Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:56 AM EST

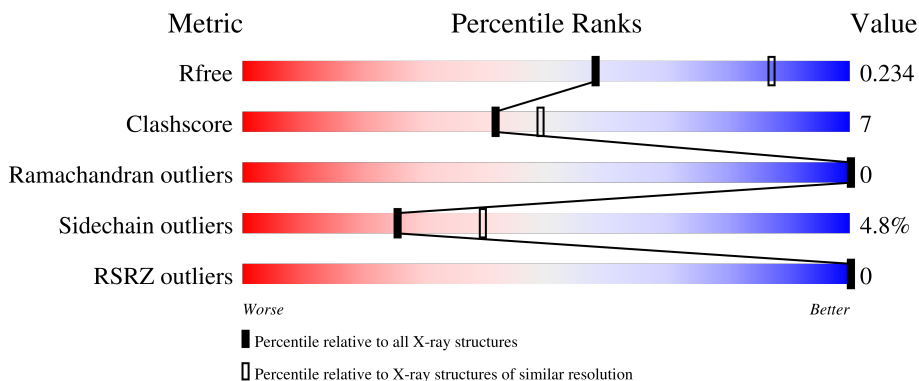|		
PDB ID	:	3G45
Title	:	Crystal structure of human phosphodiesterase 4b with regulatory domain and d155988
Authors	:	Staker, B.L.
Deposited on	:	2009-02-03
Resolution	:	2.63 Å(reported)

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 2.63 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		4.8%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	421	74% 13% 12%
1	B	421	72% 15% • 12%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6133 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total 2992	C 1881	N 509	O 581	S 21	0	0	0
1	B	370	Total 2985	C 1877	N 508	O 579	S 21	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	expression tag	UNP Q07343
A	295	LYS	-	linker	UNP Q07343
A	296	VAL	-	linker	UNP Q07343
A	297	THR	-	linker	UNP Q07343
A	298	ALA	-	linker	UNP Q07343
A	299	GLU	-	linker	UNP Q07343
A	300	GLU	-	linker	UNP Q07343
A	301	ALA	-	linker	UNP Q07343
A	302	PRO	-	linker	UNP Q07343
A	303	GLN	-	linker	UNP Q07343
A	304	PRO	-	linker	UNP Q07343
A	660	HIS	-	expression tag	UNP Q07343
A	661	HIS	-	expression tag	UNP Q07343
A	662	HIS	-	expression tag	UNP Q07343
A	663	HIS	-	expression tag	UNP Q07343
A	664	HIS	-	expression tag	UNP Q07343
A	665	HIS	-	expression tag	UNP Q07343
B	240	MET	-	expression tag	UNP Q07343
B	295	LYS	-	linker	UNP Q07343
B	296	VAL	-	linker	UNP Q07343
B	297	THR	-	linker	UNP Q07343
B	298	ALA	-	linker	UNP Q07343
B	299	GLU	-	linker	UNP Q07343
B	300	GLU	-	linker	UNP Q07343
B	301	ALA	-	linker	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	PRO	-	linker	UNP Q07343
B	303	GLN	-	linker	UNP Q07343
B	304	PRO	-	linker	UNP Q07343
B	660	HIS	-	expression tag	UNP Q07343
B	661	HIS	-	expression tag	UNP Q07343
B	662	HIS	-	expression tag	UNP Q07343
B	663	HIS	-	expression tag	UNP Q07343
B	664	HIS	-	expression tag	UNP Q07343
B	665	HIS	-	expression tag	UNP Q07343

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 8-(3-nitrophenyl)-6-(pyridin-4-ylmethyl)quinoline (three-letter code: 988) (formula: $C_{21}H_{15}N_3O_2$).
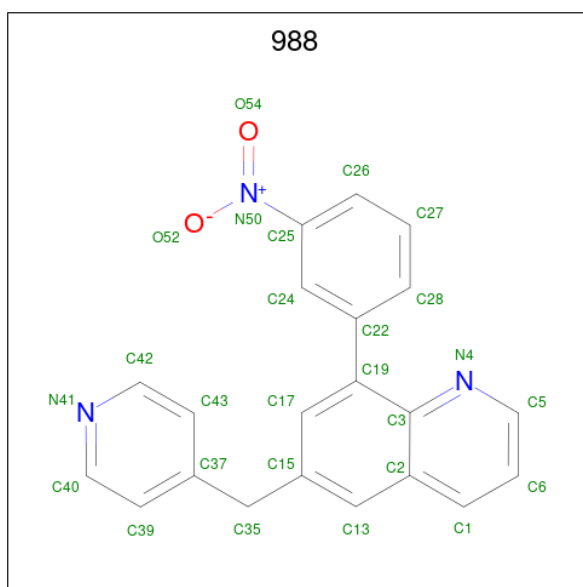
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	21	3	2		
4	B	1	Total	C	N	O	0	0
			26	21	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		
5	B	48	Total	O	0	0
			48	48		

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
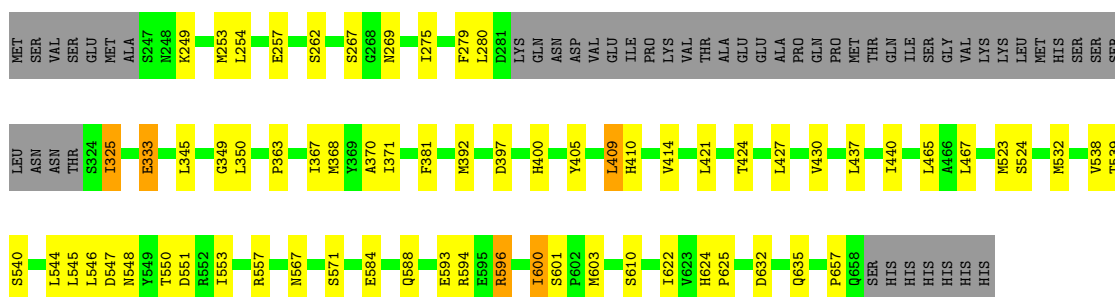
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

Chain A:
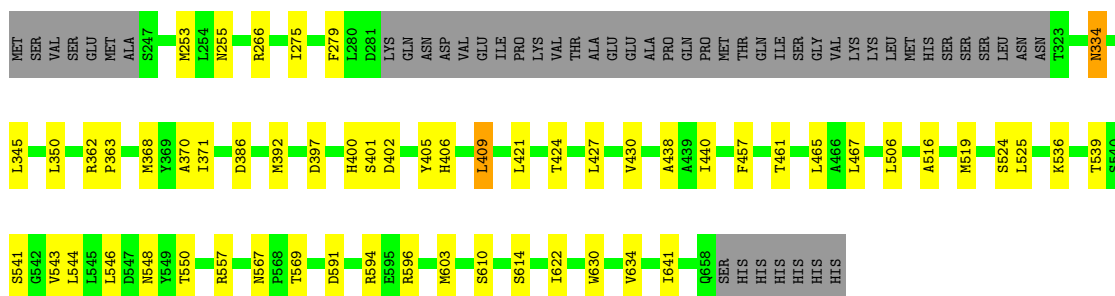
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	95.00Å 95.00Å 93.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.63 42.37 – 2.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.63) 99.7 (42.37-2.63)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.179 , 0.233 0.185 , 0.234	Depositor DCC
R_{free} test set	1413 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 9.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.449 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6133	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 988, ZN, MG

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	0.63	0/3051	0.66	1/4133 (0.0%)
1	B	0.61	0/3044	0.69	1/4123 (0.0%)
All	All	0.62	0/6095	0.68	2/8256 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	325	ILE	CG1-CB-CG2	6.45	125.59	111.40
1	A	362	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	540	SER	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	2992	0	2898	41	0
1	B	2985	0	2891	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	15	4	0
4	B	26	0	15	1	0
5	A	52	0	0	1	0
5	B	48	0	0	1	0
All	All	6133	0	5819	83	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 7.

All (83) 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:421:LEU:O	1:B:424:THR:HG22	1.71	0.90
1:B:538:VAL:HG12	1:B:539:THR:O	1.72	0.90
1:A:421:LEU:O	1:A:424:THR:HG22	1.81	0.80
1:B:279:PHE:CD1	1:B:622:ILE:HD13	2.19	0.77
1:B:539:THR:HG22	1:B:545:LEU:HD13	1.68	0.75
1:B:596:ARG:HD3	5:B:55:HOH:O	1.87	0.73
1:B:424:THR:CG2	1:B:427:LEU:HD12	2.19	0.72
1:B:280:LEU:HD23	1:B:523:MET:HG3	1.72	0.71
1:B:424:THR:HG21	1:B:427:LEU:HD12	1.75	0.68
1:B:280:LEU:CD2	1:B:523:MET:HG3	2.24	0.68
1:B:368:MET:HG3	1:B:392:MET:HE1	1.76	0.67
1:B:594:ARG:HG3	1:B:600:ILE:HD11	1.78	0.64
1:A:400:HIS:HB3	1:A:402:ASP:OD1	1.98	0.64
1:B:567:ASN:HD22	4:B:901:988:H1	1.62	0.63
1:A:279:PHE:CD1	1:A:622:ILE:HD13	2.34	0.63
1:B:279:PHE:CD1	1:B:622:ILE:CD1	2.83	0.62
1:B:603:MET:HE3	1:B:603:MET:HA	1.81	0.62
1:A:334:ASN:OD1	1:B:657:PRO:HG2	2.00	0.62
1:A:279:PHE:CE1	1:A:622:ILE:HD13	2.35	0.61
1:A:519:MET:HA	1:A:519:MET:CE	2.30	0.61
1:B:280:LEU:HD23	1:B:523:MET:CG	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:MET:HA	1:A:519:MET:HE3	1.84	0.60
1:A:548:ASN:HD22	1:A:550:THR:HB	1.66	0.60
1:B:584:GLU:OE1	1:B:588:GLN:NE2	2.34	0.59
1:A:525:LEU:HD21	1:A:557:ARG:HD2	1.85	0.58
1:B:368:MET:HG3	1:B:392:MET:CE	2.33	0.58
1:A:539:THR:HG22	1:A:543:VAL:O	2.03	0.58
1:B:371:ILE:HG21	1:B:440:ILE:HD13	1.85	0.58
1:A:591:ASP:OD1	1:A:594:ARG:NH1	2.35	0.57
1:B:279:PHE:CE1	1:B:622:ILE:HD13	2.39	0.57
1:A:424:THR:CG2	1:A:427:LEU:HD12	2.35	0.57
1:B:548:ASN:ND2	1:B:550:THR:HB	2.20	0.56
1:A:548:ASN:ND2	1:A:550:THR:HB	2.20	0.56
1:A:603:MET:HE1	4:A:901:988:H26	1.87	0.56
1:A:567:ASN:HD22	4:A:901:988:H1	1.71	0.55
1:B:345:LEU:HD22	1:B:370:ALA:HB1	1.88	0.54
1:A:630:TRP:O	1:A:634:VAL:HG22	2.08	0.54
1:B:430:VAL:HG11	1:B:546:LEU:HD12	1.90	0.53
1:A:368:MET:HG3	1:A:392:MET:HE1	1.92	0.52
1:A:275:ILE:HG12	1:A:622:ILE:HD11	1.91	0.52
1:A:438:ALA:HB2	1:A:506:LEU:HD12	1.92	0.52
1:A:279:PHE:CD1	1:A:622:ILE:CD1	2.94	0.51
1:A:368:MET:HG3	1:A:392:MET:CE	2.41	0.51
1:A:371:ILE:HG21	1:A:440:ILE:HD13	1.94	0.50
1:A:397:ASP:HB3	5:A:94:HOH:O	2.12	0.50
1:B:405:TYR:OH	1:B:567:ASN:ND2	2.42	0.50
1:A:603:MET:HE1	1:A:614:SER:HB3	1.94	0.49
1:B:624:HIS:HB3	1:B:625:PRO:HD3	1.94	0.49
1:B:603:MET:HA	1:B:603:MET:CE	2.43	0.48
1:A:424:THR:HG21	1:A:427:LEU:HD12	1.95	0.48
1:B:253:MET:O	1:B:257:GLU:HG3	2.14	0.48
1:B:548:ASN:HD22	1:B:550:THR:HB	1.79	0.47
1:A:430:VAL:HG11	1:A:546:LEU:HD12	1.98	0.46
1:A:427:LEU:HD21	1:A:544:LEU:HD12	1.98	0.45
1:A:350:LEU:C	1:A:350:LEU:HD23	2.36	0.45
1:B:381:PHE:CD2	1:B:437:LEU:HD22	2.51	0.45
1:B:275:ILE:HG12	1:B:622:ILE:HD12	1.99	0.45
1:A:406:HIS:CE1	4:A:901:988:H40	2.52	0.45
1:A:427:LEU:CD2	1:A:544:LEU:HD12	2.47	0.45
1:B:363:PRO:HG3	1:B:409:LEU:HD13	1.98	0.45
1:B:553:ILE:O	1:B:557:ARG:HG2	2.17	0.44
1:A:402:ASP:OD1	1:A:402:ASP:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:THR:HB	1:A:641:ILE:HG23	1.99	0.44
1:B:593:GLU:OE2	1:B:601:SER:OG	2.29	0.44
1:A:457:PHE:O	1:A:461:THR:HG23	2.17	0.44
1:A:516:ALA:HB2	1:A:557:ARG:HD3	2.01	0.43
1:B:427:LEU:CD2	1:B:544:LEU:HD12	2.48	0.43
1:B:254:LEU:HD11	1:B:280:LEU:HD21	1.99	0.43
1:A:345:LEU:HD22	1:A:370:ALA:HB1	2.01	0.43
1:B:262:SER:HB2	1:B:269:ASN:ND2	2.34	0.43
1:A:405:TYR:OH	1:A:567:ASN:ND2	2.52	0.42
1:A:525:LEU:HD21	1:A:557:ARG:CD	2.49	0.42
1:B:349:GLY:O	1:B:350:LEU:C	2.57	0.42
1:A:603:MET:CE	4:A:901:988:H26	2.49	0.42
1:B:371:ILE:CG2	1:B:440:ILE:HD13	2.49	0.42
1:B:367:ILE:HD12	1:B:367:ILE:HA	1.93	0.41
1:B:333:GLU:CD	1:B:333:GLU:H	2.23	0.41
1:A:275:ILE:HG12	1:A:622:ILE:CD1	2.50	0.41
1:A:363:PRO:HG3	1:A:409:LEU:HD13	2.02	0.41
1:B:262:SER:HB2	1:B:269:ASN:HD22	1.86	0.41
1:B:410:HIS:O	1:B:414:VAL:HG23	2.21	0.41
1:A:334:ASN:HD22	1:A:334:ASN:N	2.19	0.41
1:B:548:ASN:ND2	1:B:551:ASP:H	2.19	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	367/421 (87%)	361 (98%)	6 (2%)	0	100	100
1	B	366/421 (87%)	357 (98%)	9 (2%)	0	100	100
All	All	733/842 (87%)	718 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	337/385 (88%)	323 (96%)	14 (4%)	30	45
1	B	336/385 (87%)	318 (95%)	18 (5%)	22	35
All	All	673/770 (87%)	641 (95%)	32 (5%)	25	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	MET
1	A	255	ASN
1	A	266	ARG
1	A	334	ASN
1	A	386	ASP
1	A	401	SER
1	A	409	LEU
1	A	465	LEU
1	A	467	LEU
1	A	524	SER
1	A	536	LYS
1	A	541	SER
1	A	596	ARG
1	A	610	SER
1	B	249	LYS
1	B	267	SER
1	B	325	ILE
1	B	333	GLU
1	B	397	ASP
1	B	400	HIS
1	B	409	LEU
1	B	465	LEU
1	B	467	LEU
1	B	524	SER
1	B	532	MET

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Mol	Chain	Res	Type
1	B	547	ASP
1	B	571	SER
1	B	596	ARG
1	B	600	ILE
1	B	610	SER
1	B	632	ASP
1	B	635	GLN

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	269	ASN
1	A	277	ASN
1	A	567	ASN
1	A	658	GLN
1	B	269	ASN
1	B	361	ASN
1	B	548	ASN
1	B	567	ASN
1	B	577	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	#$|Z| > 2$
4	988	A	901	-	27,29,29	2.35	2 (7%)	34,40,40	1.42	4 (11%)
4	988	B	901	-	27,29,29	2.32	4 (14%)	34,40,40	1.68	6 (17%)

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
4	988	A	901	-	-	0/6/12/12	0/4/4/4
4	988	B	901	-	-	2/6/12/12	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	988	O54-N50	10.59	1.40	1.22
4	B	901	988	O54-N50	10.26	1.40	1.22
4	B	901	988	C2-C3	3.30	1.48	1.41
4	A	901	988	C2-C3	3.27	1.47	1.41
4	B	901	988	C25-N50	-2.44	1.39	1.45
4	B	901	988	C24-C22	-2.10	1.37	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	988	C19-C3-N4	4.39	122.79	118.13
4	B	901	988	C17-C15-C13	4.25	121.62	118.51
4	A	901	988	C19-C3-N4	4.12	122.51	118.13
4	B	901	988	C19-C3-C2	-3.47	117.08	119.37
4	A	901	988	C17-C15-C13	3.35	120.96	118.51
4	A	901	988	C19-C3-C2	-2.97	117.41	119.37
4	B	901	988	C17-C19-C3	2.85	120.82	118.90
4	B	901	988	C35-C15-C13	-2.23	118.35	123.40
4	A	901	988	C35-C15-C13	-2.16	118.52	123.40
4	B	901	988	C24-C22-C28	2.09	120.75	118.15

There are no chirality outliers.
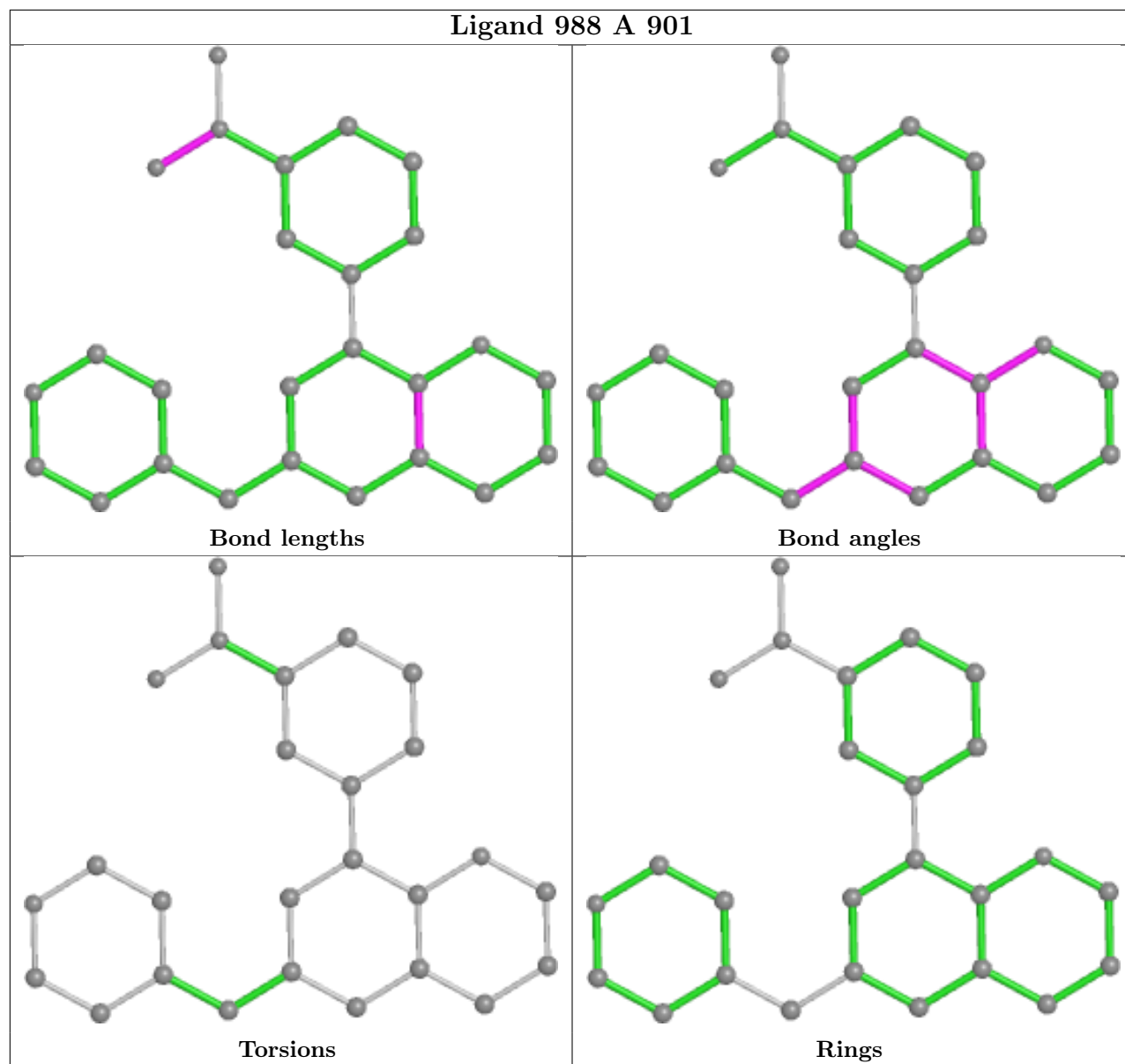
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	988	C24-C25-N50-O54
4	B	901	988	C26-C25-N50-O54

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	988	4	0
4	B	901	988	1	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 988 A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand 988 B 901

Bond lengths

Bond angles

Torsions

Rings
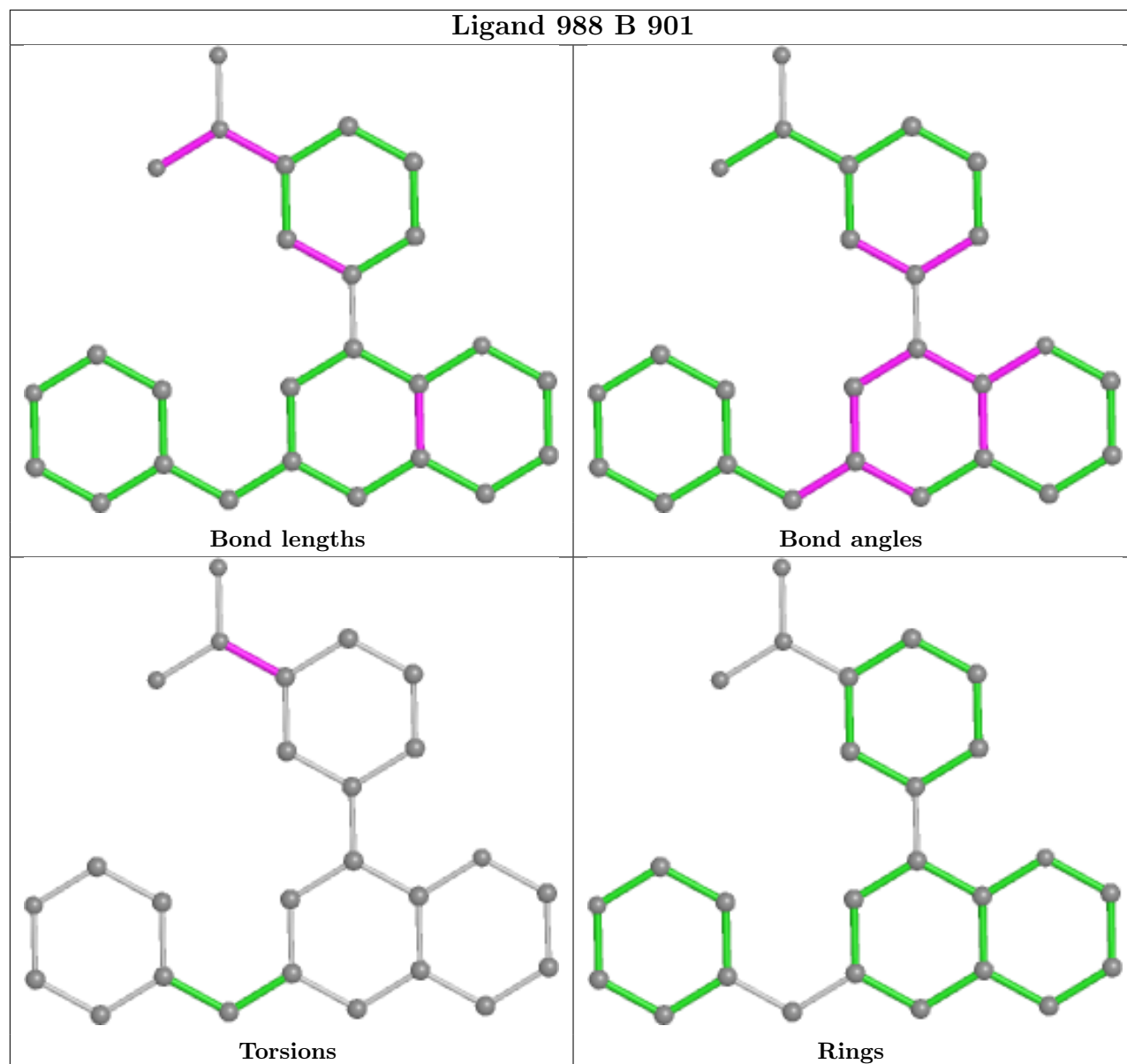
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	371/421 (88%)	-0.44	0	100	100	21, 34, 53, 63	0
1	B	370/421 (87%)	-0.41	0	100	100	22, 34, 56, 61	0
All	All	741/842 (88%)	-0.42	0	100	100	21, 34, 54, 63	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

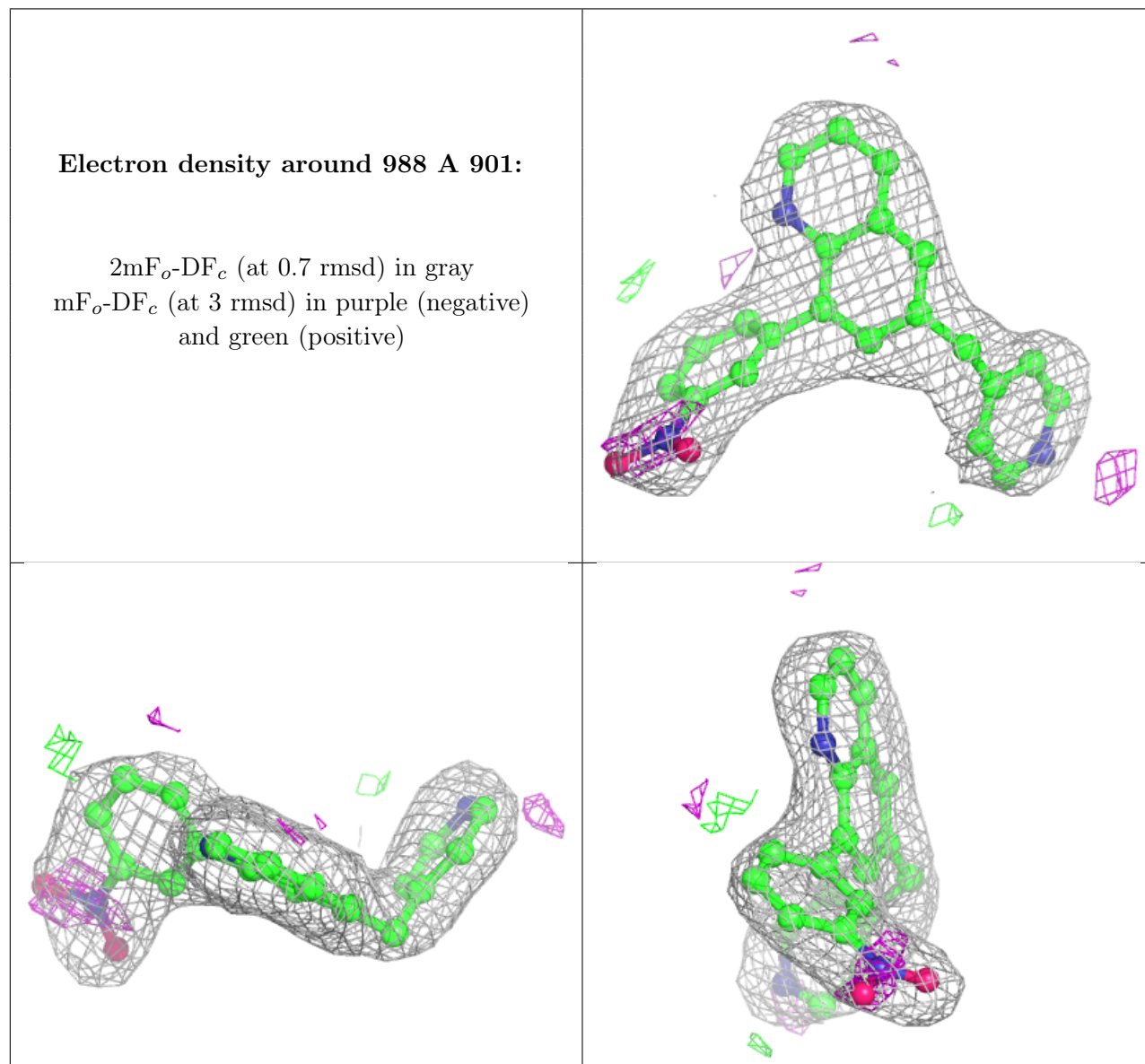There are no non-standard protein/DNA/RNA residues in this entry.

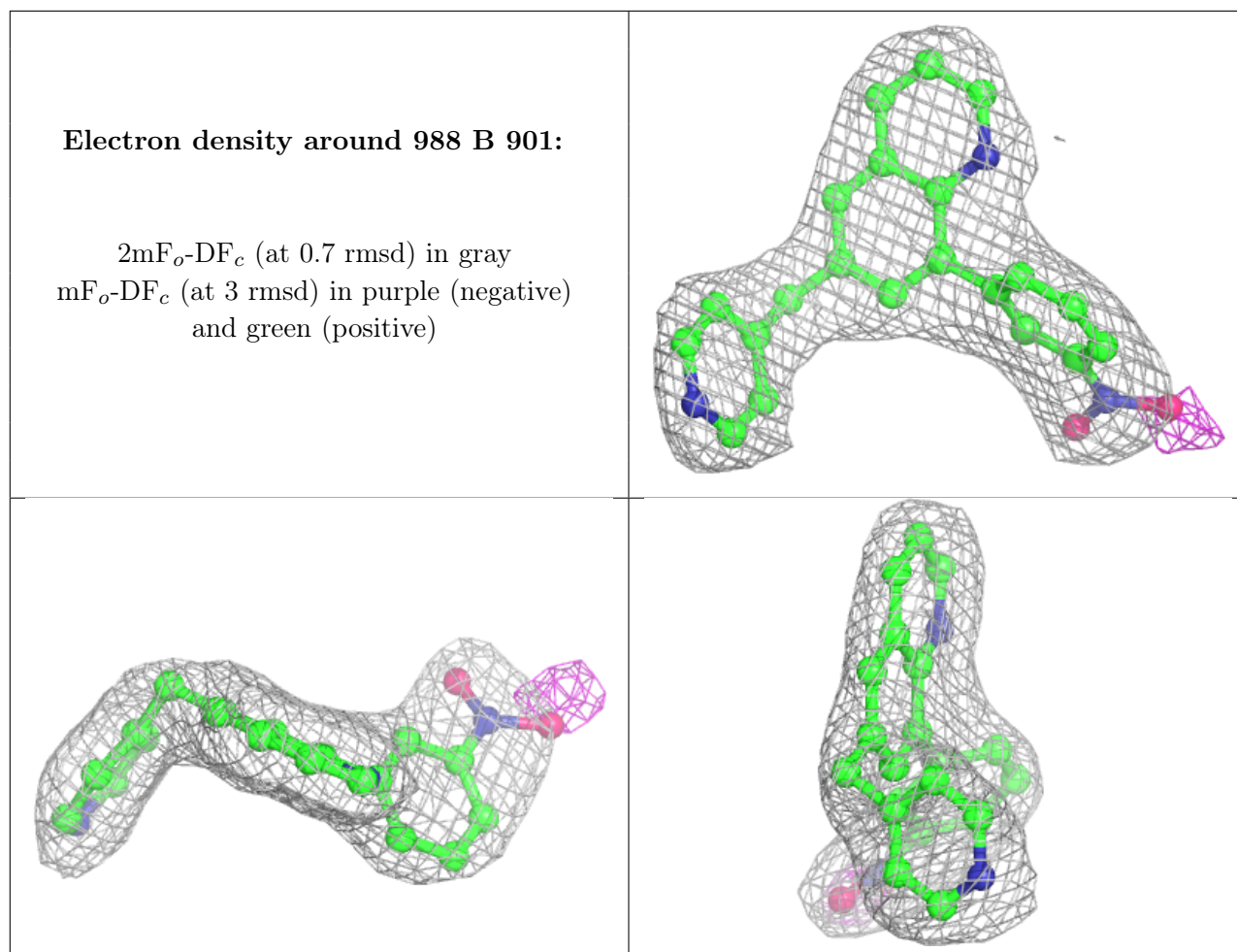## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	MG	A	802	1/1	0.91	0.35	22,22,22,22	0
4	988	A	901	26/26	0.95	0.18	32,37,44,49	0
3	MG	B	802	1/1	0.96	0.30	14,14,14,14	0
4	988	B	901	26/26	0.96	0.19	31,37,44,47	0
2	ZN	A	801	1/1	0.99	0.15	29,29,29,29	0
2	ZN	B	801	1/1	0.99	0.17	31,31,31,31	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 988 A 901:

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

Electron density around 988 B 901:

$2mF_o$-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.