



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:19 PM UTC

PDB ID : 5AKP / pdb_00005akp
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 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

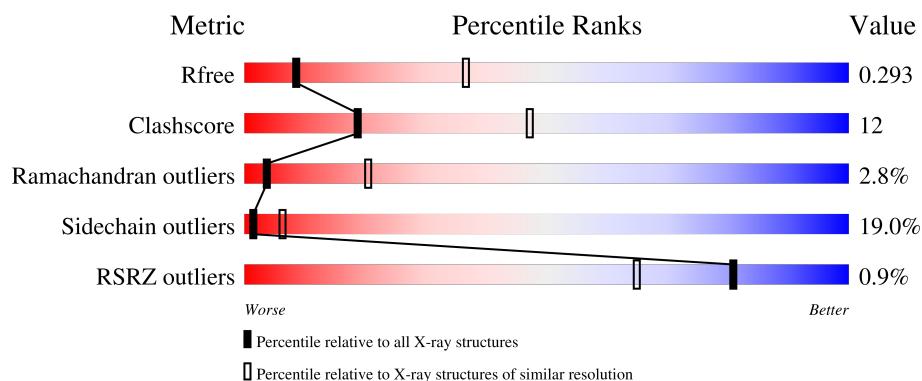
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 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	61% 24% 7% 7%
1	B	640	60% 27% 8% 5%

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.

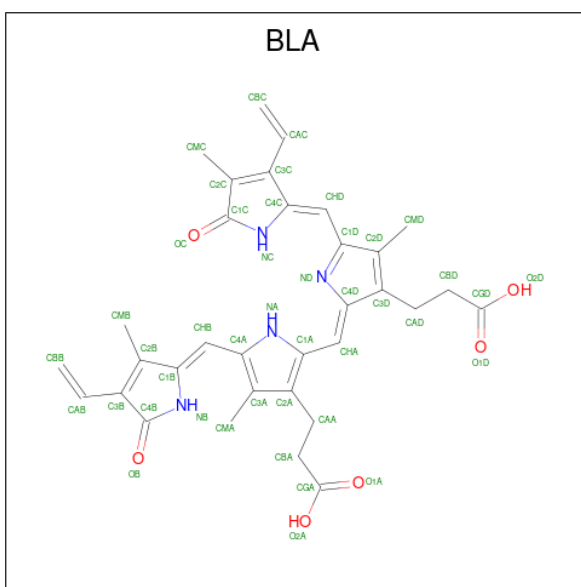
- Molecule 1 is a protein called PHYTOCHROME-LIKE PROTEIN.

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:

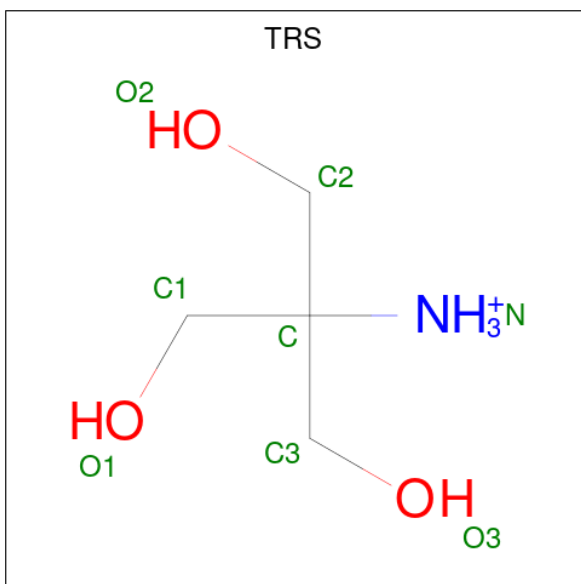
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q4UNU4
A	-4	HIS	-	expression tag	UNP Q4UNU4
A	-3	HIS	-	expression tag	UNP Q4UNU4
A	-2	HIS	-	expression tag	UNP Q4UNU4
A	-1	HIS	-	expression tag	UNP Q4UNU4
A	0	HIS	-	expression tag	UNP Q4UNU4
A	1	HIS	-	expression tag	UNP Q4UNU4
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 (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $\text{C}_4\text{H}_{12}\text{NO}_3$).



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 (CCD ID: 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		

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.

Chain A:

Chain B:

Amino Acid	Percentage
MET	60%
HIS	27%
HIS	27%
HIS	27%
HIS	27%
HIS	27%
HIS	27%
SER	27%
THR	27%
ALA	27%
ASN	27%
PRO	27%
LEU	27%
ASP	27%
LEU	27%
ASP	27%
V12	8%
C13	5%
C14	5%
R15	5%
L18	5%
P21	5%
G22	5%
G23	5%
P26	5%
Y27	5%
G28	5%
L31	5%
R39	5%
Q42	5%
T46	5%
A47	5%
A48	5%
D49	5%
L50	5%
L51	5%
W55	5%
L59	5%
P62	5%
Y63	5%
T64	5%
L67	5%
T68	5%
L84	5%
M85	5%
H86	5%
A87	5%
E88	5%
H89	5%
R90	5%
Q94	5%
A95	5%
T96	5%
P97	5%
P98	5%
W106	5%
R120	5%
D121	5%
A122	5%
R123	5%
L124	5%
L125	5%
T128	5%
L129	5%
R130	5%
E131	5%
L135	5%
L136	5%
V139	5%
E140	5%
R141	5%
D142	5%
P143	5%
G144	5%
L145	5%
A146	5%
A147	5%
R151	5%
V152	5%
I160	5%
R164	5%
I167	5%
Y168	5%
D171	5%
G176	5%

L562	R471	L381	R183
R565	R472	H387	S280
Q568	K473	I388	C281
T569	F475	E389	H282
L570	D476	S390	H283
	L477	E391	T289
			N290
R577	Q480	E394	H291
	T481	A395	A292
L587	V482	L396	M293
		R397	
G590	R487	V401	V296
R591		G402	T297
A592	S490		D298
	P491		A299
L599	L492	G410	V300
Q600	H493	E411	A301
V601	L494	V412	R302
	E495		T303
			L304
A605		A417	I216
	R498	D418	T216
Q610	V502	L419	A217
H612	L503	A420	I308
L613	I504	P421	G309
E614	E505		A310
P615	L506	V429	L311
	M507		
W626			V314
	K510	M432	A315
Q629		P433	R316
	T517	Q434	A317
D632	L518	S435	R318
PRO	L519	R436	L319
GLU	E520	S437	E320
	A521	A438	S321
	S522	L439	V322
	L523		E328
	S524	R444	
	R525		F334
	L526	Q449	
	R527	L450	L240
	D528	K451	S241
		W452	D242
		M455	E343
		PRO	L344
	I532	GLN	
	L533	LEU	D347
			M348
	R543	ALA	
	L544	LYS	
	L545	LEU	V356
	F546	GLU	
	V547	ASP	I363
	N548	ILE	
	T549	PRO	G366
	A550	ASN	A263
		SER	T264
		ARG	L265
	D558	LEU	V266
	V559	SER	
			D273

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 41.75 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.75-3.25) 99.8 (41.75-3.25)	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 0.225 , 0.293	Depositor DCC
R_{free} test set	1499 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 , 130.7	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	0.94	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, CL, 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	0.89	0/4748	1.42	38/6475 (0.6%)
1	B	0.88	0/4855	1.42	33/6624 (0.5%)
All	All	0.89	0/9603	1.42	71/13099 (0.5%)

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASP	CA-CB-CG	7.99	120.59	112.60
1	B	171	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	202	ALA	CA-C-N	7.06	129.62	120.44
1	A	202	ALA	C-N-CA	7.06	129.62	120.44
1	B	569	THR	CA-C-N	6.93	130.50	120.38
1	B	569	THR	C-N-CA	6.93	130.50	120.38
1	A	171	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	308	ILE	N-CA-CB	6.73	117.98	110.51
1	B	63	TYR	CA-C-N	6.62	129.44	120.38
1	B	63	TYR	C-N-CA	6.62	129.44	120.38
1	B	123	ARG	CA-C-N	6.39	133.74	121.54
1	B	123	ARG	C-N-CA	6.39	133.74	121.54
1	A	558	ASP	CA-C-N	6.30	128.73	120.60
1	A	558	ASP	C-N-CA	6.30	128.73	120.60
1	A	433	PRO	CA-C-N	6.23	133.44	121.54
1	A	433	PRO	C-N-CA	6.23	133.44	121.54
1	A	52	GLY	N-CA-C	6.22	120.20	112.73
1	B	558	ASP	CA-C-N	6.18	128.57	120.60
1	B	558	ASP	C-N-CA	6.18	128.57	120.60
1	A	356	VAL	N-CA-CB	-6.14	104.38	112.36
1	B	433	PRO	CA-C-N	6.12	133.23	121.54
1	B	433	PRO	C-N-CA	6.12	133.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	VAL	N-CA-CB	-6.11	104.42	112.36
1	A	52	GLY	CA-C-N	5.93	128.50	123.04
1	A	52	GLY	C-N-CA	5.93	128.50	123.04
1	B	121	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	537	THR	CA-C-N	5.88	132.77	121.54
1	A	537	THR	C-N-CA	5.88	132.77	121.54
1	B	292	ALA	CA-C-N	5.88	128.41	120.65
1	B	292	ALA	C-N-CA	5.88	128.41	120.65
1	A	587	LEU	CA-C-N	5.79	128.32	120.38
1	A	587	LEU	C-N-CA	5.79	128.32	120.38
1	A	211	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	121	ASP	CA-C-N	5.78	132.58	121.54
1	A	121	ASP	C-N-CA	5.78	132.58	121.54
1	B	121	ASP	CA-C-N	5.73	132.49	121.54
1	B	121	ASP	C-N-CA	5.73	132.49	121.54
1	B	160	ILE	N-CA-CB	5.60	119.14	111.41
1	A	548	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	53	VAL	N-CA-C	5.51	114.55	108.05
1	A	344	LEU	CD1-CG-CD2	5.39	122.67	110.80
1	B	147	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	347	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	251	VAL	CA-C-N	5.36	127.46	120.28
1	A	251	VAL	C-N-CA	5.36	127.46	120.28
1	B	251	VAL	CA-C-N	5.36	127.46	120.28
1	B	251	VAL	C-N-CA	5.36	127.46	120.28
1	B	521	ALA	CA-C-N	5.34	127.75	120.54
1	B	521	ALA	C-N-CA	5.34	127.75	120.54
1	B	587	LEU	CA-C-N	5.27	127.35	120.28
1	B	587	LEU	C-N-CA	5.27	127.35	120.28
1	A	171	ASP	CA-C-N	5.24	128.03	120.38
1	A	171	ASP	C-N-CA	5.24	128.03	120.38
1	A	37	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	121	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	147	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	521	ALA	CA-C-N	5.15	127.49	120.54
1	A	521	ALA	C-N-CA	5.15	127.49	120.54
1	B	475	PHE	CA-CB-CG	5.14	118.94	113.80
1	B	308	ILE	N-CA-CB	5.13	116.56	110.55
1	B	347	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	548	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	197	ALA	CA-C-N	5.08	127.60	120.28
1	A	197	ALA	C-N-CA	5.08	127.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	316	ARG	CA-C-N	5.06	127.37	120.54
1	B	316	ARG	C-N-CA	5.06	127.37	120.54
1	B	568	GLN	CA-C-N	5.05	127.01	120.44
1	B	568	GLN	C-N-CA	5.05	127.01	120.44
1	A	210	ARG	CA-C-N	5.03	129.12	122.42
1	A	210	ARG	C-N-CA	5.03	129.12	122.42

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	113	0
1	B	4746	0	4741	109	0
2	A	43	0	30	20	0
2	B	43	0	31	20	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	225	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 (225) 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	1.54	1.20
1:A:610:GLN:O	1:A:630:LEU:HB3	1.42	1.18
1:A:195:TYR:CD1	2:A:900:BLA:HMB2	1.78	1.17
1:A:195:TYR:CE1	2:A:900:BLA:HMB1	1.88	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE1	2:A:900:BLA:CMB	2.46	0.99
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
1:A:195:TYR:OH	2:A:900:BLA:HAB	1.69	0.91
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: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:195:TYR:CG	2:B:900:BLA:HMB3	2.18	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
1:A:401:VAL:HG13	1:A:402:GLY:H	1.53	0.73
1:A:195:TYR:CG	2:A:900:BLA:HMB2	2.23	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:A:631:ARG:HB2	1:B:527:ARG:HH22	1.55	0.71
1:B:125:LEU:O	1:B:128:THR:HG22	1.90	0.71
1:B:195:TYR:CD1	2:B:900:BLA:HMB3	2.26	0.70
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
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:629:GLN:C	1:A:630:LEU:HG	2.19	0.68
1:A:609:ARG:HE	1:A:631:ARG:C	2.02	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:NE2	2:B:900:BLA:CBA	2.48	0.62
1:B:289:THR:HB	1:B:293:MET:HE2	1.80	0.61
1:A:195:TYR:OH	2:A:900:BLA:CAB	2.45	0.61
1:B:418:ASP:C	1:B:420:ALA:H	2.08	0.61
1:A:611:PHE:CA	1:A:630:LEU:HD23	2.25	0.61
1:A:418:ASP:C	1:A:420:ALA:H	2.08	0.61
1:A:432:MET:C	1:A:434:GLN:H	2.10	0.60
1:A:535:ARG:HB2	1:A:626:TRP:CZ3	2.37	0.60
1:A:630:LEU:N	1:A:630:LEU:HD12	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:432:MET:C	1:B:434:GLN:H	2.11	0.58
1:B:145:ILE:HG12	1:B:308:ILE:HB	1.85	0.58
2:A:900:BLA:HB	2:A:900:BLA:HMA1	1.68	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:A:430:PRO:HD3	1:A:504:ILE:HG12	1.88	0.56
1:B:195:TYR:CD1	2:B:900:BLA:CMB	2.89	0.56
1:A:183:ARG:HH12	1:A:187:LEU:C	2.13	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
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:68:THR:HB	1:B:90:ARG:HB3	1.90	0.53
1:A:629:GLN:C	1:A:630:LEU:CG	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:900:BLA:HMA1	2:A:900:BLA:NB	2.24	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:A:516:PHE:CE1	1:B:519:LEU:HD22	2.45	0.52
1:B:401:VAL:HG13	1:B:402:GLY:N	2.20	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:536:GLY:C	1:A:538:ALA:H	2.19	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:208:TYR:OH	2:B:900:BLA:HAA1	2.11	0.51
1:B:401:VAL:HG13	1:B:498:ARG:HE	1.75	0.51
1:B:387:HIS:O	1:B:390:SER:HB3	2.11	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
2:B:900:BLA:CMA	2:B:900:BLA:NB	2.72	0.50
1:A:307:ARG:O	1:A:308:ILE:C	2.52	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:97:PRO:N	1:A:98:PRO:HD3	2.26	0.49
1:A:221:TYR:CE1	1:A:223:PRO:HG3	2.47	0.49
1:B:255:TYR:CD1	1:B:255:TYR:C	2.91	0.49
1:A:609:ARG:NE	1:A:631:ARG:C	2.69	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
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
2:B:900:BLA:HB	2:B:900:BLA:HMA1	1.73	0.48
2:B:900:BLA:CMA	2:B:900:BLA:CGA	2.92	0.48
2:B:900:BLA:NB	2:B:900:BLA:HMA1	2.28	0.48
1:A:28:GLY:O	1:A:46:THR:HG21	2.12	0.48
1:A:394:GLU:O	1:A:398:GLU:HG2	2.14	0.48
2:A:900:BLA:CMA	2:A:900:BLA:NB	2.71	0.48
1:B:136:LEU:HD22	1:B:303:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:HG21	1:B:298:ASP:HB2	1.96	0.48
1:B:221:TYR:O	1:B:223:PRO:HD3	2.15	0.47
1:A:255:TYR:CD1	1:A:255:TYR:C	2.92	0.47
1:A:307:ARG:NH2	1:B:273:ASP:CG	2.73	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
2:A:900:BLA:CMA	2:A:900:BLA:CGA	2.93	0.47
1:A:504:ILE:HA	1:A:507:MET:HE3	1.97	0.47
2:A:900:BLA:CGA	2:A:900:BLA:HMA2	2.45	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:504:ILE:HA	1:B:507:MET:HE3	1.97	0.46
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
2:B:900:BLA:O1A	2:B:900:BLA:HMA2	2.16	0.46
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:130:ARG:NH2	1:B:86:HIS:O	2.50	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:391:GLU:H	1:B:391:GLU:CD	2.25	0.45
1:B:420:ALA:N	1:B:421:PRO:HD2	2.31	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: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: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
1:A:501:ARG:HH12	1:B:328:GLU:CD	2.26	0.44
1:A:609:ARG:HD3	1:A:609:ARG:HA	1.78	0.44
1:B:48:ALA:HB2	1:B:55:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:HD11	2:B:900:BLA:CBB	2.47	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:A:521:ALA:O	1:A:525:ARG:HG3	2.18	0.43
2:B:900:BLA:HB	2:B:900:BLA:HMA2	1.78	0.43
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.92	0.43
1:B:152:VAL:HG21	1:B:304:LEU:HB2	2.01	0.43
1:A:84:LEU:HB2	1:A:106:TRP:HB2	2.00	0.43
1:A:424:ALA:HB3	1:A:486:ALA:HB2	2.01	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: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:449:GLN:HE22	1:A:481:THR:HG23	1.83	0.42
2:A:900:BLA:HMA2	2:A:900:BLA:O1A	2.19	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:537:THR:C	1:A:539:ASN:H	2.28	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:B:26:PRO:HD2	1:B:221:TYR:CD2	2.55	0.41
1:A:48:ALA:HB2	1:A:55:MET:HE2	2.02	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:A:523:LEU:HD12	1:B:519:LEU:HG	2.03	0.41
1:B:204:ALA:O	1:B:208:TYR:HD1	2.04	0.41
1:B:587:LEU:HA	1:B:626:TRP:CZ2	2.56	0.41
1:A:410:GLY:HA2	1:A:417:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ARG:HB3	1:B:282:HIS:HB2	2.02	0.41
1:B:255:TYR:C	1:B:255:TYR:HD1	2.28	0.41
1:B:502:VAL:O	1:B:506:LEU:HB2	2.20	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:418:ASP:C	1:B:420:ALA:N	2.78	0.40
1:B:590:GLY:HA2	1:B:626:TRP:CZ2	2.56	0.40
1:A:98:PRO:C	1:A:100:SER:H	2.29	0.40
1:A:610:GLN:H	1:A:610:GLN:HG2	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:410:GLY:HA2	1:B:417:ALA:HA	2.03	0.40
1:A:255:TYR:C	1:A:255:TYR:HD1	2.30	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%)	3	20
1	B	602/640 (94%)	543 (90%)	43 (7%)	16 (3%)	4	21
All	All	1185/1280 (93%)	1071 (90%)	81 (7%)	33 (3%)	4	20

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	LEU
1	B	241	SER

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Mol	Chain	Res	Type
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/532 (92%)	397 (81%)	92 (19%)	1	7
1	B	500/532 (94%)	404 (81%)	96 (19%)	1	6
All	All	989/1064 (93%)	801 (81%)	188 (19%)	1	6

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	23	LEU
1	A	59	LEU
1	A	65	GLN
1	A	69	LEU
1	A	77	VAL
1	A	80	GLN
1	A	94	ARG
1	A	129	LEU
1	A	131	GLU
1	A	135	LEU
1	A	136	LEU
1	A	139	VAL
1	A	141	ARG
1	A	160	ILE
1	A	167	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	212	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	238	VAL
1	A	240	LEU

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Mol	Chain	Res	Type
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	308	ILE
1	A	318	ARG
1	A	319	LEU
1	A	322	VAL
1	A	330	LEU
1	A	334	PHE
1	A	343	GLU
1	A	344	LEU
1	A	348	MET
1	A	356	VAL
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	394	GLU
1	A	396	LEU
1	A	412	VAL
1	A	419	LEU
1	A	432	MET
1	A	436	ARG
1	A	444	ARG
1	A	449	GLN
1	A	475	PHE
1	A	482	VAL
1	A	487	ARG
1	A	492	LEU
1	A	495	GLU
1	A	504	ILE
1	A	506	LEU

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Mol	Chain	Res	Type
1	A	510	LYS
1	A	518	LEU
1	A	519	LEU
1	A	524	SER
1	A	527	ARG
1	A	528	ASP
1	A	533	ILE
1	A	535	ARG
1	A	537	THR
1	A	543	ARG
1	A	545	LEU
1	A	548	ASN
1	A	577	ARG
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	18	ILE
1	B	23	LEU
1	B	39	ARG
1	B	50	LEU
1	B	59	LEU
1	B	67	LEU
1	B	69	LEU
1	B	77	VAL
1	B	94	ARG
1	B	96	THR
1	B	125	LEU
1	B	128	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

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Mol	Chain	Res	Type
1	B	188	GLU
1	B	191	LEU
1	B	207	LEU
1	B	209	LEU
1	B	210	ARG
1	B	212	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	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	308	ILE
1	B	318	ARG
1	B	319	LEU
1	B	322	VAL
1	B	334	PHE
1	B	339	HIS
1	B	343	GLU
1	B	348	MET
1	B	356	VAL
1	B	363	ILE
1	B	374	THR
1	B	375	THR
1	B	387	HIS
1	B	389	GLU
1	B	396	LEU
1	B	412	VAL
1	B	419	LEU
1	B	429	VAL

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Mol	Chain	Res	Type
1	B	432	MET
1	B	437	SER
1	B	444	ARG
1	B	449	GLN
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	504	ILE
1	B	506	LEU
1	B	510	LYS
1	B	517	THR
1	B	518	LEU
1	B	519	LEU
1	B	523	LEU
1	B	524	SER
1	B	528	ASP
1	B	533	ILE
1	B	543	ARG
1	B	544	LEU
1	B	545	LEU
1	B	565	ARG
1	B	577	ARG
1	B	599	LEU
1	B	614	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	203	GLN
1	A	211	ASN
1	A	222	GLN
1	A	231	HIS
1	A	287	HIS
1	A	335	ASN
1	A	365	HIS

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Mol	Chain	Res	Type
1	A	449	GLN
1	A	455	ASN
1	A	480	GLN
1	A	589	ASN
1	B	73	GLN
1	B	82	GLN
1	B	211	ASN
1	B	222	GLN
1	B	231	HIS
1	B	233	GLN
1	B	290	ASN
1	B	335	ASN
1	B	449	GLN
1	B	455	ASN
1	B	480	GLN
1	B	539	ASN
1	B	584	GLN
1	B	625	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.36	0	9,9,9	0.47	0
3	TRS	B	1633	-	7,7,7	0.41	0	9,9,9	0.45	0
2	BLA	B	900	1	46,46,46	2.00	12 (26%)	66,67,67	2.09	17 (25%)
2	BLA	A	900	1	46,46,46	2.11	14 (30%)	66,67,67	2.14	18 (27%)

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	-
3	TRS	B	1633	-	-	1/9/9/9	-
2	BLA	B	900	1	-	6/26/74/74	0/4/4/4
2	BLA	A	900	1	-	8/26/74/74	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	C3B-C2B	6.51	1.50	1.37
2	A	900	BLA	C3B-C2B	5.68	1.48	1.37
2	A	900	BLA	CHB-C1B	5.45	1.50	1.37
2	B	900	BLA	CHA-C4D	4.93	1.48	1.38
2	A	900	BLA	CHA-C4D	4.75	1.47	1.38
2	A	900	BLA	CHB-C4A	4.70	1.51	1.40
2	B	900	BLA	C4A-C3A	4.10	1.51	1.41
2	B	900	BLA	CHB-C1B	4.06	1.47	1.37
2	B	900	BLA	CHB-C4A	3.89	1.49	1.40
2	A	900	BLA	C4A-C3A	3.86	1.50	1.41
2	A	900	BLA	CHA-C1A	3.85	1.49	1.40
2	B	900	BLA	C2A-C3A	3.46	1.47	1.38
2	A	900	BLA	OB-C4B	3.25	1.29	1.23
2	A	900	BLA	C1B-C2B	3.14	1.50	1.45
2	B	900	BLA	C3C-C4C	3.08	1.51	1.45
2	B	900	BLA	C1B-C2B	2.90	1.50	1.45
2	B	900	BLA	CHA-C1A	2.85	1.46	1.40
2	B	900	BLA	OB-C4B	2.85	1.29	1.23
2	A	900	BLA	C2A-C3A	2.71	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C3C-C4C	2.70	1.50	1.45
2	A	900	BLA	C4D-ND	-2.60	1.33	1.38
2	B	900	BLA	C1A-C2A	2.46	1.48	1.42
2	A	900	BLA	C1B-NB	-2.37	1.33	1.37
2	A	900	BLA	C4B-NB	-2.27	1.32	1.38
2	B	900	BLA	C1A-NA	-2.26	1.34	1.37
2	A	900	BLA	C1A-C2A	2.17	1.47	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	CMA-C3A-C4A	7.49	136.50	125.62
2	B	900	BLA	C2A-C1A-NA	6.36	115.54	107.57
2	B	900	BLA	CMA-C3A-C4A	5.64	133.81	125.62
2	A	900	BLA	CMB-C2B-C1B	5.62	131.00	124.16
2	A	900	BLA	C3B-C2B-C1B	-5.24	102.08	107.92
2	B	900	BLA	CHB-C4A-NA	-5.24	113.45	125.29
2	B	900	BLA	C3A-C4A-NA	4.74	113.89	107.43
2	B	900	BLA	C3B-C2B-C1B	-4.36	103.06	107.92
2	B	900	BLA	C1A-C2A-C3A	-4.28	102.64	107.62
2	A	900	BLA	CHB-C1B-NB	-4.27	116.95	126.06
2	A	900	BLA	C3B-C4B-NB	4.17	111.37	106.13
2	B	900	BLA	C4A-C3A-C2A	-4.17	102.55	107.76
2	A	900	BLA	C2A-C1A-NA	4.14	112.77	107.57
2	A	900	BLA	C4A-C3A-C2A	-3.97	102.79	107.76
2	A	900	BLA	C3A-C4A-NA	3.74	112.53	107.43
2	A	900	BLA	CHA-C1A-C2A	-3.67	119.33	127.22
2	B	900	BLA	CMB-C2B-C1B	3.57	128.50	124.16
2	B	900	BLA	CHB-C1B-NB	-3.44	118.72	126.06
2	A	900	BLA	C2B-C1B-NB	3.36	111.86	106.97
2	B	900	BLA	CHA-C4D-ND	3.00	130.90	124.60
2	B	900	BLA	C4A-CHB-C1B	-2.90	122.47	130.82
2	A	900	BLA	CHB-C4A-NA	-2.90	118.75	125.29
2	B	900	BLA	CHA-C4D-C3D	-2.82	118.88	125.40
2	B	900	BLA	CHA-C1A-NA	-2.72	119.14	125.29
2	B	900	BLA	C4A-NA-C1A	-2.56	105.29	109.78
2	A	900	BLA	C4B-C3B-C2B	-2.47	104.75	107.92
2	A	900	BLA	OB-C4B-NB	-2.36	119.54	125.08
2	A	900	BLA	CMA-C3A-C2A	-2.32	120.69	125.62
2	B	900	BLA	CHB-C1B-C2B	2.13	131.22	126.97
2	B	900	BLA	C2B-C1B-NB	2.12	110.06	106.97
2	A	900	BLA	CHB-C1B-C2B	2.11	131.19	126.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C4A-CHB-C1B	-2.09	124.80	130.82
2	B	900	BLA	CHB-C4A-C3A	2.09	132.65	127.53
2	A	900	BLA	C1A-CHA-C4D	2.05	132.71	128.22
2	A	900	BLA	CAD-C3D-C4D	2.04	128.60	125.02

There are no chirality outliers.

All (18) 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
3	A	1632	TRS	N-C-C1-O1
3	A	1632	TRS	C2-C-C1-O1
3	A	1632	TRS	C3-C-C1-O1
2	B	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAA-CBA-CGA-O2A
2	B	900	BLA	CAA-CBA-CGA-O1A
2	A	900	BLA	CAA-CBA-CGA-O1A
2	A	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	CAD-CBD-CGD-O1D
2	A	900	BLA	CAD-CBD-CGD-O2D
2	B	900	BLA	CAD-CBD-CGD-O2D
3	B	1633	TRS	C2-C-C1-O1

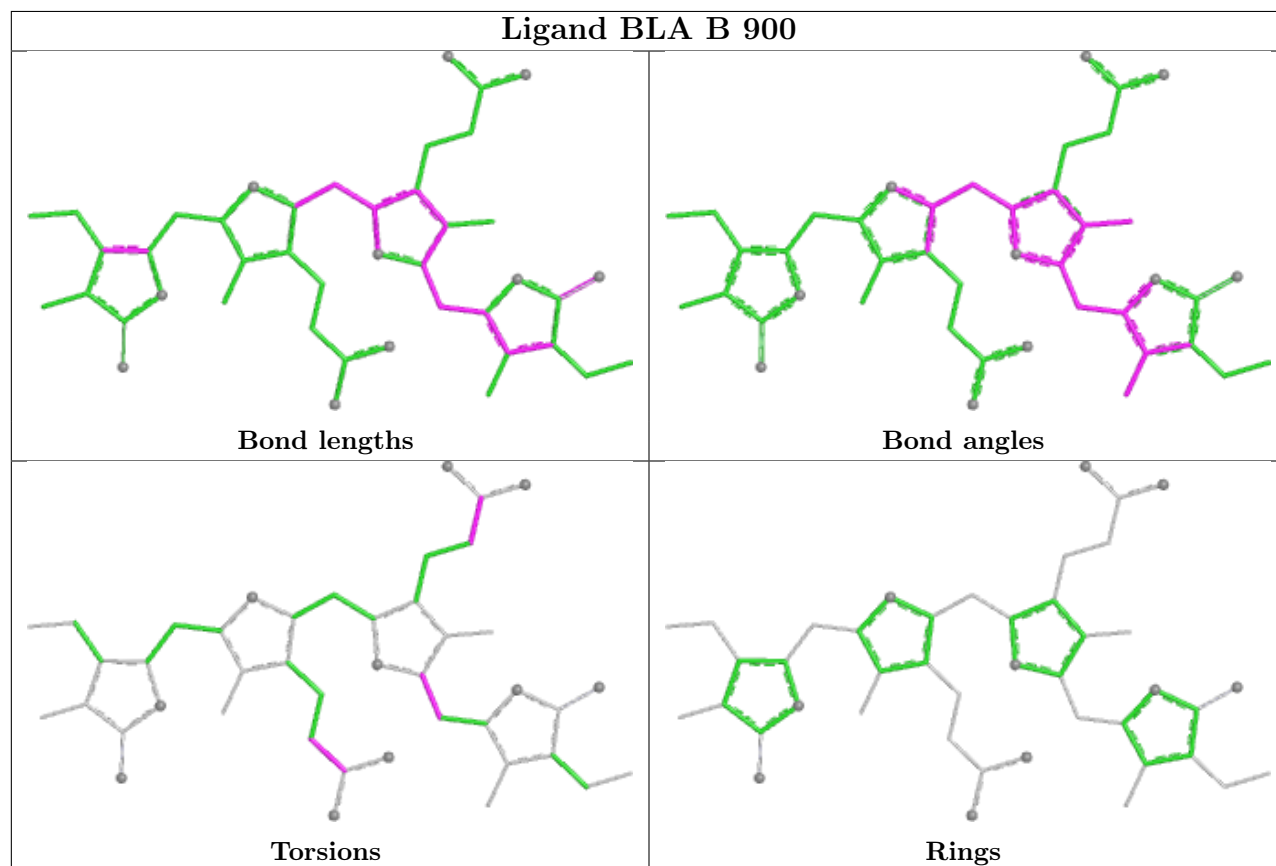
There are no ring outliers.

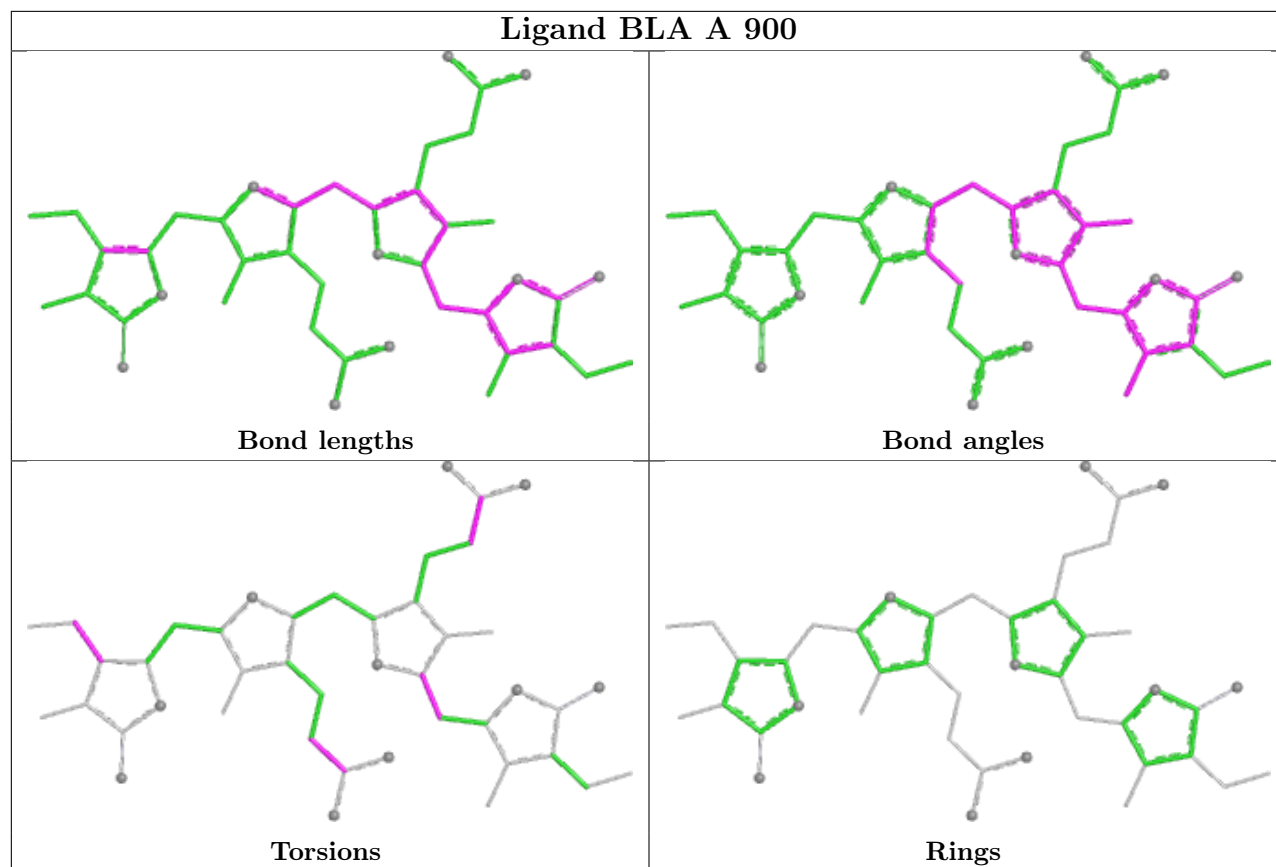
2 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	BLA	20	0
2	A	900	BLA	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	593/640 (92%)	-0.07	9 (1%) 72 53	57, 106, 165, 186	0
1	B	606/640 (94%)	-0.09	2 (0%) 90 82	60, 108, 189, 209	0
All	All	1199/1280 (93%)	-0.08	11 (0%) 81 65	57, 107, 179, 209	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	CYS	5.1
1	B	125	LEU	3.6
1	A	611	PHE	3.1
1	B	129	LEU	3.0
1	A	27	TYR	2.9
1	A	122	ALA	2.7
1	A	188	GLU	2.5
1	A	602	SER	2.3
1	A	129	LEU	2.2
1	A	630	LEU	2.2
1	A	340	MET	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

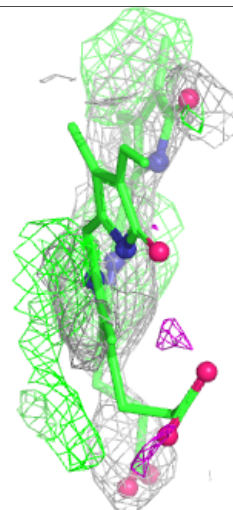
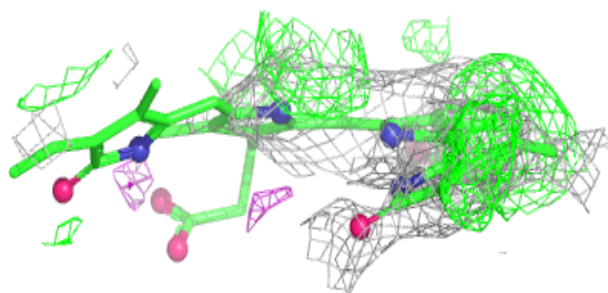
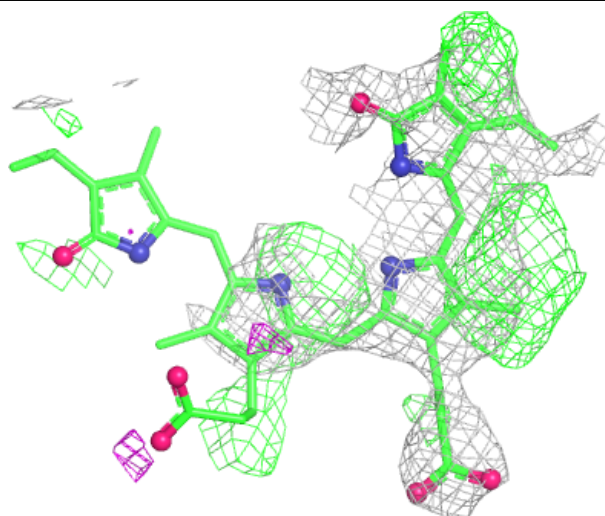
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

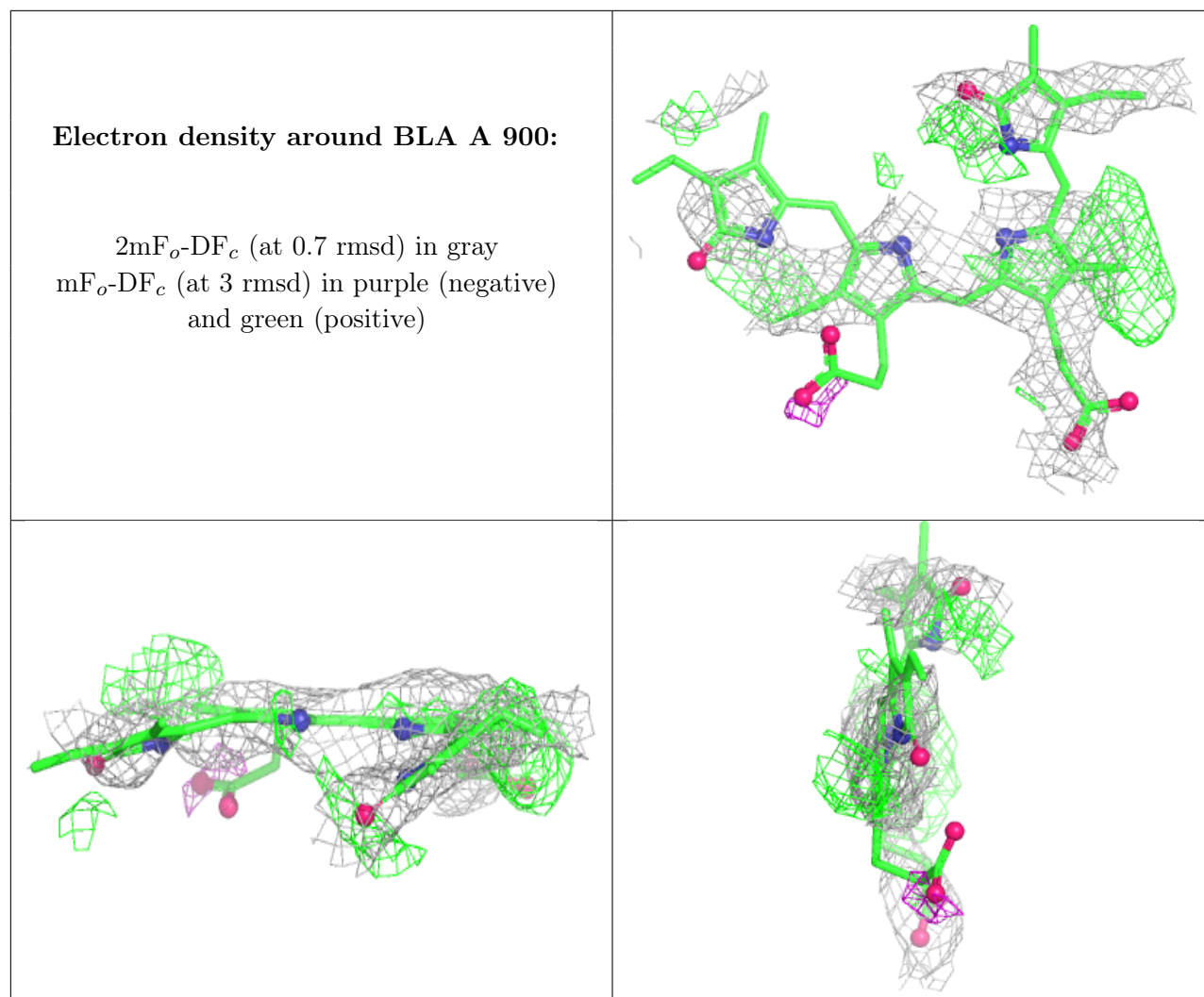
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRS	A	1632	8/8	0.80	0.13	119,122,123,123	0
2	BLA	B	900	43/43	0.82	0.34	112,135,144,157	43
3	TRS	B	1633	8/8	0.83	0.15	102,107,112,113	0
4	CL	A	1633	1/1	0.85	0.09	104,104,104,104	0
2	BLA	A	900	43/43	0.89	0.27	115,139,146,155	43

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.