



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 AM UTC

PDB ID : 9MEB / pdb_00009meb
Title : Photoactivation in Bacteriophytochrome, 100 ps structure
Authors : Schmidt, M.; Malla, T.
Deposited on : 2024-12-06
Resolution : 2.30 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

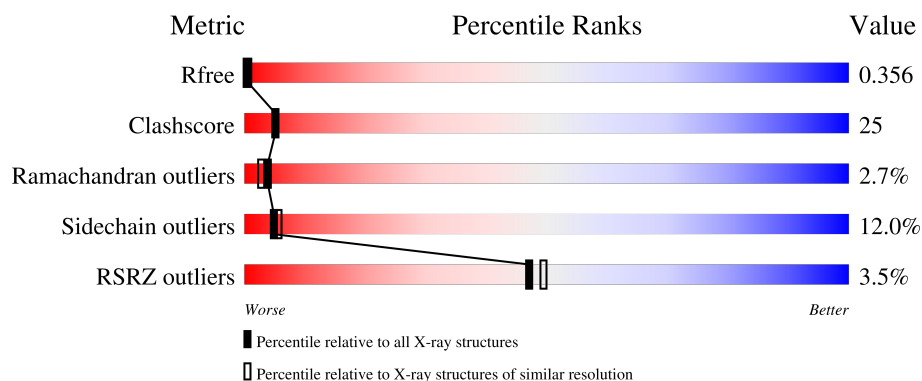
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	482	
1	B	482	

2 Entry composition [i](#)

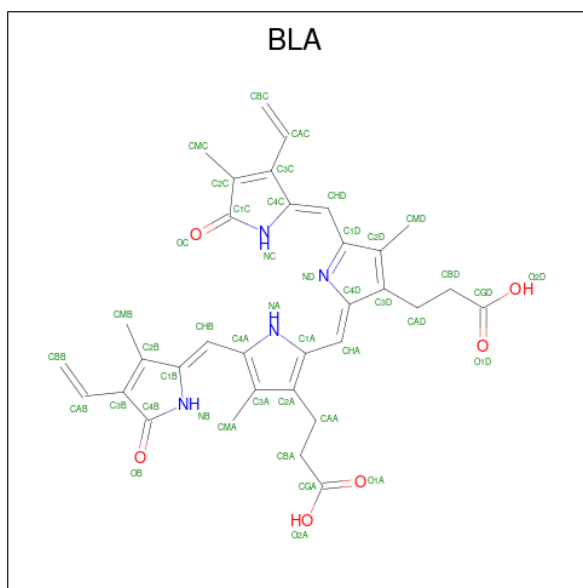
There are 4 unique types of molecules in this entry. The entry contains 7738 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Photoreceptor-histidine kinase BphP.

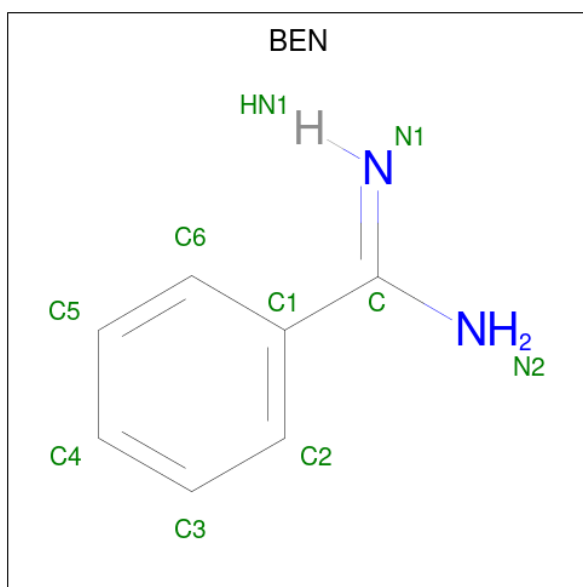
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	2	0
			3674	2327	669	667	11			
1	B	482	Total	C	N	O	S	0	0	0
			3659	2318	666	665	10			

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			86	66	8	12		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		

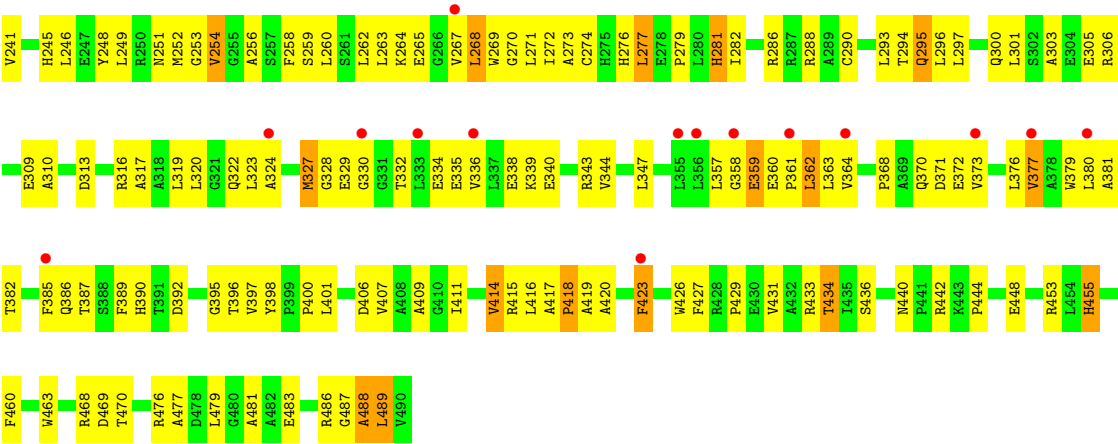
- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	0
			128	128		
4	B	139	Total	O	0	0
			139	139		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.69Å 83.40Å 86.87Å 90.00° 107.63° 90.00°	Depositor
Resolution (Å)	23.94 – 2.30 23.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.8 (23.94-2.30) 85.8 (23.94-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21_5207, PHENIX 1.21-4207	Depositor
R, R_{free}	0.271 , 0.356 0.271 , 0.356	Depositor DCC
R_{free} test set	2494 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 940.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7738	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, BEN

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	0.38	0/3759	0.63	1/5127 (0.0%)
1	B	0.38	0/3740	0.66	0/5101
All	All	0.38	0/7499	0.65	1/10228 (0.0%)

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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	ARG	Sidechain
1	B	489	LEU	Peptide

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	3674	0	3713	173	0
1	B	3659	0	3698	202	1
2	A	86	0	62	21	0
2	B	43	0	31	8	0
3	A	9	0	7	0	0
4	A	128	0	0	15	0
4	B	139	0	0	15	0
All	All	7738	0	7511	371	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 25.

All (371) 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:177:ARG:NH2	4:B:601:HOH:O	2.11	0.83
1:A:155:PHE:HE1	1:A:282:ILE:HD11	1.43	0.83
1:A:139:GLN:NE2	1:A:172:LEU:O	2.13	0.80
1:A:166:ASP:OD1	1:A:166:ASP:N	2.12	0.80
1:B:159:MET:HG3	1:B:273:ALA:HB3	1.68	0.75
1:A:159:MET:HE1	2:A:501[A]:BLA:HBB1	1.67	0.74
1:B:324:ALA:HA	1:B:327:MET:HG3	1.67	0.74
1:B:74:GLN:NE2	4:B:604:HOH:O	2.20	0.73
1:B:193:ILE:O	1:B:198:ARG:NH1	2.22	0.73
1:A:244:VAL:HG13	1:A:456:PRO:HD3	1.70	0.73
1:A:470:THR:O	4:A:601:HOH:O	2.05	0.72
1:A:155:PHE:CE1	1:A:282:ILE:HD11	2.24	0.71
1:B:316:ARG:NH1	1:B:347:LEU:O	2.24	0.71
1:B:309:GLU:HB3	1:B:476:ARG:HE	1.56	0.70
1:A:308:ALA:O	4:A:602:HOH:O	2.09	0.70
1:B:317:ALA:HA	1:B:320:LEU:HB2	1.74	0.70
1:A:159:MET:HG2	1:A:273:ALA:HB3	1.73	0.69
1:B:288:ARG:NH1	4:B:602:HOH:O	2.11	0.69
1:A:288:ARG:HB3	1:B:126:ARG:NH1	2.06	0.69
1:B:361:PRO:HD2	1:B:370:GLN:HE21	1.58	0.69
1:B:24:ILE:HG13	1:B:217:VAL:HB	1.75	0.68
1:B:416:LEU:HD22	1:B:489:LEU:HD22	1.75	0.68
1:B:319:LEU:O	1:B:323:LEU:N	2.25	0.68
1:B:159:MET:HE1	1:B:183:PHE:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:NE2	4:A:610:HOH:O	2.26	0.68
1:A:59:LEU:HD21	1:A:221:PRO:HD3	1.76	0.68
1:A:416:LEU:HD23	1:A:486:ARG:HG2	1.76	0.67
1:B:433:ARG:NH2	1:B:470:THR:OG1	2.23	0.67
1:B:204:ASN:O	1:B:207:ARG:NH2	2.27	0.67
1:A:420:ALA:O	4:A:603:HOH:O	2.13	0.67
1:A:288:ARG:HB3	1:B:126:ARG:HH12	1.61	0.66
1:B:13:CYS:O	1:B:194:PRO:HB3	1.95	0.66
1:A:134:GLY:O	1:A:137:GLY:N	2.28	0.66
1:A:177:ARG:HG3	1:A:177:ARG:HH11	1.60	0.65
1:B:129:VAL:HG23	1:B:130:SER:H	1.62	0.65
1:A:123:GLU:OE2	1:B:288:ARG:NH2	2.26	0.65
1:A:252:MET:HE2	2:A:501[A]:BLA:HAB	1.79	0.65
1:B:38:ARG:NH1	4:B:609:HOH:O	2.29	0.64
2:A:501[B]:BLA:HMA2	2:A:501[B]:BLA:HMB3	1.81	0.63
1:A:232:ASP:OD2	4:A:604:HOH:O	2.15	0.63
1:A:47:ALA:HB3	1:A:55:PRO:HG3	1.81	0.63
1:B:252:MET:HB2	1:B:254:VAL:CG1	2.29	0.63
1:B:34:ARG:HH12	1:B:39:LEU:HD12	1.64	0.62
1:A:34:ARG:HB2	1:A:103:LEU:HD22	1.82	0.62
1:A:348:THR:O	1:A:428:ARG:NH2	2.32	0.62
1:B:252:MET:HB2	1:B:254:VAL:HG12	1.80	0.62
1:A:264:LYS:O	4:A:605:HOH:O	2.16	0.61
1:A:122:LEU:O	1:A:126:ARG:HG3	1.99	0.61
1:A:303:ALA:O	1:B:306:ARG:NH1	2.30	0.61
1:A:251:ASN:HB3	1:A:458:GLY:HA2	1.82	0.60
1:B:317:ALA:HA	1:B:320:LEU:HD12	1.83	0.60
1:A:252:MET:HE2	2:A:501[A]:BLA:CBB	2.32	0.60
1:A:252:MET:HE2	2:A:501[A]:BLA:HBB2	1.82	0.60
1:B:380:LEU:HD11	1:B:389:PHE:CE2	2.36	0.60
1:B:290:CYS:HA	1:B:293:LEU:HD12	1.82	0.60
1:A:45:ALA:HB3	1:A:217:VAL:HG13	1.84	0.59
1:A:252:MET:HE2	2:A:501[A]:BLA:CAB	2.33	0.59
1:A:452:GLN:HG3	1:A:453:ARG:HG3	1.83	0.59
1:B:164:ASP:O	4:B:603:HOH:O	2.16	0.59
1:B:252:MET:SD	2:B:501:BLA:CAB	2.91	0.59
1:A:412:LEU:HD12	1:A:474:TRP:CE3	2.37	0.59
1:B:376:LEU:HD22	1:B:401:LEU:HD11	1.85	0.59
1:A:332:THR:N	1:A:335:GLU:OE1	2.33	0.59
1:B:201:TYR:OH	2:B:501:BLA:O1D	2.17	0.59
1:A:17:PRO:HB2	1:A:20:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:HD2	1:B:259:SER:OG	2.04	0.58
1:B:145:ALA:O	1:B:148:THR:OG1	2.16	0.58
1:A:254:VAL:HG21	1:A:275:HIS:HB3	1.85	0.58
1:B:162:ARG:NH2	4:B:613:HOH:O	2.37	0.58
1:B:479:LEU:O	1:B:483:GLU:HG3	2.04	0.58
1:B:184:LEU:HD12	1:B:185:GLY:H	1.68	0.58
1:B:390:HIS:CD2	1:B:479:LEU:HD21	2.39	0.58
1:A:150:ARG:NH1	4:A:617:HOH:O	2.38	0.57
1:B:416:LEU:HG	1:B:423:PHE:HA	1.85	0.57
1:A:119:GLU:HB2	1:B:118:GLU:HG2	1.85	0.57
1:A:316:ARG:HA	1:A:319:LEU:HD12	1.86	0.57
1:B:56:GLU:HG3	1:B:220:LEU:HD23	1.85	0.57
1:B:53:ARG:HE	1:B:58:LEU:HD21	1.70	0.57
1:A:62:PRO:O	1:A:66:VAL:HG22	2.05	0.56
1:A:19:HIS:H	1:A:19:HIS:CD2	2.21	0.56
1:B:180:MET:HE1	1:B:277:LEU:HD21	1.88	0.56
1:B:71:VAL:HG22	1:B:86:VAL:HG11	1.87	0.56
1:B:267:VAL:O	1:B:269:TRP:N	2.38	0.56
1:B:406:ASP:O	1:B:429:PRO:HB3	2.05	0.56
1:B:126:ARG:NH2	4:B:615:HOH:O	2.38	0.56
1:B:160:VAL:HG22	1:B:272:ILE:HG12	1.87	0.55
1:A:475:LYS:N	1:A:478:ASP:OD2	2.33	0.55
1:B:327:MET:SD	4:B:724:HOH:O	2.58	0.55
1:B:448:GLU:HG3	1:B:453:ARG:HB3	1.88	0.55
1:A:11:SER:HB2	1:A:13[A]:CYS:H	1.72	0.55
1:A:11:SER:HB2	1:A:13[B]:CYS:H	1.72	0.55
1:B:239:ARG:NH2	1:B:241:VAL:HG12	2.21	0.55
1:B:248:TYR:O	1:B:251:ASN:HB2	2.06	0.55
1:B:14:ASP:OD1	1:B:195:VAL:HG12	2.06	0.54
1:B:157:ARG:HH11	1:B:182:GLY:HA2	1.72	0.54
1:B:195:VAL:HG13	1:B:196:GLN:H	1.73	0.54
1:A:159:MET:HB2	1:A:171:VAL:HG13	1.90	0.54
1:B:47:ALA:HB3	1:B:55:PRO:HG3	1.89	0.54
1:B:272:ILE:HD12	1:B:294:THR:HG22	1.88	0.54
1:B:157:ARG:NH1	1:B:181:ASP:O	2.40	0.54
1:B:370:GLN:HA	1:B:373:VAL:HG12	1.90	0.54
1:A:195:VAL:O	1:A:198:ARG:N	2.41	0.53
1:B:56:GLU:HG3	1:B:220:LEU:CD2	2.37	0.53
1:A:260:LEU:HB3	1:A:294:THR:HG21	1.90	0.53
1:B:53:ARG:NH2	1:B:66:VAL:O	2.41	0.53
1:A:157:ARG:HD2	1:A:174:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TYR:CE2	1:A:400:PRO:HG2	2.44	0.53
1:A:38:ARG:HB2	1:A:63:VAL:HG12	1.90	0.53
1:A:249:LEU:CD2	2:A:501[B]:BLA:HBB1	2.38	0.53
1:A:261:SER:HA	1:A:271:LEU:HD23	1.91	0.53
1:A:377:VAL:O	1:A:381:ALA:N	2.41	0.52
1:B:236:SER:HB3	1:B:239:ARG:HB2	1.92	0.52
2:B:501:BLA:HHA	2:B:501:BLA:HBD1	1.91	0.52
1:A:323:LEU:HD11	1:A:343:ARG:HB2	1.90	0.52
1:B:376:LEU:O	1:B:380:LEU:HB2	2.10	0.52
1:A:14:ASP:HA	1:A:196:GLN:OE1	2.10	0.52
1:B:273:ALA:O	1:B:274:CYS:SG	2.66	0.51
1:B:252:MET:HE3	1:B:460:PHE:CD2	2.46	0.51
1:A:18:ILE:HD11	1:A:200:LEU:HD23	1.92	0.51
1:B:330:GLY:C	1:B:332:THR:H	2.18	0.51
1:A:155:PHE:CE2	1:A:276:HIS:HB2	2.45	0.51
1:B:316:ARG:HG3	1:B:477:ALA:HB1	1.93	0.51
1:A:18:ILE:HD12	2:A:501[B]:BLA:O2D	2.11	0.51
1:A:340:GLU:OE2	1:A:343:ARG:NH1	2.42	0.51
1:A:261:SER:HB3	1:A:268:LEU:HD11	1.93	0.51
1:B:487:GLY:C	1:B:489:LEU:H	2.19	0.51
1:A:399:PRO:HA	1:A:402:ALA:HB2	1.92	0.50
1:A:428:ARG:HG3	1:A:474:TRP:CH2	2.47	0.50
1:B:260:LEU:HB2	1:B:294:THR:HG21	1.94	0.50
1:B:83:SER:HB2	1:B:96:LEU:HD23	1.93	0.50
1:B:313:ASP:OD1	1:B:477:ALA:HA	2.11	0.50
1:B:414:VAL:HG23	1:B:426:TRP:HZ3	1.76	0.50
1:B:415:ARG:O	1:B:486:ARG:HD2	2.11	0.50
1:A:441:PRO:HD2	1:A:463:TRP:CE3	2.46	0.50
1:A:263:LEU:HD23	1:A:268:LEU:HD13	1.92	0.49
1:A:95:ALA:HB1	1:A:106:LEU:HD11	1.94	0.49
2:A:501[B]:BLA:HMB3	2:A:501[B]:BLA:CMA	2.42	0.49
1:A:420:ALA:HB1	1:A:422:ARG:HG2	1.93	0.49
1:B:124:VAL:HG12	1:B:127:ARG:HD3	1.95	0.49
1:A:112:GLU:HB2	1:A:283:SER:CB	2.42	0.49
1:A:267:VAL:N	4:A:605:HOH:O	2.45	0.49
1:B:386:GLN:O	1:B:386:GLN:HG3	2.12	0.49
1:B:322:GLN:HG2	1:B:343:ARG:HH21	1.78	0.49
1:A:327:MET:C	1:A:329:GLU:H	2.20	0.49
1:B:195:VAL:HG13	1:B:196:GLN:N	2.28	0.49
1:B:381:ALA:HA	1:B:415:ARG:HH21	1.77	0.49
1:A:33:PHE:O	1:A:103:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:O	1:A:340:GLU:HB2	2.13	0.49
1:B:53:ARG:NE	1:B:58:LEU:HD21	2.27	0.49
1:B:265:GLU:N	4:B:623:HOH:O	2.46	0.49
1:B:129:VAL:HG13	1:B:296:LEU:HD21	1.94	0.48
1:B:246:LEU:O	1:B:249:LEU:HB2	2.13	0.48
1:B:389:PHE:CE2	1:B:411:ILE:HD11	2.48	0.48
1:B:392:ASP:OD1	1:B:392:ASP:N	2.32	0.48
1:B:110:PRO:HG2	1:B:281:HIS:CE1	2.48	0.48
1:A:245:HIS:NE2	2:A:501[A]:BLA:HBA1	2.28	0.48
1:A:336:VAL:O	1:A:340:GLU:N	2.46	0.48
1:A:360:GLU:H	1:A:360:GLU:CD	2.20	0.48
1:A:363:LEU:HB3	1:A:367:THR:HG21	1.95	0.48
1:B:227:LEU:HB3	1:B:229:ARG:HG2	1.93	0.48
1:B:77:PRO:O	1:B:81:ARG:HG2	2.13	0.48
1:A:66:VAL:HG23	1:A:67:LEU:H	1.77	0.48
1:B:120:THR:O	1:B:124:VAL:HG22	2.14	0.48
1:A:333:LEU:O	1:A:337:LEU:HD13	2.13	0.48
1:A:124:VAL:HG23	1:A:293:LEU:HD21	1.94	0.48
1:A:244:VAL:O	1:A:248:TYR:N	2.46	0.48
1:A:417:ALA:HB3	1:A:420:ALA:HB3	1.95	0.48
1:A:418:PRO:C	1:A:420:ALA:H	2.22	0.48
1:A:162:ARG:HA	1:A:270:GLY:HA3	1.95	0.48
1:A:303:ALA:HB2	1:B:303:ALA:HB2	1.96	0.48
1:B:409:ALA:HB1	1:B:469:ASP:O	2.14	0.47
1:A:45:ALA:O	4:A:606:HOH:O	2.20	0.47
1:B:64:GLY:HA2	1:B:72:LEU:HD11	1.96	0.47
1:B:68:PRO:O	1:B:70:GLU:N	2.48	0.47
1:B:152:LEU:HD23	1:B:293:LEU:HD11	1.95	0.47
1:B:205:PRO:O	1:B:206:LEU:HD23	2.14	0.47
1:A:268:LEU:O	4:A:607:HOH:O	2.20	0.47
1:B:200:LEU:O	1:B:204:ASN:N	2.39	0.47
1:A:94:ARG:N	1:A:109:GLU:O	2.47	0.47
1:B:253:GLY:HA2	4:B:650:HOH:O	2.14	0.47
1:A:196:GLN:HG2	1:A:197:ALA:N	2.29	0.47
1:A:207:ARG:HH22	1:A:261:SER:HG	1.59	0.47
1:B:163:PHE:HD1	1:B:270:GLY:HA2	1.80	0.47
1:A:117:MET:O	1:A:120:THR:HB	2.15	0.47
1:A:450:GLY:O	1:A:451:HIS:C	2.57	0.47
1:B:282:ILE:CG2	1:B:286:ARG:HB3	2.44	0.47
1:B:363:LEU:HD21	1:B:373:VAL:HG11	1.96	0.47
1:B:431:VAL:HG22	4:B:723:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HD3	1:A:215:ARG:HA	1.74	0.47
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.73	0.47
1:B:141:LEU:HD23	1:B:301:LEU:HD23	1.96	0.47
1:B:155:PHE:HA	1:B:276:HIS:ND1	2.30	0.47
1:A:222:PRO:HG2	1:A:223:VAL:HG22	1.97	0.47
1:A:118:GLU:OE2	1:A:118:GLU:N	2.48	0.47
1:A:142:LEU:HD21	1:A:301:LEU:HD11	1.97	0.47
1:B:377:VAL:HG13	1:B:423:PHE:CZ	2.50	0.47
1:A:186:MET:HE2	1:A:186:MET:HB3	1.84	0.46
1:B:239:ARG:HH22	2:B:501:BLA:CGD	2.28	0.46
1:B:340:GLU:HB3	1:B:343:ARG:CD	2.45	0.46
1:B:377:VAL:HG13	1:B:423:PHE:HZ	1.80	0.46
1:A:59:LEU:CD2	1:A:221:PRO:HD3	2.43	0.46
1:B:335:GLU:O	1:B:338:GLU:N	2.40	0.46
1:A:199:ALA:O	1:A:202:THR:HB	2.15	0.46
1:B:126:ARG:HA	1:B:129:VAL:CG2	2.46	0.46
1:A:174:GLU:OE1	1:A:176:LYS:HE3	2.16	0.46
1:A:256:ALA:HB2	1:A:279:PRO:HA	1.96	0.46
1:B:145:ALA:CB	1:B:297:LEU:HD22	2.46	0.46
1:B:196:GLN:HG2	1:B:197:ALA:N	2.30	0.46
1:A:134:GLY:C	1:A:136:LYS:N	2.73	0.46
1:A:155:PHE:CD2	1:A:276:HIS:HB2	2.50	0.46
1:B:83:SER:OG	1:B:94:ARG:HD2	2.16	0.46
1:B:195:VAL:O	1:B:198:ARG:N	2.42	0.46
1:B:65:ARG:H	1:B:65:ARG:HG2	1.29	0.46
1:B:199:ALA:O	1:B:202:THR:HB	2.15	0.46
1:A:96:LEU:O	1:A:106:LEU:HD12	2.16	0.46
1:A:334:GLU:OE1	1:A:334:GLU:N	2.33	0.46
1:B:282:ILE:HG23	1:B:286:ARG:HD2	1.98	0.46
1:A:412:LEU:HB2	1:A:474:TRP:CE2	2.50	0.45
1:B:9:ASP:O	1:B:10:LEU:HD22	2.16	0.45
1:B:24:ILE:CG1	1:B:217:VAL:HB	2.46	0.45
1:A:34:ARG:HE	1:A:34:ARG:HB3	1.45	0.45
1:A:246:LEU:O	1:A:250:ARG:HD2	2.16	0.45
4:A:712:HOH:O	1:B:310:ALA:HB2	2.16	0.45
1:B:17:PRO:HB3	1:B:20:LEU:HD12	1.98	0.45
1:A:440:ASN:ND2	1:A:442:ARG:HB2	2.32	0.45
1:B:347:LEU:HB3	1:B:481:ALA:HB1	1.97	0.45
1:A:126:ARG:HD2	1:B:288:ARG:HH21	1.82	0.45
1:A:342:GLU:HB2	4:A:634:HOH:O	2.16	0.45
1:A:22:GLY:HA3	4:A:670:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:HB1	1:A:201:TYR:CE2	2.52	0.45
1:A:245:HIS:HE1	2:A:501[B]:BLA:CMB	2.30	0.45
1:B:245:HIS:HE1	2:B:501:BLA:HB	1.64	0.45
1:B:267:VAL:O	1:B:268:LEU:C	2.59	0.45
1:B:34:ARG:NH1	1:B:39:LEU:HD12	2.30	0.45
1:B:62:PRO:HG2	1:B:65:ARG:CG	2.47	0.45
1:A:439:GLY:O	1:A:441:PRO:HD3	2.17	0.45
1:B:62:PRO:O	1:B:66:VAL:HG12	2.17	0.45
1:A:183:PHE:O	1:A:186:MET:HG3	2.17	0.44
1:A:67:LEU:HD13	1:A:71:VAL:HG11	1.97	0.44
1:A:78:LEU:HD21	1:A:97:LEU:HD13	1.99	0.44
1:A:380:LEU:HD11	1:A:389:PHE:CD2	2.52	0.44
1:A:468:ARG:HE	1:A:468:ARG:HB3	1.40	0.44
1:B:455:HIS:N	1:B:455:HIS:CD2	2.85	0.44
1:A:34:ARG:HG2	1:A:35:GLY:N	2.32	0.44
1:A:219:LEU:O	1:A:220:LEU:HD23	2.17	0.44
1:B:124:VAL:HA	1:B:127:ARG:HG3	1.99	0.44
1:B:411:ILE:HG22	1:B:427:PHE:CD1	2.52	0.44
2:A:501[B]:BLA:HMB3	2:A:501[B]:BLA:C3A	2.47	0.44
1:B:417:ALA:HB1	1:B:418:PRO:HD2	1.99	0.44
1:B:433:ARG:NH2	1:B:470:THR:O	2.51	0.44
1:A:156:ASP:OD2	1:A:277:LEU:N	2.36	0.44
1:A:285:GLU:OE2	4:A:608:HOH:O	2.21	0.44
1:B:262:LEU:HB2	1:B:270:GLY:O	2.17	0.44
1:A:138:THR:HA	1:A:141:LEU:HD12	1.99	0.44
1:B:488:ALA:HB1	4:B:724:HOH:O	2.17	0.44
1:B:48:GLN:HG3	1:B:53:ARG:C	2.43	0.44
1:B:224:VAL:HB	1:B:227:LEU:HD12	2.00	0.44
1:A:294:THR:OG1	1:A:295:GLN:N	2.51	0.44
1:B:249:LEU:HA	1:B:249:LEU:HD23	1.63	0.44
1:A:13[B]:CYS:HA	2:A:501[B]:BLA:HBC2	1.60	0.43
1:B:249:LEU:O	1:B:254:VAL:HG13	2.18	0.43
1:B:444:PRO:HG3	4:B:697:HOH:O	2.18	0.43
1:B:68:PRO:O	1:B:69:ALA:C	2.60	0.43
1:B:76:GLU:HG3	1:B:77:PRO:HD3	2.00	0.43
1:B:264:LYS:HB2	1:B:265:GLU:H	1.67	0.43
1:A:31:LEU:HD22	1:A:67:LEU:HD21	2.01	0.43
1:A:248:TYR:HE2	2:A:501[B]:BLA:C3B	2.31	0.43
1:B:232:ASP:OD1	1:B:234:SER:OG	2.25	0.43
1:B:362:LEU:HD22	1:B:362:LEU:HA	1.70	0.43
1:B:379:TRP:HZ2	1:B:397:VAL:HG12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:PHE:HE1	1:B:415:ARG:HG2	1.84	0.43
1:A:162:ARG:HG2	1:A:163:PHE:N	2.32	0.43
1:B:16:GLU:O	1:B:18:ILE:N	2.51	0.43
1:A:147:ASP:OD1	1:A:175:SER:HB2	2.18	0.43
1:A:205:PRO:HA	1:A:261:SER:OG	2.18	0.43
1:A:245:HIS:CE1	2:A:501[B]:BLA:HMB2	2.53	0.43
1:B:117:MET:O	1:B:120:THR:HB	2.19	0.43
1:B:323:LEU:HD11	1:B:344:VAL:HG22	2.00	0.43
1:A:153:THR:HB	1:A:155:PHE:HD1	1.84	0.43
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.91	0.43
1:A:339:LYS:HA	1:A:339:LYS:HD2	1.90	0.43
1:B:48:GLN:HG3	1:B:53:ARG:O	2.18	0.43
1:B:109:GLU:HB3	1:B:238:LEU:HD21	2.01	0.43
1:B:191:THR:HB	2:B:501:BLA:HBC1	2.01	0.43
1:B:398:TYR:CE2	1:B:400:PRO:HB2	2.53	0.43
1:A:101:ASP:CG	1:A:229:ARG:HH22	2.27	0.43
1:A:356:LEU:O	1:A:422:ARG:HA	2.18	0.43
1:A:201:TYR:CE2	2:A:501[B]:BLA:HAA1	2.54	0.43
1:A:102:GLY:O	1:A:103:LEU:HD23	2.18	0.43
1:A:245:HIS:HE1	2:A:501[B]:BLA:HMB2	1.84	0.43
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.70	0.43
1:B:249:LEU:HD22	1:B:254:VAL:CG2	2.48	0.43
1:A:323:LEU:CD1	1:A:343:ARG:HB2	2.49	0.42
1:A:353:VAL:HG12	1:A:364:VAL:HG12	2.01	0.42
1:B:47:ALA:O	1:B:51:LEU:HB2	2.19	0.42
1:B:192:ASP:HA	2:B:501:BLA:C1C	2.49	0.42
1:B:359:GLU:HG2	1:B:360:GLU:HG2	2.00	0.42
1:B:126:ARG:HA	1:B:129:VAL:HG22	2.01	0.42
1:B:129:VAL:HG23	1:B:130:SER:N	2.31	0.42
1:A:119:GLU:CB	1:B:118:GLU:HG2	2.48	0.42
1:A:139:GLN:O	1:A:143:GLN:N	2.50	0.42
1:A:157:ARG:HH12	1:A:180:MET:CE	2.33	0.42
1:A:354:ALA:O	1:A:355:LEU:HD23	2.19	0.42
1:B:169:GLY:O	1:B:188:PHE:N	2.47	0.42
1:B:340:GLU:HB3	1:B:343:ARG:HD3	2.01	0.42
1:B:395:GLY:O	1:B:397:VAL:N	2.52	0.42
1:B:209:ILE:N	1:B:209:ILE:HD12	2.34	0.42
1:B:163:PHE:HE2	4:B:684:HOH:O	2.02	0.42
1:B:166:ASP:OD2	1:B:168:HIS:HB3	2.20	0.42
1:B:249:LEU:HD22	1:B:254:VAL:HG22	2.01	0.42
1:A:282:ILE:O	1:A:287:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:HA	1:B:220:LEU:O	2.20	0.42
1:B:128:LEU:HB3	1:B:296:LEU:HD23	2.02	0.42
1:B:184:LEU:HD12	1:B:185:GLY:N	2.33	0.42
1:B:206:LEU:HD22	1:B:260:LEU:HD23	2.00	0.42
1:B:216:PRO:HG3	1:B:240:SER:OG	2.19	0.42
1:B:385:PHE:CE1	1:B:415:ARG:HG2	2.54	0.42
1:A:418:PRO:HB2	1:A:419:ALA:H	1.60	0.42
1:B:40:LEU:HD21	1:B:43:VAL:HB	2.01	0.42
1:A:249:LEU:HD22	2:A:501[B]:BLA:HBB1	2.00	0.42
1:B:172:LEU:HA	1:B:172:LEU:HD23	1.80	0.42
1:B:121:ALA:HA	1:B:124:VAL:HG23	2.01	0.42
1:A:268:LEU:HD13	1:A:268:LEU:HA	1.78	0.41
1:A:398:TYR:CE1	1:A:400:PRO:HB2	2.54	0.41
2:A:501[B]:BLA:HMD1	2:A:501[B]:BLA:HHD	1.89	0.41
1:B:30:LEU:HD22	1:B:219:LEU:HD21	2.01	0.41
1:A:83:SER:OG	1:A:94:ARG:HD2	2.21	0.41
1:A:258:PHE:O	1:A:274:CYS:HB2	2.20	0.41
1:A:398:TYR:CZ	1:A:400:PRO:HG2	2.55	0.41
1:B:136:LYS:HD2	1:B:136:LYS:HA	1.78	0.41
1:B:376:LEU:HB3	1:B:398:TYR:CE2	2.55	0.41
1:B:377:VAL:O	1:B:380:LEU:HB3	2.20	0.41
1:A:32:ALA:O	1:A:40:LEU:HD12	2.21	0.41
1:A:117:MET:SD	1:A:117:MET:C	3.03	0.41
1:A:431:VAL:N	4:A:601:HOH:O	2.49	0.41
1:B:201:TYR:OH	2:B:501:BLA:HBA2	2.20	0.41
1:B:252:MET:HE3	1:B:460:PHE:CE2	2.56	0.41
1:A:452:GLN:CG	1:A:453:ARG:HG3	2.51	0.41
1:B:330:GLY:C	1:B:332:THR:N	2.79	0.41
1:B:368:PRO:HG3	1:B:407:VAL:HG23	2.02	0.41
1:B:194:PRO:HB2	1:B:196:GLN:OE1	2.20	0.41
1:B:256:ALA:HB2	1:B:279:PRO:HA	2.02	0.41
1:B:258:PHE:CZ	1:B:260:LEU:HD21	2.56	0.41
1:B:282:ILE:HG23	1:B:286:ARG:HB3	2.03	0.41
1:B:434:THR:O	1:B:434:THR:HG22	2.21	0.41
1:A:315[A]:HIS:CE1	1:A:316:ARG:HH11	2.39	0.41
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.77	0.41
1:A:100:SER:O	1:A:101:ASP:C	2.63	0.41
1:A:115:PRO:C	1:A:117:MET:H	2.29	0.41
1:A:129:VAL:HG13	1:B:295:GLN:HE21	1.86	0.41
1:B:156:ASP:O	1:B:176:LYS:HA	2.20	0.41
1:B:389:PHE:HE2	1:B:411:ILE:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:GLY:O	1:B:489:LEU:N	2.54	0.41
1:A:252:MET:CE	2:A:501[A]:BLA:HAB	2.49	0.41
1:B:476:ARG:NH2	4:B:618:HOH:O	2.43	0.41
1:A:193:ILE:HG23	2:A:501[B]:BLA:C1A	2.51	0.40
1:A:437:TRP:CG	1:A:441:PRO:HG3	2.55	0.40
1:B:139:GLN:O	1:B:140:ALA:C	2.64	0.40
1:B:382:THR:HG22	1:B:382:THR:O	2.21	0.40
1:A:48:GLN:HG3	1:A:53:ARG:N	2.37	0.40
1:A:144:THR:O	1:A:148:THR:HG23	2.21	0.40
1:A:389:PHE:CE2	1:A:411:ILE:HD11	2.56	0.40
1:A:139:GLN:HE22	1:A:172:LEU:C	2.23	0.40
1:B:442:ARG:NH1	1:B:463:TRP:HH2	2.19	0.40
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.85	0.40
1:A:145:ALA:CB	1:A:297:LEU:HD22	2.52	0.40
1:A:159:MET:HB2	1:A:171:VAL:CG1	2.50	0.40
1:A:229:ARG:NH1	1:A:230:PRO:O	2.54	0.40
1:B:67:LEU:HD11	1:B:106:LEU:HD22	2.04	0.40
1:B:141:LEU:HD21	1:B:300:GLN:HB3	2.04	0.40
1:B:363:LEU:HD11	1:B:370:GLN:N	2.37	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:B:225:PRO:O	1:B:468:ARG:NH2[2_444]	2.11	0.09

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	482/482 (100%)	416 (86%)	57 (12%)	9 (2%)	6 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	480/482 (100%)	389 (81%)	73 (15%)	18 (4%)	2	1
All	All	962/964 (100%)	805 (84%)	130 (14%)	27 (3%)	4	2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	PRO
1	B	69	ALA
1	B	115	PRO
1	B	329	GLU
1	B	396	THR
1	B	418	PRO
1	A	329	GLU
1	B	268	LEU
1	B	327	MET
1	B	49	ALA
1	B	132	LEU
1	B	359	GLU
1	B	420	ALA
1	A	13[A]	CYS
1	A	13[B]	CYS
1	A	488	ALA
1	B	419	ALA
1	B	488	ALA
1	A	14	ASP
1	A	135	VAL
1	A	451	HIS
1	B	328	GLY
1	B	358	GLY
1	B	194	PRO
1	B	222	PRO
1	B	17	PRO
1	A	361	PRO

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	377/375 (100%)	327 (87%)	50 (13%)	4	4
1	B	374/375 (100%)	333 (89%)	41 (11%)	6	7
All	All	751/750 (100%)	660 (88%)	91 (12%)	5	5

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	ASP
1	A	24	ILE
1	A	34	ARG
1	A	42	VAL
1	A	44	SER
1	A	51	LEU
1	A	63	VAL
1	A	86	VAL
1	A	119	GLU
1	A	122	LEU
1	A	132	LEU
1	A	135	VAL
1	A	136	LYS
1	A	144	THR
1	A	149	VAL
1	A	166	ASP
1	A	175	SER
1	A	181	ASP
1	A	193	ILE
1	A	195	VAL
1	A	202	THR
1	A	220	LEU
1	A	223	VAL
1	A	261	SER
1	A	268	LEU
1	A	275	HIS
1	A	292	VAL
1	A	301	LEU
1	A	311	SER
1	A	315[A]	HIS
1	A	315[B]	HIS
1	A	325	THR
1	A	332	THR
1	A	335	GLU

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Mol	Chain	Res	Type
1	A	341	SER
1	A	356	LEU
1	A	362	LEU
1	A	363	LEU
1	A	364	VAL
1	A	382	THR
1	A	386	GLN
1	A	391	THR
1	A	397	VAL
1	A	400	PRO
1	A	459	SER
1	A	463	TRP
1	A	472	LEU
1	A	486	ARG
1	A	490	VAL
1	B	41	GLU
1	B	51	LEU
1	B	56	GLU
1	B	65	ARG
1	B	66	VAL
1	B	74	GLN
1	B	78	LEU
1	B	83	SER
1	B	86	VAL
1	B	120	THR
1	B	122	LEU
1	B	124	VAL
1	B	126	ARG
1	B	132	LEU
1	B	138	THR
1	B	168	HIS
1	B	175	SER
1	B	207	ARG
1	B	254	VAL
1	B	263	LEU
1	B	271	LEU
1	B	277	LEU
1	B	281	HIS
1	B	295	GLN
1	B	305	GLU
1	B	334	GLU
1	B	336	VAL

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Mol	Chain	Res	Type
1	B	339	LYS
1	B	357	LEU
1	B	362	LEU
1	B	364	VAL
1	B	371	ASP
1	B	372	GLU
1	B	377	VAL
1	B	387	THR
1	B	414	VAL
1	B	423	PHE
1	B	434	THR
1	B	436	SER
1	B	440	ASN
1	B	455	HIS

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	139	GLN
1	A	245	HIS
1	A	251	ASN
1	A	383	GLN
1	B	27	HIS
1	B	281	HIS
1	B	295	GLN
1	B	370	GLN
1	B	455	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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BLA	B	501	1	46,46,46	0.98	1 (2%)	66,67,67	1.50	10 (15%)
2	BLA	A	501[A]	1	46,46,46	0.95	2 (4%)	66,67,67	1.02	3 (4%)
2	BLA	A	501[B]	1	46,46,46	1.04	3 (6%)	66,67,67	1.17	5 (7%)
3	BEN	A	502	-	9,9,9	0.69	0	7,11,11	1.14	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	B	501	1	-	11/26/74/74	0/4/4/4
2	BLA	A	501[A]	1	-	7/26/74/74	0/4/4/4
2	BLA	A	501[B]	1	-	9/26/74/74	0/4/4/4
3	BEN	A	502	-	-	2/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	BLA	CHD-C1D	2.48	1.46	1.40
2	A	501[B]	BLA	CHD-C1D	2.44	1.46	1.40
2	A	501[B]	BLA	CBD-CGD	2.43	1.56	1.50
2	A	501[B]	BLA	CHB-C4A	2.23	1.45	1.40
2	A	501[A]	BLA	CHD-C1D	2.14	1.45	1.40
2	A	501[A]	BLA	CBD-CGD	2.02	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	BLA	CHB-C4A-NA	4.83	136.20	125.29
2	B	501	BLA	CHB-C4A-C3A	-4.54	116.39	127.53
2	A	501[B]	BLA	CHD-C1D-C2D	-3.15	116.78	124.87
2	A	501[B]	BLA	CHD-C1D-ND	3.03	131.51	124.95
2	B	501	BLA	CAA-CBA-CGA	2.99	121.60	113.67
2	B	501	BLA	CAA-C2A-C1A	2.91	130.38	125.77
2	A	501[B]	BLA	C4C-CHD-C1D	2.85	135.06	128.06
2	B	501	BLA	CMA-C3A-C4A	2.85	129.76	125.62
3	A	502	BEN	C1-C-N2	-2.84	113.70	118.01
2	B	501	BLA	C1A-CHA-C4D	2.72	134.15	128.22
2	B	501	BLA	C4C-NC-C1C	2.71	113.99	110.66
2	A	501[A]	BLA	CHD-C1D-C2D	-2.58	118.24	124.87
2	A	501[A]	BLA	C4C-CHD-C1D	2.52	134.24	128.06
2	A	501[B]	BLA	CMB-C2B-C1B	2.36	127.02	124.16
2	A	501[A]	BLA	CHD-C1D-ND	2.23	129.78	124.95
2	B	501	BLA	CMB-C2B-C1B	-2.23	121.44	124.16
2	B	501	BLA	O2D-CGD-O1D	2.18	128.94	123.33
2	B	501	BLA	O1D-CGD-CBD	-2.06	116.56	123.09
2	A	501[B]	BLA	OB-C4B-C3B	-2.00	124.88	129.71

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[A]	BLA	C2B-C3B-CAB-CBB
2	A	501[A]	BLA	C4B-C3B-CAB-CBB
2	A	501[A]	BLA	C2C-C3C-CAC-CBC
2	A	501[A]	BLA	C4C-C3C-CAC-CBC
2	A	501[B]	BLA	C2B-C1B-CHB-C4A
2	A	501[B]	BLA	C2C-C3C-CAC-CBC
2	A	501[B]	BLA	C4C-C3C-CAC-CBC
2	B	501	BLA	C2C-C3C-CAC-CBC
2	B	501	BLA	C4C-C3C-CAC-CBC
3	A	502	BEN	N2-C-C1-C2
3	A	502	BEN	N2-C-C1-C6
2	A	501[A]	BLA	NA-C4A-CHB-C1B
2	A	501[B]	BLA	NA-C4A-CHB-C1B
2	B	501	BLA	NA-C4A-CHB-C1B
2	A	501[A]	BLA	C3A-C4A-CHB-C1B
2	A	501[B]	BLA	C3A-C4A-CHB-C1B
2	B	501	BLA	C3A-C4A-CHB-C1B
2	A	501[A]	BLA	C2A-CAA-CBA-CGA
2	A	501[B]	BLA	NB-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
2	A	501[B]	BLA	C2A-CAA-CBA-CGA
2	B	501	BLA	C4D-C3D-CAD-CBD
2	B	501	BLA	C2D-C3D-CAD-CBD
2	B	501	BLA	C2A-CAA-CBA-CGA
2	B	501	BLA	CAD-CBD-CGD-O2D
2	B	501	BLA	CAD-CBD-CGD-O1D
2	B	501	BLA	CAA-CBA-CGA-O1A
2	B	501	BLA	CAA-CBA-CGA-O2A
2	A	501[B]	BLA	CAD-CBD-CGD-O1D
2	A	501[B]	BLA	CAD-CBD-CGD-O2D

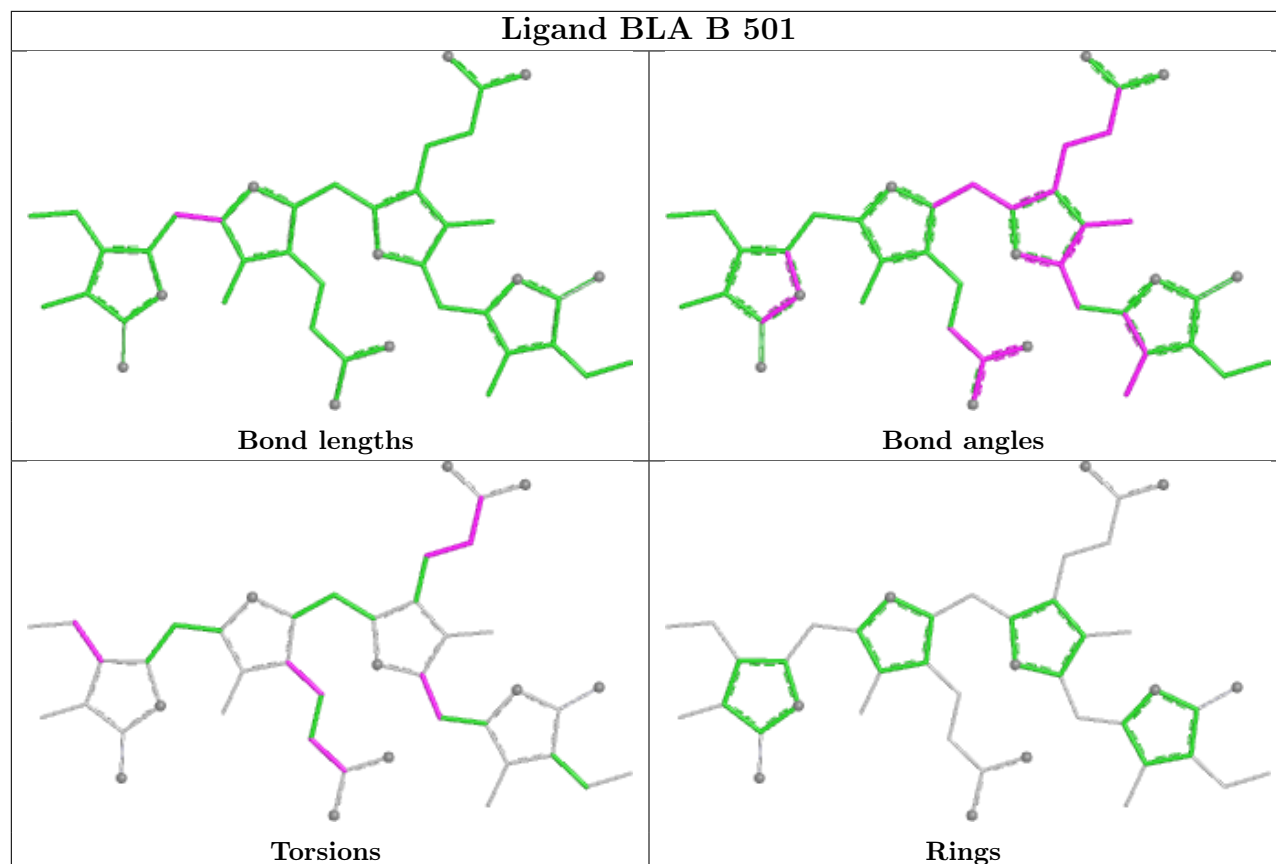
There are no ring outliers.

3 monomers are involved in 29 short contacts:

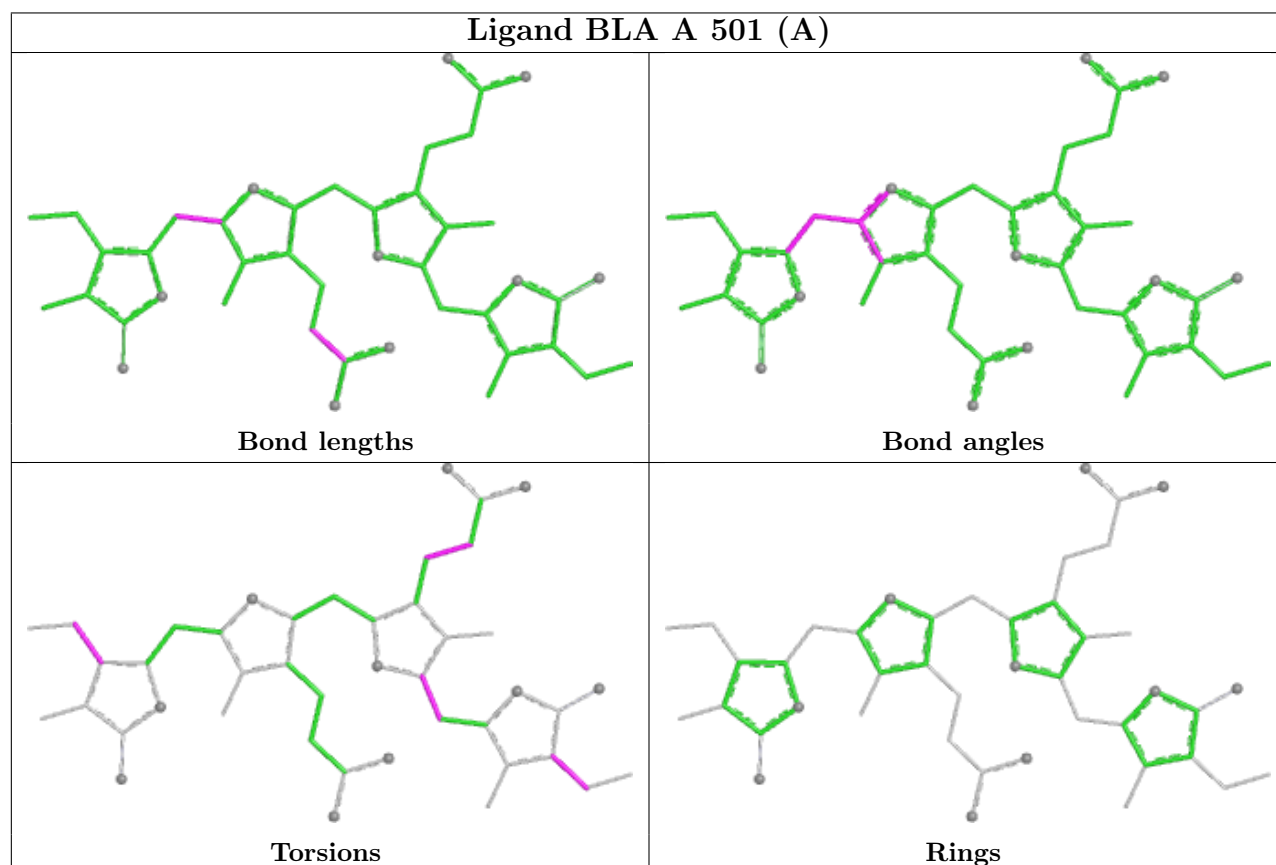
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	BLA	8	0
2	A	501[A]	BLA	7	0
2	A	501[B]	BLA	14	0

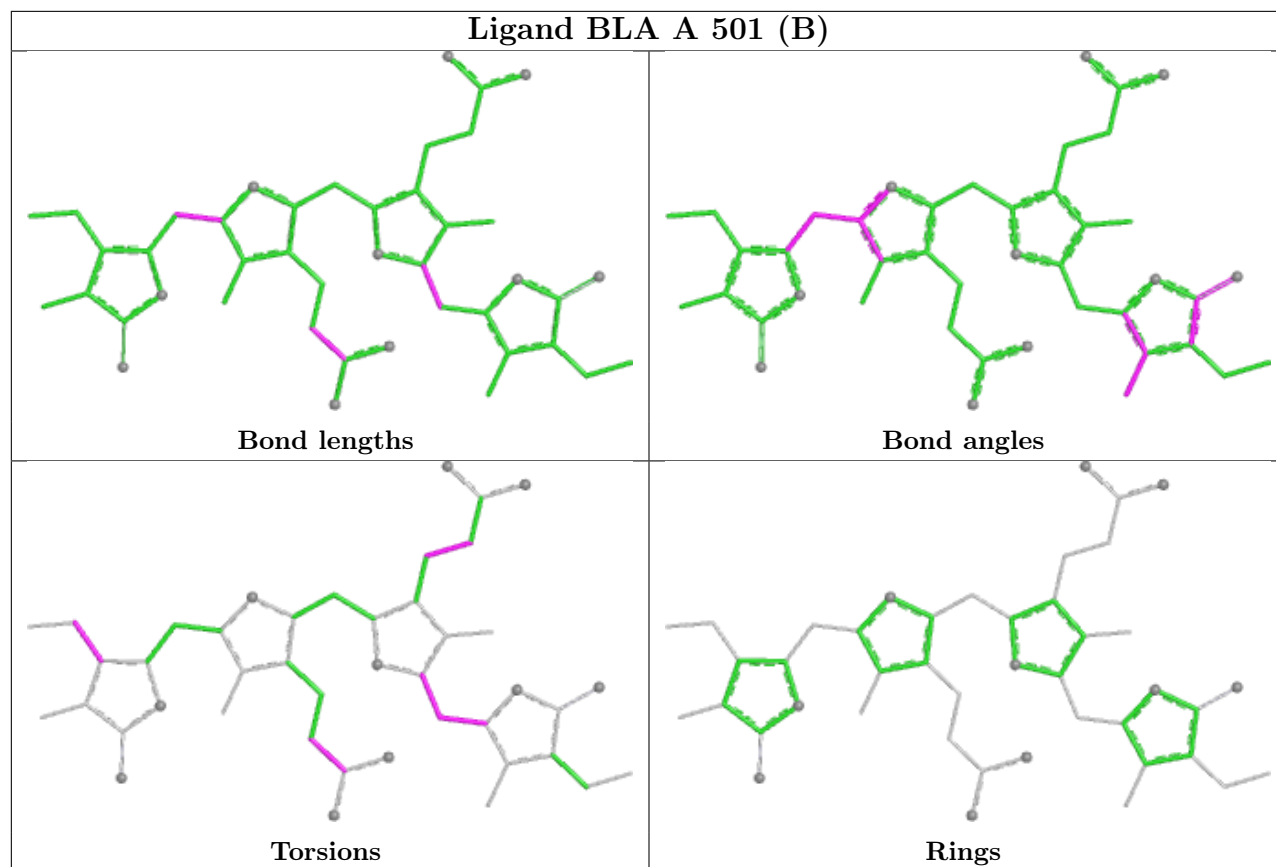
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 B 501



Ligand BLA A 501 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/482 (100%)	0.44	14 (2%) 53 56	5, 19, 42, 66	2 (0%)
1	B	482/482 (100%)	0.55	20 (4%) 41 43	7, 20, 46, 70	0
All	All	964/964 (100%)	0.50	34 (3%) 47 49	5, 20, 45, 70	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315[A]	HIS	5.4
1	A	337	LEU	3.6
1	B	358	GLY	3.2
1	A	418	PRO	3.1
1	B	364	VAL	3.1
1	A	323	LEU	3.1
1	B	133	ALA	3.0
1	B	336	VAL	2.9
1	B	9	ASP	2.6
1	B	380	LEU	2.6
1	B	132	LEU	2.6
1	B	355	LEU	2.5
1	B	361	PRO	2.5
1	B	373	VAL	2.4
1	A	420	ALA	2.4
1	B	377	VAL	2.4
1	A	379	TRP	2.4
1	B	330	GLY	2.3
1	B	324	ALA	2.3
1	A	421	ALA	2.3
1	A	423	PHE	2.3
1	A	132	LEU	2.2
1	A	131	PRO	2.2
1	A	417	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	VAL	2.2
1	A	333	LEU	2.2
1	B	333	LEU	2.2
1	B	385	PHE	2.2
1	B	423	PHE	2.2
1	B	134	GLY	2.2
1	B	356	LEU	2.1
1	A	368	PRO	2.1
1	A	380	LEU	2.1
1	B	267	VAL	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](#)

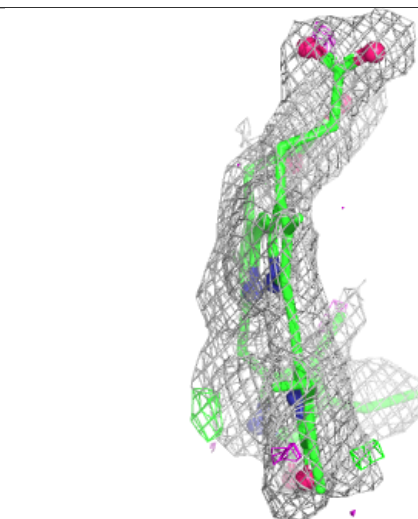
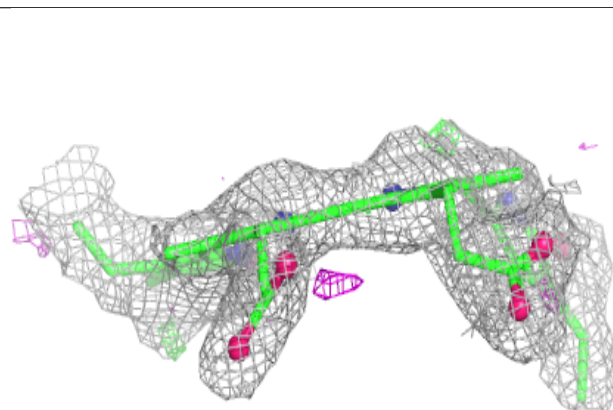
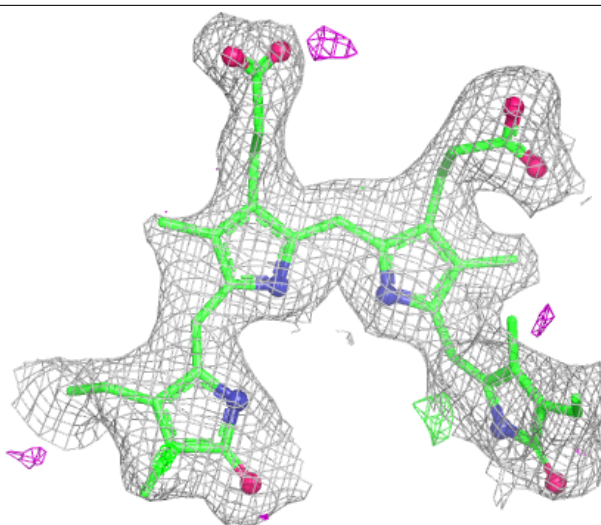
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BEN	A	502	9/9	0.71	0.15	31,35,48,48	0
2	BLA	A	501[B]	43/43	0.81	0.15	8,13,17,26	43
2	BLA	A	501[A]	43/43	0.81	0.15	10,13,17,22	43
2	BLA	B	501	43/43	0.84	0.14	2,13,27,28	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.

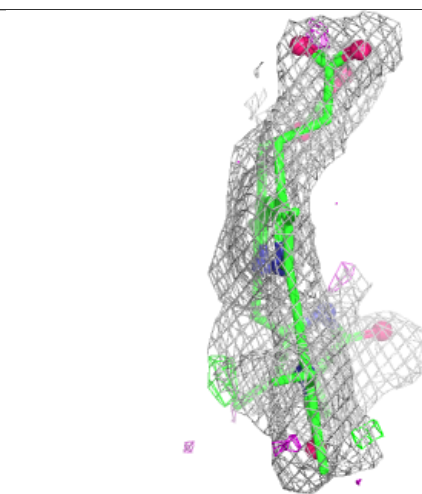
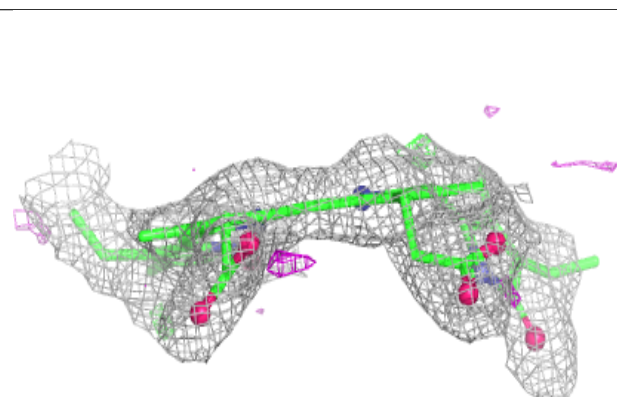
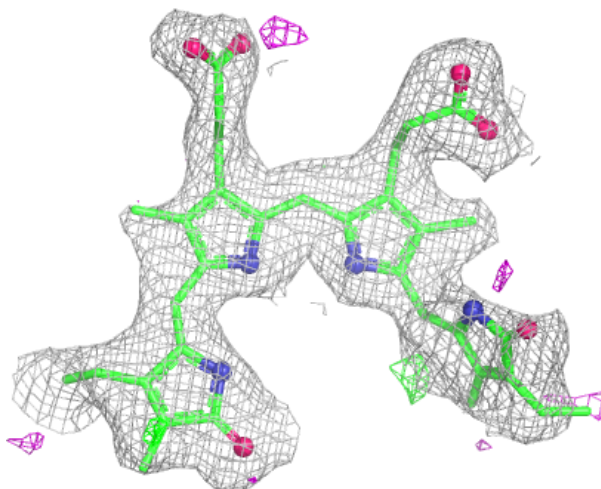
Electron density around BLA A 501 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



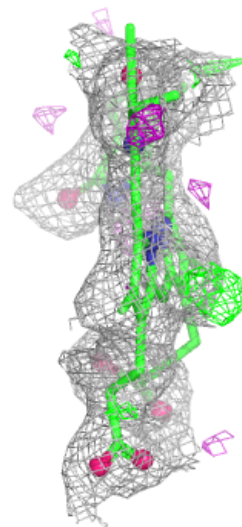
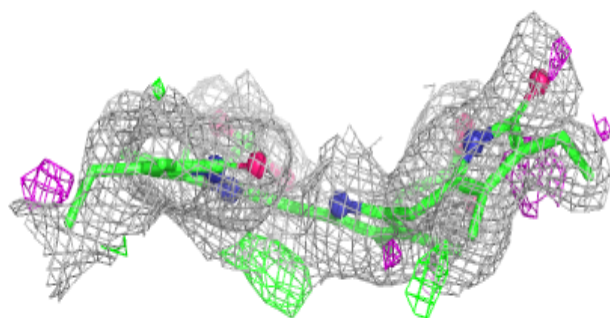
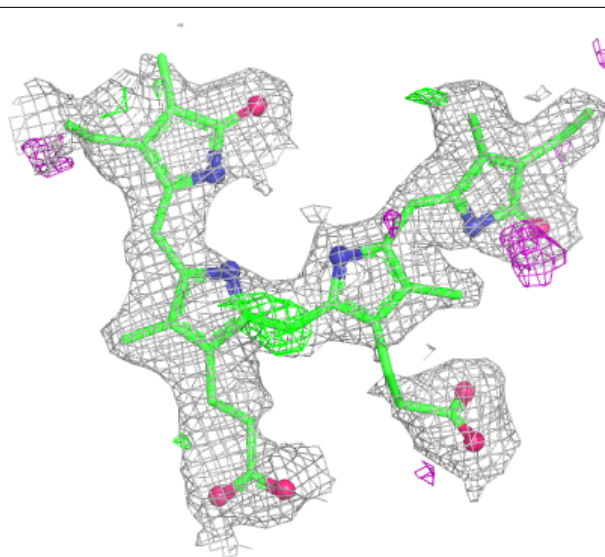
Electron density around BLA A 501 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLA B 501:

$2mF_o-DF_c$ (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.