



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:15 PM UTC

PDB ID : 6NDP / pdb_00006ndp
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP mutant L193Q from Xanthomonas campestris
Authors : Otero, L.H.; Sirigu, S.; Klinke, S.; Rinaldi, J.; Conforte, V.; Malamud, F.; Goldbaum, F.A.; Chavas, L.; Bonomi, H.R.
Deposited on : 2018-12-14
Resolution : 3.89 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

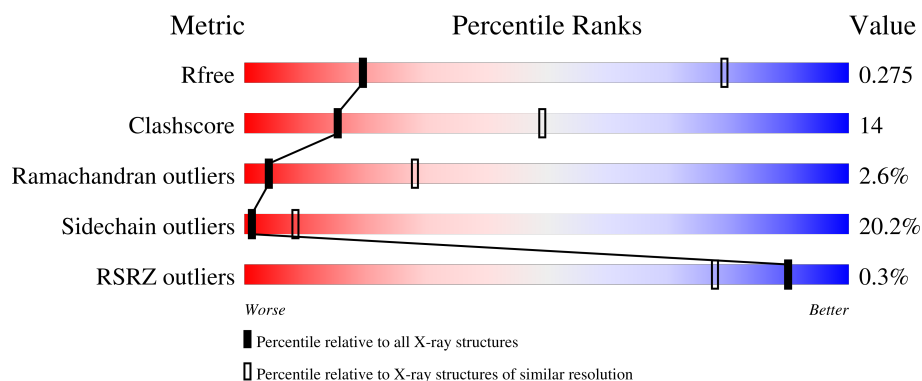
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	640	
1	B	640	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9407 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.

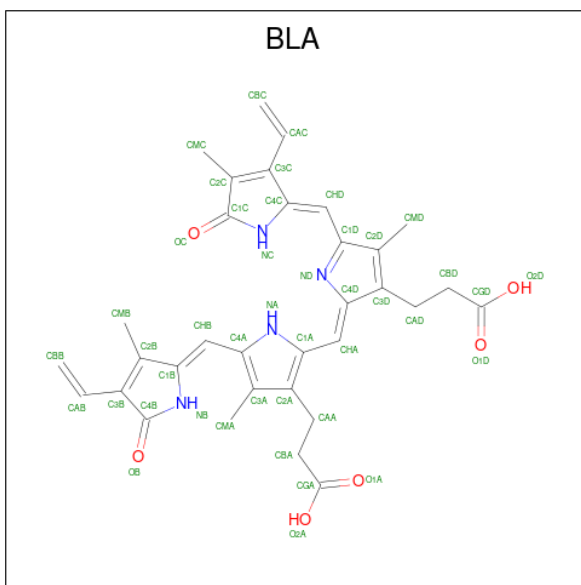
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4605	2913	838	838	16			
1	B	602	Total	C	N	O	S	0	0	0
			4716	2982	859	859	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A0H2XCS3
A	-4	HIS	-	expression tag	UNP A0A0H2XCS3
A	-3	HIS	-	expression tag	UNP A0A0H2XCS3
A	-2	HIS	-	expression tag	UNP A0A0H2XCS3
A	-1	HIS	-	expression tag	UNP A0A0H2XCS3
A	0	HIS	-	expression tag	UNP A0A0H2XCS3
A	1	HIS	-	expression tag	UNP A0A0H2XCS3
A	193	GLN	LEU	engineered mutation	UNP A0A0H2XCS3
B	-5	MET	-	initiating methionine	UNP A0A0H2XCS3
B	-4	HIS	-	expression tag	UNP A0A0H2XCS3
B	-3	HIS	-	expression tag	UNP A0A0H2XCS3
B	-2	HIS	-	expression tag	UNP A0A0H2XCS3
B	-1	HIS	-	expression tag	UNP A0A0H2XCS3
B	0	HIS	-	expression tag	UNP A0A0H2XCS3
B	1	HIS	-	expression tag	UNP A0A0H2XCS3
B	193	GLN	LEU	engineered mutation	UNP A0A0H2XCS3

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).

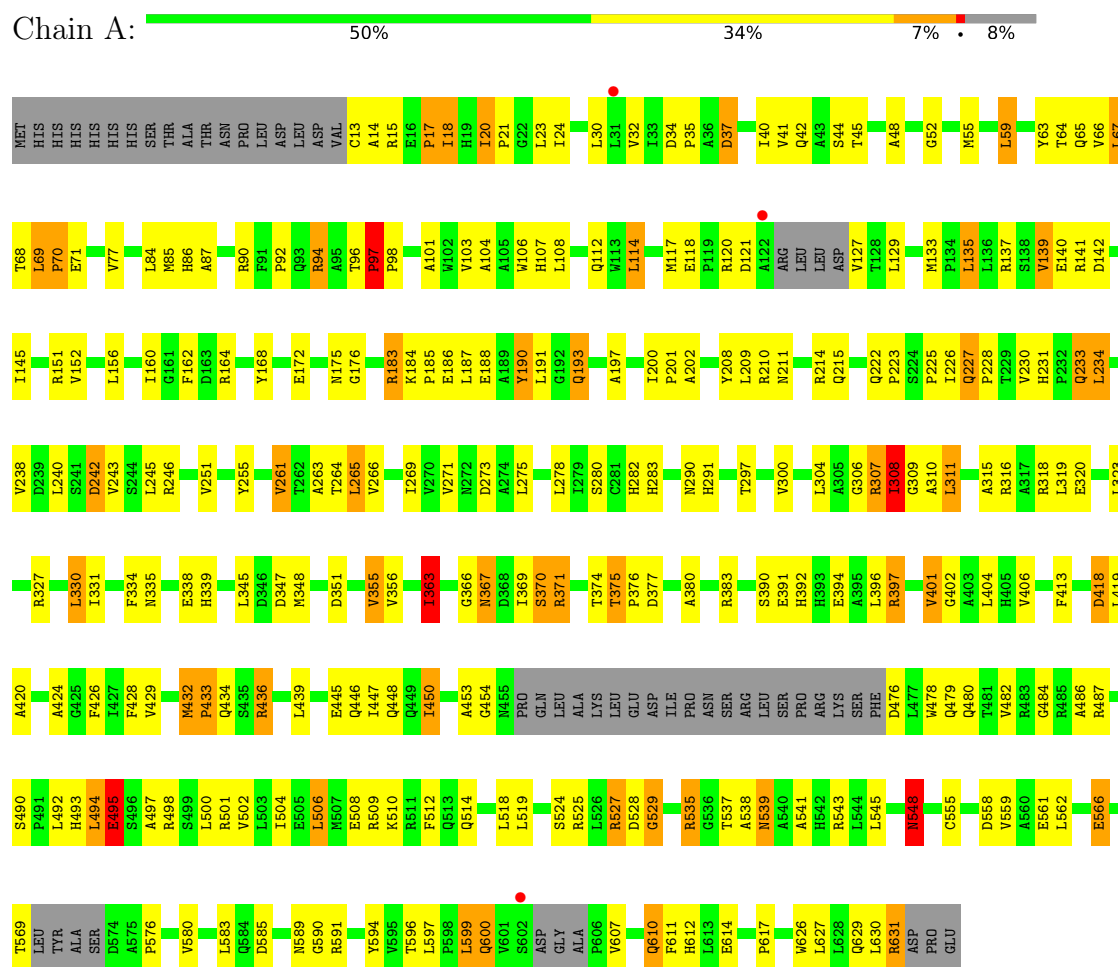


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0

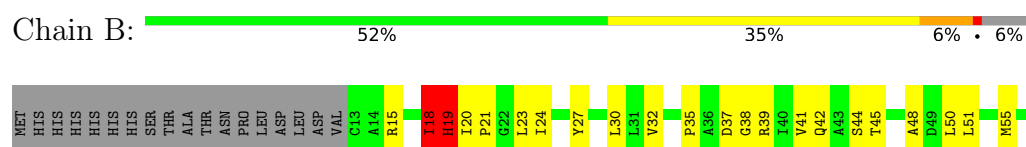
3 Residue-property plots

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: Bacteriophytochrome



• Molecule 1: Bacteriophytochrome





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.22Å 103.22Å 344.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 3.89 49.43 – 3.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.43-3.89) 99.7 (49.43-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.213 , 0.270 (Not available) , 0.275	Depositor DCC
R_{free} test set	895 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	187.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 191.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å ²)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: 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	0.88	3/4708 (0.1%)	1.46	45/6420 (0.7%)
1	B	0.89	1/4824 (0.0%)	1.45	42/6579 (0.6%)
All	All	0.89	4/9532 (0.0%)	1.45	87/12999 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	VAL	CA-C	5.17	1.59	1.52
1	A	97	PRO	CA-C	5.16	1.56	1.52
1	A	600	GLN	CA-C	5.07	1.59	1.53
1	A	121	ASP	CA-C	5.03	1.57	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASP	CA-CB-CG	9.76	122.36	112.60
1	A	142	ASP	CA-CB-CG	9.43	122.03	112.60
1	B	419	LEU	CA-C-N	7.31	129.22	120.09
1	B	419	LEU	C-N-CA	7.31	129.22	120.09
1	A	308	ILE	N-CA-CB	7.05	120.67	110.52
1	A	419	LEU	CA-C-N	7.00	128.84	120.09
1	A	419	LEU	C-N-CA	7.00	128.84	120.09
1	A	548	ASN	CA-CB-CG	6.60	119.20	112.60
1	A	539	ASN	CA-CB-CG	6.45	119.05	112.60
1	A	211	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	428	PHE	CA-C-N	6.42	128.91	123.33
1	A	428	PHE	C-N-CA	6.42	128.91	123.33
1	A	245	LEU	CA-C-N	6.37	129.80	120.82
1	A	245	LEU	C-N-CA	6.37	129.80	120.82
1	B	558	ASP	CA-C-N	6.36	128.81	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	558	ASP	C-N-CA	6.36	128.81	120.60
1	A	175	ASN	CA-CB-CG	6.36	118.96	112.60
1	A	433	PRO	CA-C-N	6.35	129.42	120.28
1	A	433	PRO	C-N-CA	6.35	129.42	120.28
1	B	367	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	18	ILE	N-CA-CB	6.21	121.48	111.23
1	A	367	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	160	ILE	N-CA-CB	6.12	117.81	110.95
1	B	73	GLN	CB-CG-CD	6.09	122.95	112.60
1	B	63	TYR	CA-C-N	6.00	129.13	120.38
1	B	63	TYR	C-N-CA	6.00	129.13	120.38
1	A	172	GLU	CB-CG-CD	5.98	122.77	112.60
1	B	197	ALA	CA-C-N	5.96	130.13	120.60
1	B	197	ALA	C-N-CA	5.96	130.13	120.60
1	B	433	PRO	CA-C-N	5.95	128.85	120.28
1	B	433	PRO	C-N-CA	5.95	128.85	120.28
1	B	601	VAL	CA-C-N	5.94	128.24	120.28
1	B	601	VAL	C-N-CA	5.94	128.24	120.28
1	B	142	ASP	N-CA-C	5.81	116.28	109.60
1	A	64	THR	CA-C-N	5.80	128.05	120.28
1	A	64	THR	C-N-CA	5.80	128.05	120.28
1	B	495	GLU	CB-CG-CD	5.77	122.41	112.60
1	B	569	THR	CA-C-N	5.72	129.40	120.82
1	B	569	THR	C-N-CA	5.72	129.40	120.82
1	B	548	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	558	ASP	CA-C-N	5.68	128.21	120.77
1	A	558	ASP	C-N-CA	5.68	128.21	120.77
1	B	290	ASN	CA-CB-CG	5.67	118.27	112.60
1	B	391	GLU	CB-CG-CD	5.63	122.17	112.60
1	A	308	ILE	N-CA-C	-5.62	105.36	110.82
1	A	273	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	18	ILE	CA-C-N	5.56	132.16	121.54
1	B	18	ILE	C-N-CA	5.56	132.16	121.54
1	B	264	THR	CA-C-N	5.53	129.08	121.33
1	B	264	THR	C-N-CA	5.53	129.08	121.33
1	A	202	ALA	CA-C-N	5.45	127.90	120.54
1	A	202	ALA	C-N-CA	5.45	127.90	120.54
1	B	397	ARG	CA-C-N	5.45	127.53	120.44
1	B	397	ARG	C-N-CA	5.45	127.53	120.44
1	A	17	PRO	CA-C-N	5.41	131.71	121.97
1	A	17	PRO	C-N-CA	5.41	131.71	121.97
1	A	476	ASP	CA-CB-CG	5.39	117.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	TYR	N-CA-C	-5.37	106.04	112.59
1	A	495	GLU	CB-CG-CD	5.36	121.71	112.60
1	B	190	TYR	N-CA-C	-5.33	106.09	112.59
1	A	453	ALA	N-CA-C	-5.33	106.62	113.23
1	B	390	SER	CA-C-N	5.31	127.39	120.28
1	B	390	SER	C-N-CA	5.31	127.39	120.28
1	A	397	ARG	CA-C-N	5.30	127.33	120.44
1	A	397	ARG	C-N-CA	5.30	127.33	120.44
1	A	242	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	197	ALA	CA-C-N	5.28	129.54	120.72
1	A	197	ALA	C-N-CA	5.28	129.54	120.72
1	A	390	SER	CA-C-N	5.26	127.33	120.28
1	A	390	SER	C-N-CA	5.26	127.33	120.28
1	B	242	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	134	PRO	CA-C-N	5.23	127.29	120.28
1	B	134	PRO	C-N-CA	5.23	127.29	120.28
1	A	37	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	315	ALA	CA-C-N	5.16	127.51	120.54
1	A	315	ALA	C-N-CA	5.16	127.51	120.54
1	B	631	ARG	CA-C-N	5.16	130.98	121.70
1	B	631	ARG	C-N-CA	5.16	130.98	121.70
1	B	273	ASP	CA-C-N	5.12	131.16	121.69
1	B	273	ASP	C-N-CA	5.12	131.16	121.69
1	A	363	ILE	N-CA-CB	5.09	116.81	111.00
1	A	370	SER	CA-C-N	5.09	128.78	121.50
1	A	370	SER	C-N-CA	5.09	128.78	121.50
1	B	411	GLU	CA-C-N	5.03	126.89	120.56
1	B	411	GLU	C-N-CA	5.03	126.89	120.56
1	B	315	ALA	CA-C-N	5.01	127.31	120.54
1	B	315	ALA	C-N-CA	5.01	127.31	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4605	0	4594	132	0
1	B	4716	0	4702	125	0
2	A	43	0	31	10	0
2	B	43	0	31	11	0
All	All	9407	0	9358	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:TYR:OH	2:B:900:BLA:HAA1	1.52	1.09
1:A:599:LEU:HG	1:A:600:GLN:H	1.25	0.98
1:B:21:PRO:HD2	1:B:240:LEU:HD23	1.55	0.89
1:A:599:LEU:HG	1:A:600:GLN:N	1.90	0.86
1:B:42:GLN:HA	1:B:228:PRO:HG2	1.56	0.86
1:A:42:GLN:HA	1:A:228:PRO:HG2	1.57	0.84
1:B:271:VAL:HG21	1:B:308:ILE:HD11	1.59	0.84
1:A:255:TYR:OH	2:A:900:BLA:CMB	2.26	0.82
1:A:94:ARG:HB3	1:A:97:PRO:HG3	1.62	0.81
1:B:439:LEU:HB2	1:B:504:ILE:HD11	1.62	0.81
1:B:454:GLY:HA2	1:B:478:TRP:CD1	2.16	0.80
1:B:450:ILE:HD12	1:B:452:TRP:HE1	1.47	0.80
1:A:454:GLY:HA2	1:A:478:TRP:HD1	1.46	0.77
1:B:251:VAL:HG11	2:B:900:BLA:HBC1	1.66	0.75
1:A:35:PRO:HD3	1:A:112:GLN:HA	1.67	0.75
1:A:70:PRO:HG3	1:A:90:ARG:HH21	1.53	0.74
1:B:35:PRO:HD3	1:B:112:GLN:HA	1.69	0.74
2:A:900:BLA:HB	2:A:900:BLA:CMA	2.00	0.74
1:A:310:ALA:HB1	1:B:272:ASN:HA	1.70	0.73
1:A:255:TYR:OH	2:A:900:BLA:HMB3	1.90	0.72
1:B:51:LEU:HG	1:B:66:VAL:HG21	1.72	0.71
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.56	0.70
1:A:208:TYR:OH	2:A:900:BLA:HAA1	1.91	0.70
1:A:454:GLY:HA2	1:A:478:TRP:CD1	2.27	0.69
1:A:307:ARG:HB3	1:A:307:ARG:CZ	2.21	0.69
1:B:610:GLN:HB2	1:B:632:ASP:HB2	1.75	0.69
1:B:601:VAL:HG11	1:B:605:ALA:O	1.93	0.67
1:A:494:LEU:HD23	1:A:498:ARG:HH21	1.60	0.67
1:A:255:TYR:OH	2:A:900:BLA:HMB1	1.92	0.67
1:A:96:THR:C	1:A:98:PRO:HD3	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:HG2	1:B:185:PRO:HD2	1.76	0.66
1:A:263:ALA:HB3	1:A:283:HIS:HB3	1.78	0.66
1:B:97:PRO:HB2	1:B:98:PRO:HD3	1.78	0.66
1:A:133:MET:HE2	1:B:295:ASP:HB3	1.78	0.65
1:B:204:ALA:O	1:B:208:TYR:HD1	1.80	0.65
1:A:509:ARG:HD3	1:B:508:GLU:HB3	1.79	0.65
1:B:263:ALA:HB3	1:B:283:HIS:HB3	1.79	0.65
1:A:535:ARG:HB2	1:A:626:TRP:CZ3	2.33	0.64
1:B:195:TYR:CZ	2:B:900:BLA:HAB	2.32	0.64
1:A:184:LYS:HG2	1:A:185:PRO:HD2	1.78	0.64
1:B:450:ILE:HD12	1:B:452:TRP:NE1	2.13	0.63
1:B:265:LEU:HD21	1:B:297:THR:HG21	1.79	0.63
1:A:17:PRO:HB2	1:A:20:ILE:HG13	1.81	0.63
1:A:183:ARG:HG3	1:A:183:ARG:NH1	2.14	0.62
1:B:394:GLU:HG3	1:B:397:ARG:HH21	1.64	0.61
1:B:183:ARG:HH11	1:B:183:ARG:CG	2.14	0.61
1:A:265:LEU:HD21	1:A:297:THR:HG21	1.82	0.60
1:B:18:ILE:HG12	1:B:203:GLN:HE21	1.66	0.60
1:A:137:ARG:HH12	1:B:85:MET:HE3	1.65	0.60
1:B:555:CYS:HA	1:B:599:LEU:HD21	1.84	0.60
1:B:345:LEU:HD13	1:B:363:ILE:HD13	1.84	0.60
1:B:208:TYR:CZ	2:B:900:BLA:HAA1	2.36	0.59
1:A:251:VAL:HG11	2:A:900:BLA:HBC1	1.86	0.58
1:B:183:ARG:HH11	1:B:183:ARG:HG3	1.69	0.58
1:A:345:LEU:HD22	1:A:363:ILE:HD13	1.86	0.58
1:B:429:VAL:HG21	1:B:501:ARG:HG2	1.87	0.57
1:B:32:VAL:HG22	1:B:114:LEU:HG	1.87	0.57
1:B:19:HIS:CD2	1:B:20:ILE:HG12	2.39	0.56
1:A:495:GLU:HG2	1:A:498:ARG:NH1	2.20	0.56
1:A:266:VAL:HG12	1:A:280:SER:HA	1.87	0.56
1:A:371:ARG:HH21	1:A:377:ASP:HA	1.70	0.56
1:B:394:GLU:HA	1:B:397:ARG:HE	1.70	0.56
1:B:70:PRO:HG3	1:B:90:ARG:HH22	1.71	0.56
1:A:32:VAL:HG22	1:A:114:LEU:HG	1.87	0.56
1:A:543:ARG:HG3	1:A:566:GLU:HG3	1.88	0.56
1:B:327:ARG:O	1:B:331:ILE:HG12	2.07	0.55
1:B:477:LEU:HD22	1:B:477:LEU:O	2.07	0.55
1:A:418:ASP:C	1:A:420:ALA:H	2.15	0.55
1:A:156:LEU:HD11	1:A:297:THR:HG22	1.89	0.55
1:A:231:HIS:CD2	1:A:234:LEU:H	2.25	0.54
1:B:183:ARG:HG3	1:B:183:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:O	1:A:187:LEU:HB2	2.07	0.54
1:B:454:GLY:HA2	1:B:478:TRP:HD1	1.67	0.54
1:A:327:ARG:O	1:A:331:ILE:HG12	2.06	0.54
1:A:266:VAL:HG11	2:A:900:BLA:HMA3	1.90	0.54
1:A:555:CYS:HA	1:A:599:LEU:HD21	1.88	0.54
1:A:135:LEU:O	1:A:139:VAL:HG22	2.07	0.54
1:B:231:HIS:CD2	1:B:234:LEU:H	2.26	0.54
1:B:190:TYR:O	1:B:193:GLN:HB2	2.08	0.54
1:B:327:ARG:HD3	1:B:499:SER:HB3	1.89	0.54
1:B:30:LEU:HD11	1:B:114:LEU:HD23	1.90	0.54
1:B:418:ASP:C	1:B:420:ALA:H	2.15	0.54
1:A:190:TYR:O	1:A:193:GLN:HB2	2.08	0.53
1:A:334:PHE:HD2	1:A:506:LEU:HD22	1.72	0.53
1:A:394:GLU:HA	1:A:397:ARG:HE	1.73	0.53
1:A:14:ALA:HB2	1:A:201:PRO:HB3	1.90	0.53
1:A:394:GLU:HG3	1:A:397:ARG:HH21	1.74	0.53
1:A:525:ARG:HE	1:B:617:PRO:HD3	1.74	0.53
1:B:363:ILE:HD12	1:B:370:SER:HB3	1.91	0.52
1:A:612:HIS:HB3	1:A:629:GLN:HG3	1.90	0.52
1:A:524:SER:HA	1:A:548:ASN:HB2	1.92	0.52
1:A:52:GLY:HA2	1:A:94:ARG:HG2	1.92	0.52
1:B:599:LEU:HG	1:B:600:GLN:N	2.24	0.52
1:A:304:LEU:O	1:A:308:ILE:HG23	2.10	0.51
1:B:551:PHE:CE2	1:B:630:LEU:HD11	2.45	0.51
1:A:338:GLU:HA	1:A:510:LYS:HE3	1.92	0.51
1:A:30:LEU:HD11	1:A:114:LEU:HD23	1.91	0.51
2:A:900:BLA:CMA	2:A:900:BLA:NB	2.71	0.51
2:B:900:BLA:NB	2:B:900:BLA:CMA	2.73	0.51
1:A:363:ILE:HD12	1:A:370:SER:HB3	1.92	0.51
1:A:617:PRO:HD3	1:B:525:ARG:NH1	2.26	0.51
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.46	0.50
1:A:537:THR:C	1:A:539:ASN:H	2.19	0.50
1:B:453:ALA:HB3	1:B:472:ARG:HH22	1.77	0.50
1:A:94:ARG:CB	1:A:97:PRO:HG3	2.38	0.50
1:A:86:HIS:HB2	1:A:291:HIS:CD2	2.45	0.50
1:B:91:PHE:HB2	1:B:97:PRO:HG2	1.93	0.50
1:A:23:LEU:HD22	1:A:223:PRO:HB2	1.94	0.50
1:B:101:ALA:HB3	1:B:120:ARG:HB2	1.93	0.50
1:B:334:PHE:HD2	1:B:506:LEU:HD22	1.76	0.50
1:A:21:PRO:HD2	1:A:240:LEU:HD13	1.93	0.50
1:A:45:THR:HA	1:A:55:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:900:BLA:HB	2:A:900:BLA:HMA2	1.73	0.50
1:A:401:VAL:HG13	1:A:402:GLY:H	1.77	0.50
1:B:213:VAL:C	1:B:214:ARG:HG3	2.37	0.50
1:A:103:VAL:HG12	1:A:118:GLU:O	2.12	0.49
1:B:338:GLU:HA	1:B:510:LYS:HE3	1.94	0.49
1:A:502:VAL:O	1:A:506:LEU:HB2	2.12	0.49
1:B:351:ASP:O	1:B:355:VAL:HG22	2.11	0.49
1:A:543:ARG:HA	1:A:566:GLU:HA	1.95	0.49
1:B:23:LEU:HD22	1:B:223:PRO:HB2	1.95	0.49
1:B:156:LEU:HD11	1:B:297:THR:HG22	1.94	0.49
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.47	0.49
1:B:231:HIS:HD2	1:B:233:GLN:H	1.59	0.49
1:A:308:ILE:HG13	1:A:309:GLY:N	2.27	0.49
2:B:900:BLA:HBB1	2:B:900:BLA:OB	2.12	0.49
1:A:594:TYR:HA	1:A:611:PHE:O	2.13	0.49
1:B:45:THR:HA	1:B:55:MET:HE3	1.95	0.49
1:B:502:VAL:O	1:B:506:LEU:HB2	2.13	0.48
1:A:231:HIS:HD2	1:A:233:GLN:H	1.60	0.48
1:A:156:LEU:HD13	1:A:300:VAL:HG21	1.96	0.48
1:A:307:ARG:HG2	1:A:311:LEU:HD12	1.96	0.48
1:B:55:MET:HG2	1:B:227:GLN:HG3	1.95	0.48
1:B:122:ALA:HB3	1:B:123:ARG:HH11	1.78	0.48
1:A:104:ALA:HB2	1:A:117:MET:HB3	1.95	0.48
1:B:401:VAL:HG13	1:B:402:GLY:H	1.79	0.48
1:A:40:ILE:HD11	1:A:66:VAL:HG11	1.95	0.47
1:B:568:GLN:HA	1:B:571:TYR:CE2	2.49	0.47
1:A:450:ILE:HG13	1:A:480:GLN:HB3	1.96	0.47
1:A:629:GLN:HE22	1:B:526:LEU:HA	1.79	0.47
1:A:596:THR:HA	1:A:610:GLN:HA	1.96	0.47
1:B:84:LEU:HB2	1:B:106:TRP:HB2	1.96	0.47
1:B:308:ILE:O	1:B:312:GLN:HG3	2.15	0.47
1:B:159:LEU:HB3	1:B:160:ILE:HD12	1.97	0.47
1:A:351:ASP:O	1:A:355:VAL:HG22	2.15	0.46
1:B:330:LEU:O	1:B:334:PHE:HB2	2.15	0.46
1:B:104:ALA:HB2	1:B:117:MET:HB3	1.96	0.46
1:A:84:LEU:HB2	1:A:106:TRP:HB2	1.98	0.46
1:B:184:LYS:H	1:B:187:LEU:HD11	1.80	0.46
1:A:240:LEU:HD23	1:A:246:ARG:HA	1.97	0.46
1:B:107:HIS:HD2	1:B:243:VAL:HG22	1.81	0.46
1:B:41:VAL:HG21	1:B:231:HIS:CE1	2.51	0.46
1:A:413:PHE:HE2	1:A:426:PHE:HZ	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LEU:HD12	1:B:526:LEU:HD12	1.98	0.46
1:B:23:LEU:HA	1:B:225:PRO:HA	1.97	0.46
1:A:114:LEU:HD21	1:A:238:VAL:CG1	2.46	0.46
1:B:32:VAL:HB	1:B:42:GLN:HB2	1.99	0.45
1:B:432:MET:C	1:B:434:GLN:H	2.24	0.45
1:B:156:LEU:HD13	1:B:300:VAL:HG21	1.99	0.45
1:A:32:VAL:HB	1:A:42:GLN:HB2	1.98	0.45
1:B:173:GLU:O	1:B:174:TRP:HB2	2.17	0.45
1:B:340:MET:HA	1:B:344:LEU:HD23	1.98	0.45
1:A:41:VAL:HG21	1:A:231:HIS:CE1	2.51	0.45
1:B:42:GLN:HG2	1:B:228:PRO:HB2	1.99	0.45
1:B:183:ARG:HB2	1:B:187:LEU:CD1	2.46	0.45
1:A:23:LEU:HA	1:A:225:PRO:HA	1.98	0.45
1:B:80:GLN:HE21	1:B:80:GLN:HA	1.82	0.45
1:A:594:TYR:CE1	1:A:610:GLN:HB2	2.52	0.45
1:A:164:ARG:HH21	1:A:183:ARG:HD2	1.81	0.45
1:A:24:ILE:HD11	1:A:30:LEU:HD22	2.00	0.44
1:A:68:THR:HG23	1:A:92:PRO:HG3	1.99	0.44
1:A:330:LEU:O	1:A:334:PHE:HB2	2.17	0.44
1:B:429:VAL:HG22	1:B:430:PRO:HA	1.99	0.44
1:B:24:ILE:HD11	1:B:30:LEU:HD22	2.00	0.44
1:B:51:LEU:CG	1:B:66:VAL:HG21	2.44	0.44
1:A:42:GLN:HG2	1:A:228:PRO:HB2	2.00	0.44
1:A:44:SER:HA	1:A:226:ILE:HA	2.00	0.44
1:A:67:LEU:HA	1:A:92:PRO:HD2	1.98	0.44
1:A:227:GLN:HB3	1:A:228:PRO:HD3	1.99	0.44
1:A:48:ALA:HB2	1:A:55:MET:HE2	2.00	0.44
1:A:71:GLU:HB2	1:A:87:ALA:HB1	2.00	0.44
2:B:900:BLA:NB	2:B:900:BLA:HMA2	2.33	0.44
1:A:589:ASN:ND2	1:A:591:ARG:HH21	2.16	0.44
1:B:246:ARG:HH22	2:B:900:BLA:CGD	2.31	0.44
1:B:44:SER:HA	1:B:226:ILE:HA	2.00	0.44
1:B:48:ALA:HB2	1:B:55:MET:HE2	2.00	0.44
1:B:424:ALA:HB3	1:B:486:ALA:HB2	2.00	0.44
1:A:307:ARG:HA	1:A:310:ALA:HB3	2.00	0.43
1:A:375:THR:HG22	1:A:376:PRO:HD2	2.00	0.43
1:A:424:ALA:HB3	1:A:486:ALA:HB2	2.00	0.43
1:B:71:GLU:HB2	1:B:87:ALA:HB1	1.99	0.43
1:B:143:PRO:O	1:B:147:GLU:HB2	2.18	0.43
1:B:208:TYR:OH	2:B:900:BLA:HHA	2.18	0.43
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:MET:HE3	1:B:137:ARG:NH2	2.33	0.43
1:A:576:PRO:O	1:A:580:VAL:HG23	2.18	0.43
1:B:100:SER:O	1:B:102:TRP:HD1	2.02	0.43
1:B:316:ARG:HG2	1:B:320:GLU:OE1	2.18	0.43
1:A:34:ASP:HB3	1:A:37:ASP:OD1	2.18	0.43
1:A:541:ALA:HB3	1:A:566:GLU:HG2	2.00	0.43
1:B:376:PRO:HB2	1:B:380:ALA:HB3	2.00	0.43
1:A:59:LEU:HD21	1:A:228:PRO:HG3	2.01	0.43
2:A:900:BLA:NB	2:A:900:BLA:HMA1	2.34	0.43
1:B:243:VAL:HG12	1:B:245:LEU:H	1.84	0.43
1:A:432:MET:C	1:A:434:GLN:H	2.25	0.43
1:B:114:LEU:HD21	1:B:238:VAL:CG1	2.48	0.43
1:B:266:VAL:HG22	1:B:280:SER:HA	2.01	0.43
1:B:612:HIS:HB3	1:B:629:GLN:HB2	2.01	0.43
1:A:164:ARG:HH12	1:A:187:LEU:HD22	1.84	0.43
1:B:97:PRO:CB	1:B:98:PRO:HD3	2.47	0.43
1:B:413:PHE:HE2	1:B:426:PHE:HZ	1.66	0.42
1:A:445:GLU:HG3	1:A:484:GLY:H	1.84	0.42
2:B:900:BLA:HMA2	2:B:900:BLA:HB	1.83	0.42
1:A:275:LEU:HD21	1:A:278:LEU:HD21	2.01	0.42
1:A:490:SER:HB3	1:A:493:HIS:ND1	2.35	0.42
1:B:615:PRO:HA	1:B:626:TRP:CD1	2.54	0.42
1:A:107:HIS:HD2	1:A:243:VAL:HG22	1.84	0.42
1:A:512:PHE:CD1	1:B:513:GLN:HA	2.54	0.42
1:A:397:ARG:HH12	1:A:433:PRO:HB3	1.84	0.42
1:A:617:PRO:HD3	1:B:525:ARG:CZ	2.50	0.42
1:B:208:TYR:HA	1:B:214:ARG:HE	1.83	0.42
1:B:375:THR:HG22	1:B:376:PRO:HD2	2.01	0.42
1:A:162:PHE:CE2	1:A:283:HIS:HB2	2.54	0.42
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.89	0.42
1:A:376:PRO:HB2	1:A:380:ALA:HB3	2.02	0.42
1:B:164:ARG:HH21	1:B:183:ARG:HD2	1.84	0.41
1:B:215:GLN:HG2	1:B:216:ILE:N	2.34	0.41
1:A:269:ILE:HG12	1:A:304:LEU:HD23	2.02	0.41
1:A:13:CYS:C	1:A:15:ARG:H	2.27	0.41
1:A:97:PRO:N	1:A:98:PRO:HD3	2.35	0.41
1:A:231:HIS:HD2	1:A:234:LEU:H	1.67	0.41
1:A:307:ARG:HG2	1:A:307:ARG:O	2.19	0.41
1:B:59:LEU:HD21	1:B:228:PRO:HG3	2.02	0.41
1:A:527:ARG:NH1	1:A:631:ARG:HG3	2.35	0.41
1:B:494:LEU:HD23	1:B:498:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HB3	1:A:120:ARG:HB2	2.02	0.41
1:A:497:ALA:O	1:A:500:LEU:HB2	2.20	0.41
1:B:576:PRO:O	1:B:580:VAL:HG23	2.20	0.41
1:A:141:ARG:HD3	1:B:212:ARG:NH1	2.36	0.41
1:A:316:ARG:HG2	1:A:320:GLU:OE1	2.21	0.41
1:A:429:VAL:HG13	1:A:501:ARG:HG2	2.02	0.41
1:A:529:GLY:HA2	1:A:548:ASN:OD1	2.21	0.41
1:A:590:GLY:HA2	1:A:626:TRP:HZ2	1.85	0.41
1:A:271:VAL:HG21	1:A:308:ILE:HD11	2.03	0.41
1:A:335:ASN:HA	1:A:506:LEU:HD21	2.03	0.41
1:B:403:ALA:HA	1:B:431:LEU:HG	2.03	0.41
1:B:103:VAL:HG12	1:B:118:GLU:O	2.21	0.40
1:B:327:ARG:HD3	1:B:499:SER:CB	2.52	0.40
1:A:63:TYR:HE2	1:A:69:LEU:HD21	1.87	0.40
1:A:508:GLU:HB3	1:B:509:ARG:HD3	2.04	0.40
1:B:252:HIS:NE2	2:B:900:BLA:HBA2	2.37	0.40
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.95	0.40
1:B:533:ILE:HG12	1:B:567:LEU:HD13	2.03	0.40
1:B:578:ALA:O	1:B:582:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

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	578/640 (90%)	496 (86%)	68 (12%)	14 (2%)	4	29
1	B	596/640 (93%)	519 (87%)	60 (10%)	17 (3%)	3	26
All	All	1174/1280 (92%)	1015 (86%)	128 (11%)	31 (3%)	4	28

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	VAL
1	B	19	HIS
1	B	401	VAL
1	A	140	GLU
1	A	366	GLY
1	A	529	GLY
1	B	18	ILE
1	B	97	PRO
1	B	174	TRP
1	B	241	SER
1	B	366	GLY
1	B	436	ARG
1	A	70	PRO
1	A	306	GLY
1	A	418	ASP
1	A	436	ARG
1	A	538	ALA
1	B	418	ASP
1	B	38	GLY
1	B	70	PRO
1	B	475	PHE
1	A	97	PRO
1	B	187	LEU
1	B	474	SER
1	A	261	VAL
1	A	607	VAL
1	B	261	VAL
1	B	144	GLY
1	A	18	ILE
1	B	152	VAL
1	A	152	VAL

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	485/532 (91%)	388 (80%)	97 (20%)	1 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	496/532 (93%)	395 (80%)	101 (20%)	1	8
All	All	981/1064 (92%)	783 (80%)	198 (20%)	1	8

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	59	LEU
1	A	65	GLN
1	A	67	LEU
1	A	69	LEU
1	A	77	VAL
1	A	85	MET
1	A	94	ARG
1	A	108	LEU
1	A	114	LEU
1	A	127	VAL
1	A	129	LEU
1	A	135	LEU
1	A	139	VAL
1	A	145	ILE
1	A	151	ARG
1	A	183	ARG
1	A	188	GLU
1	A	191	LEU
1	A	193	GLN
1	A	200	ILE
1	A	209	LEU
1	A	210	ARG
1	A	214	ARG
1	A	215	GLN
1	A	222	GLN
1	A	227	GLN
1	A	230	VAL
1	A	233	GLN
1	A	234	LEU
1	A	242	ASP
1	A	261	VAL
1	A	264	THR
1	A	265	LEU
1	A	282	HIS
1	A	290	ASN

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Mol	Chain	Res	Type
1	A	307	ARG
1	A	308	ILE
1	A	311	LEU
1	A	318	ARG
1	A	319	LEU
1	A	323	LEU
1	A	330	LEU
1	A	339	HIS
1	A	347	ASP
1	A	348	MET
1	A	355	VAL
1	A	356	VAL
1	A	363	ILE
1	A	367	ASN
1	A	369	ILE
1	A	371	ARG
1	A	374	THR
1	A	375	THR
1	A	383	ARG
1	A	391	GLU
1	A	392	HIS
1	A	396	LEU
1	A	404	LEU
1	A	406	VAL
1	A	432	MET
1	A	436	ARG
1	A	439	LEU
1	A	446	GLN
1	A	447	ILE
1	A	448	GLN
1	A	450	ILE
1	A	479	GLN
1	A	482	VAL
1	A	487	ARG
1	A	492	LEU
1	A	494	LEU
1	A	495	GLU
1	A	504	ILE
1	A	506	LEU
1	A	514	GLN
1	A	518	LEU
1	A	519	LEU

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Mol	Chain	Res	Type
1	A	527	ARG
1	A	528	ASP
1	A	535	ARG
1	A	545	LEU
1	A	548	ASN
1	A	559	VAL
1	A	561	GLU
1	A	562	LEU
1	A	566	GLU
1	A	569	THR
1	A	583	LEU
1	A	585	ASP
1	A	597	LEU
1	A	599	LEU
1	A	610	GLN
1	A	614	GLU
1	A	627	LEU
1	A	630	LEU
1	A	631	ARG
1	B	15	ARG
1	B	19	HIS
1	B	27	TYR
1	B	37	ASP
1	B	39	ARG
1	B	50	LEU
1	B	59	LEU
1	B	64	THR
1	B	67	LEU
1	B	68	THR
1	B	69	LEU
1	B	73	GLN
1	B	77	VAL
1	B	85	MET
1	B	96	THR
1	B	108	LEU
1	B	114	LEU
1	B	121	ASP
1	B	123	ARG
1	B	129	LEU
1	B	135	LEU
1	B	140	GLU
1	B	141	ARG

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Mol	Chain	Res	Type
1	B	142	ASP
1	B	151	ARG
1	B	169	ARG
1	B	171	ASP
1	B	179	ILE
1	B	183	ARG
1	B	187	LEU
1	B	188	GLU
1	B	191	LEU
1	B	193	GLN
1	B	200	ILE
1	B	203	GLN
1	B	209	LEU
1	B	210	ARG
1	B	213	VAL
1	B	214	ARG
1	B	215	GLN
1	B	222	GLN
1	B	227	GLN
1	B	230	VAL
1	B	234	LEU
1	B	242	ASP
1	B	261	VAL
1	B	264	THR
1	B	282	HIS
1	B	293	MET
1	B	303	THR
1	B	308	ILE
1	B	318	ARG
1	B	319	LEU
1	B	330	LEU
1	B	343	GLU
1	B	346	ASP
1	B	347	ASP
1	B	348	MET
1	B	355	VAL
1	B	356	VAL
1	B	363	ILE
1	B	367	ASN
1	B	369	ILE
1	B	374	THR
1	B	375	THR

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Mol	Chain	Res	Type
1	B	383	ARG
1	B	392	HIS
1	B	396	LEU
1	B	404	LEU
1	B	406	VAL
1	B	432	MET
1	B	436	ARG
1	B	439	LEU
1	B	446	GLN
1	B	447	ILE
1	B	448	GLN
1	B	450	ILE
1	B	473	LYS
1	B	477	LEU
1	B	479	GLN
1	B	482	VAL
1	B	487	ARG
1	B	492	LEU
1	B	494	LEU
1	B	495	GLU
1	B	504	ILE
1	B	506	LEU
1	B	514	GLN
1	B	518	LEU
1	B	519	LEU
1	B	528	ASP
1	B	545	LEU
1	B	559	VAL
1	B	565	ARG
1	B	577	ARG
1	B	583	LEU
1	B	597	LEU
1	B	599	LEU
1	B	608	TYR
1	B	614	GLU
1	B	627	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	107	HIS

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	175	ASN
1	A	203	GLN
1	A	222	GLN
1	A	227	GLN
1	A	231	HIS
1	A	290	ASN
1	A	291	HIS
1	A	393	HIS
1	A	405	HIS
1	A	455	ASN
1	A	479	GLN
1	A	584	GLN
1	A	589	ASN
1	B	80	GLN
1	B	93	GLN
1	B	107	HIS
1	B	112	GLN
1	B	203	GLN
1	B	215	GLN
1	B	222	GLN
1	B	227	GLN
1	B	231	HIS
1	B	233	GLN
1	B	272	ASN
1	B	393	HIS
1	B	405	HIS
1	B	455	ASN
1	B	479	GLN
1	B	584	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](#)

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	BLA	A	900	1	46,46,46	1.82	10 (21%)	66,67,67	2.18	17 (25%)
2	BLA	B	900	1	46,46,46	1.57	10 (21%)	66,67,67	2.56	20 (30%)

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	BLA	A	900	1	-	8/26/74/74	0/4/4/4
2	BLA	B	900	1	-	8/26/74/74	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C3B-C2B	5.75	1.48	1.37
2	A	900	BLA	CHB-C1B	4.68	1.49	1.37
2	B	900	BLA	CHA-C4D	4.28	1.46	1.38
2	B	900	BLA	C3B-C2B	4.18	1.45	1.37
2	A	900	BLA	CHB-C4A	4.09	1.49	1.40
2	A	900	BLA	C4A-C3A	3.86	1.50	1.41
2	B	900	BLA	CHB-C1B	3.68	1.46	1.37
2	A	900	BLA	C2A-C3A	3.39	1.47	1.38
2	A	900	BLA	CHA-C1A	3.16	1.47	1.40
2	A	900	BLA	C3C-C4C	3.06	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	C2A-C3A	3.04	1.46	1.38
2	B	900	BLA	C3C-C4C	2.89	1.51	1.45
2	A	900	BLA	C1B-C2B	2.80	1.50	1.45
2	A	900	BLA	OB-C4B	2.75	1.28	1.23
2	B	900	BLA	CHB-C4A	2.60	1.46	1.40
2	B	900	BLA	C4A-C3A	2.60	1.47	1.41
2	A	900	BLA	C1A-C2A	2.40	1.48	1.42
2	B	900	BLA	CHA-C1A	2.25	1.45	1.40
2	B	900	BLA	C1A-NA	-2.22	1.34	1.37
2	B	900	BLA	C1A-C2A	2.05	1.47	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C3B-C4B-NB	8.19	116.42	106.13
2	B	900	BLA	C2A-C1A-NA	6.57	115.81	107.57
2	B	900	BLA	C1B-NB-C4B	-6.50	102.68	110.66
2	B	900	BLA	C3A-C4A-NA	6.36	116.11	107.43
2	B	900	BLA	C2B-C1B-NB	5.96	115.66	106.97
2	A	900	BLA	C3B-C2B-C1B	-5.82	101.44	107.92
2	A	900	BLA	C3B-C4B-NB	5.77	113.38	106.13
2	A	900	BLA	CMA-C3A-C4A	5.08	133.00	125.62
2	A	900	BLA	C2A-C1A-NA	5.07	113.92	107.57
2	A	900	BLA	C2B-C1B-NB	5.02	114.28	106.97
2	B	900	BLA	C3B-C2B-C1B	-4.67	102.71	107.92
2	B	900	BLA	C4A-C3A-C2A	-4.62	101.98	107.76
2	A	900	BLA	C3A-C4A-NA	4.57	113.67	107.43
2	B	900	BLA	OB-C4B-C3B	-4.24	119.48	129.71
2	B	900	BLA	C4B-C3B-C2B	-4.22	102.50	107.92
2	A	900	BLA	CMB-C2B-C1B	4.21	129.28	124.16
2	B	900	BLA	CMB-C2B-C1B	4.20	129.26	124.16
2	A	900	BLA	C4A-C3A-C2A	-4.17	102.54	107.76
2	B	900	BLA	C1A-C2A-C3A	-4.06	102.89	107.62
2	A	900	BLA	CHB-C4A-NA	-3.95	116.37	125.29
2	A	900	BLA	CHB-C1B-NB	-3.93	117.68	126.06
2	B	900	BLA	C4A-NA-C1A	-3.76	103.17	109.78
2	A	900	BLA	CBA-CAA-C2A	-3.56	102.69	112.53
2	B	900	BLA	C4A-CHB-C1B	-3.52	120.69	130.82
2	A	900	BLA	C1B-NB-C4B	-3.36	106.53	110.66
2	A	900	BLA	C1A-C2A-C3A	-3.07	104.05	107.62
2	B	900	BLA	CHB-C4A-C3A	-2.79	120.69	127.53
2	A	900	BLA	C4B-C3B-C2B	-2.78	104.36	107.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C4A-CHB-C1B	-2.65	123.18	130.82
2	B	900	BLA	CAA-CBA-CGA	-2.62	106.70	113.67
2	B	900	BLA	CHB-C1B-NB	-2.52	120.67	126.06
2	B	900	BLA	CHA-C1A-C2A	-2.27	122.34	127.22
2	A	900	BLA	C4A-NA-C1A	-2.26	105.81	109.78
2	B	900	BLA	CBA-CAA-C2A	-2.12	106.66	112.53
2	B	900	BLA	CMA-C3A-C2A	2.08	130.03	125.62
2	B	900	BLA	C4C-CHD-C1D	2.05	133.10	128.06
2	A	900	BLA	CHA-C1A-C2A	-2.00	122.92	127.22

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	ND-C1D-CHD-C4C
2	B	900	BLA	C4C-C3C-CAC-CBC
2	A	900	BLA	C4C-C3C-CAC-CBC
2	B	900	BLA	CAA-CBA-CGA-O2A
2	B	900	BLA	CAA-CBA-CGA-O1A
2	B	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	CAD-CBD-CGD-O1D
2	A	900	BLA	CAA-CBA-CGA-O1A

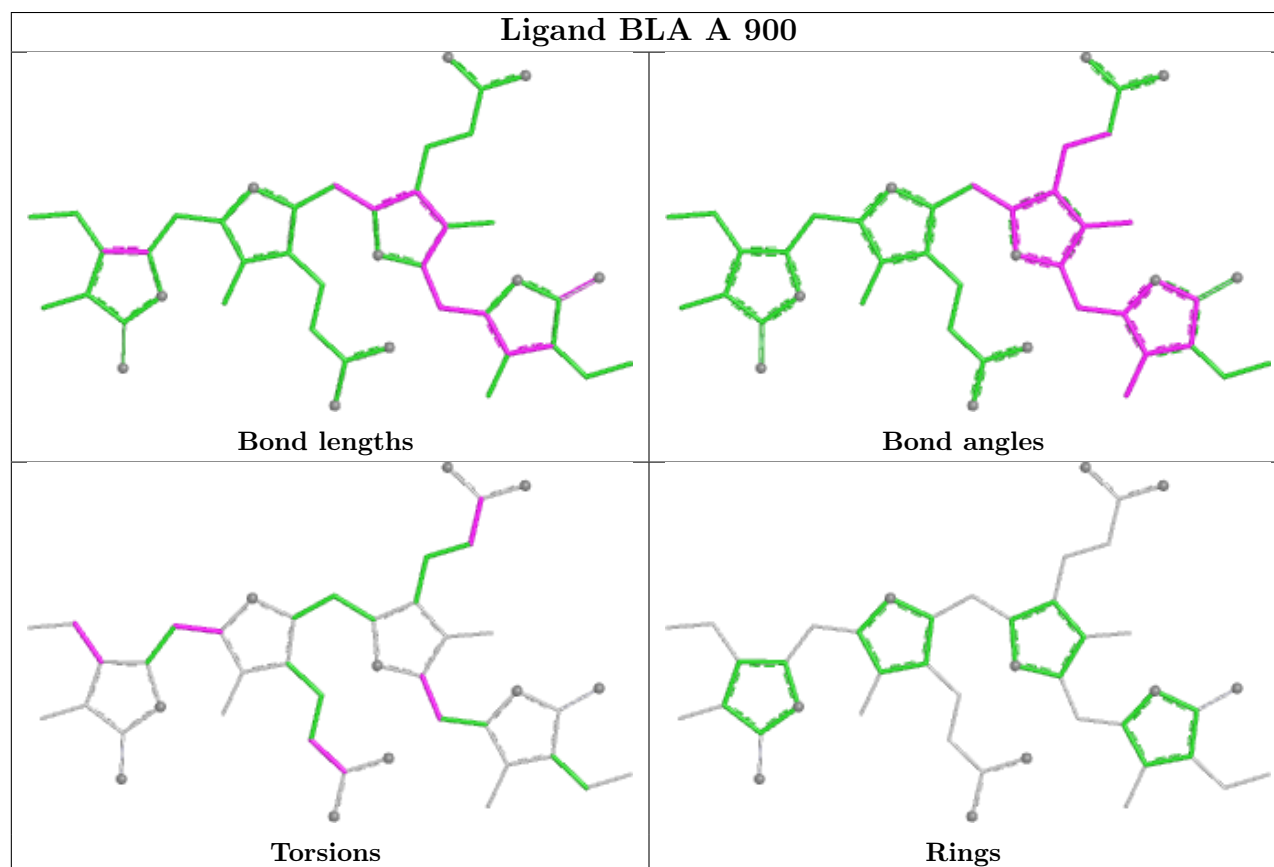
There are no ring outliers.

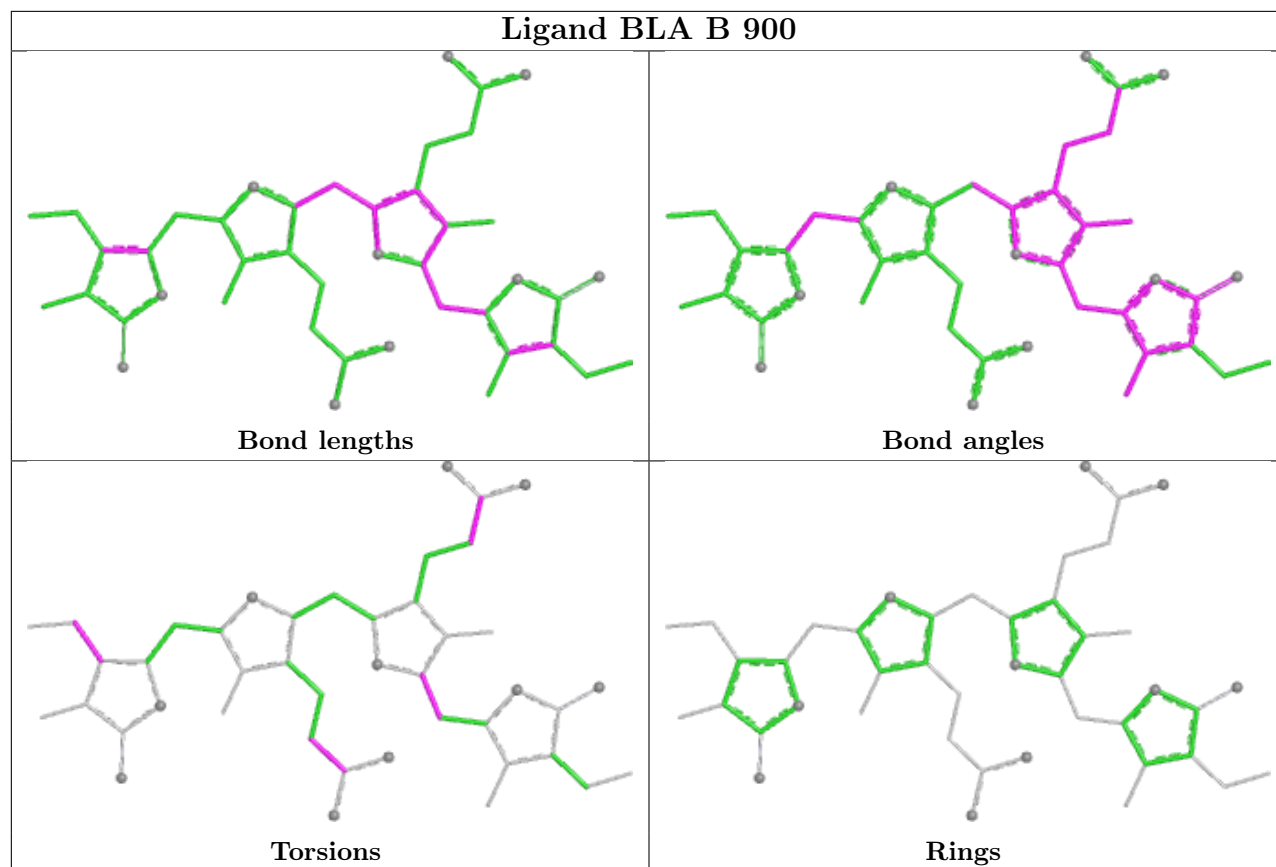
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	10	0
2	B	900	BLA	11	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	588/640 (91%)	-0.33	3 (0%) 87 72	141, 211, 257, 280	0
1	B	602/640 (94%)	-0.44	0 100 100	147, 213, 268, 280	0
All	All	1190/1280 (92%)	-0.38	3 (0%) 90 78	141, 212, 266, 280	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	2.3
1	A	31	LEU	2.2
1	A	602	SER	2.1

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

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

6.3 Carbohydrates [i](#)

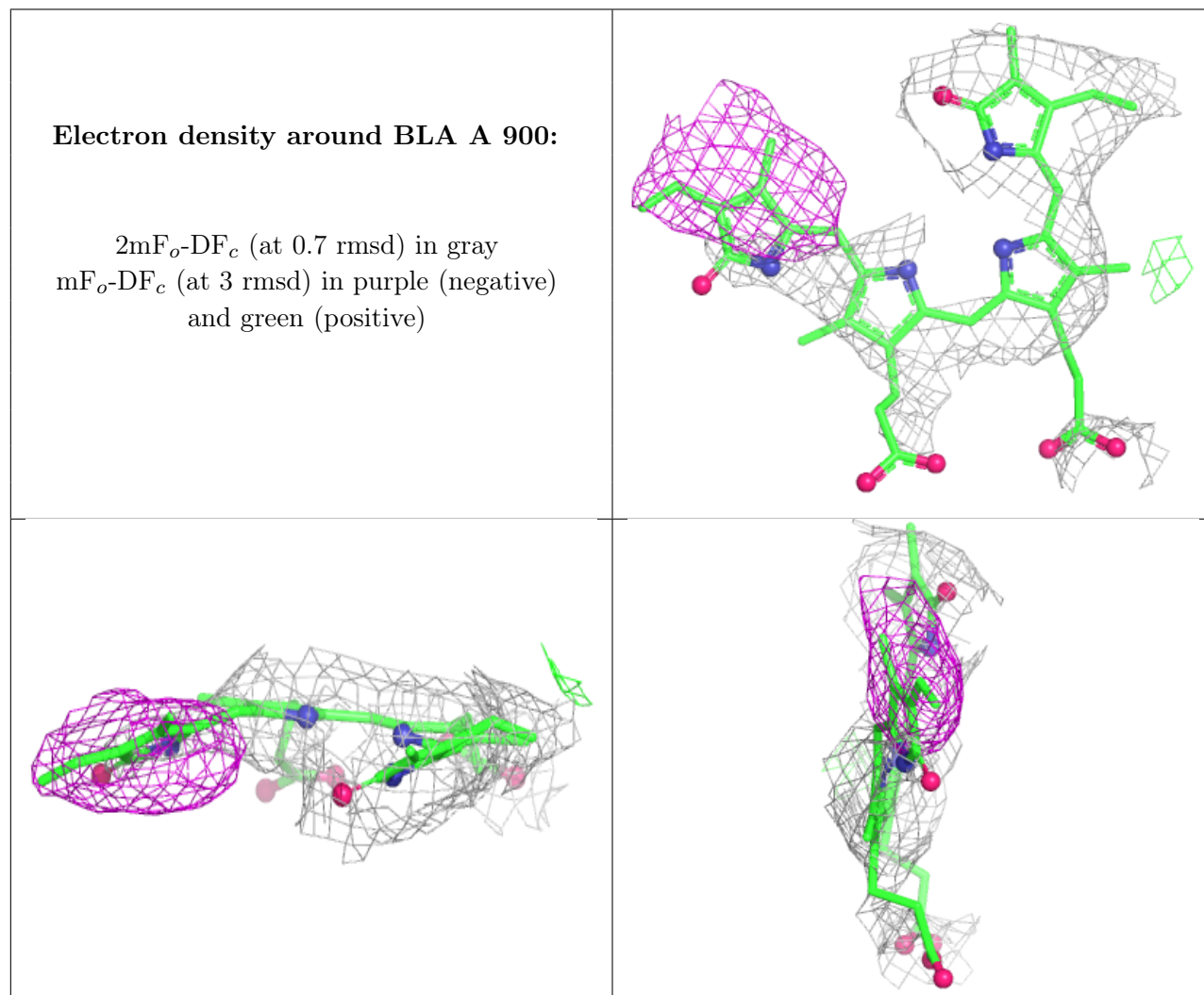
There are no oligosaccharides in this entry.

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.

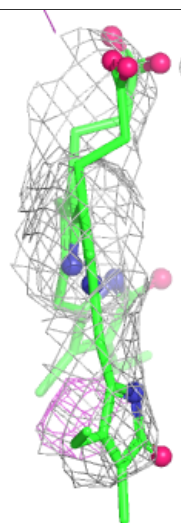
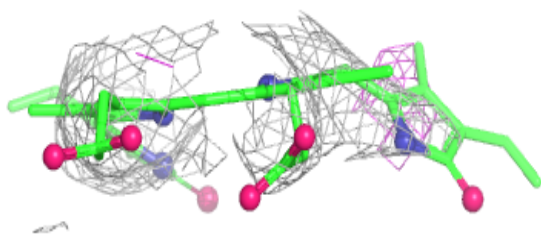
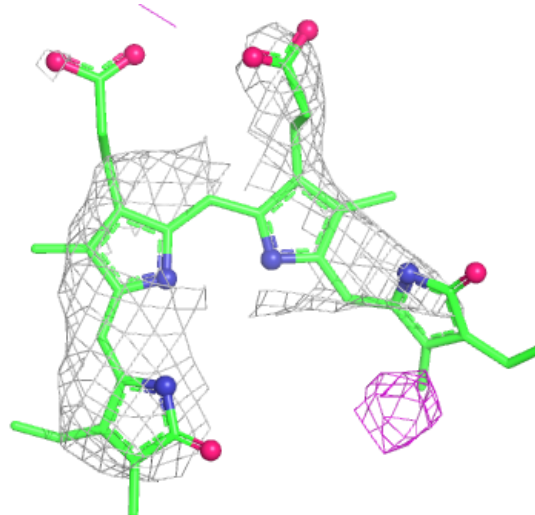
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	A	900	43/43	0.87	0.11	178,184,186,187	0
2	BLA	B	900	43/43	0.92	0.10	213,218,221,222	0

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 BLA B 900:

$2mF_o-DF_c$ (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.