



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:04 pm BST

PDB ID : 5XKM
Title : Crystal structure of human phosphodiesterase 2A in complex with 6-methyl-N-(1-(4-(trifluoromethoxy)phenyl)propyl)pyrazolo[1,5-a]pyrimidine-3-carboxamide
Authors : Oki, H.; Kondo, M.; Snell, G.; Lane, W.
Deposited on : 2017-05-08
Resolution : 2.16 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

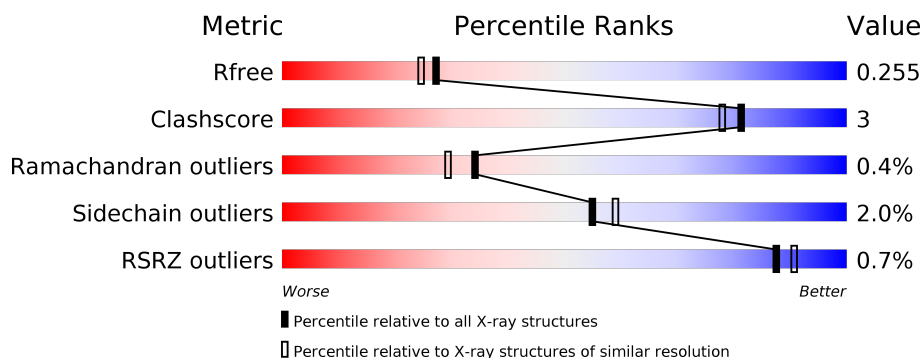
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	345	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	345	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	C	345	<div> <div></div> <div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	D	345	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
1	E	345	<div> <div></div> <div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>
1	F	345	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17394 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2784	1772	476	511	25			
1	B	345	Total	C	N	O	S	0	0	0
			2818	1791	483	519	25			
1	C	343	Total	C	N	O	S	0	1	0
			2806	1785	482	514	25			
1	D	337	Total	C	N	O	S	0	0	0
			2759	1759	473	502	25			
1	E	319	Total	C	N	O	S	0	0	0
			2618	1667	451	475	25			
1	F	321	Total	C	N	O	S	0	0	0
			2638	1680	455	478	25			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP O00408
A	576	HIS	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
B	575	GLY	-	expression tag	UNP O00408
B	576	HIS	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	UNP O00408
C	575	GLY	-	expression tag	UNP O00408
C	576	HIS	-	expression tag	UNP O00408
C	577	ALA	-	expression tag	UNP O00408
D	575	GLY	-	expression tag	UNP O00408
D	576	HIS	-	expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
E	575	GLY	-	expression tag	UNP O00408
E	576	HIS	-	expression tag	UNP O00408
E	577	ALA	-	expression tag	UNP O00408
F	575	GLY	-	expression tag	UNP O00408
F	576	HIS	-	expression tag	UNP O00408

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Chain	Residue	Modelled	Actual	Comment	Reference
F	577	ALA	-	expression tag	UNP O00408

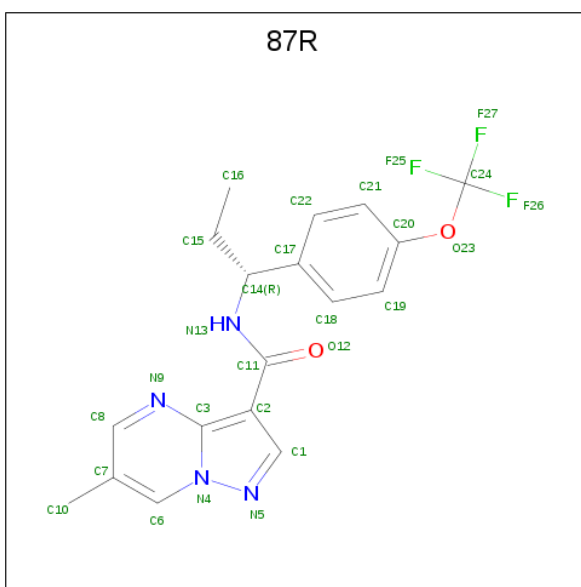
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Mg 2 2	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	2	Total Mg 2 2	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is 6-methyl-N-[(1R)-1-[4-(trifluoromethoxy)phenyl]propyl]pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: 87R) (formula: C₁₈H₁₇F₃N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
4	B	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
4	C	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
4	D	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
4	E	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
4	F	1	Total	C	F	N	O	0	0
			27	18	3	4	2		

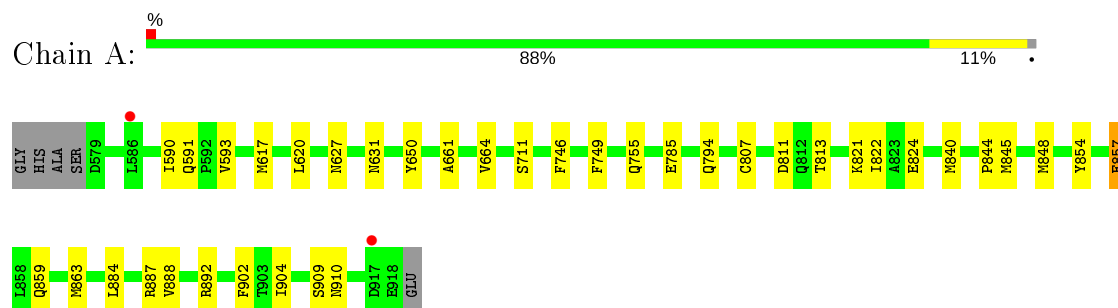
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	0
			144	144		
5	B	136	Total	O	0	0
			136	136		
5	C	144	Total	O	0	0
			144	144		
5	D	135	Total	O	0	0
			135	135		
5	E	113	Total	O	0	0
			113	113		
5	F	123	Total	O	0	0
			123	123		

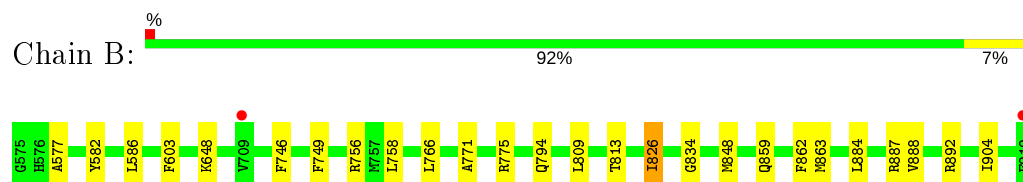
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

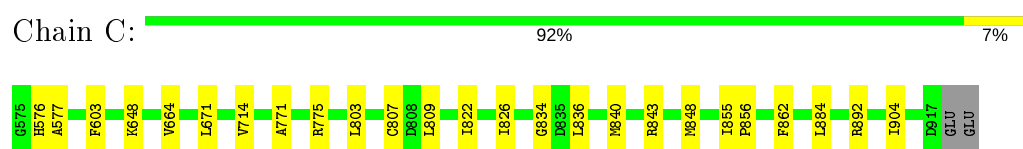
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



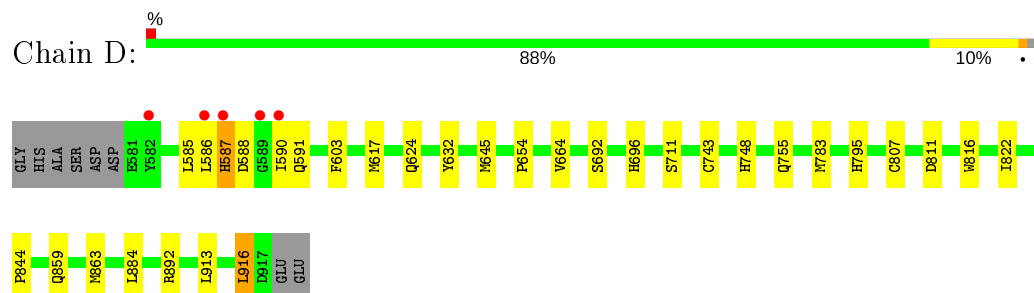
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



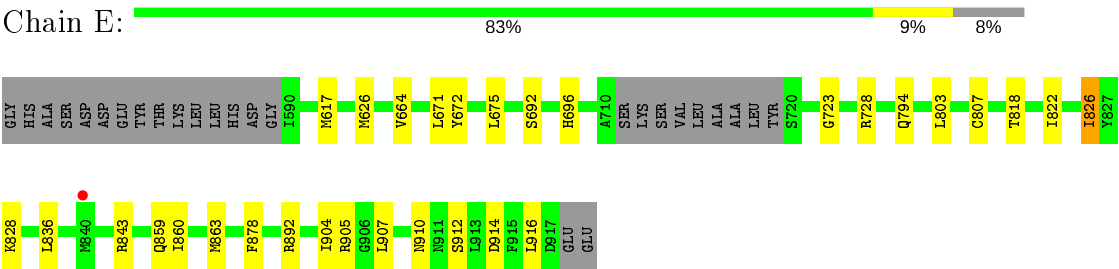
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



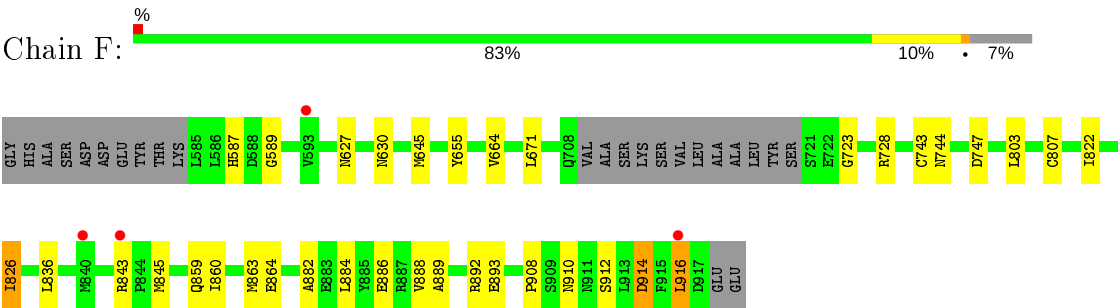
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



● Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.92Å 89.77Å 90.36Å 107.31° 113.85° 89.84°	Depositor
Resolution (Å)	84.82 – 2.16 49.06 – 2.16	Depositor EDS
% Data completeness (in resolution range)	95.0 (84.82-2.16) 95.0 (49.06-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.202 , 0.256 0.202 , 0.255	Depositor DCC
R_{free} test set	5035 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 10.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17394	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1506e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, 87R, 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	0.29	0/2851	0.46	0/3847
1	B	0.29	0/2886	0.47	0/3894
1	C	0.29	0/2877	0.46	0/3882
1	D	0.29	0/2826	0.48	1/3813 (0.0%)
1	E	0.29	0/2681	0.47	0/3615
1	F	0.30	0/2702	0.47	0/3643
All	All	0.29	0/16823	0.47	1/22694 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	587	HIS	CB-CA-C	5.47	121.34	110.40

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	2784	0	2719	18	0
1	B	2818	0	2745	13	0
1	C	2806	0	2741	14	0
1	D	2759	0	2705	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2618	0	2560	12	0
1	F	2638	0	2577	16	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	27	0	0	0	0
4	B	27	0	0	1	0
4	C	27	0	0	1	0
4	D	27	0	0	0	0
4	E	27	0	0	1	0
4	F	27	0	0	1	0
5	A	144	0	0	2	0
5	B	136	0	0	2	0
5	C	144	0	0	0	0
5	D	135	0	0	1	0
5	E	113	0	0	0	0
5	F	123	0	0	1	0
All	All	17394	0	16047	86	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 3.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:GLN:O	1:A:863:MET:HG2	1.84	0.77
1:B:859:GLN:O	1:B:863:MET:HG2	1.89	0.72
1:C:826:ILE:HD13	4:C:2003:87R:C1	2.23	0.68
1:B:904:ILE:HD11	1:C:904:ILE:HD11	1.81	0.62
1:D:590:ILE:HD11	1:D:624:GLN:HB2	1.83	0.60
1:C:822:ILE:HG22	1:C:826:ILE:HD12	1.81	0.60
1:E:859:GLN:O	1:E:863:MET:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:859:GLN:O	1:F:863:MET:HG2	2.04	0.58
1:B:826:ILE:HD13	4:B:2003:87R:C1	2.34	0.58
1:F:826:ILE:HD13	4:F:2003:87R:C1	2.35	0.56
1:A:617:MET:HG3	5:A:2222:HOH:O	2.07	0.54
1:D:913:LEU:HB3	1:D:916:LEU:HD22	1.90	0.54
1:D:654:PRO:HD2	1:D:829:GLU:HG3	1.89	0.53
1:D:859:GLN:O	1:D:863:MET:HG2	2.09	0.53
1:A:794:GLN:NE2	5:A:2102:HOH:O	2.41	0.52
1:D:632:TYR:O	1:D:748:HIS:NE2	2.27	0.52
1:F:645:MET:HG3	1:F:743:CYS:SG	2.49	0.52
1:D:816:TRP:HZ2	1:F:916:LEU:HD13	1.75	0.52
1:F:723:GLY:O	1:F:728:ARG:NH1	2.43	0.51
1:D:617:MET:HG3	5:D:2208:HOH:O	2.11	0.51
1:C:671:LEU:HD13	1:C:803:LEU:HD22	1.93	0.51
1:E:826:ILE:HD13	4:E:2003:87R:C1	2.41	0.50
1:F:882:ALA:O	1:F:886:GLU:HG2	2.13	0.49
1:D:645:MET:HG3	1:D:743:CYS:SG	2.52	0.48
1:D:811:ASP:HB3	1:D:822:ILE:HG13	1.95	0.48
1:D:711:SER:HA	1:D:840:MET:HE1	1.96	0.47
1:D:783:MET:HG3	1:D:795:HIS:CE1	2.49	0.47
1:F:671:LEU:HD13	1:F:803:LEU:HD22	1.95	0.47
1:A:813:THR:O	1:A:887:ARG:HD2	2.14	0.47
1:E:723:GLY:O	1:E:728:ARG:NH1	2.48	0.47
1:A:664:VAL:HG13	1:A:807:CYS:HB3	1.97	0.47
1:C:855:ILE:HB	1:C:856:PRO:HD3	1.97	0.46
1:D:664:VAL:HG13	1:D:807:CYS:HB3	1.97	0.46
1:B:582:TYR:O	1:B:586:LEU:HB2	2.15	0.46
5:B:2140:HOH:O	1:C:855:ILE:HG12	2.15	0.46
1:F:884:LEU:O	1:F:888:VAL:HG23	2.15	0.46
1:E:671:LEU:HD13	1:E:803:LEU:HD22	1.97	0.46
1:A:811:ASP:HB3	1:A:822:ILE:HG13	1.97	0.46
1:C:843:ARG:HD3	1:C:843:ARG:HA	1.83	0.46
1:D:585:LEU:C	1:D:587:HIS:H	2.19	0.46
1:E:664:VAL:HG13	1:E:807:CYS:HB3	1.99	0.45
1:D:587:HIS:O	1:D:588:ASP:C	2.54	0.45
1:A:854:TYR:HD2	1:A:857:GLU:HB2	1.82	0.45
1:E:626:MET:HG2	1:E:672:TYR:CD2	2.52	0.45
1:A:627:ASN:O	1:A:631:ASN:HB2	2.17	0.45
1:C:809:LEU:HD22	1:C:862:PHE:HZ	1.81	0.44
1:E:692:SER:O	1:E:696:HIS:HB3	2.16	0.44
1:A:650:TYR:CZ	1:A:661:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:860:ILE:O	1:F:864:GLU:HG2	2.18	0.44
1:C:771:ALA:O	1:C:775:ARG:HG3	2.18	0.44
1:A:711:SER:HA	1:A:840:MET:HE1	1.99	0.44
1:A:845:MET:HG2	1:A:848:MET:CG	2.48	0.43
1:A:884:LEU:O	1:A:888:VAL:HG23	2.17	0.43
1:F:912:SER:OG	1:F:914:ASP:HB2	2.18	0.43
1:A:904:ILE:HD11	1:E:904:ILE:HG12	2.01	0.43
1:D:843:ARG:HA	1:D:844:PRO:HD3	1.91	0.43
1:C:577:ALA:HB3	1:C:648:LYS:HE3	2.01	0.43
1:C:834:GLY:HA3	1:C:848:MET:O	2.19	0.43
1:F:664:VAL:HG13	1:F:807:CYS:HB3	1.99	0.43
1:B:834:GLY:HA3	1:B:848:MET:O	2.19	0.42
1:B:809:LEU:HD22	1:B:862:PHE:HZ	1.84	0.42
1:C:603:PHE:CD1	1:C:884:LEU:HD21	2.54	0.42
1:C:664:VAL:HG13	1:C:807:CYS:HB3	2.00	0.42
1:F:627:ASN:HD21	1:F:630:ASN:HD22	1.66	0.42
1:B:813:THR:O	1:B:887:ARG:HD2	2.20	0.42
1:F:587:HIS:HA	5:F:4083:HOH:O	2.18	0.42
1:F:655:TYR:CE1	1:F:822:ILE:HG23	2.54	0.42
1:A:746:PHE:O	1:A:749:PHE:HB2	2.20	0.42
1:B:746:PHE:O	1:B:749:PHE:HB2	2.20	0.42
1:E:818:THR:O	1:E:822:ILE:HG12	2.19	0.41
1:E:912:SER:OG	1:E:914:ASP:HB2	2.20	0.41
1:B:603:PHE:CD1	1:B:884:LEU:HD21	2.56	0.41
1:B:771:ALA:O	1:B:775:ARG:HG3	2.21	0.41
1:D:603:PHE:CD1	1:D:884:LEU:HD21	2.56	0.41
1:F:889:ALA:O	1:F:893:GLU:HG2	2.21	0.41
1:A:821:LYS:O	1:A:824:GLU:HB2	2.20	0.41
1:A:844:PRO:HB2	1:A:848:MET:HB2	2.02	0.41
1:B:756:ARG:NE	5:B:2101:HOH:O	2.36	0.41
1:B:884:LEU:O	1:B:888:VAL:HG23	2.21	0.41
1:A:617:MET:HE1	1:A:620:LEU:HD12	2.02	0.41
1:B:577:ALA:HB3	1:B:648:LYS:HE3	2.03	0.40
1:C:836:LEU:O	1:C:840:MET:HG2	2.21	0.40
1:D:692:SER:O	1:D:696:HIS:HB3	2.21	0.40
1:F:744:ASN:HB3	1:F:747:ASP:HB3	2.03	0.40
1:E:675:LEU:HD22	1:E:878:PHE:HB3	2.03	0.40
1:A:902:PHE:CE2	1:E:916:LEU:HD21	2.56	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	338/345 (98%)	331 (98%)	5 (2%)	2 (1%)	25	18
1	B	343/345 (99%)	334 (97%)	9 (3%)	0	100	100
1	C	342/345 (99%)	337 (98%)	4 (1%)	1 (0%)	41	37
1	D	335/345 (97%)	327 (98%)	7 (2%)	1 (0%)	41	37
1	E	315/345 (91%)	306 (97%)	8 (2%)	1 (0%)	41	37
1	F	317/345 (92%)	308 (97%)	7 (2%)	2 (1%)	25	18
All	All	1990/2070 (96%)	1943 (98%)	40 (2%)	7 (0%)	34	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	908	PRO
1	C	576	HIS
1	A	910	ASN
1	D	586	LEU
1	E	910	ASN
1	A	909	SER
1	F	589	GLY

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	307/310 (99%)	300 (98%)	7 (2%)	50	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	310/310 (100%)	305 (98%)	5 (2%)	62	67
1	C	309/310 (100%)	307 (99%)	2 (1%)	86	90
1	D	304/310 (98%)	300 (99%)	4 (1%)	69	74
1	E	289/310 (93%)	279 (96%)	10 (4%)	36	34
1	F	291/310 (94%)	283 (97%)	8 (3%)	44	46
All	All	1810/1860 (97%)	1774 (98%)	36 (2%)	55	59

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	590	ILE
1	A	591	GLN
1	A	593	VAL
1	A	755	GLN
1	A	785	GLU
1	A	857	GLU
1	A	892	ARG
1	B	758	LEU
1	B	766	LEU
1	B	794	GLN
1	B	826	ILE
1	B	892	ARG
1	C	714	VAL
1	C	892	ARG
1	D	591	GLN
1	D	755	GLN
1	D	892	ARG
1	D	916	LEU
1	E	617	MET
1	E	794	GLN
1	E	826	ILE
1	E	828	LYS
1	E	836	LEU
1	E	843	ARG
1	E	860	ILE
1	E	892	ARG
1	E	905	ARG
1	E	907	LEU
1	F	826	ILE
1	F	836	LEU

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Mol	Chain	Res	Type
1	F	843	ARG
1	F	845	MET
1	F	892	ARG
1	F	910	ASN
1	F	914	ASP
1	F	916	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	GLN
1	A	794	GLN
1	A	859	GLN
1	B	708	GLN
1	B	900	HIS
1	B	911	ASN
1	C	679	ASN
1	C	911	ASN
1	D	708	GLN
1	D	755	GLN
1	E	624	GLN
1	E	733	GLN
1	E	859	GLN
1	E	911	ASN
1	F	627	ASN
1	F	910	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 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	87R	F	2003	-	24,29,29	1.53	3 (12%)	32,42,42	1.61	5 (15%)
4	87R	D	2004	-	24,29,29	1.51	4 (16%)	32,42,42	1.55	5 (15%)
4	87R	A	2004	-	24,29,29	1.48	4 (16%)	32,42,42	1.45	4 (12%)
4	87R	E	2003	-	24,29,29	1.53	3 (12%)	32,42,42	1.68	4 (12%)
4	87R	C	2003	-	24,29,29	1.51	3 (12%)	32,42,42	1.54	3 (9%)
4	87R	B	2003	-	24,29,29	1.51	3 (12%)	32,42,42	1.56	5 (15%)

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	87R	F	2003	-	-	0/17/19/19	0/3/3/3
4	87R	D	2004	-	-	0/17/19/19	0/3/3/3
4	87R	A	2004	-	-	0/17/19/19	0/3/3/3
4	87R	E	2003	-	-	0/17/19/19	0/3/3/3
4	87R	C	2003	-	-	0/17/19/19	0/3/3/3
4	87R	B	2003	-	-	0/17/19/19	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2004	87R	C6-C7	4.45	1.47	1.39
4	F	2003	87R	C6-C7	4.40	1.47	1.39
4	E	2003	87R	C6-C7	4.38	1.47	1.39
4	B	2003	87R	C6-C7	4.36	1.47	1.39
4	D	2004	87R	C6-C7	4.34	1.47	1.39
4	C	2003	87R	C6-C7	4.27	1.47	1.39
4	E	2003	87R	C2-C11	-3.94	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2003	87R	C2-C11	-3.83	1.44	1.50
4	C	2003	87R	C2-C11	-3.82	1.44	1.50
4	D	2004	87R	C2-C11	-3.76	1.44	1.50
4	B	2003	87R	C2-C11	-3.68	1.44	1.50
4	A	2004	87R	C2-C11	-3.59	1.44	1.50
4	B	2003	87R	C8-C7	-2.05	1.34	1.38
4	A	2004	87R	C8-C7	-2.04	1.34	1.38
4	C	2003	87R	C8-C7	-2.04	1.34	1.38
4	D	2004	87R	C8-C7	-2.03	1.34	1.38
4	E	2003	87R	C8-C7	-2.03	1.34	1.38
4	F	2003	87R	C8-C7	-2.02	1.34	1.38
4	A	2004	87R	O23-C24	2.00	1.43	1.31
4	D	2004	87R	O23-C24	2.00	1.43	1.31

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2003	87R	C15-C14-C17	-6.15	105.73	112.52
4	F	2003	87R	C15-C14-C17	-5.13	106.86	112.52
4	F	2003	87R	C6-C7-C8	5.10	123.63	115.93
4	E	2003	87R	C6-C7-C8	5.09	123.61	115.93
4	A	2004	87R	C6-C7-C8	5.06	123.58	115.93
4	C	2003	87R	C6-C7-C8	5.04	123.55	115.93
4	D	2004	87R	C6-C7-C8	5.02	123.51	115.93
4	C	2003	87R	C15-C14-C17	-4.96	107.05	112.52
4	B	2003	87R	C6-C7-C8	4.88	123.31	115.93
4	B	2003	87R	C15-C14-C17	-4.87	107.15	112.52
4	D	2004	87R	C15-C14-C17	-4.29	107.79	112.52
4	A	2004	87R	C15-C14-C17	-4.01	108.09	112.52
4	D	2004	87R	C16-C15-C14	-2.83	110.56	113.70
4	A	2004	87R	C24-O23-C20	-2.41	110.05	118.01
4	D	2004	87R	C10-C7-C6	-2.39	116.39	120.51
4	F	2003	87R	C10-C7-C6	-2.37	116.42	120.51
4	B	2003	87R	C16-C15-C14	-2.36	111.08	113.70
4	E	2003	87R	C10-C7-C6	-2.23	116.66	120.51
4	D	2004	87R	C24-O23-C20	-2.23	110.66	118.01
4	B	2003	87R	C24-O23-C20	-2.22	110.68	118.01
4	A	2004	87R	C10-C7-C6	-2.21	116.69	120.51
4	B	2003	87R	C10-C7-C6	-2.18	116.74	120.51
4	F	2003	87R	C16-C15-C14	-2.18	111.28	113.70
4	C	2003	87R	C24-O23-C20	-2.11	111.03	118.01
4	E	2003	87R	C24-O23-C20	-2.07	111.17	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2003	87R	C24-O23-C20	-2.02	111.34	118.01

There are no chirality outliers.

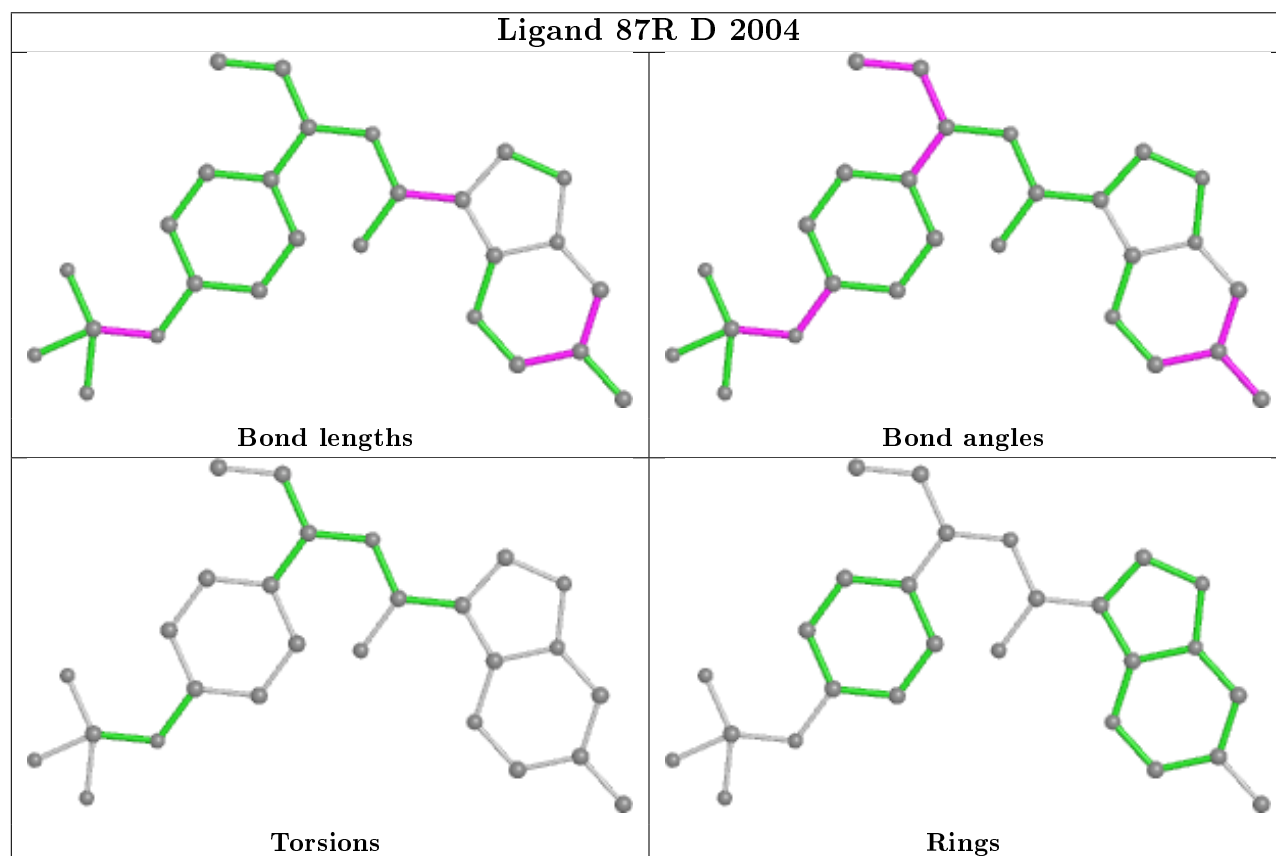
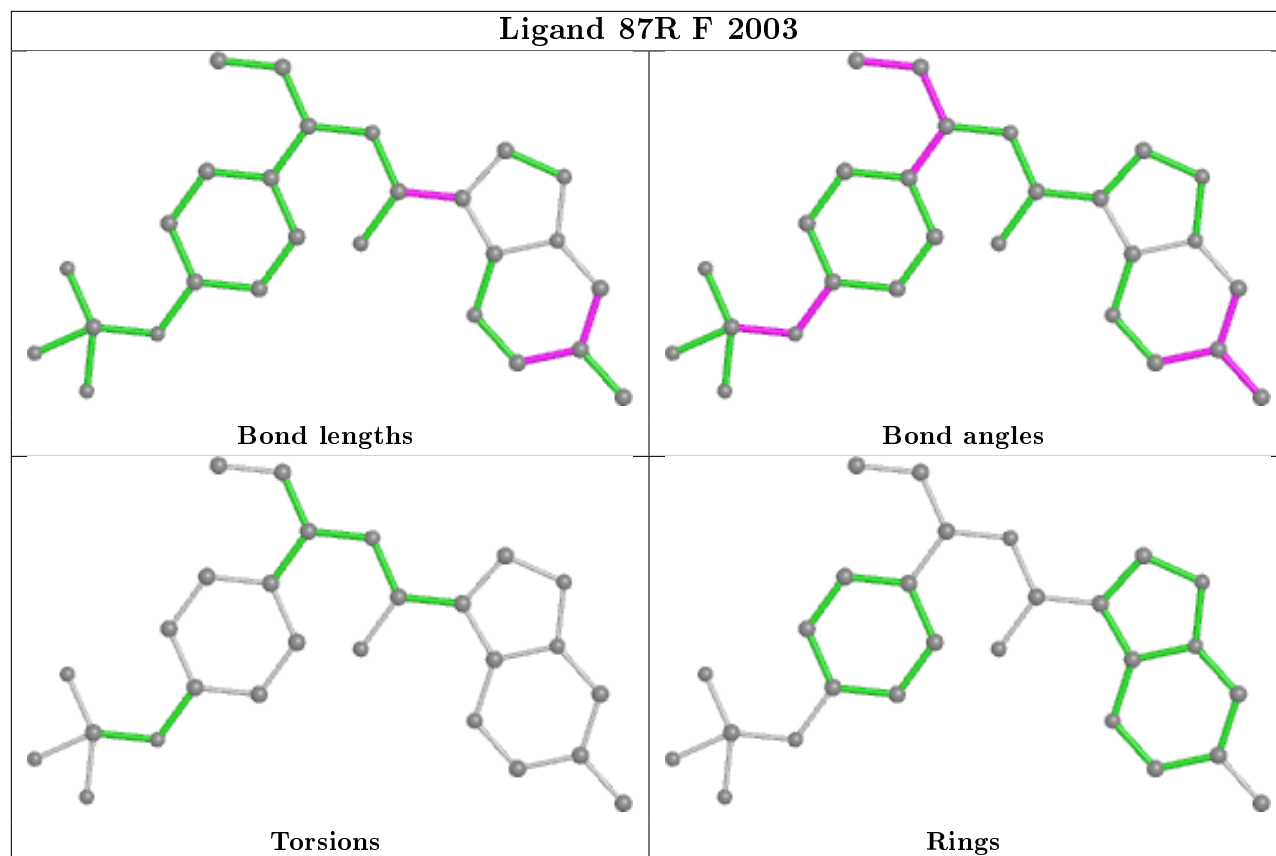
There are no torsion outliers.

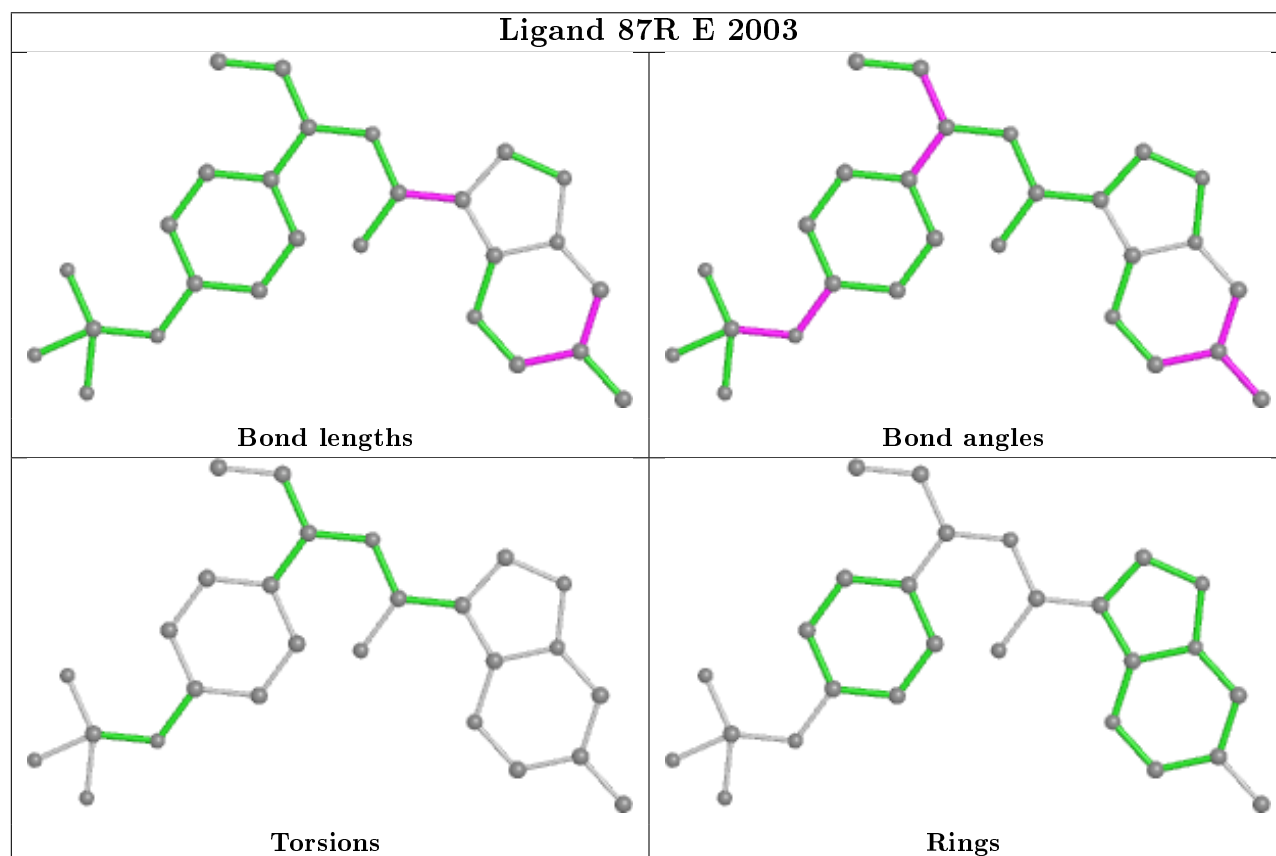
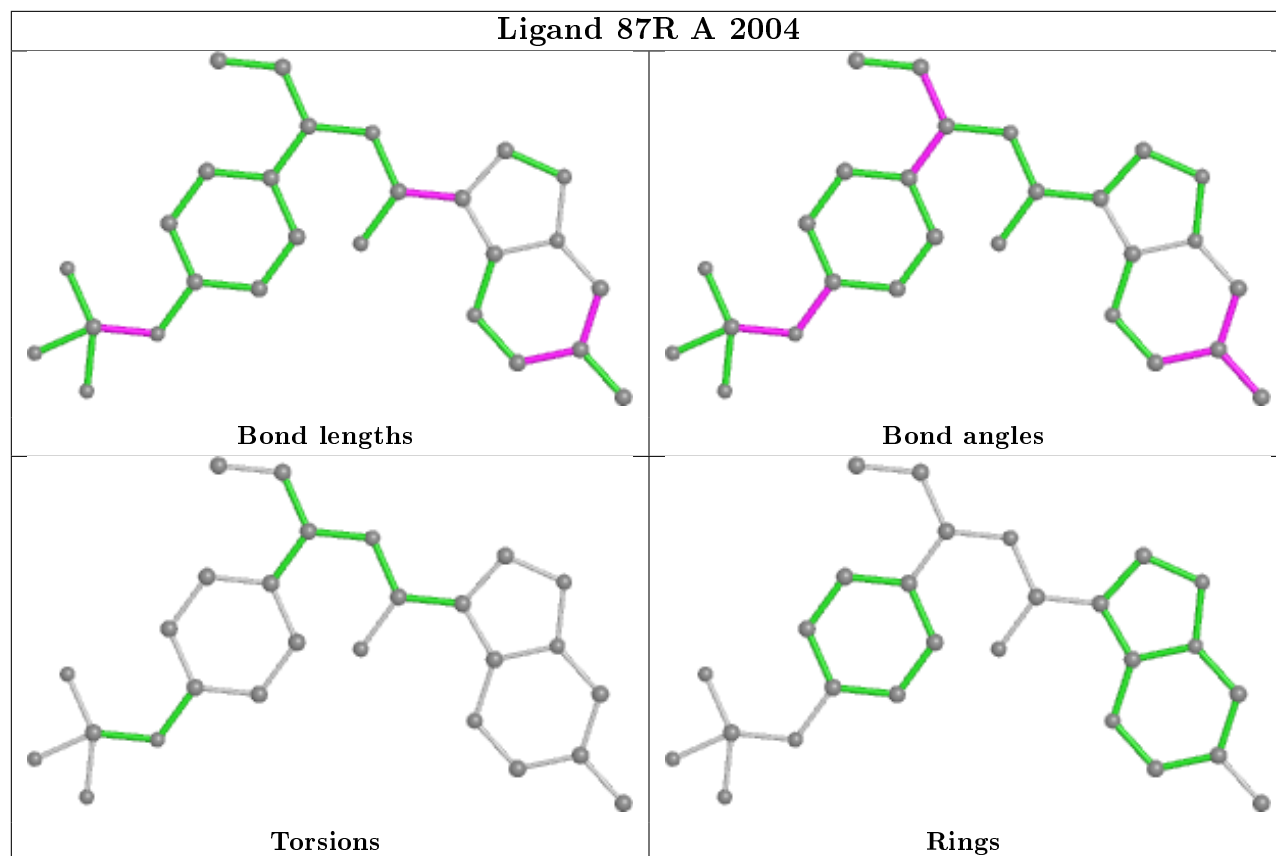
There are no ring outliers.

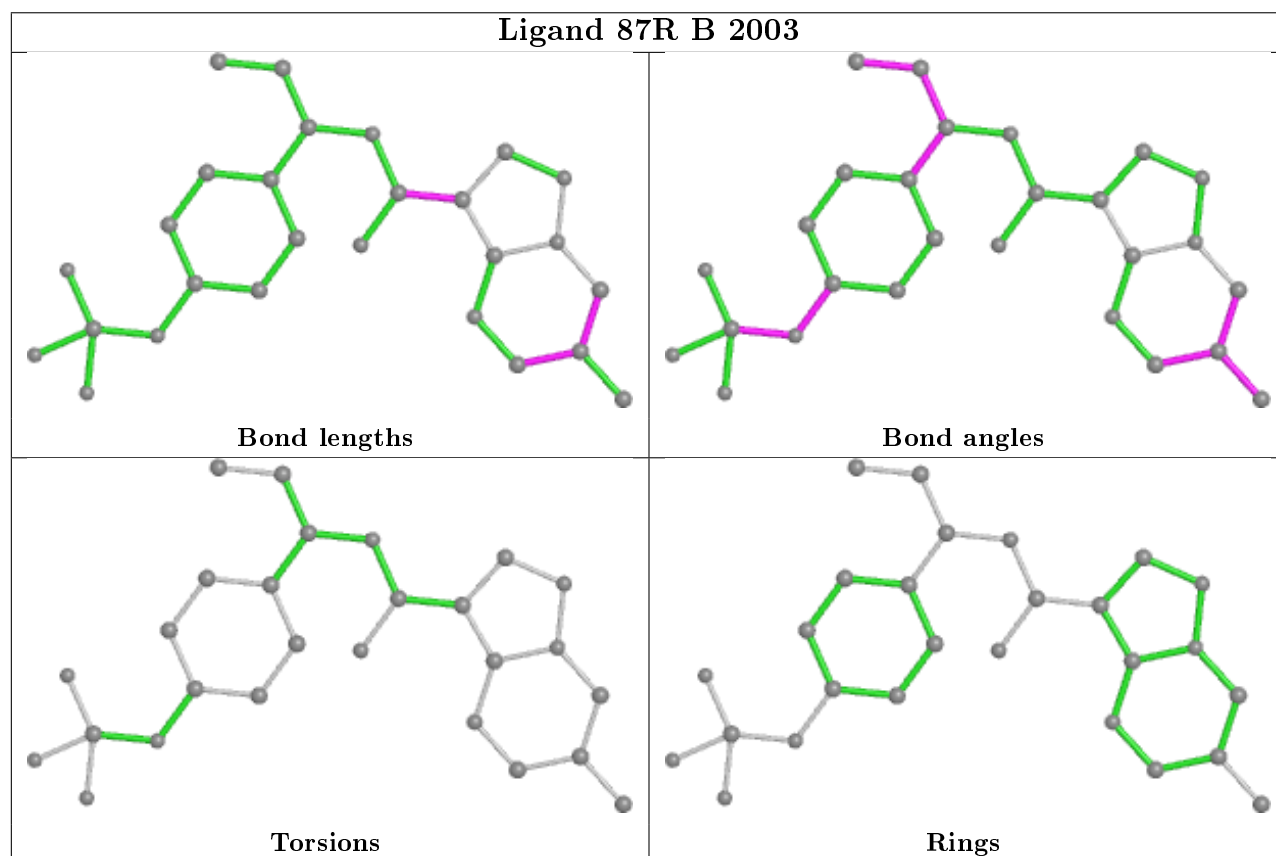
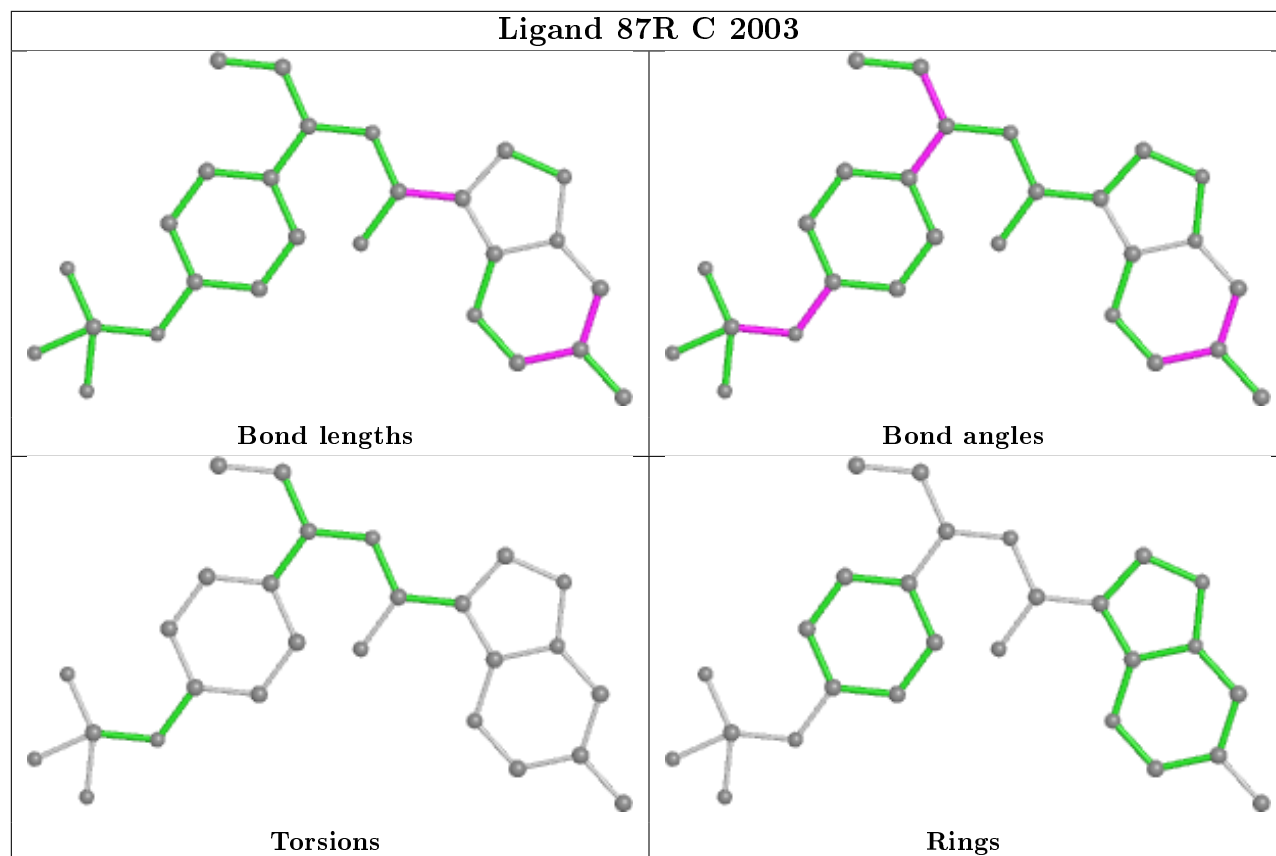
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2003	87R	1	0
4	E	2003	87R	1	0
4	C	2003	87R	1	0
4	B	2003	87R	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.







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	340/345 (98%)	-0.18	2 (0%) 89 91	11, 23, 46, 74	0
1	B	345/345 (100%)	-0.15	2 (0%) 89 91	10, 23, 44, 93	0
1	C	343/345 (99%)	-0.21	0 100 100	10, 23, 42, 62	0
1	D	337/345 (97%)	-0.15	5 (1%) 73 79	11, 24, 47, 93	0
1	E	319/345 (92%)	-0.11	1 (0%) 94 95	13, 27, 49, 83	0
1	F	321/345 (93%)	-0.06	4 (1%) 79 83	13, 26, 53, 78	0
All	All	2005/2070 (96%)	-0.14	14 (0%) 87 91	10, 24, 47, 93	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	589	GLY	4.1
1	B	709	VAL	3.3
1	D	582	TYR	3.2
1	F	593	VAL	3.1
1	E	840	MET	2.8
1	D	586	LEU	2.8
1	A	586	LEU	2.4
1	D	587	HIS	2.4
1	B	919	GLU	2.4
1	D	590	ILE	2.3
1	F	916	LEU	2.2
1	F	843	ARG	2.2
1	F	840	MET	2.1
1	A	917	ASP	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

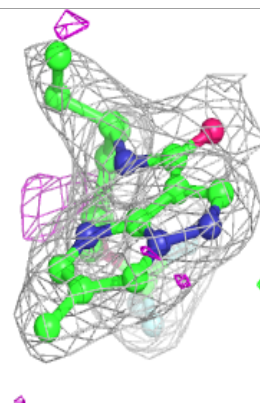
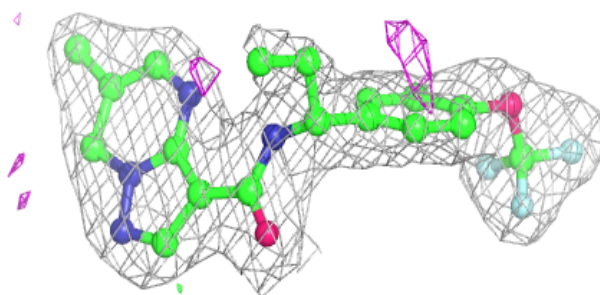
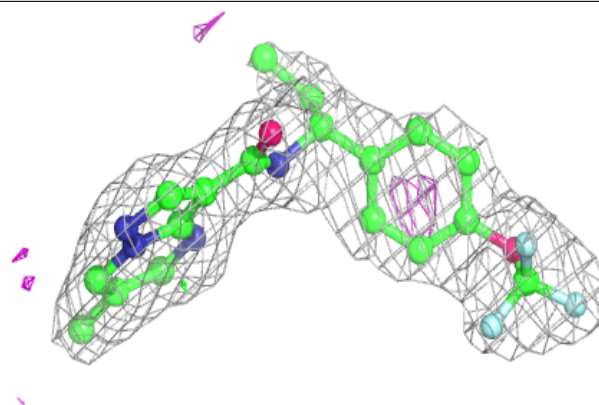
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	2003	1/1	0.93	0.07	35,35,35,35	0
4	87R	C	2003	27/27	0.95	0.12	19,22,26,28	0
2	MG	C	2001	1/1	0.95	0.16	15,15,15,15	0
4	87R	D	2004	27/27	0.96	0.10	20,23,28,32	0
4	87R	A	2004	27/27	0.96	0.10	18,20,23,25	0
4	87R	E	2003	27/27	0.96	0.10	20,22,27,32	0
4	87R	F	2003	27/27	0.96	0.10	19,21,30,32	0
2	MG	F	2001	1/1	0.96	0.06	14,14,14,14	0
4	87R	B	2003	27/27	0.96	0.12	19,21,23,25	0
2	MG	B	2001	1/1	0.97	0.09	17,17,17,17	0
2	MG	D	2003	1/1	0.97	0.06	26,26,26,26	0
2	MG	E	2001	1/1	0.98	0.11	15,15,15,15	0
2	MG	D	2001	1/1	0.98	0.11	14,14,14,14	0
2	MG	A	2001	1/1	0.99	0.06	15,15,15,15	0
3	ZN	E	2002	1/1	1.00	0.06	19,19,19,19	0
3	ZN	B	2002	1/1	1.00	0.07	17,17,17,17	0
3	ZN	A	2002	1/1	1.00	0.08	15,15,15,15	0
3	ZN	C	2002	1/1	1.00	0.08	17,17,17,17	0
3	ZN	F	2002	1/1	1.00	0.08	17,17,17,17	0
3	ZN	D	2002	1/1	1.00	0.06	15,15,15,15	0

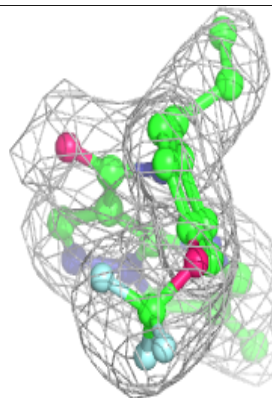
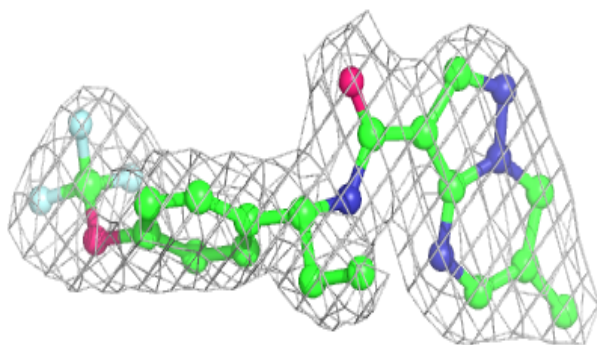
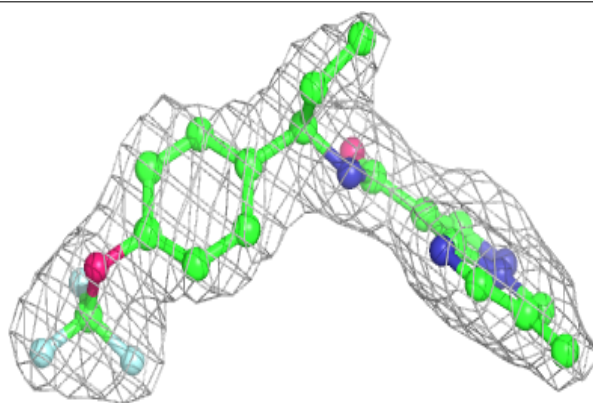
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 87R C 2003:

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

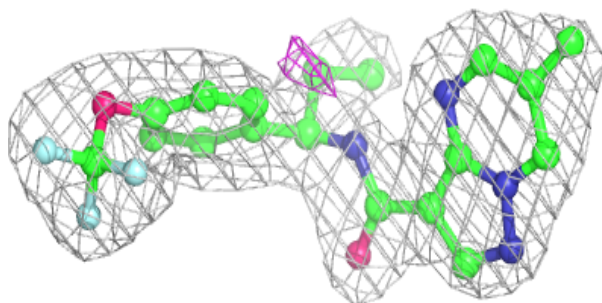
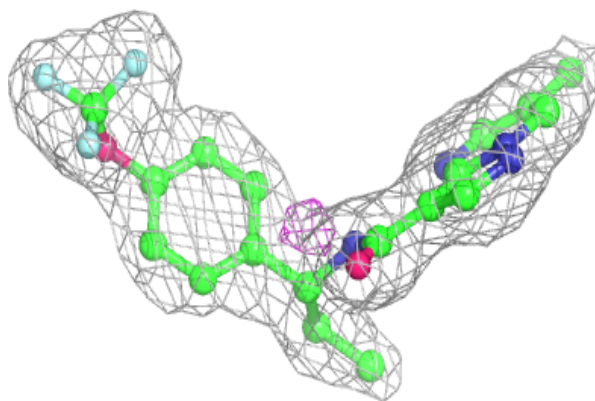
**Electron density around 87R D 2004:**

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

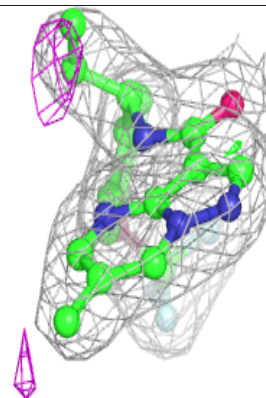
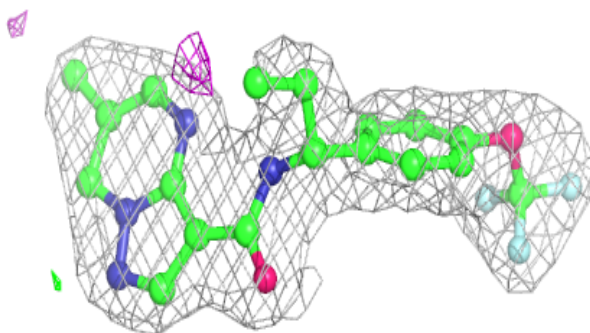
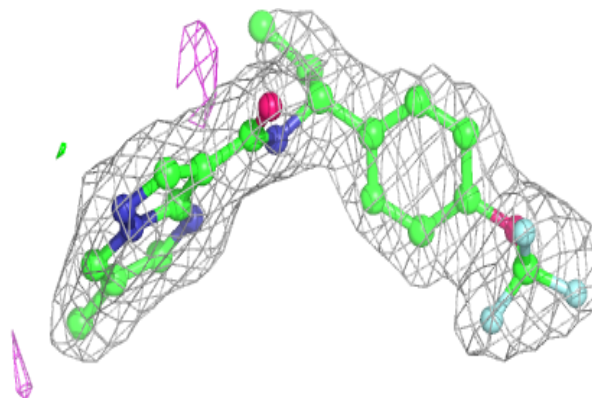


Electron density around 87R A 2004:

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

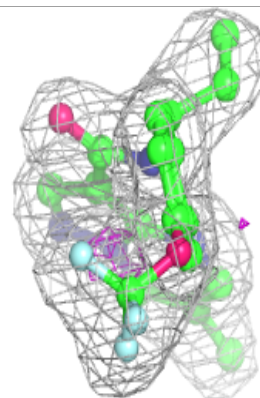
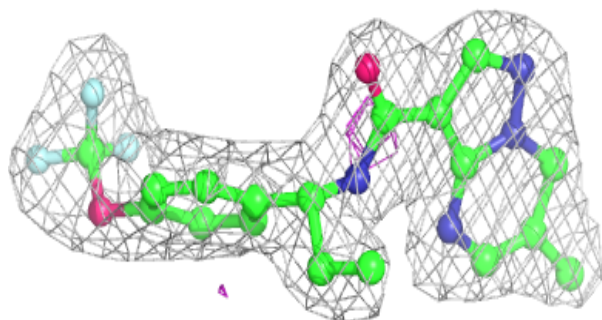
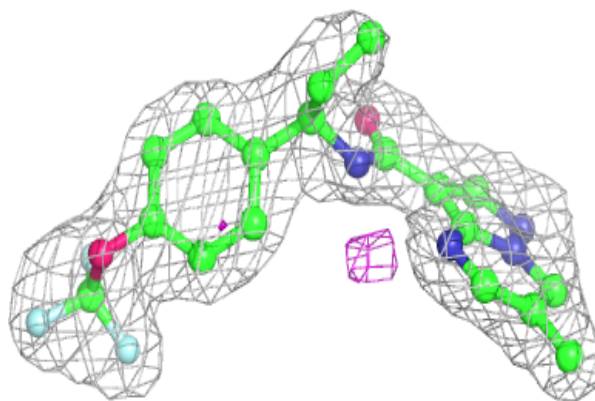
**Electron density around 87R E 2003:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

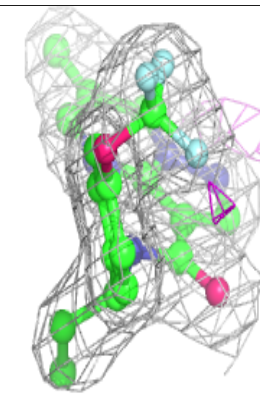
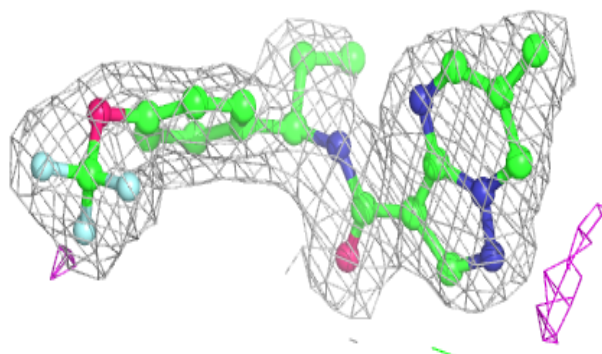
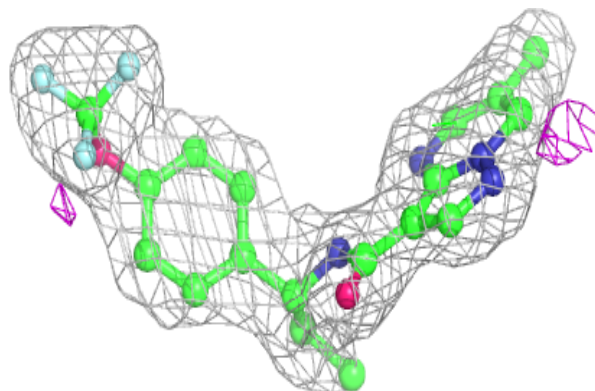


Electron density around 87R F 2003:

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

**Electron density around 87R B 2003:**

$2mF_o-DF_c$ (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.