Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 09:03 PM EDT

PDB ID	:	5OY5
Title	:	Monomeric crystal structure of RpBphP1 photosensory core domain from the bacterium Rhodopseudomonas palustris
Authors	:	Papiz, M.Z.; Bellini, D.
Deposited on	:	2017-09-07
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

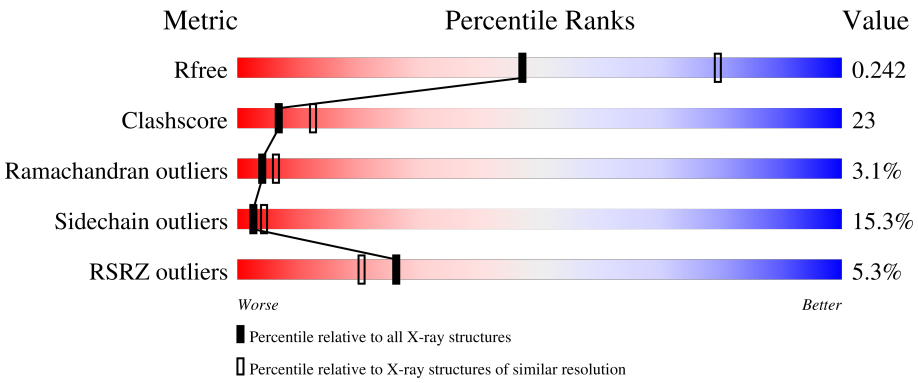
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

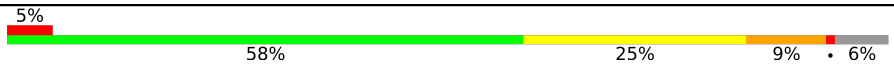
The reported resolution of this entry is 2.60 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	525	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4057 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.

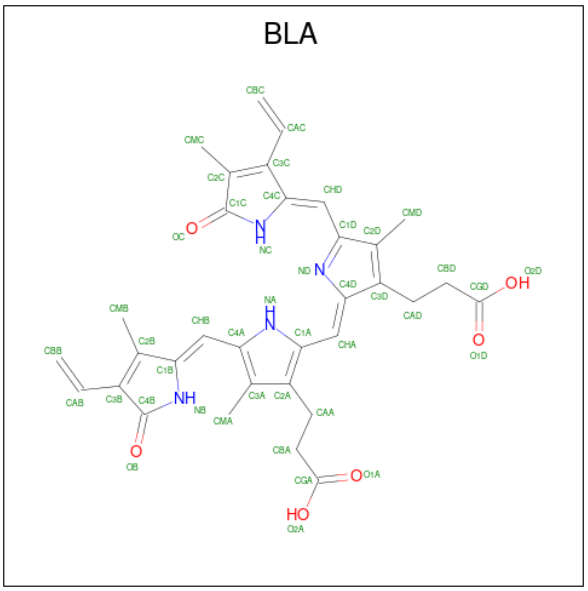
- Molecule 1 is a protein called BphP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	3796	2392	678	707	19	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A161I5N6
A	-18	GLY	-	expression tag	UNP A0A161I5N6
A	-17	SER	-	expression tag	UNP A0A161I5N6
A	-16	SER	-	expression tag	UNP A0A161I5N6
A	-15	HIS	-	expression tag	UNP A0A161I5N6
A	-14	HIS	-	expression tag	UNP A0A161I5N6
A	-13	HIS	-	expression tag	UNP A0A161I5N6
A	-12	HIS	-	expression tag	UNP A0A161I5N6
A	-11	HIS	-	expression tag	UNP A0A161I5N6
A	-10	HIS	-	expression tag	UNP A0A161I5N6
A	-9	SER	-	expression tag	UNP A0A161I5N6
A	-8	SER	-	expression tag	UNP A0A161I5N6
A	-7	GLY	-	expression tag	UNP A0A161I5N6
A	-6	LEU	-	expression tag	UNP A0A161I5N6
A	-5	VAL	-	expression tag	UNP A0A161I5N6
A	-4	PRO	-	expression tag	UNP A0A161I5N6
A	-3	ARG	-	expression tag	UNP A0A161I5N6
A	-2	GLY	-	expression tag	UNP A0A161I5N6
A	-1	SER	-	expression tag	UNP A0A161I5N6
A	0	HIS	-	expression tag	UNP A0A161I5N6
A	1	MET	-	expression tag	UNP A0A161I5N6
A	2	VAL	MET	conflict	UNP A0A161I5N6
A	291	ILE	MET	conflict	UNP A0A161I5N6
A	360	ASP	ALA	conflict	UNP A0A161I5N6

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

- Molecule 3 is water.

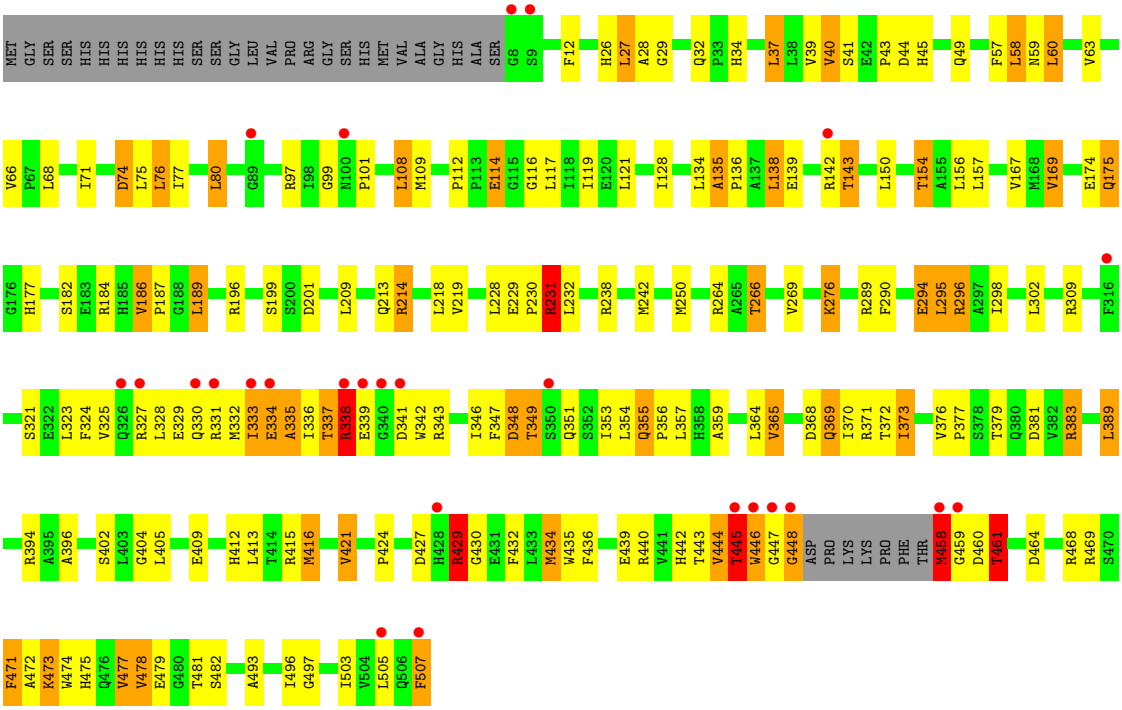
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	218	218	218	0	0

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: BphP1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	92.78Å 92.78Å 449.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.09 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (79.09-2.60) 99.9 (19.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.192 , 0.242 0.192 , 0.242	Depositor DCC
R_{free} test set	1840 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4057	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.65	4/3882 (0.1%)	0.91	12/5284 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	MET	CG-SD	6.81	1.98	1.81
1	A	448	GLY	N-CA	5.75	1.54	1.46
1	A	458	MET	N-CA	5.30	1.56	1.46
1	A	447	GLY	N-CA	5.19	1.53	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	A	264	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	A	264	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	74	ASP	N-CA-C	6.87	129.55	111.00
1	A	37	LEU	CA-CB-CG	6.86	131.09	115.30
1	A	229	GLU	C-N-CD	-6.44	106.43	120.60
1	A	448	GLY	N-CA-C	5.83	127.67	113.10
1	A	296	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	447	GLY	N-CA-C	5.24	126.21	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	445	THR	N-CA-C	5.24	125.14	111.00
1	A	383	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	458	MET	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3796	0	3754	172	1
2	A	43	0	30	7	0
3	A	218	0	0	22	0
All	All	4057	0	3784	177	1

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 23.

All (177) 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:119:ILE:HA	3:A:701:HOH:O	1.28	1.25
1:A:458:MET:HB2	3:A:705:HOH:O	1.43	1.16
1:A:338:ARG:O	1:A:339:GLU:HG2	1.49	1.13
1:A:448:GLY:O	1:A:468:ARG:NH1	1.82	1.12
1:A:338:ARG:HH11	1:A:338:ARG:HB2	1.11	1.08
1:A:276:LYS:HA	1:A:276:LYS:HE2	1.37	1.06
1:A:329:GLU:O	1:A:333:ILE:HG13	1.63	0.98
1:A:109:MET:HA	3:A:701:HOH:O	1.62	0.97
1:A:289:ARG:HD2	3:A:703:HOH:O	1.60	0.97
1:A:77:ILE:HD12	3:A:898:HOH:O	1.64	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:O	1:A:44:ASP:HB2	1.66	0.95
1:A:169:VAL:HG13	1:A:182:SER:HB2	1.48	0.95
1:A:77:ILE:CD1	3:A:898:HOH:O	2.17	0.92
1:A:177:HIS:HD2	1:A:199:SER:H	1.15	0.91
1:A:184:ARG:HD2	3:A:868:HOH:O	1.73	0.88
1:A:29:GLY:N	1:A:242:MET:HE3	1.92	0.84
1:A:338:ARG:HB2	1:A:338:ARG:NH1	1.91	0.83
2:A:600:BLA:HMA2	2:A:600:BLA:HMB3	1.60	0.81
1:A:347:PHE:CD1	1:A:373:ILE:HG12	2.15	0.81
1:A:150:LEU:O	1:A:154:THR:HG23	1.81	0.80
1:A:404:GLY:O	1:A:405:LEU:HB3	1.82	0.80
2:A:600:BLA:HMB3	2:A:600:BLA:CMA	2.11	0.79
1:A:276:LYS:HA	1:A:276:LYS:CE	2.14	0.77
1:A:230:PRO:O	1:A:231:ARG:HB2	1.85	0.77
1:A:439:GLU:OE2	1:A:479:GLU:O	2.03	0.77
1:A:108:LEU:O	3:A:701:HOH:O	2.03	0.77
1:A:177:HIS:HD2	1:A:199:SER:N	1.83	0.77
1:A:330:GLN:HA	1:A:333:ILE:HD12	1.67	0.77
1:A:230:PRO:O	1:A:231:ARG:CB	2.34	0.76
1:A:177:HIS:CD2	1:A:199:SER:H	2.03	0.75
1:A:336:ILE:HD11	1:A:342:TRP:HB3	1.68	0.74
1:A:139:GLU:O	1:A:143:THR:HB	1.86	0.74
1:A:29:GLY:H	1:A:242:MET:HE3	1.52	0.73
1:A:445:THR:O	1:A:446:TRP:HB2	1.88	0.73
1:A:477:VAL:O	1:A:478:VAL:HB	1.88	0.73
1:A:478:VAL:O	1:A:481:THR:HB	1.87	0.73
1:A:507:PHE:HA	3:A:852:HOH:O	1.90	0.72
1:A:347:PHE:HD1	1:A:373:ILE:HG12	1.56	0.70
1:A:334:GLU:O	1:A:337:THR:N	2.24	0.69
1:A:266:THR:HG21	3:A:712:HOH:O	1.94	0.67
1:A:328:LEU:HA	1:A:331:ARG:HG2	1.74	0.67
1:A:330:GLN:HA	1:A:333:ILE:CD1	2.25	0.66
1:A:328:LEU:HD12	1:A:331:ARG:HB2	1.78	0.65
1:A:230:PRO:O	3:A:702:HOH:O	2.15	0.65
1:A:396:ALA:O	1:A:424:PRO:HD2	1.97	0.64
1:A:383:ARG:HD2	3:A:845:HOH:O	1.97	0.64
1:A:338:ARG:O	1:A:339:GLU:CG	2.37	0.64
1:A:348:ASP:O	1:A:349:THR:HG23	1.99	0.63
1:A:266:THR:HG22	3:A:745:HOH:O	1.98	0.63
1:A:334:GLU:C	1:A:336:ILE:H	2.00	0.63
1:A:421:VAL:HG13	1:A:435:TRP:HB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LYS:NZ	3:A:704:HOH:O	2.32	0.63
1:A:446:TRP:CZ3	3:A:832:HOH:O	2.51	0.63
1:A:135:ALA:HB3	1:A:136:PRO:CD	2.28	0.62
1:A:377:PRO:HA	1:A:416:MET:HG3	1.80	0.62
1:A:134:LEU:HD23	1:A:298:ILE:HD13	1.81	0.61
1:A:334:GLU:O	1:A:336:ILE:N	2.30	0.61
1:A:377:PRO:CA	1:A:416:MET:HG3	2.31	0.60
1:A:328:LEU:HA	1:A:331:ARG:CG	2.32	0.59
1:A:40:VAL:HG13	1:A:45:HIS:HA	1.84	0.59
1:A:57:PHE:HD2	1:A:58:LEU:HD13	1.65	0.59
1:A:289:ARG:NH1	3:A:703:HOH:O	2.30	0.59
1:A:448:GLY:O	1:A:458:MET:HB2	2.02	0.59
1:A:26:HIS:CD2	1:A:27:LEU:HD13	2.39	0.58
1:A:34:HIS:CE1	1:A:219:VAL:HG13	2.38	0.58
1:A:334:GLU:OE2	1:A:335:ALA:N	2.37	0.58
1:A:443:THR:C	1:A:444:VAL:HG13	2.23	0.58
2:A:600:BLA:HMA1	2:A:600:BLA:C1B	2.33	0.57
1:A:134:LEU:O	1:A:134:LEU:HD12	2.03	0.57
1:A:415:ARG:HH11	1:A:442:HIS:CD2	2.23	0.57
1:A:460:ASP:O	1:A:460:ASP:OD1	2.22	0.57
1:A:348:ASP:O	1:A:349:THR:CG2	2.54	0.56
1:A:135:ALA:HB3	1:A:136:PRO:HD3	1.87	0.56
1:A:266:THR:CG2	3:A:745:HOH:O	2.54	0.55
1:A:29:GLY:H	1:A:242:MET:CE	2.18	0.55
1:A:351:GLN:O	1:A:351:GLN:HG3	2.06	0.55
1:A:336:ILE:HD11	1:A:342:TRP:CB	2.37	0.55
1:A:114:GLU:OE2	1:A:238:ARG:NH2	2.38	0.54
1:A:338:ARG:HH11	1:A:338:ARG:CB	2.02	0.54
2:A:600:BLA:HMA1	2:A:600:BLA:C2B	2.37	0.54
1:A:347:PHE:CE1	1:A:373:ILE:HG12	2.42	0.54
1:A:134:LEU:CD2	1:A:298:ILE:HD13	2.36	0.54
1:A:381:ASP:OD2	1:A:413:LEU:HD21	2.07	0.54
1:A:404:GLY:O	1:A:405:LEU:CB	2.51	0.53
1:A:460:ASP:CB	1:A:469:ARG:HH21	2.20	0.53
1:A:150:LEU:O	1:A:154:THR:CG2	2.56	0.53
1:A:357:LEU:HD21	1:A:493:ALA:HB2	1.90	0.53
1:A:186:VAL:HG23	1:A:187:PRO:HD2	1.91	0.53
1:A:58:LEU:HB3	1:A:60:LEU:HD22	1.91	0.52
1:A:372:THR:HB	1:A:376:VAL:HG11	1.91	0.52
1:A:330:GLN:CA	1:A:333:ILE:HD12	2.37	0.52
1:A:29:GLY:N	1:A:242:MET:CE	2.68	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASP:OD2	1:A:343:ARG:HG3	2.08	0.52
1:A:330:GLN:HA	1:A:333:ILE:CG1	2.40	0.52
1:A:109:MET:CA	3:A:701:HOH:O	2.36	0.52
1:A:365:VAL:HG22	1:A:432:PHE:H	1.74	0.52
1:A:128:ILE:HG13	1:A:294:GLU:CG	2.40	0.52
1:A:128:ILE:HG13	1:A:294:GLU:HG3	1.92	0.51
1:A:459:GLY:O	1:A:469:ARG:NE	2.37	0.51
1:A:440:ARG:HD2	1:A:481:THR:HG22	1.93	0.51
1:A:134:LEU:O	1:A:135:ALA:HB2	2.10	0.51
1:A:355:GLN:N	1:A:356:PRO:CD	2.75	0.49
1:A:415:ARG:NH1	1:A:442:HIS:CD2	2.80	0.49
2:A:600:BLA:CMA	2:A:600:BLA:CMB	2.89	0.49
1:A:289:ARG:HD3	1:A:290:PHE:O	2.13	0.49
1:A:353:ILE:HG22	1:A:373:ILE:HD11	1.94	0.49
1:A:59:ASN:HB3	1:A:101:PRO:HD2	1.95	0.49
1:A:379:THR:HG23	3:A:716:HOH:O	2.13	0.49
1:A:444:VAL:HG23	1:A:445:THR:N	2.28	0.49
1:A:228:LEU:HD11	1:A:242:MET:HE1	1.96	0.48
1:A:415:ARG:HB3	1:A:416:MET:HE1	1.95	0.48
1:A:112:PRO:HD2	1:A:116:GLY:O	2.14	0.48
1:A:365:VAL:HG23	1:A:430:GLY:O	2.13	0.48
1:A:332:MET:O	1:A:333:ILE:C	2.52	0.48
1:A:323:LEU:HG	1:A:327:ARG:HD3	1.96	0.47
1:A:415:ARG:NH1	1:A:442:HIS:CG	2.82	0.47
1:A:213:GLN:NE2	3:A:706:HOH:O	2.35	0.47
1:A:330:GLN:HG3	1:A:331:ARG:NH1	2.29	0.47
1:A:43:PRO:O	1:A:44:ASP:CB	2.41	0.47
1:A:295:LEU:HD22	1:A:295:LEU:O	2.15	0.47
1:A:186:VAL:HG13	1:A:189:LEU:HD22	1.97	0.47
1:A:396:ALA:O	1:A:424:PRO:CD	2.62	0.47
1:A:324:PHE:C	1:A:324:PHE:CD1	2.89	0.46
1:A:175:GLN:H	1:A:175:GLN:HG2	1.60	0.46
1:A:346:ILE:HG22	1:A:347:PHE:CD2	2.50	0.46
1:A:39:VAL:HB	1:A:49:GLN:HB2	1.97	0.46
1:A:394:ARG:H	1:A:429:ARG:HH22	1.64	0.46
1:A:389:LEU:HB3	1:A:432:PHE:CZ	2.51	0.46
1:A:250:MET:HG3	2:A:600:BLA:O1D	2.16	0.46
1:A:12:PHE:CG	1:A:28:ALA:HA	2.51	0.45
1:A:346:ILE:HD13	1:A:346:ILE:HA	1.80	0.45
1:A:446:TRP:CH2	3:A:832:HOH:O	2.69	0.45
1:A:458:MET:CB	3:A:705:HOH:O	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.59	0.44
1:A:323:LEU:HG	1:A:327:ARG:HH11	1.82	0.44
1:A:357:LEU:HD13	1:A:435:TRP:CE2	2.52	0.44
1:A:354:LEU:HG	1:A:359:ALA:O	2.16	0.44
1:A:458:MET:HB3	1:A:459:GLY:H	1.68	0.44
1:A:196:ARG:HG3	1:A:474:TRP:CZ2	2.52	0.44
1:A:334:GLU:C	1:A:336:ILE:N	2.70	0.43
1:A:330:GLN:C	1:A:332:MET:N	2.72	0.43
1:A:364:LEU:O	1:A:370:ILE:HA	2.18	0.43
1:A:443:THR:C	1:A:444:VAL:CG1	2.85	0.43
1:A:477:VAL:O	1:A:478:VAL:CB	2.61	0.43
1:A:409:GLU:O	1:A:412:HIS:HE1	2.01	0.43
1:A:347:PHE:O	1:A:349:THR:HG22	2.18	0.42
1:A:434:MET:HE2	1:A:436:PHE:HZ	1.84	0.42
1:A:461:THR:HG22	1:A:464:ASP:OD2	2.19	0.42
1:A:330:GLN:CB	1:A:333:ILE:HD12	2.50	0.42
1:A:343:ARG:O	1:A:346:ILE:HB	2.19	0.42
1:A:32:GLN:HE22	1:A:218:LEU:HA	1.84	0.42
1:A:63:VAL:O	1:A:66:VAL:HG13	2.20	0.42
1:A:460:ASP:HB2	1:A:469:ARG:HH21	1.83	0.42
1:A:460:ASP:HB3	1:A:469:ARG:HH21	1.85	0.42
1:A:60:LEU:CD1	1:A:99:GLY:HA2	2.49	0.42
1:A:228:LEU:HD11	1:A:242:MET:CE	2.50	0.42
1:A:228:LEU:CD1	1:A:242:MET:HE1	2.50	0.42
1:A:327:ARG:HA	1:A:330:GLN:OE1	2.20	0.42
1:A:332:MET:O	1:A:334:GLU:N	2.53	0.42
1:A:416:MET:HE2	1:A:416:MET:H	1.84	0.41
1:A:427:ASP:C	1:A:429:ARG:N	2.72	0.41
1:A:448:GLY:CA	1:A:472:ALA:HB2	2.50	0.41
1:A:338:ARG:NH1	1:A:338:ARG:CB	2.72	0.41
1:A:76:LEU:HD22	1:A:80:LEU:CD2	2.50	0.41
1:A:40:VAL:HG21	1:A:68:LEU:HD22	2.01	0.41
1:A:77:ILE:HD12	1:A:77:ILE:H	1.85	0.41
1:A:471:PHE:O	1:A:475:HIS:HD2	2.04	0.41
1:A:330:GLN:HA	1:A:333:ILE:HG13	2.01	0.41
1:A:496:ILE:O	1:A:497:GLY:C	2.59	0.41
1:A:60:LEU:HD13	1:A:99:GLY:HA2	2.02	0.41
1:A:201:ASP:HB3	2:A:600:BLA:HHB	2.02	0.41
1:A:381:ASP:CG	1:A:413:LEU:HD21	2.41	0.41
1:A:409:GLU:O	1:A:412:HIS:CE1	2.73	0.41
1:A:369:GLN:HE21	1:A:369:GLN:HB2	1.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:O	1:A:45:HIS:HA	2.20	0.40
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.90	0.40
1:A:481:THR:CG2	1:A:482:SER:N	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:THR:OG1	1:A:372:THR:OG1[10_665]	2.00	0.20

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	489/525 (93%)	437 (89%)	37 (8%)	15 (3%)	4 6

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	135	ALA
1	A	231	ARG
1	A	338	ARG
1	A	444	VAL
1	A	445	THR
1	A	446	TRP
1	A	458	MET
1	A	461	THR
1	A	478	VAL
1	A	325	VAL
1	A	333	ILE
1	A	335	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	ASP
1	A	429	ARG

5.3.2 Protein sidechains (i)

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	405/434 (93%)	343 (85%)	62 (15%)	2 4

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	LEU
1	A	40	VAL
1	A	58	LEU
1	A	60	LEU
1	A	71	ILE
1	A	75	LEU
1	A	76	LEU
1	A	80	LEU
1	A	97	ARG
1	A	108	LEU
1	A	114	GLU
1	A	117	LEU
1	A	121	LEU
1	A	138	LEU
1	A	142	ARG
1	A	143	THR
1	A	154	THR
1	A	156	LEU
1	A	157	LEU
1	A	167	VAL
1	A	169	VAL
1	A	174	GLU
1	A	175	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	186	VAL
1	A	189	LEU
1	A	209	LEU
1	A	231	ARG
1	A	232	LEU
1	A	266	THR
1	A	269	VAL
1	A	276	LYS
1	A	294	GLU
1	A	295	LEU
1	A	296	ARG
1	A	302	LEU
1	A	309	ARG
1	A	321	SER
1	A	334	GLU
1	A	337	THR
1	A	338	ARG
1	A	349	THR
1	A	355	GLN
1	A	365	VAL
1	A	368	ASP
1	A	369	GLN
1	A	371	ARG
1	A	373	ILE
1	A	389	LEU
1	A	402	SER
1	A	416	MET
1	A	421	VAL
1	A	429	ARG
1	A	434	MET
1	A	458	MET
1	A	461	THR
1	A	471	PHE
1	A	473	LYS
1	A	477	VAL
1	A	503	ILE
1	A	505	LEU
1	A	507	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	34	HIS
1	A	177	HIS
1	A	195	ASN
1	A	355	GLN
1	A	369	GLN
1	A	428	HIS
1	A	442	HIS
1	A	475	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	600	1	42,46,46	3.31	12 (28%)	53,67,67	2.62	22 (41%)

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	600	1	-	8/26/74/74	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	BLA	CHA-C4D	15.34	1.47	1.35
2	A	600	BLA	CHB-C1B	6.69	1.48	1.34
2	A	600	BLA	C3D-C2D	5.59	1.48	1.36
2	A	600	BLA	C3C-C2C	5.26	1.47	1.37
2	A	600	BLA	C3B-C2B	5.03	1.47	1.37
2	A	600	BLA	CHD-C4C	3.94	1.47	1.38
2	A	600	BLA	C2A-C3A	3.24	1.47	1.37
2	A	600	BLA	CHD-C1D	3.21	1.47	1.40
2	A	600	BLA	OC-C1C	2.92	1.29	1.23
2	A	600	BLA	C1B-C2B	2.74	1.50	1.45
2	A	600	BLA	OB-C4B	2.66	1.28	1.23
2	A	600	BLA	C4D-C3D	2.38	1.49	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	BLA	CMB-C2B-C1B	5.83	131.44	124.17
2	A	600	BLA	C3B-C2B-C1B	-5.74	101.09	108.03
2	A	600	BLA	C4C-NC-C1C	-5.15	104.12	110.67
2	A	600	BLA	CHB-C1B-NB	-4.70	114.60	130.40
2	A	600	BLA	CHA-C4D-ND	-4.68	122.34	128.83
2	A	600	BLA	C3B-C4B-NB	4.64	111.43	106.19
2	A	600	BLA	C2B-C1B-NB	4.46	113.52	106.99
2	A	600	BLA	C3C-C4C-NC	4.36	113.61	106.80
2	A	600	BLA	C1B-NB-C4B	-4.03	105.54	110.67
2	A	600	BLA	C2C-C1C-NC	3.66	116.23	106.45
2	A	600	BLA	C1D-C2D-C3D	-3.41	102.59	106.51
2	A	600	BLA	C1A-CHA-C4D	-3.19	125.00	128.81
2	A	600	BLA	CMC-C2C-C1C	3.18	128.87	121.39
2	A	600	BLA	OB-C4B-C3B	-3.07	122.51	129.46
2	A	600	BLA	C3D-C4D-ND	2.98	114.38	110.05
2	A	600	BLA	C4D-C3D-C2D	-2.88	103.59	106.78
2	A	600	BLA	OB-C4B-NB	-2.83	118.50	125.08
2	A	600	BLA	C4B-C3B-C2B	-2.62	104.57	107.92
2	A	600	BLA	CBA-CAA-C2A	-2.58	108.21	112.62
2	A	600	BLA	O2A-CGA-CBA	2.21	121.14	114.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	BLA	CHD-C4C-NC	-2.19	121.36	126.06
2	A	600	BLA	CAD-CBD-CGD	-2.02	109.25	113.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	BLA	C2A-C1A-CHA-C4D
2	A	600	BLA	NA-C4A-CHB-C1B
2	A	600	BLA	NB-C1B-CHB-C4A
2	A	600	BLA	C2B-C1B-CHB-C4A
2	A	600	BLA	C2B-C3B-CAB-CBB
2	A	600	BLA	CAD-CBD-CGD-O1D
2	A	600	BLA	CAD-CBD-CGD-O2D
2	A	600	BLA	CAA-CBA-CGA-O1A

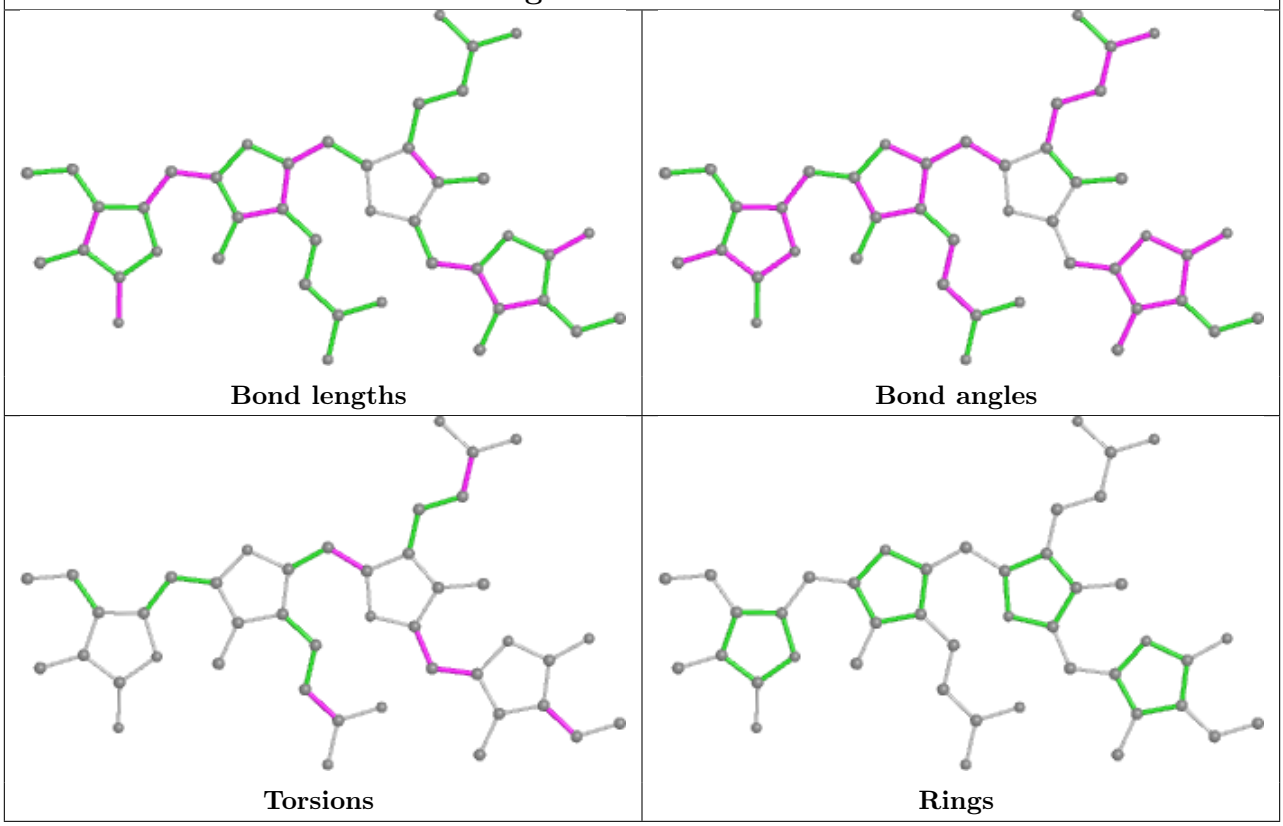
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	BLA	7	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 then 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 600



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	491/525 (93%)	-0.22	26 (5%) 26 20	37, 70, 147, 237	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	448	GLY	9.5
1	A	447	GLY	8.9
1	A	458	MET	6.3
1	A	340	GLY	4.3
1	A	446	TRP	4.0
1	A	339	GLU	3.8
1	A	8	GLY	3.7
1	A	505	LEU	3.5
1	A	338	ARG	3.4
1	A	341	ASP	3.4
1	A	445	THR	3.1
1	A	428	HIS	2.9
1	A	350	SER	2.8
1	A	507	PHE	2.8
1	A	331	ARG	2.7
1	A	327	ARG	2.5
1	A	326	GLN	2.5
1	A	333	ILE	2.3
1	A	459	GLY	2.2
1	A	9	SER	2.2
1	A	334	GLU	2.2
1	A	100	ASN	2.1
1	A	316	PHE	2.1
1	A	89	GLY	2.1
1	A	142	ARG	2.1
1	A	330	GLN	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)

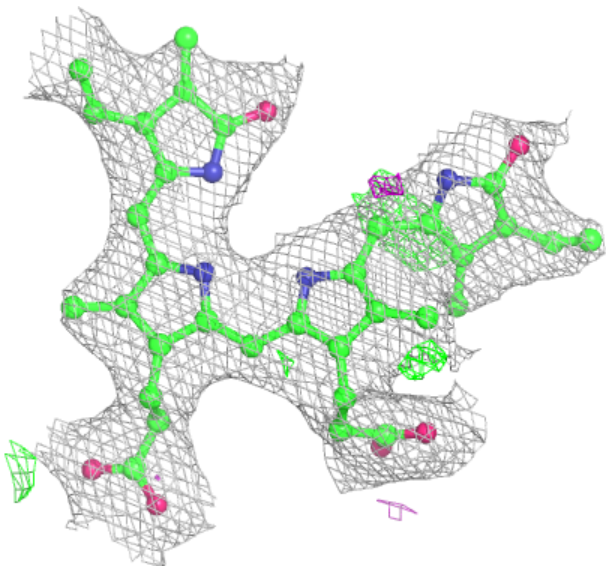
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

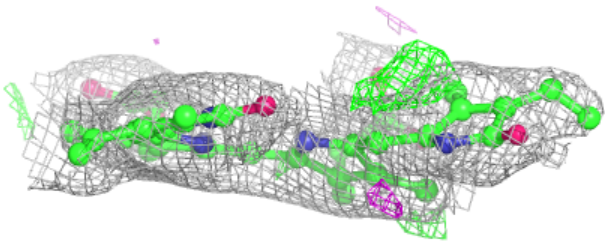
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BLA	A	600	43/43	0.98	0.21	28,44,66,76	0

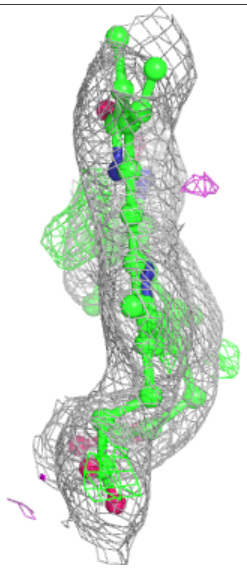
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BLA A 600:

$2mF_o$-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.