



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2021 – 02:12 PM EST

PDB ID : 5UYR
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP mutant D199A from Xanthomonas campestris
Authors : Otero, L.H.; Klinke, S.; Goldbaum, F.A.; Bonomi, H.R.
Deposited on : 2017-02-24
Resolution : 3.45 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 : 2.23.2
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) : 2.23.2

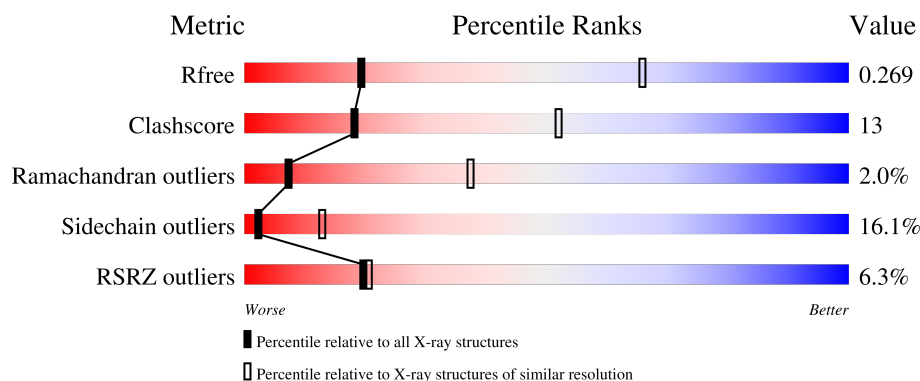
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	<div> <div>3%</div> <div>63%</div> <div>27%</div> <div>•</div> <div>7%</div> </div>
1	B	640	<div> <div>9%</div> <div>62%</div> <div>27%</div> <div>5%</div> <div>6%</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	B	900	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9455 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.

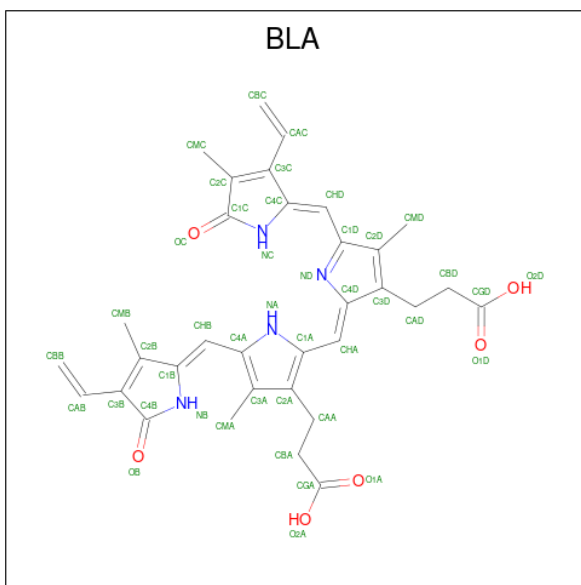
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4674	2959	853	846	16			
1	B	600	Total	C	N	O	S	0	0	0
			4693	2972	852	853	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	199	ALA	ASP	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	199	ALA	ASP	engineered mutation	UNP A0A0H2XCS3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: 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

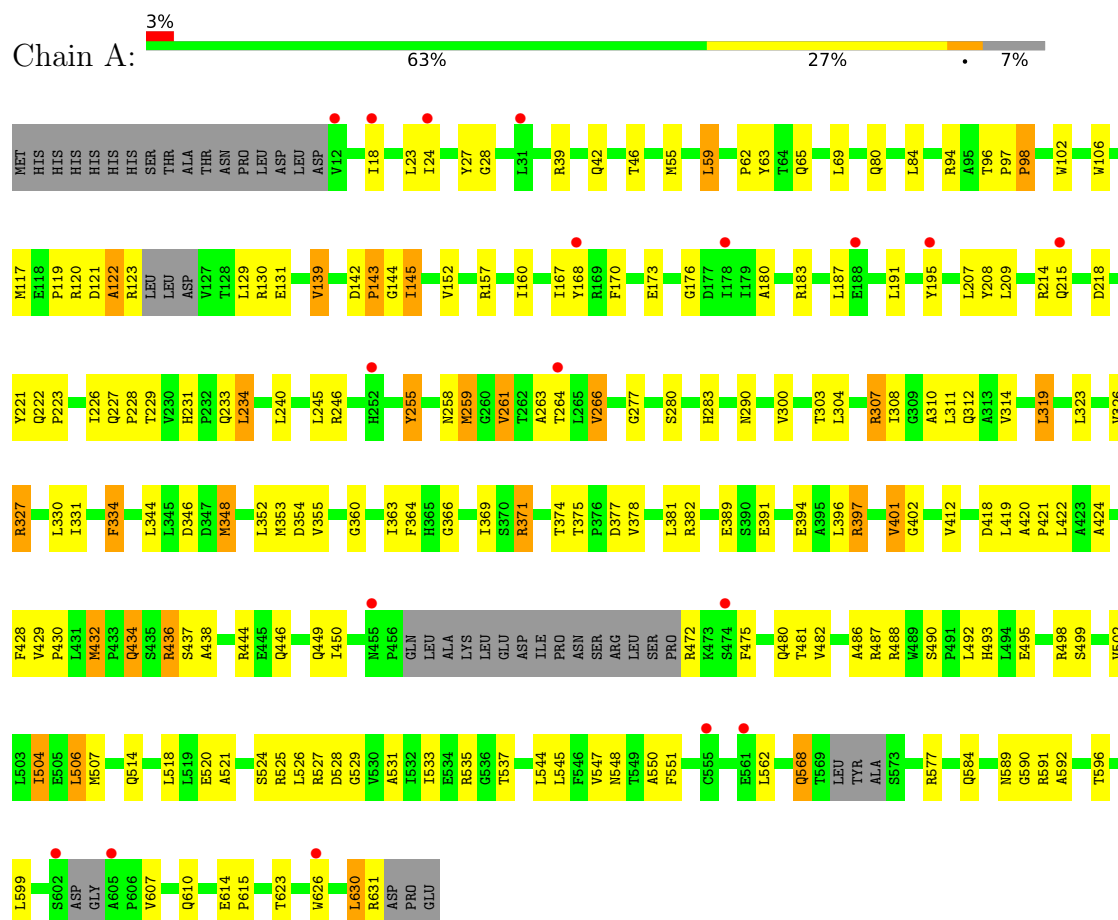
- Molecule 3 is water.

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

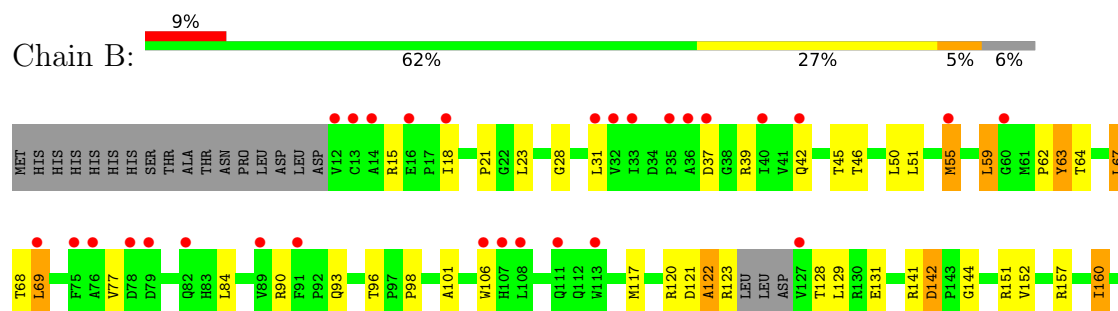
3 Residue-property plots [i](#)

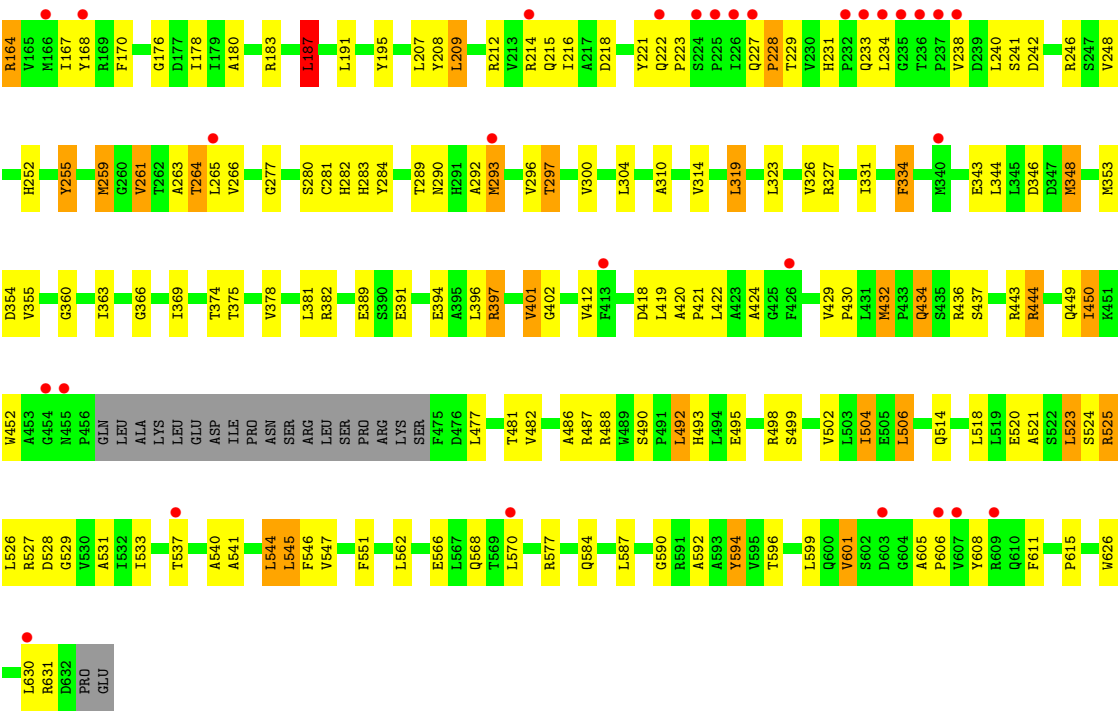
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 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	103.86Å 103.86Å 342.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.27 – 3.45 47.27 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.27-3.45) 100.0 (47.27-3.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.230 , 0.250 0.250 , 0.269	Depositor DCC
R_{free} test set	1258 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	126.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9455	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	0.51	0/4779	0.74	0/6516
1	B	0.50	0/4801	0.74	0/6552
All	All	0.51	0/9580	0.74	0/13068

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	4674	0	4676	130	0
1	B	4693	0	4683	111	0
2	A	43	0	30	19	0
2	B	43	0	31	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9455	0	9420	252	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 13.

All (252) 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	1.77	1.19
1:B:252:HIS:NE2	2:B:900:BLA:HBA1	1.63	1.14
1:A:551:PHE:CE2	1:A:630:LEU:HD11	1.88	1.08
1:A:551:PHE:HE2	1:A:630:LEU:HD11	1.23	1.03
1:A:544:LEU:HD13	1:A:547:VAL:HG11	1.40	1.00
1:B:195:TYR:CZ	2:B:900:BLA:HAB	1.97	0.99
1:A:307:ARG:HG2	1:A:307:ARG:HH21	1.28	0.98
2:A:900:BLA:HMA1	2:A:900:BLA:HB	1.30	0.96
2:A:900:BLA:HMA1	2:A:900:BLA:NB	1.83	0.93
1:A:195:TYR:CD1	2:A:900:BLA:HMB1	2.05	0.91
2:B:900:BLA:HMA1	2:B:900:BLA:HB	1.35	0.90
2:B:900:BLA:HMA1	2:B:900:BLA:NB	1.89	0.87
2:A:900:BLA:HB	2:A:900:BLA:CMA	1.88	0.86
1:A:371:ARG:HH21	1:A:377:ASP:HA	1.42	0.84
1:A:195:TYR:CZ	2:A:900:BLA:HAB	2.13	0.84
2:B:900:BLA:HB	2:B:900:BLA:CMA	1.92	0.83
1:A:195:TYR:CD1	2:A:900:BLA:CMB	2.61	0.82
1:B:195:TYR:CD1	2:B:900:BLA:HMB1	2.17	0.80
1:A:307:ARG:HD2	1:A:311:LEU:HD11	1.65	0.79
1:A:142:ASP:OD1	1:A:143:PRO:CD	2.30	0.79
1:A:195:TYR:OH	2:A:900:BLA:HAB	1.84	0.77
1:B:160:ILE:HG12	1:B:293:MET:SD	2.25	0.77
1:B:209:LEU:O	1:B:212:ARG:NH1	2.18	0.77
1:A:145:ILE:HG12	1:A:308:ILE:HG23	1.66	0.76
1:B:152:VAL:HG11	1:B:304:LEU:HD22	1.68	0.76
1:B:531:ALA:CB	1:B:547:VAL:HG12	2.17	0.75
1:A:214:ARG:HE	1:A:246:ARG:HH21	1.34	0.74
1:B:216:ILE:HB	1:B:264:THR:HB	1.69	0.74
1:A:145:ILE:CD1	1:A:308:ILE:HG23	2.20	0.72
1:B:214:ARG:HH21	1:B:246:ARG:NH2	1.88	0.71
1:B:42:GLN:HA	1:B:228:PRO:HG2	1.74	0.69
1:A:521:ALA:O	1:A:525:ARG:HG3	1.93	0.69
1:A:568:GLN:HE21	1:A:584:GLN:HE22	1.42	0.68
1:A:42:GLN:HA	1:A:228:PRO:HG2	1.76	0.68
1:A:24:ILE:HG12	1:A:226:ILE:HD11	1.75	0.68
1:A:424:ALA:HB3	1:A:486:ALA:HB2	1.76	0.68
1:B:531:ALA:HB1	1:B:547:VAL:HG12	1.74	0.68
1:B:424:ALA:HB3	1:B:486:ALA:HB2	1.76	0.67
1:A:371:ARG:NH2	1:A:377:ASP:HA	2.09	0.67
1:B:541:ALA:HB1	1:B:566:GLU:HG3	1.77	0.67
1:B:568:GLN:HE21	1:B:584:GLN:HE22	1.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:CE1	2:B:900:BLA:HBA1	2.30	0.67
1:A:531:ALA:CB	1:A:547:VAL:HG12	2.25	0.66
1:B:401:VAL:HG13	1:B:402:GLY:H	1.61	0.66
1:A:122:ALA:O	1:A:123:ARG:HG2	1.95	0.65
1:A:214:ARG:HH21	1:A:246:ARG:NH2	1.93	0.65
1:A:145:ILE:CG1	1:A:308:ILE:HG23	2.27	0.65
1:A:307:ARG:HH21	1:A:307:ARG:CG	2.07	0.65
1:A:371:ARG:HG3	1:A:381:LEU:HD11	1.79	0.65
1:A:531:ALA:HB1	1:A:547:VAL:HG12	1.79	0.65
1:A:551:PHE:CD2	1:A:630:LEU:HD11	2.31	0.65
1:B:265:LEU:HD21	1:B:297:THR:HG21	1.77	0.64
1:A:307:ARG:CD	1:A:311:LEU:HD11	2.28	0.64
1:A:121:ASP:CG	1:A:122:ALA:H	2.00	0.63
1:B:533:ILE:HG22	1:B:626:TRP:HE3	1.63	0.63
1:A:401:VAL:HG13	1:A:402:GLY:H	1.63	0.63
1:A:142:ASP:OD1	1:A:143:PRO:HD2	1.98	0.62
1:B:537:THR:H	1:B:540:ALA:HB3	1.65	0.62
1:A:430:PRO:HD3	1:A:504:ILE:HG12	1.82	0.61
1:B:521:ALA:O	1:B:525:ARG:HG2	2.00	0.61
1:A:255:TYR:OH	2:A:900:BLA:HMB3	2.01	0.60
1:B:195:TYR:CG	2:B:900:BLA:HMB1	2.37	0.60
2:B:900:BLA:CGA	2:B:900:BLA:HMA2	2.31	0.60
1:B:326:VAL:HG12	1:B:355:VAL:HG13	1.85	0.59
1:B:122:ALA:O	1:B:123:ARG:HB3	2.02	0.59
1:A:590:GLY:HA2	1:A:626:TRP:HZ2	1.67	0.59
1:B:142:ASP:OD2	1:B:151:ARG:HD2	2.03	0.59
1:A:450:ILE:HG13	1:A:480:GLN:HB3	1.84	0.59
1:A:195:TYR:CD1	2:A:900:BLA:HMB2	2.38	0.58
1:A:263:ALA:HB3	1:A:283:HIS:HB3	1.84	0.58
1:B:123:ARG:O	1:B:123:ARG:HG2	2.02	0.58
1:B:327:ARG:O	1:B:331:ILE:HG12	2.04	0.58
1:A:327:ARG:O	1:A:331:ILE:HG12	2.02	0.58
1:A:394:GLU:HA	1:A:397:ARG:HE	1.67	0.58
1:B:208:TYR:OH	2:B:900:BLA:HAA1	2.04	0.58
1:A:308:ILE:O	1:A:312:GLN:HG3	2.02	0.58
1:B:231:HIS:HD2	1:B:233:GLN:H	1.52	0.57
1:A:121:ASP:O	1:A:122:ALA:HB2	2.05	0.57
1:A:142:ASP:OD1	1:A:143:PRO:HD3	2.03	0.57
1:B:167:ILE:HB	1:B:180:ALA:HB3	1.86	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:TYR:CE1	1:B:214:ARG:HD3	2.40	0.56
1:A:307:ARG:HG2	1:A:307:ARG:NH2	2.08	0.56
1:A:432:MET:C	1:A:434:GLN:H	2.09	0.56
1:B:68:THR:HB	1:B:90:ARG:HB3	1.87	0.56
1:B:64:THR:HA	1:B:67:LEU:HB3	1.88	0.56
1:B:263:ALA:HB3	1:B:283:HIS:HB3	1.87	0.56
1:B:601:VAL:HG11	1:B:605:ALA:O	2.06	0.56
1:A:102:TRP:CZ2	1:A:119:PRO:HD3	2.41	0.55
1:A:121:ASP:OD1	1:A:122:ALA:N	2.39	0.55
1:A:227:GLN:HB3	1:A:228:PRO:HD3	1.89	0.55
1:A:214:ARG:NH2	2:A:900:BLA:O1D	2.40	0.55
1:A:214:ARG:HE	1:A:246:ARG:NH2	2.04	0.54
1:B:531:ALA:HB2	1:B:547:VAL:HG12	1.90	0.54
1:A:214:ARG:HH21	1:A:246:ARG:HH22	1.55	0.54
1:A:592:ALA:HB2	1:A:615:PRO:HD3	1.90	0.53
1:B:432:MET:C	1:B:434:GLN:H	2.10	0.53
1:A:195:TYR:CZ	2:A:900:BLA:CAB	2.88	0.53
1:A:307:ARG:CD	1:A:311:LEU:CD1	2.86	0.53
1:B:430:PRO:HD3	1:B:504:ILE:HG12	1.90	0.53
1:B:327:ARG:HD3	1:B:499:SER:HB3	1.91	0.53
1:A:208:TYR:CE1	1:A:214:ARG:HD3	2.43	0.52
1:B:227:GLN:HB3	1:B:228:PRO:HD3	1.91	0.52
1:B:214:ARG:NH2	2:B:900:BLA:O1D	2.42	0.52
1:B:394:GLU:HA	1:B:397:ARG:HE	1.74	0.52
1:B:551:PHE:CE2	1:B:630:LEU:HD12	2.44	0.52
1:A:326:VAL:HG12	1:A:355:VAL:HG13	1.91	0.52
1:A:214:ARG:NH2	1:A:246:ARG:HH22	2.06	0.52
1:A:307:ARG:HD3	1:A:311:LEU:HG	1.92	0.52
1:B:23:LEU:HD22	1:B:223:PRO:HB2	1.91	0.52
1:A:214:ARG:NH2	1:A:246:ARG:NH2	2.58	0.51
1:B:592:ALA:HB2	1:B:615:PRO:HD3	1.90	0.51
1:A:23:LEU:HD22	1:A:223:PRO:HB2	1.91	0.51
1:A:97:PRO:N	1:A:98:PRO:HD3	2.25	0.51
1:A:215:GLN:O	1:A:215:GLN:HG2	2.11	0.50
1:A:334:PHE:HE1	1:A:348:MET:HG2	1.74	0.50
1:A:437:SER:HB3	1:A:507:MET:HE3	1.92	0.50
1:B:152:VAL:HG21	1:B:304:LEU:HD13	1.92	0.50
1:B:289:THR:HB	1:B:293:MET:HE2	1.93	0.50
1:A:120:ARG:O	1:A:121:ASP:HB3	2.12	0.49
1:A:266:VAL:HG21	2:A:900:BLA:HBA2	1.94	0.49
1:B:195:TYR:CE1	2:B:900:BLA:HAB	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASP:C	1:B:420:ALA:H	2.15	0.49
1:A:195:TYR:OH	2:A:900:BLA:CAB	2.58	0.49
1:A:429:VAL:HG12	1:A:504:ILE:HD13	1.94	0.49
1:B:214:ARG:NH2	1:B:248:VAL:HG12	2.28	0.49
1:A:231:HIS:CD2	1:A:234:LEU:H	2.31	0.49
1:A:353:MET:SD	1:A:360:GLY:HA2	2.53	0.49
1:B:450:ILE:HD12	1:B:452:TRP:HE1	1.77	0.49
1:A:259:MET:HB3	1:A:261:VAL:HG12	1.94	0.49
1:A:418:ASP:C	1:A:420:ALA:H	2.16	0.49
1:A:589:ASN:HD22	1:A:591:ARG:HH21	1.58	0.48
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.47	0.48
1:A:401:VAL:HG11	1:A:498:ARG:HH21	1.78	0.48
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.48	0.48
1:B:334:PHE:HE1	1:B:348:MET:HG2	1.77	0.48
1:A:490:SER:HB3	1:A:493:HIS:ND1	2.28	0.48
1:A:551:PHE:CD2	1:A:630:LEU:CD1	2.95	0.48
1:A:142:ASP:O	1:A:307:ARG:NE	2.47	0.48
1:A:215:GLN:OE1	1:A:215:GLN:N	2.46	0.48
1:A:533:ILE:HG22	1:A:626:TRP:HE3	1.79	0.48
1:B:28:GLY:O	1:B:46:THR:HG21	2.14	0.48
1:B:259:MET:HB3	1:B:261:VAL:HG12	1.94	0.48
1:B:212:ARG:HG3	1:B:212:ARG:HH11	1.78	0.48
1:A:183:ARG:HH12	1:A:187:LEU:C	2.16	0.48
1:A:327:ARG:HD2	1:A:499:SER:HB3	1.94	0.48
1:A:28:GLY:O	1:A:46:THR:HG21	2.13	0.47
1:A:102:TRP:CH2	1:A:119:PRO:HD3	2.49	0.47
1:A:258:ASN:HA	1:A:472:ARG:HE	1.79	0.47
1:A:323:LEU:O	1:A:327:ARG:HB2	2.14	0.47
1:B:59:LEU:HD11	1:B:228:PRO:HG3	1.96	0.47
1:A:27:TYR:OH	1:A:215:GLN:NE2	2.48	0.47
1:A:152:VAL:HG21	1:A:304:LEU:HB2	1.95	0.47
1:A:195:TYR:CE1	2:A:900:BLA:CMB	2.68	0.47
1:B:323:LEU:O	1:B:327:ARG:HB2	2.14	0.47
1:A:24:ILE:HG23	1:A:245:LEU:HB3	1.96	0.47
1:B:374:THR:HG22	1:B:422:LEU:HD22	1.96	0.47
1:B:353:MET:SD	1:B:360:GLY:HA2	2.55	0.47
1:B:490:SER:HB3	1:B:493:HIS:HB2	1.97	0.47
1:B:545:LEU:HD22	1:B:546:PHE:CE2	2.50	0.47
1:A:374:THR:HG22	1:A:422:LEU:HD22	1.97	0.47
1:B:289:THR:HB	1:B:293:MET:CE	2.45	0.47
1:A:307:ARG:HD2	1:A:311:LEU:CD1	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:VAL:O	1:A:506:LEU:HB2	2.16	0.46
1:B:214:ARG:NH2	1:B:246:ARG:NH2	2.61	0.46
1:B:490:SER:HB3	1:B:493:HIS:ND1	2.31	0.46
1:B:31:LEU:HD11	1:B:51:LEU:HD21	1.96	0.46
1:B:606:PRO:HB2	1:B:608:TYR:CE2	2.51	0.46
1:B:401:VAL:HG11	1:B:498:ARG:HH21	1.80	0.45
1:B:326:VAL:HG12	1:B:355:VAL:CG1	2.46	0.45
1:B:327:ARG:HD3	1:B:499:SER:CB	2.46	0.45
1:A:548:ASN:OD1	1:A:551:PHE:HB3	2.16	0.45
1:A:208:TYR:OH	2:A:900:BLA:HAA1	2.16	0.45
1:A:369:ILE:HD11	1:A:382:ARG:HG3	1.99	0.45
2:A:900:BLA:HMA2	2:A:900:BLA:CGA	2.47	0.45
1:B:450:ILE:O	1:B:452:TRP:HD1	1.99	0.45
1:A:526:LEU:O	1:A:550:ALA:HB2	2.15	0.45
1:A:544:LEU:HD13	1:A:547:VAL:CG1	2.29	0.45
1:A:420:ALA:N	1:A:421:PRO:HD2	2.31	0.45
1:B:590:GLY:HA2	1:B:626:TRP:HZ2	1.81	0.45
1:B:255:TYR:CD1	1:B:255:TYR:C	2.91	0.44
1:A:531:ALA:HB2	1:A:547:VAL:HG12	1.98	0.44
1:B:214:ARG:HH21	1:B:246:ARG:HH21	1.63	0.44
1:B:420:ALA:N	1:B:421:PRO:HD2	2.32	0.44
1:B:541:ALA:HB1	1:B:566:GLU:CG	2.46	0.44
1:A:310:ALA:O	1:A:314:VAL:HG23	2.17	0.44
1:B:369:ILE:HD11	1:B:382:ARG:HG3	1.99	0.44
1:A:330:LEU:HD11	1:A:352:LEU:HA	2.00	0.44
1:A:548:ASN:OD1	1:A:551:PHE:CB	2.66	0.44
1:B:326:VAL:CG1	1:B:355:VAL:HG13	2.48	0.44
1:B:502:VAL:O	1:B:506:LEU:HB2	2.18	0.44
1:A:59:LEU:HD11	1:A:228:PRO:HG3	1.98	0.44
1:A:428:PHE:CE1	1:A:438:ALA:HB1	2.53	0.44
1:A:490:SER:HB3	1:A:493:HIS:HB2	2.00	0.44
1:B:551:PHE:CE2	1:B:630:LEU:CD1	3.00	0.43
1:B:290:ASN:ND2	1:B:292:ALA:HB3	2.32	0.43
1:B:265:LEU:HB3	1:B:281:CYS:HB2	2.01	0.43
1:A:319:LEU:O	1:A:323:LEU:HB2	2.19	0.43
1:B:21:PRO:HD2	1:B:240:LEU:HD23	2.00	0.43
1:B:378:VAL:HA	1:B:381:LEU:HD12	2.01	0.43
1:B:544:LEU:HD11	1:B:570:LEU:HD11	2.01	0.43
1:A:144:GLY:O	1:A:145:ILE:C	2.57	0.43
1:B:310:ALA:O	1:B:314:VAL:HG23	2.18	0.43
1:A:255:TYR:CD1	1:A:255:TYR:C	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:HB3	1:B:120:ARG:HB3	1.99	0.43
1:A:139:VAL:HG22	1:A:303:THR:HG22	2.00	0.43
1:A:231:HIS:CG	1:A:234:LEU:HB2	2.54	0.42
1:B:231:HIS:CD2	1:B:234:LEU:H	2.36	0.42
2:B:900:BLA:HBB1	2:B:900:BLA:OB	2.20	0.42
1:A:364:PHE:HB2	1:A:438:ALA:HB3	2.01	0.42
1:B:164:ARG:HB3	1:B:282:HIS:HB2	2.00	0.42
1:A:195:TYR:CE1	2:A:900:BLA:HAB	2.52	0.42
1:A:590:GLY:HA2	1:A:626:TRP:CZ2	2.51	0.42
1:B:449:GLN:NE2	1:B:481:THR:HG23	2.33	0.42
1:B:587:LEU:HA	1:B:626:TRP:CZ2	2.55	0.42
1:A:307:ARG:CG	1:A:307:ARG:NH2	2.72	0.42
1:A:548:ASN:ND2	1:A:550:ALA:HB3	2.34	0.42
1:A:84:LEU:HB2	1:A:106:TRP:HB2	2.01	0.42
1:B:187:LEU:HD22	1:B:284:TYR:CE2	2.54	0.42
1:B:121:ASP:OD1	1:B:122:ALA:N	2.52	0.42
1:B:84:LEU:HB2	1:B:106:TRP:HB2	2.01	0.42
1:A:535:ARG:HD3	1:A:623:THR:O	2.20	0.42
1:A:378:VAL:HA	1:A:381:LEU:HD12	2.02	0.41
1:B:67:LEU:HD12	1:B:69:LEU:HG	2.01	0.41
1:B:121:ASP:O	1:B:122:ALA:CB	2.68	0.41
1:A:214:ARG:NE	1:A:246:ARG:NH2	2.68	0.41
1:A:419:LEU:C	1:A:421:PRO:HD2	2.41	0.41
1:A:170:PHE:CD2	1:A:277:GLY:HA2	2.55	0.41
1:B:541:ALA:CB	1:B:566:GLU:HG3	2.47	0.41
1:A:168:TYR:CE1	1:A:176:GLY:HA3	2.56	0.41
1:B:45:THR:HA	1:B:55:MET:HE1	2.02	0.41
1:A:39:ARG:HA	1:A:62:PRO:HA	2.02	0.41
1:B:63:TYR:CE2	1:B:67:LEU:HD13	2.56	0.41
1:B:128:THR:HG22	1:B:296:VAL:HG21	2.02	0.41
1:B:523:LEU:HA	1:B:526:LEU:HD12	2.02	0.41
1:A:449:GLN:NE2	1:A:481:THR:HG23	2.36	0.41
1:B:195:TYR:CE1	2:B:900:BLA:HMB1	2.55	0.41
1:B:214:ARG:HE	1:B:246:ARG:HH21	1.69	0.41
1:B:221:TYR:O	1:B:223:PRO:HD3	2.20	0.41
1:B:443:ARG:HB3	1:B:486:ALA:HB1	2.03	0.41
1:B:594:TYR:HA	1:B:611:PHE:O	2.21	0.41
2:B:900:BLA:HMA2	2:B:900:BLA:O1A	2.21	0.41
2:A:900:BLA:NB	2:A:900:BLA:CMA	2.61	0.41
1:B:419:LEU:C	1:B:421:PRO:HD2	2.41	0.41
1:B:170:PHE:CD2	1:B:277:GLY:HA2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HA	1:B:62:PRO:HA	2.02	0.40
1:A:221:TYR:CE1	1:A:223:PRO:HG3	2.56	0.40
1:B:319:LEU:HD13	1:B:492:LEU:HD12	2.02	0.40
1:B:421:PRO:O	1:B:444:ARG:HB2	2.22	0.40
1:A:307:ARG:O	1:A:310:ALA:N	2.55	0.40
1:B:178:ILE:HD11	2:B:900:BLA:CBB	2.51	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	587/640 (92%)	532 (91%)	42 (7%)	13 (2%)	6	35
1	B	594/640 (93%)	535 (90%)	48 (8%)	11 (2%)	8	38
All	All	1181/1280 (92%)	1067 (90%)	90 (8%)	24 (2%)	7	37

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	VAL
1	B	122	ALA
1	B	241	SER
1	A	18	ILE
1	A	143	PRO
1	A	366	GLY
1	A	529	GLY
1	B	18	ILE
1	B	187	LEU
1	B	366	GLY
1	B	401	VAL
1	A	98	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	434	GLN
1	A	436	ARG
1	A	568	GLN
1	B	144	GLY
1	A	55	MET
1	A	607	VAL
1	B	55	MET
1	B	98	PRO
1	B	434	GLN
1	A	122	ALA
1	B	529	GLY
1	A	145	ILE

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	492/531 (93%)	417 (85%)	75 (15%)	3	15
1	B	493/531 (93%)	409 (83%)	84 (17%)	2	10
All	All	985/1062 (93%)	826 (84%)	159 (16%)	2	13

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	63	TYR
1	A	65	GLN
1	A	69	LEU
1	A	80	GLN
1	A	94	ARG
1	A	96	THR
1	A	117	MET
1	A	129	LEU
1	A	130	ARG
1	A	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	VAL
1	A	157	ARG
1	A	160	ILE
1	A	173	GLU
1	A	191	LEU
1	A	207	LEU
1	A	209	LEU
1	A	218	ASP
1	A	222	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
1	A	266	VAL
1	A	280	SER
1	A	290	ASN
1	A	300	VAL
1	A	307	ARG
1	A	319	LEU
1	A	327	ARG
1	A	334	PHE
1	A	344	LEU
1	A	346	ASP
1	A	348	MET
1	A	354	ASP
1	A	363	ILE
1	A	371	ARG
1	A	375	THR
1	A	389	GLU
1	A	391	GLU
1	A	396	LEU
1	A	397	ARG
1	A	412	VAL
1	A	432	MET
1	A	436	ARG
1	A	444	ARG
1	A	446	GLN
1	A	475	PHE
1	A	482	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	487	ARG
1	A	488	ARG
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	520	GLU
1	A	524	SER
1	A	527	ARG
1	A	528	ASP
1	A	537	THR
1	A	545	LEU
1	A	562	LEU
1	A	577	ARG
1	A	596	THR
1	A	599	LEU
1	A	610	GLN
1	A	614	GLU
1	A	630	LEU
1	A	631	ARG
1	B	15	ARG
1	B	37	ASP
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	93	GLN
1	B	96	THR
1	B	117	MET
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	191	LEU
1	B	207	LEU
1	B	209	LEU
1	B	215	GLN
1	B	218	ASP
1	B	222	GLN
1	B	228	PRO
1	B	229	THR
1	B	238	VAL
1	B	242	ASP
1	B	255	TYR
1	B	259	MET
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	319	LEU
1	B	334	PHE
1	B	343	GLU
1	B	344	LEU
1	B	346	ASP
1	B	348	MET
1	B	354	ASP
1	B	363	ILE
1	B	375	THR
1	B	389	GLU
1	B	391	GLU
1	B	396	LEU
1	B	397	ARG
1	B	412	VAL
1	B	429	VAL
1	B	432	MET
1	B	436	ARG
1	B	437	SER
1	B	444	ARG
1	B	450	ILE
1	B	477	LEU
1	B	482	VAL
1	B	487	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	488	ARG
1	B	492	LEU
1	B	495	GLU
1	B	504	ILE
1	B	506	LEU
1	B	514	GLN
1	B	518	LEU
1	B	520	GLU
1	B	523	LEU
1	B	524	SER
1	B	525	ARG
1	B	527	ARG
1	B	528	ASP
1	B	544	LEU
1	B	545	LEU
1	B	562	LEU
1	B	577	ARG
1	B	594	TYR
1	B	596	THR
1	B	599	LEU
1	B	601	VAL
1	B	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	215	GLN
1	A	231	HIS
1	A	365	HIS
1	A	480	GLN
1	A	584	GLN
1	A	589	ASN
1	B	82	GLN
1	B	231	HIS
1	B	233	GLN
1	B	290	ASN
1	B	480	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	900	1	36,46,46	1.36	2 (5%)	47,67,67	0.88	3 (6%)
2	BLA	A	900	1	36,46,46	1.08	3 (8%)	47,67,67	0.96	3 (6%)

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	B	900	1	-	2/22/74/74	0/4/4/4
2	BLA	A	900	1	-	4/22/74/74	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CHA-C4D	6.55	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	CHA-C4D	4.44	1.38	1.35
2	B	900	BLA	C3C-C4C	3.54	1.51	1.45
2	A	900	BLA	C3C-C4C	2.89	1.50	1.45
2	A	900	BLA	CHB-C1B	2.17	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C1A-CHA-C4D	3.74	133.28	128.81
2	B	900	BLA	C1A-CHA-C4D	3.64	133.15	128.81
2	A	900	BLA	CHA-C4D-ND	-3.16	124.44	128.83
2	A	900	BLA	CHB-C1B-NB	-2.46	122.15	130.40
2	B	900	BLA	CHB-C1B-NB	-2.45	122.18	130.40
2	B	900	BLA	C4C-CHD-C1D	2.20	133.45	128.08

There are no chirality outliers.

All (6) 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

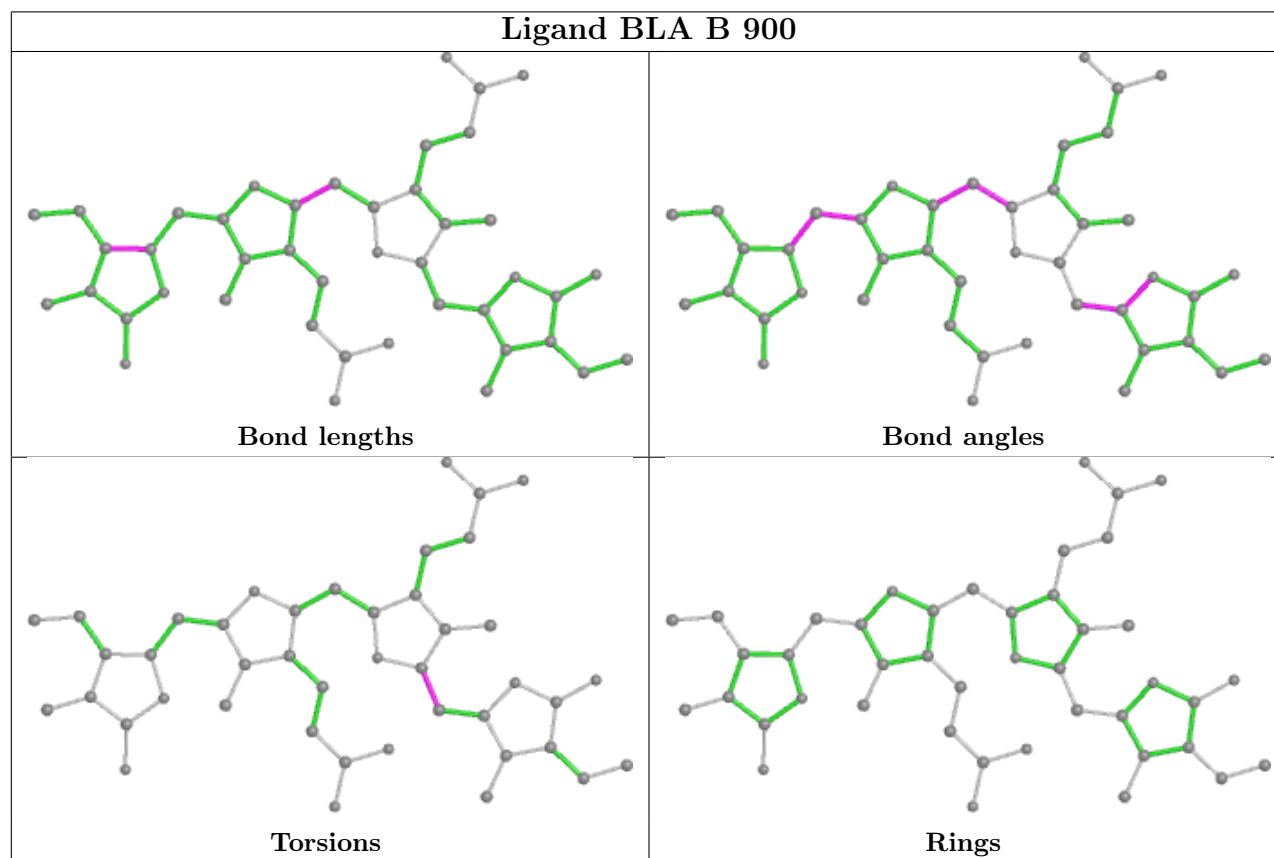
There are no ring outliers.

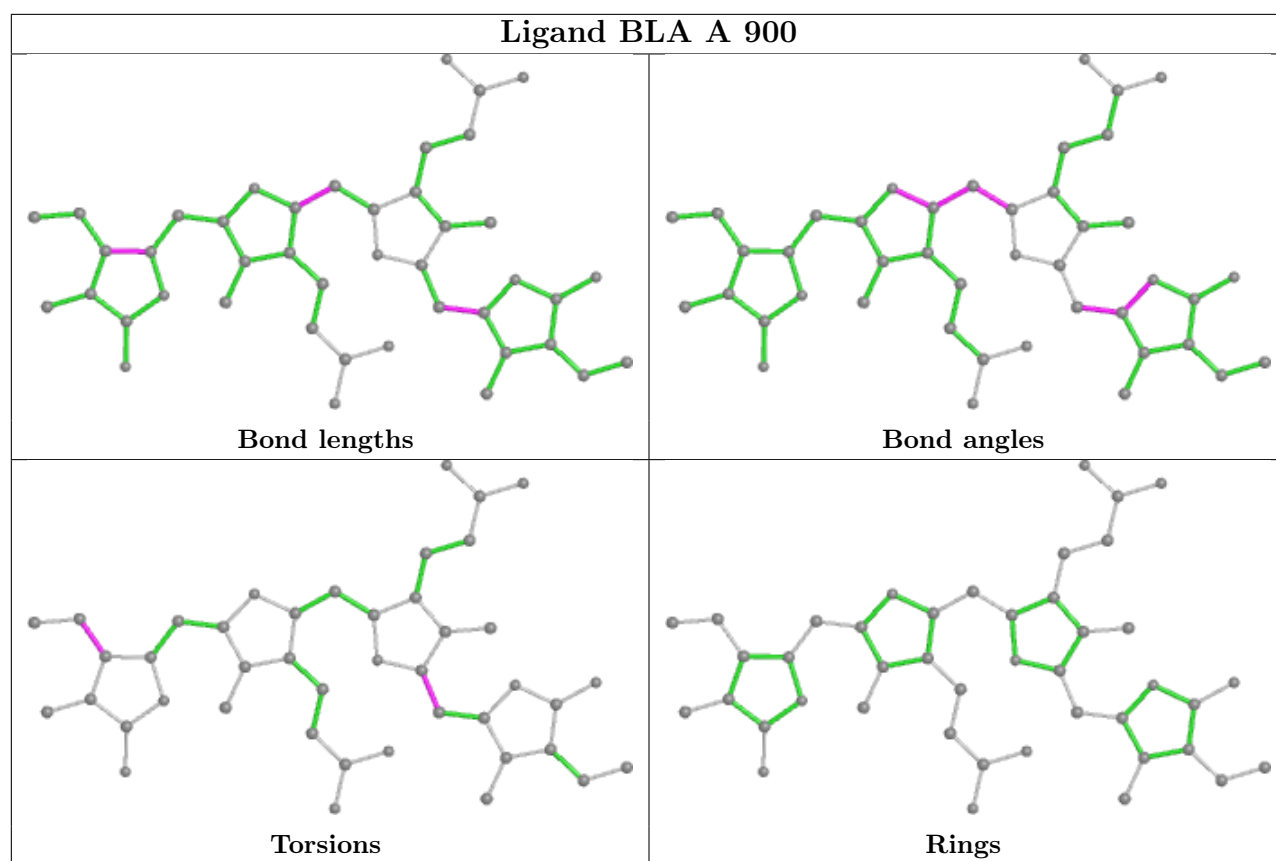
2 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	BLA	16	0
2	A	900	BLA	19	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	597/640 (93%)	0.32	18 (3%)	50 48	81, 125, 178, 196	0
1	B	600/640 (93%)	0.58	58 (9%)	7 10	76, 127, 211, 231	0
All	All	1197/1280 (93%)	0.45	76 (6%)	20 20	76, 126, 204, 231	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	CYS	7.1
1	B	35	PRO	6.7
1	B	33	ILE	5.7
1	B	12	VAL	5.2
1	A	555	CYS	5.1
1	B	236	THR	4.6
1	B	413	PHE	4.5
1	B	108	LEU	4.4
1	B	89	VAL	4.3
1	B	40	ILE	4.0
1	B	238	VAL	4.0
1	B	91	PHE	3.8
1	B	76	ALA	3.8
1	B	237	PRO	3.8
1	A	195	TYR	3.5
1	A	215	GLN	3.4
1	B	113	TRP	3.4
1	B	222	GLN	3.3
1	B	75	PHE	3.3
1	B	69	LEU	3.2
1	B	570	LEU	3.2
1	B	18	ILE	3.1
1	B	36	ALA	3.1
1	B	106	TRP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	561	GLU	3.0
1	B	127	VAL	3.0
1	B	224	SER	3.0
1	B	31	LEU	3.0
1	B	37	ASP	2.9
1	B	42	GLN	2.8
1	B	232	PRO	2.8
1	B	14	ALA	2.8
1	B	78	ASP	2.8
1	B	32	VAL	2.7
1	A	455	ASN	2.7
1	B	55	MET	2.7
1	B	60	GLY	2.7
1	A	474	SER	2.6
1	A	12	VAL	2.6
1	B	603	ASP	2.6
1	A	252	HIS	2.6
1	B	82	GLN	2.6
1	B	293	MET	2.5
1	A	605	ALA	2.5
1	B	233	GLN	2.5
1	B	168	TYR	2.4
1	B	455	ASN	2.4
1	B	226	ILE	2.4
1	B	235	GLY	2.3
1	A	178	ILE	2.3
1	B	454	GLY	2.3
1	B	234	LEU	2.3
1	A	602	SER	2.3
1	A	264	THR	2.3
1	B	79	ASP	2.3
1	A	18	ILE	2.2
1	A	168	TYR	2.2
1	B	16	GLU	2.2
1	B	537	THR	2.2
1	B	606	PRO	2.2
1	B	426	PHE	2.2
1	B	265	LEU	2.2
1	B	609	ARG	2.2
1	A	188	GLU	2.1
1	B	166	MET	2.1
1	A	626	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	340	MET	2.1
1	B	214	ARG	2.1
1	B	630	LEU	2.1
1	B	225	PRO	2.0
1	B	107	HIS	2.0
1	B	227	GLN	2.0
1	B	607	VAL	2.0
1	B	111	GLN	2.0
1	A	24	ILE	2.0
1	A	31	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

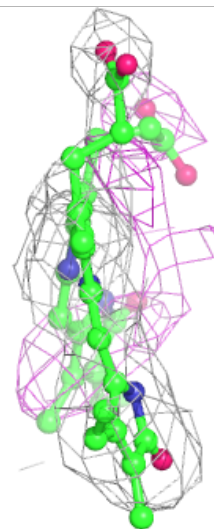
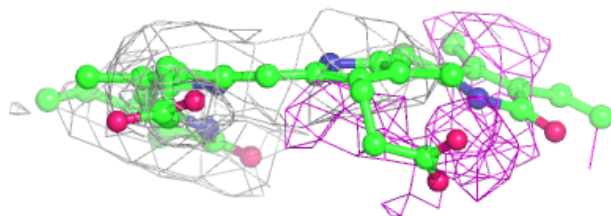
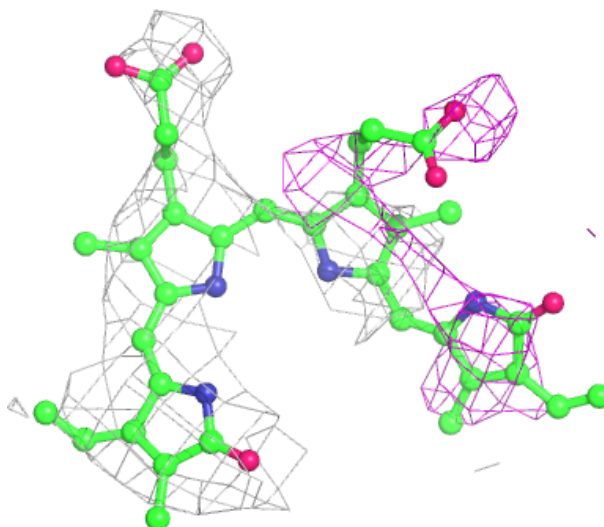
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

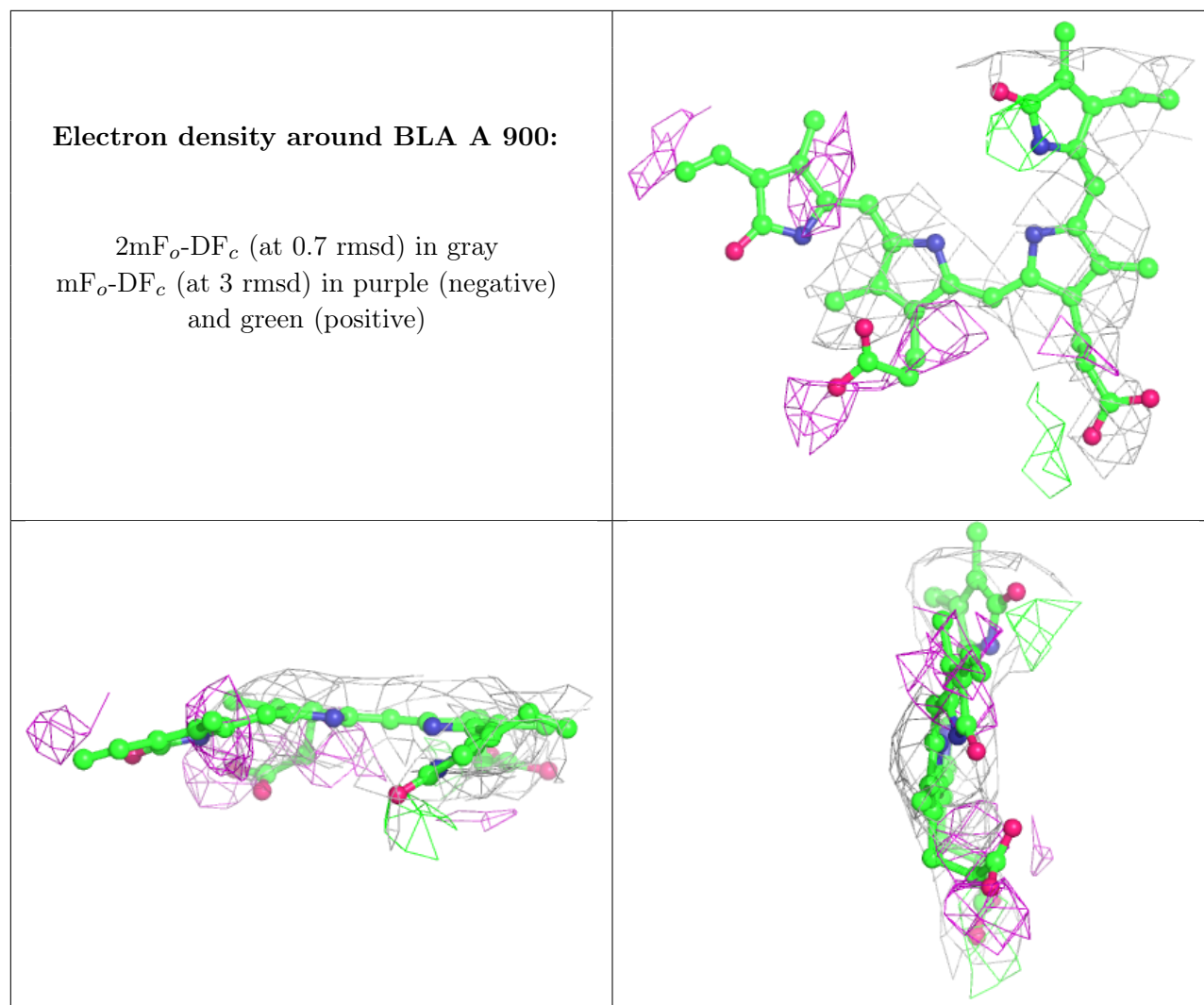
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BLA	B	900	43/43	0.73	0.68	173,186,203,208	0
2	BLA	A	900	43/43	0.83	0.55	131,159,198,202	0

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.