



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:57 AM UTC

PDB ID : 6BAO / pdb_00006bao
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

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

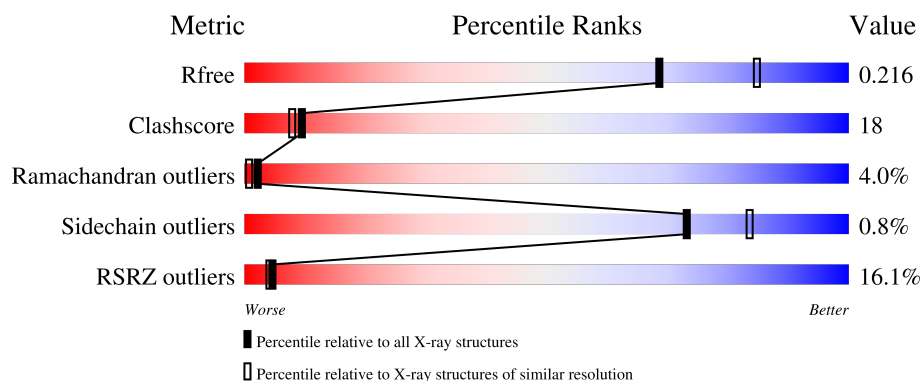
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (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 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	513	20% 63% 30% .
1	B	513	12% 69% 24% 5% .

2 Entry composition [i](#)

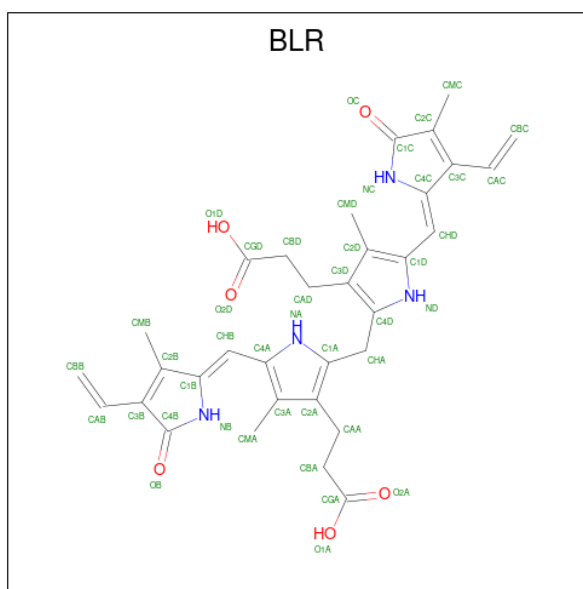
There are 3 unique types of molecules in this entry. The entry contains 8281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	503	Total	C	N	O	S	0	0	0
			3962	2500	722	727	13			
1	B	503	Total	C	N	O	S	0	0	0
			3962	2500	722	727	13			

- 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 (CCD ID: BLR) (formula: C₃₃H₃₆N₄O₆).

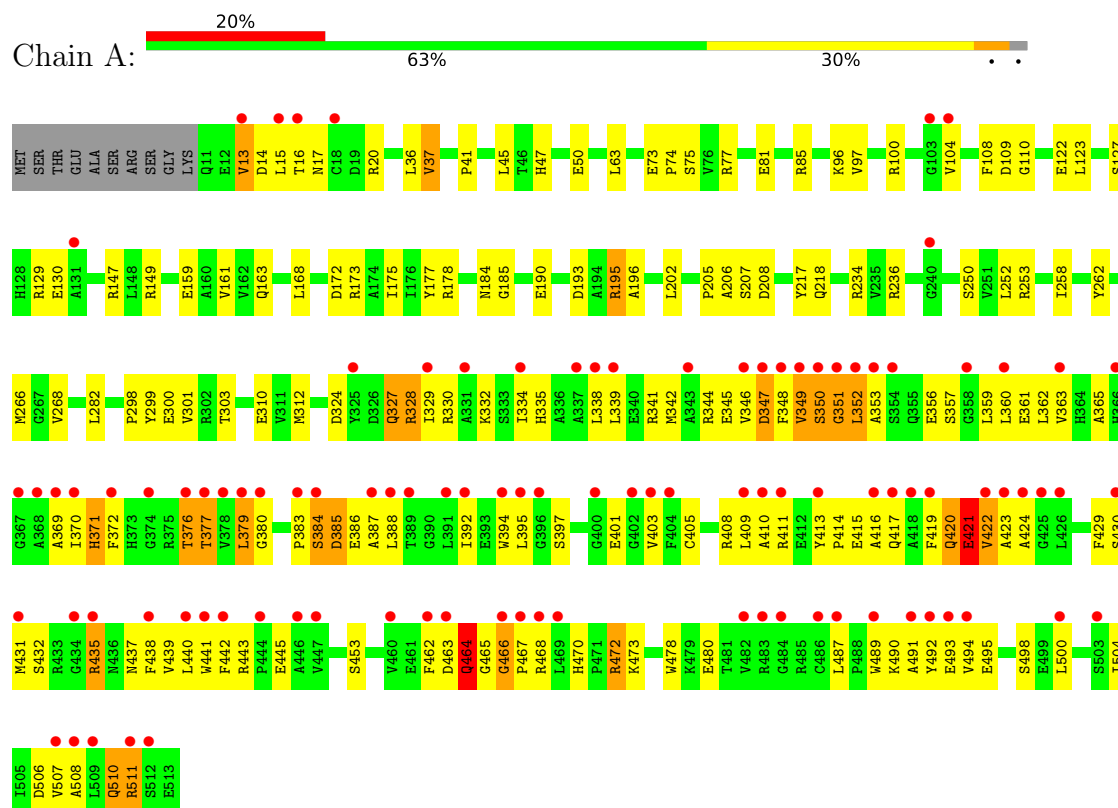


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total 134	O 134	0	0
3	B	137	Total 137	O 137	0	0

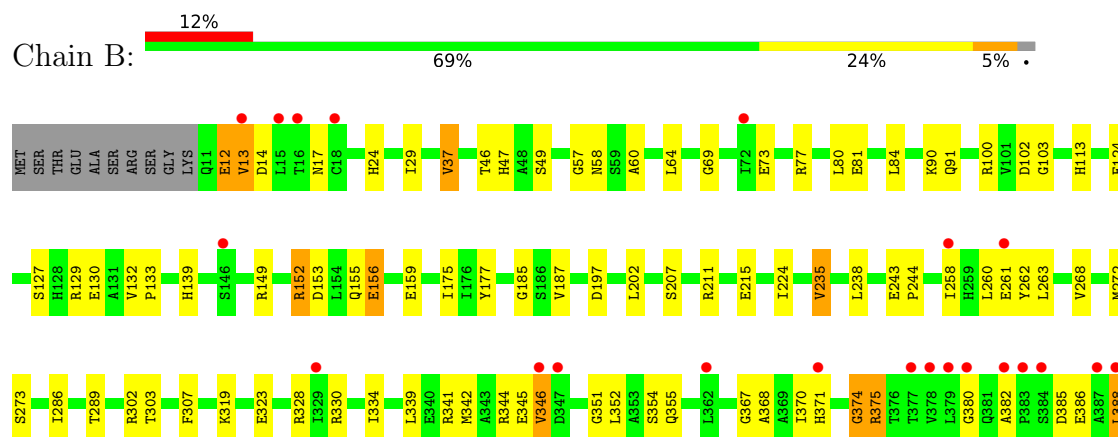
3 Residue-property plots [i](#)

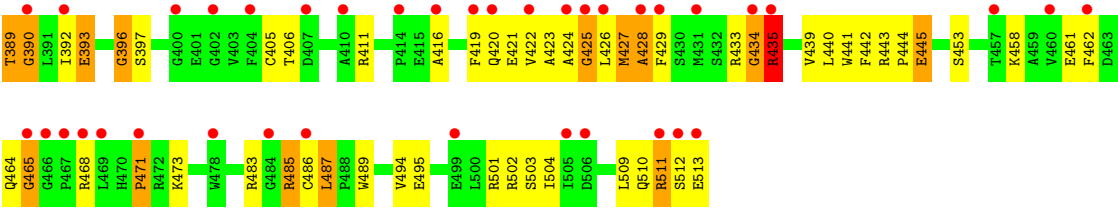
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photoreceptor-histidine kinase BphP



• Molecule 1: Photoreceptor-histidine kinase BphP





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.220 , 0.262 0.218 , 0.216	Depositor DCC
R_{free} test set	2903 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: 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	0.52	5/4054 (0.1%)	0.79	11/5501 (0.2%)
1	B	0.63	8/4054 (0.2%)	0.75	10/5501 (0.2%)
All	All	0.58	13/8108 (0.2%)	0.77	21/11002 (0.2%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	PRO	N-CD	-18.47	1.21	1.47
1	A	511	ARG	NE-CZ	-10.69	1.21	1.33
1	B	435	ARG	NE-CZ	-9.40	1.22	1.33
1	B	435	ARG	CZ-NH2	-9.12	1.21	1.33
1	B	435	ARG	CD-NE	-8.61	1.34	1.46
1	A	511	ARG	CZ-NH1	-8.48	1.20	1.32
1	B	152	ARG	CZ-NH1	-8.32	1.21	1.32
1	A	110	GLY	CA-C	-8.16	1.46	1.52
1	B	435	ARG	CZ-NH1	-6.17	1.24	1.32
1	B	152	ARG	CD-NE	-5.49	1.38	1.46
1	A	109	ASP	C-N	-5.47	1.29	1.33
1	B	152	ARG	NE-CZ	-5.36	1.27	1.33
1	A	511	ARG	CZ-NH2	-5.25	1.26	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	THR	CA-C-N	8.31	136.66	121.70
1	A	376	THR	C-N-CA	8.31	136.66	121.70
1	A	511	ARG	NE-CZ-NH1	-8.20	113.31	121.50
1	B	152	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	B	374	GLY	CA-C-N	5.90	132.31	121.70
1	B	374	GLY	C-N-CA	5.90	132.31	121.70
1	B	152	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	B	487	LEU	CA-CB-CG	5.71	136.30	116.30
1	B	425	GLY	N-CA-C	-5.47	97.43	113.30
1	A	421	GLU	CA-C-N	5.30	131.25	121.70
1	A	421	GLU	C-N-CA	5.30	131.25	121.70
1	A	379	LEU	N-CA-C	5.30	122.08	110.80
1	A	13	VAL	CA-C-N	5.15	130.96	121.70
1	A	13	VAL	C-N-CA	5.15	130.96	121.70
1	B	156	GLU	CB-CG-CD	-5.13	103.88	112.60
1	A	464	GLN	CA-C-N	5.12	130.91	121.70
1	A	464	GLN	C-N-CA	5.12	130.91	121.70
1	B	510	GLN	CA-C-N	5.10	130.88	121.70
1	B	510	GLN	C-N-CA	5.10	130.88	121.70
1	A	110	GLY	O-C-N	-5.06	119.71	123.61
1	B	152	ARG	CA-CB-CG	5.06	124.22	114.10

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	168	1
1	B	3962	0	3908	128	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	285	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 18.

All (285) 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:HA	1:B:435:ARG:HH11	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:O	1:A:341:ARG:NH1	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:37:VAL:HG13	1:B:47:HIS:HB2	1.65	0.78
1:B:341:ARG:NH2	1:B:355:GLN:HG2	1.97	0.78
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:492:TYR:HA	1:A:495:GLU:CD	2.12	0.74
1:B:512:SER:OG	1:B:513:GLU:N	2.17	0.74
1:A:266:MET:HB2	3:A:705:HOH:O	1.87	0.73
1:A:208:ASP:CG	1:A:472:ARG:HH12	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:352:LEU:C	1:A:352:LEU:HD12	2.14	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:B:374:GLY:CA	1:B:375:ARG:HB2	2.22	0.69
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
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:HA	1:A:468:ARG:NE	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:B:342:MET:HE3	1:B:352:LEU:HD11	1.82	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:VAL:C	1:A:351:GLY:H	2.09	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:A:405:CYS:HG	1:A:489:TRP:CD1	2.21	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
1:B:392:ILE:O	1:B:393:GLU:HG2	2.05	0.56
1:A:351:GLY:C	1:A:353:ALA:H	2.13	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:416:ALA:C	1:A:420:GLN:HA	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:324:ASP:CG	1:A:490:LYS:HZ3	2.15	0.53
1:A:147:ARG:HA	1:B:91:GLN:HG2	1.90	0.52
1:B:435:ARG:HA	1:B:435:ARG:NH1	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:383:PRO:C	1:A:385:ASP:H	2.17	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: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
1:A:478:TRP:HZ3	1:A:480:GLU:HB2	1.76	0.51
1:B:77:ARG:O	1:B:81:GLU:HG3	2.11	0.51
1:B:345:GLU:O	3:B:704:HOH:O	2.19	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:B:427:MET:HE1	1:B:494:VAL:HA	1.93	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:356:GLU:OE1	1:A:357:SER:OG	2.18	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:A:401:GLU:CG	1:A:435:ARG:HH21	2.25	0.50
1:A:352:LEU:C	1:A:352:LEU:CD1	2.85	0.50
1:A:408:ARG:C	1:A:410:ALA:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:330:ARG:HH21	1:A:361:GLU:CD	2.21	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:342:MET:HB3	1:A:507:VAL:HG11	1.96	0.47
1:A:384:SER:HB2	1:A:387:ALA:HB3	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
1:A:129:ARG:NH2	1:A:298:PRO:HB3	2.30	0.47
1:B:124:GLU:CD	1:B:302:ARG:HH22	2.22	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: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:B:386:GLU:C	1:B:388:LEU:N	2.74	0.45
1:A:352:LEU:HD11	1:A:370:ILE:CD1	2.31	0.45
1:A:217:TYR:OH	2:A:601:BLR:H33	2.17	0.45
1:B:485:ARG:HB3	1:B:485:ARG:NH2	2.32	0.45
1:A:172:ASP:OD1	1:A:195:ARG:NH1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLY:C	1:A:353:ALA:N	2.72	0.45
1:B:396:GLY:HA2	1:B:435:ARG:HD3	1.99	0.45
1:A:74:PRO:HA	1:A:77:ARG:HG3	1.98	0.45
1:A:351:GLY:O	1:A:353:ALA:N	2.50	0.45
1:A:511:ARG:HH22	1:B:511:ARG:C	2.24	0.44
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:A:73:GLU:OE2	1:A:75:SER:OG	2.25	0.44
1:B:80:LEU:HD23	1:B:84:LEU:HD12	2.00	0.44
1:B:177:TYR:OH	1:B:185:GLY:HA3	2.18	0.44
1:A:335:HIS:NE2	1:A:339:LEU:HD23	2.33	0.43
1:B:439:VAL:C	1:B:440:LEU:HD12	2.43	0.43
1:B:60:ALA:O	1:B:64:LEU:HG	2.18	0.43
1:B:429:PHE:CE2	1:B:501:ARG:HB2	2.52	0.43
1:B:202:LEU:HD13	1:B:453:SER:HB3	2.00	0.43
1:A:352:LEU:H	1:A:352:LEU:HG	1.52	0.43
1:A:388:LEU:HD12	1:A:388:LEU:O	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:A:490:LYS:O	1:A:491:ALA:C	2.61	0.43
1:B:330:ARG:O	1:B:334:ILE:HD12	2.19	0.43
1:B:427:MET:HE1	1:B:494:VAL:HG22	1.99	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:A:429:PHE:CD1	1:A:429:PHE:C	2.96	0.43
1:B:215:GLU:OE1	3:B:708:HOH:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:B:421:GLU:N	2.52	0.42
1:A:218:GLN:HG3	1:A:282:LEU:HB2	2.01	0.42
1:B:342:MET:HE1	1:B:504:ILE:HG23	2.00	0.42
1:A:252:LEU:O	1:A:253:ARG:C	2.63	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
1:B:433:ARG:HD3	1:B:433:ARG:C	2.45	0.41
1:A:473:LYS:HB3	1:A:473:LYS:HE3	1.87	0.41
1:B:113:HIS:HE1	3:B:784:HOH:O	2.03	0.41
1:A:130:GLU:H	1:A:130:GLU:CD	2.24	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:A:349:VAL:C	1:A:351:GLY:N	2.78	0.41
1:A:356:GLU:HB2	1:A:379:LEU:CD2	2.48	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:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:PRO:C	1:A:416:ALA:N	2.79	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: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 [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	501/513 (98%)	433 (86%)	47 (9%)	21 (4%)	2	0
1	B	501/513 (98%)	444 (89%)	38 (8%)	19 (4%)	2	1
All	All	1002/1026 (98%)	877 (88%)	85 (8%)	40 (4%)	2	1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	327	GLN
1	A	328	ARG

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Mol	Chain	Res	Type
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
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%)	414 (99%)	3 (1%)	76	86
1	B	417/425 (98%)	413 (99%)	4 (1%)	68	79
All	All	834/850 (98%)	827 (99%)	7 (1%)	73	83

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

Mol	Chain	Res	Type
1	A	37	VAL
1	A	268	VAL
1	A	472	ARG
1	B	37	VAL
1	B	235	VAL
1	B	427	MET
1	B	435	ARG

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	91	GLN
1	A	128	HIS
1	A	184	ASN
1	A	335	HIS
1	B	128	HIS
1	B	203	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	46,46,46	3.40	20 (43%)	66,67,67	1.82	18 (27%)
2	BLR	A	601	1	46,46,46	3.52	22 (47%)	66,67,67	1.74	16 (24%)

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	-	10/26/58/58	0/4/4/4
2	BLR	A	601	1	-	10/26/58/58	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BLR	C4C-NC	9.47	1.54	1.37
2	A	601	BLR	C1B-NB	8.91	1.53	1.37
2	B	601	BLR	C1B-NB	8.87	1.52	1.37
2	B	601	BLR	C4C-NC	8.37	1.52	1.37
2	B	601	BLR	C1D-ND	7.42	1.50	1.37
2	A	601	BLR	C1D-ND	7.31	1.50	1.37
2	A	601	BLR	C4B-NB	6.96	1.54	1.38
2	B	601	BLR	C4D-ND	6.90	1.52	1.37
2	A	601	BLR	C4D-ND	6.63	1.51	1.37
2	A	601	BLR	C1C-NC	6.63	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BLR	C4B-NB	6.60	1.53	1.38
2	B	601	BLR	C1C-NC	6.42	1.53	1.38
2	A	601	BLR	CHD-C1D	5.65	1.53	1.40
2	A	601	BLR	CHB-C4A	5.51	1.52	1.40
2	B	601	BLR	C4D-C3D	5.31	1.52	1.39
2	A	601	BLR	C4D-C3D	5.05	1.52	1.39
2	B	601	BLR	CHB-C4A	5.05	1.51	1.40
2	B	601	BLR	CHD-C1D	4.71	1.51	1.40
2	B	601	BLR	CHA-C4D	-4.38	1.32	1.49
2	A	601	BLR	CHA-C4D	-4.35	1.32	1.49
2	A	601	BLR	C3D-C2D	3.19	1.47	1.38
2	B	601	BLR	CHB-C1B	-3.16	1.30	1.37
2	A	601	BLR	OC-C1C	-3.12	1.17	1.23
2	A	601	BLR	C3B-C2B	3.05	1.43	1.37
2	B	601	BLR	CHD-C4C	-3.04	1.30	1.37
2	B	601	BLR	C3D-C2D	3.01	1.46	1.38
2	B	601	BLR	C3C-C2C	2.87	1.43	1.37
2	A	601	BLR	CHB-C1B	-2.86	1.31	1.37
2	B	601	BLR	OB-C4B	-2.79	1.18	1.23
2	A	601	BLR	C1D-C2D	2.77	1.48	1.41
2	B	601	BLR	OC-C1C	-2.67	1.18	1.23
2	A	601	BLR	C3C-C2C	2.62	1.42	1.37
2	B	601	BLR	CAC-C3C	2.55	1.54	1.47
2	A	601	BLR	OB-C4B	-2.45	1.18	1.23
2	A	601	BLR	C3C-C4C	2.39	1.50	1.45
2	B	601	BLR	C1D-C2D	2.36	1.47	1.41
2	B	601	BLR	CAB-C3B	2.34	1.53	1.47
2	A	601	BLR	CAB-C3B	2.26	1.53	1.47
2	A	601	BLR	CAC-C3C	2.23	1.53	1.47
2	A	601	BLR	CHD-C4C	-2.16	1.32	1.37
2	B	601	BLR	C3B-C2B	2.12	1.41	1.37
2	A	601	BLR	CMA-C3A	2.03	1.54	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	BLR	CHA-C4D-ND	6.08	134.39	122.04
2	B	601	BLR	CHA-C4D-ND	5.28	132.77	122.04
2	A	601	BLR	CHA-C4D-C3D	-4.62	121.23	130.07
2	B	601	BLR	C1B-NB-C4B	-4.28	105.41	110.66
2	B	601	BLR	CHA-C4D-C3D	-4.25	121.95	130.07
2	A	601	BLR	C4D-CHA-C1A	3.59	129.60	115.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BLR	CHD-C1D-C2D	-3.39	119.23	127.53
2	A	601	BLR	C1B-NB-C4B	-3.36	106.53	110.66
2	B	601	BLR	CBD-CAD-C3D	-3.32	103.35	112.53
2	B	601	BLR	C4D-CHA-C1A	3.32	128.56	115.77
2	A	601	BLR	C4D-C3D-C2D	3.23	111.18	107.33
2	A	601	BLR	C4C-NC-C1C	-2.79	107.23	110.66
2	B	601	BLR	C4D-C3D-C2D	2.73	110.59	107.33
2	B	601	BLR	CHA-C1A-C2A	-2.72	124.87	130.07
2	A	601	BLR	CAD-CBD-CGD	-2.67	106.59	113.67
2	B	601	BLR	CAD-CBD-CGD	-2.63	106.69	113.67
2	B	601	BLR	CMA-C3A-C4A	2.58	129.37	125.62
2	B	601	BLR	C4A-CHB-C1B	-2.57	123.42	130.82
2	B	601	BLR	C4C-NC-C1C	-2.52	107.57	110.66
2	A	601	BLR	C3B-C2B-C1B	2.46	110.66	107.92
2	B	601	BLR	C3B-C2B-C1B	2.40	110.59	107.92
2	A	601	BLR	C3D-C4D-ND	-2.38	104.35	107.77
2	A	601	BLR	CHD-C1D-C2D	-2.36	121.73	127.53
2	B	601	BLR	C2D-C1D-ND	2.35	110.64	107.43
2	B	601	BLR	O1D-CGD-CBD	2.31	121.30	114.00
2	A	601	BLR	CHA-C1A-C2A	-2.23	125.81	130.07
2	A	601	BLR	C1D-CHD-C4C	-2.18	124.56	130.82
2	B	601	BLR	C1D-CHD-C4C	-2.17	124.58	130.82
2	B	601	BLR	CHD-C1D-ND	2.14	130.12	125.29
2	A	601	BLR	O1A-CGA-CBA	2.10	120.63	114.00
2	A	601	BLR	CBD-CAD-C3D	-2.10	106.73	112.53
2	A	601	BLR	C4A-CHB-C1B	-2.09	124.81	130.82
2	A	601	BLR	CMA-C3A-C4A	2.02	128.56	125.62
2	B	601	BLR	CHA-C1A-NA	2.01	126.13	122.04

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BLR	C2C-C3C-CAC-CBC
2	B	601	BLR	C2C-C3C-CAC-CBC
2	A	601	BLR	NA-C4A-CHB-C1B
2	B	601	BLR	NA-C4A-CHB-C1B
2	A	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	C2B-C1B-CHB-C4A
2	B	601	BLR	NB-C1B-CHB-C4A
2	A	601	BLR	NB-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
2	A	601	BLR	C4C-C3C-CAC-CBC
2	B	601	BLR	C4C-C3C-CAC-CBC
2	A	601	BLR	C2B-C1B-CHB-C4A
2	B	601	BLR	CAD-CBD-CGD-O2D
2	B	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	CAA-CBA-CGA-O2A
2	A	601	BLR	CAA-CBA-CGA-O1A
2	A	601	BLR	CAD-CBD-CGD-O2D
2	B	601	BLR	CAA-CBA-CGA-O2A
2	B	601	BLR	CAA-CBA-CGA-O1A

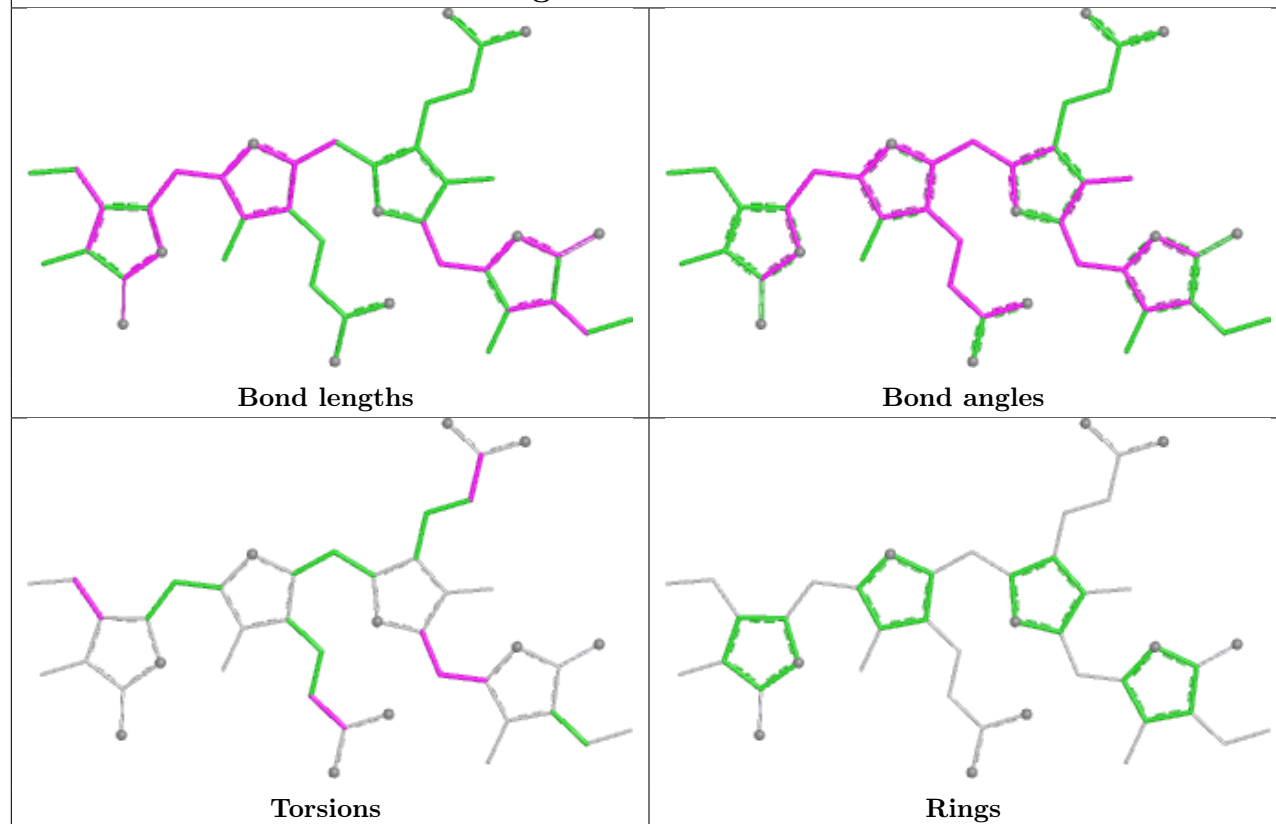
There are no ring outliers.

2 monomers are involved in 2 short contacts:

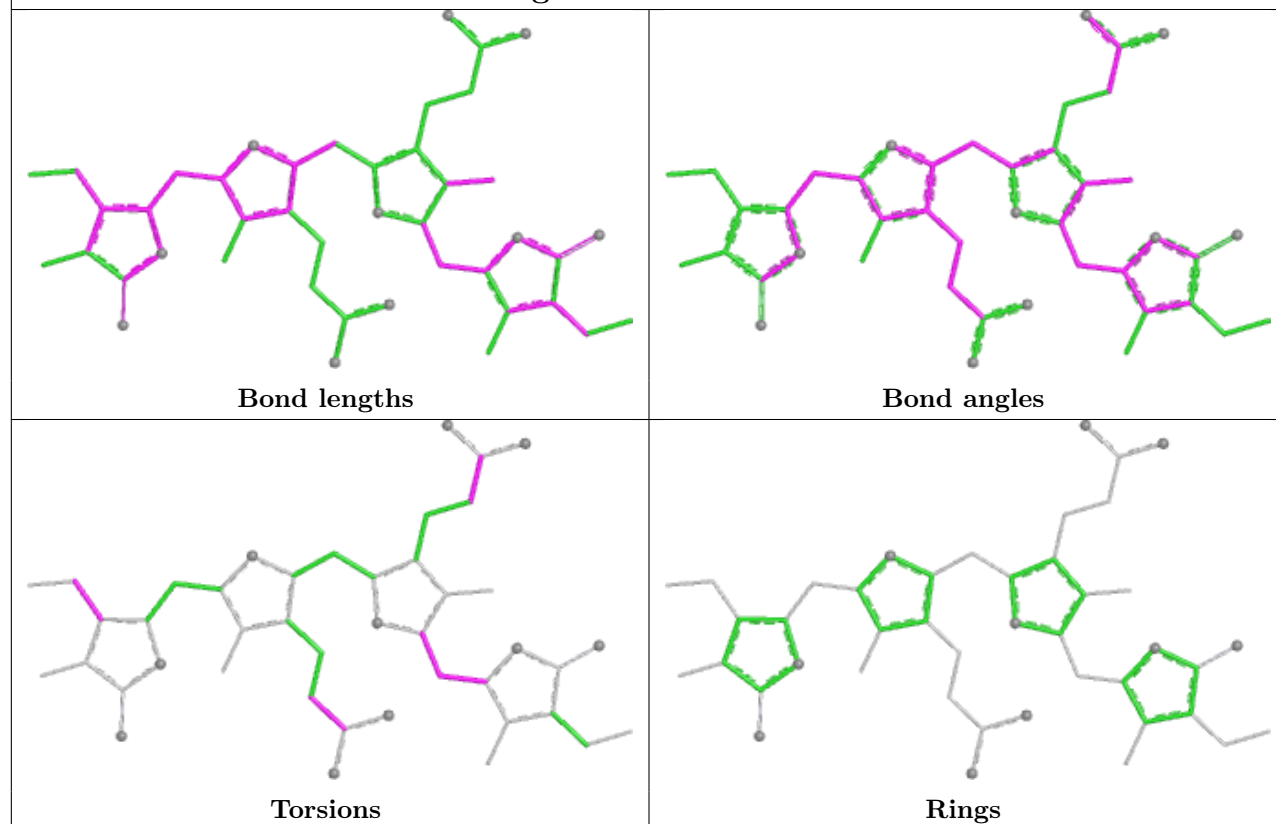
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	BLR	1	0
2	A	601	BLR	1	0

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, 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	503/513 (98%)	1.03	102 (20%) 3 2	39, 60, 122, 135	0
1	B	503/513 (98%)	0.87	60 (11%) 9 8	39, 65, 97, 128	1 (0%)
All	All	1006/1026 (98%)	0.95	162 (16%) 4 4	39, 63, 115, 135	1 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	LEU	8.8
1	A	419	PHE	6.9
1	A	418	ALA	6.7
1	B	15	LEU	6.6
1	A	423	ALA	5.6
1	B	428	ALA	5.3
1	A	15	LEU	5.3
1	B	469	LEU	5.3
1	A	349	VAL	5.1
1	B	400	GLY	5.0
1	A	348	PHE	4.9
1	B	424	ALA	4.9
1	B	425	GLY	4.7
1	A	492	TYR	4.7
1	B	383	PRO	4.4
1	A	329	ILE	4.4
1	B	16	THR	4.3
1	A	16	THR	4.3
1	A	372	PHE	4.2
1	A	402	GLY	4.2
1	A	392	ILE	4.2
1	A	484	GLY	4.1
1	B	511	ARG	4.1
1	A	410	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	402	GLY	4.1
1	A	493	GLU	4.1
1	A	422	VAL	4.0
1	B	462	PHE	3.9
1	A	395	LEU	3.9
1	A	400	GLY	3.9
1	B	512	SER	3.9
1	A	376	THR	3.9
1	A	434	GLY	3.9
1	A	394	TRP	3.7
1	A	435	ARG	3.7
1	A	404	PHE	3.6
1	A	486	CYS	3.6
1	A	387	ALA	3.5
1	A	13	VAL	3.5
1	A	347	ASP	3.5
1	A	383	PRO	3.4
1	B	13	VAL	3.4
1	A	396	GLY	3.3
1	A	467	PRO	3.3
1	A	446	ALA	3.2
1	A	444	PRO	3.2
1	A	462	PHE	3.2
1	A	337	ALA	3.2
1	A	469	LEU	3.2
1	A	354	SER	3.2
1	B	466	GLY	3.1
1	A	131	ALA	3.1
1	A	343	ALA	3.1
1	A	346	VAL	3.1
1	A	409	LEU	3.1
1	B	258	ILE	3.1
1	A	104	VAL	3.1
1	A	339	LEU	3.1
1	A	350	SER	3.1
1	A	369	ALA	3.0
1	A	482	VAL	3.0
1	B	457	THR	3.0
1	A	413	TYR	3.0
1	B	388	LEU	2.9
1	A	103	GLY	2.9
1	A	425	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	465	GLY	2.9
1	A	366	HIS	2.9
1	B	431	MET	2.9
1	B	419	PHE	2.9
1	A	391	LEU	2.9
1	A	463	ASP	2.8
1	A	438	PHE	2.8
1	B	72	ILE	2.8
1	B	505	ILE	2.8
1	A	442	PHE	2.7
1	A	353	ALA	2.7
1	A	325	TYR	2.7
1	B	362	LEU	2.7
1	A	384	SER	2.7
1	B	146	SER	2.7
1	B	387	ALA	2.7
1	A	379	LEU	2.7
1	A	426	LEU	2.7
1	A	468	ARG	2.7
1	B	426	LEU	2.7
1	B	422	VAL	2.7
1	B	460	VAL	2.7
1	A	483	ARG	2.6
1	A	411	ARG	2.6
1	A	494	VAL	2.6
1	B	329	ILE	2.6
1	A	367	GLY	2.6
1	B	499	GLU	2.6
1	B	346	VAL	2.6
1	B	380	GLY	2.6
1	B	486	CYS	2.6
1	A	360	LEU	2.5
1	B	513	GLU	2.5
1	A	18	CYS	2.5
1	B	407	ASP	2.5
1	A	503	SER	2.5
1	A	388	LEU	2.5
1	A	374	GLY	2.5
1	B	434	GLY	2.5
1	A	430	SER	2.5
1	A	416	ALA	2.5
1	A	487	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	431	MET	2.5
1	B	468	ARG	2.5
1	B	379	LEU	2.4
1	A	370	ILE	2.4
1	A	508	ALA	2.4
1	A	511	ARG	2.4
1	A	380	GLY	2.4
1	A	338	LEU	2.4
1	B	392	ILE	2.4
1	B	414	PRO	2.4
1	B	471	PRO	2.4
1	A	378	VAL	2.3
1	A	512	SER	2.3
1	A	377	THR	2.3
1	B	467	PRO	2.3
1	B	478	TRP	2.3
1	A	491	ALA	2.3
1	B	347	ASP	2.3
1	B	371	HIS	2.3
1	A	334	ILE	2.3
1	A	403	VAL	2.3
1	A	389	THR	2.3
1	A	424	ALA	2.3
1	A	466	GLY	2.3
1	B	261	GLU	2.2
1	B	378	VAL	2.2
1	A	331	ALA	2.2
1	A	358	GLY	2.2
1	B	390	GLY	2.2
1	B	429	PHE	2.2
1	A	440	LEU	2.2
1	A	500	LEU	2.2
1	A	363	VAL	2.2
1	B	484	GLY	2.2
1	B	18	CYS	2.2
1	B	377	THR	2.2
1	B	404	PHE	2.1
1	B	384	SER	2.1
1	A	351	GLY	2.1
1	B	382	ALA	2.1
1	B	416	ALA	2.1
1	B	435	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	489	TRP	2.1
1	B	410	ALA	2.1
1	A	509	LEU	2.1
1	B	506	ASP	2.1
1	A	417	GLN	2.1
1	A	460	VAL	2.1
1	A	447	VAL	2.0
1	A	507	VAL	2.0
1	A	368	ALA	2.0
1	A	441	TRP	2.0
1	B	420	GLN	2.0
1	A	240	GLY	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 [i](#)

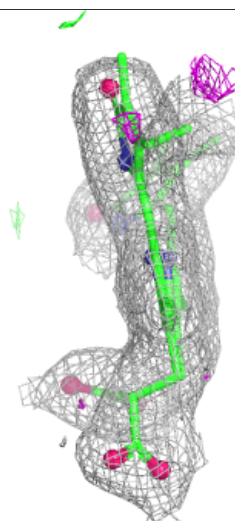
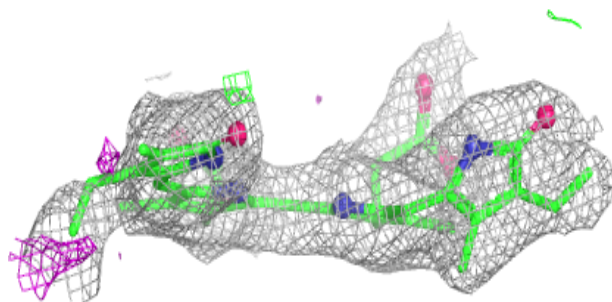
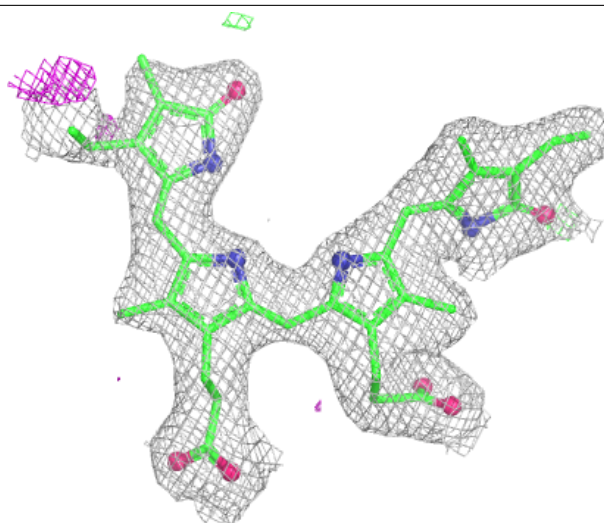
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

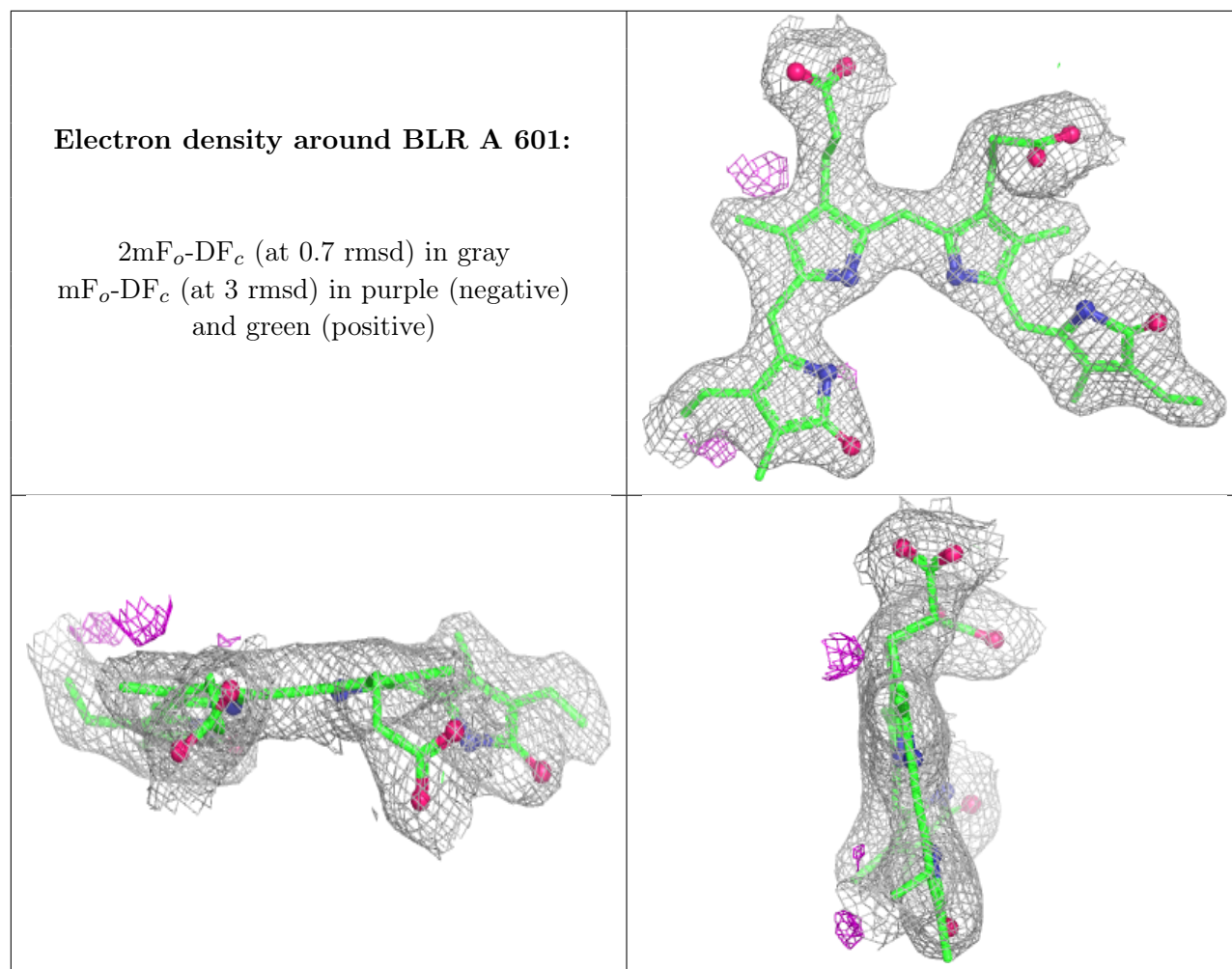
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BLR	B	601	43/43	0.95	0.09	39,50,63,72	1
2	BLR	A	601	43/43	0.96	0.09	41,49,64,75	0

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 ⓘ

There are no such residues in this entry.