



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:47 PM UTC

PDB ID : 5UYR / pdb_00005uyr
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

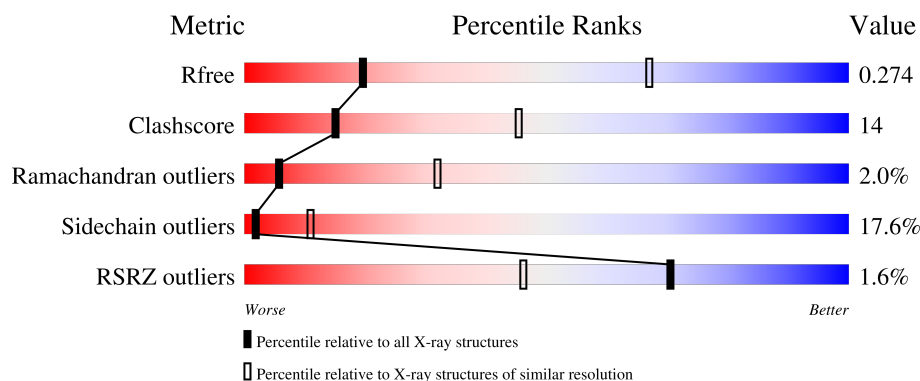
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	2% 59%28%6%7%
1	B	640	% 59%28%7%6%

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.

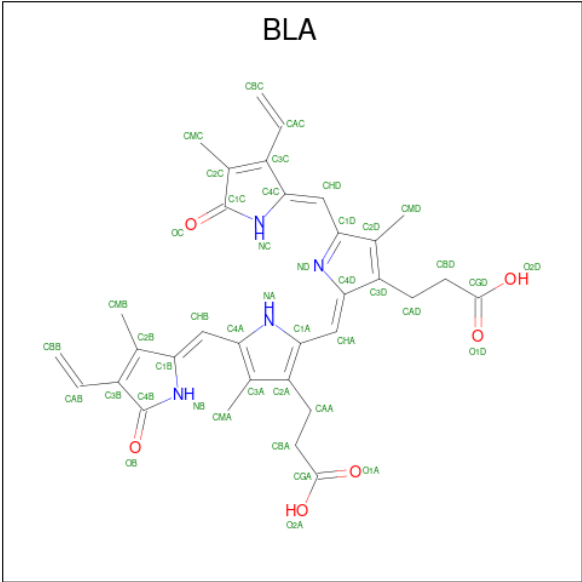
- Molecule 1 is a protein called Bacteriophytochrome.

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 (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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		

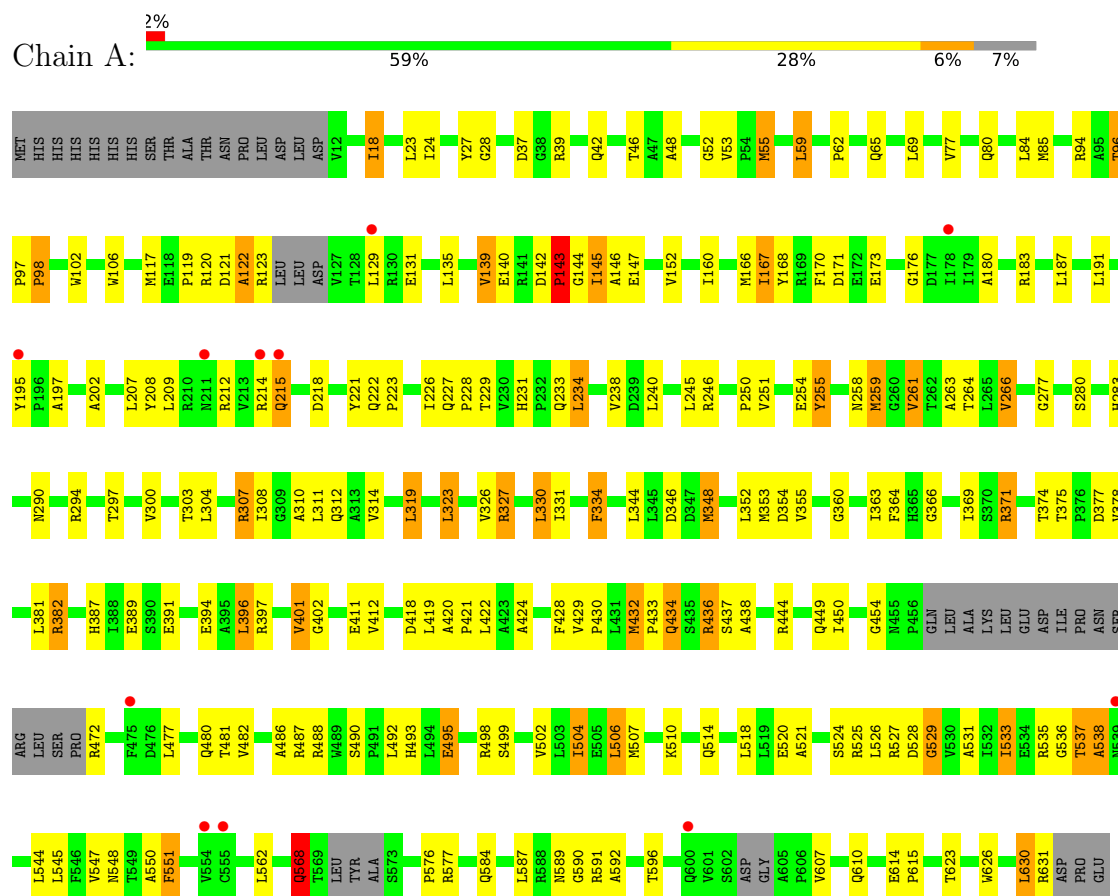
- Molecule 3 is water.

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

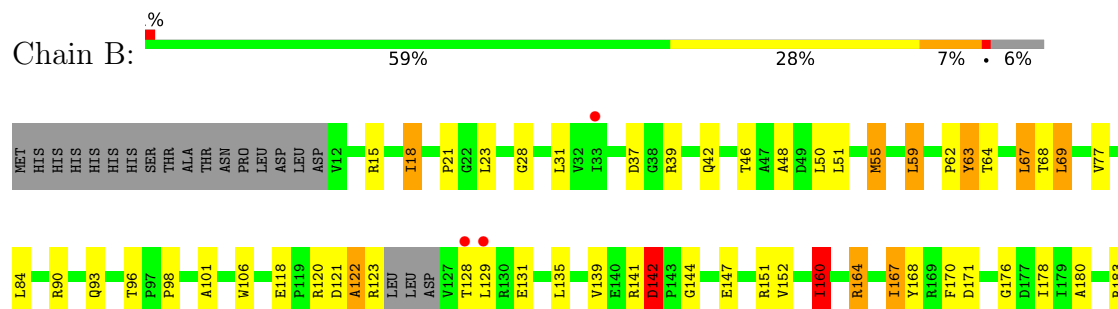
3 Residue-property plots

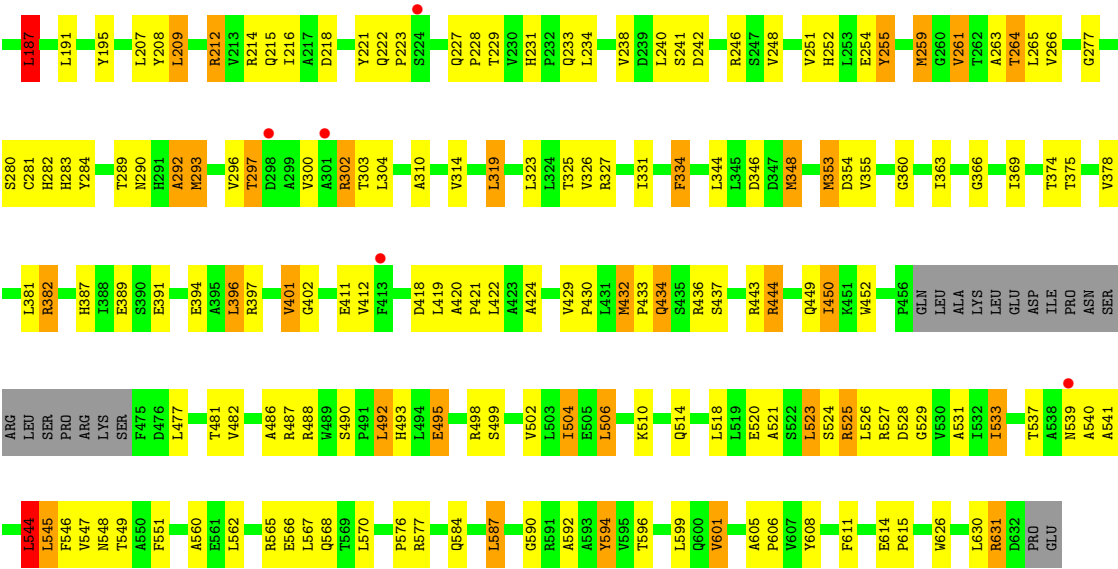
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	103.86Å 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) 99.9 (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 0.252 , 0.274	Depositor DCC
R_{free} test set	1258 reflections (4.89%)	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)	0.31 , 100.4	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	0.88	0/4779	1.40	39/6516 (0.6%)
1	B	0.87	0/4801	1.39	39/6552 (0.6%)
All	All	0.88	0/9580	1.40	78/13068 (0.6%)

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ARG	N-CA-C	10.05	122.32	111.36
1	A	215	GLN	N-CA-C	8.17	121.74	108.34
1	B	171	ASP	CA-CB-CG	7.49	120.09	112.60
1	B	142	ASP	N-CA-C	6.98	117.62	109.60
1	A	538	ALA	CA-C-N	6.85	129.69	120.65
1	A	538	ALA	C-N-CA	6.85	129.69	120.65
1	B	302	ARG	N-CA-C	6.66	119.54	111.82
1	A	171	ASP	CA-CB-CG	6.63	119.23	112.60
1	B	539	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	568	GLN	CA-C-N	6.39	133.20	121.70
1	A	568	GLN	C-N-CA	6.39	133.20	121.70
1	B	303	THR	N-CA-C	-6.34	104.45	111.36
1	A	202	ALA	CA-C-N	6.19	128.58	120.28
1	A	202	ALA	C-N-CA	6.19	128.58	120.28
1	A	537	THR	CA-C-N	6.13	133.25	121.54
1	A	537	THR	C-N-CA	6.13	133.25	121.54
1	A	433	PRO	CA-C-N	6.08	133.16	121.54
1	A	433	PRO	C-N-CA	6.08	133.16	121.54
1	A	52	GLY	N-CA-C	6.08	120.02	112.73
1	B	544	LEU	CA-C-N	6.04	128.65	120.44
1	B	544	LEU	C-N-CA	6.04	128.65	120.44
1	B	560	ALA	CA-C-N	6.03	132.93	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	560	ALA	C-N-CA	6.03	132.93	122.56
1	A	551	PHE	N-CA-C	5.97	117.87	111.36
1	B	631	ARG	CA-C-N	5.90	132.32	121.70
1	B	631	ARG	C-N-CA	5.90	132.32	121.70
1	B	325	THR	CA-C-N	5.82	127.89	120.56
1	B	325	THR	C-N-CA	5.82	127.89	120.56
1	B	292	ALA	CA-C-N	5.78	128.28	120.65
1	B	292	ALA	C-N-CA	5.78	128.28	120.65
1	B	433	PRO	CA-C-N	5.72	132.46	121.54
1	B	433	PRO	C-N-CA	5.72	132.46	121.54
1	B	160	ILE	N-CA-CB	5.70	119.28	111.41
1	B	212	ARG	N-CA-C	5.64	117.50	111.36
1	A	454	GLY	N-CA-C	5.51	121.60	112.89
1	A	495	GLU	CB-CG-CD	5.42	121.81	112.60
1	B	495	GLU	CB-CG-CD	5.41	121.79	112.60
1	B	118	GLU	CA-C-N	-5.32	114.29	119.76
1	B	118	GLU	C-N-CA	-5.32	114.29	119.76
1	A	143	PRO	CA-N-CD	-5.31	104.57	112.00
1	A	146	ALA	CA-C-N	5.30	127.33	120.44
1	A	146	ALA	C-N-CA	5.30	127.33	120.44
1	A	37	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	587	LEU	CA-C-N	5.29	127.32	120.44
1	B	587	LEU	C-N-CA	5.29	127.32	120.44
1	B	396	LEU	CA-C-N	5.26	127.64	120.54
1	B	396	LEU	C-N-CA	5.26	127.64	120.54
1	A	587	LEU	CA-C-N	5.24	127.57	120.44
1	A	587	LEU	C-N-CA	5.24	127.57	120.44
1	A	330	LEU	CA-C-N	5.20	127.20	120.70
1	A	330	LEU	C-N-CA	5.20	127.20	120.70
1	B	251	VAL	CA-C-N	5.19	127.23	120.28
1	B	251	VAL	C-N-CA	5.19	127.23	120.28
1	B	63	TYR	CA-C-N	5.18	127.74	120.28
1	B	63	TYR	C-N-CA	5.18	127.74	120.28
1	A	396	LEU	CA-C-N	5.17	127.21	120.28
1	A	396	LEU	C-N-CA	5.17	127.21	120.28
1	B	576	PRO	CA-C-N	5.17	127.72	120.28
1	B	576	PRO	C-N-CA	5.17	127.72	120.28
1	A	251	VAL	CA-C-N	5.16	127.19	120.28
1	A	251	VAL	C-N-CA	5.16	127.19	120.28
1	B	548	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	250	PRO	CA-C-N	5.12	127.48	120.77
1	A	250	PRO	C-N-CA	5.12	127.48	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	LEU	CA-C-N	5.12	127.39	120.38
1	B	567	LEU	C-N-CA	5.12	127.39	120.38
1	B	353	MET	CA-C-N	5.11	127.08	120.44
1	B	353	MET	C-N-CA	5.11	127.08	120.44
1	A	53	VAL	N-CA-C	5.10	114.07	108.05
1	A	197	ALA	CA-C-N	5.09	127.61	120.28
1	A	197	ALA	C-N-CA	5.09	127.61	120.28
1	A	294	ARG	CA-C-N	5.08	127.08	120.28
1	A	294	ARG	C-N-CA	5.08	127.08	120.28
1	A	576	PRO	CA-C-N	5.07	127.57	120.28
1	A	576	PRO	C-N-CA	5.07	127.57	120.28
1	B	525	ARG	CB-CG-CD	5.05	122.93	111.30
1	B	147	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	147	GLU	CB-CG-CD	5.01	121.12	112.60

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	137	0
1	B	4693	0	4683	113	0
2	A	43	0	30	18	0
2	B	43	0	31	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9455	0	9420	258	0

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

All (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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
1:A:195:TYR:CD1	2:A:900:BLA:HMB2	2.03	0.93
1:A:195:TYR:CE1	2:A:900:BLA:HMB1	2.07	0.90
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:CMA	2:B:900:BLA:HB	1.92	0.83
1:A:195:TYR:CD1	2:A:900:BLA:CMB	2.61	0.82
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:A:195:TYR:CE1	2:A:900:BLA:CMB	2.68	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
2:B:900:BLA:HB	2:B:900:BLA:HMA2	1.54	0.72
1:B:214:ARG:HH21	1:B:246:ARG:NH2	1.88	0.71
2:A:900:BLA:HB	2:A:900:BLA:HMA2	1.54	0.70
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:121:ASP:CG	1:A:122:ALA:H	2.00	0.68
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
1:B:252:HIS:CE1	2:B:900:BLA:HBA1	2.30	0.67
1:B:195:TYR:CG	2:B:900:BLA:HMB3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:437:SER:HB3	1:A:507:MET:HE3	1.78	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: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:B:289:THR:HB	1:B:293:MET:HE2	1.80	0.62
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
2:A:900:BLA:CMA	2:A:900:BLA:NB	2.61	0.61
1:A:432:MET:C	1:A:434:GLN:H	2.09	0.61
1:B:521:ALA:O	1:B:525:ARG:HG2	2.00	0.61
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
2:B:900:BLA:CMA	2:B:900:BLA:NB	2.65	0.59
1:A:450:ILE:HG13	1:A:480:GLN:HB3	1.84	0.59
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:432:MET:C	1:B:434:GLN:H	2.10	0.58
1:B:195:TYR:CD1	2:B:900:BLA:HMB3	2.39	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: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:121:ASP:O	1:A:122:ALA:HB2	2.05	0.57
1:A:231:HIS:HD2	1:A:233:GLN:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HB	1:A:180:ALA:HB3	1.86	0.57
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: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:A:418:ASP:C	1:A:420:ALA:H	2.16	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:B:418:ASP:C	1:B:420:ALA:H	2.15	0.54
2:A:900:BLA:NB	2:A:900:BLA:HMA1	2.22	0.54
1:A:592:ALA:HB2	1:A:615:PRO:HD3	1.90	0.53
1:A:183:ARG:HH12	1:A:187:LEU:C	2.16	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:A:121:ASP:CG	1:A:122:ALA:N	2.67	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:A:166:MET:HE3	2:A:900:BLA:OB	2.10	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:195:TYR:CG	2:A:900:BLA:HMB2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG21	1:B:304:LEU:HD13	1.92	0.50
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
1:B:255:TYR:CD1	1:B:255:TYR:C	2.91	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:120:ARG:O	1:A:121:ASP:HB3	2.12	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: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: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:144:GLY:O	1:A:145:ILE:C	2.57	0.47
1:A:102:TRP:CH2	1:A:119:PRO:HD3	2.49	0.47
1:A:255:TYR:CD1	1:A:255:TYR:C	2.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:HG22	1:A:422:LEU:HD22	1.97	0.47
2:B:900:BLA:NB	2:B:900:BLA:HMA1	2.29	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
1:A:419:LEU:C	1:A:421:PRO:HD2	2.41	0.46
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:B:419:LEU:C	1:B:421:PRO:HD2	2.41	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
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:A:96:THR:C	1:A:98:PRO:HD3	2.42	0.45
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:48:ALA:HB2	1:B:55:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:GLU:CD	1:B:302:ARG:HE	2.27	0.43
1:B:310:ALA:O	1:B:314:VAL:HG23	2.18	0.43
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:B:195:TYR:CD1	2:B:900:BLA:CMB	3.02	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:307:ARG:O	1:A:308:ILE:C	2.59	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:48:ALA:HB2	1:A:55:MET:HE2	2.02	0.42
1:A:535:ARG:HD3	1:A:623:THR:O	2.20	0.42
1:A:536:GLY:C	1:A:538:ALA:H	2.28	0.41
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:255:TYR:C	1:B:255:TYR:HD1	2.29	0.41
1:B:170:PHE:CD2	1:B:277:GLY:HA2	2.57	0.40
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:529:GLY:C	1:A:551:PHE:HB2	2.46	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%)	5	30
1	B	594/640 (93%)	535 (90%)	48 (8%)	11 (2%)	6	33
All	All	1181/1280 (92%)	1067 (90%)	90 (8%)	24 (2%)	6	32

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

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Mol	Chain	Res	Type
1	B	18	ILE
1	B	187	LEU
1	B	366	GLY
1	B	401	VAL
1	A	98	PRO
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%)	409 (83%)	83 (17%)	2	13
1	B	493/531 (93%)	403 (82%)	90 (18%)	2	10
All	All	985/1062 (93%)	812 (82%)	173 (18%)	2	11

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	59	LEU
1	A	65	GLN
1	A	69	LEU
1	A	77	VAL
1	A	80	GLN

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Mol	Chain	Res	Type
1	A	85	MET
1	A	94	ARG
1	A	96	THR
1	A	117	MET
1	A	129	LEU
1	A	131	GLU
1	A	135	LEU
1	A	139	VAL
1	A	160	ILE
1	A	167	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	238	VAL
1	A	240	LEU
1	A	254	GLU
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	297	THR
1	A	300	VAL
1	A	307	ARG
1	A	319	LEU
1	A	323	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

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Mol	Chain	Res	Type
1	A	382	ARG
1	A	387	HIS
1	A	389	GLU
1	A	391	GLU
1	A	396	LEU
1	A	411	GLU
1	A	412	VAL
1	A	432	MET
1	A	436	ARG
1	A	444	ARG
1	A	477	LEU
1	A	482	VAL
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	510	LYS
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	533	ILE
1	A	537	THR
1	A	545	LEU
1	A	562	LEU
1	A	577	ARG
1	A	596	THR
1	A	610	GLN
1	A	614	GLU
1	A	630	LEU
1	A	631	ARG
1	B	15	ARG
1	B	18	ILE
1	B	37	ASP
1	B	50	LEU
1	B	59	LEU
1	B	67	LEU
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	77	VAL
1	B	93	GLN
1	B	96	THR
1	B	129	LEU
1	B	131	GLU
1	B	135	LEU
1	B	139	VAL
1	B	141	ARG
1	B	142	ASP
1	B	160	ILE
1	B	164	ARG
1	B	167	ILE
1	B	183	ARG
1	B	187	LEU
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	229	THR
1	B	238	VAL
1	B	242	ASP
1	B	254	GLU
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	344	LEU
1	B	346	ASP
1	B	348	MET
1	B	354	ASP
1	B	363	ILE
1	B	375	THR
1	B	382	ARG

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Mol	Chain	Res	Type
1	B	387	HIS
1	B	389	GLU
1	B	391	GLU
1	B	396	LEU
1	B	411	GLU
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
1	B	488	ARG
1	B	492	LEU
1	B	495	GLU
1	B	504	ILE
1	B	506	LEU
1	B	510	LYS
1	B	514	GLN
1	B	518	LEU
1	B	520	GLU
1	B	523	LEU
1	B	524	SER
1	B	527	ARG
1	B	528	ASP
1	B	533	ILE
1	B	544	LEU
1	B	545	LEU
1	B	549	THR
1	B	562	LEU
1	B	565	ARG
1	B	577	ARG
1	B	594	TYR
1	B	596	THR
1	B	599	LEU
1	B	601	VAL
1	B	614	GLU
1	B	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	93	GLN
1	A	215	GLN
1	A	222	GLN
1	A	231	HIS
1	A	233	GLN
1	A	258	ASN
1	A	287	HIS
1	A	335	ASN
1	A	339	HIS
1	A	365	HIS
1	A	434	GLN
1	A	446	GLN
1	A	449	GLN
1	A	480	GLN
1	A	579	ASN
1	A	584	GLN
1	A	589	ASN
1	B	222	GLN
1	B	231	HIS
1	B	233	GLN
1	B	339	HIS
1	B	434	GLN
1	B	446	GLN
1	B	449	GLN
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 oligosaccharides 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	A	900	1	46,46,46	0.65	1 (2%)	66,67,67	0.69	1 (1%)
2	BLA	B	900	1	46,46,46	0.67	1 (2%)	66,67,67	0.78	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	A	900	1	-	8/26/74/74	0/4/4/4
2	BLA	B	900	1	-	6/26/74/74	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	C3C-C4C	3.04	1.51	1.45
2	A	900	BLA	C3C-C4C	2.45	1.50	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C1A-CHA-C4D	2.32	133.28	128.22
2	B	900	BLA	C1A-CHA-C4D	2.26	133.15	128.22
2	B	900	BLA	C4C-CHD-C1D	2.20	133.45	128.06

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	C4C-C3C-CAC-CBC
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	CAA-CBA-CGA-O1A
2	A	900	BLA	CAA-CBA-CGA-O1A
2	B	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAA-CBA-CGA-O2A
2	B	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAD-CBD-CGD-O1D

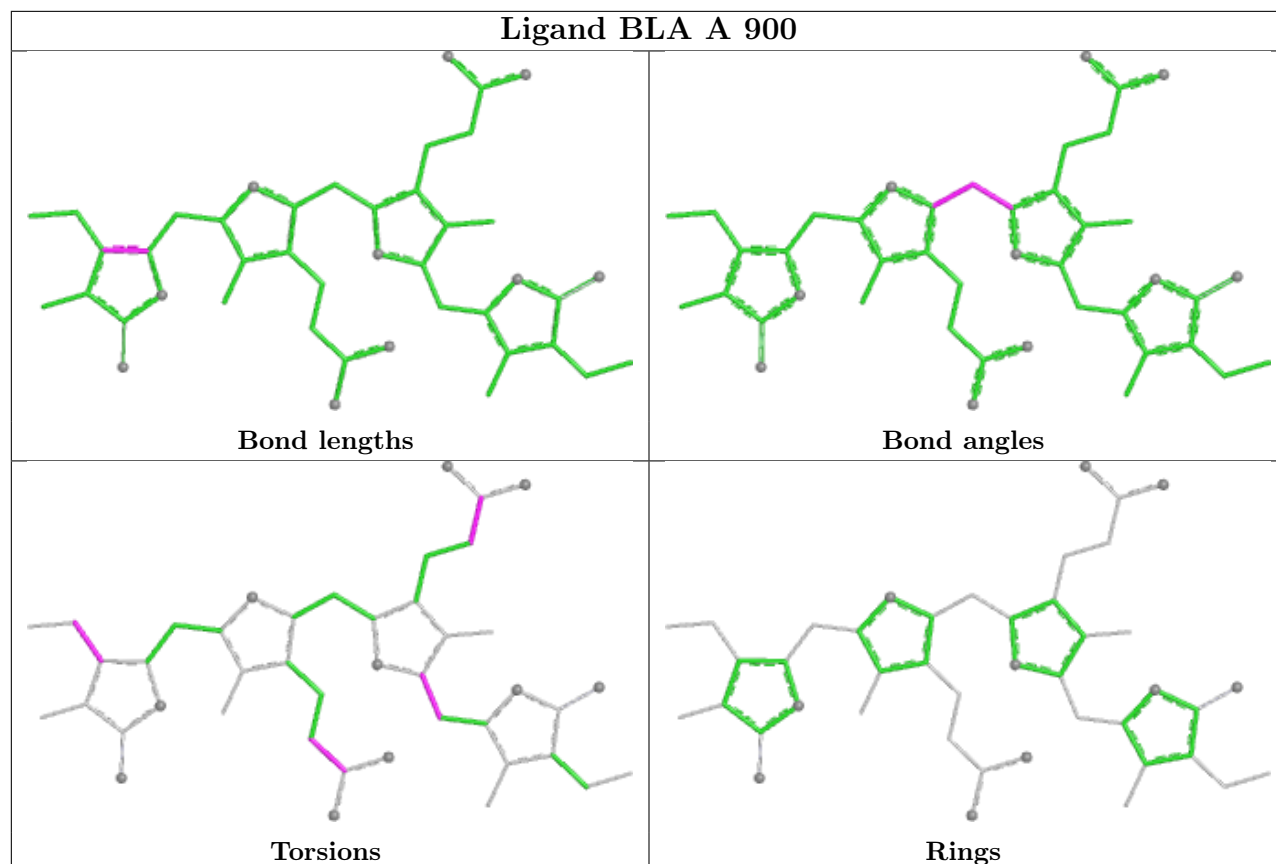
There are no ring outliers.

2 monomers are involved in 33 short contacts:

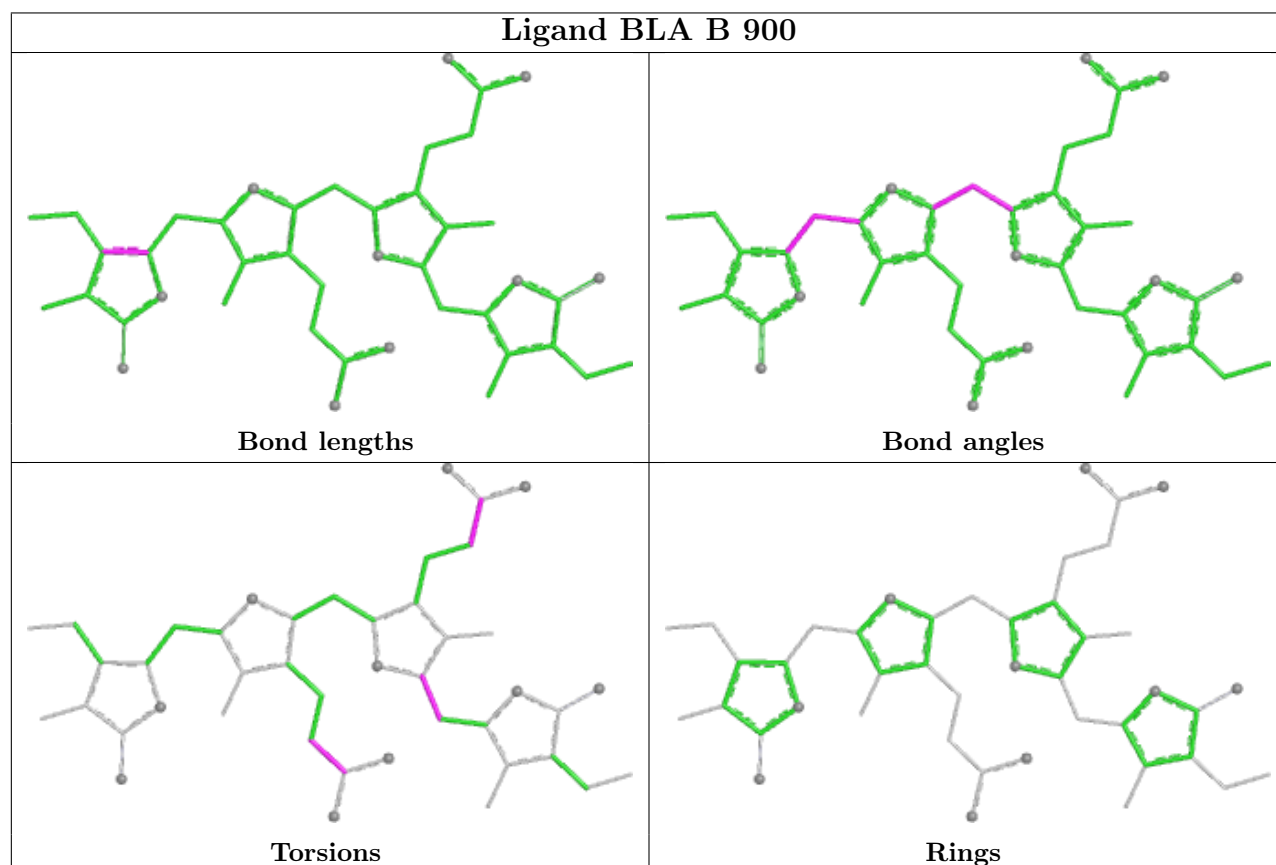
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	18	0
2	B	900	BLA	15	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	597/640 (93%)	0.08	11 (1%) 67 43	81, 125, 178, 196	0
1	B	600/640 (93%)	0.03	8 (1%) 75 51	76, 127, 211, 231	0
All	All	1197/1280 (93%)	0.05	19 (1%) 70 46	76, 126, 204, 231	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	GLN	4.6
1	A	555	CYS	4.4
1	B	129	LEU	4.1
1	A	195	TYR	3.7
1	A	214	ARG	3.3
1	A	129	LEU	2.8
1	B	301	ALA	2.5
1	B	128	THR	2.5
1	B	298	ASP	2.4
1	A	178	ILE	2.3
1	A	475	PHE	2.3
1	B	539	ASN	2.3
1	A	554	VAL	2.2
1	B	413	PHE	2.1
1	B	224	SER	2.1
1	A	539	ASN	2.1
1	A	211	ASN	2.1
1	A	600	GLN	2.0
1	B	33	ILE	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](#)

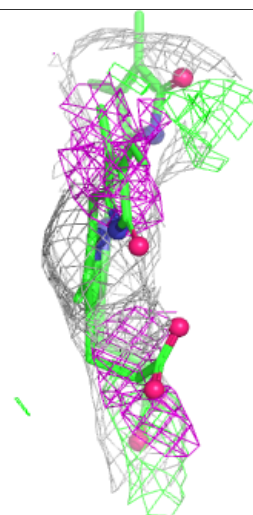
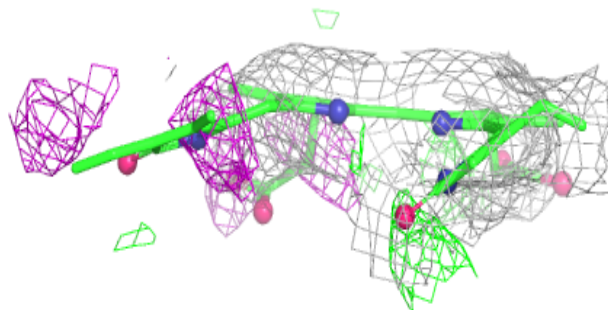
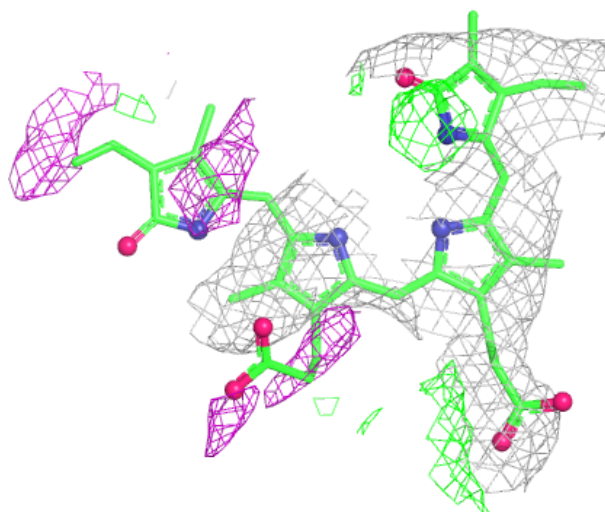
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.84	0.21	131,159,198,202	0
2	BLA	B	900	43/43	0.85	0.21	173,186,203,208	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.

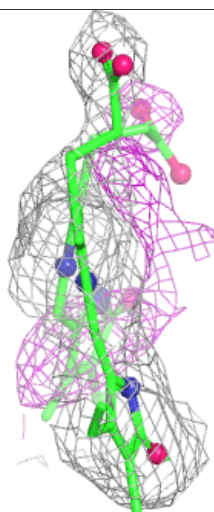
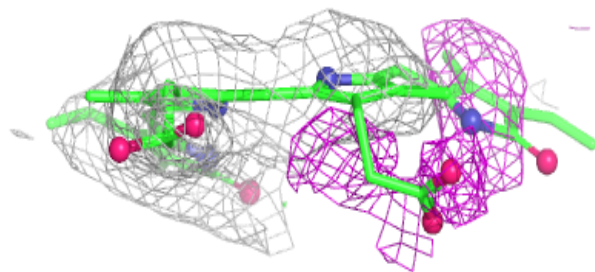
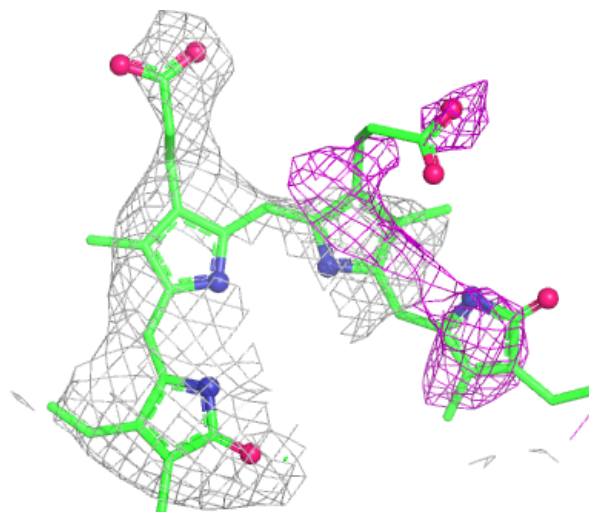
Electron density around BLA A 900:

$2mF_o-DF_c$ (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.