:B:332:THR:CG2	1:B:335:GLU:HG3	2.45	0.46
1:B:96:LEU:HD21	1:B:284:HIS:ND1	2.30	0.46
1:B:323:LEU:O	1:B:327:MET:HG3	2.15	0.46
1:B:70:GLU:OE1	1:B:70:GLU:N	2.38	0.46
1:B:174:GLU:OE2	1:B:182:GLY:HA3	2.16	0.46
1:B:332:THR:HG22	1:B:335:GLU:H	1.80	0.46
1:B:462:ALA:HB1	3:B:612:HOH:O	2.14	0.46
1:A:452:GLN:NE2	3:A:637:HOH:O	2.48	0.46
1:A:135:VAL:O	1:A:136:LYS:HD3	2.16	0.46
1:A:387:THR:O	3:A:606:HOH:O	2.21	0.45
1:A:341:SER:O	1:A:345:LEU:HD22	2.17	0.45
1:B:440:ASN:OD1	1:B:442:ARG:N	2.47	0.45
1:A:415:ARG:N	3:A:606:HOH:O	2.49	0.45
1:A:183:PHE:HA	1:A:186:MET:HE3	1.98	0.44
1:B:309:GLU:HA	1:B:476:ARG:NH2	2.32	0.44
1:A:385:PHE:HE1	3:A:606:HOH:O	2.00	0.44
1:B:398:TYR:CE2	1:B:400:PRO:HB2	2.53	0.44
1:A:224:VAL:HG21	1:A:227:LEU:HD12	1.98	0.44
1:B:248:TYR:N	1:B:456:PRO:HG3	2.33	0.44
1:A:339:LYS:HE3	1:A:340:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:NH2	3:A:612:HOH:O	2.28	0.43
1:A:128:LEU:HB3	1:A:296:LEU:HD23	2.01	0.43
1:A:133:ALA:HB3	1:A:300:GLN:HE22	1.83	0.43
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.90	0.43
1:A:48:GLN:CG	1:A:54:PRO:HA	2.49	0.43
1:B:129:VAL:HG23	1:B:296:LEU:HD11	2.00	0.43
1:B:130:SER:HA	3:B:675:HOH:O	2.18	0.43
1:B:56:GLU:H	1:B:56:GLU:CD	2.26	0.43
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.89	0.43
1:B:155:PHE:CD2	1:B:276:HIS:HB2	2.54	0.42
1:B:101:ASP:HB3	1:B:227:LEU:HD11	2.02	0.42
1:B:246:LEU:O	1:B:250:ARG:HD2	2.20	0.42
1:A:206:LEU:HD21	1:A:260:LEU:HD23	2.00	0.42
1:A:48:GLN:HG3	1:A:55:PRO:HD3	2.00	0.42
1:A:136:LYS:HD3	1:A:136:LYS:HA	1.78	0.42
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.85	0.42
1:B:205:PRO:C	1:B:206:LEU:HD12	2.44	0.42
1:A:394:LEU:HD22	1:A:411:ILE:HG23	2.02	0.42
1:B:247:GLU:CA	1:B:250:ARG:HH11	2.33	0.42
1:A:128:LEU:HB3	1:A:296:LEU:CD2	2.50	0.42
1:B:332:THR:O	1:B:336:VAL:HG23	2.19	0.42
1:A:12:GLN:OE1	3:A:608:HOH:O	2.22	0.42
1:A:415:ARG:HG3	3:A:606:HOH:O	2.20	0.42
1:A:326:ALA:C	1:A:336:VAL:HG11	2.45	0.41
1:A:196:GLN:OE1	1:A:196:GLN:N	2.53	0.41
1:A:448:GLU:HG3	1:A:453:ARG:HB2	2.02	0.41
1:A:153:THR:HB	1:A:155:PHE:HD2	1.86	0.41
1:A:70:GLU:HG2	1:A:87:VAL:O	2.21	0.41
1:A:385:PHE:O	1:A:387:THR:N	2.54	0.41
1:A:81:ARG:NH1	3:A:641:HOH:O	2.53	0.41
1:B:180:MET:HE3	1:B:180:MET:HB3	1.77	0.41
1:B:216:PRO:HB3	1:B:240:SER:OG	2.21	0.41
1:B:309:GLU:HA	1:B:476:ARG:HH21	1.85	0.41
1:B:356:LEU:CD1	1:B:377:VAL:HG21	2.44	0.41
1:A:332:THR:O	1:A:336:VAL:HG23	2.21	0.41
1:A:38:ARG:NH2	1:A:75:TRP:HE1	2.19	0.40
1:A:41:GLU:OE1	3:A:607:HOH:O	2.21	0.40
1:A:130:SER:OG	1:A:133:ALA:HB2	2.22	0.40
1:B:206:LEU:HD23	1:B:287:ARG:HB3	2.02	0.40
1:A:479:LEU:H	1:A:479:LEU:HG	1.68	0.40
1:B:159:MET:HB3	1:B:171:VAL:HG13	2.03	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	479/481 (100%)	454 (95%)	20 (4%)	5 (1%)	12	11
1	B	479/481 (100%)	447 (93%)	27 (6%)	5 (1%)	12	11
All	All	958/962 (100%)	901 (94%)	47 (5%)	10 (1%)	12	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	359	GLU
1	A	454	LEU
1	B	132	LEU
1	B	331	GLY
1	A	386	GLN
1	B	131	PRO
1	B	418	PRO
1	A	10	LEU
1	A	418	PRO
1	A	384	PRO

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	374/374 (100%)	370 (99%)	4 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	374/374 (100%)	371 (99%)	3 (1%)	73	85
All	All	748/748 (100%)	741 (99%)	7 (1%)	70	84

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

Mol	Chain	Res	Type
1	A	345	LEU
1	A	366	CYS
1	A	393	ARG
1	A	433	ARG
1	B	122	LEU
1	B	207	ARG
1	B	300	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	48	GLN
1	A	300	GLN
1	B	12	GLN
1	B	74	GLN
1	B	461	GLN

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

2 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
2	EL5	A	501	1	46,46,46	3.59	19 (41%)	58,67,67	1.56	9 (15%)
2	EL5	B	501	1	46,46,46	3.64	20 (43%)	58,67,67	1.56	11 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EL5	A	501	1	-	8/26/74/74	0/4/4/4
2	EL5	B	501	1	-	10/26/74/74	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	EL5	C1A-NA	12.47	1.54	1.37
2	A	501	EL5	C1A-NA	11.87	1.53	1.37
2	B	501	EL5	C4A-NA	8.95	1.53	1.37
2	B	501	EL5	C1D-ND	8.51	1.52	1.37
2	A	501	EL5	C4A-NA	8.32	1.52	1.37
2	A	501	EL5	C1D-ND	8.27	1.51	1.37
2	B	501	EL5	C4D-ND	6.46	1.53	1.38
2	A	501	EL5	C4B-NB	6.35	1.52	1.38
2	A	501	EL5	C4D-ND	5.94	1.51	1.38
2	A	501	EL5	C1B-NB	5.66	1.49	1.36
2	A	501	EL5	CHD-C4C	5.45	1.52	1.40
2	B	501	EL5	C4B-NB	5.42	1.50	1.38
2	B	501	EL5	C1B-NB	5.12	1.48	1.36
2	B	501	EL5	CHC-C1C	5.10	1.51	1.40
2	A	501	EL5	CHC-C1C	5.09	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EL5	CHB-C1B	4.92	1.52	1.40
2	B	501	EL5	CHD-C4C	4.85	1.51	1.40
2	A	501	EL5	C3B-C2B	4.56	1.46	1.36
2	B	501	EL5	CHB-C1B	4.53	1.51	1.40
2	A	501	EL5	C4B-C3B	4.49	1.52	1.45
2	B	501	EL5	C3B-C2B	4.27	1.46	1.36
2	B	501	EL5	C4B-C3B	3.93	1.51	1.45
2	B	501	EL5	CHC-C4B	-3.64	1.31	1.38
2	B	501	EL5	CHD-C1D	-3.29	1.30	1.37
2	B	501	EL5	CHB-C4A	-3.12	1.30	1.37
2	A	501	EL5	CHC-C4B	-2.99	1.33	1.38
2	A	501	EL5	CHB-C4A	-2.94	1.30	1.37
2	A	501	EL5	C3D-C2D	2.77	1.42	1.37
2	A	501	EL5	CHD-C1D	-2.73	1.31	1.37
2	B	501	EL5	C3D-C2D	2.56	1.42	1.37
2	B	501	EL5	OA-C1A	-2.56	1.18	1.23
2	B	501	EL5	C2A-C1A	-2.54	1.49	1.52
2	A	501	EL5	OD-C4D	-2.37	1.19	1.23
2	A	501	EL5	OA-C1A	-2.36	1.18	1.23
2	B	501	EL5	OD-C4D	-2.32	1.19	1.23
2	A	501	EL5	C4A-C3A	2.23	1.49	1.45
2	B	501	EL5	C4A-C3A	2.15	1.48	1.45
2	A	501	EL5	CAD-C3D	2.11	1.53	1.47
2	B	501	EL5	CAD-C3D	2.11	1.53	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	EL5	CHC-C4B-NB	4.00	133.01	124.60
2	B	501	EL5	CAB-CBB-CGB	-3.60	104.13	113.67
2	B	501	EL5	C4B-C3B-C2B	3.59	110.61	106.73
2	A	501	EL5	CAA-C3A-C4A	-3.58	122.03	126.36
2	A	501	EL5	C3B-C4B-NB	-3.47	105.13	110.04
2	A	501	EL5	C4B-C3B-C2B	3.42	110.43	106.73
2	B	501	EL5	CHC-C4B-NB	3.32	131.56	124.60
2	B	501	EL5	C3B-C4B-NB	-3.28	105.41	110.04
2	A	501	EL5	CHB-C1B-NB	3.02	131.48	124.95
2	B	501	EL5	C1D-ND-C4D	-2.95	107.05	110.66
2	A	501	EL5	CHB-C1B-C2B	-2.74	117.85	124.87
2	A	501	EL5	CAB-CBB-CGB	-2.64	106.67	113.67
2	A	501	EL5	CMC-C3C-C4C	2.58	129.36	125.62
2	B	501	EL5	CAA-C3A-C4A	-2.38	123.48	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	EL5	C3D-C2D-C1D	2.36	110.55	107.92
2	B	501	EL5	C3D-C2D-C1D	2.27	110.44	107.92
2	B	501	EL5	CMD-C2D-C1D	-2.20	121.48	124.16
2	B	501	EL5	CAB-C3B-C2B	-2.09	123.95	127.87
2	B	501	EL5	CHB-C4A-NA	2.08	130.49	126.06
2	B	501	EL5	C4C-NC-C1C	-2.03	106.22	109.78

There are no chirality outliers.

All (18) torsion outliers are listed below:

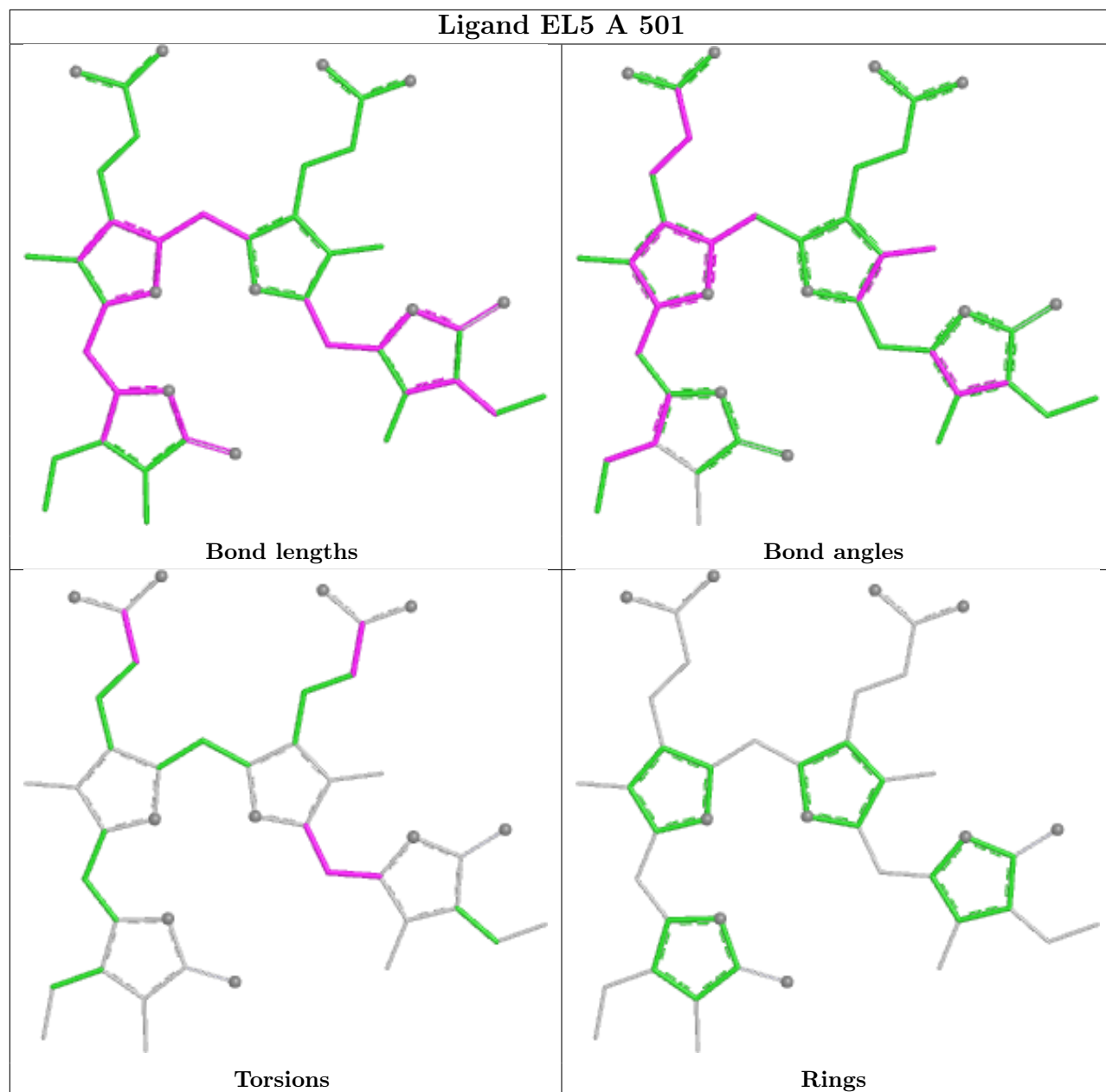
Mol	Chain	Res	Type	Atoms
2	B	501	EL5	C2A-C3A-CAA-CBA
2	B	501	EL5	C4A-C3A-CAA-CBA
2	B	501	EL5	NC-C4C-CHD-C1D
2	B	501	EL5	C3C-C4C-CHD-C1D
2	A	501	EL5	C3C-C4C-CHD-C1D
2	A	501	EL5	NC-C4C-CHD-C1D
2	A	501	EL5	ND-C1D-CHD-C4C
2	B	501	EL5	ND-C1D-CHD-C4C
2	A	501	EL5	C2D-C1D-CHD-C4C
2	B	501	EL5	C2D-C1D-CHD-C4C
2	B	501	EL5	CAC-CBC-CGC-O2C
2	B	501	EL5	CAC-CBC-CGC-O1C
2	B	501	EL5	CAB-CBB-CGB-O2B
2	A	501	EL5	CAB-CBB-CGB-O2B
2	B	501	EL5	CAB-CBB-CGB-O1B
2	A	501	EL5	CAC-CBC-CGC-O2C
2	A	501	EL5	CAB-CBB-CGB-O1B
2	A	501	EL5	CAC-CBC-CGC-O1C

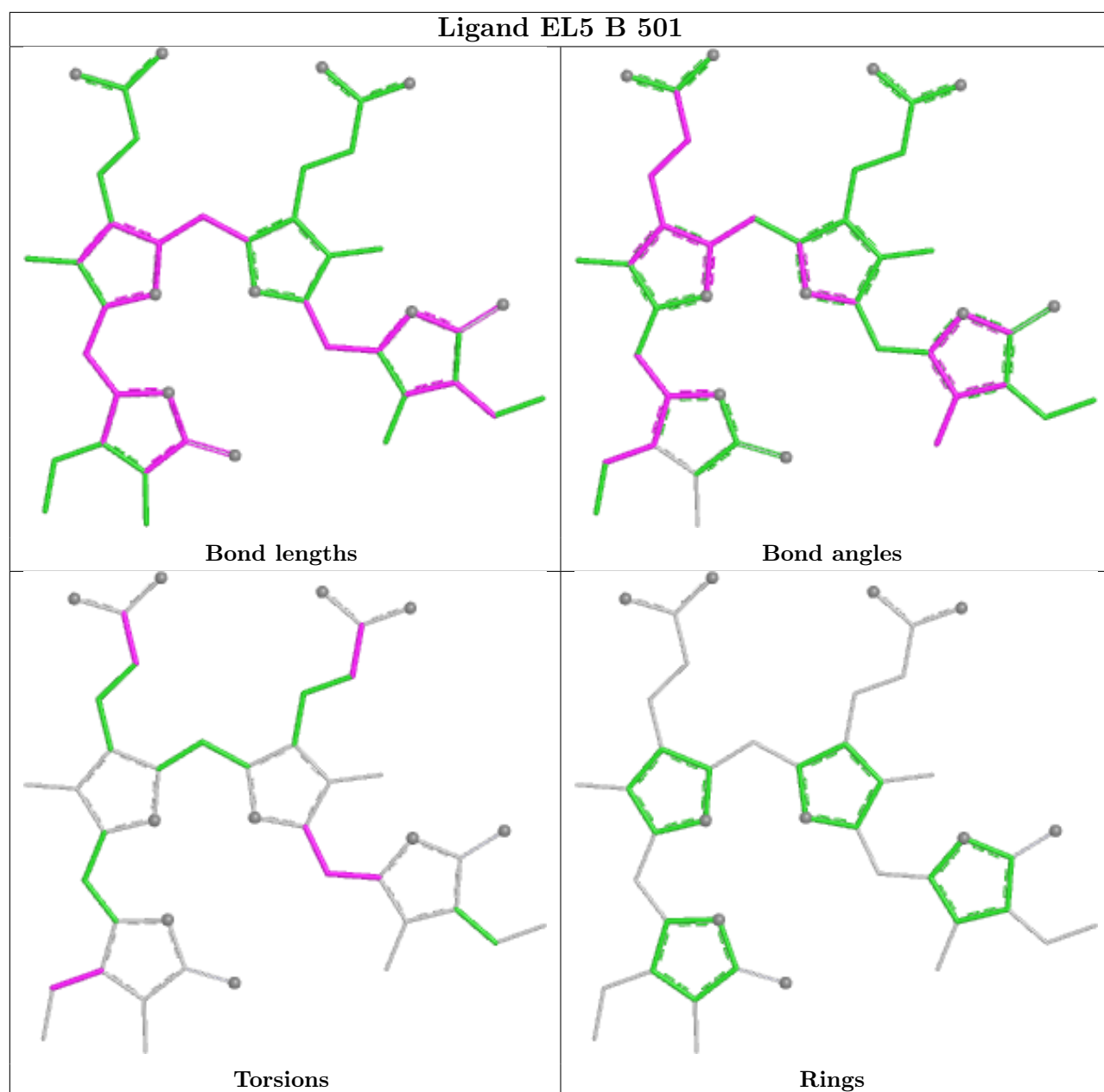
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/481 (100%)	0.41	24 (4%) 34 31	18, 28, 50, 65	0
1	B	481/481 (100%)	0.44	29 (6%) 27 24	18, 28, 53, 82	0
All	All	962/962 (100%)	0.42	53 (5%) 30 27	18, 28, 52, 82	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	VAL	5.4
1	A	133	ALA	4.5
1	B	358	GLY	4.4
1	B	10	LEU	4.3
1	A	10	LEU	4.2
1	B	331	GLY	3.7
1	B	131	PRO	3.4
1	B	9	ASP	3.3
1	A	51	LEU	3.3
1	A	385	PHE	3.0
1	B	134	GLY	3.0
1	A	451	HIS	2.9
1	B	51	LEU	2.8
1	A	358	GLY	2.8
1	A	418	PRO	2.8
1	B	265	GLU	2.8
1	B	417	ALA	2.8
1	A	132	LEU	2.8
1	A	9	ASP	2.7
1	B	328	GLY	2.7
1	B	89	PRO	2.7
1	A	220	LEU	2.7
1	A	382	THR	2.6
1	A	420	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	419	ALA	2.6
1	B	384	PRO	2.6
1	B	179	GLY	2.6
1	B	381	ALA	2.6
1	B	132	LEU	2.5
1	A	331	GLY	2.5
1	A	135	VAL	2.5
1	B	377	VAL	2.5
1	A	419	ALA	2.5
1	A	356	LEU	2.4
1	B	378	ALA	2.4
1	B	136	LYS	2.3
1	A	136	LYS	2.3
1	A	50	LEU	2.2
1	B	55	PRO	2.2
1	B	418	PRO	2.2
1	A	396	THR	2.2
1	B	359	GLU	2.2
1	A	383	GLN	2.2
1	B	91	GLY	2.1
1	A	11	SER	2.1
1	B	382	THR	2.1
1	A	58	LEU	2.1
1	B	50	LEU	2.1
1	B	130	SER	2.1
1	B	49	ALA	2.1
1	A	338	GLU	2.1
1	B	423	PHE	2.0
1	A	80	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

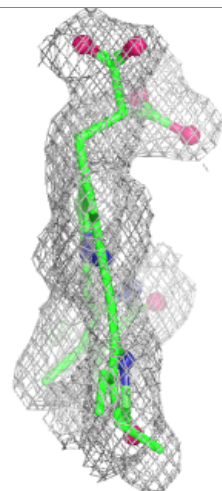
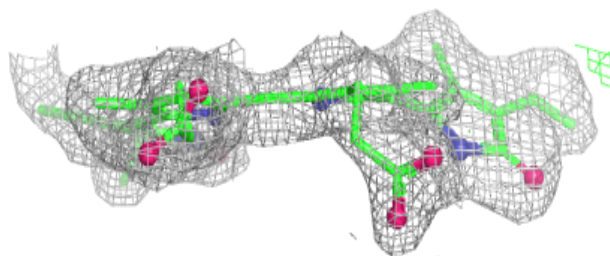
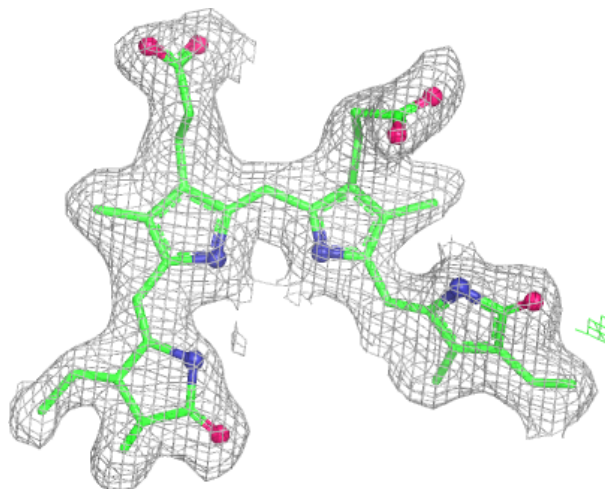
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EL5	A	501	43/43	0.94	0.08	18,21,27,37	0
2	EL5	B	501	43/43	0.94	0.08	16,20,26,37	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.

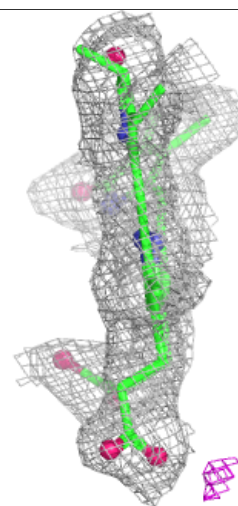
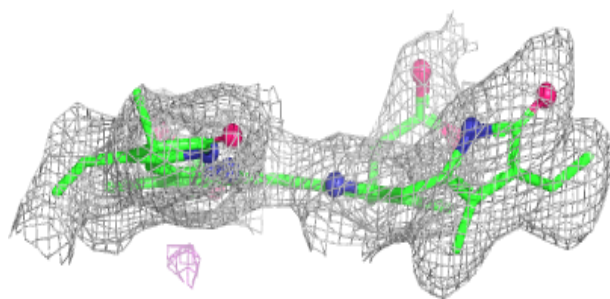
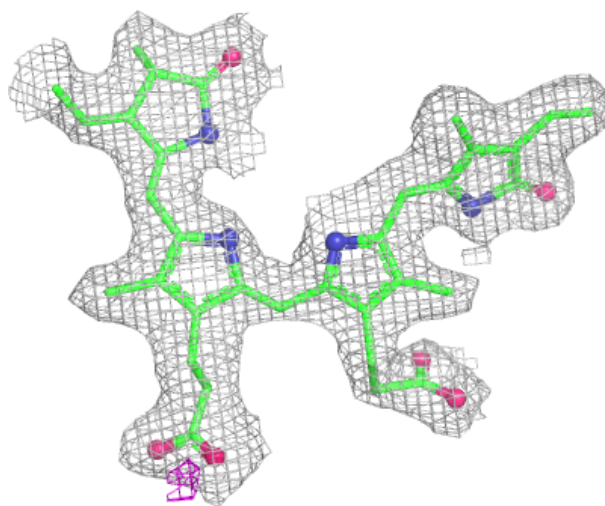
Electron density around EL5 A 501:

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 501:

$2mF_o-DF_c$ (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.