



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:29 PM UTC

PDB ID : 6PL0 / pdb_00006pl0
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP from Xanthomonas campestris in the Pr state bound to BV chromophore
Authors : Otero, L.H.; Sirigu, S.; Klinke, S.; Goldbaum, F.; Chavas, L.; Rinaldi, J.; Bonomi, H.R.
Deposited on : 2019-06-30
Resolution : 2.96 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](#) ①) were used in the production of this report:

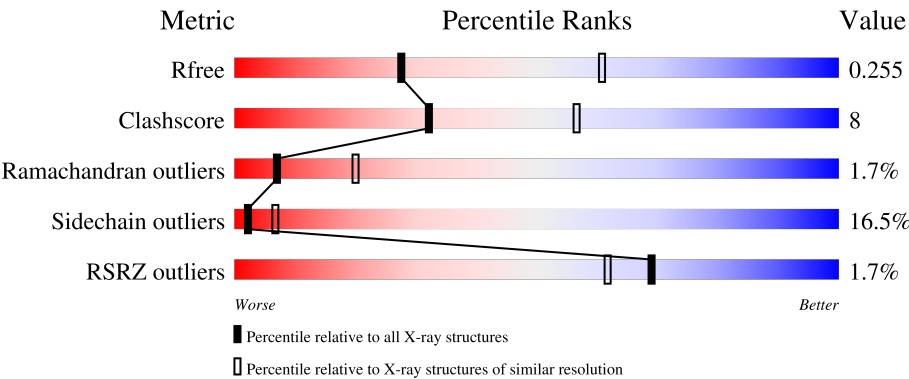
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 3 unique types of molecules in this entry. The entry contains 9597 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.

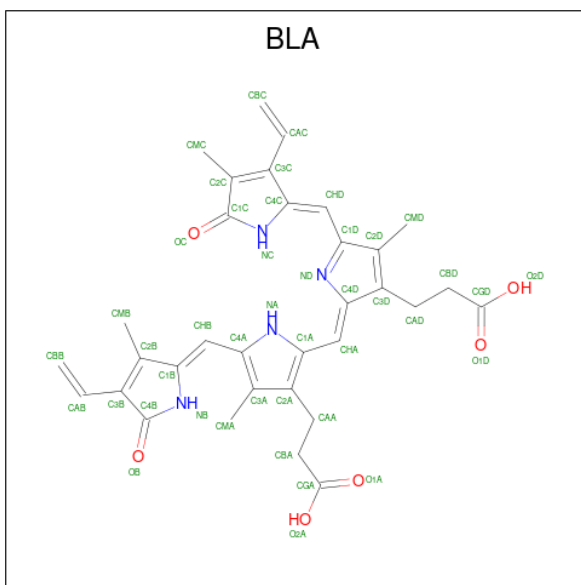
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	0	0
			4748	3004	862	866	16			
1	B	608	Total	C	N	O	S	0	0	0
			4761	3011	864	870	16			

There are 14 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
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

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



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

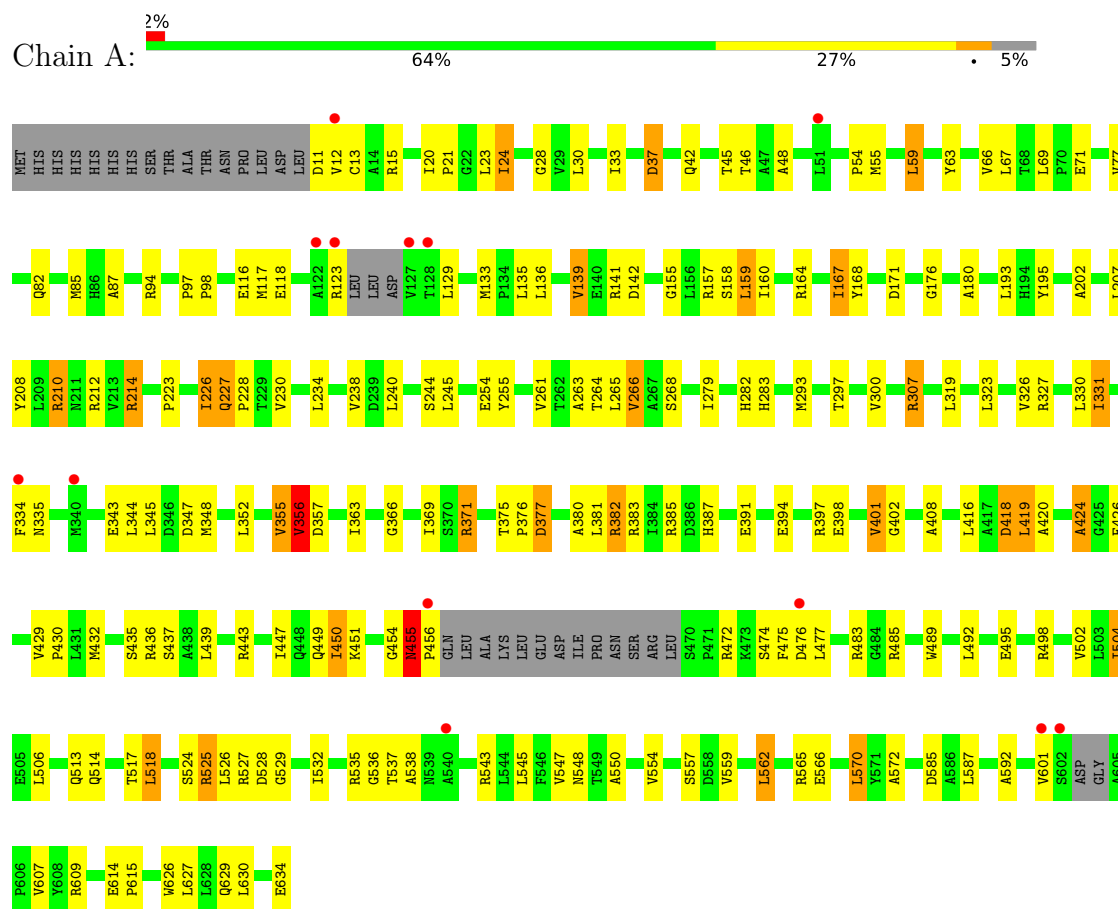
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0

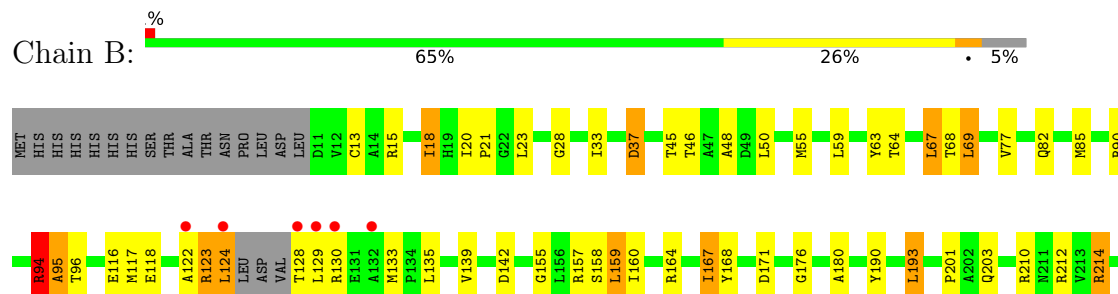
3 Residue-property plots

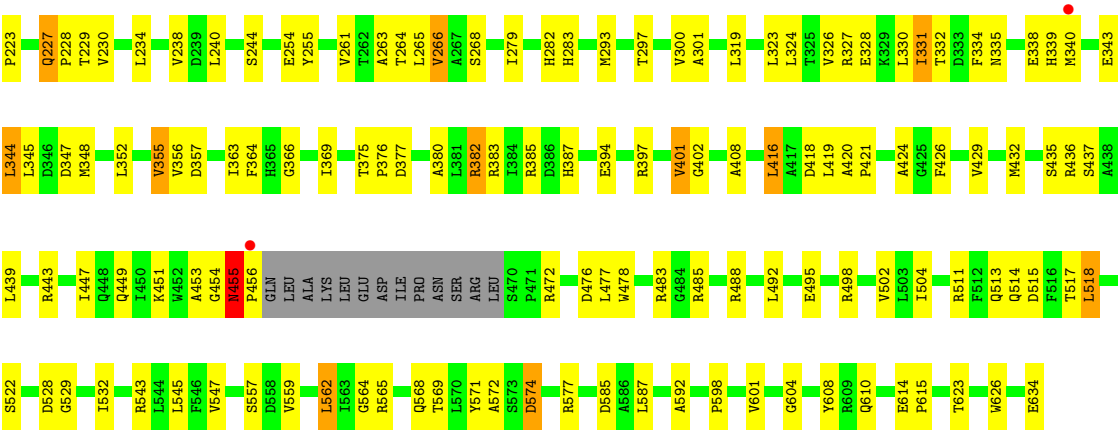
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	103.53Å 103.53Å 346.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.96 49.60 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.60-2.96) 99.9 (49.60-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.206 , 0.248 0.223 , 0.255	Depositor DCC
R_{free} test set	2021 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	112.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9597	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.91	2/4857 (0.0%)	1.40	34/6625 (0.5%)
1	B	0.89	1/4871 (0.0%)	1.39	29/6645 (0.4%)
All	All	0.90	3/9728 (0.0%)	1.39	63/13270 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	MET	SD-CE	6.18	1.95	1.79
1	B	455	ASN	CA-C	5.23	1.59	1.52
1	A	455	ASN	CA-C	5.02	1.59	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASP	CA-CB-CG	7.27	119.87	112.60
1	B	171	ASP	CA-CB-CG	6.86	119.46	112.60
1	B	95	ALA	CA-C-N	6.62	129.98	122.83
1	B	95	ALA	C-N-CA	6.62	129.98	122.83
1	A	171	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	569	THR	CA-C-N	6.37	128.81	120.28
1	B	569	THR	C-N-CA	6.37	128.81	120.28
1	B	122	ALA	CA-C-N	6.36	133.69	121.54
1	B	122	ALA	C-N-CA	6.36	133.69	121.54
1	B	37	ASP	CA-CB-CG	6.33	118.92	112.60
1	A	37	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	301	ALA	CA-C-N	6.06	128.32	120.44
1	B	301	ALA	C-N-CA	6.06	128.32	120.44
1	A	202	ALA	CA-C-N	6.01	128.65	120.54
1	A	202	ALA	C-N-CA	6.01	128.65	120.54
1	B	335	ASN	CA-C-N	5.95	128.53	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	ASN	C-N-CA	5.95	128.53	120.38
1	A	335	ASN	CA-C-N	5.92	128.50	120.38
1	A	335	ASN	C-N-CA	5.92	128.50	120.38
1	A	450	ILE	CB-CA-C	5.87	118.06	110.96
1	B	610	GLN	CA-C-N	5.84	130.69	121.99
1	B	610	GLN	C-N-CA	5.84	130.69	121.99
1	A	525	ARG	CA-C-N	5.83	132.67	121.54
1	A	525	ARG	C-N-CA	5.83	132.67	121.54
1	B	347	ASP	CA-C-N	5.78	128.02	120.28
1	B	347	ASP	C-N-CA	5.78	128.02	120.28
1	A	419	LEU	CA-C-N	5.76	128.19	120.58
1	A	419	LEU	C-N-CA	5.76	128.19	120.58
1	A	538	ALA	CA-C-N	5.74	128.98	120.95
1	A	538	ALA	C-N-CA	5.74	128.98	120.95
1	B	171	ASP	CA-C-N	5.72	128.22	120.38
1	B	171	ASP	C-N-CA	5.72	128.22	120.38
1	B	419	LEU	CA-C-N	5.50	126.61	120.06
1	B	419	LEU	C-N-CA	5.50	126.61	120.06
1	B	377	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	377	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	416	LEU	CA-C-N	5.45	127.85	120.38
1	A	416	LEU	C-N-CA	5.45	127.85	120.38
1	B	577	ARG	CA-C-N	5.45	128.36	120.79
1	B	577	ARG	C-N-CA	5.45	128.36	120.79
1	A	171	ASP	CA-C-N	5.40	128.27	120.38
1	A	171	ASP	C-N-CA	5.40	128.27	120.38
1	B	515	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	347	ASP	CA-C-N	5.39	127.51	120.28
1	A	347	ASP	C-N-CA	5.39	127.51	120.28
1	A	475	PHE	CA-C-N	5.37	128.47	120.90
1	A	475	PHE	C-N-CA	5.37	128.47	120.90
1	B	574	ASP	CA-CB-CG	5.33	117.94	112.60
1	A	210	ARG	CA-C-N	5.24	129.39	122.42
1	A	210	ARG	C-N-CA	5.24	129.39	122.42
1	A	528	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	416	LEU	CA-C-N	5.19	128.61	120.82
1	B	416	LEU	C-N-CA	5.19	128.61	120.82
1	A	426	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	364	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	63	TYR	CA-C-N	5.13	127.88	120.38
1	A	63	TYR	C-N-CA	5.13	127.88	120.38
1	A	356	VAL	N-CA-CB	-5.09	105.69	112.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	GLY	CA-C-N	5.09	131.26	121.54
1	A	536	GLY	C-N-CA	5.09	131.26	121.54
1	B	426	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	424	ALA	CA-C-N	5.02	125.64	122.18
1	A	424	ALA	C-N-CA	5.02	125.64	122.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4748	0	4734	72	0
1	B	4761	0	4744	73	0
2	A	43	0	30	9	0
2	B	43	0	31	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9597	0	9539	153	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 8.

All (153) 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:455:ASN:HB3	1:A:456:PRO:HD3	1.47	0.96
1:B:455:ASN:HB3	1:B:456:PRO:HD3	1.51	0.89
1:A:524:SER:HA	1:A:548:ASN:HB2	1.59	0.85
2:A:900:BLA:HHD	2:A:900:BLA:HBC1	1.58	0.83
1:B:164:ARG:HG2	1:B:282:HIS:HB2	1.64	0.79
1:A:394:GLU:HG2	1:A:397:ARG:HH22	1.49	0.77
1:B:63:TYR:HE2	1:B:67:LEU:HD13	1.48	0.77
2:A:900:BLA:OB	2:A:900:BLA:HBB1	1.87	0.74
1:A:455:ASN:HB3	1:A:456:PRO:CD	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ARG:HH21	1:A:377:ASP:HA	1.53	0.72
1:B:63:TYR:CE2	1:B:67:LEU:HD13	2.26	0.71
1:B:123:ARG:HG2	1:B:124:LEU:HG	1.71	0.70
1:B:455:ASN:HB3	1:B:456:PRO:CD	2.21	0.69
1:A:227:GLN:HB3	1:A:228:PRO:HD3	1.75	0.68
1:B:227:GLN:HB3	1:B:228:PRO:HD3	1.78	0.65
2:B:900:BLA:HBB1	2:B:900:BLA:OB	1.98	0.63
2:A:900:BLA:HHD	2:A:900:BLA:CBC	2.28	0.63
1:A:447:ILE:HG12	1:A:483:ARG:HG2	1.80	0.63
1:B:326:VAL:HG12	1:B:355:VAL:HG13	1.79	0.63
2:A:900:BLA:HB	2:A:900:BLA:CMA	2.12	0.62
1:B:282:HIS:CE1	2:B:900:BLA:OB	2.52	0.62
1:B:401:VAL:HG13	1:B:402:GLY:H	1.65	0.61
1:A:455:ASN:CB	1:A:456:PRO:HD3	2.24	0.61
1:A:371:ARG:HG3	1:A:381:LEU:HD11	1.83	0.61
1:A:23:LEU:HD22	1:A:223:PRO:HB2	1.82	0.61
1:B:455:ASN:CB	1:B:456:PRO:HD3	2.26	0.60
1:A:164:ARG:HG2	1:A:282:HIS:HB2	1.83	0.60
1:A:327:ARG:O	1:A:331:ILE:HG12	2.02	0.60
1:A:451:LYS:HB3	1:A:477:LEU:HD11	1.82	0.60
2:B:900:BLA:CMA	2:B:900:BLA:HB	2.15	0.60
1:A:345:LEU:HD22	1:A:363:ILE:HD13	1.84	0.59
1:B:265:LEU:HD21	1:B:297:THR:HG21	1.85	0.59
1:B:345:LEU:HD22	1:B:363:ILE:HD13	1.85	0.58
1:B:557:SER:HB3	1:B:562:LEU:HD13	1.84	0.58
1:A:24:ILE:HD12	1:A:245:LEU:HB2	1.84	0.58
2:A:900:BLA:HB	2:A:900:BLA:HMA2	1.67	0.58
1:A:326:VAL:HG12	1:A:355:VAL:HG13	1.85	0.58
1:A:565:ARG:HH12	1:A:570:LEU:HB3	1.68	0.57
1:A:265:LEU:HD21	1:A:297:THR:HG21	1.85	0.57
2:B:900:BLA:HB	2:B:900:BLA:HMA2	1.69	0.57
1:A:401:VAL:HG13	1:A:402:GLY:H	1.69	0.56
1:A:371:ARG:NH2	1:A:377:ASP:HA	2.19	0.56
1:B:401:VAL:HG11	1:B:498:ARG:HH21	1.70	0.56
1:A:557:SER:HB3	1:A:562:LEU:HD13	1.87	0.56
1:A:401:VAL:HG11	1:A:498:ARG:NH2	2.21	0.56
1:A:160:ILE:HD13	1:A:293:MET:HG3	1.88	0.56
1:A:21:PRO:HD2	1:A:240:LEU:HD12	1.89	0.55
1:B:394:GLU:HG2	1:B:397:ARG:HH21	1.71	0.54
1:B:447:ILE:HG22	1:B:483:ARG:HG2	1.89	0.54
2:B:900:BLA:HBC1	2:B:900:BLA:HHD	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB2	1:A:485:ARG:HG2	1.88	0.54
2:A:900:BLA:CMA	2:A:900:BLA:NB	2.70	0.54
1:B:21:PRO:HD2	1:B:240:LEU:HD12	1.88	0.54
1:B:451:LYS:HB3	1:B:477:LEU:HD11	1.90	0.53
1:A:380:ALA:HB1	1:A:419:LEU:HD23	1.90	0.53
1:A:454:GLY:O	1:A:455:ASN:HB2	2.08	0.53
1:B:408:ALA:HB2	1:B:485:ARG:HG2	1.90	0.53
1:A:394:GLU:O	1:A:398:GLU:HG2	2.09	0.53
2:B:900:BLA:CMA	2:B:900:BLA:NB	2.72	0.53
1:A:139:VAL:O	1:A:307:ARG:HD2	2.11	0.52
1:A:513:GLN:O	1:A:517:THR:HG23	2.10	0.52
1:B:327:ARG:O	1:B:331:ILE:HG12	2.10	0.52
1:B:23:LEU:HD22	1:B:223:PRO:HB2	1.92	0.51
1:B:263:ALA:HB3	1:B:283:HIS:HB3	1.91	0.51
1:B:513:GLN:O	1:B:517:THR:HG23	2.10	0.51
1:B:48:ALA:HB2	1:B:55:MET:HE2	1.92	0.51
1:B:357:ASP:HB3	1:B:443:ARG:HH21	1.75	0.51
2:B:900:BLA:HHD	2:B:900:BLA:CBC	2.41	0.51
1:A:293:MET:O	1:A:297:THR:HG23	2.11	0.51
1:A:30:LEU:HD23	1:A:226:ILE:HD12	1.93	0.51
1:B:293:MET:O	1:B:297:THR:HG23	2.11	0.51
1:A:71:GLU:HB2	1:A:87:ALA:HB1	1.92	0.50
1:B:418:ASP:C	1:B:420:ALA:H	2.20	0.50
1:A:45:THR:HA	1:A:55:MET:HE1	1.94	0.50
1:A:401:VAL:HG11	1:A:498:ARG:HH21	1.76	0.50
1:A:547:VAL:HG13	1:A:559:VAL:HG13	1.94	0.49
1:B:45:THR:HA	1:B:55:MET:HE1	1.95	0.49
1:A:42:GLN:HA	1:A:228:PRO:HD2	1.94	0.49
1:B:420:ALA:O	1:B:424:ALA:HB2	2.12	0.49
1:A:48:ALA:HB1	1:A:54:PRO:HA	1.94	0.49
1:B:547:VAL:HG13	1:B:559:VAL:HG13	1.93	0.49
1:A:263:ALA:HB3	1:A:283:HIS:HB3	1.93	0.49
1:B:587:LEU:HA	1:B:626:TRP:CZ2	2.48	0.48
1:B:68:THR:HB	1:B:90:ARG:HB2	1.94	0.48
1:A:587:LEU:HA	1:A:626:TRP:CZ2	2.49	0.48
1:A:45:THR:HA	1:A:55:MET:CE	2.44	0.48
1:B:454:GLY:O	1:B:478:TRP:CD1	2.67	0.48
1:A:208:TYR:OH	2:A:900:BLA:HAA1	2.14	0.47
1:B:420:ALA:N	1:B:421:PRO:HD2	2.28	0.47
1:A:592:ALA:HB2	1:A:615:PRO:HD3	1.96	0.47
1:B:592:ALA:HB2	1:B:615:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:PRO:HB2	1:B:380:ALA:HB3	1.96	0.47
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.49	0.47
1:B:45:THR:HA	1:B:55:MET:CE	2.45	0.47
1:B:324:LEU:HD12	1:B:327:ARG:HH12	1.80	0.46
1:B:193:LEU:HG	1:B:453:ALA:HB2	1.97	0.46
1:B:167:ILE:HB	1:B:180:ALA:HB3	1.97	0.46
1:A:357:ASP:HB3	1:A:443:ARG:HH21	1.79	0.46
1:B:190:TYR:O	1:B:193:LEU:HB2	2.15	0.46
1:A:59:LEU:HD11	1:A:228:PRO:HD3	1.98	0.46
1:A:155:GLY:O	1:A:159:LEU:HD12	2.15	0.46
1:A:418:ASP:C	1:A:420:ALA:H	2.24	0.45
1:B:568:GLN:HA	1:B:571:TYR:CE2	2.50	0.45
1:A:214:ARG:NH2	1:A:266:VAL:HG22	2.32	0.45
1:A:167:ILE:HB	1:A:180:ALA:HB3	1.99	0.45
1:A:609:ARG:HG2	1:A:630:LEU:HB3	1.98	0.45
1:B:340:MET:HA	1:B:344:LEU:HD22	1.98	0.45
1:B:543:ARG:HD2	1:B:564:GLY:O	2.16	0.45
1:B:572:ALA:C	1:B:574:ASP:H	2.25	0.45
1:A:356:VAL:HG13	1:A:489:TRP:CZ3	2.51	0.44
1:B:326:VAL:CG1	1:B:355:VAL:HG13	2.47	0.44
1:A:266:VAL:HA	1:A:279:ILE:O	2.18	0.44
1:A:369:ILE:HD11	1:A:382:ARG:HG3	2.00	0.44
1:A:376:PRO:HB2	1:A:380:ALA:HB3	1.98	0.44
1:A:627:LEU:HD13	1:B:522:SER:HB3	2.00	0.43
1:B:155:GLY:O	1:B:159:LEU:HD12	2.17	0.43
1:B:416:LEU:O	1:B:418:ASP:O	2.37	0.43
1:A:28:GLY:O	1:A:46:THR:HG21	2.19	0.43
1:A:430:PRO:HD3	1:A:504:ILE:HG12	2.01	0.43
1:B:214:ARG:HG3	2:B:900:BLA:O2A	2.19	0.43
1:B:255:TYR:CD2	2:B:900:BLA:OC	2.70	0.43
1:A:330:LEU:O	1:A:334:PHE:HB2	2.19	0.43
1:B:130:ARG:HA	1:B:133:MET:HE3	2.01	0.43
1:A:97:PRO:HD2	1:A:98:PRO:HD3	2.01	0.43
1:A:502:VAL:HG23	1:B:502:VAL:HA	2.00	0.43
1:A:518:LEU:HD22	1:B:532:ILE:HG21	2.00	0.42
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.53	0.42
1:B:201:PRO:HB2	1:B:203:GLN:OE1	2.18	0.42
1:A:529:GLY:O	1:A:629:GLN:HA	2.20	0.42
1:B:330:LEU:O	1:B:334:PHE:HB2	2.20	0.42
1:B:94:ARG:NH1	1:B:95:ALA:H	2.17	0.42
1:B:266:VAL:HA	1:B:279:ILE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:VAL:CG1	1:A:498:ARG:HH21	2.33	0.42
1:B:615:PRO:HB2	1:B:623:THR:HG21	2.01	0.41
1:A:255:TYR:CD2	2:A:900:BLA:OC	2.73	0.41
1:A:352:LEU:HD21	1:A:439:LEU:HD21	2.02	0.41
1:A:12:VAL:HA	1:A:15:ARG:HD2	2.02	0.41
1:B:94:ARG:CZ	1:B:95:ALA:H	2.33	0.41
1:A:532:ILE:HG21	1:B:518:LEU:HD22	2.03	0.41
1:A:420:ALA:O	1:A:424:ALA:HB2	2.19	0.41
1:B:369:ILE:HD11	1:B:382:ARG:HG3	2.02	0.41
1:A:550:ALA:O	1:A:554:VAL:HG23	2.21	0.41
1:B:64:THR:HA	1:B:67:LEU:HB3	2.03	0.41
1:B:67:LEU:HD11	1:B:69:LEU:HB2	2.03	0.41
1:A:97:PRO:CD	1:A:98:PRO:HD3	2.51	0.41
1:B:328:GLU:O	1:B:332:THR:HG23	2.21	0.41
1:B:436:ARG:CZ	1:B:511:ARG:HG2	2.51	0.41
1:B:28:GLY:O	1:B:46:THR:HG21	2.21	0.40
1:A:195:TYR:CZ	2:A:900:BLA:HAB	2.56	0.40
1:B:352:LEU:HD21	1:B:439:LEU:HD21	2.02	0.40
1:B:615:PRO:CB	1:B:623:THR:HG21	2.52	0.40
1:B:598:PRO:HA	1:B:608:TYR:HA	2.04	0.40
1:B:282:HIS:HE1	2:B:900:BLA:OB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/640 (93%)	542 (91%)	45 (8%)	11 (2%)	6	19
1	B	602/640 (94%)	550 (91%)	43 (7%)	9 (2%)	8	23
All	All	1200/1280 (94%)	1092 (91%)	88 (7%)	20 (2%)	7	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	SER
1	A	455	ASN
1	A	526	LEU
1	A	537	THR
1	B	455	ASN
1	A	366	GLY
1	B	18	ILE
1	B	366	GLY
1	B	529	GLY
1	A	572	ALA
1	B	435	SER
1	B	94	ARG
1	A	436	ARG
1	A	227	GLN
1	A	418	ASP
1	A	607	VAL
1	A	401	VAL
1	B	401	VAL
1	B	227	GLN
1	B	604	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	501/532 (94%)	416 (83%)	85 (17%)	2	5
1	B	502/532 (94%)	422 (84%)	80 (16%)	2	8
All	All	1003/1064 (94%)	838 (84%)	165 (16%)	2	7

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	13	CYS
1	A	20	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	ILE
1	A	33	ILE
1	A	37	ASP
1	A	59	LEU
1	A	66	VAL
1	A	67	LEU
1	A	69	LEU
1	A	77	VAL
1	A	82	GLN
1	A	94	ARG
1	A	116	GLU
1	A	117	MET
1	A	118	GLU
1	A	123	ARG
1	A	129	LEU
1	A	133	MET
1	A	135	LEU
1	A	136	LEU
1	A	139	VAL
1	A	141	ARG
1	A	157	ARG
1	A	158	SER
1	A	159	LEU
1	A	167	ILE
1	A	193	LEU
1	A	207	LEU
1	A	210	ARG
1	A	212	ARG
1	A	214	ARG
1	A	226	ILE
1	A	230	VAL
1	A	234	LEU
1	A	238	VAL
1	A	244	SER
1	A	254	GLU
1	A	261	VAL
1	A	264	THR
1	A	266	VAL
1	A	268	SER
1	A	300	VAL
1	A	307	ARG
1	A	319	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	LEU
1	A	331	ILE
1	A	343	GLU
1	A	344	LEU
1	A	348	MET
1	A	355	VAL
1	A	356	VAL
1	A	371	ARG
1	A	375	THR
1	A	382	ARG
1	A	383	ARG
1	A	385	ARG
1	A	387	HIS
1	A	391	GLU
1	A	429	VAL
1	A	432	MET
1	A	437	SER
1	A	449	GLN
1	A	450	ILE
1	A	472	ARG
1	A	474	SER
1	A	476	ASP
1	A	492	LEU
1	A	495	GLU
1	A	504	ILE
1	A	506	LEU
1	A	514	GLN
1	A	518	LEU
1	A	525	ARG
1	A	527	ARG
1	A	535	ARG
1	A	543	ARG
1	A	545	LEU
1	A	562	LEU
1	A	566	GLU
1	A	570	LEU
1	A	585	ASP
1	A	601	VAL
1	A	614	GLU
1	A	634	GLU
1	B	13	CYS
1	B	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	18	ILE
1	B	20	ILE
1	B	33	ILE
1	B	37	ASP
1	B	50	LEU
1	B	59	LEU
1	B	67	LEU
1	B	69	LEU
1	B	77	VAL
1	B	82	GLN
1	B	85	MET
1	B	94	ARG
1	B	96	THR
1	B	116	GLU
1	B	117	MET
1	B	118	GLU
1	B	123	ARG
1	B	124	LEU
1	B	128	THR
1	B	129	LEU
1	B	135	LEU
1	B	139	VAL
1	B	142	ASP
1	B	157	ARG
1	B	158	SER
1	B	159	LEU
1	B	160	ILE
1	B	167	ILE
1	B	193	LEU
1	B	210	ARG
1	B	212	ARG
1	B	214	ARG
1	B	229	THR
1	B	230	VAL
1	B	234	LEU
1	B	238	VAL
1	B	244	SER
1	B	254	GLU
1	B	261	VAL
1	B	264	THR
1	B	266	VAL
1	B	268	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	300	VAL
1	B	319	LEU
1	B	323	LEU
1	B	331	ILE
1	B	338	GLU
1	B	339	HIS
1	B	343	GLU
1	B	344	LEU
1	B	348	MET
1	B	355	VAL
1	B	356	VAL
1	B	375	THR
1	B	382	ARG
1	B	383	ARG
1	B	385	ARG
1	B	387	HIS
1	B	429	VAL
1	B	432	MET
1	B	437	SER
1	B	449	GLN
1	B	472	ARG
1	B	476	ASP
1	B	488	ARG
1	B	492	LEU
1	B	495	GLU
1	B	504	ILE
1	B	514	GLN
1	B	518	LEU
1	B	528	ASP
1	B	545	LEU
1	B	562	LEU
1	B	565	ARG
1	B	585	ASP
1	B	601	VAL
1	B	614	GLU
1	B	634	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	222	GLN
1	A	287	HIS
1	A	335	ASN
1	A	455	ASN
1	A	514	GLN
1	A	584	GLN
1	B	82	GLN
1	B	222	GLN
1	B	258	ASN
1	B	291	HIS
1	B	455	ASN
1	B	610	GLN

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 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	1.70	10 (21%)	66,67,67	2.06	19 (28%)
2	BLA	B	900	1	46,46,46	1.65	9 (19%)	66,67,67	2.29	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	-	4/26/74/74	0/4/4/4
2	BLA	B	900	1	-	4/26/74/74	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C3D-C2D	5.36	1.48	1.36
2	A	900	BLA	C3B-C2B	4.99	1.47	1.37
2	B	900	BLA	C3B-C2B	4.93	1.47	1.37
2	A	900	BLA	CHA-C1A	4.05	1.49	1.40
2	B	900	BLA	CHB-C1B	4.04	1.47	1.37
2	B	900	BLA	CHA-C1A	3.73	1.48	1.40
2	B	900	BLA	C2A-C3A	3.43	1.47	1.38
2	B	900	BLA	CHB-C4A	3.23	1.47	1.40
2	A	900	BLA	C2A-C3A	3.16	1.47	1.38
2	B	900	BLA	C4A-C3A	2.94	1.48	1.41
2	B	900	BLA	C1A-C2A	2.46	1.48	1.42
2	A	900	BLA	C1A-C2A	2.41	1.48	1.42
2	A	900	BLA	OB-C4B	2.40	1.28	1.23
2	A	900	BLA	C4A-C3A	2.40	1.47	1.41
2	B	900	BLA	OB-C4B	2.39	1.28	1.23
2	A	900	BLA	C1B-C2B	2.31	1.49	1.45
2	A	900	BLA	C4D-C3D	2.20	1.49	1.45
2	A	900	BLA	C3C-C4C	2.10	1.49	1.45
2	B	900	BLA	C3C-C4C	2.06	1.49	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C3B-C4B-NB	6.41	114.19	106.13
2	B	900	BLA	C3B-C2B-C1B	-6.07	101.16	107.92
2	B	900	BLA	C3A-C4A-NA	5.92	115.50	107.43
2	B	900	BLA	C2B-C1B-NB	5.86	115.51	106.97
2	A	900	BLA	C3B-C2B-C1B	-5.79	101.47	107.92
2	A	900	BLA	C3B-C4B-NB	5.64	113.22	106.13
2	B	900	BLA	C4A-C3A-C2A	-5.10	101.38	107.76
2	B	900	BLA	C2A-C1A-NA	5.01	113.85	107.57
2	B	900	BLA	C1B-NB-C4B	-4.82	104.74	110.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C3A-C4A-NA	4.64	113.77	107.43
2	A	900	BLA	C2A-C1A-NA	4.60	113.34	107.57
2	A	900	BLA	C2B-C1B-NB	4.52	113.56	106.97
2	A	900	BLA	CMB-C2B-C1B	4.16	129.22	124.16
2	A	900	BLA	C4A-C3A-C2A	-3.49	103.39	107.76
2	A	900	BLA	C1A-C2A-C3A	-3.39	103.68	107.62
2	A	900	BLA	C1B-NB-C4B	-3.31	106.60	110.66
2	A	900	BLA	OB-C4B-C3B	-2.90	122.71	129.71
2	B	900	BLA	C4A-NA-C1A	-2.88	104.73	109.78
2	B	900	BLA	CMB-C2B-C1B	2.88	127.66	124.16
2	B	900	BLA	CHB-C4A-NA	-2.86	118.82	125.29
2	B	900	BLA	OB-C4B-C3B	-2.84	122.86	129.71
2	B	900	BLA	C4B-C3B-C2B	-2.75	104.39	107.92
2	A	900	BLA	CHA-C1A-C2A	-2.72	121.38	127.22
2	B	900	BLA	C1A-C2A-C3A	-2.69	104.49	107.62
2	B	900	BLA	CHB-C1B-NB	-2.66	120.39	126.06
2	B	900	BLA	CHA-C1A-C2A	-2.62	121.58	127.22
2	A	900	BLA	C4D-C3D-C2D	-2.61	103.90	106.73
2	B	900	BLA	CMA-C3A-C4A	2.55	129.33	125.62
2	A	900	BLA	CHB-C1B-NB	-2.47	120.79	126.06
2	B	900	BLA	CAA-CBA-CGA	-2.46	107.14	113.67
2	A	900	BLA	CBB-CAB-C3B	-2.44	115.32	127.53
2	A	900	BLA	C4C-CHD-C1D	2.35	133.82	128.06
2	B	900	BLA	C4C-CHD-C1D	2.30	133.71	128.06
2	A	900	BLA	C4A-NA-C1A	-2.26	105.82	109.78
2	B	900	BLA	CBB-CAB-C3B	-2.20	116.53	127.53
2	B	900	BLA	C4A-CHB-C1B	-2.20	124.50	130.82
2	A	900	BLA	CBA-CAA-C2A	-2.19	106.48	112.53
2	A	900	BLA	C4B-C3B-C2B	-2.17	105.14	107.92
2	A	900	BLA	C1D-C2D-C3D	-2.14	104.05	106.48

There are no chirality outliers.

All (8) 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	CAD-CBD-CGD-O1D
2	A	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	900	BLA	CAD-CBD-CGD-O2D

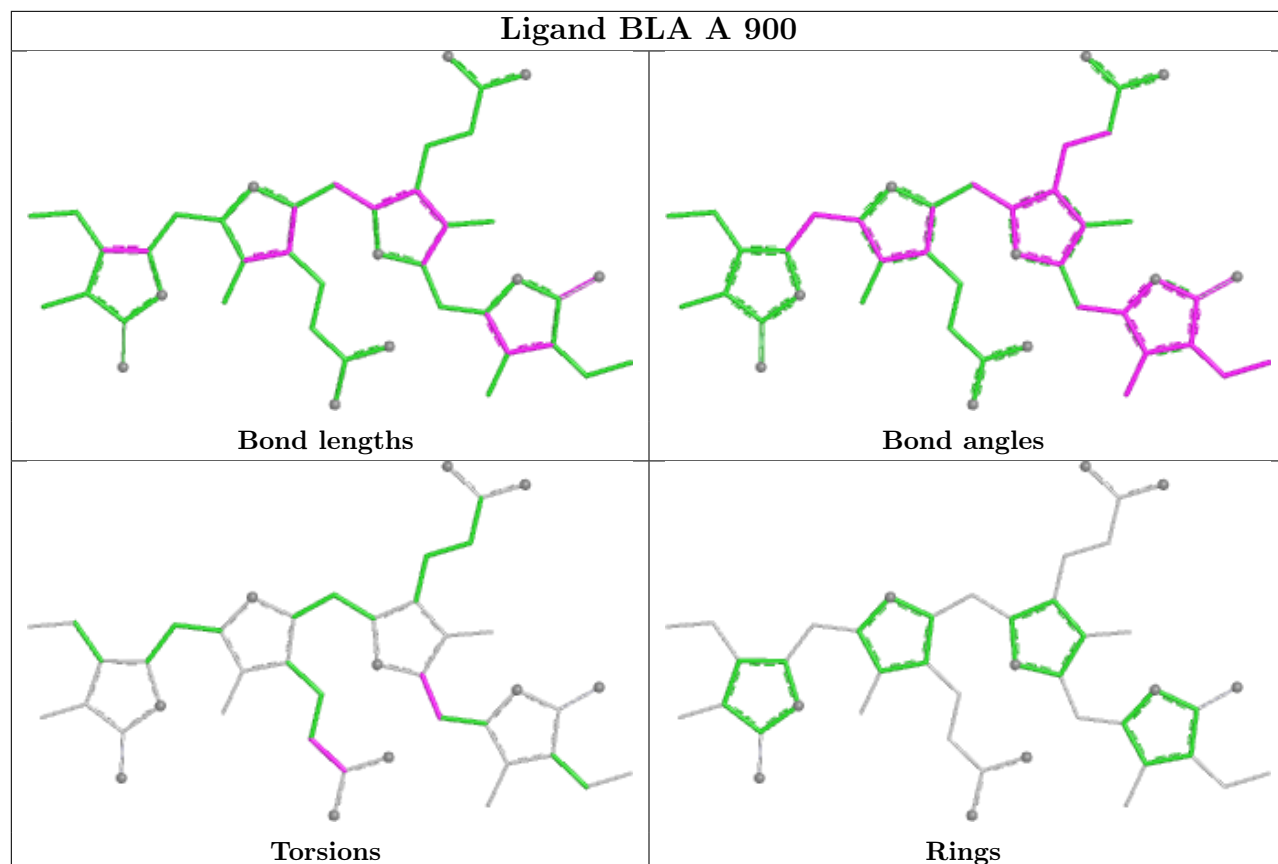
There are no ring outliers.

2 monomers are involved in 19 short contacts:

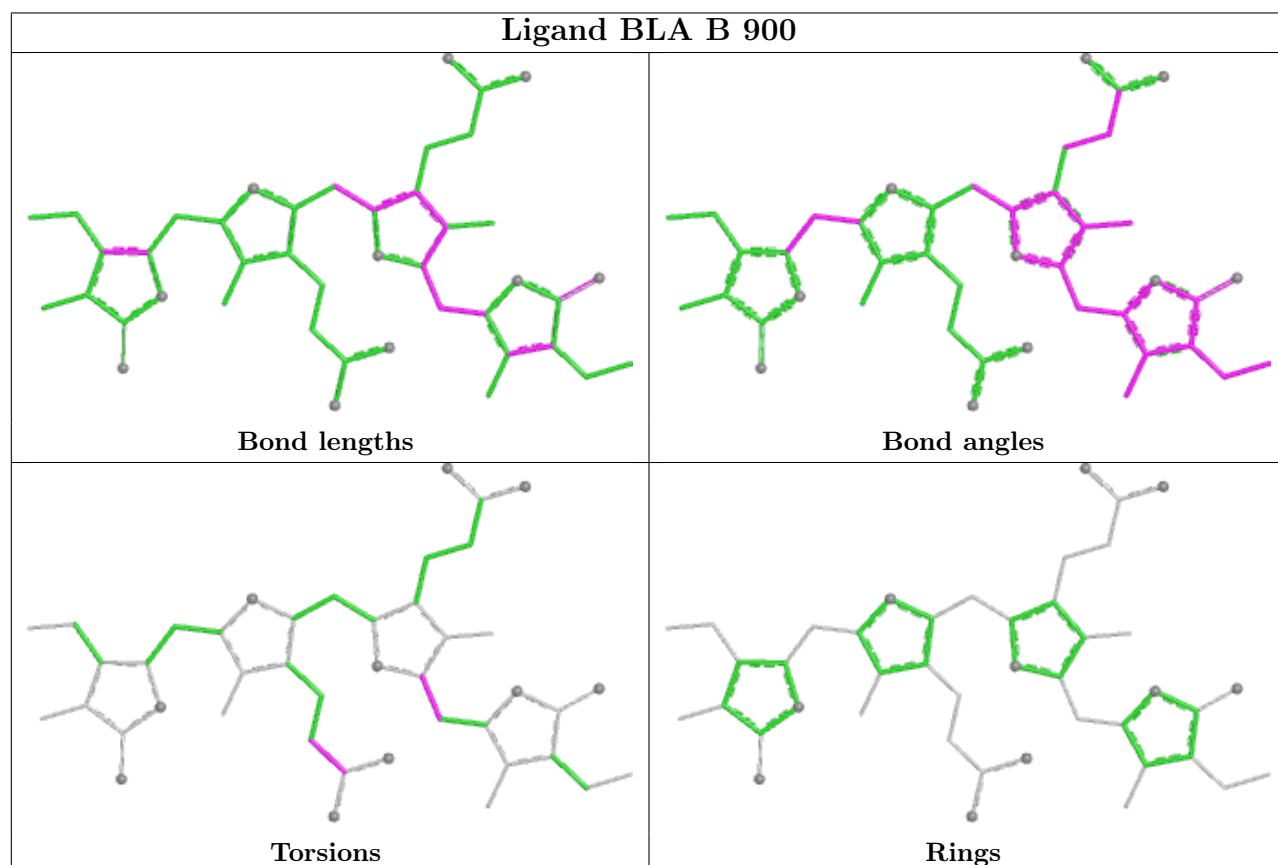
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	9	0
2	B	900	BLA	10	0

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 BLA A 900



Ligand BLA B 900



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	606/640 (94%)	0.17	13 (2%) 63 55	79, 116, 167, 184	0
1	B	608/640 (95%)	0.03	8 (1%) 75 69	77, 115, 172, 203	0
All	All	1214/1280 (94%)	0.10	21 (1%) 69 62	77, 116, 170, 203	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	THR	4.8
1	B	124	LEU	4.6
1	A	602	SER	4.5
1	B	456	PRO	4.0
1	A	456	PRO	3.7
1	B	129	LEU	3.6
1	A	122	ALA	3.5
1	A	127	VAL	3.3
1	A	51	LEU	3.2
1	A	128	THR	2.6
1	A	601	VAL	2.4
1	B	132	ALA	2.3
1	B	340	MET	2.3
1	A	340	MET	2.3
1	B	130	ARG	2.3
1	B	122	ALA	2.2
1	A	540	ALA	2.1
1	A	476	ASP	2.1
1	A	12	VAL	2.0
1	A	123	ARG	2.0
1	A	334	PHE	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](#)

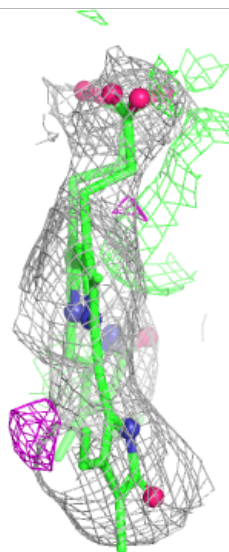
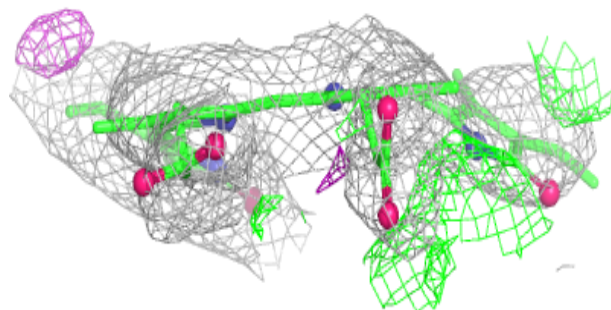
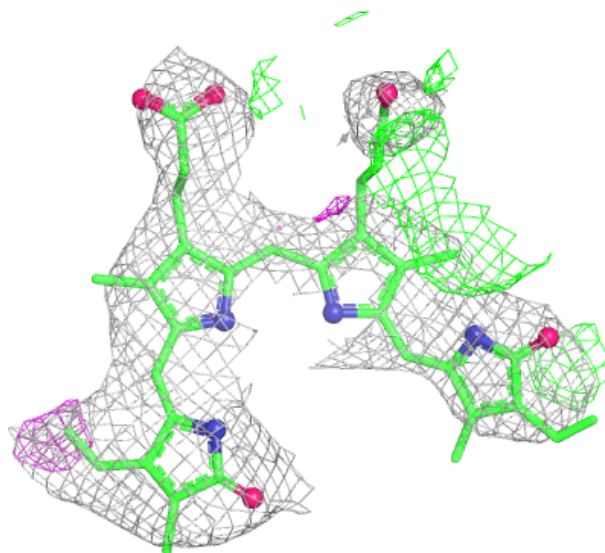
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BLA	A	900	43/43	0.89	0.15	122,129,145,159	0
2	BLA	B	900	43/43	0.91	0.16	116,123,137,151	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.

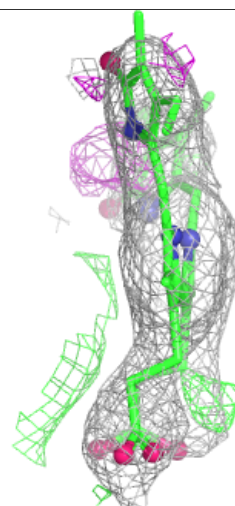
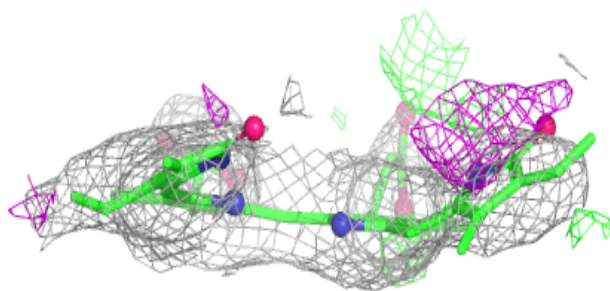
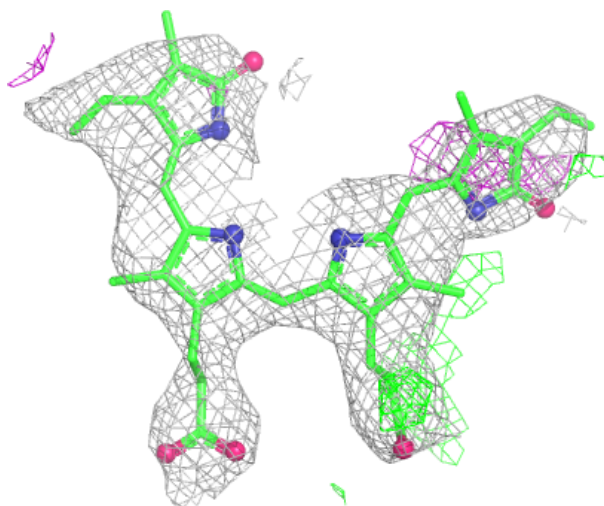
Electron density around BLA A 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.