



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:56 pm BST

PDB ID : 6BAO  
Title : Stigmatella aurantiaca phytochrome photosensory core module, wild type  
Authors : Schmidt, M.; Stojkovic, E.  
Deposited on : 2017-10-14  
Resolution : 2.18 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

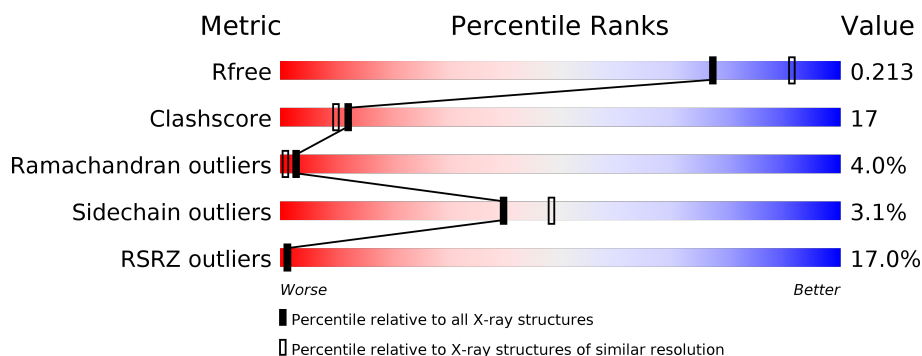
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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))
$R_{free}$	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	513	<div> <div>20%</div> <div>63%</div> <div>30%</div> <div>...</div> </div>
1	B	513	<div> <div>13%</div> <div>69%</div> <div>24%</div> <div>5%</div> <div>...</div> </div>

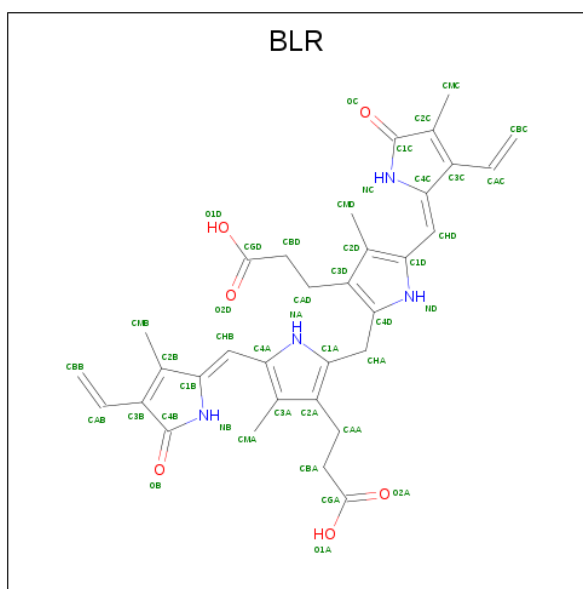


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total 3962	C 2500	N 722	O 727	S 13	0	0	0
1	B	503	Total 3962	C 2500	N 722	O 727	S 13	0	0	0

- Molecule 2 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: BLR) (formula: C<sub>33</sub>H<sub>36</sub>N<sub>4</sub>O<sub>6</sub>).



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	134	Total 134	O 134	0	0
3	B	137	Total 137	O 137	0	0

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

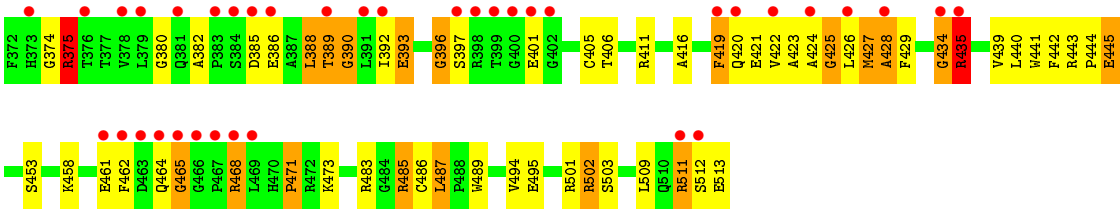
Chain A:

Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 300. A color scale at the top indicates conservation levels: 13% (red), 69% (green), 24% (yellow), and 5% (grey).

Key residues and their conservation levels (approximate bits):

- Position 1: MET (0.13 bits)
- Position 2: SER (0.13 bits)
- Position 3: THR (0.13 bits)
- Position 4: GLU (0.13 bits)
- Position 5: ALA (0.13 bits)
- Position 6: SER (0.13 bits)
- Position 7: ARG (0.13 bits)
- Position 8: SER (0.13 bits)
- Position 9: GLY (0.13 bits)
- Position 10: LYS (0.13 bits)
- Position 11: Q11 (0.13 bits)
- Position 12: E12 (0.13 bits)
- Position 13: V13 (0.13 bits)
- Position 14: D14 (0.13 bits)
- Position 15: L15 (0.13 bits)
- Position 16: T16 (0.13 bits)
- Position 17: N17 (0.13 bits)
- Position 18: H24 (0.13 bits)
- Position 19: I29 (0.13 bits)
- Position 20: L36 (0.13 bits)
- Position 21: V37 (0.13 bits)
- Position 22: T46 (0.13 bits)
- Position 23: H47 (0.13 bits)
- Position 24: A48 (0.13 bits)
- Position 25: S49 (0.13 bits)
- Position 26: G57 (0.13 bits)
- Position 27: N58 (0.13 bits)
- Position 28: S59 (0.13 bits)
- Position 29: A60 (0.13 bits)
- Position 30: L64 (0.13 bits)
- Position 31: G69 (0.13 bits)
- Position 32: E73 (0.13 bits)
- Position 33: R77 (0.13 bits)
- Position 34: L80 (0.13 bits)
- Position 35: E81 (0.13 bits)
- Position 36: L84 (0.13 bits)
- Position 37: K90 (0.13 bits)
- Position 38: Q91 (0.13 bits)
- Position 39: R100 (0.13 bits)
- Position 40: V101 (0.13 bits)
- Position 41: D102 (0.13 bits)
- Position 42: G103 (0.13 bits)
- Position 43: I111 (0.13 bits)
- Position 44: A112 (0.13 bits)
- Position 45: H113 (0.13 bits)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.51Å 134.99Å 113.18Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	38.40 – 2.18 38.40 – 2.18	Depositor EDS
% Data completeness (in resolution range)	78.7 (38.40-2.18) 96.1 (38.40-2.18)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.220 , 0.262 0.216 , 0.213	Depositor DCC
$R_{free}$ test set	2903 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BLR

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	0.53	2/4054 (0.0%)	0.77	8/5501 (0.1%)
1	B	0.66	7/4054 (0.2%)	0.74	6/5501 (0.1%)
All	All	0.60	9/8108 (0.1%)	0.76	14/11002 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	PRO	N-CD	-18.54	1.21	1.47
1	A	511	ARG	CZ-NH1	-9.37	1.20	1.33
1	B	152	ARG	CZ-NH1	-9.19	1.21	1.33
1	A	511	ARG	NE-CZ	-9.04	1.21	1.33
1	B	435	ARG	CZ-NH2	-8.81	1.21	1.33
1	B	156	GLU	CD-OE1	-8.66	1.16	1.25
1	B	435	ARG	NE-CZ	-7.96	1.22	1.33
1	B	435	ARG	CD-NE	-7.21	1.34	1.46
1	B	435	ARG	CZ-NH1	-6.88	1.24	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	ARG	NE-CZ-NH1	-13.99	113.31	120.30
1	B	152	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	A	302	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	487	LEU	CA-CB-CG	9.13	136.30	115.30
1	B	152	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	A	472	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	302	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	425	GLY	N-CA-C	-6.27	97.43	113.10
1	A	376	THR	C-N-CA	5.99	136.66	121.70
1	B	487	LEU	CB-CG-CD1	5.71	120.71	111.00
1	A	339	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	502	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	15	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	511	ARG	NH1-CZ-NH2	5.13	125.04	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466	GLY	Peptide
1	A	510	GLN	Peptide
1	B	485	ARG	Peptide

## 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	3962	0	3908	160	1
1	B	3962	0	3908	121	1
2	A	43	0	32	1	0
2	B	43	0	32	1	0
3	A	134	0	0	11	0
3	B	137	0	0	22	0
All	All	8281	0	7880	271	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 17.

All (271) 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:352:LEU:HD11	1:A:370:ILE:HD11	1.45	0.98
1:A:37:VAL:HG13	1:A:47:HIS:HB2	1.50	0.93
1:A:352:LEU:HD13	1:A:359:LEU:HD22	1.52	0.91
1:A:45:LEU:HD12	1:A:63:LEU:HB3	1.50	0.91
1:B:435:ARG:HH11	1:B:435:ARG:HA	1.38	0.86
1:B:424:ALA:HB2	1:B:486:CYS:SG	2.14	0.86
1:A:462:PHE:HB3	1:A:467:PRO:HB2	1.58	0.85
1:B:367:GLY:HA2	1:B:380:GLY:HA3	1.59	0.85
1:A:341:ARG:NH1	1:A:341:ARG:O	2.09	0.85
1:B:374:GLY:HA3	1:B:375:ARG:HB2	1.57	0.83
1:A:41:PRO:O	1:A:85:ARG:NH1	2.13	0.82
1:A:432:SER:O	1:A:435:ARG:NH1	2.14	0.81
1:A:495:GLU:OE1	1:A:495:GLU:N	2.13	0.79
1:B:152:ARG:HG2	1:B:156:GLU:OE1	1.82	0.79
1:B:261:GLU:OE1	1:B:471:PRO:HG3	1.82	0.79
1:B:341:ARG:NH2	1:B:355:GLN:HG2	1.97	0.78
1:B:37:VAL:HG13	1:B:47:HIS:HB2	1.65	0.78
1:B:512:SER:OG	1:B:513:GLU:N	2.17	0.76
1:A:417:GLN:NE2	3:A:704:HOH:O	2.17	0.76
1:B:177:TYR:CZ	1:B:185:GLY:HA3	2.21	0.76
1:A:324:ASP:OD1	1:A:490:LYS:NZ	2.19	0.75
1:A:208:ASP:OD1	1:A:472:ARG:NH1	2.20	0.74
1:B:24:HIS:ND1	3:B:706:HOH:O	2.21	0.74
1:A:266:MET:HB2	3:A:705:HOH:O	1.87	0.73
1:B:69:GLY:O	1:B:77:ARG:NH1	2.22	0.72
1:A:395:LEU:HB2	1:A:438:PHE:HZ	1.54	0.72
1:B:424:ALA:HB3	1:B:443:ARG:HB2	1.71	0.72
1:A:328:ARG:O	1:A:332:LYS:N	2.23	0.72
1:A:372:PHE:O	3:A:701:HOH:O	2.07	0.72
1:A:430:SER:OG	1:A:435:ARG:NH1	2.21	0.72
1:B:468:ARG:NH1	3:B:709:HOH:O	2.21	0.72
1:A:97:VAL:HG21	1:A:123:LEU:HD22	1.72	0.71
1:A:149:ARG:HD3	1:B:307:PHE:CD1	2.25	0.71
1:A:409:LEU:HD21	1:A:413:TYR:HB3	1.73	0.71
1:B:344:ARG:NH1	3:B:710:HOH:O	2.22	0.69
1:A:492:TYR:HA	1:A:495:GLU:CD	2.12	0.69
1:B:374:GLY:CA	1:B:375:ARG:HB2	2.22	0.69
1:A:208:ASP:CG	1:A:472:ARG:HH12	1.96	0.68
1:A:352:LEU:HD12	1:A:352:LEU:C	2.14	0.68
1:B:73:GLU:OE1	1:B:100:ARG:NH1	2.27	0.68
1:A:184:ASN:HD22	1:A:206:ALA:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:MET:HB3	1:B:441:TRP:HB2	1.77	0.66
1:B:328:ARG:NH1	1:B:495:GLU:OE1	2.29	0.66
1:B:130:GLU:HB2	1:B:132:VAL:O	1.95	0.66
1:B:511:ARG:HE	1:B:512:SER:HB3	1.62	0.65
1:A:149:ARG:HD3	1:B:307:PHE:HD1	1.62	0.65
1:B:207:SER:OG	3:B:701:HOH:O	2.14	0.65
1:A:299:TYR:O	1:A:303:THR:HG23	1.96	0.65
1:A:310:GLU:OE1	3:A:702:HOH:O	2.14	0.65
1:B:132:VAL:HA	3:B:763:HOH:O	1.97	0.64
1:B:370:ILE:HG12	1:B:439:VAL:HG23	1.78	0.64
1:A:184:ASN:HD22	1:A:206:ALA:N	1.96	0.63
1:A:468:ARG:NE	1:A:468:ARG:HA	2.12	0.63
1:B:411:ARG:NH2	3:B:713:HOH:O	2.31	0.63
1:B:424:ALA:HB1	1:B:489:TRP:CZ2	2.33	0.63
1:B:405:CYS:HA	1:B:426:LEU:O	1.98	0.63
1:A:443:ARG:NH1	1:A:487:LEU:O	2.31	0.63
1:A:356:GLU:HB2	1:A:379:LEU:HD21	1.82	0.62
1:A:494:VAL:O	1:A:498:SER:N	2.30	0.61
1:A:352:LEU:HD12	1:A:353:ALA:N	2.14	0.61
1:A:495:GLU:HA	1:A:498:SER:HB2	1.81	0.61
1:A:383:PRO:O	1:A:385:ASP:N	2.33	0.60
1:B:422:VAL:HG23	1:B:422:VAL:O	2.02	0.60
1:A:207:SER:OG	3:A:703:HOH:O	2.16	0.60
1:A:365:ALA:HB1	1:A:442:PHE:O	2.01	0.60
1:B:12:GLU:HG2	1:B:13:VAL:HG12	1.84	0.60
1:A:97:VAL:CG2	1:A:108:PHE:HB2	2.32	0.60
1:A:408:ARG:CZ	1:A:411:ARG:HH12	2.14	0.60
1:B:422:VAL:HG12	1:B:442:PHE:HB3	1.84	0.60
1:B:355:GLN:OE1	3:B:702:HOH:O	2.16	0.59
1:A:347:ASP:OD2	1:A:348:PHE:N	2.29	0.59
1:A:508:ALA:O	1:A:511:ARG:HB3	2.03	0.59
1:A:356:GLU:OE1	1:A:357:SER:OG	2.18	0.59
1:A:363:VAL:HB	1:A:493:GLU:HG2	1.85	0.59
1:A:511:ARG:HH12	1:B:511:ARG:HG3	1.68	0.58
1:B:346:VAL:O	3:B:703:HOH:O	2.17	0.58
1:A:178:ARG:NH1	3:A:708:HOH:O	2.25	0.58
1:B:133:PRO:HA	3:B:763:HOH:O	2.03	0.58
1:A:193:ASP:OD1	1:A:195:ARG:HB2	2.04	0.57
1:A:422:VAL:HG23	1:A:445:GLU:HG3	1.87	0.57
1:A:384:SER:O	1:A:386:GLU:N	2.38	0.57
1:A:36:LEU:HD22	1:A:45:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ILE:O	1:B:393:GLU:HG2	2.05	0.56
1:B:511:ARG:CZ	1:B:511:ARG:HB3	2.36	0.56
1:A:341:ARG:NH1	1:A:351:GLY:HA2	2.21	0.56
1:A:330:ARG:NH2	1:A:361:GLU:OE2	2.37	0.56
1:A:369:ALA:HB3	1:A:440:LEU:HB2	1.88	0.56
1:A:376:THR:HA	1:A:377:THR:HB	1.88	0.55
1:A:360:LEU:HD23	1:A:441:TRP:HD1	1.71	0.55
1:B:386:GLU:HA	1:B:388:LEU:HD12	1.88	0.55
1:B:341:ARG:HH21	1:B:355:GLN:HG2	1.69	0.55
1:A:462:PHE:HA	1:A:468:ARG:O	2.07	0.55
1:B:339:LEU:HD13	1:B:503:SER:HB3	1.88	0.55
1:A:500:LEU:O	1:A:504:ILE:HG22	2.07	0.55
1:B:341:ARG:HH12	1:B:354:SER:HB2	1.71	0.55
1:B:57:GLY:O	1:B:58:ASN:ND2	2.41	0.54
1:A:300:GLU:OE2	1:B:139:HIS:NE2	2.32	0.54
1:A:379:LEU:N	1:A:380:GLY:HA2	2.23	0.54
1:A:177:TYR:CZ	1:A:185:GLY:HA3	2.42	0.54
1:A:327:GLN:O	1:A:329:ILE:N	2.40	0.54
1:A:349:VAL:C	1:A:351:GLY:H	2.09	0.54
1:B:49:SER:HA	1:B:235:VAL:HA	1.89	0.54
1:B:352:LEU:HD12	1:B:352:LEU:H	1.73	0.54
1:B:419:PHE:CD2	1:B:422:VAL:HG22	2.43	0.53
1:A:379:LEU:H	1:A:380:GLY:HA2	1.74	0.53
1:A:385:ASP:HA	1:A:388:LEU:HD23	1.90	0.53
1:A:341:ARG:NH2	1:A:350:SER:O	2.41	0.53
1:A:421:GLU:OE2	1:A:423:ALA:N	2.42	0.53
1:A:258:ILE:HD12	1:A:258:ILE:H	1.72	0.53
1:A:490:LYS:NZ	3:A:712:HOH:O	2.39	0.53
1:A:147:ARG:HA	1:B:91:GLN:HG2	1.90	0.52
1:B:435:ARG:NH1	1:B:435:ARG:HA	2.18	0.52
1:A:184:ASN:ND2	1:A:206:ALA:H	2.05	0.52
1:B:388:LEU:O	1:B:390:GLY:N	2.41	0.52
1:A:491:ALA:O	1:A:494:VAL:HG22	2.10	0.52
1:A:351:GLY:C	1:A:353:ALA:H	2.13	0.52
1:A:401:GLU:HG2	1:A:435:ARG:HH21	1.75	0.52
1:B:153:ASP:HB2	1:B:323:GLU:HG2	1.92	0.51
1:B:427:MET:HB3	1:B:441:TRP:HE3	1.75	0.51
1:A:370:ILE:HG22	1:A:371:HIS:H	1.75	0.51
1:A:416:ALA:C	1:A:420:GLN:HA	2.31	0.51
1:B:424:ALA:HB1	1:B:489:TRP:HZ2	1.76	0.51
1:A:492:TYR:HA	1:A:495:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TRP:HZ3	1:A:480:GLU:HB2	1.76	0.51
1:B:345:GLU:O	3:B:704:HOH:O	2.19	0.51
1:B:77:ARG:O	1:B:81:GLU:HG3	2.11	0.51
1:B:289:THR:HG22	3:B:721:HOH:O	2.09	0.51
1:A:96:LYS:HG3	3:A:801:HOH:O	2.11	0.50
1:B:129:ARG:NE	3:B:719:HOH:O	2.41	0.50
1:B:406:THR:HG22	1:B:425:GLY:O	2.12	0.50
1:A:430:SER:HB2	1:A:438:PHE:CZ	2.45	0.50
1:A:202:LEU:HD13	1:A:453:SER:HB2	1.94	0.50
1:A:376:THR:O	1:A:376:THR:OG1	2.27	0.50
1:B:155:GLN:O	1:B:159:GLU:HG2	2.12	0.50
1:A:262:TYR:O	3:A:705:HOH:O	2.19	0.50
1:B:427:MET:HE1	1:B:494:VAL:HG22	1.93	0.50
1:A:401:GLU:CG	1:A:435:ARG:HH21	2.25	0.50
1:B:149:ARG:NH2	3:B:724:HOH:O	2.45	0.50
1:B:261:GLU:OE1	1:B:262:TYR:N	2.45	0.50
1:B:90:LYS:NZ	3:B:723:HOH:O	2.45	0.49
1:A:17:ASN:HA	1:A:20:ARG:HD3	1.94	0.49
1:B:367:GLY:HA3	1:B:382:ALA:HB3	1.94	0.49
1:B:428:ALA:HB1	1:B:429:PHE:CD2	2.46	0.49
1:B:439:VAL:HB	3:B:817:HOH:O	2.13	0.49
1:A:173:ARG:NH1	1:A:196:ALA:HB1	2.27	0.49
1:B:341:ARG:HH12	1:B:354:SER:CB	2.26	0.49
1:A:334:ILE:O	1:A:338:LEU:HD12	2.14	0.48
1:A:413:TYR:O	1:A:415:GLU:N	2.46	0.48
1:A:370:ILE:HG23	1:A:439:VAL:HG22	1.94	0.48
1:B:389:THR:HA	1:B:392:ILE:HG23	1.96	0.48
1:A:401:GLU:HG2	1:A:435:ARG:HE	1.78	0.48
1:A:384:SER:HB2	1:A:387:ALA:HB3	1.96	0.47
1:A:342:MET:HB3	1:A:507:VAL:HG11	1.96	0.47
1:A:100:ARG:HA	1:A:104:VAL:O	2.14	0.47
1:B:17:ASN:HB2	3:B:772:HOH:O	2.13	0.47
1:B:464:GLN:H	1:B:465:GLY:HA3	1.79	0.47
1:A:362:LEU:HD23	1:A:363:VAL:HG13	1.95	0.47
1:A:463:ASP:HB2	1:A:470:HIS:CD2	2.50	0.47
1:B:258:ILE:HD13	2:B:601:BLR:H24	1.97	0.47
1:A:388:LEU:HD12	1:A:392:ILE:HD11	1.97	0.47
1:A:416:ALA:O	1:A:420:GLN:HA	2.14	0.47
1:A:511:ARG:NH1	1:B:511:ARG:HG3	2.29	0.47
1:A:329:ILE:HA	1:A:332:LYS:HB3	1.97	0.47
1:B:416:ALA:HA	1:B:419:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	1:A:298:PRO:HB3	2.30	0.47
1:A:168:LEU:HG	1:A:301:VAL:HG13	1.97	0.46
1:A:205:PRO:HG2	1:A:208:ASP:OD1	2.15	0.46
1:A:464:GLN:HB3	1:A:465:GLY:HA3	1.97	0.46
1:B:416:ALA:HA	1:B:419:PHE:CE2	2.50	0.46
1:A:360:LEU:HD22	1:A:365:ALA:HB3	1.98	0.46
1:A:443:ARG:NH2	1:A:493:GLU:OE1	2.48	0.46
1:A:466:GLY:O	1:A:468:ARG:NH2	2.49	0.46
1:A:383:PRO:C	1:A:385:ASP:H	2.17	0.46
1:A:408:ARG:NH2	1:A:411:ARG:HH12	2.14	0.46
1:B:29:ILE:HG23	3:B:791:HOH:O	2.15	0.46
1:A:511:ARG:HH12	1:B:511:ARG:CG	2.28	0.46
1:A:376:THR:HA	1:A:377:THR:CB	2.45	0.45
1:A:50:GLU:OE1	1:A:236:ARG:HD3	2.16	0.45
1:A:81:GLU:O	1:A:85:ARG:HG3	2.16	0.45
1:B:14:ASP:O	1:B:211:ARG:HD3	2.17	0.45
1:B:462:PHE:HB3	1:B:465:GLY:O	2.16	0.45
1:A:352:LEU:C	1:A:352:LEU:CD1	2.85	0.45
1:A:352:LEU:HD11	1:A:370:ILE:CD1	2.31	0.45
1:A:408:ARG:C	1:A:410:ALA:H	2.20	0.45
1:A:217:TYR:OH	2:A:601:BLR:H33	2.17	0.45
1:A:73:GLU:OE2	1:A:75:SER:OG	2.25	0.45
1:B:485:ARG:NH2	1:B:485:ARG:HB3	2.32	0.45
1:A:172:ASP:OD1	1:A:195:ARG:NH1	2.41	0.45
1:B:396:GLY:HA2	1:B:435:ARG:HD3	1.99	0.45
1:A:351:GLY:O	1:A:353:ALA:N	2.50	0.45
1:A:74:PRO:HA	1:A:77:ARG:HG3	1.98	0.45
1:B:424:ALA:CB	1:B:443:ARG:HB2	2.46	0.44
1:B:420:GLN:OE1	1:B:483:ARG:NH2	2.51	0.44
1:A:360:LEU:HD23	1:A:441:TRP:CD1	2.51	0.44
1:A:403:VAL:HG23	1:A:403:VAL:O	2.18	0.44
1:B:224:ILE:HB	1:B:272:MET:HG3	2.00	0.44
1:A:16:THR:OG1	1:A:17:ASN:N	2.49	0.44
1:A:234:ARG:H	1:A:234:ARG:HG2	1.57	0.44
1:B:319:LYS:HA	1:B:319:LYS:HD3	1.71	0.44
1:B:434:GLY:O	1:B:435:ARG:HB2	2.18	0.44
1:A:438:PHE:HB3	1:A:440:LEU:CD1	2.48	0.44
1:B:258:ILE:O	1:B:261:GLU:OE1	2.36	0.44
1:A:492:TYR:HA	1:A:495:GLU:OE1	2.17	0.44
1:B:177:TYR:OH	1:B:185:GLY:HA3	2.18	0.44
1:B:80:LEU:HD23	1:B:84:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:HIS:NE2	1:A:339:LEU:HD23	2.33	0.43
1:B:429:PHE:CE2	1:B:501:ARG:HB2	2.52	0.43
1:B:60:ALA:O	1:B:64:LEU:HG	2.18	0.43
1:B:202:LEU:HD13	1:B:453:SER:HB3	2.00	0.43
1:A:352:LEU:HG	1:A:352:LEU:H	1.52	0.43
1:A:388:LEU:O	1:A:388:LEU:HD12	2.19	0.43
1:A:445:GLU:HB3	3:A:714:HOH:O	2.18	0.43
1:B:273:SER:HA	1:B:286:ILE:O	2.18	0.43
1:A:421:GLU:O	1:A:424:ALA:HB2	2.18	0.43
1:B:37:VAL:HG22	1:B:46:THR:OG1	2.18	0.43
1:A:347:ASP:O	1:A:507:VAL:HG11	2.18	0.43
1:B:330:ARG:O	1:B:334:ILE:HD12	2.19	0.43
1:B:175:ILE:HB	1:B:187:VAL:HG13	2.00	0.43
1:A:395:LEU:HB2	1:A:438:PHE:CZ	2.43	0.43
1:B:215:GLU:OE1	3:B:708:HOH:O	2.21	0.43
1:A:324:ASP:CG	1:A:490:LYS:HZ3	2.15	0.43
1:B:303:THR:HG22	3:B:741:HOH:O	2.19	0.43
1:B:371:HIS:HA	1:B:375:ARG:O	2.18	0.43
1:B:423:ALA:HB2	1:B:445:GLU:HB2	2.00	0.43
1:A:422:VAL:HA	1:A:423:ALA:HA	1.80	0.43
1:A:347:ASP:OD2	1:A:349:VAL:HG23	2.19	0.42
1:A:346:VAL:HG13	1:A:348:PHE:N	2.34	0.42
1:A:394:TRP:O	3:A:706:HOH:O	2.21	0.42
1:A:506:ASP:OD2	1:B:502:ARG:NH2	2.53	0.42
1:B:243:GLU:HG3	1:B:244:PRO:HD2	2.01	0.42
1:B:421:GLU:N	1:B:421:GLU:OE1	2.52	0.42
1:B:124:GLU:CD	1:B:302:ARG:HH22	2.22	0.42
1:A:218:GLN:HG3	1:A:282:LEU:HB2	2.01	0.42
1:A:159:GLU:HG3	1:A:163:GLN:NE2	2.35	0.42
1:A:388:LEU:CD1	1:A:392:ILE:HD11	2.50	0.42
1:A:511:ARG:NH1	1:B:509:LEU:O	2.52	0.42
1:B:444:PRO:O	1:B:445:GLU:HB3	2.18	0.42
1:B:473:LYS:HE3	1:B:473:LYS:HB3	1.76	0.42
1:A:491:ALA:O	1:A:495:GLU:OE1	2.38	0.42
1:B:458:LYS:HB2	1:B:461:GLU:HG2	2.02	0.42
1:A:377:THR:O	1:A:377:THR:HG23	2.20	0.41
1:A:338:LEU:HD23	1:A:352:LEU:HB3	2.03	0.41
1:B:427:MET:HA	1:B:428:ALA:HA	1.66	0.41
1:A:161:VAL:HG21	1:A:312:MET:SD	2.60	0.41
1:B:263:LEU:HD22	1:B:268:VAL:HG21	2.03	0.41
1:B:341:ARG:NH2	1:B:351:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LYS:HE3	1:A:473:LYS:HB3	1.87	0.41
1:B:113:HIS:HE1	3:B:784:HOH:O	2.03	0.41
1:A:330:ARG:HH21	1:A:361:GLU:CD	2.21	0.41
1:A:376:THR:HA	1:A:377:THR:HG22	2.02	0.41
1:A:464:GLN:CB	1:A:465:GLY:HA3	2.51	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.91	0.41
1:A:431:MET:CG	1:A:437:ASN:HB2	2.51	0.41
1:B:149:ARG:NH1	3:B:733:HOH:O	2.51	0.41
1:B:424:ALA:N	1:B:486:CYS:HB3	2.36	0.41
1:B:197:ASP:OD1	3:B:707:HOH:O	2.21	0.41
1:B:386:GLU:C	1:B:388:LEU:N	2.74	0.41
1:A:356:GLU:HB2	1:A:379:LEU:CD2	2.48	0.41
1:A:17:ASN:O	1:A:20:ARG:HG2	2.20	0.41
1:B:368:ALA:HA	1:B:440:LEU:O	2.21	0.41
1:B:468:ARG:HE	1:B:468:ARG:H	1.69	0.41
1:A:122:GLU:OE1	1:A:250:SER:HB3	2.20	0.40
1:A:341:ARG:NH2	1:A:345:GLU:OE2	2.54	0.40
1:A:13:VAL:HA	1:A:14:ASP:HB3	2.03	0.40
1:A:510:GLN:N	1:A:510:GLN:OE1	2.54	0.40
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.85	0.40
1:B:427:MET:CB	1:B:441:TRP:HB2	2.48	0.40
1:A:175:ILE:HG22	1:A:190:GLU:HG3	2.02	0.40
1:A:363:VAL:HB	1:A:493:GLU:CG	2.51	0.40
1:A:351:GLY:C	1:A:353:ALA:N	2.72	0.40
1:A:511:ARG:HH12	1:B:511:ARG:CB	2.35	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:A:344:ARG:NH2	1:B:103:GLY:O[3_545]	2.18	0.02

## 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	501/513 (98%)	433 (86%)	47 (9%)	21 (4%)	3	1
1	B	501/513 (98%)	444 (89%)	38 (8%)	19 (4%)	3	1
All	All	1002/1026 (98%)	877 (88%)	85 (8%)	40 (4%)	3	1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	327	GLN
1	A	328	ARG
1	A	347	ASP
1	A	349	VAL
1	A	351	GLY
1	A	377	THR
1	A	385	ASP
1	A	435	ARG
1	A	464	GLN
1	B	346	VAL
1	B	375	ARG
1	B	385	ASP
1	B	393	GLU
1	A	195	ARG
1	A	352	LEU
1	A	419	PHE
1	A	422	VAL
1	B	12	GLU
1	B	127	SER
1	B	389	THR
1	B	445	GLU
1	B	487	LEU
1	A	350	SER
1	A	371	HIS
1	A	384	SER
1	B	102	ASP
1	B	388	LEU
1	B	428	ALA
1	B	434	GLY
1	A	420	GLN
1	A	421	GLU
1	B	390	GLY

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Mol	Chain	Res	Type
1	B	511	ARG
1	A	15	LEU
1	A	397	SER
1	B	13	VAL
1	B	397	SER
1	B	396	GLY
1	B	465	GLY

### 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	417/425 (98%)	406 (97%)	11 (3%)	46	55
1	B	417/425 (98%)	402 (96%)	15 (4%)	35	42
All	All	834/850 (98%)	808 (97%)	26 (3%)	40	48

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	ARG
1	A	223	ARG
1	A	295	ARG
1	A	341	ARG
1	A	366	HIS
1	A	375	ARG
1	A	385	ASP
1	A	404	PHE
1	A	436	ASN
1	A	472	ARG
1	A	492	TYR
1	B	47	HIS
1	B	129	ARG
1	B	152	ARG
1	B	223	ARG
1	B	231	GLN

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Mol	Chain	Res	Type
1	B	261	GLU
1	B	340	GLU
1	B	356	GLU
1	B	375	ARG
1	B	401	GLU
1	B	419	PHE
1	B	427	MET
1	B	435	ARG
1	B	468	ARG
1	B	502	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	335	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	BLR	B	601	1	34,46,46	5.56	16 (47%)	38,67,67	1.75	7 (18%)
2	BLR	A	601	1	34,46,46	5.62	16 (47%)	38,67,67	1.91	6 (15%)

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	BLR	B	601	1	-	8/20/58/58	0/4/4/4
2	BLR	A	601	1	-	8/20/58/58	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BLR	CHA-C4D	-25.01	1.32	1.51
2	A	601	BLR	CHA-C4D	-24.84	1.32	1.51
2	A	601	BLR	C4C-NC	9.67	1.54	1.37
2	B	601	BLR	C3D-C4D	9.13	1.52	1.39
2	A	601	BLR	C1B-NB	9.09	1.53	1.37
2	B	601	BLR	C1B-NB	9.05	1.52	1.37
2	A	601	BLR	C3D-C4D	8.69	1.52	1.39
2	B	601	BLR	C4C-NC	8.54	1.52	1.37
2	A	601	BLR	C4B-NB	7.73	1.54	1.38
2	A	601	BLR	C1C-NC	7.36	1.53	1.38
2	B	601	BLR	C4B-NB	7.33	1.53	1.38
2	B	601	BLR	C1C-NC	7.14	1.53	1.38
2	A	601	BLR	C3D-C2D	3.22	1.47	1.37
2	A	601	BLR	OC-C1C	-3.12	1.17	1.23
2	A	601	BLR	C1D-CHD	3.10	1.53	1.41
2	B	601	BLR	C3D-C2D	3.07	1.46	1.37
2	A	601	BLR	C4A-CHB	3.02	1.52	1.41
2	A	601	BLR	C3B-C2B	3.00	1.43	1.37
2	B	601	BLR	C3C-C2C	2.82	1.43	1.37
2	A	601	BLR	C3C-C4C	2.81	1.50	1.45
2	B	601	BLR	OB-C4B	-2.80	1.18	1.23
2	B	601	BLR	C4A-CHB	2.74	1.51	1.41
2	B	601	BLR	OC-C1C	-2.68	1.18	1.23
2	A	601	BLR	C3C-C2C	2.57	1.42	1.37
2	B	601	BLR	C1D-CHD	2.55	1.51	1.41
2	B	601	BLR	CAC-C3C	2.48	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BLR	OB-C4B	-2.46	1.18	1.23
2	B	601	BLR	CAB-C3B	2.27	1.53	1.47
2	B	601	BLR	C3C-C4C	2.23	1.49	1.45
2	A	601	BLR	CAB-C3B	2.20	1.53	1.47
2	A	601	BLR	CAC-C3C	2.17	1.53	1.47
2	B	601	BLR	C3B-C2B	2.06	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	BLR	CAD-C3D-C4D	-8.02	121.66	127.30
2	B	601	BLR	CBD-CAD-C3D	-4.95	103.35	112.49
2	B	601	BLR	CAD-C3D-C4D	-4.79	123.93	127.30
2	B	601	BLR	C1B-NB-C4B	-4.13	105.41	110.67
2	A	601	BLR	CAD-CBD-CGD	-3.63	106.59	112.67
2	B	601	BLR	CAD-CBD-CGD	-3.56	106.69	112.67
2	A	601	BLR	C1B-NB-C4B	-3.25	106.53	110.67
2	A	601	BLR	CBD-CAD-C3D	-3.12	106.73	112.49
2	A	601	BLR	C4C-NC-C1C	-2.70	107.23	110.67
2	B	601	BLR	C4C-NC-C1C	-2.44	107.57	110.67
2	B	601	BLR	CAA-CBA-CGA	-2.41	108.62	112.67
2	A	601	BLR	C3B-C2B-C1B	2.18	110.66	108.03
2	B	601	BLR	C3B-C2B-C1B	2.12	110.59	108.03

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	BLR	C2A-C1A-CHA-C4D
2	B	601	BLR	NA-C4A-CHB-C1B
2	B	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	NB-C1B-CHB-C4A
2	B	601	BLR	C2B-C1B-CHB-C4A
2	B	601	BLR	C2C-C3C-CAC-CBC
2	A	601	BLR	C2A-C1A-CHA-C4D
2	A	601	BLR	NA-C4A-CHB-C1B
2	A	601	BLR	C3A-C4A-CHB-C1B
2	A	601	BLR	NB-C1B-CHB-C4A
2	A	601	BLR	C2C-C3C-CAC-CBC
2	B	601	BLR	C4C-C3C-CAC-CBC
2	A	601	BLR	C4C-C3C-CAC-CBC
2	B	601	BLR	C3D-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
2	A	601	BLR	C3D-C4D-CHA-C1A
2	A	601	BLR	C2B-C1B-CHB-C4A

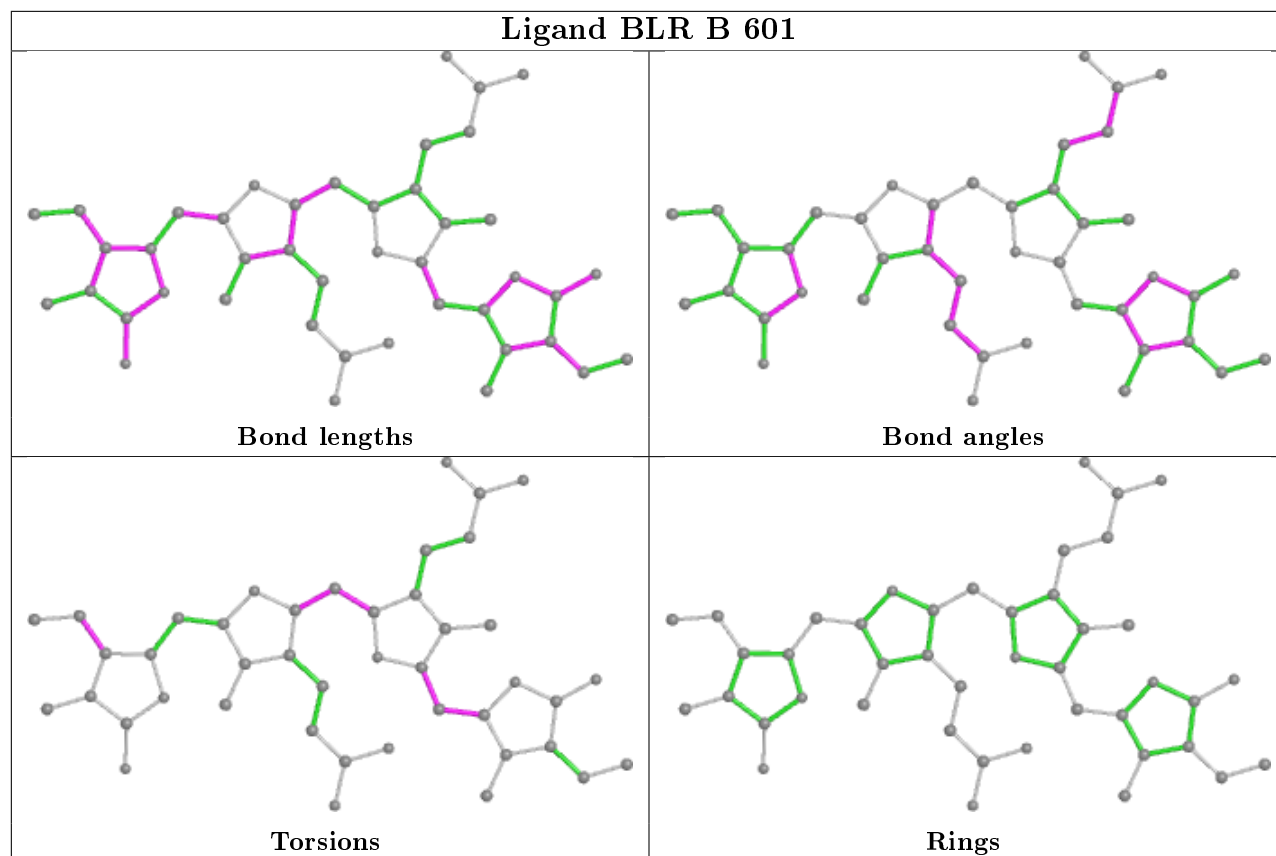
There are no ring outliers.

2 monomers are involved in 2 short contacts:

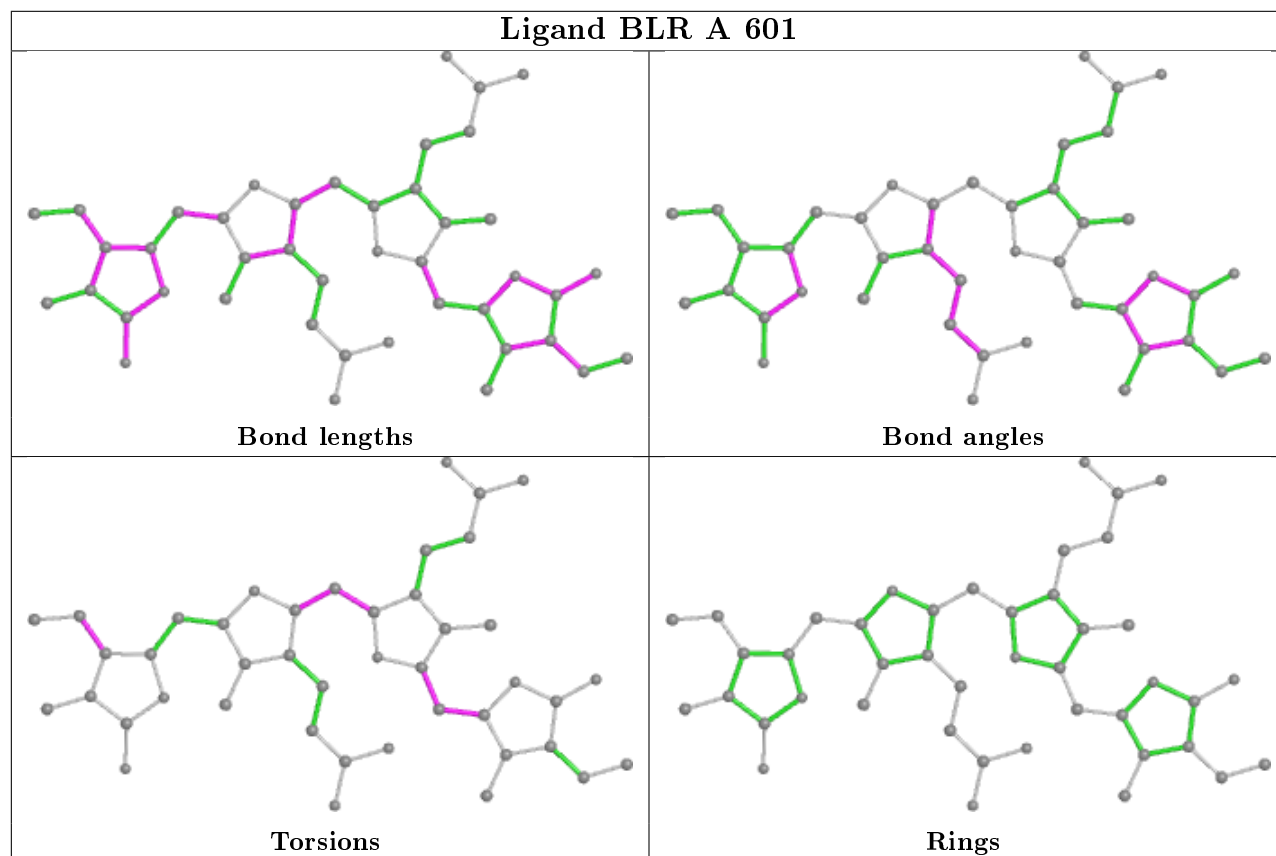
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	BLR	1	0
2	A	601	BLR	1	0

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 BLR B 601



## Ligand BLR A 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	503/513 (98%)	1.44	105 (20%) 1 1	39, 60, 122, 135	0
1	B	503/513 (98%)	0.87	66 (13%) 3 3	39, 65, 97, 128	1 (0%)
All	All	1006/1026 (98%)	1.15	171 (16%) 1 1	39, 63, 115, 135	1 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	PHE	22.7
1	A	15	LEU	17.0
1	A	13	VAL	10.6
1	B	15	LEU	10.2
1	A	411	ARG	10.1
1	A	352	LEU	9.4
1	A	399	THR	9.2
1	A	391	LEU	8.9
1	A	418	ALA	8.8
1	B	11	GLN	8.5
1	B	13	VAL	8.3
1	A	375	ARG	8.1
1	A	12	GLU	8.1
1	A	422	VAL	8.1
1	A	395	LEU	7.9
1	B	466	GLY	7.5
1	A	11	GLN	7.4
1	A	389	THR	7.4
1	B	462	PHE	7.4
1	A	343	ALA	7.3
1	A	394	TRP	7.2
1	A	420	GLN	6.8
1	A	435	ARG	6.7
1	B	469	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	14	ASP	6.6
1	A	465	GLY	6.6
1	B	16	THR	6.6
1	A	329	ILE	6.5
1	A	14	ASP	6.4
1	A	412	GLU	6.4
1	A	325	TYR	6.3
1	A	377	THR	6.2
1	B	464	GLN	6.2
1	B	463	ASP	6.1
1	A	484	GLY	6.1
1	A	417	GLN	6.1
1	A	386	GLU	6.0
1	A	446	ALA	6.0
1	A	16	THR	5.9
1	B	399	THR	5.7
1	B	467	PRO	5.7
1	A	462	PHE	5.7
1	A	383	PRO	5.6
1	A	410	ALA	5.5
1	A	398	ARG	5.2
1	B	383	PRO	5.2
1	B	12	GLU	5.1
1	A	348	PHE	5.1
1	A	425	GLY	5.1
1	A	387	ALA	5.1
1	A	463	ASP	5.1
1	A	326	ASP	5.0
1	A	376	THR	5.0
1	A	467	PRO	5.0
1	A	344	ARG	4.8
1	A	336	ALA	4.8
1	A	483	ARG	4.7
1	A	460	VAL	4.6
1	B	346	VAL	4.6
1	A	397	SER	4.6
1	A	392	ILE	4.4
1	B	378	VAL	4.4
1	B	435	ARG	4.4
1	A	374	GLY	4.4
1	A	414	PRO	4.3
1	A	416	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	325	TYR	4.2
1	A	388	LEU	4.1
1	B	400	GLY	4.1
1	A	328	ARG	4.1
1	B	401	GLU	4.0
1	A	390	GLY	4.0
1	A	492	TYR	4.0
1	A	369	ALA	4.0
1	B	468	ARG	4.0
1	B	422	VAL	4.0
1	A	350	SER	3.8
1	A	487	LEU	3.8
1	B	347	ASP	3.8
1	A	337	ALA	3.8
1	B	402	GLY	3.7
1	A	423	ALA	3.7
1	B	329	ILE	3.6
1	B	465	GLY	3.6
1	A	404	PHE	3.5
1	A	195	ARG	3.5
1	A	274	ILE	3.5
1	A	485	ARG	3.5
1	A	400	GLY	3.4
1	A	468	ARG	3.4
1	A	347	ASP	3.4
1	B	511	ARG	3.3
1	B	343	ALA	3.3
1	A	339	LEU	3.2
1	A	464	GLN	3.2
1	A	381	GLN	3.2
1	A	349	VAL	3.2
1	B	461	GLU	3.1
1	B	381	GLN	3.1
1	A	413	TYR	3.1
1	A	324	ASP	3.1
1	A	469	LEU	3.1
1	B	356	GLU	3.1
1	B	384	SER	3.0
1	A	372	PHE	3.0
1	A	286	ILE	2.9
1	A	434	GLY	2.9
1	A	444	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	438	PHE	2.8
1	B	389	THR	2.8
1	A	252	LEU	2.8
1	B	385	ASP	2.7
1	B	428	ALA	2.7
1	A	384	SER	2.6
1	A	424	ALA	2.6
1	B	512	SER	2.6
1	B	398	ARG	2.6
1	A	440	LEU	2.6
1	B	353	ALA	2.6
1	A	493	GLU	2.5
1	B	274	ILE	2.5
1	B	376	THR	2.5
1	A	285	LEU	2.5
1	A	304	ALA	2.5
1	B	252	LEU	2.5
1	A	461	GLU	2.5
1	A	488	PRO	2.4
1	A	447	VAL	2.4
1	B	37	VAL	2.4
1	B	251	VAL	2.4
1	A	340	GLU	2.4
1	A	357	SER	2.4
1	B	391	LEU	2.4
1	A	222	LEU	2.3
1	A	322	ASN	2.3
1	A	436	ASN	2.3
1	B	424	ALA	2.3
1	A	175	ILE	2.3
1	A	442	PHE	2.3
1	B	305	CYS	2.3
1	B	273	SER	2.3
1	B	426	LEU	2.2
1	B	101	VAL	2.2
1	A	445	GLU	2.2
1	A	333	SER	2.2
1	A	176	ILE	2.2
1	A	373	HIS	2.2
1	B	373	HIS	2.2
1	B	397	SER	2.2
1	A	288	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	131	ALA	2.2
1	B	362	LEU	2.2
1	B	434	GLY	2.2
1	B	328	ARG	2.2
1	B	222	LEU	2.1
1	B	247	LEU	2.1
1	B	379	LEU	2.1
1	B	386	GLU	2.1
1	B	111	ILE	2.1
1	A	466	GLY	2.1
1	B	224	ILE	2.1
1	B	344	ARG	2.1
1	B	420	GLN	2.1
1	B	36	LEU	2.1
1	B	419	PHE	2.1
1	A	457	THR	2.1
1	B	119	LEU	2.1
1	A	482	VAL	2.0
1	B	392	ILE	2.0
1	A	273	SER	2.0
1	A	378	VAL	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

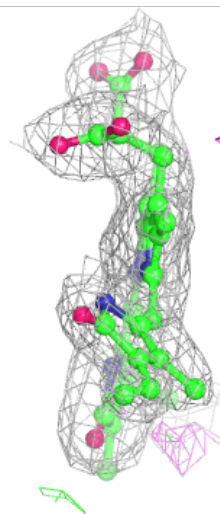
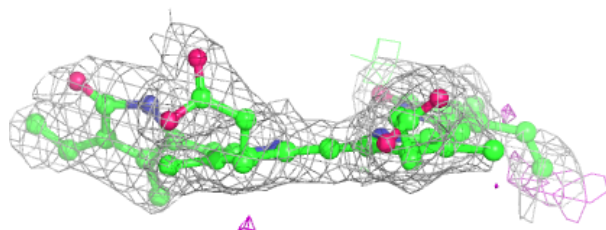
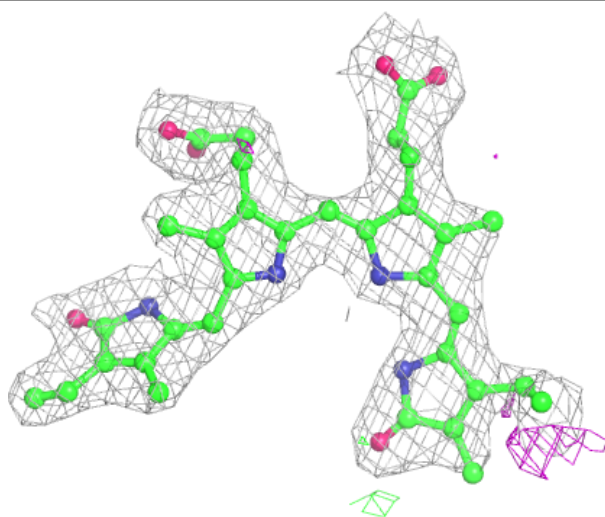
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

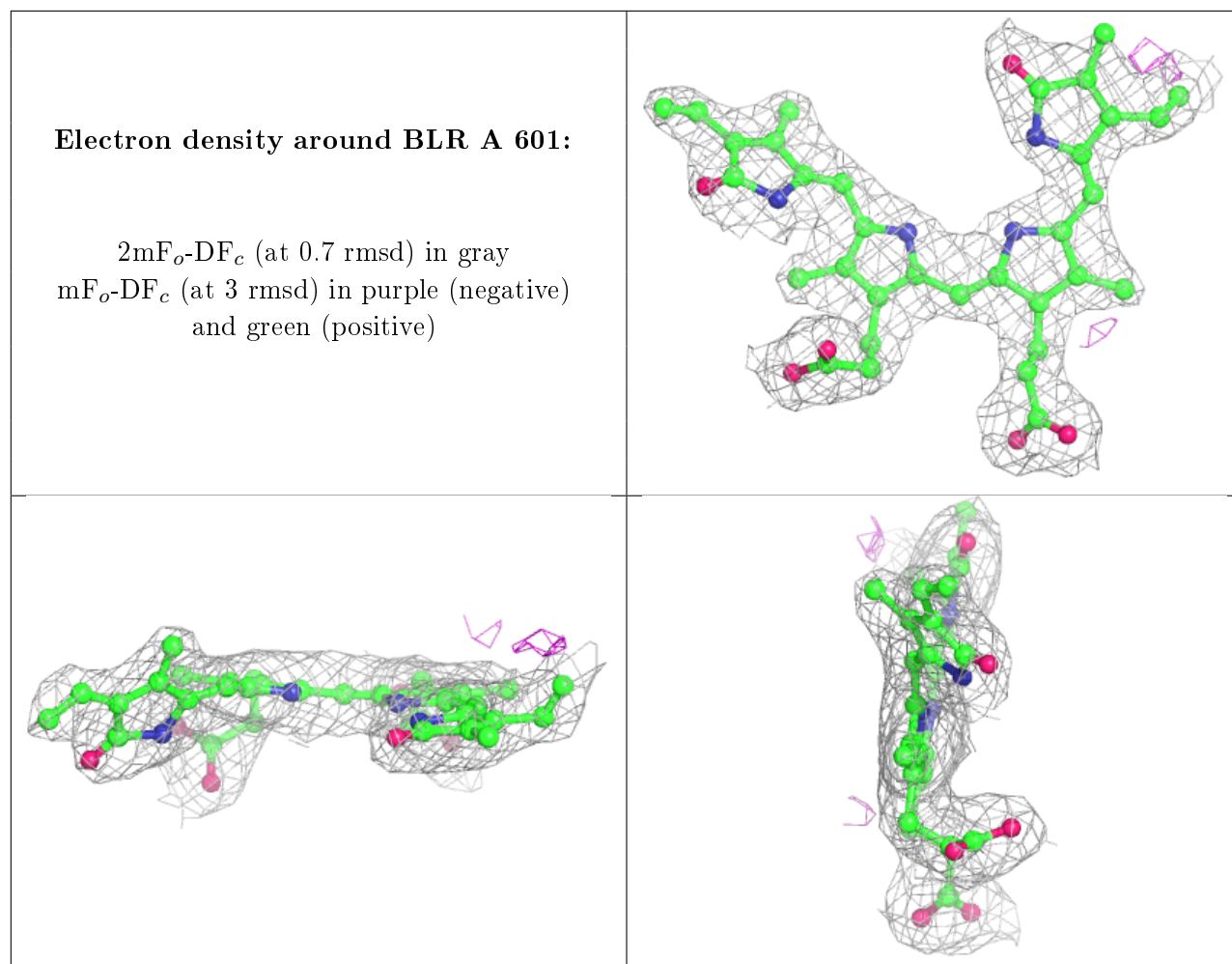
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BLR	B	601	43/43	0.93	0.18	39,50,63,72	1
2	BLR	A	601	43/43	0.94	0.17	41,49,64,75	0

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 BLR 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.