



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:02 am BST

PDB ID : 2FM0  
Title : Crystal structure of PDE4D in complex with L-869298  
Authors : Huai, Q.; Sun, Y.; Wang, H.; Macdonald, D.; Aspiotis, R.; Robinson, H.;  
Huang, Z.; Ke, H.  
Deposited on : 2006-01-06  
Resolution : 2.00 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](mailto: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.

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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

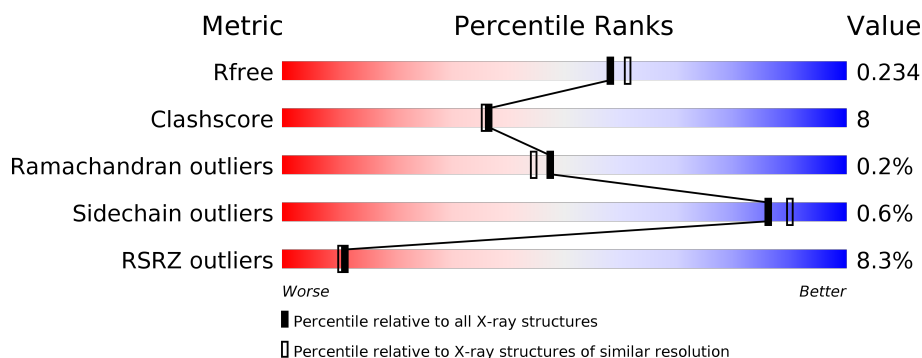
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	361	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	B	361	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>9%</div> </div> </div>
1	C	361	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>9%</div> </div> </div>
1	D	361	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11236 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	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			

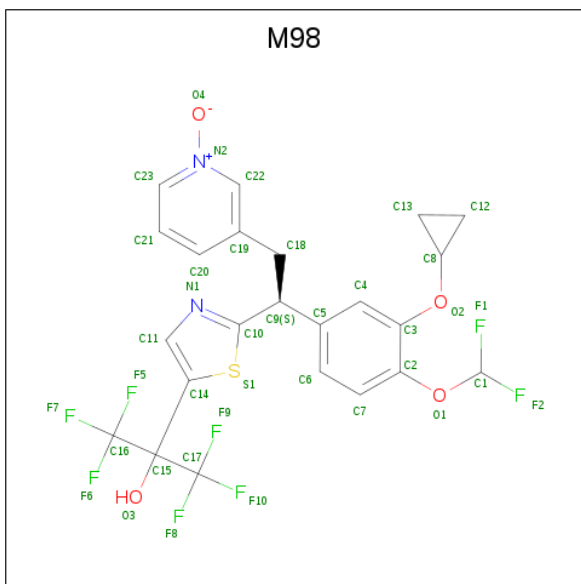
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is (S)-3-(2-(3-CYCLOPROPOXY-4-(DIFLUOROMETHOXY)PHENYL)-2-(5-(1,1,1,3,3,3-HEXAFLUORO-2-HYDROXYPROPAN-2-YL)THIAZOL-2-YL)ETHYL)PYRIDINE 1-OXIDE (three-letter code: M98) (formula:  $C_{23}H_{18}F_8N_2O_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		
4	B	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		
4	C	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		
4	D	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		

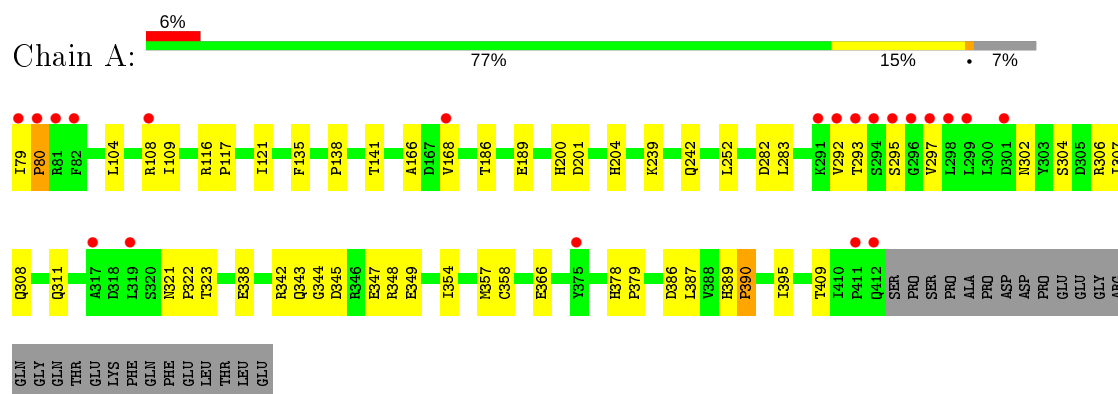
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	81	Total	O	0	0
			81	81		
5	C	76	Total	O	0	0
			76	76		
5	D	116	Total	O	0	0
			116	116		

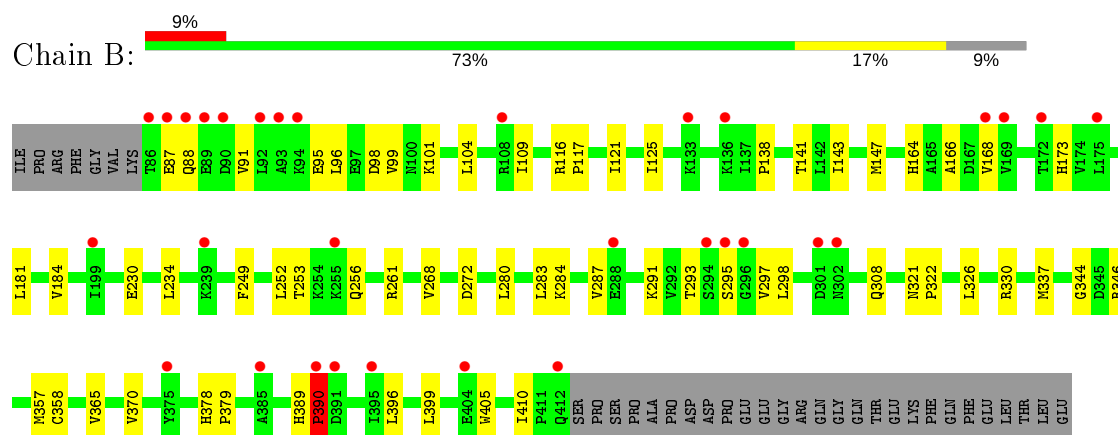
### 3 Residue-property plots [i](#)

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.

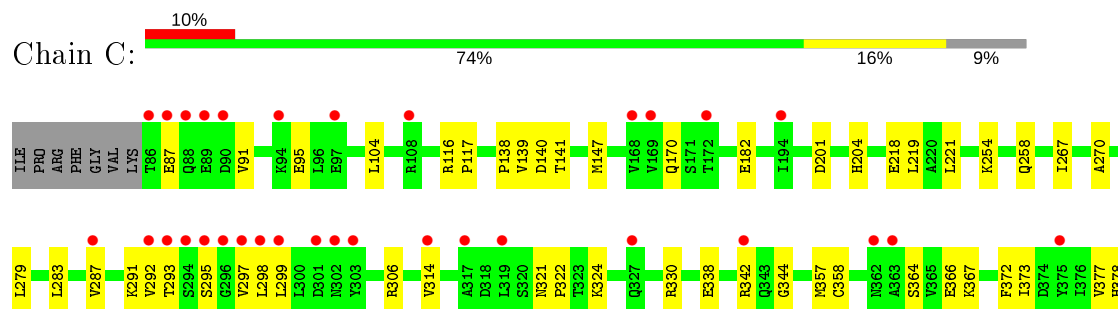
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

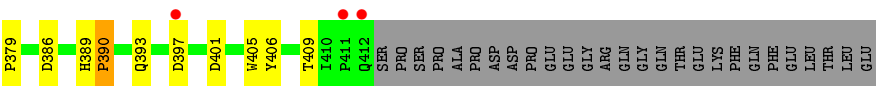


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

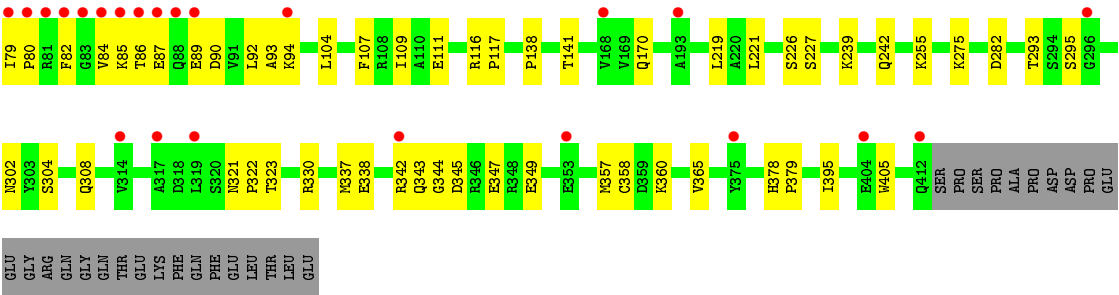
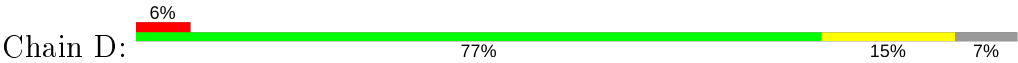


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





● 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, $\alpha$ , $\beta$ , $\gamma$	99.51Å 112.18Å 160.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 96.0 (29.43-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.245 0.212 , 0.234	Depositor DCC
$R_{free}$ test set	12121 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M98, 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	0.32	0/2760	0.54	0/3749
1	B	0.31	0/2701	0.53	0/3670
1	C	0.29	0/2701	0.51	0/3670
1	D	0.32	0/2760	0.55	0/3749
All	All	0.31	0/10922	0.53	0/14838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2704	0	2664	44	0
1	B	2647	0	2599	44	0
1	C	2647	0	2599	43	0
1	D	2704	0	2664	45	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	38	0	17	1	0
4	B	38	0	17	2	0
4	C	38	0	17	4	0
4	D	38	0	17	1	0
5	A	101	0	0	1	0
5	B	81	0	0	2	0
5	C	76	0	0	1	0
5	D	116	0	0	3	0
All	All	11236	0	10594	170	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 8.

All (170) 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:292:VAL:HG12	1:A:293:THR:H	1.34	0.91
1:D:282:ASP:HB3	1:D:308:GLN:NE2	1.95	0.81
1:A:282:ASP:HB3	1:A:308:GLN:NE2	1.97	0.79
1:C:293:THR:HG23	1:C:295:SER:H	1.48	0.78
1:B:104:LEU:HD11	1:B:109:ILE:HD11	1.70	0.73
1:B:96:LEU:O	1:B:99:VAL:HG23	1.89	0.72
1:C:292:VAL:HG22	1:C:293:THR:H	1.53	0.72
1:D:79:ILE:N	1:D:80:PRO:HD2	2.07	0.69
1:C:221:LEU:O	1:C:221:LEU:HD23	1.94	0.68
1:A:292:VAL:HG12	1:A:293:THR:N	2.08	0.68
1:D:337:MET:CE	1:D:365:VAL:HG22	2.24	0.67
1:D:275:LYS:HE2	5:D:679:HOH:O	1.94	0.67
1:D:86:THR:HG21	1:D:92:LEU:HD23	1.77	0.67
1:A:79:ILE:N	1:A:80:PRO:HD2	2.11	0.66
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.31	0.65
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.15	0.64
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.78	0.64
5:B:642:HOH:O	1:D:84:VAL:HG13	1.97	0.64
1:C:357:MET:SD	4:C:603:M98:H122	2.38	0.64
1:D:337:MET:HE2	1:D:365:VAL:HG22	1.79	0.63
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.80	0.63
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HZ3	1:D:239:LYS:HZ3	1.46	0.62
1:A:357:MET:SD	4:A:601:M98:H122	2.38	0.62
1:C:293:THR:HG22	1:C:297:VAL:O	1.99	0.61
1:C:366:GLU:HG2	1:C:409:THR:HG22	1.81	0.61
1:C:291:LYS:O	1:C:299:LEU:HB3	2.00	0.61
1:D:282:ASP:HB3	1:D:308:GLN:HE22	1.62	0.61
1:D:345:ASP:O	1:D:349:GLU:HG3	2.01	0.60
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.83	0.60
1:B:184:VAL:HG22	1:B:297:VAL:CG1	2.32	0.59
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.84	0.59
1:D:79:ILE:N	1:D:79:ILE:HD12	2.17	0.59
1:C:292:VAL:HG22	1:C:293:THR:N	2.17	0.58
1:B:337:MET:HE2	1:B:365:VAL:HG22	1.86	0.57
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.40	0.57
1:A:79:ILE:N	1:A:80:PRO:CD	2.67	0.57
1:D:86:THR:O	1:D:89:GLU:HB2	2.05	0.57
1:C:254:LYS:O	1:C:258:GLN:HG3	2.06	0.56
1:A:295:SER:C	1:A:297:VAL:H	2.09	0.56
1:D:344:GLY:HA3	1:D:358:CYS:O	2.06	0.56
1:B:396:LEU:O	1:B:396:LEU:HD23	2.05	0.55
1:C:338:GLU:OE2	1:C:342:ARG:NH2	2.40	0.55
1:C:366:GLU:CD	1:C:366:GLU:H	2.10	0.53
1:D:79:ILE:N	1:D:80:PRO:CD	2.71	0.53
1:A:121:ILE:HD12	1:A:166:ALA:HB1	1.90	0.53
1:B:125:ILE:HD13	1:B:173:HIS:HB2	1.91	0.53
5:A:684:HOH:O	1:B:261:ARG:HD3	2.08	0.53
1:B:291:LYS:O	1:B:298:LEU:HD12	2.09	0.53
1:C:344:GLY:HA3	1:C:358:CYS:O	2.08	0.53
1:B:337:MET:CE	1:B:365:VAL:HG22	2.38	0.53
1:B:357:MET:SD	4:B:602:M98:H122	2.48	0.52
1:B:87:GLU:HG3	1:B:88:GLN:N	2.25	0.52
1:C:393:GLN:HE21	1:C:397:ASP:CG	2.12	0.52
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.45	0.52
1:A:345:ASP:O	1:A:349:GLU:HG3	2.08	0.52
1:A:239:LYS:HE3	1:C:218:GLU:HB2	1.92	0.52
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.92	0.52
1:B:138:PRO:HG2	1:B:141:THR:OG1	2.10	0.52
1:B:138:PRO:HG2	1:B:141:THR:CB	2.41	0.51
1:D:337:MET:HE1	1:D:365:VAL:HG22	1.92	0.51
1:A:292:VAL:CG1	1:A:293:THR:H	2.16	0.51
1:A:344:GLY:HA3	1:A:358:CYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:GLU:OE2	1:D:342:ARG:NH2	2.44	0.51
1:D:107:PHE:O	1:D:111:GLU:HG3	2.10	0.51
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.40	0.51
1:C:116:ARG:N	1:C:117:PRO:CD	2.74	0.51
1:C:297:VAL:HG12	1:C:298:LEU:N	2.26	0.51
1:C:324:LYS:HE2	5:C:655:HOH:O	2.11	0.51
1:B:91:VAL:O	1:B:95:GLU:HG2	2.11	0.50
1:D:87:GLU:C	1:D:89:GLU:H	2.15	0.50
1:A:186:THR:OG1	1:A:189:GLU:HG3	2.11	0.50
1:D:357:MET:SD	4:D:604:M98:H122	2.52	0.50
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.93	0.50
1:D:116:ARG:N	1:D:117:PRO:CD	2.75	0.49
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.60	0.49
1:C:182:GLU:O	1:C:297:VAL:HG11	2.12	0.49
1:B:249:PHE:HA	1:B:252:LEU:HD13	1.94	0.49
5:B:659:HOH:O	1:D:85:LYS:HD2	2.13	0.49
1:D:221:LEU:O	1:D:221:LEU:HD23	2.12	0.49
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.95	0.49
1:B:346:ARG:HD2	5:D:624:HOH:O	2.13	0.49
1:B:138:PRO:HG2	1:B:141:THR:HB	1.95	0.48
1:A:239:LYS:HZ3	1:D:239:LYS:NZ	2.11	0.48
1:B:87:GLU:HG3	1:B:88:GLN:HG3	1.95	0.48
1:C:138:PRO:HG2	1:C:141:THR:OG1	2.12	0.48
1:A:138:PRO:HG2	1:A:141:THR:OG1	2.13	0.48
1:D:221:LEU:C	1:D:221:LEU:HD23	2.33	0.48
1:B:283:LEU:O	1:B:287:VAL:HG23	2.14	0.48
1:D:104:LEU:HD22	1:D:170:GLN:HG3	1.96	0.48
1:B:389:HIS:CD2	1:B:390:PRO:HB3	2.49	0.47
1:D:255:LYS:HA	1:D:255:LYS:HD2	1.70	0.47
1:B:280:LEU:HG	1:B:284:LYS:HE3	1.95	0.47
1:B:378:HIS:HB3	1:B:379:PRO:HD3	1.95	0.47
1:B:116:ARG:N	1:B:117:PRO:CD	2.78	0.47
1:A:302:ASN:O	1:A:306:ARG:HG3	2.13	0.47
1:A:307:ILE:O	1:A:311:GLN:HG3	2.15	0.47
1:A:338:GLU:OE2	1:A:342:ARG:NH2	2.48	0.47
1:B:181:LEU:HA	1:B:184:VAL:HG21	1.97	0.46
1:C:283:LEU:O	1:C:287:VAL:HG23	2.15	0.46
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.97	0.46
1:A:116:ARG:N	1:A:117:PRO:CD	2.79	0.46
1:A:348:ARG:HD3	1:A:354:ILE:HD11	1.97	0.45
1:C:364:SER:HB3	1:C:367:LYS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:THR:O	1:D:295:SER:O	2.34	0.45
1:D:138:PRO:HG2	1:D:141:THR:OG1	2.16	0.45
1:A:302:ASN:OD1	1:A:304:SER:HB3	2.17	0.45
1:C:372:PHE:HB2	4:C:603:M98:H132	1.98	0.45
1:C:87:GLU:O	1:C:91:VAL:HG23	2.17	0.45
1:C:287:VAL:HG11	1:C:386:ASP:HB3	1.99	0.45
1:B:181:LEU:C	1:B:184:VAL:HG23	2.37	0.45
1:B:330:ARG:HH11	1:B:405:TRP:HH2	1.65	0.45
1:C:406:TYR:O	1:C:409:THR:HB	2.17	0.45
1:B:184:VAL:CG2	1:B:297:VAL:CG1	2.94	0.44
1:C:221:LEU:C	1:C:221:LEU:HD23	2.37	0.44
1:D:378:HIS:HB3	1:D:379:PRO:HD3	1.98	0.44
1:A:135:PHE:HB3	1:A:252:LEU:HD11	1.99	0.44
1:B:184:VAL:HG22	1:B:297:VAL:HG11	1.99	0.44
1:C:293:THR:HG22	1:C:297:VAL:N	2.32	0.44
1:D:302:ASN:OD1	1:D:304:SER:HB3	2.17	0.44
1:A:349:GLU:HB3	1:C:147:MET:HE1	2.00	0.44
1:A:378:HIS:HB3	1:A:379:PRO:HD3	2.00	0.43
1:A:283:LEU:HD11	1:A:387:LEU:HD22	1.99	0.43
1:B:87:GLU:HG3	1:B:88:GLN:H	1.83	0.43
1:D:85:LYS:HG3	5:D:714:HOH:O	2.18	0.43
1:B:230:GLU:HG2	1:B:272:ASP:HB2	2.00	0.43
1:B:253:THR:OG1	1:B:256:GLN:HG3	2.18	0.43
1:D:226:SER:O	1:D:227:SER:C	2.56	0.43
1:B:147:MET:CE	1:D:349:GLU:HB3	2.49	0.43
1:B:234:LEU:HG	1:B:268:VAL:HG11	2.01	0.43
1:C:201:ASP:O	1:C:204:HIS:HB2	2.19	0.43
1:C:293:THR:HG23	1:C:295:SER:N	2.26	0.43
1:D:90:ASP:O	1:D:94:LYS:HG3	2.19	0.43
1:A:108:ARG:HG2	1:A:108:ARG:HH11	1.84	0.43
1:B:143:ILE:O	1:B:147:MET:HG3	2.20	0.42
1:A:239:LYS:NZ	1:D:239:LYS:HZ3	2.16	0.42
1:A:409:THR:HG22	1:A:409:THR:O	2.17	0.42
1:C:267:ILE:HG21	1:C:314:VAL:HG21	2.01	0.42
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.89	0.42
1:A:366:GLU:HG2	1:A:409:THR:HG22	2.01	0.42
1:D:323:THR:HB	1:D:395:ILE:HG23	2.00	0.42
1:A:282:ASP:HB3	1:A:308:GLN:CD	2.40	0.42
1:C:373:ILE:HA	1:C:377:VAL:HB	2.01	0.42
1:C:139:VAL:HG13	1:C:140:ASP:N	2.35	0.42
4:B:602:M98:H4	4:B:602:M98:S1	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:603:M98:H4	4:C:603:M98:S1	2.60	0.42
1:C:91:VAL:O	1:C:95:GLU:HG2	2.20	0.42
1:A:168:VAL:HG21	1:A:200:HIS:CE1	2.55	0.42
1:A:345:ASP:OD1	1:A:348:ARG:NH2	2.52	0.42
1:B:234:LEU:HD21	1:B:268:VAL:HB	2.01	0.42
1:C:372:PHE:CG	4:C:603:M98:H132	2.55	0.41
1:B:344:GLY:HA3	1:B:358:CYS:O	2.20	0.41
1:A:323:THR:HB	1:A:395:ILE:HG23	2.01	0.41
1:B:293:THR:C	1:B:295:SER:H	2.24	0.41
1:C:389:HIS:CE1	1:C:390:PRO:HB3	2.55	0.41
1:C:219:LEU:HA	1:C:219:LEU:HD12	1.94	0.41
1:B:181:LEU:HA	1:B:184:VAL:CG2	2.50	0.41
1:B:370:VAL:HG21	1:B:410:ILE:HD11	2.02	0.41
1:B:378:HIS:HA	1:B:399:LEU:HD21	2.02	0.41
1:D:345:ASP:OD1	1:D:360:LYS:HE2	2.21	0.41
1:B:98:ASP:OD1	1:B:101:LYS:HD2	2.20	0.41
1:C:297:VAL:HG12	1:C:298:LEU:H	1.85	0.41
1:A:295:SER:O	1:A:297:VAL:N	2.54	0.41
1:C:270:ALA:HB1	1:C:279:LEU:HD11	2.02	0.41
1:A:282:ASP:HB3	1:A:308:GLN:HE22	1.82	0.40
1:A:343:GLN:O	1:A:347:GLU:HG3	2.21	0.40
1:D:343:GLN:O	1:D:347:GLU:HG3	2.21	0.40
1:A:201:ASP:O	1:A:204:HIS:HB2	2.21	0.40
1:B:164:HIS:O	1:B:168:VAL:HG23	2.21	0.40
1:D:82:PHE:CZ	1:D:93:ALA:HA	2.56	0.40

There are no symmetry-related clashes.

## 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	332/361 (92%)	321 (97%)	10 (3%)	1 (0%)	41 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	325/361 (90%)	310 (95%)	13 (4%)	2 (1%)	25	19
1	C	325/361 (90%)	309 (95%)	16 (5%)	0	100	100
1	D	332/361 (92%)	322 (97%)	10 (3%)	0	100	100
All	All	1314/1444 (91%)	1262 (96%)	49 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	LEU
1	A	80	PRO
1	B	390	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/329 (93%)	303 (99%)	2 (1%)	84	88
1	B	299/329 (91%)	297 (99%)	2 (1%)	84	88
1	C	299/329 (91%)	296 (99%)	3 (1%)	76	81
1	D	305/329 (93%)	305 (100%)	0	100	100
All	All	1208/1316 (92%)	1201 (99%)	7 (1%)	86	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	ASP
1	A	390	PRO
1	B	308	GLN
1	B	390	PRO
1	C	306	ARG
1	C	390	PRO
1	C	401	ASP

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	123	HIS
1	A	245	ASN
1	A	308	GLN
1	B	245	ASN
1	B	250	GLN
1	B	258	GLN
1	B	278	ASN
1	B	407	GLN
1	C	242	GLN
1	C	245	ASN
1	C	278	ASN
1	C	393	GLN
1	D	123	HIS
1	D	127	GLN
1	D	245	ASN
1	D	308	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	M98	B	602	-	36,41,41	1.42	4 (11%)	47,63,63	0.79	0
4	M98	C	603	-	36,41,41	1.43	3 (8%)	47,63,63	0.74	0
4	M98	D	604	-	36,41,41	1.42	3 (8%)	47,63,63	0.83	1 (2%)
4	M98	A	601	-	36,41,41	1.45	4 (11%)	47,63,63	0.78	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
4	M98	B	602	-	-	3/34/46/46	0/4/4/4
4	M98	C	603	-	-	4/34/46/46	0/4/4/4
4	M98	D	604	-	-	3/34/46/46	0/4/4/4
4	M98	A	601	-	-	3/34/46/46	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	M98	C11-N1	6.01	1.45	1.36
4	C	603	M98	C11-N1	5.90	1.44	1.36
4	A	601	M98	C11-N1	5.68	1.44	1.36
4	B	602	M98	C11-N1	5.30	1.44	1.36
4	A	601	M98	C14-S1	-3.52	1.67	1.74
4	B	602	M98	C14-S1	-3.41	1.67	1.74
4	C	603	M98	C14-S1	-2.82	1.68	1.74
4	D	604	M98	C14-S1	-2.75	1.69	1.74
4	D	604	M98	C22-N2	2.57	1.40	1.35
4	A	601	M98	C22-N2	2.46	1.40	1.35
4	C	603	M98	C22-N2	2.45	1.40	1.35
4	B	602	M98	C22-N2	2.29	1.39	1.35
4	B	602	M98	C10-S1	-2.19	1.66	1.73
4	A	601	M98	C10-S1	-2.08	1.67	1.73

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	D	604	M98	C16-C15-C14	-2.62	106.97	110.88

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	M98	C13-C8-O2-C3
4	C	603	M98	C12-C8-O2-C3
4	C	603	M98	C13-C8-O2-C3
4	D	604	M98	C13-C8-O2-C3
4	A	601	M98	C13-C8-O2-C3
4	A	601	M98	C4-C5-C9-C10
4	B	602	M98	C4-C5-C9-C10
4	C	603	M98	C4-C5-C9-C10
4	D	604	M98	C4-C5-C9-C10
4	B	602	M98	C6-C5-C9-C10
4	A	601	M98	C6-C5-C9-C10
4	C	603	M98	C6-C5-C9-C10
4	D	604	M98	C6-C5-C9-C10

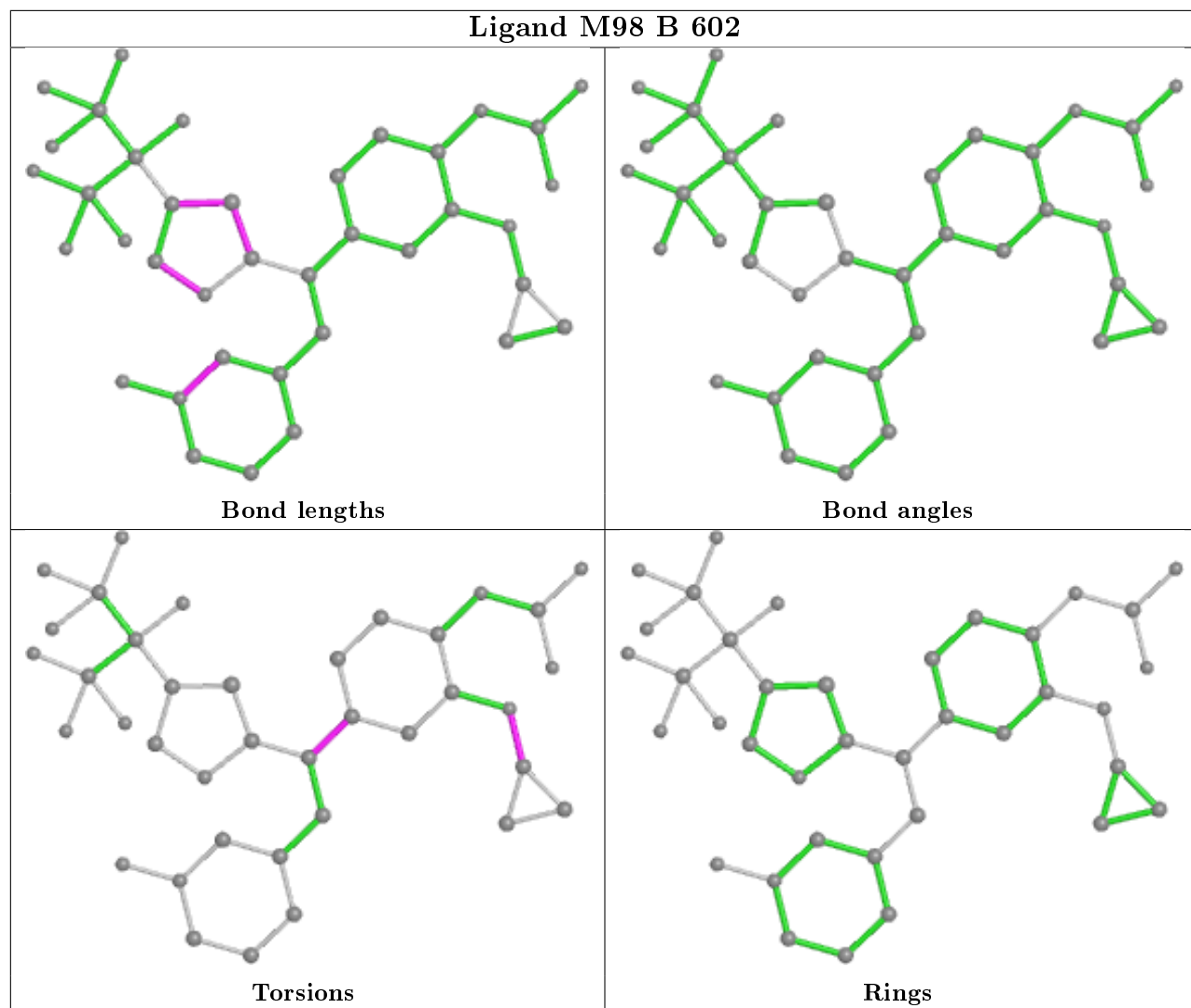
There are no ring outliers.

4 monomers are involved in 8 short contacts:

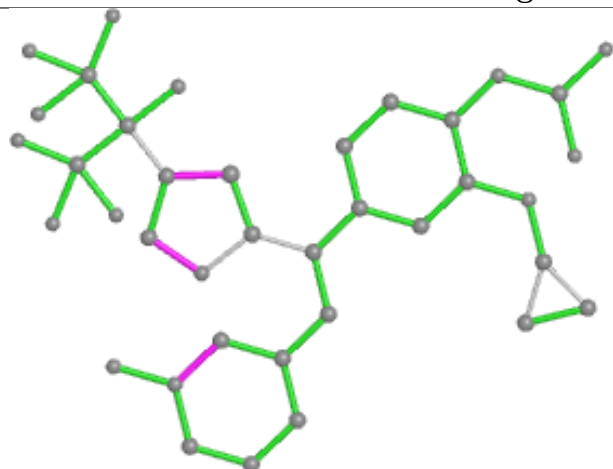
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	M98	2	0
4	C	603	M98	4	0
4	D	604	M98	1	0
4	A	601	M98	1	0

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.

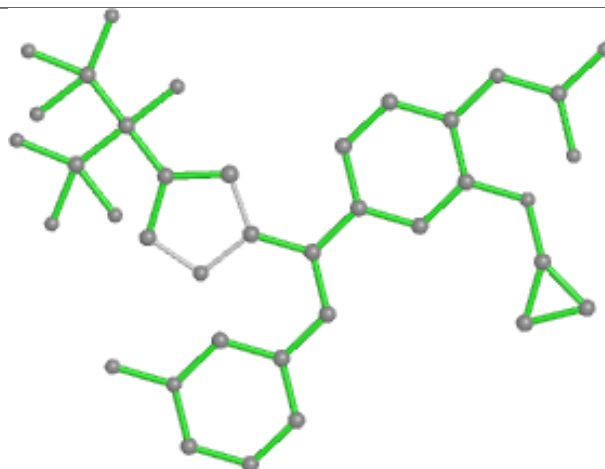
## Ligand M98 B 602



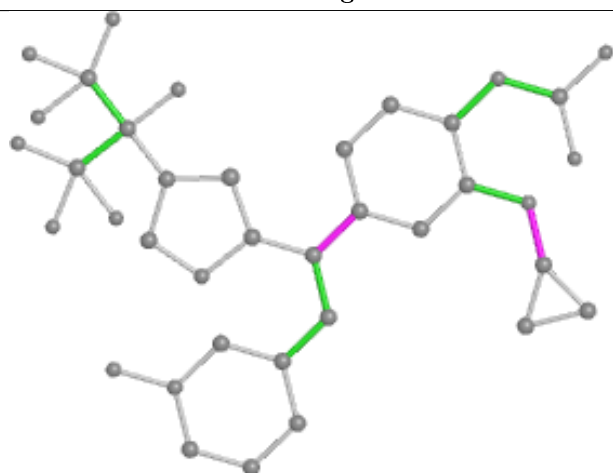
## Ligand M98 C 603



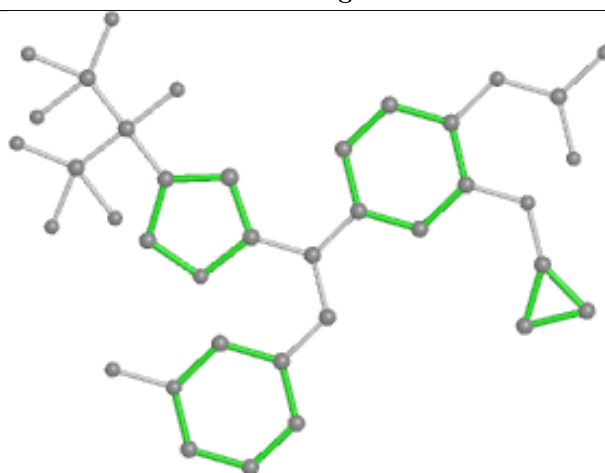
Bond lengths



Bond angles

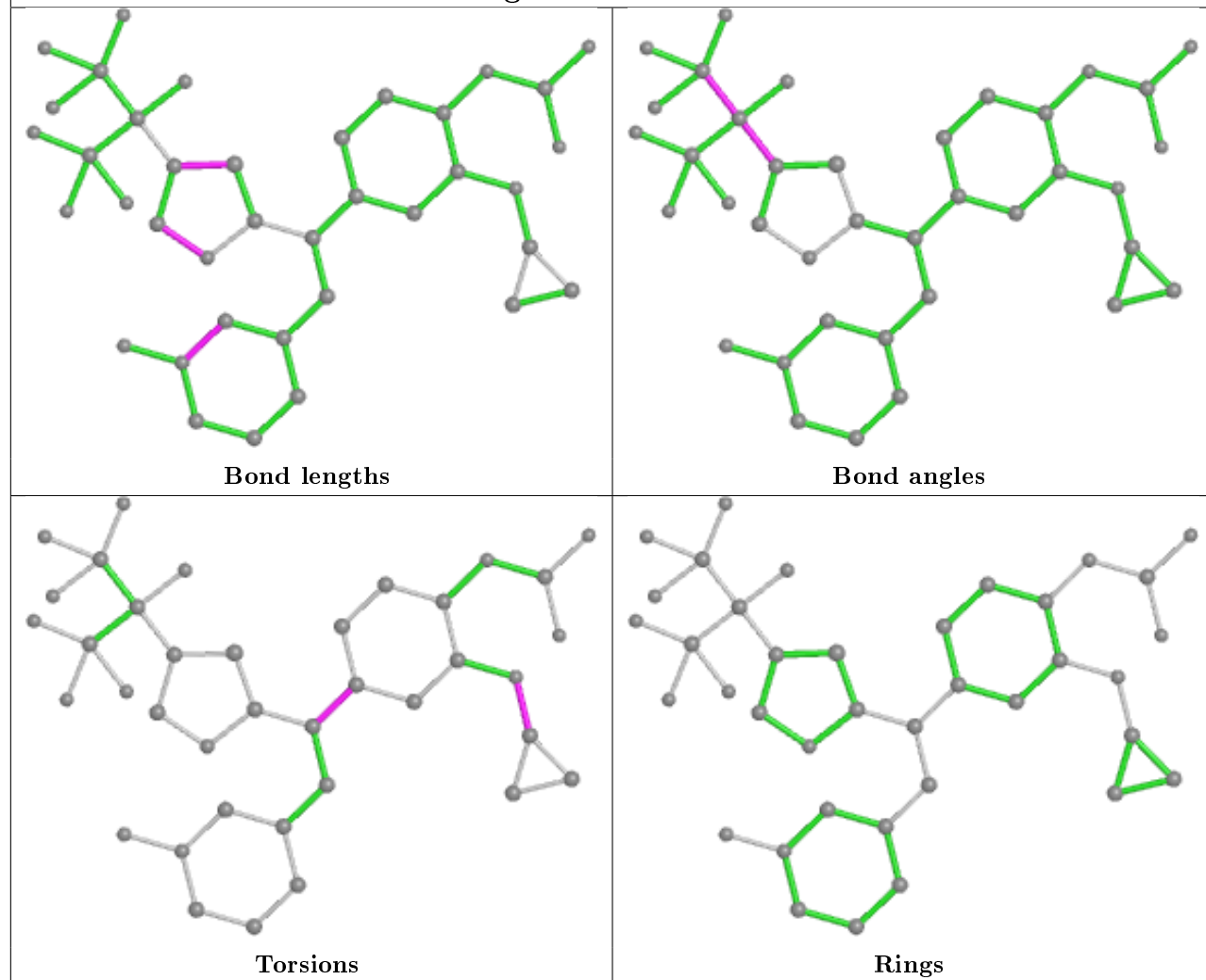


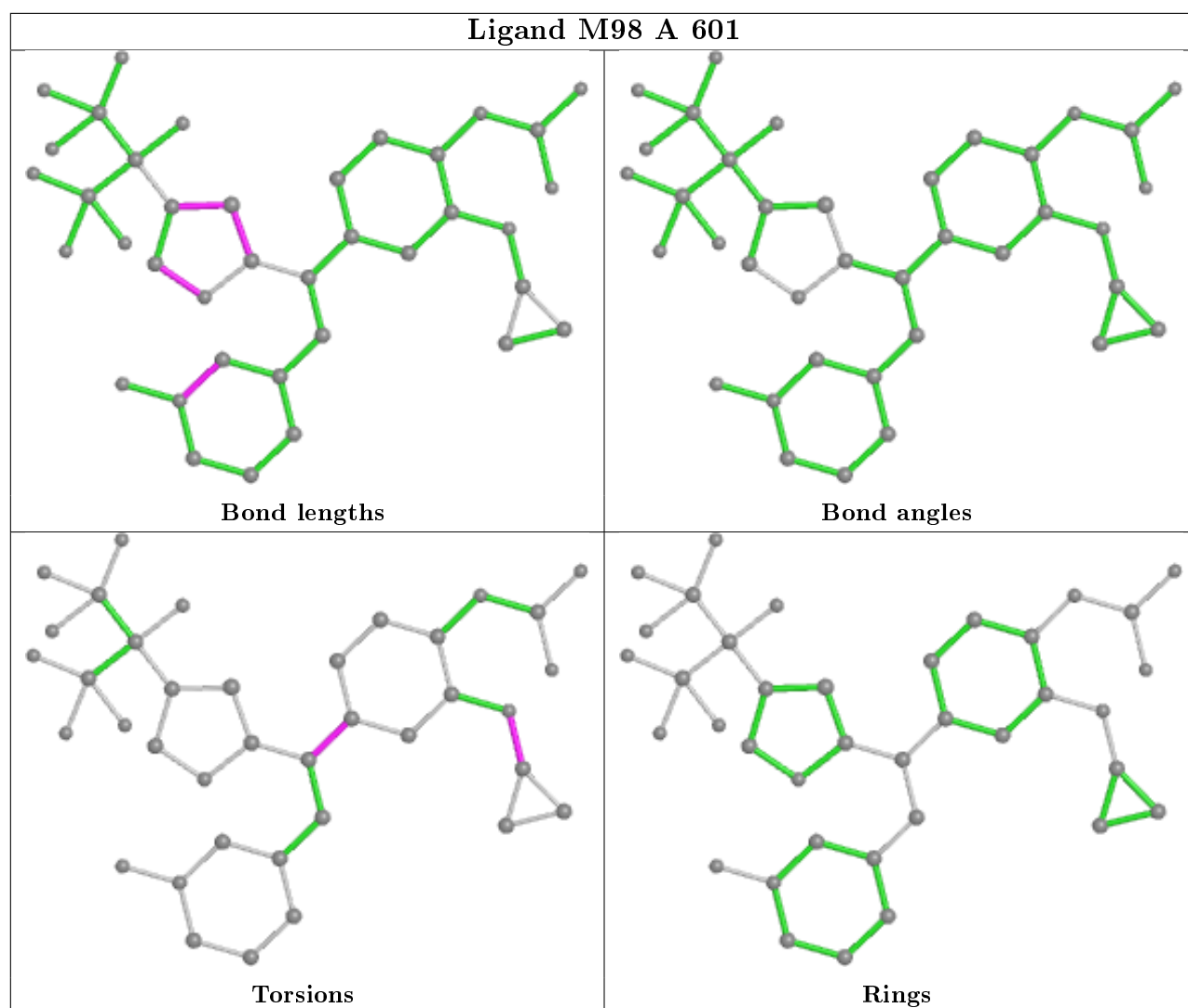
Torsions



Rings

## Ligand M98 D 604





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/361 (92%)	0.36	21 (6%) 20 19	17, 27, 62, 85	0
1	B	327/361 (90%)	0.63	31 (9%) 8 7	19, 35, 57, 91	0
1	C	327/361 (90%)	0.52	35 (10%) 6 5	19, 35, 69, 80	0
1	D	334/361 (92%)	0.33	23 (6%) 16 16	17, 27, 47, 83	0
All	All	1322/1444 (91%)	0.46	110 (8%) 11 10	17, 31, 61, 91	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	SER	13.9
1	A	79	ILE	10.0
1	B	86	THR	9.4
1	A	296	GLY	8.6
1	D	84	VAL	7.5
1	D	79	ILE	7.5
1	A	80	PRO	7.5
1	D	82	PHE	7.4
1	A	293	THR	7.3
1	D	87	GLU	6.9
1	B	88	GLN	6.7
1	D	80	PRO	6.7
1	B	412	GLN	6.3
1	D	86	THR	6.3
1	B	87	GLU	6.1
1	A	295	SER	5.8
1	C	297	VAL	5.8
1	D	85	LYS	5.5
1	C	294	SER	5.4
1	A	81	ARG	5.4
1	C	293	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	5.2
1	A	411	PRO	5.1
1	C	412	GLN	5.0
1	A	412	GLN	5.0
1	C	292	VAL	4.9
1	D	81	ARG	4.8
1	B	391	ASP	4.6
1	A	297	VAL	4.5
1	D	412	GLN	4.4
1	B	168	VAL	4.1
1	C	296	GLY	3.9
1	C	411	PRO	3.8
1	A	301	ASP	3.6
1	C	87	GLU	3.6
1	A	298	LEU	3.6
1	A	292	VAL	3.5
1	B	108	ARG	3.5
1	C	298	LEU	3.4
1	D	296	GLY	3.4
1	B	295	SER	3.3
1	B	302	ASN	3.3
1	D	89	GLU	3.3
1	B	93	ALA	3.3
1	C	303	TYR	3.3
1	C	86	THR	3.3
1	C	90	ASP	3.3
1	B	296	GLY	3.2
1	A	319	LEU	3.2
1	A	299	LEU	3.2
1	B	136	LYS	3.1
1	B	92	LEU	3.1
1	A	168	VAL	3.1
1	B	89	GLU	3.1
1	B	169	VAL	3.1
1	D	404	GLU	3.0
1	C	168	VAL	2.9
1	C	314	VAL	2.9
1	D	94	LYS	2.9
1	D	88	GLN	2.9
1	A	291	LYS	2.9
1	B	90	ASP	2.9
1	B	301	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	317	ALA	2.9
1	C	295	SER	2.9
1	C	317	ALA	2.8
1	D	342	ARG	2.8
1	B	133	LYS	2.8
1	B	255	LYS	2.7
1	C	327	GLN	2.7
1	C	169	VAL	2.7
1	B	172	THR	2.7
1	D	314	VAL	2.7
1	B	294	SER	2.6
1	D	168	VAL	2.6
1	D	353	GLU	2.6
1	C	172	THR	2.6
1	A	108	ARG	2.5
1	D	317	ALA	2.5
1	C	319	LEU	2.5
1	C	94	LYS	2.5
1	C	108	ARG	2.5
1	C	88	GLN	2.5
1	C	97	GLU	2.5
1	C	287	VAL	2.4
1	C	375	TYR	2.4
1	C	302	ASN	2.4
1	C	342	ARG	2.4
1	C	301	ASP	2.3
1	C	397	ASP	2.3
1	B	288	GLU	2.3
1	B	390	PRO	2.3
1	D	83	GLY	2.3
1	C	89	GLU	2.2
1	A	375	TYR	2.2
1	B	404	GLU	2.2
1	C	194	ILE	2.2
1	B	385	ALA	2.2
1	B	175	LEU	2.1
1	C	363	ALA	2.1
1	B	239	LYS	2.1
1	B	199	ILE	2.1
1	D	375	TYR	2.1
1	C	362	ASN	2.1
1	B	375	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	193	ALA	2.0
1	D	319	LEU	2.0
1	B	395	ILE	2.0
1	C	299	LEU	2.0
1	B	94	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

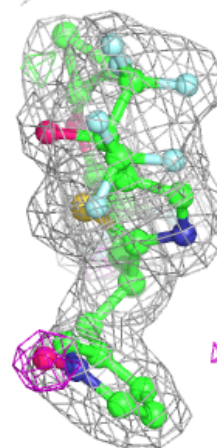
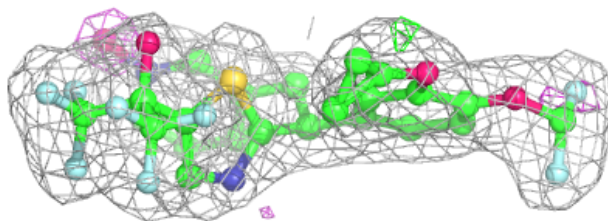
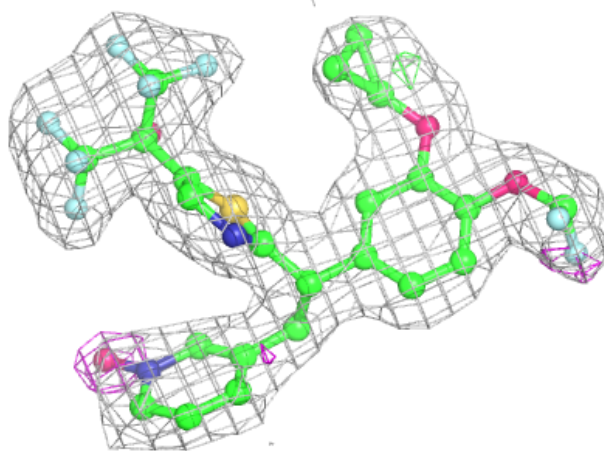
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	M98	C	603	38/38	0.90	0.15	32,36,44,46	0
3	MG	C	506	1/1	0.91	0.07	25,25,25,25	0
4	M98	A	601	38/38	0.93	0.17	25,29,39,41	0
4	M98	D	604	38/38	0.94	0.15	25,31,42,44	0
4	M98	B	602	38/38	0.95	0.14	29,32,41,43	0
3	MG	D	508	1/1	0.96	0.07	24,24,24,24	0
3	MG	B	504	1/1	0.96	0.06	26,26,26,26	0
2	ZN	B	503	1/1	0.97	0.06	30,30,30,30	0
3	MG	A	502	1/1	0.98	0.10	21,21,21,21	0
2	ZN	C	505	1/1	0.99	0.05	27,27,27,27	0
2	ZN	A	501	1/1	0.99	0.07	24,24,24,24	0
2	ZN	D	507	1/1	0.99	0.07	24,24,24,24	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.

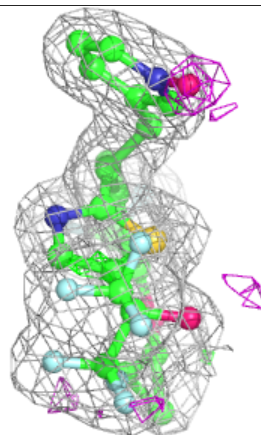
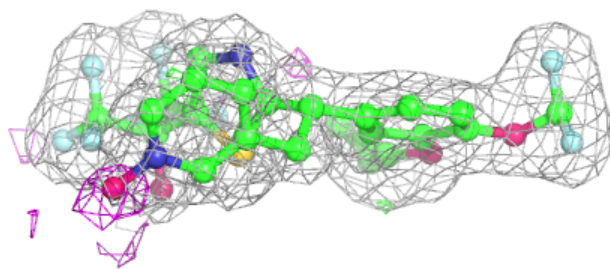
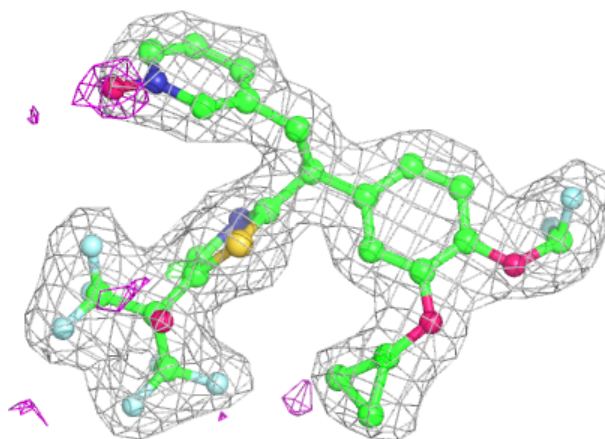
**Electron density around M98 C 603:**

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



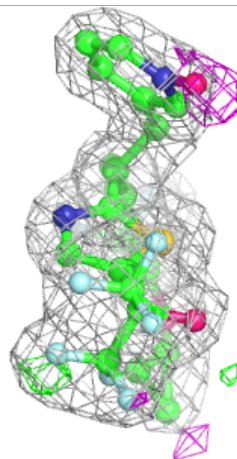
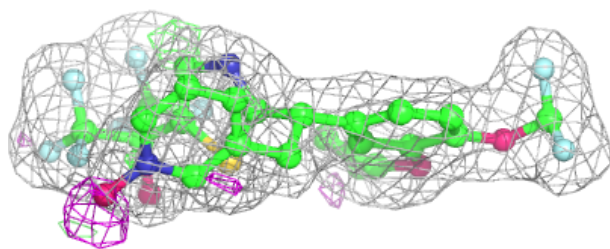
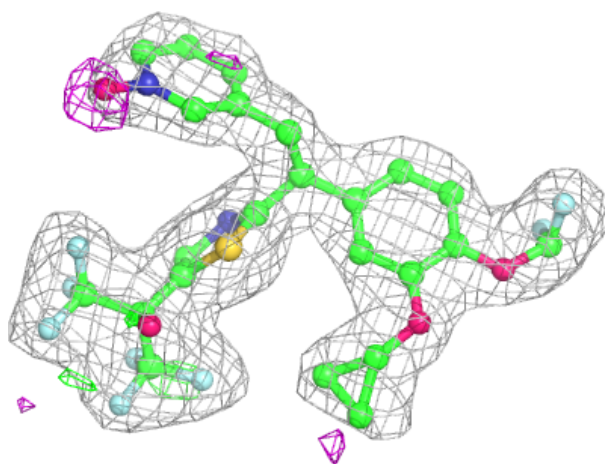
**Electron density around M98 A 601:**

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



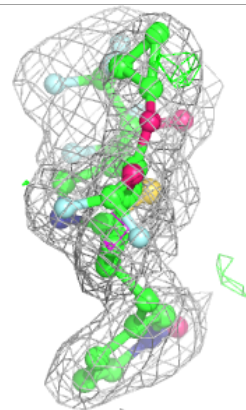
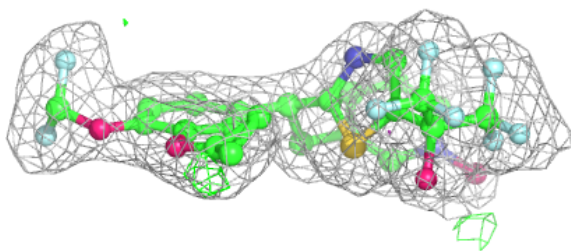
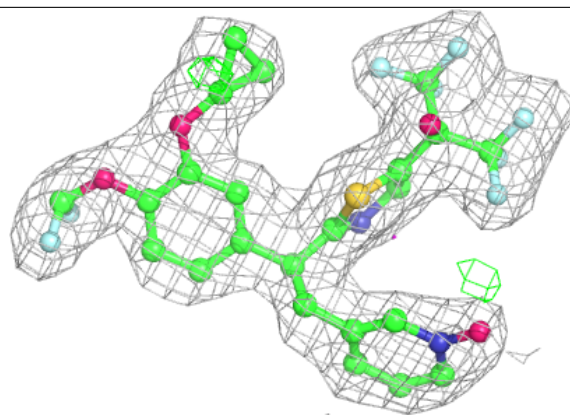
**Electron density around M98 D 604:**

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



**Electron density around M98 B 602:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.