



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2025 – 10:07 AM EDT

PDB ID : 9MD9 / pdb_00009md9
Title : Photoactivation in Bacteriophytochromes; 3ps TR-SFX structure
Authors : Schmidt, M.; Malla, T.
Deposited on : 2024-12-05
Resolution : 2.30 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

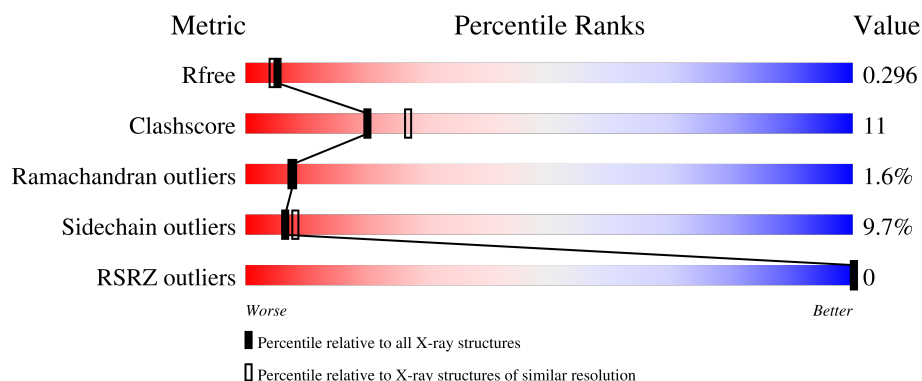
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	482	 69% 27% .
1	B	482	 71% 26% .

2 Entry composition [i](#)

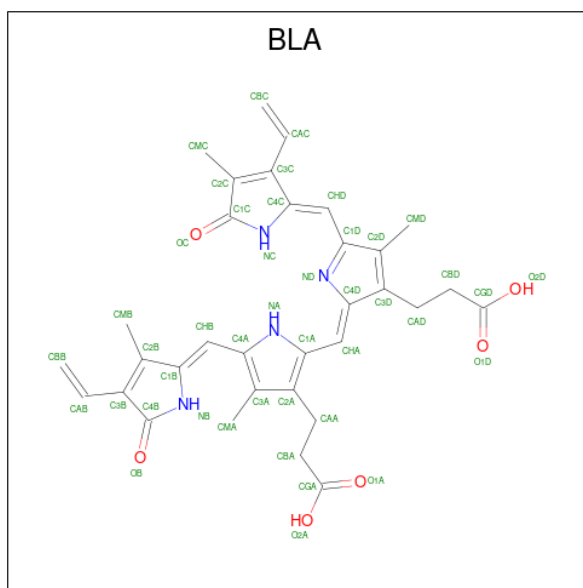
There are 4 unique types of molecules in this entry. The entry contains 7481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

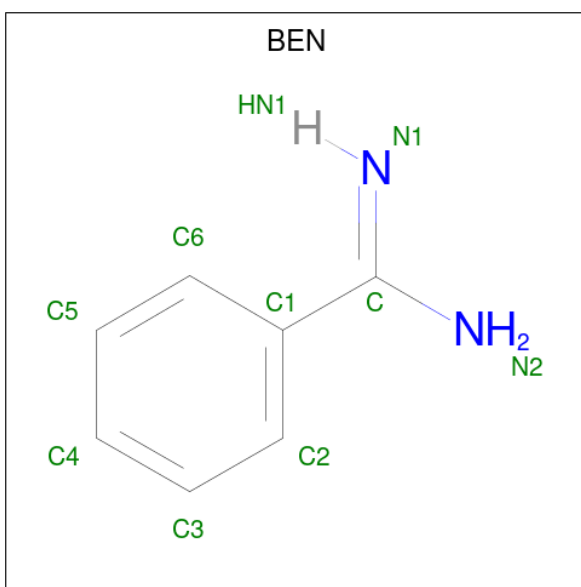
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3671	2325	669	667	10			
1	B	482	Total	C	N	O	S	0	0	0
			3659	2318	666	665	10			

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		

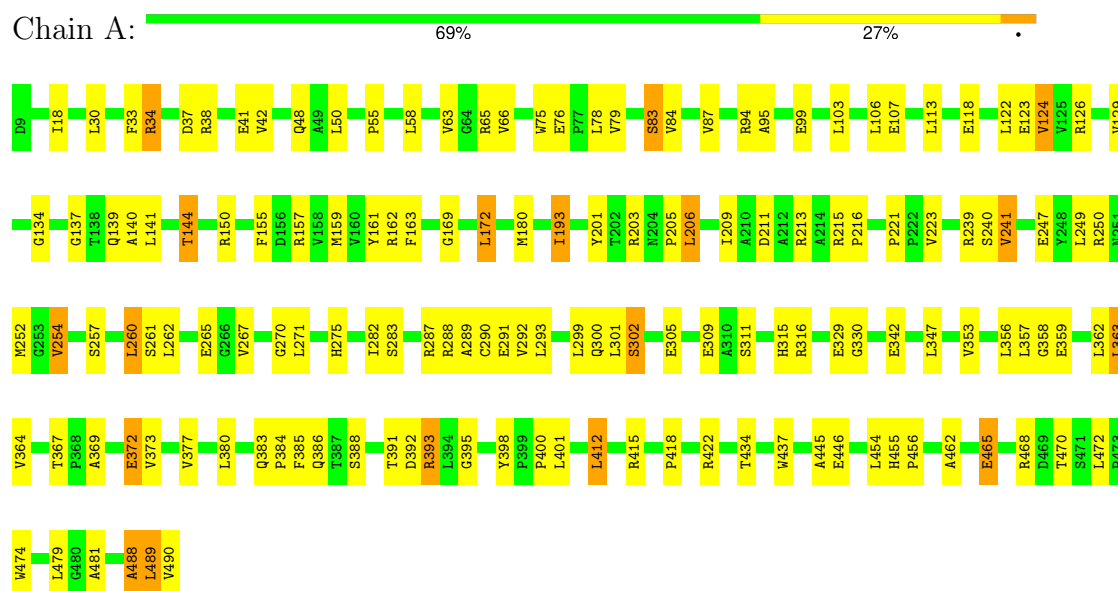
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	26	Total	O	0	0
			26	26		

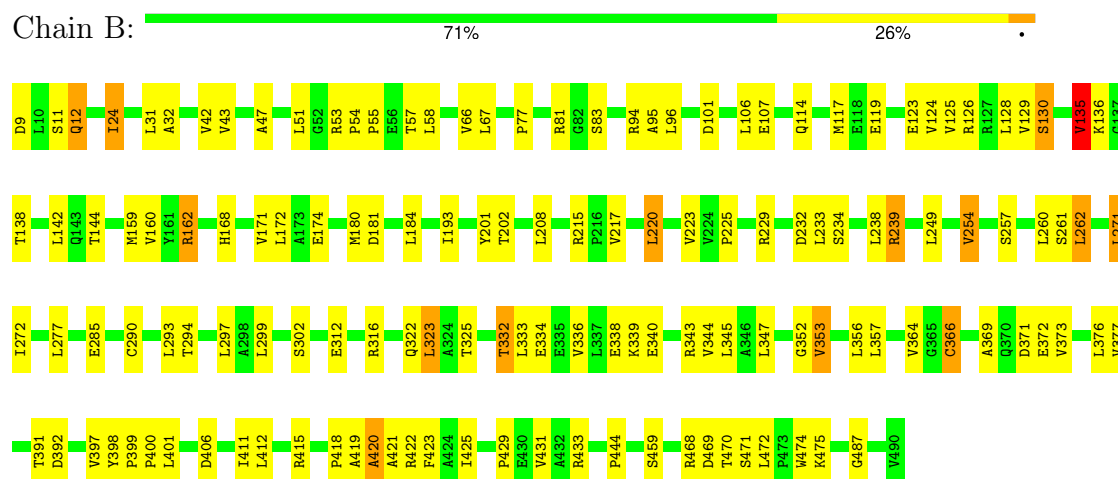
3 Residue-property plots

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	83.69Å 83.40Å 86.87Å 90.00° 107.63° 90.00°	Depositor
Resolution (Å)	24.33 – 2.30 24.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	74.6 (24.33-2.30) 74.6 (24.33-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.21_5207, PHENIX 1.21	Depositor
R, R_{free}	0.224 , 0.296 0.224 , 0.296	Depositor DCC
R_{free} test set	2054 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 117.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7481	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: BEN, BLA

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	0.39	0/3753	0.56	0/5119
1	B	0.37	0/3740	0.56	0/5101
All	All	0.38	0/7493	0.56	0/10220

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	ARG	Sidechain

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	3671	0	3709	84	0
1	B	3659	0	3698	85	1
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	9	0	7	0	0
4	A	30	0	0	1	0
4	B	26	0	0	5	0
All	All	7481	0	7474	167	1

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 (167) 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:252:MET:HG2	2:A:501:BLA:HBB2	1.50	0.93
1:A:206:LEU:HD12	1:A:260:LEU:HD23	1.53	0.88
1:B:372:GLU:HB3	1:B:401:LEU:HD21	1.58	0.85
1:B:32:ALA:HB3	1:B:42:VAL:HB	1.62	0.81
1:A:150:ARG:NH1	4:A:601:HOH:O	2.13	0.80
1:A:140:ALA:O	1:A:144:THR:OG1	2.02	0.78
1:A:385:PHE:O	1:A:415:ARG:NH2	2.17	0.77
1:A:347:LEU:HD22	1:A:481:ALA:HB1	1.65	0.77
1:B:444:PRO:O	4:B:601:HOH:O	2.04	0.76
1:A:290:CYS:HA	1:A:293:LEU:HD12	1.69	0.74
1:A:206:LEU:HD11	1:A:291:GLU:HB2	1.71	0.72
1:B:322:GLN:OE1	1:B:343:ARG:NE	2.21	0.72
1:A:265:GLU:OE1	1:A:302:SER:OG	2.07	0.72
1:A:372:GLU:HB3	1:A:401:LEU:HD21	1.74	0.70
1:A:363:LEU:HB3	1:A:367:THR:HG21	1.74	0.69
1:A:155:PHE:CE1	1:A:282:ILE:HD11	2.29	0.68
1:A:48:GLN:HB2	1:A:55:PRO:HD3	1.74	0.68
1:A:141:LEU:HD21	1:A:300:GLN:HB3	1.75	0.67
1:B:11:SER:OG	1:B:12:GLN:N	2.27	0.67
1:A:380:LEU:HA	1:A:383:GLN:HG2	1.78	0.66
1:B:232:ASP:OD1	1:B:234:SER:OG	2.14	0.65
1:B:400:PRO:O	4:B:602:HOH:O	2.13	0.65
1:B:336:VAL:HA	1:B:339:LYS:HG2	1.80	0.64
1:A:353:VAL:HG12	1:A:364:VAL:HB	1.80	0.64
1:B:124:VAL:HG23	1:B:293:LEU:HD21	1.78	0.64
1:B:159:MET:HG3	1:B:174:GLU:HG3	1.79	0.64
1:B:125:VAL:O	1:B:129:VAL:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:HD2	1:B:58:LEU:HD21	1.81	0.62
1:B:272:ILE:HD12	1:B:294:THR:HG22	1.80	0.62
1:B:54:PRO:HB2	1:B:57:THR:HG23	1.80	0.62
1:A:412:LEU:HD11	1:A:479:LEU:HD23	1.82	0.61
1:A:261:SER:HA	1:A:271:LEU:HD23	1.83	0.61
1:A:118:GLU:HG2	1:B:119:GLU:HA	1.82	0.60
1:B:162:ARG:NE	1:B:172:LEU:HD11	2.17	0.59
1:B:107:GLU:OE1	4:B:603:HOH:O	2.16	0.59
1:B:332:THR:O	1:B:336:VAL:HG22	2.03	0.59
1:A:33:PHE:CZ	1:A:63:VAL:HG23	2.38	0.59
1:B:129:VAL:HG23	1:B:130:SER:H	1.68	0.58
1:B:369:ALA:HB3	1:B:372:GLU:HG3	1.85	0.58
1:A:34:ARG:HG2	1:A:41:GLU:OE1	2.03	0.57
1:A:42:VAL:HG13	1:A:221:PRO:HD2	1.87	0.57
1:B:249:LEU:HD22	1:B:254:VAL:HG21	1.85	0.57
1:B:391:THR:HG22	1:B:411:ILE:HG12	1.85	0.56
1:A:155:PHE:HE1	1:A:282:ILE:HD11	1.70	0.56
1:A:162:ARG:HD3	1:A:172:LEU:HD11	1.87	0.56
1:A:392:ASP:C	1:A:393:ARG:HG3	2.31	0.56
1:B:433:ARG:NH2	1:B:471:SER:O	2.33	0.55
1:B:261:SER:HA	1:B:271:LEU:HD12	1.89	0.54
1:A:311:SER:O	1:A:315[B]:HIS:ND1	2.40	0.54
1:A:75:TRP:O	1:A:79:VAL:HG23	2.06	0.54
1:B:47:ALA:HB3	1:B:55:PRO:HG3	1.90	0.54
1:A:299:LEU:HD23	1:B:299:LEU:HD23	1.88	0.54
1:B:83:SER:HB2	1:B:96:LEU:HD23	1.89	0.53
1:B:124:VAL:HG21	1:B:293:LEU:HD11	1.91	0.53
1:B:233:LEU:O	1:B:239:ARG:HD3	2.08	0.53
1:A:157:ARG:HH11	1:A:180:MET:HE3	1.72	0.52
1:A:316:ARG:NH1	1:A:347:LEU:O	2.42	0.52
1:A:445:ALA:HB1	1:A:454:LEU:HD22	1.91	0.52
1:B:431:VAL:HG21	1:B:472:LEU:HG	1.91	0.52
1:A:288:ARG:NH1	1:B:123:GLU:OE2	2.39	0.52
1:B:339:LYS:HG3	1:B:340:GLU:HG2	1.91	0.52
1:A:215:ARG:HG2	1:A:216:PRO:HD2	1.92	0.51
2:B:501:BLA:OB	2:B:501:BLA:HBB1	2.10	0.51
1:B:249:LEU:CD2	2:B:501:BLA:HBB1	2.41	0.51
1:A:123:GLU:OE2	1:A:126:ARG:HD2	2.11	0.51
1:A:373:VAL:O	1:A:377:VAL:HG23	2.12	0.50
1:A:252:MET:HG2	2:A:501:BLA:CBB	2.33	0.50
1:B:77:PRO:O	1:B:81:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:CYS:O	1:B:294:THR:HG23	2.12	0.50
1:A:157:ARG:HB2	1:A:180:MET:HE1	1.92	0.50
1:B:162:ARG:HE	1:B:172:LEU:HD11	1.75	0.50
1:B:353:VAL:HG12	1:B:364:VAL:HB	1.94	0.50
1:A:392:ASP:OD1	1:A:393:ARG:HG3	2.12	0.50
1:B:344:VAL:HA	1:B:347:LEU:HD12	1.93	0.50
1:A:157:ARG:HB2	1:A:180:MET:CE	2.42	0.49
1:A:412:LEU:HD12	1:A:474:TRP:CE3	2.47	0.49
1:B:366:CYS:O	1:B:366:CYS:SG	2.70	0.49
1:B:58:LEU:HD13	1:B:66:VAL:HG23	1.94	0.49
1:A:437:TRP:O	1:A:462:ALA:HA	2.13	0.48
1:A:78:LEU:HD13	1:A:84:VAL:HG12	1.95	0.48
1:A:95:ALA:HB1	1:A:106:LEU:HD11	1.96	0.48
1:A:446:GLU:O	1:A:455:HIS:HB2	2.14	0.48
1:A:468:ARG:O	1:A:470:THR:HG23	2.13	0.48
1:B:352:GLY:HA3	1:B:366:CYS:O	2.13	0.48
1:A:34:ARG:HB3	1:A:103:LEU:HD22	1.96	0.47
1:B:135:VAL:HG23	1:B:136:LYS:H	1.78	0.47
1:A:211:ASP:C	1:A:213:ARG:H	2.22	0.47
1:B:47:ALA:HB1	1:B:51:LEU:HD12	1.95	0.47
1:A:392:ASP:OD1	1:A:393:ARG:NE	2.48	0.47
1:B:142:LEU:HD22	1:B:160:VAL:HG11	1.95	0.47
1:A:124:VAL:HG23	1:A:293:LEU:HD21	1.96	0.47
1:A:247:GLU:HB3	1:A:456:PRO:HG3	1.97	0.47
1:B:412:LEU:HD12	1:B:474:TRP:CE3	2.48	0.47
1:A:213:ARG:NE	1:A:250:ARG:HG2	2.30	0.46
1:B:101:ASP:CG	1:B:229:ARG:HH12	2.24	0.46
1:B:142:LEU:HD23	1:B:297:LEU:HD11	1.96	0.46
1:B:468:ARG:O	1:B:470:THR:N	2.49	0.46
1:A:58:LEU:HB3	1:A:66:VAL:HG12	1.98	0.46
1:B:397:VAL:O	1:B:399:PRO:HD3	2.15	0.46
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.81	0.46
1:A:369:ALA:HB3	1:A:372:GLU:HG3	1.98	0.46
1:A:488:ALA:HA	1:B:487:GLY:O	2.16	0.45
1:A:398:TYR:CE2	1:A:400:PRO:HB2	2.50	0.45
1:A:201:TYR:OH	2:A:501:BLA:HAA1	2.16	0.45
1:A:83:SER:OG	1:A:94:ARG:HD2	2.16	0.45
1:A:358:GLY:HA2	1:A:422:ARG:CZ	2.46	0.45
1:B:312:GLU:O	1:B:316:ARG:HG2	2.17	0.45
1:B:475:LYS:HD3	1:B:475:LYS:HA	1.72	0.45
1:B:334:GLU:O	1:B:338:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD11	1:A:241:VAL:HG11	1.99	0.45
1:A:37:ASP:O	1:A:38:ARG:C	2.60	0.45
1:A:489:LEU:H	1:A:489:LEU:HG	1.35	0.44
1:B:180:MET:HE3	1:B:277:LEU:HD11	1.99	0.44
1:B:193:ILE:HG12	2:B:501:BLA:C4A	2.47	0.44
1:A:163:PHE:HE1	1:A:193:ILE:HD12	1.82	0.44
1:B:83:SER:HA	1:B:95:ALA:O	2.17	0.44
1:B:128:LEU:HD13	1:B:144:THR:HG22	1.99	0.44
1:A:163:PHE:CD2	1:A:270:GLY:HA2	2.52	0.44
1:B:415:ARG:HD3	1:B:423:PHE:CE1	2.53	0.44
1:A:357:LEU:HD12	1:A:359:GLU:OE2	2.17	0.44
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.77	0.44
1:B:369:ALA:O	1:B:372:GLU:N	2.44	0.44
1:A:30:LEU:HD12	1:A:107:GLU:HG2	1.98	0.44
1:A:213:ARG:CZ	1:A:250:ARG:HG2	2.48	0.44
1:B:344:VAL:O	1:B:347:LEU:HB2	2.17	0.44
1:B:468:ARG:C	1:B:470:THR:H	2.26	0.43
1:A:301:LEU:O	1:A:305:GLU:HB2	2.17	0.43
1:B:94:ARG:NE	1:B:285:GLU:OE2	2.35	0.43
1:A:18:ILE:O	1:A:239:ARG:NH1	2.50	0.43
1:B:107:GLU:HG2	1:B:238:LEU:HD12	2.01	0.43
2:B:501:BLA:C3A	2:B:501:BLA:HB	2.28	0.43
1:A:393:ARG:HH11	1:A:393:ARG:CG	2.31	0.43
1:B:323:LEU:HD21	1:B:347:LEU:HD11	2.00	0.43
1:B:94:ARG:HE	1:B:285:GLU:CD	2.25	0.42
1:A:161:TYR:CZ	1:A:169:GLY:HA3	2.54	0.42
1:B:159:MET:CG	1:B:174:GLU:HG3	2.47	0.42
1:B:42:VAL:HA	1:B:220:LEU:O	2.20	0.42
1:A:205:PRO:C	1:A:206:LEU:HD13	2.44	0.42
1:A:221:PRO:HG2	1:A:223:VAL:O	2.18	0.42
1:A:249:LEU:HD22	1:A:254:VAL:HG21	2.02	0.42
1:B:24:ILE:HG13	1:B:217:VAL:HB	2.01	0.42
1:B:31:LEU:HD13	1:B:106:LEU:HD23	2.01	0.42
1:B:159:MET:HG2	1:B:171:VAL:HG11	2.02	0.42
1:B:397:VAL:C	1:B:399:PRO:HD3	2.45	0.42
1:B:233:LEU:HG	4:B:604:HOH:O	2.20	0.41
1:B:398:TYR:CE2	1:B:401:LEU:HD12	2.55	0.41
1:B:117:MET:HE3	1:B:117:MET:HB3	1.89	0.41
1:B:420:ALA:O	1:B:422:ARG:HG2	2.20	0.41
1:B:249:LEU:HD22	1:B:254:VAL:CG2	2.49	0.41
1:B:101:ASP:OD2	1:B:229:ARG:NH1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HA	1:A:221:PRO:HD3	2.03	0.41
1:A:283:SER:O	1:A:287:ARG:HG3	2.20	0.41
1:B:262:LEU:HD21	1:B:297:LEU:HD23	2.01	0.41
1:A:99:GLU:HA	1:A:103:LEU:O	2.20	0.41
1:A:211:ASP:C	1:A:213:ARG:N	2.78	0.41
1:A:434:THR:HA	1:A:465:GLU:O	2.21	0.41
1:B:123:GLU:CD	1:B:126:ARG:HE	2.29	0.41
1:B:201:TYR:OH	2:B:501:BLA:HAA1	2.20	0.41
1:B:468:ARG:O	1:B:470:THR:HG23	2.20	0.41
1:A:159:MET:HE1	1:A:275:HIS:CE1	2.55	0.40
1:B:129:VAL:HG23	1:B:130:SER:N	2.33	0.40
1:A:163:PHE:CE1	1:A:193:ILE:HD12	2.56	0.40
1:A:289:ALA:O	1:A:292:VAL:HB	2.22	0.40
1:B:215:ARG:NH2	4:B:610:HOH:O	2.54	0.40
1:A:134:GLY:HA2	1:A:137:GLY:O	2.20	0.40
1:B:223:VAL:O	1:B:225:PRO:HD3	2.21	0.40
1:B:406:ASP:O	1:B:429:PRO:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:SER:OG	1:B:136:LYS:NZ[2_444]	2.12	0.08

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	481/482 (100%)	445 (92%)	30 (6%)	6 (1%)	11	12
1	B	480/482 (100%)	429 (89%)	42 (9%)	9 (2%)	6	6
All	All	961/964 (100%)	874 (91%)	72 (8%)	15 (2%)	8	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	VAL
1	A	386	GLN
1	A	418	PRO
1	B	333	LEU
1	B	419	ALA
1	B	421	ALA
1	B	130	SER
1	B	418	PRO
1	B	420	ALA
1	A	488	ALA
1	B	332	THR
1	B	469	ASP
1	A	330	GLY
1	A	395	GLY
1	A	384	PRO

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	376/375 (100%)	338 (90%)	38 (10%)	6	7
1	B	374/375 (100%)	339 (91%)	35 (9%)	7	9
All	All	750/750 (100%)	677 (90%)	73 (10%)	6	8

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	50	LEU
1	A	65	ARG
1	A	76	GLU
1	A	83	SER
1	A	87	VAL
1	A	113	LEU
1	A	124	VAL

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Mol	Chain	Res	Type
1	A	129	VAL
1	A	139	GLN
1	A	144	THR
1	A	172	LEU
1	A	193	ILE
1	A	203	ARG
1	A	206	LEU
1	A	240	SER
1	A	241	VAL
1	A	254	VAL
1	A	257	SER
1	A	260	LEU
1	A	262	LEU
1	A	267	VAL
1	A	302	SER
1	A	309	GLU
1	A	329	GLU
1	A	342	GLU
1	A	356	LEU
1	A	362	LEU
1	A	363	LEU
1	A	372	GLU
1	A	388	SER
1	A	391	THR
1	A	393	ARG
1	A	412	LEU
1	A	465	GLU
1	A	472	LEU
1	A	489	LEU
1	A	490	VAL
1	B	9	ASP
1	B	12	GLN
1	B	24	ILE
1	B	43	VAL
1	B	67	LEU
1	B	114	GLN
1	B	135	VAL
1	B	138	THR
1	B	162	ARG
1	B	168	HIS
1	B	181	ASP
1	B	184	LEU

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Mol	Chain	Res	Type
1	B	202	THR
1	B	208	LEU
1	B	220	LEU
1	B	254	VAL
1	B	257	SER
1	B	260	LEU
1	B	262	LEU
1	B	271	LEU
1	B	302	SER
1	B	323	LEU
1	B	325	THR
1	B	345	LEU
1	B	353	VAL
1	B	356	LEU
1	B	357	LEU
1	B	366	CYS
1	B	371	ASP
1	B	373	VAL
1	B	376	LEU
1	B	377	VAL
1	B	392	ASP
1	B	425	ILE
1	B	459	SER

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	143	GLN
1	A	300	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	BEN	A	502	-	9,9,9	0.69	0	7,11,11	1.07	1 (14%)
2	BLA	A	501	1	42,46,46	1.21	4 (9%)	54,67,67	1.37	7 (12%)
2	BLA	B	501	1	42,46,46	1.27	6 (14%)	54,67,67	1.58	7 (12%)

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
3	BEN	A	502	-	-	0/4/4/4	0/1/1/1
2	BLA	A	501	1	-	4/26/74/74	0/4/4/4
2	BLA	B	501	1	-	6/26/74/74	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	BLA	CHA-C4D	3.82	1.38	1.35
2	B	501	BLA	CHA-C4D	3.57	1.38	1.35
2	A	501	BLA	O2A-CGA	-2.74	1.21	1.30
2	B	501	BLA	CHD-C1D	2.69	1.46	1.40
2	B	501	BLA	C3C-C4C	2.11	1.49	1.45
2	B	501	BLA	O2A-CGA	-2.08	1.23	1.30
2	A	501	BLA	CBA-CGA	2.06	1.55	1.50
2	A	501	BLA	CHD-C1D	2.03	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	BLA	C4B-NB	-2.01	1.33	1.38
2	B	501	BLA	CBD-CGD	2.01	1.55	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	BLA	C1A-CHA-C4D	6.35	137.23	128.73
2	B	501	BLA	CHB-C1B-C2B	4.33	135.60	126.99
2	A	501	BLA	C1A-CHA-C4D	4.14	134.27	128.73
2	B	501	BLA	CHB-C1B-NB	-3.81	116.88	130.33
3	A	502	BEN	C1-C-N2	-2.76	113.82	118.01
2	A	501	BLA	CHA-C4D-C3D	-2.46	119.72	125.40
2	B	501	BLA	O1D-CGD-CBD	-2.46	115.29	123.09
2	B	501	BLA	C3B-C2B-C1B	-2.32	105.33	107.92
2	B	501	BLA	C1B-NB-C4B	2.24	113.42	110.66
2	A	501	BLA	CHB-C1B-NB	-2.23	122.45	130.33
2	B	501	BLA	O2D-CGD-CBD	2.20	120.94	114.00
2	A	501	BLA	CMB-C2B-C1B	-2.18	121.50	124.16
2	A	501	BLA	CMC-C2C-C1C	-2.16	116.70	121.21
2	A	501	BLA	O2D-CGD-O1D	2.05	128.62	123.33
2	A	501	BLA	OC-C1C-NC	2.05	129.90	125.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

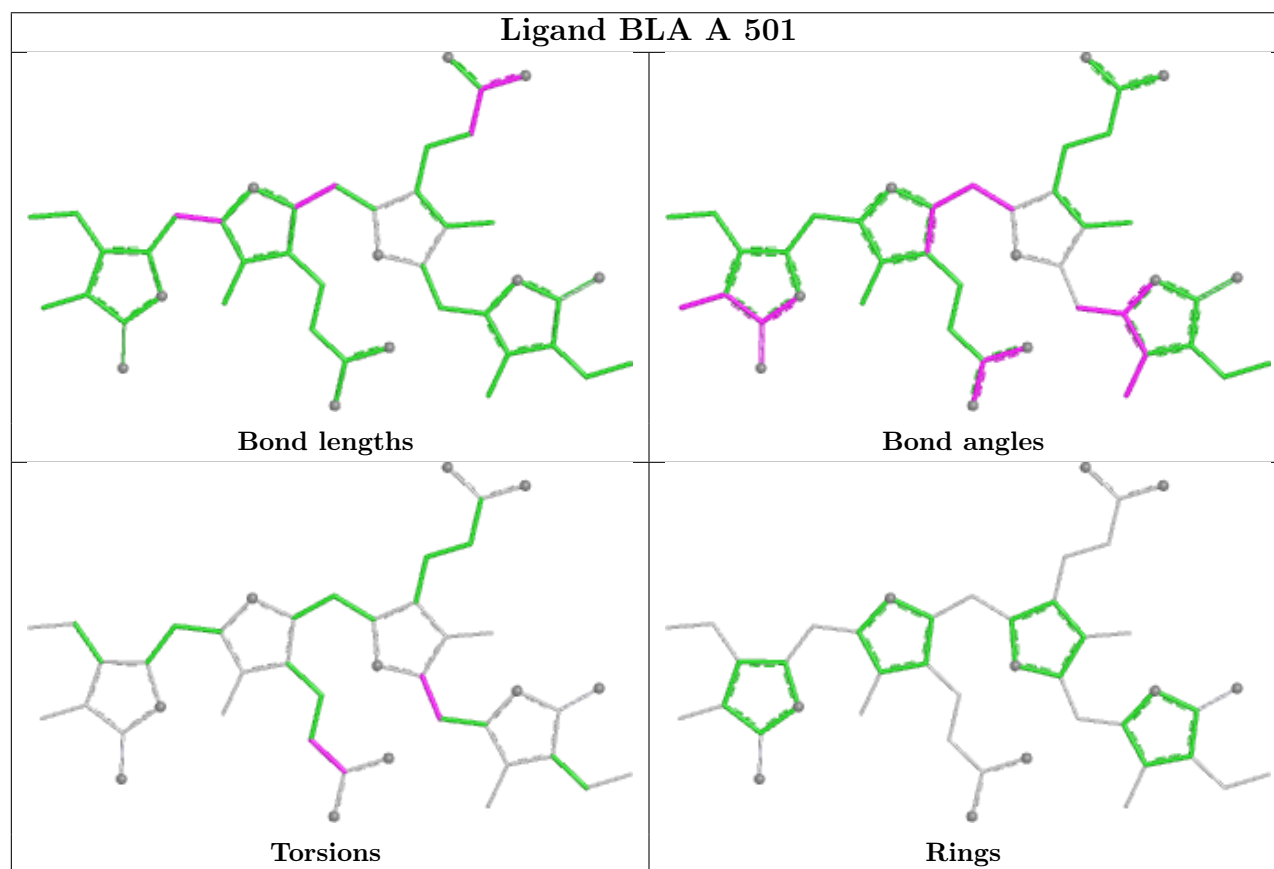
Mol	Chain	Res	Type	Atoms
2	A	501	BLA	NA-C4A-CHB-C1B
2	A	501	BLA	C3A-C4A-CHB-C1B
2	B	501	BLA	NA-C4A-CHB-C1B
2	B	501	BLA	C3A-C4A-CHB-C1B
2	B	501	BLA	CAD-CBD-CGD-O2D
2	B	501	BLA	CAD-CBD-CGD-O1D
2	B	501	BLA	CAA-CBA-CGA-O1A
2	B	501	BLA	CAA-CBA-CGA-O2A
2	A	501	BLA	CAD-CBD-CGD-O1D
2	A	501	BLA	CAD-CBD-CGD-O2D

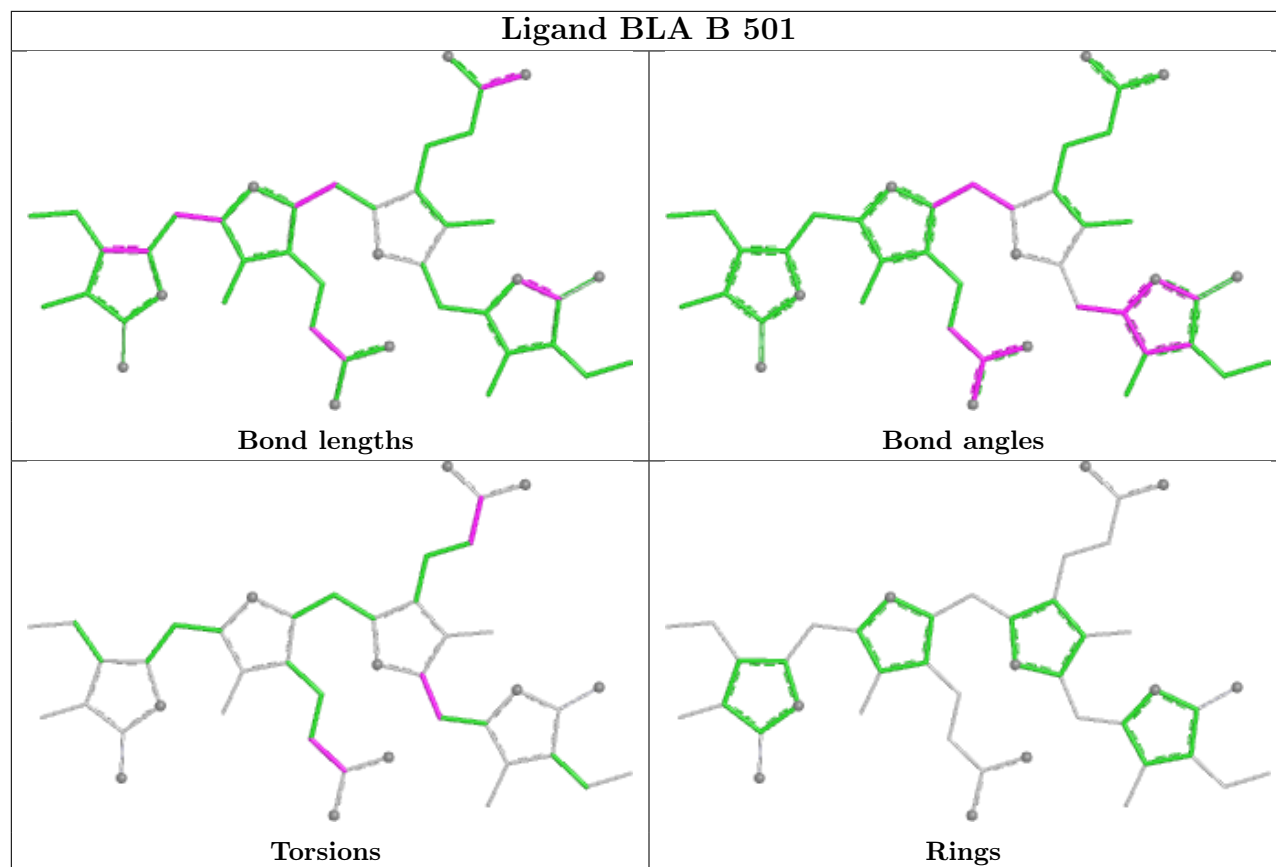
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BLA	3	0
2	B	501	BLA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/482 (100%)	-0.41	0 100 100	9, 23, 44, 58	1 (0%)
1	B	482/482 (100%)	-0.33	0 100 100	10, 24, 50, 62	0
All	All	964/964 (100%)	-0.37	0 100 100	9, 24, 47, 62	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

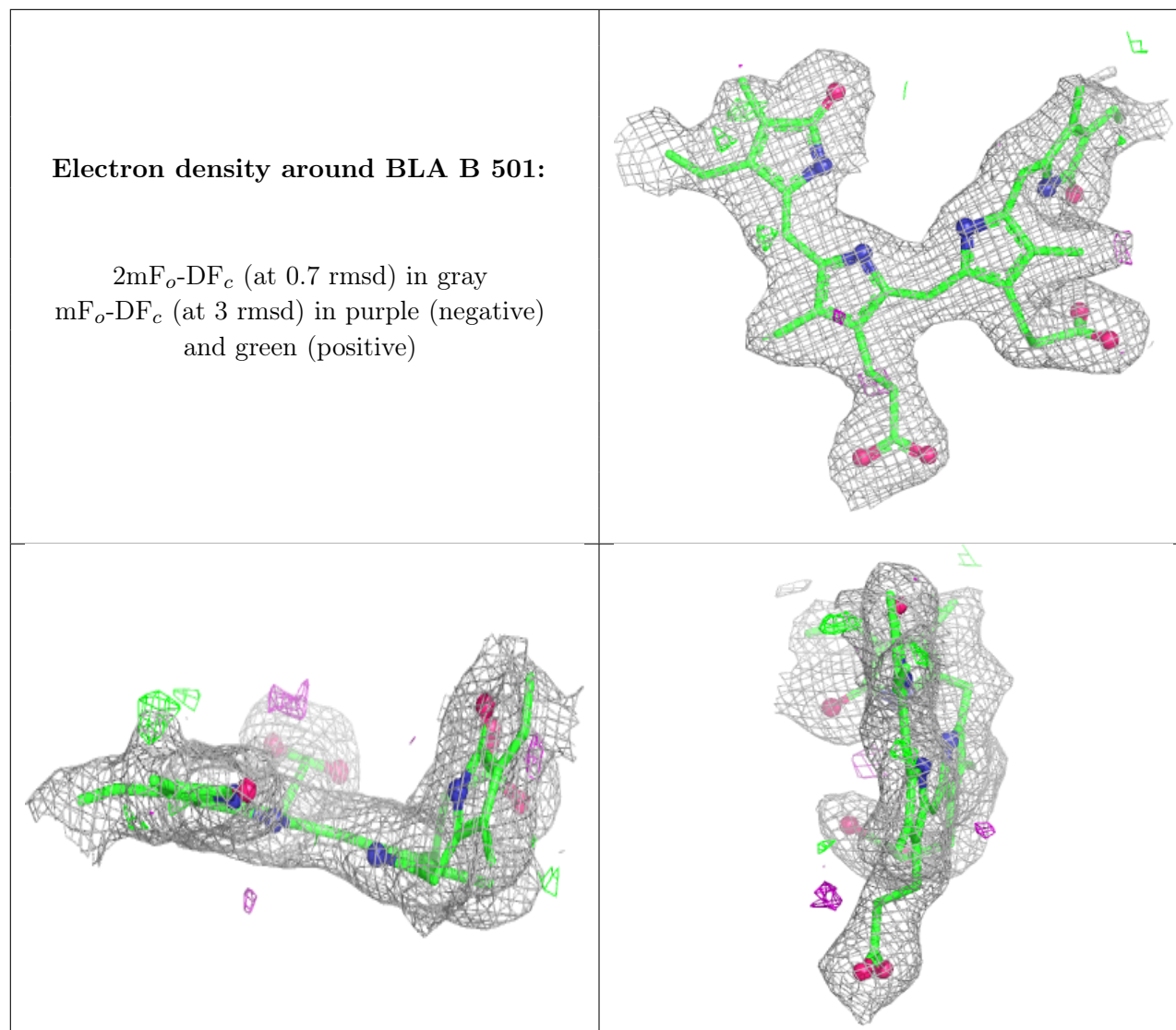
6.4 Ligands [i](#)

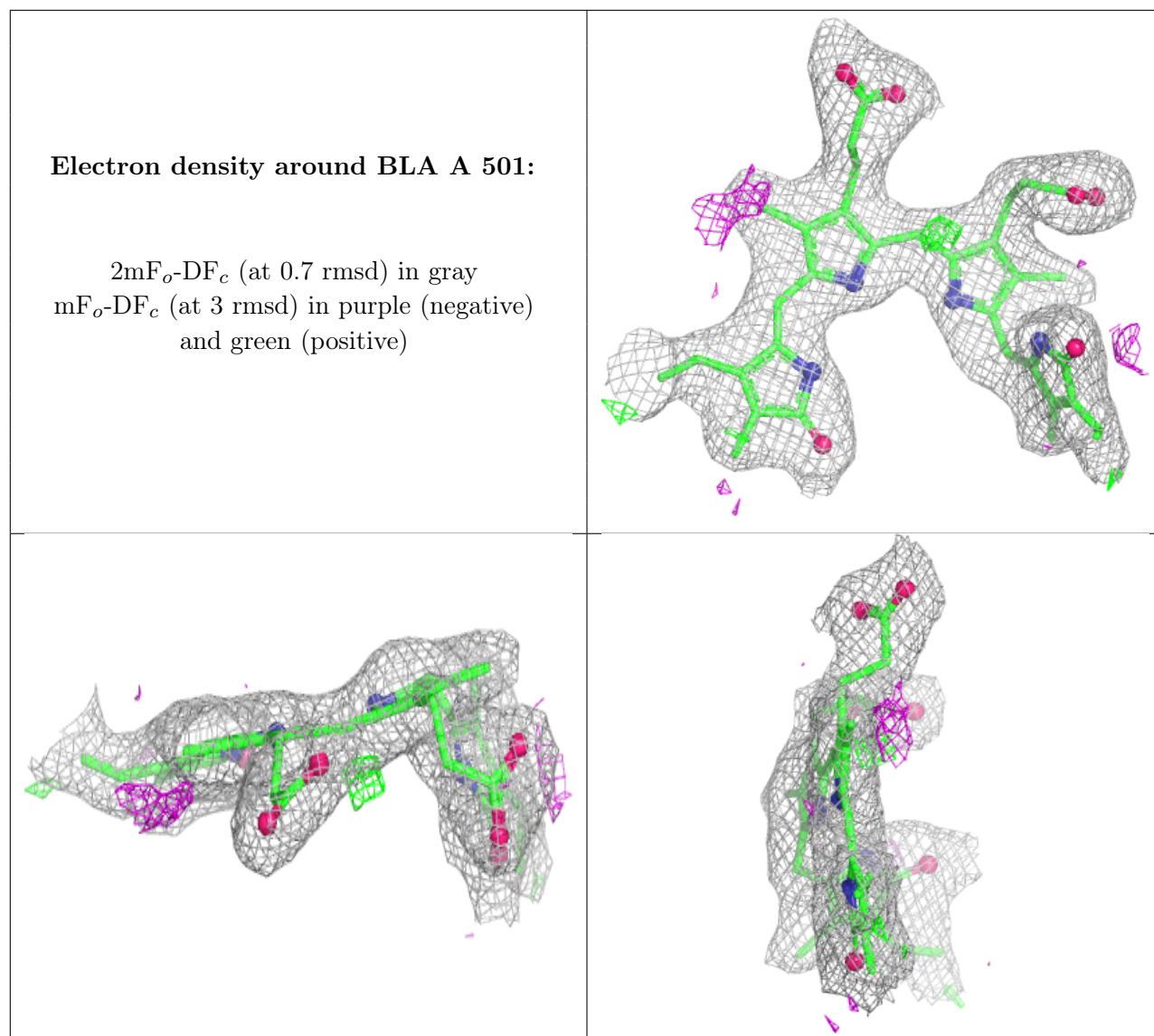
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BEN	A	502	9/9	0.85	0.13	27,53,58,59	0
2	BLA	B	501	43/43	0.94	0.08	5,9,17,25	0
2	BLA	A	501	43/43	0.95	0.07	3,9,14,20	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.