



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:09 PM UTC

PDB ID : 3G58 / pdb_00003g58
Title : Crystal structure of human phosphodiesterase 4d with d155988/pmnpq
Authors : Staker, B.L.
Deposited on : 2009-02-04
Resolution : 2.05 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

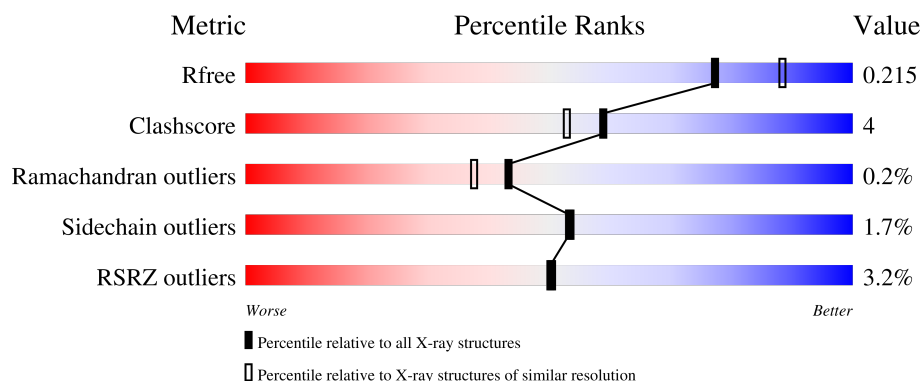
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	381	4% 80% 8% • 12%
1	B	381	% 79% 7% 14%
1	C	381	2% 76% 9% 14%
1	D	381	5% 81% 8% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	D	11	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12091 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 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2696	1706	461	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2633	1665	448	506	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	345	Total	C	N	O	S	0	0	0
			2786	1765	476	531	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	expression tag	UNP Q08499
A	579	ALA	SER	engineered mutation	UNP Q08499
A	581	ALA	SER	engineered mutation	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	expression tag	UNP Q08499
B	579	ALA	SER	engineered mutation	UNP Q08499
B	581	ALA	SER	engineered mutation	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	expression tag	UNP Q08499
C	579	ALA	SER	engineered mutation	UNP Q08499
C	581	ALA	SER	engineered mutation	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	expression tag	UNP Q08499
D	579	ALA	SER	engineered mutation	UNP Q08499
D	581	ALA	SER	engineered mutation	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

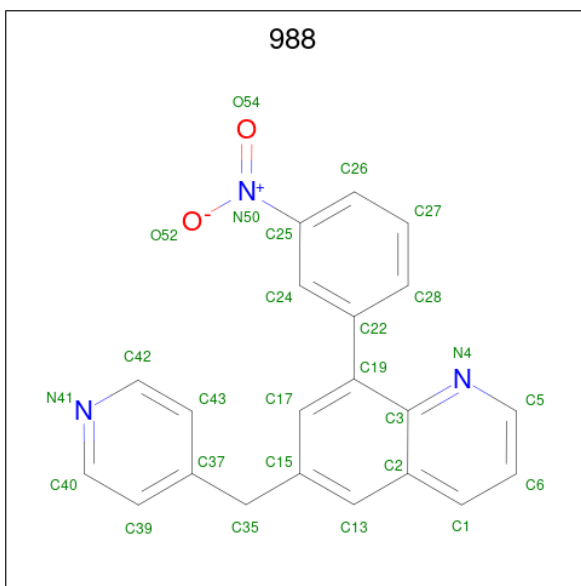
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 8-(3-nitrophenyl)-6-(pyridin-4-ylmethyl)quinoline (CCD ID: 988) (formula: C₂₁H₁₅N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			26	21	3	2		
5	B	1	Total	C	N	O	0	0
			26	21	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			26	21	3	2		
5	D	1	Total	C	N	O	0	0
			26	21	3	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

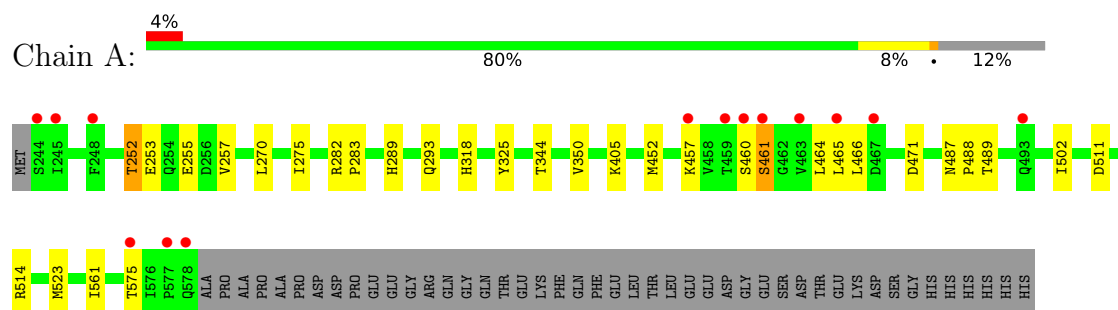
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	294	Total O 294 294	0	0
7	B	284	Total O 284 284	0	0
7	C	259	Total O 259 259	0	0
7	D	307	Total O 307 307	0	0

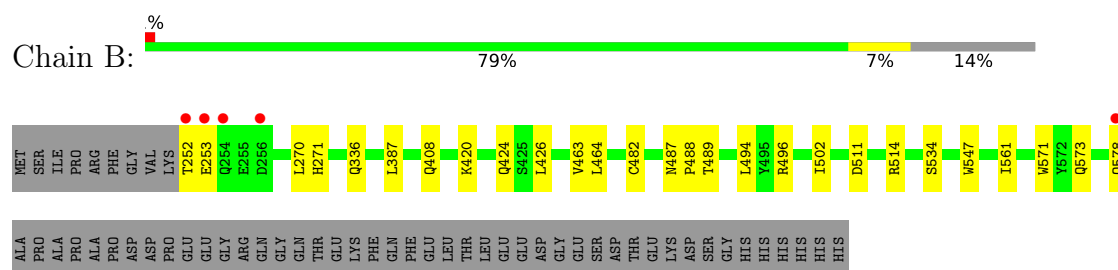
3 Residue-property plots [i](#)

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.

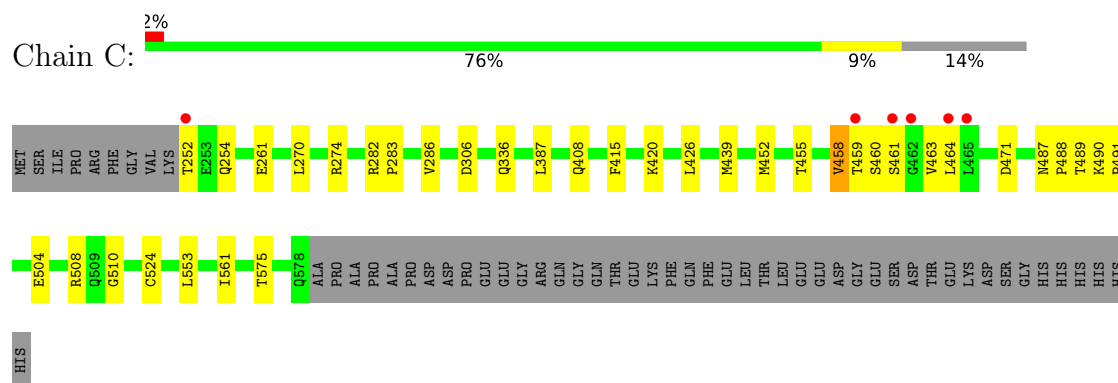
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



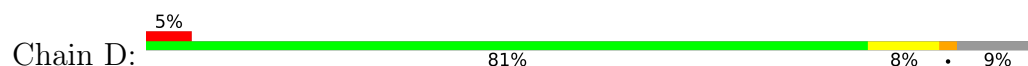
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

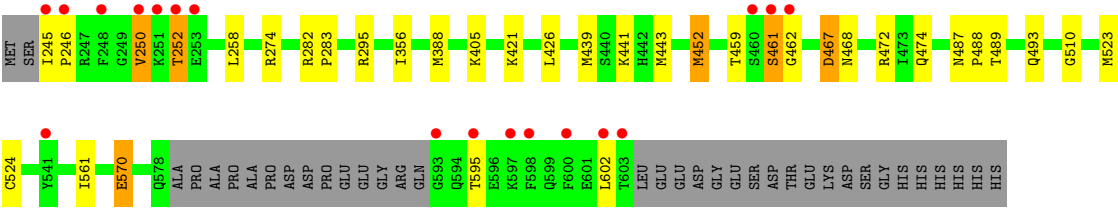


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.39Å 113.57Å 161.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.05 49.21 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.21-2.05) 90.1 (49.21-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.171 , 0.213 0.174 , 0.215	Depositor DCC
R_{free} test set	5158 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12091	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: EDO, SO4, MG, ZN, 988

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	0/2751	0.76	0/3739
1	B	0.63	0/2687	0.77	0/3654
1	C	0.65	0/2701	0.79	0/3670
1	D	0.67	0/2843	0.79	3/3859 (0.1%)
All	All	0.65	0/10982	0.78	3/14922 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	ILE	CA-C-N	7.77	129.55	119.84
1	D	245	ILE	C-N-CA	7.77	129.55	119.84
1	D	461	SER	N-CA-C	-5.53	103.19	110.33

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	2696	0	2645	21	0
1	B	2633	0	2573	16	0
1	C	2647	0	2599	25	0
1	D	2786	0	2731	36	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
5	A	26	0	15	0	0
5	B	26	0	15	1	0
5	C	26	0	15	0	0
5	D	26	0	15	0	0
6	A	16	0	24	1	0
6	B	16	0	24	3	0
6	C	16	0	24	0	0
6	D	20	0	30	7	0
7	A	294	0	0	1	1
7	B	284	0	0	4	0
7	C	259	0	0	2	0
7	D	307	0	0	5	0
All	All	12091	0	10710	96	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 4.

All (96) 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:D:439:MET:HE2	1:D:602:LEU:CD1	1.81	1.10
1:D:439:MET:HE2	1:D:602:LEU:HD11	1.43	1.00
1:D:439:MET:CE	1:D:602:LEU:CD1	2.51	0.89
1:D:439:MET:HE2	1:D:602:LEU:HD13	1.54	0.86
1:A:575:THR:HG21	7:A:774:HOH:O	1.76	0.85
1:D:356:ILE:HD13	6:D:14:EDO:H22	1.61	0.81
1:D:439:MET:CE	1:D:602:LEU:HD13	2.08	0.81
1:D:493:GLN:HE22	6:D:11:EDO:C1	1.95	0.80
1:C:464:LEU:HD21	1:C:553:LEU:HD11	1.65	0.78
1:D:493:GLN:HE22	6:D:11:EDO:H12	1.46	0.77
1:A:252:THR:HG22	1:A:255:GLU:H	1.51	0.75
1:C:306:ASP:OD2	7:C:1059:HOH:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:HA	6:B:10:EDO:H11	1.69	0.73
1:D:459:THR:O	1:D:461:SER:O	2.05	0.73
1:D:472:ARG:CZ	7:D:931:HOH:O	2.39	0.71
1:B:489:THR:HB	1:B:561:ILE:HG23	1.73	0.69
1:A:523:MET:HA	1:A:523:MET:HE2	1.74	0.68
1:D:523:MET:HE1	1:D:595:THR:HA	1.75	0.67
1:C:387:LEU:HD23	1:C:387:LEU:O	1.95	0.67
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.27	0.66
1:B:496:ARG:HD3	1:B:571:TRP:CZ3	2.30	0.66
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.30	0.65
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.31	0.63
1:D:472:ARG:NE	7:D:931:HOH:O	2.31	0.62
1:A:457:LYS:HG2	1:A:465:LEU:HD23	1.84	0.58
1:B:387:LEU:HG	7:B:698:HOH:O	2.04	0.58
1:C:387:LEU:HD23	1:C:387:LEU:C	2.29	0.57
1:D:570:GLU:OE1	7:D:849:HOH:O	2.17	0.57
1:A:252:THR:CG2	1:A:255:GLU:H	2.17	0.57
1:A:489:THR:HB	1:A:561:ILE:HG23	1.88	0.55
1:A:575:THR:HG22	1:A:575:THR:O	2.07	0.54
1:C:452:MET:HE1	1:C:471:ASP:HA	1.88	0.54
1:B:271:HIS:CA	6:B:10:EDO:H11	2.38	0.54
1:A:460:SER:O	1:A:461:SER:CB	2.55	0.54
1:C:489:THR:HB	1:C:561:ILE:HG23	1.90	0.54
1:C:252:THR:N	7:C:1085:HOH:O	2.40	0.53
1:D:493:GLN:NE2	6:D:11:EDO:H12	2.18	0.53
1:A:405:LYS:NZ	1:D:405:LYS:NZ	2.57	0.53
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.91	0.52
1:C:487:ASN:HB2	1:C:488:PRO:HD3	1.92	0.52
1:A:452:MET:HE1	1:A:471:ASP:HA	1.92	0.52
1:B:496:ARG:HD2	7:B:854:HOH:O	2.09	0.52
1:B:494:LEU:HD21	6:B:10:EDO:H12	1.95	0.49
1:D:493:GLN:NE2	6:D:11:EDO:C1	2.72	0.49
1:C:282:ARG:N	1:C:283:PRO:CD	2.76	0.49
1:C:459:THR:HG23	1:C:461:SER:N	2.27	0.49
1:C:282:ARG:O	1:C:286:VAL:HG22	2.13	0.49
1:D:489:THR:HB	1:D:561:ILE:HG23	1.95	0.48
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.46	0.48
1:B:420:LYS:HE2	1:B:424:GLN:HE22	1.79	0.47
1:D:282:ARG:N	1:D:283:PRO:CD	2.78	0.47
1:D:439:MET:HE3	1:D:602:LEU:HD13	1.95	0.47
1:D:295:ARG:HB3	6:D:14:EDO:H21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:THR:C	1:D:461:SER:O	2.58	0.47
1:C:575:THR:O	1:C:575:THR:HG22	2.14	0.46
1:A:487:ASN:HB2	1:A:488:PRO:HD3	1.97	0.46
1:C:459:THR:HG23	1:C:461:SER:H	1.80	0.46
1:A:464:LEU:HD21	1:A:466:LEU:HD21	1.96	0.46
1:C:261:GLU:OE2	1:C:274:ARG:NH1	2.48	0.46
1:D:439:MET:CE	1:D:602:LEU:HD11	2.26	0.46
1:D:523:MET:HE1	1:D:595:THR:CA	2.45	0.46
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.98	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.98	0.46
1:C:510:GLY:HA3	1:C:524:CYS:O	2.16	0.45
1:D:443:MET:HG2	7:D:767:HOH:O	2.15	0.45
1:D:510:GLY:HA3	1:D:524:CYS:O	2.16	0.45
1:C:455:THR:O	1:C:455:THR:HG22	2.16	0.45
1:D:439:MET:HE3	1:D:439:MET:HA	1.97	0.45
1:D:441:LYS:HE2	7:D:741:HOH:O	2.17	0.45
1:A:253:GLU:O	1:A:257:VAL:HG23	2.17	0.44
1:B:482:CYS:HB3	1:B:547:TRP:CZ2	2.52	0.44
1:A:289:HIS:CE1	1:A:293:GLN:HE21	2.36	0.44
1:C:420:LYS:HB2	1:C:420:LYS:HE2	1.87	0.44
1:C:490:LYS:O	1:C:491:PRO:C	2.60	0.44
1:B:408:GLN:OE1	1:C:408:GLN:OE1	2.35	0.44
1:A:270:LEU:HD11	1:A:275:ILE:CD1	2.48	0.43
1:B:534:SER:HB3	5:B:902:988:H26	2.01	0.43
1:D:388:MET:HA	1:D:388:MET:HE2	2.00	0.43
1:A:325:TYR:CG	1:A:502:ILE:HD13	2.54	0.43
1:B:487:ASN:HB2	1:B:488:PRO:HD3	2.00	0.43
1:A:350:VAL:HG11	1:A:466:LEU:HD12	2.01	0.43
1:C:439:MET:HE3	1:C:439:MET:HA	2.00	0.43
1:D:252:THR:HG21	1:D:258:LEU:HD23	2.01	0.42
1:A:318:HIS:HE1	6:A:6:EDO:C1	2.32	0.42
1:D:467:ASP:HB3	1:D:468:ASN:HD22	1.83	0.42
1:C:459:THR:HG22	1:C:463:VAL:H	1.84	0.42
1:C:415:PHE:CE1	1:C:426:LEU:HD21	2.54	0.42
1:D:452:MET:HE3	1:D:474:GLN:NE2	2.35	0.41
1:C:458:VAL:HG13	1:C:459:THR:O	2.20	0.41
1:D:452:MET:HE3	1:D:452:MET:HB2	1.85	0.41
1:A:282:ARG:N	1:A:283:PRO:CD	2.83	0.41
1:D:295:ARG:HH11	6:D:14:EDO:H11	1.86	0.41
1:D:487:ASN:HB2	1:D:488:PRO:HD3	2.01	0.41
1:B:252:THR:HG22	7:B:951:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ASP:CB	1:D:468:ASN:HD22	2.34	0.40
7:B:134:HOH:O	1:D:250:VAL:HG22	2.22	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:D:462:GLY:N	7:A:695:HOH:O[4_455]	2.02	0.18

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	333/381 (87%)	325 (98%)	7 (2%)	1 (0%)	36	30
1	B	325/381 (85%)	319 (98%)	6 (2%)	0	100	100
1	C	325/381 (85%)	316 (97%)	9 (3%)	0	100	100
1	D	341/381 (90%)	326 (96%)	14 (4%)	1 (0%)	36	30
All	All	1324/1524 (87%)	1286 (97%)	36 (3%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	246	PRO
1	A	461	SER

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	302/345 (88%)	300 (99%)	2 (1%)	76	80
1	B	296/345 (86%)	289 (98%)	7 (2%)	43	40
1	C	299/345 (87%)	296 (99%)	3 (1%)	68	72
1	D	312/345 (90%)	304 (97%)	8 (3%)	40	37
All	All	1209/1380 (88%)	1189 (98%)	20 (2%)	53	53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	THR
1	A	344	THR
1	B	253	GLU
1	B	426	LEU
1	B	463	VAL
1	B	464	LEU
1	B	502	ILE
1	B	573	GLN
1	B	578	GLN
1	C	254	GLN
1	C	458	VAL
1	C	460	SER
1	D	250	VAL
1	D	252	THR
1	D	274	ARG
1	D	421	LYS
1	D	426	LEU
1	D	452	MET
1	D	467	ASP
1	D	570	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	424	GLN
1	A	493	GLN
1	A	535	GLN
1	B	289	HIS

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Mol	Chain	Res	Type
1	B	376	GLN
1	B	380	ASN
1	B	424	GLN
1	B	497	GLN
1	B	535	GLN
1	B	555	HIS
1	C	376	GLN
1	C	535	GLN
1	C	559	GLN
1	C	573	GLN
1	D	289	HIS
1	D	293	GLN
1	D	468	ASN
1	D	474	GLN
1	D	497	GLN
1	D	535	GLN

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 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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
6	EDO	C	16	-	3,3,3	0.49	0	2,2,2	0.28	0
6	EDO	C	5	-	3,3,3	0.43	0	2,2,2	0.25	0
6	EDO	C	13	-	3,3,3	0.28	0	2,2,2	0.59	0
5	988	B	902	-	29,29,29	2.24	3 (10%)	38,40,40	1.53	9 (23%)
6	EDO	D	14	-	3,3,3	0.52	0	2,2,2	0.21	0
5	988	C	903	-	29,29,29	2.13	4 (13%)	38,40,40	1.64	9 (23%)
6	EDO	B	10	-	3,3,3	0.28	0	2,2,2	0.57	0
5	988	A	901	-	29,29,29	2.25	3 (10%)	38,40,40	1.80	12 (31%)
6	EDO	B	17	-	3,3,3	0.46	0	2,2,2	0.38	0
6	EDO	A	7	-	3,3,3	0.44	0	2,2,2	0.30	0
6	EDO	B	3	-	3,3,3	0.40	0	2,2,2	0.45	0
6	EDO	D	4	-	3,3,3	0.41	0	2,2,2	0.54	0
6	EDO	A	9	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	C	18	-	3,3,3	0.36	0	2,2,2	0.34	0
6	EDO	A	12	-	3,3,3	0.47	0	2,2,2	0.17	0
6	EDO	D	11	-	3,3,3	0.22	0	2,2,2	0.69	0
6	EDO	A	6	-	3,3,3	0.34	0	2,2,2	0.34	0
5	988	D	904	-	29,29,29	2.29	3 (10%)	38,40,40	1.71	7 (18%)
4	SO4	A	1	-	4,4,4	0.18	0	6,6,6	0.42	0
6	EDO	B	8	-	3,3,3	0.38	0	2,2,2	0.35	0
6	EDO	D	15	-	3,3,3	0.39	0	2,2,2	0.53	0
6	EDO	D	2	-	3,3,3	0.46	0	2,2,2	0.20	0

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
6	EDO	C	16	-	-	0/1/1/1	-
6	EDO	C	5	-	-	0/1/1/1	-
6	EDO	C	13	-	-	0/1/1/1	-
5	988	B	902	-	-	0/10/12/12	0/4/4/4
6	EDO	D	14	-	-	1/1/1/1	-
5	988	C	903	-	-	0/10/12/12	0/4/4/4
6	EDO	B	10	-	-	0/1/1/1	-
5	988	A	901	-	-	0/10/12/12	0/4/4/4
6	EDO	B	17	-	-	1/1/1/1	-
6	EDO	A	7	-	-	1/1/1/1	-
6	EDO	B	3	-	-	0/1/1/1	-
6	EDO	D	4	-	-	0/1/1/1	-
6	EDO	A	9	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	18	-	-	0/1/1/1	-
6	EDO	A	12	-	-	0/1/1/1	-
6	EDO	D	11	-	-	1/1/1/1	-
6	EDO	A	6	-	-	0/1/1/1	-
5	988	D	904	-	-	0/10/12/12	0/4/4/4
6	EDO	B	8	-	-	0/1/1/1	-
6	EDO	D	15	-	-	1/1/1/1	-
6	EDO	D	2	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	904	988	O54-N50	9.60	1.39	1.22
5	A	901	988	O54-N50	9.59	1.39	1.22
5	B	902	988	O54-N50	9.52	1.39	1.22
5	C	903	988	O54-N50	8.97	1.38	1.22
5	D	904	988	C2-C3	5.06	1.49	1.42
5	B	902	988	C2-C3	4.62	1.48	1.42
5	A	901	988	C2-C3	4.47	1.48	1.42
5	C	903	988	C2-C3	4.21	1.47	1.42
5	D	904	988	C19-C3	3.71	1.49	1.43
5	A	901	988	C19-C3	3.58	1.49	1.43
5	B	902	988	C19-C3	3.55	1.49	1.43
5	C	903	988	C19-C3	3.44	1.48	1.43
5	C	903	988	C25-N50	-2.04	1.40	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904	988	C19-C3-N4	5.72	123.76	118.69
5	A	901	988	C19-C3-N4	5.08	123.20	118.69
5	C	903	988	C19-C3-N4	5.04	123.16	118.69
5	B	902	988	C19-C3-N4	4.62	122.79	118.69
5	A	901	988	C24-C25-N50	4.12	122.29	118.74
5	D	904	988	C5-N4-C3	3.71	121.68	117.31
5	A	901	988	C19-C3-C2	-3.41	116.57	119.31
5	C	903	988	C24-C25-N50	3.31	121.59	118.74
5	C	903	988	C19-C3-C2	-3.10	116.82	119.31
5	D	904	988	C19-C3-C2	-3.08	116.84	119.31
5	D	904	988	C2-C3-N4	-3.07	119.39	122.63
5	A	901	988	C5-N4-C3	2.99	120.83	117.31
5	B	902	988	C5-N4-C3	2.84	120.65	117.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903	988	C5-N4-C3	2.67	120.45	117.31
5	A	901	988	C28-C22-C24	2.57	121.77	118.23
5	B	902	988	C2-C3-N4	-2.55	119.94	122.63
5	B	902	988	C19-C3-C2	-2.54	117.27	119.31
5	C	903	988	C2-C3-N4	-2.48	120.02	122.63
5	D	904	988	C26-C25-N50	2.47	121.50	119.34
5	A	901	988	C42-N41-C40	2.33	122.19	116.86
5	B	902	988	C13-C15-C17	2.31	121.17	118.84
5	A	901	988	C2-C3-N4	-2.27	120.23	122.63
5	C	903	988	C22-C19-C3	-2.25	119.36	122.19
5	A	901	988	C28-C22-C19	-2.20	117.22	120.87
5	A	901	988	C22-C19-C3	-2.20	119.43	122.19
5	B	902	988	C24-C25-N50	2.19	120.63	118.74
5	C	903	988	C35-C15-C13	-2.17	117.52	122.51
5	A	901	988	C43-C42-N41	-2.15	119.94	123.60
5	D	904	988	C6-C5-N4	-2.13	120.85	123.97
5	B	902	988	C43-C42-N41	-2.10	120.02	123.60
5	A	901	988	C39-C40-N41	-2.09	120.03	123.60
5	C	903	988	C42-N41-C40	2.09	121.65	116.86
5	B	902	988	C42-N41-C40	2.07	121.60	116.86
5	A	901	988	C6-C5-N4	-2.02	121.01	123.97
5	B	902	988	C22-C19-C3	-2.02	119.66	122.19
5	C	903	988	C39-C40-N41	-2.00	120.18	123.60
5	D	904	988	C42-N41-C40	2.00	121.44	116.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	11	EDO	O1-C1-C2-O2
6	D	15	EDO	O1-C1-C2-O2
6	A	7	EDO	O1-C1-C2-O2
6	B	17	EDO	O1-C1-C2-O2
6	D	14	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	988	1	0
6	D	14	EDO	3	0

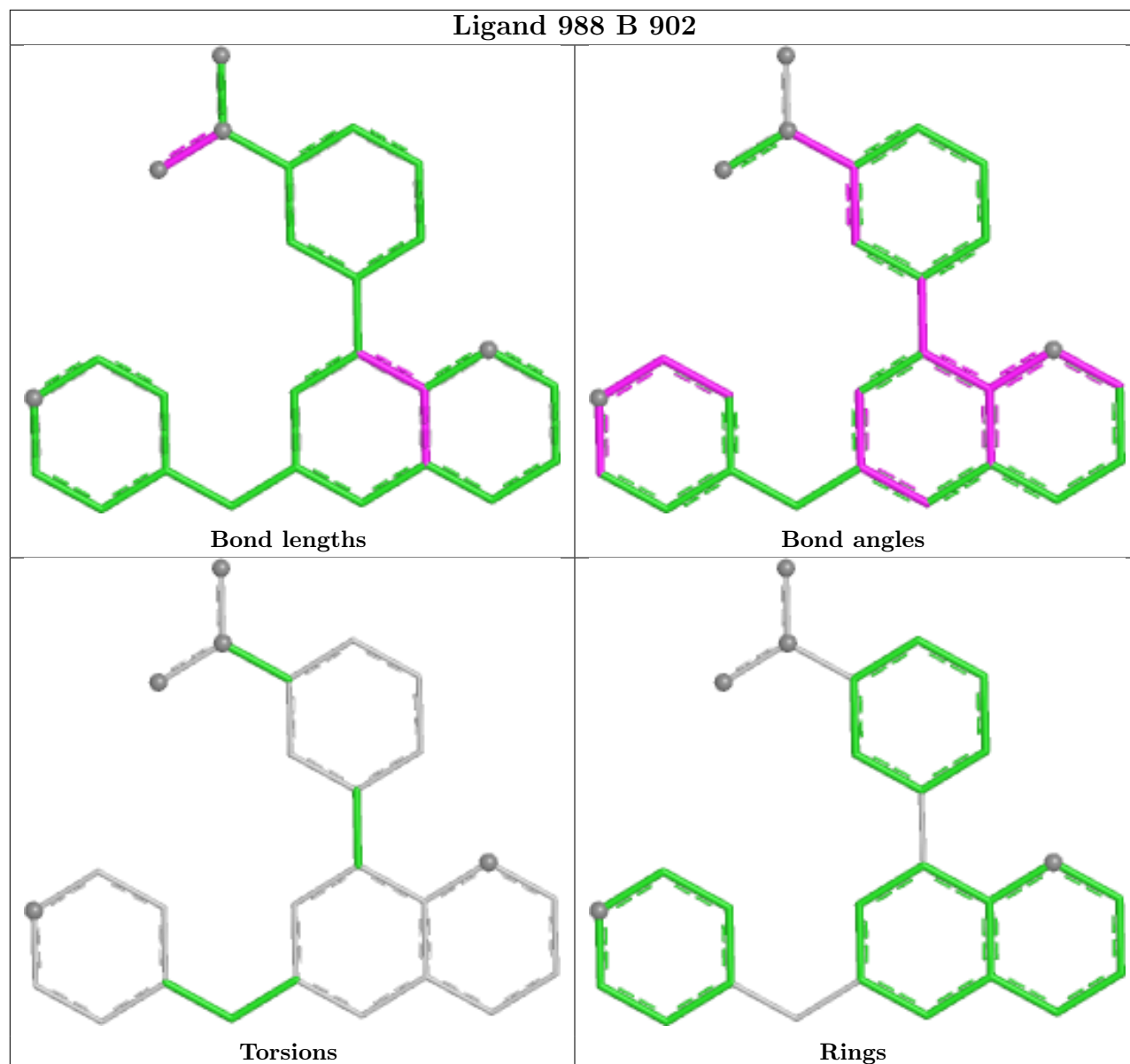
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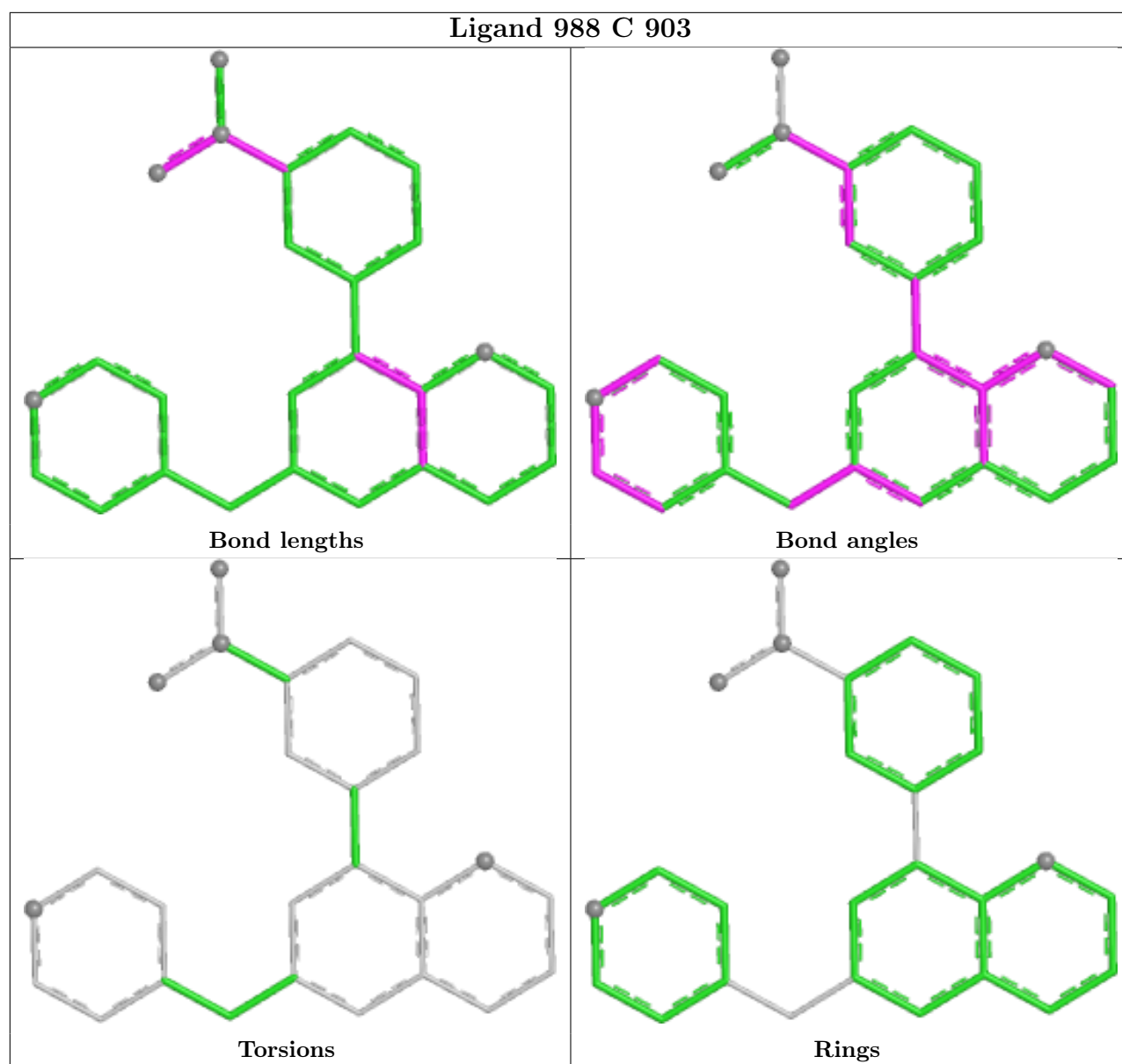
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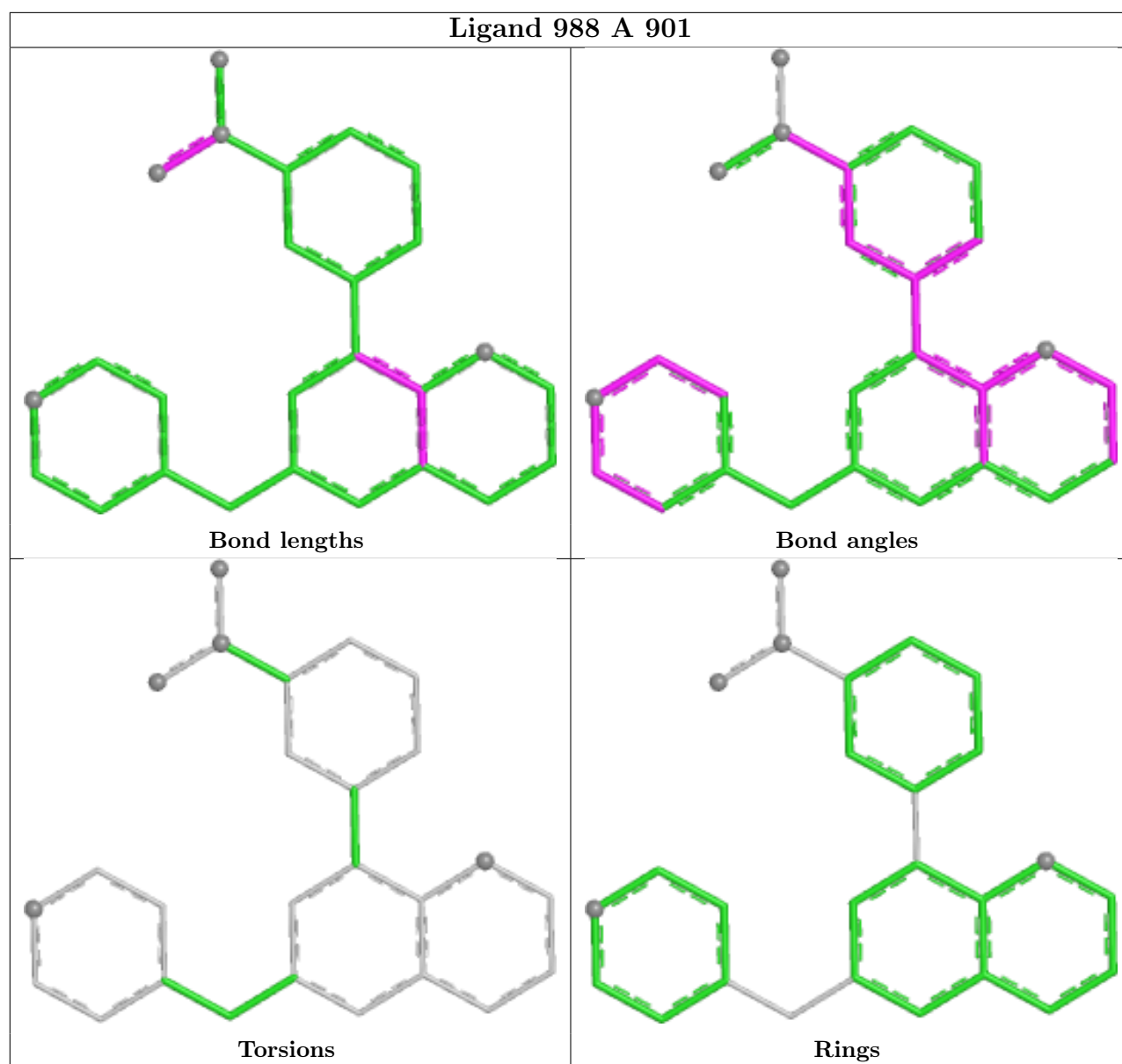
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	10	EDO	3	0
6	D	11	EDO	4	0
6	A	6	EDO	1	0

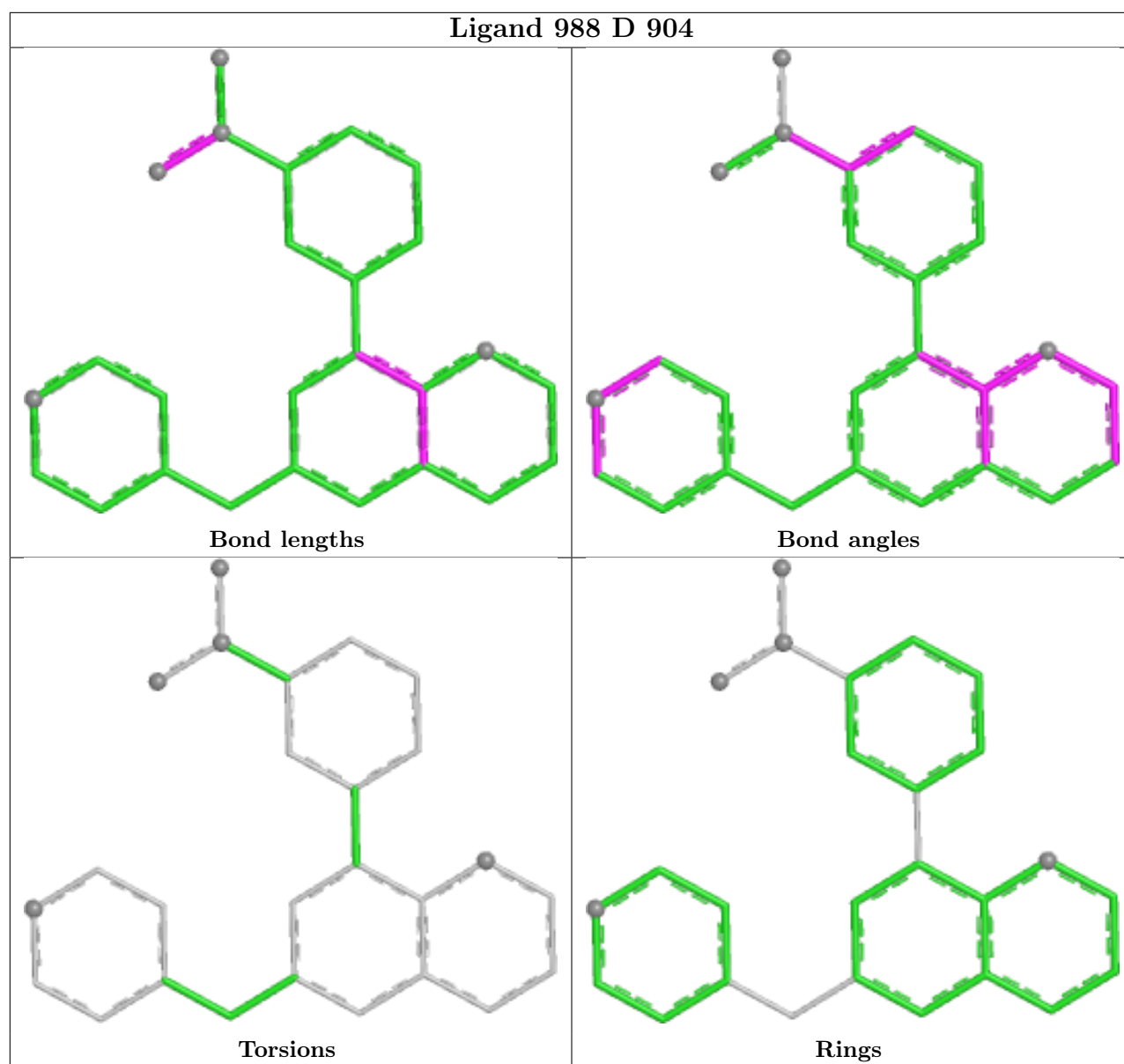
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 988 B 902









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	335/381 (87%)	-0.12	14 (4%) 40 40	15, 24, 57, 67	0
1	B	327/381 (85%)	-0.14	5 (1%) 72 73	16, 27, 43, 75	0
1	C	327/381 (85%)	-0.05	6 (1%) 67 69	15, 26, 58, 69	0
1	D	345/381 (90%)	-0.13	18 (5%) 33 33	15, 25, 60, 66	0
All	All	1334/1524 (87%)	-0.11	43 (3%) 50 50	15, 26, 54, 75	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	VAL	4.6
1	A	461	SER	4.6
1	A	460	SER	4.4
1	D	245	ILE	4.4
1	A	465	LEU	4.1
1	A	577	PRO	3.9
1	A	467	ASP	3.5
1	A	578	GLN	3.5
1	D	593	GLY	3.4
1	A	245	ILE	3.4
1	D	246	PRO	3.4
1	D	600	PHE	3.3
1	D	461	SER	3.2
1	D	595	THR	3.1
1	B	252	THR	3.1
1	D	603	THR	2.9
1	D	248	PHE	2.9
1	D	598	PHE	2.9
1	D	460	SER	2.7
1	C	462	GLY	2.7
1	C	465	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	602	LEU	2.7
1	D	251	LYS	2.6
1	A	457	LYS	2.6
1	B	253	GLU	2.5
1	A	248	PHE	2.5
1	C	459	THR	2.5
1	D	462	GLY	2.5
1	C	252	THR	2.5
1	D	541	TYR	2.4
1	C	464	LEU	2.4
1	A	493	GLN	2.3
1	B	254	GLN	2.3
1	A	459	THR	2.3
1	B	578	GLN	2.2
1	D	597	LYS	2.2
1	A	575	THR	2.2
1	A	463	VAL	2.1
1	A	244	SER	2.1
1	C	461	SER	2.1
1	D	253	GLU	2.1
1	D	252	THR	2.0
1	B	256	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	D	14	4/4	0.79	0.22	38,38,40,42	0

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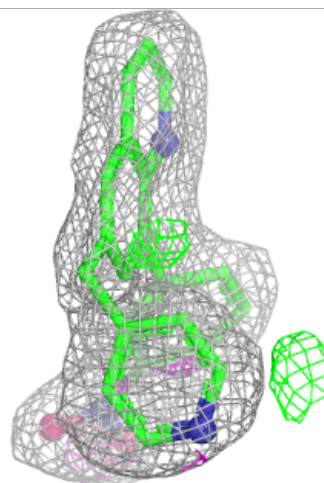
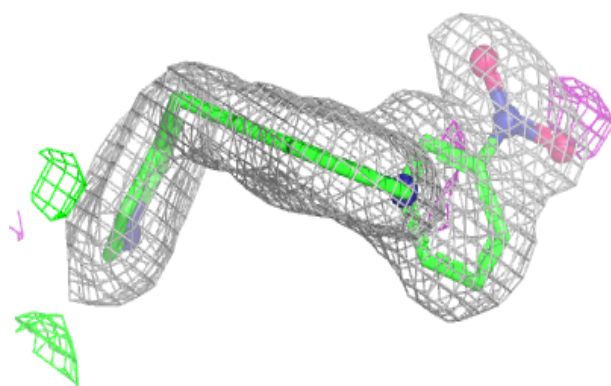
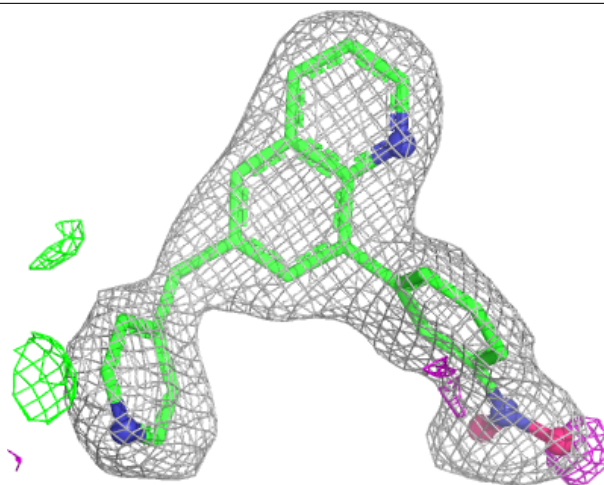
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	10	4/4	0.81	0.19	31,34,38,41	0
6	EDO	A	6	4/4	0.82	0.22	44,44,44,46	0
6	EDO	D	4	4/4	0.87	0.15	42,43,44,44	0
6	EDO	D	11	4/4	0.89	0.17	23,30,35,40	0
6	EDO	C	18	4/4	0.90	0.16	49,49,50,50	0
5	988	A	901	26/26	0.90	0.09	30,35,40,40	0
6	EDO	D	15	4/4	0.90	0.14	40,41,41,42	0
6	EDO	C	13	4/4	0.91	0.16	19,29,32,37	0
5	988	B	902	26/26	0.91	0.10	33,36,39,41	0
5	988	C	903	26/26	0.92	0.08	25,31,35,37	0
6	EDO	B	17	4/4	0.92	0.11	40,40,41,41	0
4	SO4	A	1	5/5	0.93	0.14	38,43,47,48	0
6	EDO	A	9	4/4	0.94	0.08	37,37,37,39	0
6	EDO	B	3	4/4	0.94	0.09	32,33,33,35	0
6	EDO	D	2	4/4	0.95	0.09	24,24,25,25	0
6	EDO	A	7	4/4	0.95	0.07	28,32,33,35	0
6	EDO	C	5	4/4	0.95	0.08	27,29,29,30	0
6	EDO	B	8	4/4	0.95	0.07	25,26,27,28	0
5	988	D	904	26/26	0.95	0.06	23,27,32,36	0
6	EDO	C	16	4/4	0.96	0.09	27,27,28,29	0
6	EDO	A	12	4/4	0.97	0.06	24,27,29,30	0
3	MG	B	625	1/1	0.98	0.02	22,22,22,22	0
3	MG	C	625	1/1	0.98	0.02	24,24,24,24	0
3	MG	A	625	1/1	0.99	0.07	22,22,22,22	0
3	MG	D	625	1/1	0.99	0.02	22,22,22,22	0
2	ZN	B	624	1/1	0.99	0.07	34,34,34,34	0
2	ZN	D	624	1/1	1.00	0.06	32,32,32,32	0
2	ZN	A	624	1/1	1.00	0.07	33,33,33,33	0
2	ZN	C	624	1/1	1.00	0.07	32,32,32,32	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.

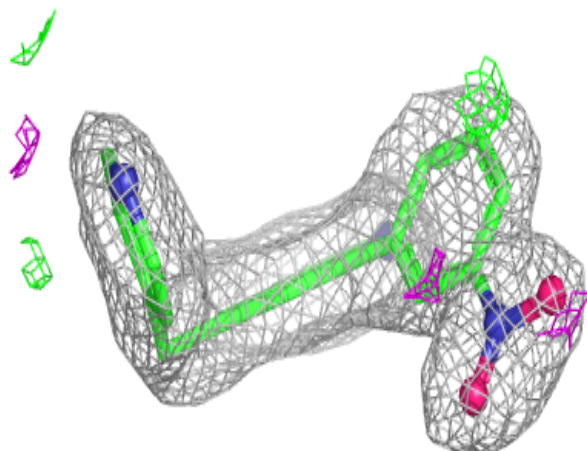
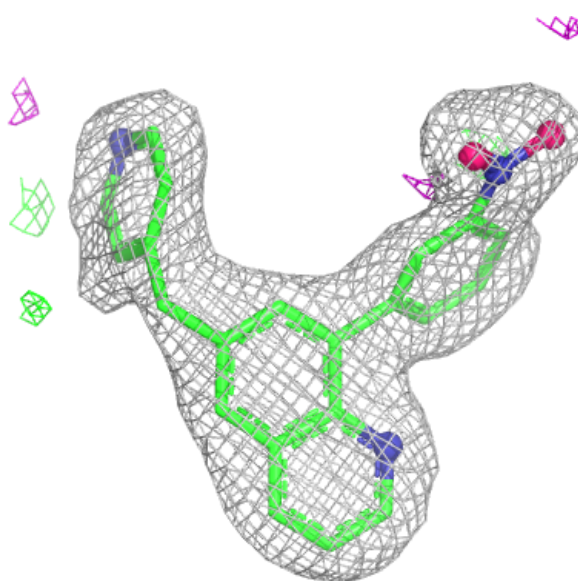
Electron density around 988 A 901:

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



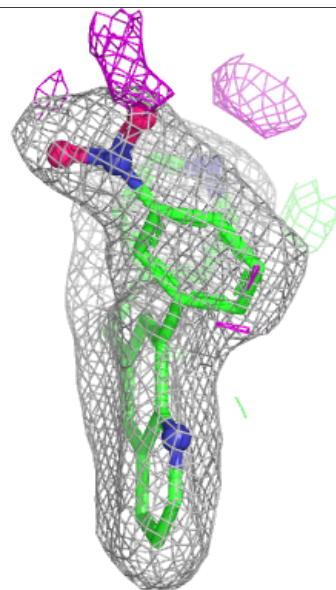
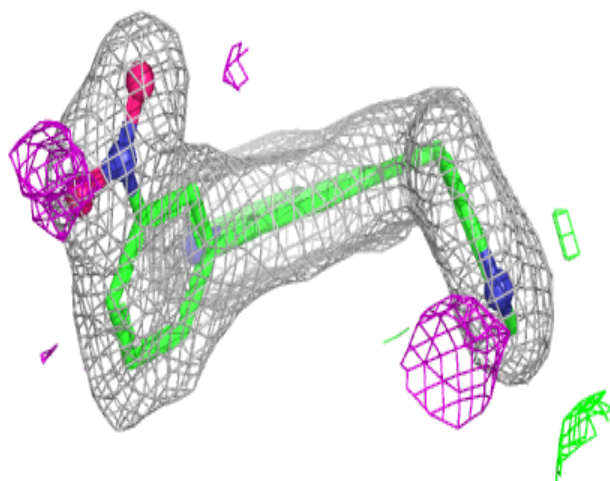
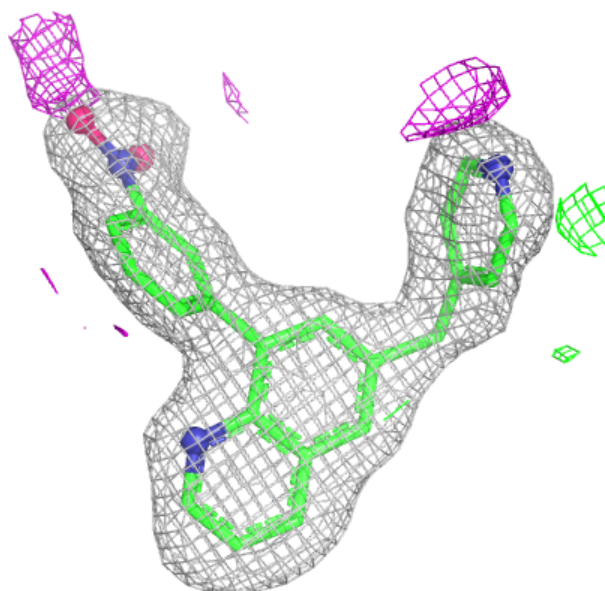
Electron density around 988 B 902:

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



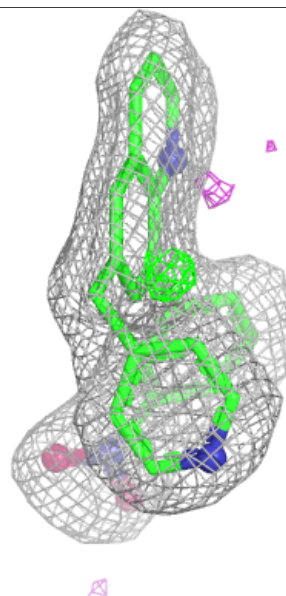
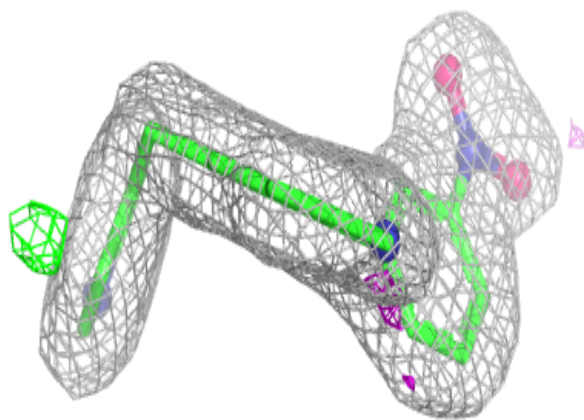
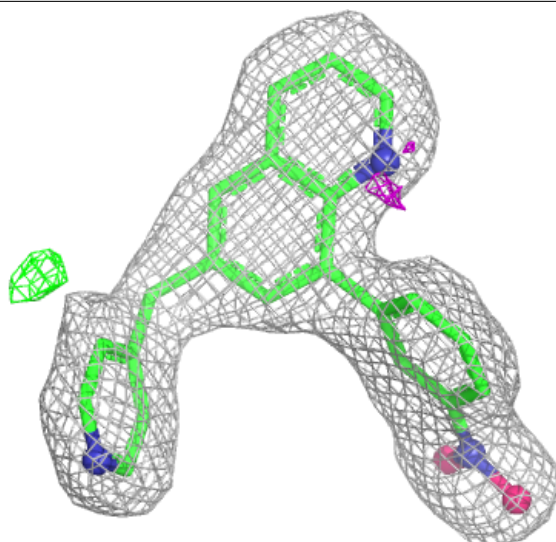
Electron density around 988 C 903:

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



Electron density around 988 D 904:

$2mF_o-DF_c$ (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.