



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:36 am BST

PDB ID : 5AKP
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP from Xanthomonas campestris bound to BV chromophore
Authors : Otero, L.H.; Klinke, S.; Goldbaum, F.A.; Bonomi, H.R.
Deposited on : 2015-03-04
Resolution : 3.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

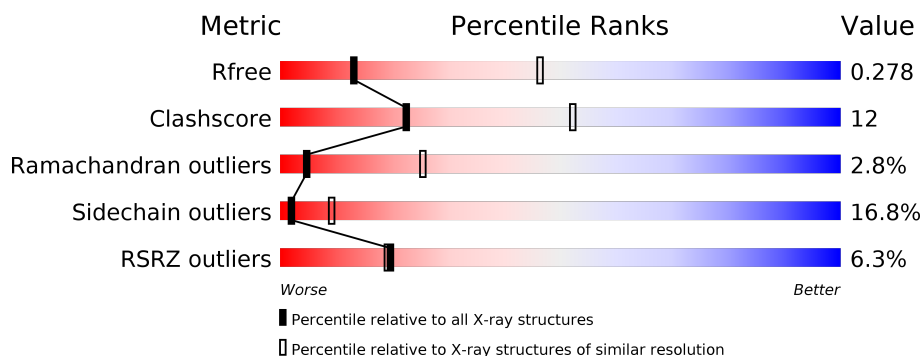
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>2%</div> <div>64%</div> <div>24%</div> <div>5%</div> <div>7%</div> </div>
1	B	640	<div> <div>10%</div> <div>63%</div> <div>26%</div> <div>6%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BLA	A	900	-	-	X	X
2	BLA	B	900	-	-	X	X
3	TRS	B	1633	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9495 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.

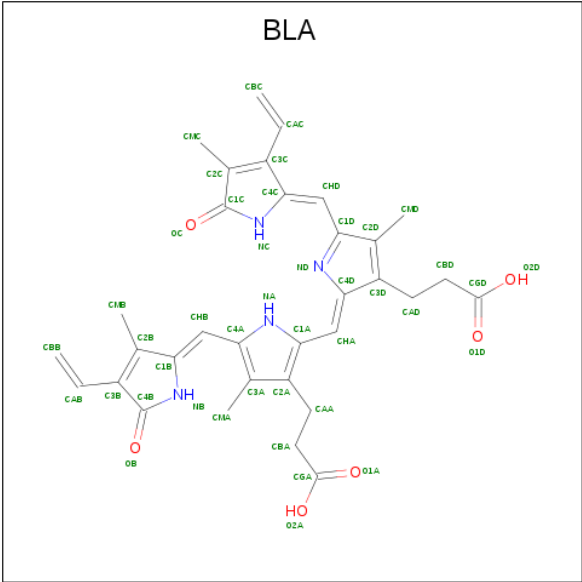
- Molecule 1 is a protein called PHYTOCHROME-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4644	2940	845	843	16			
1	B	606	Total	C	N	O	S	0	0	0
			4746	3004	862	864	16			

There are 14 discrepancies between the modelled and reference sequences:

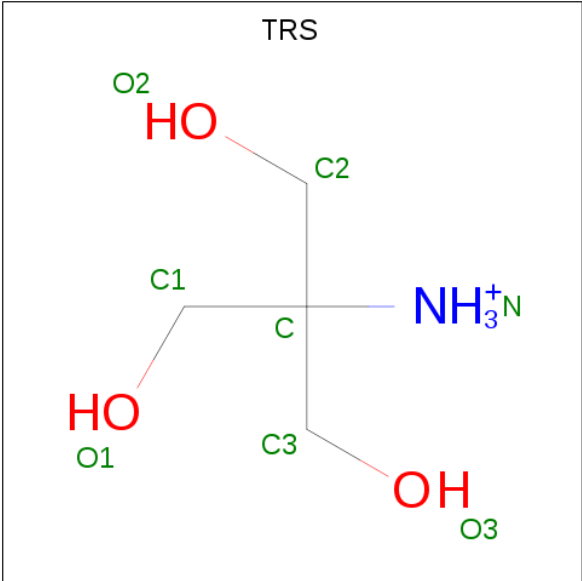
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q4UNU4
A	-4	HIS	-	expression tag	UNP Q4UNU4
A	-3	HIS	-	expression tag	UNP Q4UNU4
A	-2	HIS	-	expression tag	UNP Q4UNU4
A	-1	HIS	-	expression tag	UNP Q4UNU4
A	0	HIS	-	expression tag	UNP Q4UNU4
A	1	HIS	-	expression tag	UNP Q4UNU4
B	-5	MET	-	expression tag	UNP Q4UNU4
B	-4	HIS	-	expression tag	UNP Q4UNU4
B	-3	HIS	-	expression tag	UNP Q4UNU4
B	-2	HIS	-	expression tag	UNP Q4UNU4
B	-1	HIS	-	expression tag	UNP Q4UNU4
B	0	HIS	-	expression tag	UNP Q4UNU4
B	1	HIS	-	expression tag	UNP Q4UNU4

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

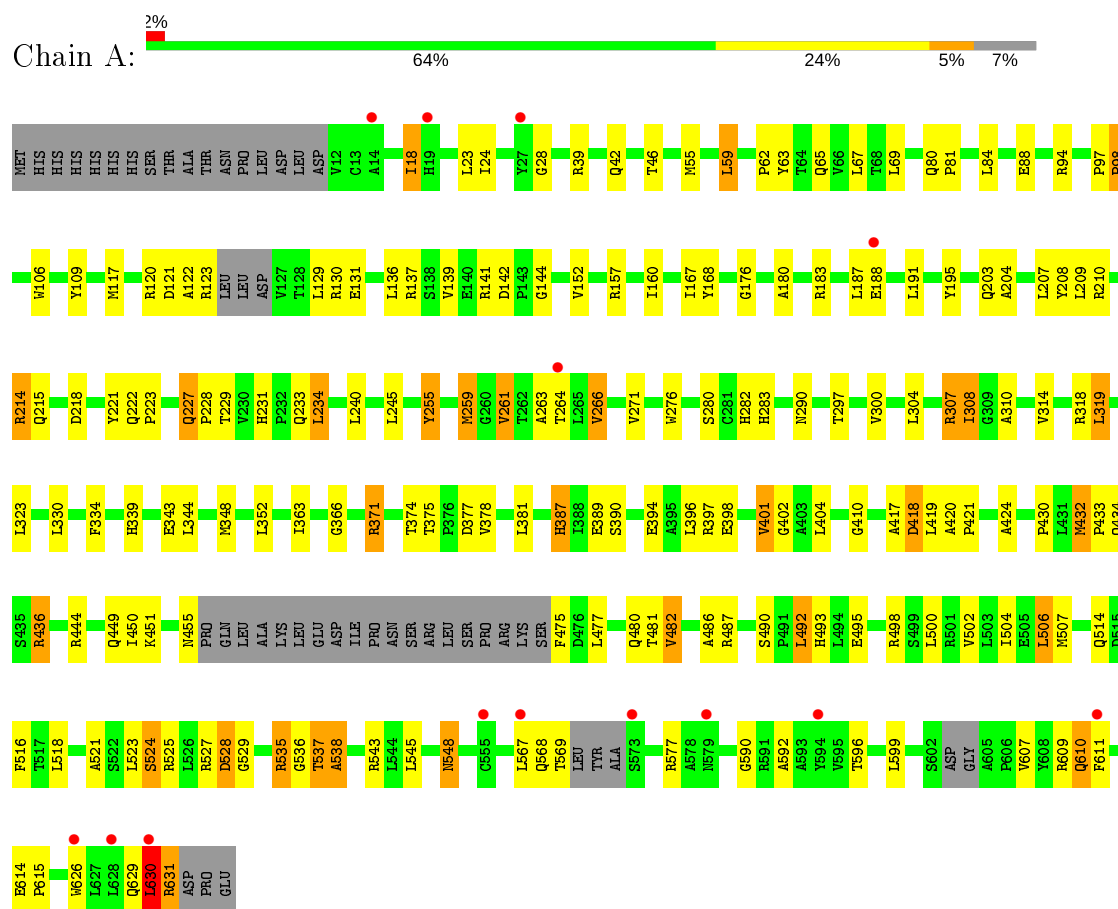
- Molecule 5 is water.

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

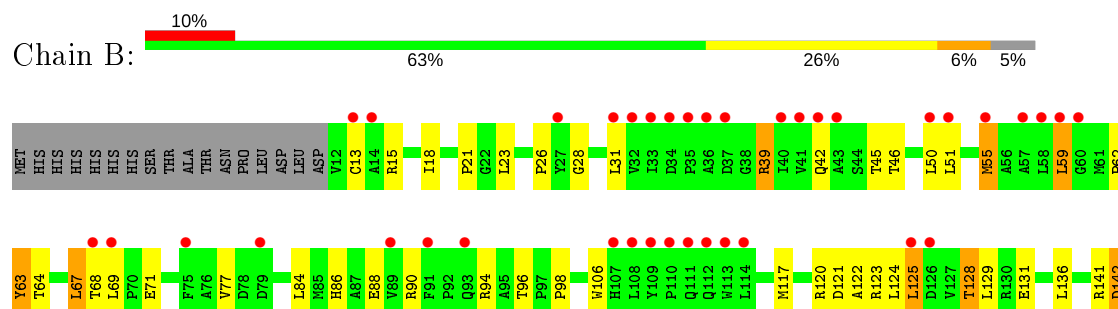
3 Residue-property plots [i](#)

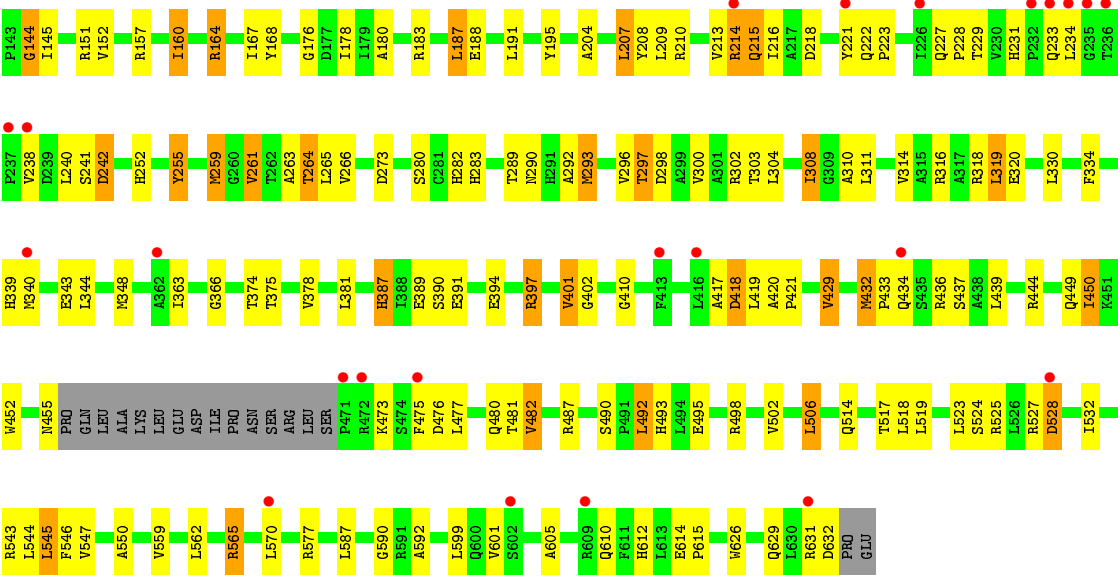
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PHYTOCHROME-LIKE PROTEIN



• Molecule 1: PHYTOCHROME-LIKE PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.94Å 103.94Å 344.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.75 – 3.25 49.22 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.75-3.25) 99.9 (49.22-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.255 0.224 , 0.278	Depositor DCC
R_{free} test set	1498 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 94.9	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	0.92	EDS
Total number of atoms	9495	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: TRS, BLA, CL

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	0/4748	0.74	0/6475
1	B	0.51	0/4855	0.74	0/6624
All	All	0.51	0/9603	0.74	0/13099

There are no bond length outliers.

There are no bond angle outliers.

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	4644	0	4637	110	0
1	B	4746	0	4741	107	0
2	A	43	0	30	21	0
2	B	43	0	31	21	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	9495	0	9463	219	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 12.

All (219) 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:195:TYR:CE1	2:A:900:BLA:HMB1	1.57	1.39
1:B:252:HIS:NE2	2:B:900:BLA:HBA1	1.54	1.20
1:A:610:GLN:O	1:A:630:LEU:HB3	1.42	1.18
1:B:195:TYR:CZ	2:B:900:BLA:HAB	1.89	1.07
1:A:195:TYR:CD1	2:A:900:BLA:CMB	2.39	1.05
1:A:611:PHE:HA	1:A:630:LEU:HD23	1.37	1.04
1:A:195:TYR:CD1	2:A:900:BLA:HMB1	1.94	1.00
1:A:195:TYR:CE1	2:A:900:BLA:CMB	2.46	0.99
2:A:900:BLA:HMA1	2:A:900:BLA:HB	1.28	0.98
1:A:195:TYR:CZ	2:A:900:BLA:HAB	1.98	0.97
1:A:614:GLU:HG2	1:B:525:ARG:HH21	1.27	0.96
2:B:900:BLA:HMA1	2:B:900:BLA:HB	1.32	0.92
1:B:195:TYR:CD1	2:B:900:BLA:HMB1	2.05	0.91
1:A:195:TYR:OH	2:A:900:BLA:HAB	1.69	0.91
1:A:195:TYR:CD1	2:A:900:BLA:HMB2	2.08	0.88
2:A:900:BLA:HMA1	2:A:900:BLA:NB	1.92	0.85
1:B:13:CYS:SG	2:B:900:BLA:HBC1	2.15	0.84
1:B:252:HIS:CE1	2:B:900:BLA:HBA1	2.14	0.83
1:A:610:GLN:O	1:A:630:LEU:CB	2.24	0.82
2:B:900:BLA:HMA1	2:B:900:BLA:NB	1.94	0.82
2:A:900:BLA:HB	2:A:900:BLA:CMA	1.94	0.80
2:B:900:BLA:CMA	2:B:900:BLA:HB	1.95	0.79
1:B:401:VAL:HG13	1:B:402:GLY:H	1.48	0.78
1:B:128:THR:HG23	1:B:296:VAL:HG21	1.63	0.77
1:A:371:ARG:HH21	1:A:377:ASP:HA	1.49	0.77
2:A:900:BLA:HMA2	2:A:900:BLA:CGA	2.15	0.76
2:B:900:BLA:HMA2	2:B:900:BLA:CGA	2.16	0.76
1:A:401:VAL:HG13	1:A:402:GLY:H	1.53	0.73
1:B:160:ILE:HG12	1:B:293:MET:SD	2.29	0.72
1:A:142:ASP:O	1:A:307:ARG:NH1	2.23	0.72
1:B:125:LEU:O	1:B:128:THR:HG22	1.90	0.71
1:A:631:ARG:HB2	1:B:527:ARG:HH22	1.55	0.71
1:B:195:TYR:CG	2:B:900:BLA:HMB1	2.26	0.71
1:A:307:ARG:NH2	1:B:273:ASP:OD1	2.24	0.70
1:B:42:GLN:HA	1:B:228:PRO:HG2	1.73	0.70
1:A:42:GLN:HA	1:A:228:PRO:HG2	1.74	0.69
1:A:629:GLN:O	1:A:630:LEU:HG	1.93	0.69
1:A:631:ARG:HB2	1:B:527:ARG:NH2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:CG	1:B:525:ARG:HH21	2.04	0.69
1:B:319:LEU:HD13	1:B:492:LEU:HD12	1.74	0.69
1:B:544:LEU:HD11	1:B:570:LEU:HD11	1.74	0.68
1:B:216:ILE:HB	1:B:264:THR:HB	1.73	0.68
1:A:255:TYR:OH	2:A:900:BLA:HMB3	1.94	0.68
1:B:265:LEU:HD21	1:B:297:THR:HG21	1.76	0.66
1:B:480:GLN:HE21	1:B:482:VAL:HG22	1.59	0.66
1:A:195:TYR:CZ	2:A:900:BLA:CAB	2.76	0.65
1:A:319:LEU:HD13	1:A:492:LEU:HD12	1.78	0.64
1:B:195:TYR:CE1	2:B:900:BLA:HAB	2.33	0.64
2:B:900:BLA:HMA2	2:B:900:BLA:O1A	1.98	0.64
1:A:629:GLN:C	1:A:630:LEU:HG	2.19	0.63
1:A:480:GLN:HE21	1:A:482:VAL:HG22	1.63	0.63
1:A:263:ALA:HB3	1:A:283:HIS:HB3	1.79	0.63
1:A:609:ARG:HE	1:A:631:ARG:C	2.02	0.62
1:B:252:HIS:NE2	2:B:900:BLA:CBA	2.48	0.62
1:A:195:TYR:OH	2:A:900:BLA:CAB	2.45	0.61
1:A:611:PHE:CA	1:A:630:LEU:HD23	2.25	0.61
1:A:535:ARG:HB2	1:A:626:TRP:CZ3	2.37	0.60
1:A:630:LEU:HD12	1:A:630:LEU:N	2.16	0.59
1:B:527:ARG:O	1:B:550:ALA:HB1	2.01	0.59
1:B:142:ASP:OD2	1:B:151:ARG:HD2	2.02	0.59
1:B:231:HIS:HD2	1:B:233:GLN:H	1.51	0.59
1:B:601:VAL:HG11	1:B:605:ALA:O	2.03	0.59
1:B:532:ILE:HG12	1:B:546:PHE:HB2	1.85	0.59
1:B:167:ILE:HB	1:B:180:ALA:HB3	1.85	0.58
1:B:145:ILE:HG12	1:B:308:ILE:HB	1.85	0.58
1:A:231:HIS:HD2	1:A:233:GLN:H	1.51	0.57
1:A:167:ILE:HB	1:A:180:ALA:HB3	1.86	0.57
1:B:418:ASP:C	1:B:420:ALA:H	2.08	0.57
1:A:418:ASP:C	1:A:420:ALA:H	2.08	0.56
1:A:430:PRO:HD3	1:A:504:ILE:HG12	1.88	0.56
1:A:432:MET:C	1:A:434:GLN:H	2.10	0.55
1:B:610:GLN:HB2	1:B:632:ASP:HB2	1.88	0.55
1:B:592:ALA:HB2	1:B:615:PRO:HD3	1.88	0.55
1:A:227:GLN:HB3	1:A:228:PRO:HD3	1.88	0.55
1:A:451:LYS:HB3	1:A:477:LEU:HD11	1.89	0.54
1:B:207:LEU:HB3	1:B:214:ARG:HH21	1.71	0.54
1:B:304:LEU:O	1:B:308:ILE:HG23	2.08	0.54
1:B:418:ASP:O	1:B:420:ALA:N	2.37	0.54
1:A:271:VAL:HG21	1:A:308:ILE:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ALA:HB2	1:A:615:PRO:HD3	1.88	0.54
1:A:450:ILE:HG13	1:A:480:GLN:HB3	1.89	0.54
1:A:195:TYR:CE1	2:A:900:BLA:HAB	2.42	0.54
1:B:378:VAL:HA	1:B:381:LEU:HD12	1.90	0.54
1:B:432:MET:C	1:B:434:GLN:H	2.11	0.53
1:B:68:THR:HB	1:B:90:ARG:HB3	1.90	0.53
1:B:263:ALA:HB3	1:B:283:HIS:HB3	1.90	0.53
1:A:378:VAL:HA	1:A:381:LEU:HD12	1.91	0.53
1:A:401:VAL:HG13	1:A:402:GLY:N	2.24	0.53
1:B:562:LEU:O	1:B:565:ARG:HB2	2.08	0.52
1:B:450:ILE:HD12	1:B:452:TRP:HE1	1.73	0.52
1:A:418:ASP:O	1:A:420:ALA:N	2.38	0.52
1:B:401:VAL:HG13	1:B:402:GLY:N	2.20	0.52
1:A:516:PHE:CE1	1:B:519:LEU:HD22	2.45	0.52
1:A:387:HIS:O	1:A:390:SER:HB3	2.10	0.52
1:A:271:VAL:HG21	1:A:308:ILE:HG12	1.92	0.51
1:A:214:ARG:HB3	1:A:266:VAL:HG23	1.92	0.51
1:A:396:LEU:HD22	1:A:404:LEU:HD11	1.92	0.51
1:B:401:VAL:HG13	1:B:498:ARG:HE	1.75	0.51
1:B:208:TYR:OH	2:B:900:BLA:HAA1	2.11	0.51
1:B:387:HIS:O	1:B:390:SER:HB3	2.11	0.51
1:B:289:THR:HB	1:B:293:MET:HE2	1.91	0.51
1:A:183:ARG:HH12	1:A:187:LEU:C	2.13	0.51
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.46	0.51
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.46	0.50
1:A:23:LEU:HD22	1:A:223:PRO:HB2	1.92	0.50
1:B:88:GLU:HB2	1:B:120:ARG:HH21	1.76	0.50
1:A:401:VAL:HG13	1:A:498:ARG:HE	1.75	0.50
1:A:266:VAL:HG21	2:A:900:BLA:HBA2	1.94	0.49
1:A:371:ARG:HG3	1:A:381:LEU:HD11	1.94	0.49
1:B:23:LEU:HD22	1:B:223:PRO:HB2	1.93	0.49
1:A:221:TYR:CE1	1:A:223:PRO:HG3	2.47	0.49
1:A:97:PRO:N	1:A:98:PRO:HD3	2.26	0.49
1:B:28:GLY:O	1:B:46:THR:HG21	2.12	0.49
1:A:88:GLU:HB2	1:A:120:ARG:HH21	1.78	0.49
1:A:596:THR:HA	1:A:609:ARG:O	2.11	0.49
2:A:900:BLA:HMA2	2:A:900:BLA:O1A	2.13	0.49
1:B:64:THR:HA	1:B:67:LEU:HB3	1.95	0.49
1:A:231:HIS:CD2	1:A:234:LEU:H	2.31	0.48
1:B:527:ARG:HG3	1:B:528:ASP:N	2.28	0.48
1:A:528:ASP:OD1	1:A:631:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:O	1:A:398:GLU:HG2	2.14	0.48
1:A:28:GLY:O	1:A:46:THR:HG21	2.12	0.48
1:B:213:VAL:HG21	1:B:298:ASP:HB2	1.96	0.48
1:B:136:LEU:HD22	1:B:303:THR:OG1	2.13	0.48
1:B:221:TYR:O	1:B:223:PRO:HD3	2.15	0.47
1:B:59:LEU:HD11	1:B:228:PRO:HG3	1.96	0.47
1:A:259:MET:HB3	1:A:261:VAL:HG13	1.96	0.47
1:A:371:ARG:NH2	1:A:377:ASP:HA	2.24	0.47
1:A:629:GLN:C	1:A:630:LEU:CG	2.80	0.47
1:B:289:THR:HB	1:B:293:MET:CE	2.45	0.47
1:B:394:GLU:HA	1:B:397:ARG:HE	1.79	0.47
1:A:137:ARG:HG2	1:B:302:ARG:NH2	2.30	0.47
1:B:259:MET:HB3	1:B:261:VAL:HG12	1.96	0.47
1:B:290:ASN:ND2	1:B:292:ALA:HB3	2.30	0.46
1:A:24:ILE:HG23	1:A:245:LEU:HB3	1.97	0.46
1:A:59:LEU:HD11	1:A:228:PRO:HG3	1.97	0.46
1:B:195:TYR:CE1	2:B:900:BLA:HMB1	2.47	0.46
1:A:307:ARG:O	1:A:308:ILE:C	2.52	0.45
1:A:504:ILE:HA	1:A:507:MET:HE3	1.98	0.45
1:A:81:PRO:HB3	1:A:109:TYR:CD1	2.51	0.45
1:B:215:GLN:HG2	1:B:216:ILE:N	2.31	0.45
1:A:525:ARG:HH12	1:B:614:GLU:HG2	1.82	0.45
1:A:152:VAL:HG21	1:A:304:LEU:HB2	1.97	0.45
1:A:490:SER:HB3	1:A:493:HIS:ND1	2.31	0.45
1:A:420:ALA:N	1:A:421:PRO:HD2	2.32	0.45
1:A:527:ARG:HH11	1:A:631:ARG:HD3	1.80	0.45
1:B:31:LEU:HD11	1:B:51:LEU:HD21	1.97	0.45
1:B:340:MET:HA	1:B:344:LEU:HD23	1.99	0.45
1:B:420:ALA:N	1:B:421:PRO:HD2	2.31	0.45
1:A:130:ARG:NH2	1:B:86:HIS:O	2.50	0.45
1:A:609:ARG:NE	1:A:631:ARG:O	2.36	0.45
1:A:310:ALA:O	1:A:314:VAL:HG23	2.17	0.45
1:A:609:ARG:NE	1:A:631:ARG:C	2.69	0.45
1:A:524:SER:HA	1:A:548:ASN:HB2	1.98	0.45
1:B:547:VAL:HG13	1:B:559:VAL:HG13	1.98	0.45
1:B:527:ARG:O	1:B:550:ALA:CB	2.64	0.44
1:B:195:TYR:CG	2:B:900:BLA:CMB	3.00	0.44
1:B:255:TYR:CD1	1:B:255:TYR:C	2.91	0.44
1:B:310:ALA:O	1:B:314:VAL:HG23	2.17	0.44
1:A:214:ARG:HH21	2:A:900:BLA:HBD1	1.83	0.44
2:A:900:BLA:CGA	2:A:900:BLA:CMA	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ARG:HD3	1:A:609:ARG:HA	1.78	0.44
1:B:432:MET:HG2	1:B:433:PRO:HD2	2.00	0.44
1:B:449:GLN:HE22	1:B:481:THR:HG23	1.82	0.44
1:B:178:ILE:HD11	2:B:900:BLA:CBB	2.47	0.44
1:A:521:ALA:O	1:A:525:ARG:HG3	2.18	0.43
1:B:195:TYR:CD1	2:B:900:BLA:CMB	2.89	0.43
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.92	0.43
1:A:195:TYR:CG	2:A:900:BLA:HMB2	2.50	0.43
1:B:152:VAL:HG21	1:B:304:LEU:HB2	2.01	0.43
1:A:424:ALA:HB3	1:A:486:ALA:HB2	2.01	0.43
1:A:84:LEU:HB2	1:A:106:TRP:HB2	2.00	0.43
1:B:21:PRO:HD2	1:B:240:LEU:HD23	1.99	0.43
1:B:84:LEU:HB2	1:B:106:TRP:HB2	2.00	0.43
1:A:255:TYR:C	1:A:255:TYR:CD1	2.92	0.43
1:B:240:LEU:O	1:B:242:ASP:N	2.37	0.43
1:B:195:TYR:CE2	2:B:900:BLA:HAB	2.49	0.42
1:A:307:ARG:NH2	1:B:273:ASP:CG	2.73	0.42
1:A:449:GLN:HE22	1:A:481:THR:HG23	1.83	0.42
1:B:45:THR:HA	1:B:55:MET:HE1	2.01	0.42
1:B:450:ILE:HD12	1:B:452:TRP:NE1	2.33	0.42
1:B:545:LEU:HD22	1:B:546:PHE:CE2	2.54	0.42
1:A:631:ARG:HA	1:A:631:ARG:HD2	1.80	0.42
1:B:231:HIS:CD2	1:B:234:LEU:H	2.36	0.42
1:A:432:MET:HG2	1:A:433:PRO:HD2	2.02	0.42
1:A:502:VAL:O	1:A:506:LEU:HB2	2.20	0.42
1:A:567:LEU:O	1:A:569:THR:N	2.53	0.42
1:B:429:VAL:HG12	1:B:439:LEU:HB2	2.02	0.42
1:B:490:SER:HB3	1:B:493:HIS:ND1	2.34	0.42
1:A:319:LEU:HD22	1:A:323:LEU:HD22	2.01	0.42
1:A:590:GLY:HA2	1:A:626:TRP:HZ2	1.84	0.42
2:B:900:BLA:HBB1	2:B:900:BLA:OB	2.20	0.42
1:A:536:GLY:C	1:A:538:ALA:H	2.19	0.41
1:B:26:PRO:HD2	1:B:221:TYR:CD2	2.55	0.41
1:A:168:TYR:CE1	1:A:176:GLY:HA3	2.56	0.41
1:B:449:GLN:NE2	1:B:481:THR:HG23	2.34	0.41
1:B:612:HIS:HB3	1:B:629:GLN:HB2	2.01	0.41
1:A:208:TYR:OH	2:A:900:BLA:HAA1	2.20	0.41
1:B:144:GLY:H	1:B:311:LEU:HD22	1.86	0.41
1:A:276:TRP:NE1	1:A:308:ILE:HD13	2.35	0.41
1:A:449:GLN:NE2	1:A:481:THR:HG23	2.35	0.41
1:B:204:ALA:O	1:B:208:TYR:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD12	1:B:519:LEU:HG	2.03	0.41
2:B:900:BLA:CMA	2:B:900:BLA:CGA	2.92	0.41
1:B:587:LEU:HA	1:B:626:TRP:CZ2	2.56	0.41
1:B:164:ARG:HB3	1:B:282:HIS:HB2	2.02	0.41
1:B:502:VAL:O	1:B:506:LEU:HB2	2.20	0.41
1:A:410:GLY:HA2	1:A:417:ALA:HA	2.02	0.41
1:A:204:ALA:O	1:A:208:TYR:HD1	2.03	0.41
1:B:316:ARG:O	1:B:320:GLU:HB2	2.21	0.41
1:B:527:ARG:CG	1:B:528:ASP:N	2.84	0.41
1:B:39:ARG:HA	1:B:62:PRO:HA	2.02	0.40
1:B:590:GLY:HA2	1:B:626:TRP:CZ2	2.56	0.40
1:A:610:GLN:HG2	1:A:610:GLN:H	1.73	0.40
1:A:39:ARG:HA	1:A:62:PRO:HA	2.03	0.40
1:A:330:LEU:HD11	1:A:352:LEU:HA	2.03	0.40
1:B:391:GLU:CD	1:B:391:GLU:H	2.25	0.40
1:B:410:GLY:HA2	1:B:417:ALA:HA	2.03	0.40
1:B:63:TYR:CE2	1:B:67:LEU:HD13	2.57	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	583/640 (91%)	528 (91%)	38 (6%)	17 (3%)	4	25
1	B	602/640 (94%)	543 (90%)	43 (7%)	16 (3%)	5	26
All	All	1185/1280 (93%)	1071 (90%)	81 (7%)	33 (3%)	5	25

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	LEU

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Mol	Chain	Res	Type
1	B	241	SER
1	A	18	ILE
1	A	366	GLY
1	A	529	GLY
1	A	537	THR
1	A	568	GLN
1	A	630	LEU
1	B	18	ILE
1	B	144	GLY
1	B	187	LEU
1	B	366	GLY
1	B	401	VAL
1	A	98	PRO
1	A	121	ASP
1	A	122	ALA
1	A	401	VAL
1	A	418	ASP
1	A	436	ARG
1	B	98	PRO
1	B	121	ASP
1	B	122	ALA
1	B	418	ASP
1	B	475	PHE
1	A	55	MET
1	A	144	GLY
1	A	419	LEU
1	A	538	ALA
1	B	55	MET
1	B	419	LEU
1	B	436	ARG
1	A	607	VAL
1	B	71	GLU

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	489/532 (92%)	408 (83%)	81 (17%)	2	9
1	B	500/532 (94%)	415 (83%)	85 (17%)	2	9
All	All	989/1064 (93%)	823 (83%)	166 (17%)	2	9

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	59	LEU
1	A	63	TYR
1	A	65	GLN
1	A	67	LEU
1	A	69	LEU
1	A	80	GLN
1	A	94	ARG
1	A	117	MET
1	A	123	ARG
1	A	129	LEU
1	A	131	GLU
1	A	136	LEU
1	A	139	VAL
1	A	141	ARG
1	A	157	ARG
1	A	160	ILE
1	A	188	GLU
1	A	191	LEU
1	A	203	GLN
1	A	207	LEU
1	A	209	LEU
1	A	210	ARG
1	A	214	ARG
1	A	215	GLN
1	A	218	ASP
1	A	222	GLN
1	A	227	GLN
1	A	229	THR
1	A	234	LEU
1	A	240	LEU
1	A	255	TYR
1	A	259	MET
1	A	261	VAL
1	A	264	THR

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Mol	Chain	Res	Type
1	A	266	VAL
1	A	280	SER
1	A	282	HIS
1	A	290	ASN
1	A	297	THR
1	A	300	VAL
1	A	307	ARG
1	A	308	ILE
1	A	318	ARG
1	A	319	LEU
1	A	334	PHE
1	A	339	HIS
1	A	343	GLU
1	A	344	LEU
1	A	348	MET
1	A	363	ILE
1	A	371	ARG
1	A	374	THR
1	A	375	THR
1	A	387	HIS
1	A	389	GLU
1	A	397	ARG
1	A	432	MET
1	A	436	ARG
1	A	444	ARG
1	A	455	ASN
1	A	475	PHE
1	A	482	VAL
1	A	487	ARG
1	A	492	LEU
1	A	495	GLU
1	A	506	LEU
1	A	514	GLN
1	A	518	LEU
1	A	524	SER
1	A	528	ASP
1	A	535	ARG
1	A	537	THR
1	A	543	ARG
1	A	545	LEU
1	A	548	ASN
1	A	577	ARG

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Mol	Chain	Res	Type
1	A	599	LEU
1	A	610	GLN
1	A	630	LEU
1	A	631	ARG
1	B	15	ARG
1	B	39	ARG
1	B	50	LEU
1	B	59	LEU
1	B	63	TYR
1	B	67	LEU
1	B	69	LEU
1	B	77	VAL
1	B	94	ARG
1	B	96	THR
1	B	117	MET
1	B	123	ARG
1	B	125	LEU
1	B	128	THR
1	B	129	LEU
1	B	131	GLU
1	B	141	ARG
1	B	142	ASP
1	B	157	ARG
1	B	160	ILE
1	B	164	ARG
1	B	183	ARG
1	B	187	LEU
1	B	188	GLU
1	B	191	LEU
1	B	207	LEU
1	B	209	LEU
1	B	210	ARG
1	B	214	ARG
1	B	215	GLN
1	B	218	ASP
1	B	222	GLN
1	B	227	GLN
1	B	229	THR
1	B	238	VAL
1	B	242	ASP
1	B	255	TYR
1	B	259	MET

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Mol	Chain	Res	Type
1	B	261	VAL
1	B	264	THR
1	B	266	VAL
1	B	280	SER
1	B	293	MET
1	B	297	THR
1	B	300	VAL
1	B	308	ILE
1	B	318	ARG
1	B	319	LEU
1	B	330	LEU
1	B	334	PHE
1	B	339	HIS
1	B	343	GLU
1	B	348	MET
1	B	363	ILE
1	B	374	THR
1	B	375	THR
1	B	387	HIS
1	B	389	GLU
1	B	397	ARG
1	B	429	VAL
1	B	432	MET
1	B	437	SER
1	B	444	ARG
1	B	450	ILE
1	B	455	ASN
1	B	473	LYS
1	B	476	ASP
1	B	477	LEU
1	B	482	VAL
1	B	487	ARG
1	B	492	LEU
1	B	495	GLU
1	B	506	LEU
1	B	514	GLN
1	B	517	THR
1	B	518	LEU
1	B	523	LEU
1	B	524	SER
1	B	528	ASP
1	B	543	ARG

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Mol	Chain	Res	Type
1	B	545	LEU
1	B	565	ARG
1	B	577	ARG
1	B	599	LEU
1	B	631	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	365	HIS
1	A	455	ASN
1	A	480	GLN
1	B	73	GLN
1	B	82	GLN
1	B	231	HIS
1	B	233	GLN
1	B	290	ASN
1	B	480	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRS	A	1632	-	7,7,7	0.31	0	9,9,9	0.38	0
2	BLA	A	900	1	36,46,46	3.30	12 (33%)	47,67,67	2.01	12 (25%)
2	BLA	B	900	1	36,46,46	3.21	8 (22%)	47,67,67	1.37	7 (14%)
3	TRS	B	1633	-	7,7,7	0.34	0	9,9,9	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	A	1632	-	-	3/9/9/9	-
2	BLA	A	900	1	-	4/22/74/74	0/4/4/4
2	BLA	B	900	1	-	2/22/74/74	0/4/4/4
3	TRS	B	1633	-	-	0/9/9/9	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CHA-C4D	15.43	1.48	1.35
2	A	900	BLA	CHA-C4D	15.01	1.47	1.35
2	A	900	BLA	CHB-C1B	7.93	1.50	1.34
2	B	900	BLA	C3B-C2B	6.47	1.50	1.37
2	B	900	BLA	CHB-C1B	6.34	1.47	1.34
2	A	900	BLA	C3B-C2B	5.64	1.48	1.37
2	B	900	BLA	C3C-C4C	3.58	1.51	1.45
2	B	900	BLA	C2A-C3A	3.46	1.47	1.37
2	A	900	BLA	OB-C4B	3.23	1.29	1.23
2	A	900	BLA	C3C-C4C	3.16	1.50	1.45
2	A	900	BLA	C1B-C2B	3.10	1.50	1.45
2	B	900	BLA	C1B-C2B	2.86	1.50	1.45
2	B	900	BLA	OB-C4B	2.83	1.29	1.23
2	A	900	BLA	C2A-C3A	2.80	1.46	1.37
2	A	900	BLA	C4D-ND	-2.57	1.33	1.38
2	A	900	BLA	C4A-CHB	2.54	1.51	1.41
2	A	900	BLA	C4B-NB	-2.46	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C1B-NB	-2.41	1.33	1.37
2	B	900	BLA	C4A-CHB	2.07	1.49	1.41
2	A	900	BLA	C1A-CHA	2.05	1.49	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	CMB-C2B-C1B	5.47	131.00	124.17
2	A	900	BLA	CHA-C4D-ND	-5.40	121.34	128.83
2	A	900	BLA	C3B-C2B-C1B	-4.92	102.08	108.03
2	A	900	BLA	C3B-C4B-NB	4.59	111.37	106.19
2	B	900	BLA	C3B-C2B-C1B	-4.11	103.06	108.03
2	A	900	BLA	CHB-C1B-NB	-4.00	116.95	130.40
2	B	900	BLA	CHB-C1B-NB	-3.48	118.72	130.40
2	B	900	BLA	CMB-C2B-C1B	3.47	128.50	124.17
2	A	900	BLA	C2B-C1B-NB	3.33	111.86	106.99
2	A	900	BLA	C1A-CHA-C4D	3.26	132.71	128.81
2	B	900	BLA	CHA-C4D-C3D	-2.79	118.88	125.32
2	A	900	BLA	C4B-C3B-C2B	-2.47	104.75	107.92
2	A	900	BLA	OB-C4B-NB	-2.38	119.54	125.08
2	A	900	BLA	CMA-C3A-C2A	-2.25	120.69	124.94
2	B	900	BLA	CHB-C1B-C2B	2.15	131.22	126.97
2	A	900	BLA	CHB-C1B-C2B	2.14	131.19	126.97
2	B	900	BLA	C2B-C1B-NB	2.10	110.06	106.99
2	B	900	BLA	C3B-C4B-NB	2.05	108.51	106.19
2	A	900	BLA	CAD-C3D-C4D	2.03	128.60	125.01

There are no chirality outliers.

All (9) torsion outliers are listed below:

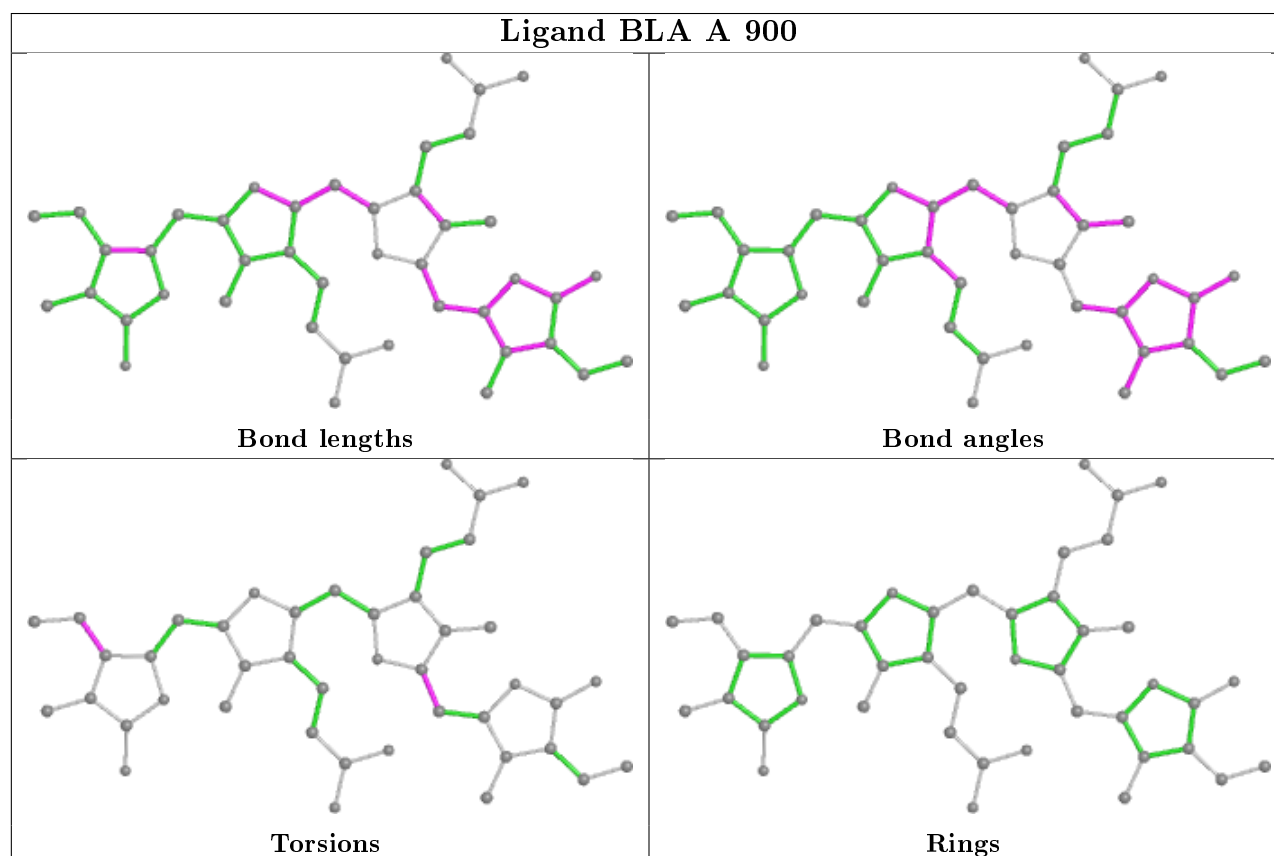
Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	A	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	C4C-C3C-CAC-CBC
2	B	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
3	A	1632	TRS	N-C-C1-O1
3	A	1632	TRS	C2-C-C1-O1
3	A	1632	TRS	C3-C-C1-O1

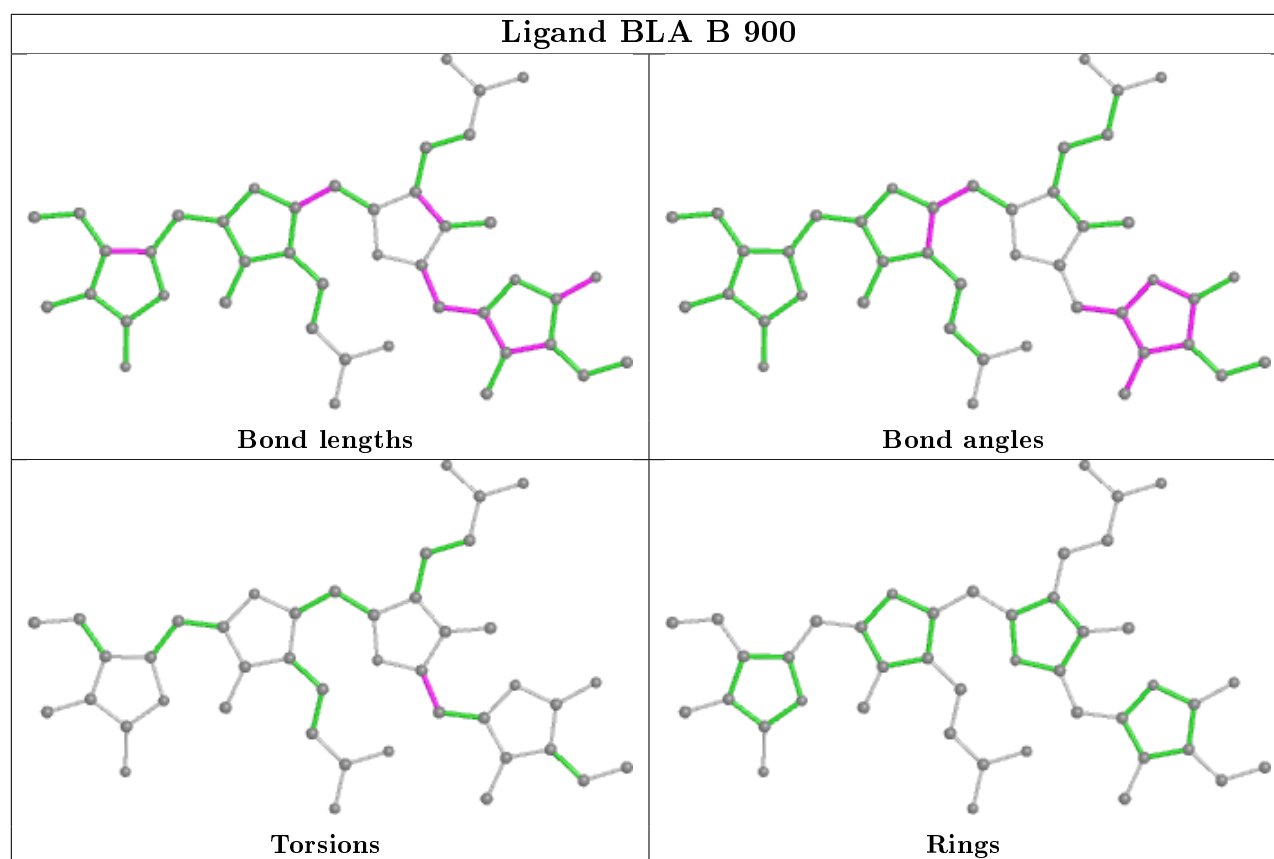
There are no ring outliers.

2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	21	0
2	B	900	BLA	21	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

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	593/640 (92%)	0.20	14 (2%) 59 55	57, 106, 165, 186	0
1	B	606/640 (94%)	0.53	61 (10%) 7 7	60, 108, 189, 209	0
All	All	1199/1280 (93%)	0.37	75 (6%) 20 19	57, 107, 179, 209	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	PHE	6.0
1	B	33	ILE	5.6
1	B	35	PRO	5.2
1	B	236	THR	5.0
1	B	113	TRP	4.9
1	B	40	ILE	4.8
1	A	630	LEU	4.5
1	B	55	MET	4.2
1	A	555	CYS	4.2
1	B	60	GLY	4.2
1	B	37	ASP	4.1
1	B	59	LEU	3.8
1	B	226	ILE	3.7
1	B	125	LEU	3.6
1	B	471	PRO	3.5
1	B	528	ASP	3.3
1	B	51	LEU	3.3
1	B	570	LEU	3.2
1	A	611	PHE	3.2
1	B	233	GLN	3.2
1	B	58	LEU	3.1
1	B	413	PHE	3.1
1	B	93	GLN	3.0
1	B	235	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	69	LEU	3.0
1	A	27	TYR	2.9
1	B	31	LEU	2.9
1	B	126	ASP	2.9
1	B	111	GLN	2.9
1	B	41	VAL	2.9
1	B	238	VAL	2.8
1	B	36	ALA	2.8
1	B	50	LEU	2.8
1	B	13	CYS	2.8
1	B	14	ALA	2.8
1	B	221	TYR	2.8
1	B	68	THR	2.8
1	B	237	PRO	2.7
1	B	32	VAL	2.7
1	A	594	TYR	2.7
1	B	42	GLN	2.6
1	B	434	GLN	2.6
1	B	79	ASP	2.6
1	B	114	LEU	2.6
1	B	609	ARG	2.6
1	A	567	LEU	2.4
1	B	108	LEU	2.4
1	B	89	VAL	2.4
1	B	57	ALA	2.4
1	A	14	ALA	2.4
1	B	232	PRO	2.4
1	B	107	HIS	2.4
1	A	188	GLU	2.4
1	B	472	ARG	2.4
1	B	340	MET	2.4
1	B	234	LEU	2.4
1	B	112	GLN	2.3
1	B	475	PHE	2.3
1	A	579	ASN	2.3
1	B	27	TYR	2.3
1	B	631	ARG	2.3
1	B	110	PRO	2.2
1	A	573	SER	2.2
1	B	43	ALA	2.2
1	B	416	LEU	2.2
1	A	628	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	2.2
1	B	602	SER	2.2
1	B	214	ARG	2.1
1	A	264	THR	2.1
1	A	626	TRP	2.1
1	B	34	ASP	2.0
1	A	19	HIS	2.0
1	B	75	PHE	2.0
1	B	109	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

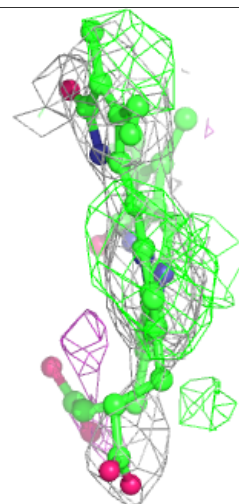
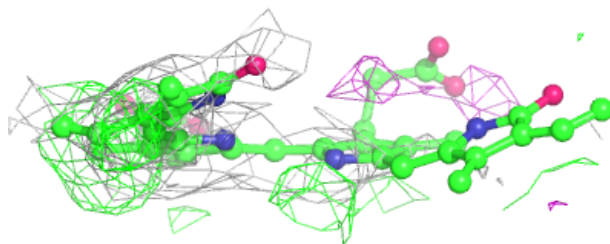
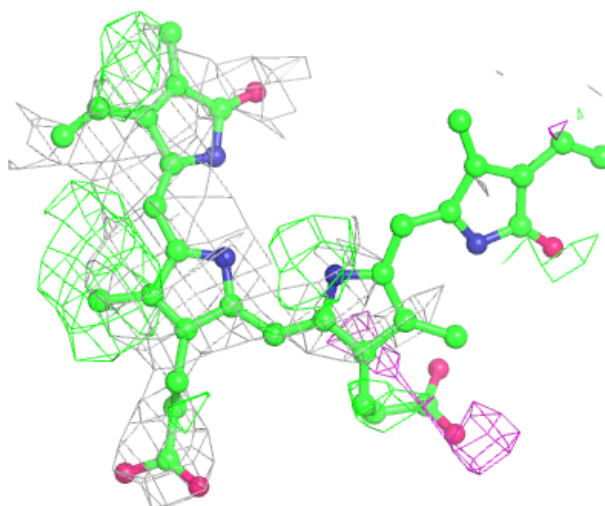
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

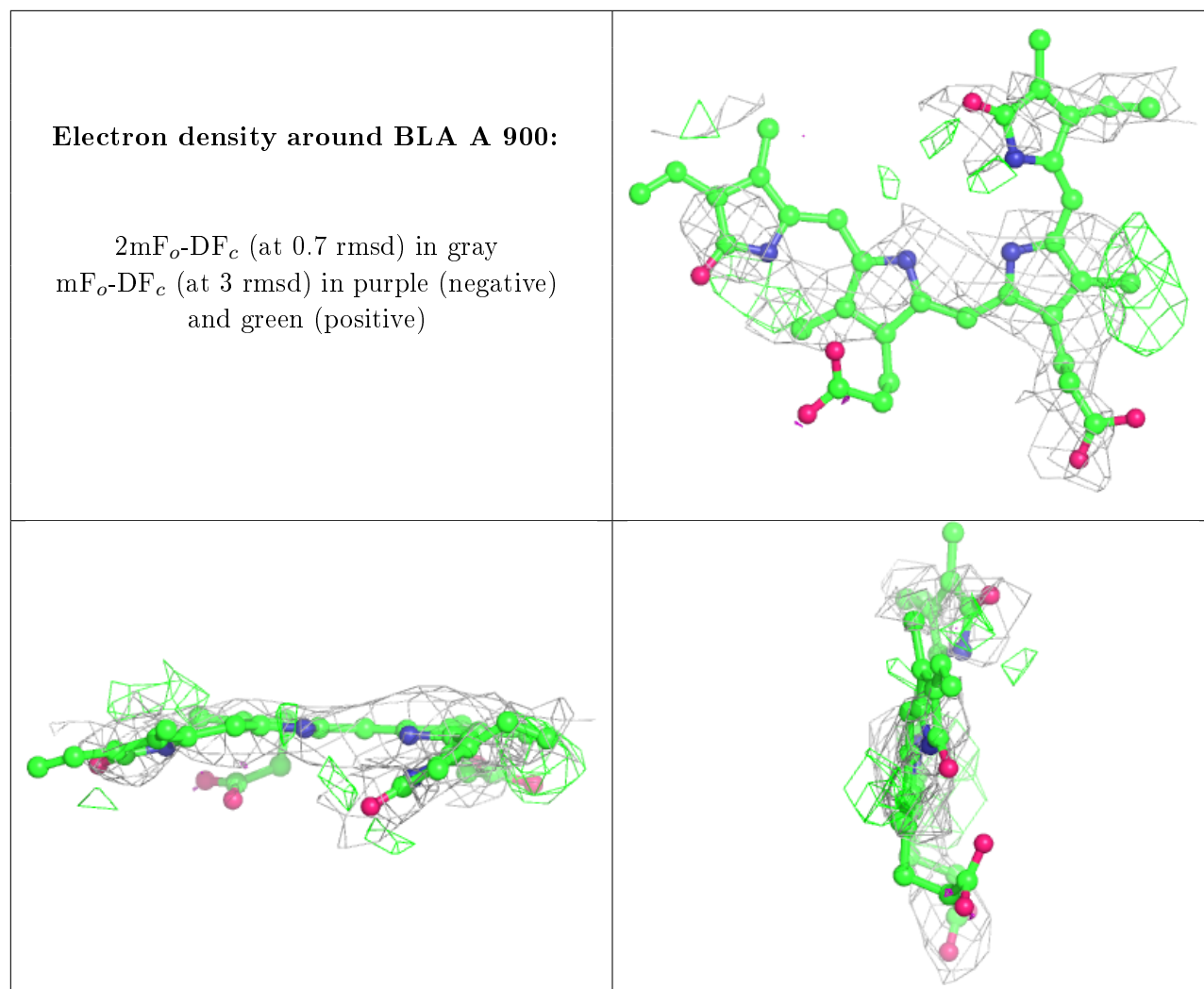
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TRS	A	1632	8/8	0.68	0.39	119,122,123,123	0
2	BLA	B	900	43/43	0.68	0.61	112,135,144,157	43
4	CL	A	1633	1/1	0.69	0.22	104,104,104,104	0
3	TRS	B	1633	8/8	0.73	0.41	102,107,112,113	0
2	BLA	A	900	43/43	0.79	0.65	115,139,146,155	43

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 ⓘ

There are no such residues in this entry.