



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:25 pm BST

PDB ID : 6GXW
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with an hydroxamate 4
Authors : Shaik, T.B.; Marek, M.; Romier, C.
Deposited on : 2018-06-27
Resolution : 2.07 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

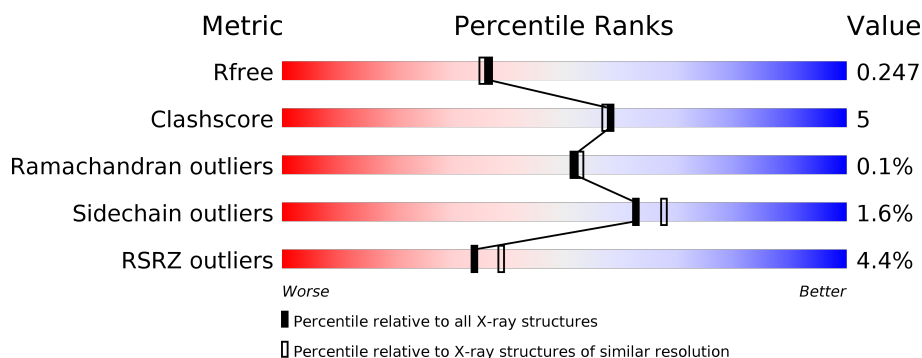
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	447	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>11%</div> </div> </div>
1	B	447	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	C	447	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
1	D	447	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>11%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FGN	B	504	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13831 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 Histone deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3180	2052	530	584	14			
1	B	411	Total	C	N	O	S	0	1	0
			3282	2115	549	601	17			
1	C	411	Total	C	N	O	S	0	0	0
			3279	2113	549	601	16			
1	D	399	Total	C	N	O	S	0	1	0
			3196	2063	531	586	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A5H660
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	0	HIS	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	0	HIS	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

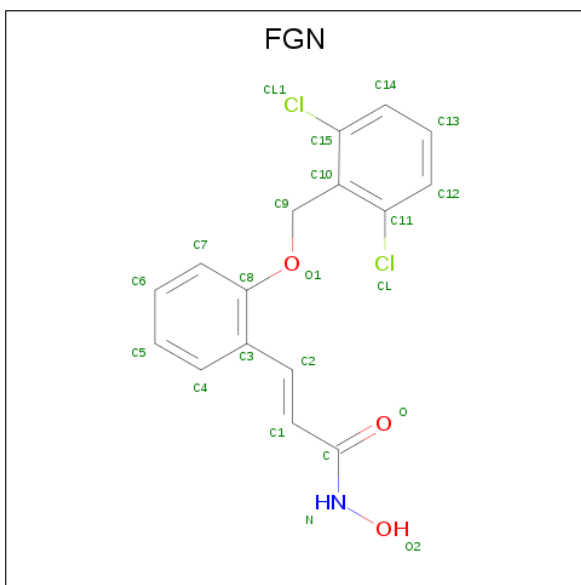
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

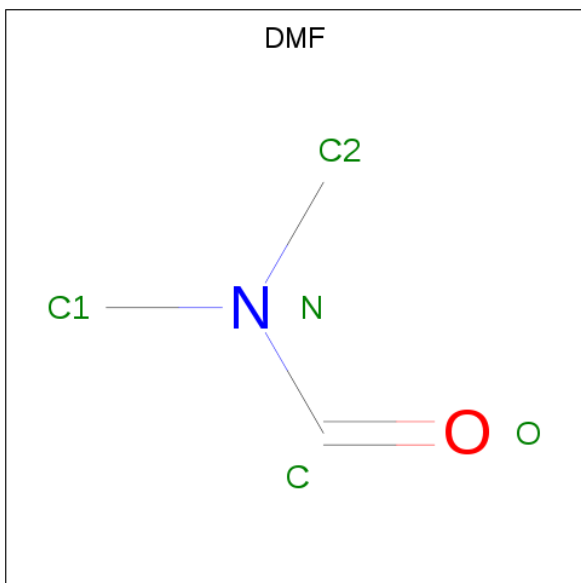
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is ({E})-3-[2-[[2,6-bis(chloranyl)phenyl]methoxy]phenyl]- {N}-oxidanyl-prop-2-enamide (three-letter code: FGN) (formula: C₁₆H₁₃Cl₂NO₃) (labeled as "Ligand of Interest" by author).



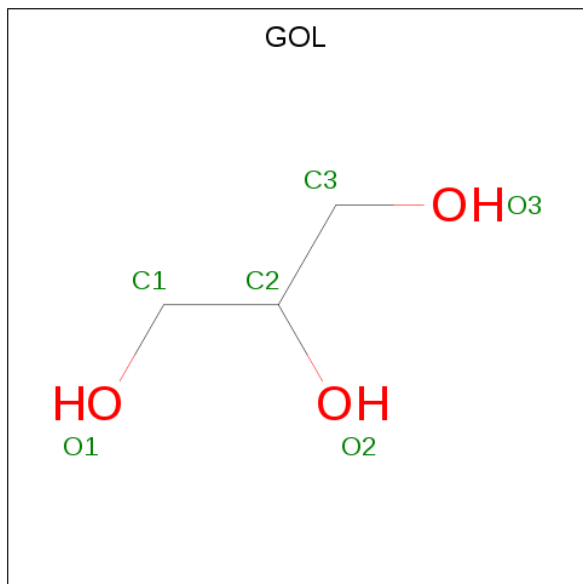
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			22	16	2	1	3		
4	B	1	Total	C	Cl	N	O	0	0
			22	16	2	1	3		
4	C	1	Total	C	Cl	N	O	0	0
			22	16	2	1	3		
4	D	1	Total	C	Cl	N	O	0	0
			22	16	2	1	3		

- Molecule 5 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

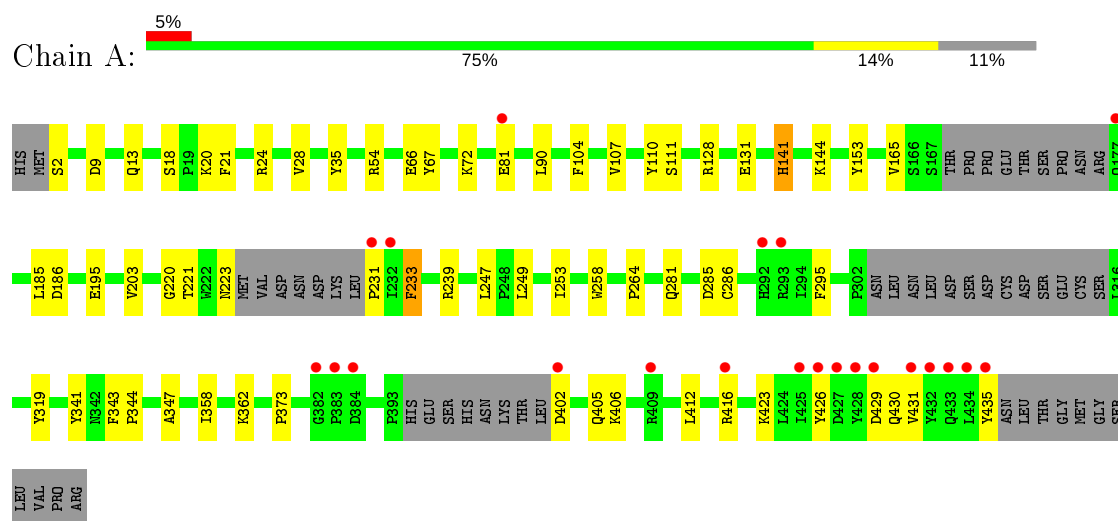
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	162	Total	O	0	0
			162	162		
7	B	216	Total	O	0	0
			216	216		
7	C	203	Total	O	0	0
			203	203		
7	D	180	Total	O	0	0
			180	180		

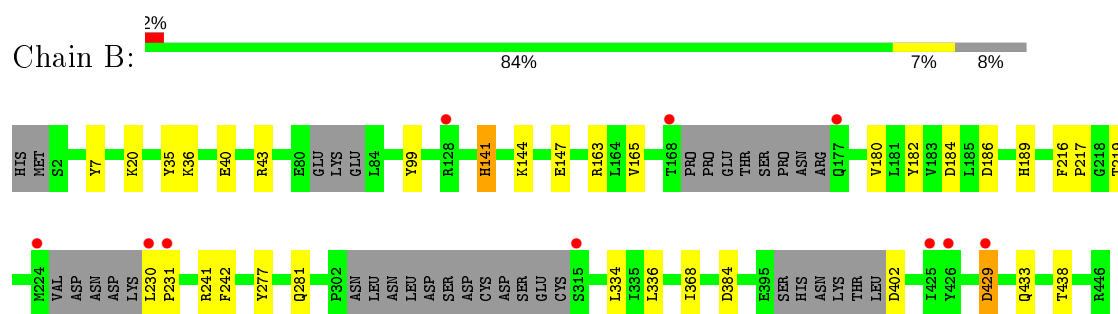
3 Residue-property plots [i](#)

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.

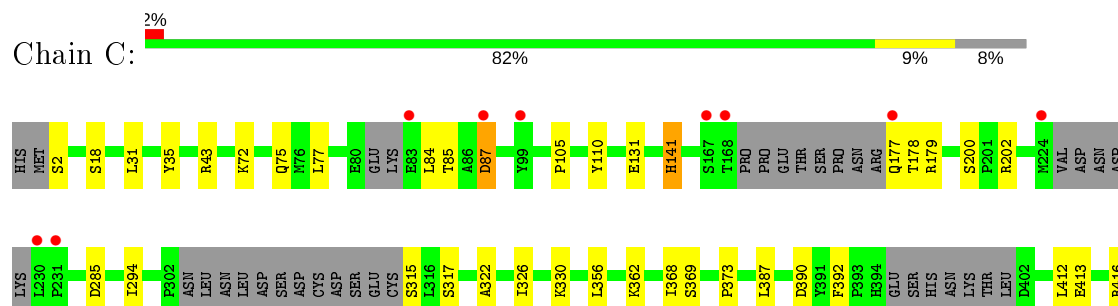
- Molecule 1: Histone deacetylase

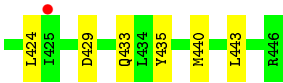


- Molecule 1: Histone deacetylase

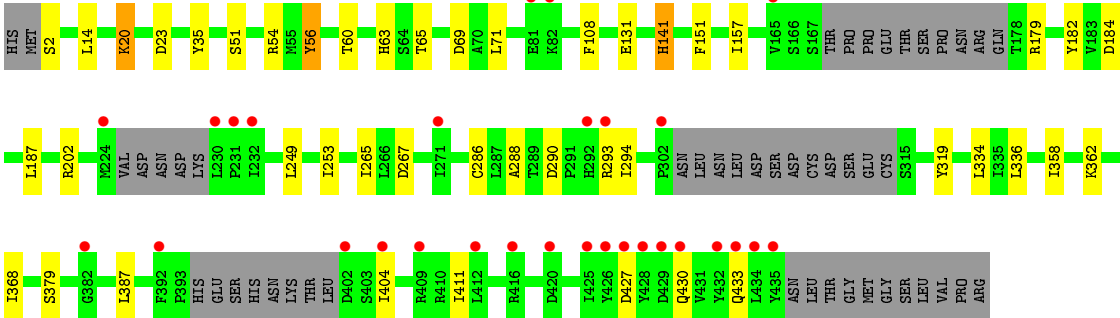
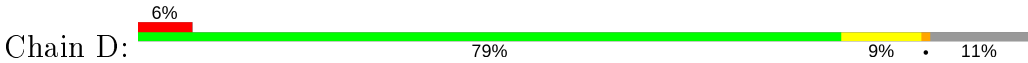


- Molecule 1: Histone deacetylase





● Molecule 1: Histone deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.80Å 70.99Å 98.20Å 75.58° 77.93° 85.56°	Depositor
Resolution (Å)	48.13 – 2.07 48.13 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.13-2.07) 94.4 (48.13-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.189 , 0.247 0.189 , 0.247	Depositor DCC
R_{free} test set	5198 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.116 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13831	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, FGN, K, DMF

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	0.42	0/3270	0.54	0/4447
1	B	0.43	0/3376	0.58	0/4591
1	C	0.43	0/3370	0.56	0/4583
1	D	0.43	0/3289	0.55	0/4473
All	All	0.43	0/13305	0.56	0/18094

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	3180	0	3071	43	0
1	B	3282	0	3179	21	0
1	C	3279	0	3174	30	0
1	D	3196	0	3092	30	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	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	22	0	0	1	0
4	B	22	0	0	0	0
4	C	22	0	0	0	0
4	D	22	0	0	1	0
5	A	10	0	14	2	0
5	C	5	0	7	2	0
6	A	6	0	8	2	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	162	0	0	5	0
7	B	216	0	0	5	0
7	C	203	0	0	6	0
7	D	180	0	0	5	0
All	All	13831	0	12561	122	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 5.

All (122) 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:20:LYS:NZ	4:D:504:FGN:CL	2.41	0.91
1:A:20:LYS:NZ	4:A:504:FGN:CL1	2.48	0.83
1:C:390:ASP:HA	5:C:801:DMF:HC	1.65	0.77
1:D:56:TYR:OH	1:D:69:ASP:OD1	2.05	0.75
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.23	0.74
1:A:220:GLY:H	6:A:507:GOL:H31	1.55	0.70
1:A:412:LEU:HD13	1:A:435:TYR:HE2	1.61	0.66
1:D:267:ASP:OD1	7:D:601:HOH:O	2.13	0.66
1:A:24:ARG:HH21	5:A:506:DMF:H22	1.61	0.66
1:A:220:GLY:N	6:A:507:GOL:H31	2.11	0.65
1:B:429:ASP:O	1:B:433:GLN:HG2	1.98	0.63
1:D:2:SER:N	1:D:131:GLU:OE2	2.31	0.63
1:B:402:ASP:N	7:B:603:HOH:O	2.32	0.61
1:A:430:GLN:OE1	7:A:601:HOH:O	2.16	0.61
1:D:60:THR:HG21	1:D:65:THR:HG22	1.82	0.61
1:C:178:THR:HB	1:C:202:ARG:HH21	1.67	0.59
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ASP:O	1:C:433:GLN:HG2	2.05	0.57
1:D:249:LEU:HD13	1:D:253:ILE:HD13	1.85	0.56
1:C:294:ILE:HD11	1:D:51:SER:HA	1.87	0.56
1:B:182:TYR:CE2	1:B:184:ASP:HB2	2.41	0.55
1:C:178:THR:HB	1:C:202:ARG:NH2	2.22	0.55
1:D:54:ARG:NH1	7:D:604:HOH:O	2.39	0.54
1:A:20:LYS:HE3	1:A:341:TYR:CE1	2.44	0.53
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.43	0.53
1:A:28:VAL:HG22	1:A:347:ALA:HA	1.89	0.52
1:A:9:ASP:O	1:A:13:GLN:HG2	2.09	0.52
1:B:241:ARG:HG2	1:B:242:PHE:CE2	2.45	0.52
1:D:427:ASP:HB3	1:D:430:GLN:HB3	1.93	0.51
1:C:77:LEU:HD13	1:C:84:LEU:HD22	1.93	0.51
1:A:128:ARG:NH1	7:A:609:HOH:O	2.44	0.51
1:D:427:ASP:OD1	1:D:430:GLN:N	2.26	0.51
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.46	0.50
1:A:223:ASN:O	1:A:231:PRO:HA	2.12	0.50
1:A:249:LEU:HD13	1:A:253:ILE:HD13	1.94	0.49
1:D:290:ASP:O	1:D:293:ARG:HG3	2.12	0.49
1:A:20:LYS:HE3	1:A:341:TYR:HE1	1.77	0.49
1:A:24:ARG:NH2	5:A:506:DMF:H22	2.26	0.49
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.13	0.48
1:A:54:ARG:NE	7:A:610:HOH:O	2.46	0.48
1:A:423:LYS:HD2	1:A:423:LYS:N	2.29	0.48
1:B:141:HIS:CD2	1:B:141:HIS:H	2.31	0.47
1:B:384:ASP:OD2	7:B:602:HOH:O	2.20	0.47
1:C:179:ARG:NH2	1:C:424:LEU:HD21	2.29	0.47
1:C:43:ARG:NH2	7:C:905:HOH:O	2.47	0.47
1:B:186:ASP:HB2	1:B:281:GLN:OE1	2.14	0.47
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.49	0.47
1:B:144:LYS:HB2	1:B:147:GLU:HB3	1.96	0.47
1:C:179:ARG:HD2	7:C:904:HOH:O	2.14	0.47
1:A:20:LYS:HD3	1:A:21:PHE:CE2	2.51	0.46
1:B:7:TYR:O	1:B:43:ARG:NH1	2.41	0.46
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.50	0.46
1:C:368:ILE:CG2	1:C:387:LEU:HD22	2.45	0.46
1:B:36:LYS:NZ	7:B:612:HOH:O	2.46	0.46
1:C:368:ILE:HG21	1:C:387:LEU:CD2	2.45	0.46
1:D:141:HIS:CD2	1:D:141:HIS:H	2.33	0.46
1:B:334:LEU:HD11	1:B:336:LEU:HD21	1.98	0.46
1:A:358:ILE:HG23	1:A:362:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:TYR:HB3	7:D:657:HOH:O	2.16	0.46
1:D:23:ASP:OD2	7:D:602:HOH:O	2.20	0.46
1:C:2:SER:N	1:C:131:GLU:OE1	2.49	0.45
1:C:440:MET:HE3	1:C:443:LEU:HD12	1.98	0.45
1:A:111:SER:OG	1:A:153:TYR:HB2	2.17	0.44
1:A:416:ARG:HG3	1:A:426:TYR:OH	2.17	0.44
1:A:264:PRO:HB2	1:A:435:TYR:CD1	2.51	0.44
1:C:85:THR:OG1	1:C:87:ASP:OD1	2.31	0.44
1:A:402:ASP:N	1:A:405:GLN:OE1	2.50	0.44
1:B:216:PHE:HA	1:B:217:PRO:HA	1.78	0.44
1:B:230:LEU:HG	1:B:231:PRO:HD2	2.00	0.44
1:B:40:GLU:OE2	7:B:601:HOH:O	2.20	0.43
1:A:165:VAL:HG11	1:A:203:VAL:CG2	2.49	0.43
1:D:71:LEU:HG	1:D:108:PHE:HD1	1.82	0.43
1:A:141:HIS:H	1:A:141:HIS:CD2	2.36	0.43
1:A:247:LEU:HD21	1:A:249:LEU:HD21	1.99	0.43
1:B:189:HIS:CE1	1:B:219:THR:HG1	2.32	0.43
1:D:368:ILE:HG21	1:D:387:LEU:HD22	2.00	0.43
1:A:18:SER:HB3	1:A:110:TYR:CE1	2.54	0.43
1:C:177:GLN:N	7:C:910:HOH:O	2.51	0.43
1:C:315:SER:HB3	7:C:1058:HOH:O	2.18	0.43
1:B:180:VAL:HG22	1:B:277:TYR:HB2	2.01	0.42
1:D:288:ALA:O	1:D:293:ARG:HG2	2.19	0.42
1:B:163:ARG:HB2	7:B:679:HOH:O	2.19	0.42
1:C:413:GLU:OE2	1:C:416:ARG:NH2	2.52	0.42
1:C:412:LEU:HD11	1:C:435:TYR:CZ	2.54	0.42
1:D:179:ARG:HE	1:D:202:ARG:NH1	2.17	0.42
1:A:239:ARG:HD3	1:C:392:PHE:CD2	2.55	0.42
1:D:202:ARG:NH2	7:D:612:HOH:O	2.50	0.42
1:D:265:ILE:HD13	1:D:411:ILE:HD13	2.02	0.42
1:A:2:SER:N	1:A:131:GLU:OE2	2.53	0.42
1:A:185:LEU:HD22	1:A:258:TRP:HH2	1.84	0.42
1:A:239:ARG:HH22	5:C:801:DMF:H12	1.84	0.42
1:C:72:LYS:HE3	1:C:72:LYS:HB2	1.48	0.42
1:D:157:ILE:HG12	1:D:336:LEU:HD13	2.02	0.42
1:B:20:LYS:HD3	1:B:20:LYS:HA	1.85	0.42
1:C:362:LYS:HE3	7:C:988:HOH:O	2.19	0.42
1:D:60:THR:HA	1:D:63:HIS:O	2.20	0.42
1:D:20:LYS:HE3	1:D:151:PHE:HB2	2.01	0.42
1:A:72:LYS:HG2	7:A:679:HOH:O	2.18	0.41
1:C:330:LYS:NZ	7:C:906:HOH:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HA	1:D:14:LEU:HD23	1.92	0.41
1:A:253:ILE:HG22	1:A:295:PHE:CD1	2.55	0.41
1:B:189:HIS:ND1	1:B:219:THR:OG1	2.37	0.41
1:D:286:CYS:HB2	1:D:319:TYR:OH	2.20	0.41
1:C:75:GLN:HG3	1:C:105:PRO:O	2.19	0.41
1:D:358:ILE:HG23	1:D:362:LYS:HD3	2.03	0.41
1:A:286:CYS:HB2	1:A:319:TYR:OH	2.20	0.41
1:A:66:GLU:HG2	1:A:67:TYR:N	2.36	0.41
1:C:322:ALA:O	1:C:326:ILE:HG13	2.20	0.41
1:A:144:LYS:NZ	1:A:195:GLU:OE1	2.43	0.41
1:A:426:TYR:HE2	1:A:431:VAL:HG21	1.86	0.41
1:C:18:SER:HB3	1:C:110:TYR:CE1	2.55	0.41
1:D:182:TYR:CE2	1:D:184:ASP:HB2	2.55	0.41
1:D:187:LEU:HD11	1:D:294:ILE:HB	2.03	0.41
1:A:54:ARG:HD3	7:A:708:HOH:O	2.21	0.41
1:C:141:HIS:H	1:C:141:HIS:CD2	2.39	0.41
1:C:35:TYR:CZ	1:C:373:PRO:HD3	2.55	0.41
1:C:31:LEU:HA	1:C:31:LEU:HD12	1.91	0.40
1:A:104:PHE:CE2	1:A:107:VAL:HA	2.56	0.40
1:A:402:ASP:O	1:A:406:LYS:HD2	2.21	0.40
1:A:221:THR:HA	1:A:233:PHE:CZ	2.56	0.40
1:A:343:PHE:HB2	1:A:344:PRO:HD3	2.04	0.40
1:D:404:ILE:HA	1:D:404:ILE:HD12	1.91	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	387/447 (87%)	380 (98%)	7 (2%)	0	100	100
1	B	400/447 (90%)	389 (97%)	10 (2%)	1 (0%)	41	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	399/447 (89%)	391 (98%)	8 (2%)	0	100	100
1	D	390/447 (87%)	383 (98%)	7 (2%)	0	100	100
All	All	1576/1788 (88%)	1543 (98%)	32 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	TYR

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	344/392 (88%)	338 (98%)	6 (2%)	60	65
1	B	357/392 (91%)	353 (99%)	4 (1%)	73	78
1	C	356/392 (91%)	349 (98%)	7 (2%)	55	59
1	D	347/392 (88%)	341 (98%)	6 (2%)	60	65
All	All	1404/1568 (90%)	1381 (98%)	23 (2%)	62	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	90	LEU
1	A	141	HIS
1	A	233	PHE
1	A	285	ASP
1	A	429	ASP
1	B	141	HIS
1	B	165	VAL
1	B	429	ASP
1	B	438	THR
1	C	87	ASP

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Mol	Chain	Res	Type
1	C	141	HIS
1	C	200	SER
1	C	285	ASP
1	C	317	SER
1	C	356	LEU
1	C	369	SER
1	D	20	LYS
1	D	56	TYR
1	D	141	HIS
1	D	334	LEU
1	D	379	SER
1	D	433	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	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 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	$\# Z > 2$
5	DMF	A	505	-	4,4,4	0.34	0	4,4,4	0.39	0
5	DMF	C	801	-	4,4,4	0.28	0	4,4,4	0.35	0
4	FGN	D	504	2	23,23,23	0.27	0	30,30,30	0.67	0
4	FGN	A	504	2	23,23,23	0.29	0	30,30,30	0.36	0
4	FGN	B	504	2	23,23,23	0.25	0	30,30,30	0.57	0
4	FGN	C	805	2	23,23,23	0.29	0	30,30,30	0.72	0
5	DMF	A	506	-	4,4,4	0.34	0	4,4,4	0.49	0
6	GOL	C	806	-	5,5,5	0.40	0	5,5,5	0.79	0
6	GOL	D	505	-	5,5,5	0.40	0	5,5,5	0.34	0
6	GOL	A	507	-	5,5,5	0.22	0	5,5,5	1.05	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
5	DMF	A	505	-	-	0/2/2/2	-
5	DMF	C	801	-	-	0/2/2/2	-
4	FGN	D	504	2	-	4/12/12/12	0/2/2/2
4	FGN	A	504	2	-	5/12/12/12	0/2/2/2
4	FGN	B	504	2	-	4/12/12/12	0/2/2/2
4	FGN	C	805	2	-	2/12/12/12	0/2/2/2
5	DMF	A	506	-	-	2/2/2/2	-
6	GOL	C	806	-	-	4/4/4/4	-
6	GOL	D	505	-	-	0/4/4/4	-
6	GOL	A	507	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	504	FGN	C1-C-N-O2
4	D	504	FGN	O-C-N-O2

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Mol	Chain	Res	Type	Atoms
4	C	805	FGN	C11-C10-C9-O1
4	C	805	FGN	C15-C10-C9-O1
6	C	806	GOL	O1-C1-C2-C3
6	C	806	GOL	C1-C2-C3-O3
6	C	806	GOL	O2-C2-C3-O3
4	B	504	FGN	C1-C-N-O2
4	B	504	FGN	O-C-N-O2
4	A	504	FGN	C1-C-N-O2
4	A	504	FGN	O-C-N-O2
6	A	507	GOL	C1-C2-C3-O3
5	A	506	DMF	O-C-N-C2
6	C	806	GOL	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
5	A	506	DMF	O-C-N-C1
4	A	504	FGN	C10-C9-O1-C8
4	D	504	FGN	C11-C10-C9-O1
4	D	504	FGN	C15-C10-C9-O1
4	B	504	FGN	C11-C10-C9-O1
4	B	504	FGN	C15-C10-C9-O1
4	A	504	FGN	C11-C10-C9-O1
4	A	504	FGN	C15-C10-C9-O1

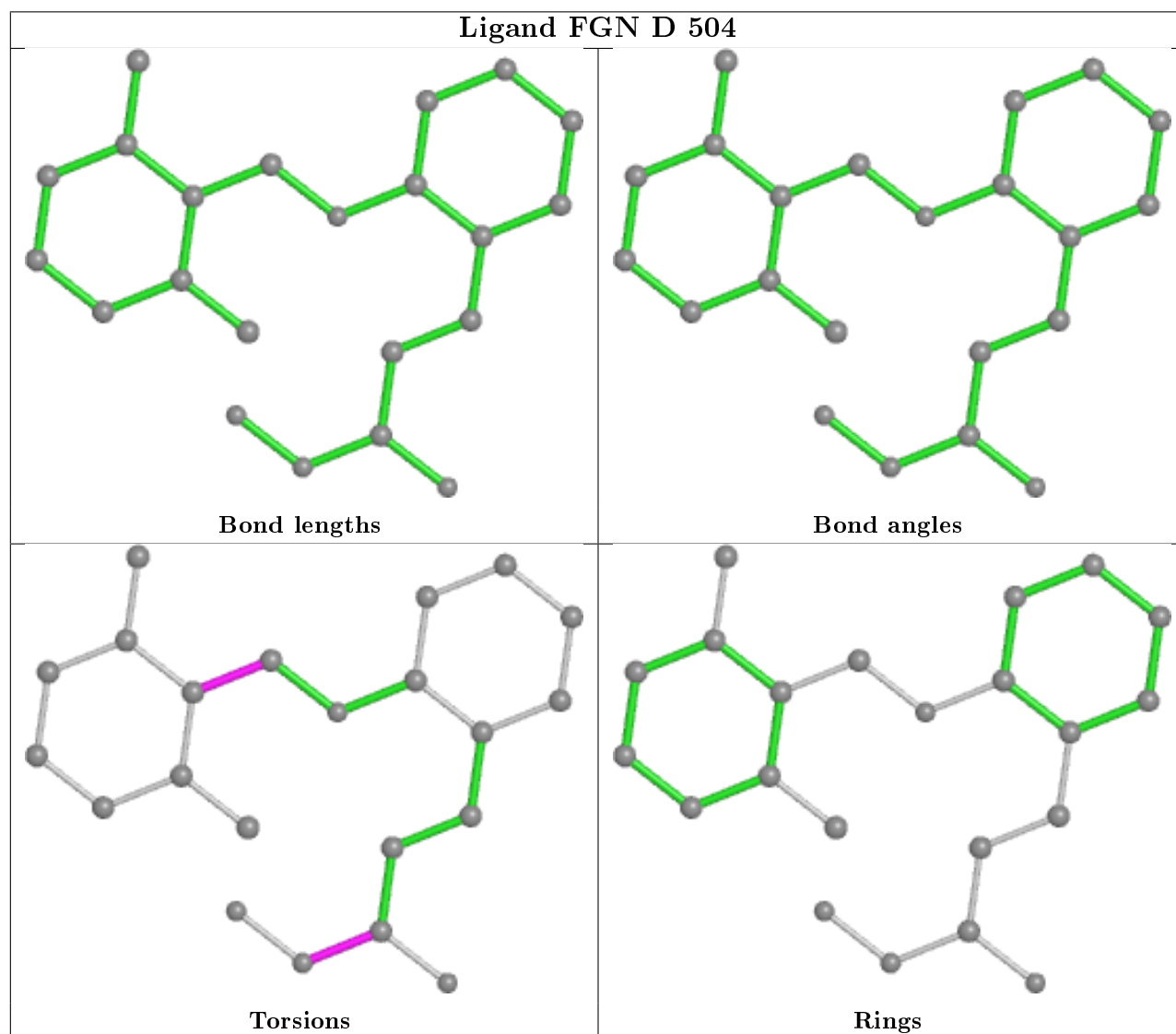
There are no ring outliers.

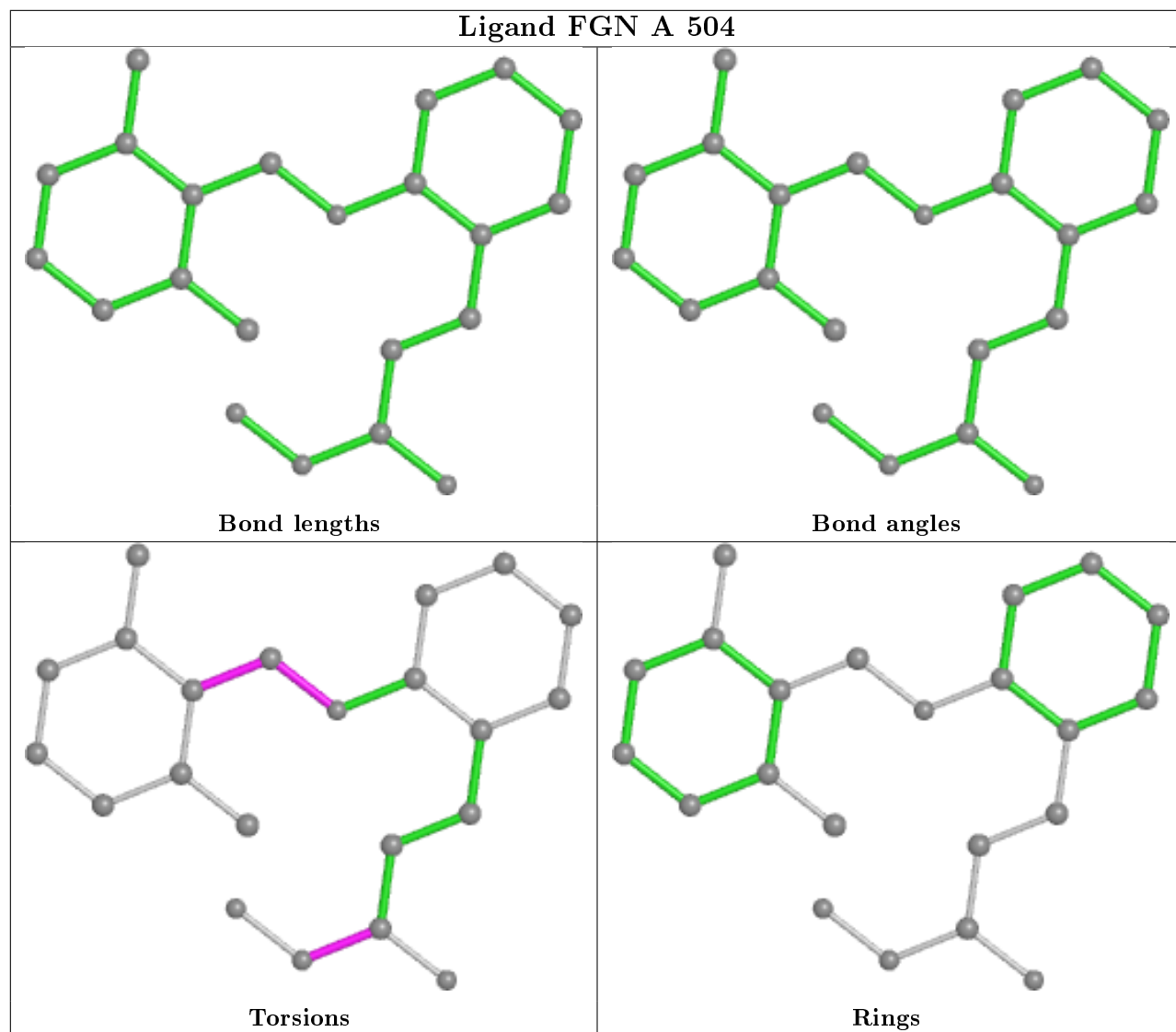
5 monomers are involved in 8 short contacts:

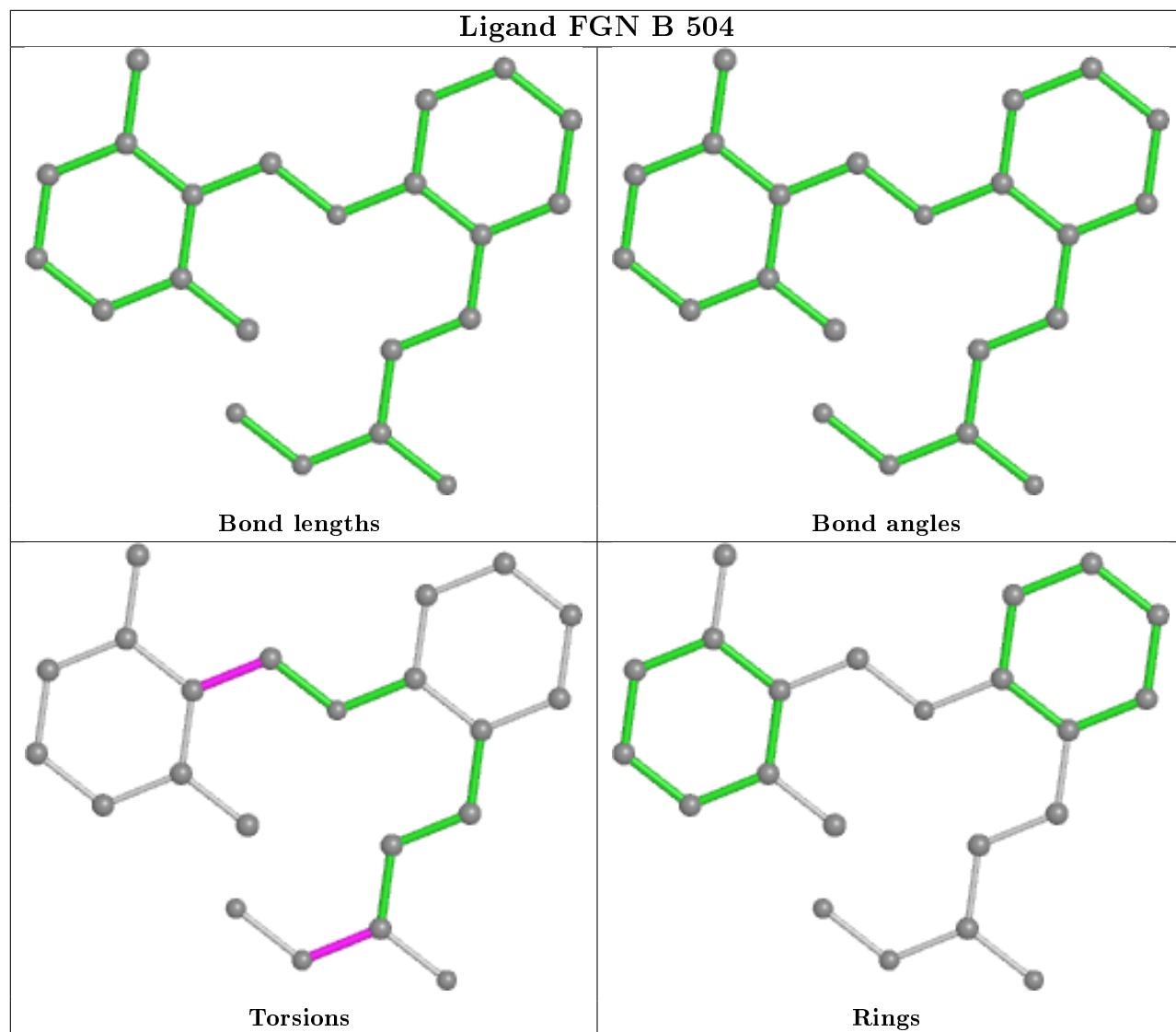
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	801	DMF	2	0
4	D	504	FGN	1	0
4	A	504	FGN	1	0
5	A	506	DMF	2	0
6	A	507	GOL	2	0

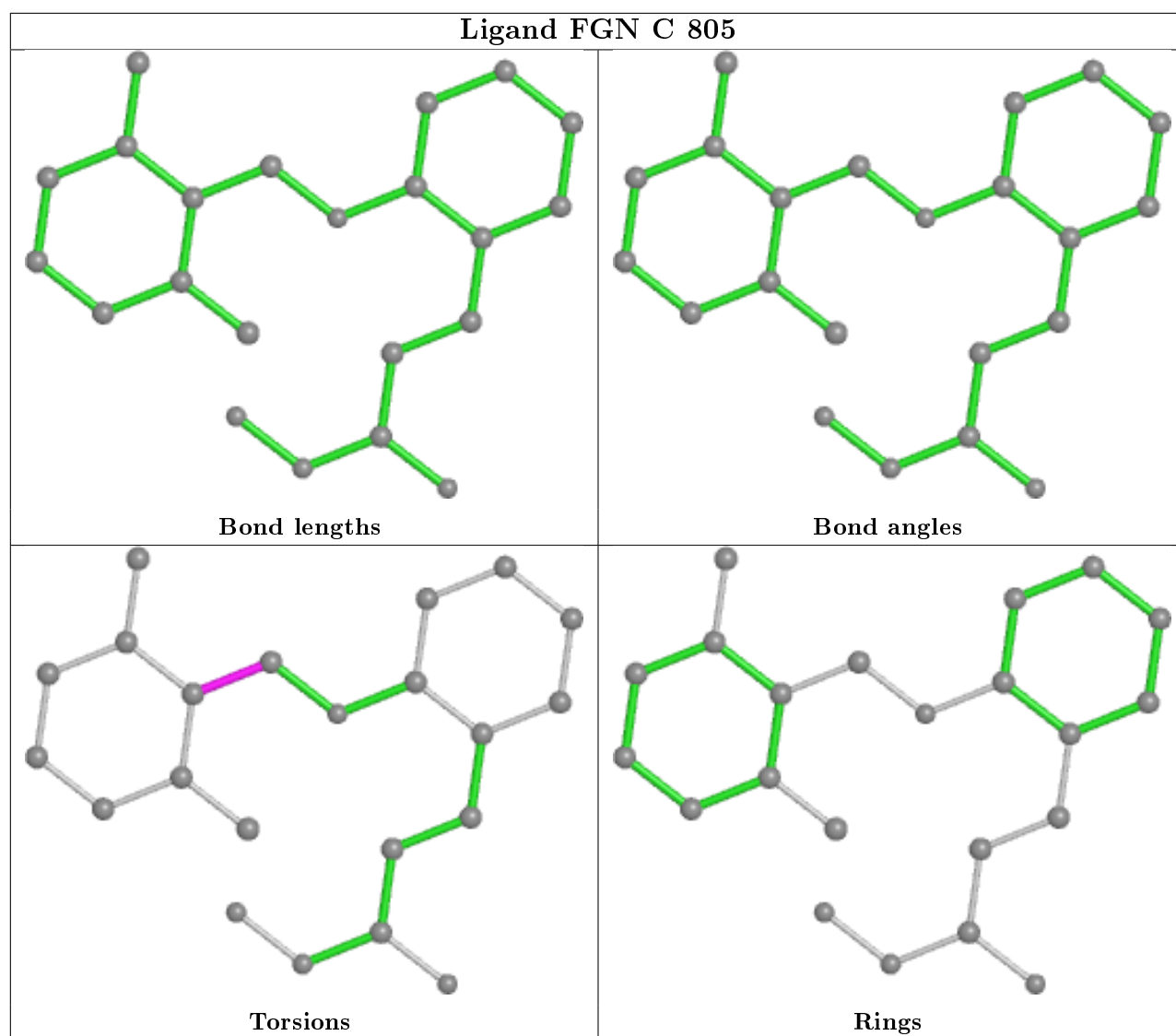
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	397/447 (88%)	0.49	22 (5%) 25 30	15, 27, 56, 110	0
1	B	411/447 (91%)	0.29	10 (2%) 59 63	12, 24, 47, 79	0
1	C	411/447 (91%)	0.35	10 (2%) 59 63	15, 24, 45, 106	0
1	D	399/447 (89%)	0.50	29 (7%) 15 18	16, 27, 66, 104	0
All	All	1618/1788 (90%)	0.41	71 (4%) 34 39	12, 26, 53, 110	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	TYR	9.5
1	D	434	LEU	9.5
1	A	428	TYR	9.5
1	D	432	TYR	9.3
1	A	434	LEU	8.9
1	D	435	TYR	8.1
1	A	426	TYR	8.1
1	B	230	LEU	7.6
1	A	435	TYR	7.4
1	D	426	TYR	7.0
1	D	429	ASP	6.9
1	A	425	ILE	6.6
1	D	425	ILE	6.0
1	D	428	TYR	5.9
1	D	224	MET	5.6
1	C	230	LEU	5.6
1	B	425	ILE	5.5
1	A	429	ASP	5.0
1	B	168	THR	4.9
1	D	230	LEU	4.9
1	A	293	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	168	THR	4.7
1	D	433	GLN	4.2
1	C	83	GLU	4.2
1	A	177	GLN	4.1
1	D	81	GLU	4.0
1	D	409	ARG	3.8
1	A	81	GLU	3.8
1	D	165	VAL	3.7
1	D	392	PHE	3.7
1	A	232	ILE	3.6
1	A	409	ARG	3.6
1	B	426	TYR	3.6
1	A	384	ASP	3.4
1	B	231	PRO	3.4
1	C	224	MET	3.3
1	A	402	ASP	3.3
1	A	383	PRO	3.2
1	D	82	LYS	3.1
1	D	232	ILE	3.1
1	A	431	VAL	3.1
1	D	293	ARG	2.9
1	D	420	ASP	2.9
1	D	412	LEU	2.9
1	B	429	ASP	2.7
1	D	427	ASP	2.6
1	B	224	MET	2.6
1	D	292	HIS	2.6
1	D	404	ILE	2.6
1	C	167	SER	2.5
1	D	416	ARG	2.5
1	C	231	PRO	2.5
1	D	231	PRO	2.5
1	D	402	ASP	2.5
1	C	425	ILE	2.5
1	A	231	PRO	2.4
1	D	271	ILE	2.4
1	C	99	TYR	2.3
1	B	315	SER	2.3
1	B	177	GLN	2.3
1	A	292	HIS	2.3
1	D	382	GLY	2.3
1	B	128	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	302	PRO	2.2
1	C	87	ASP	2.2
1	A	382	GLY	2.1
1	C	177	GLN	2.1
1	A	433	GLN	2.1
1	A	427	ASP	2.1
1	A	416	ARG	2.0
1	D	430	GLN	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.

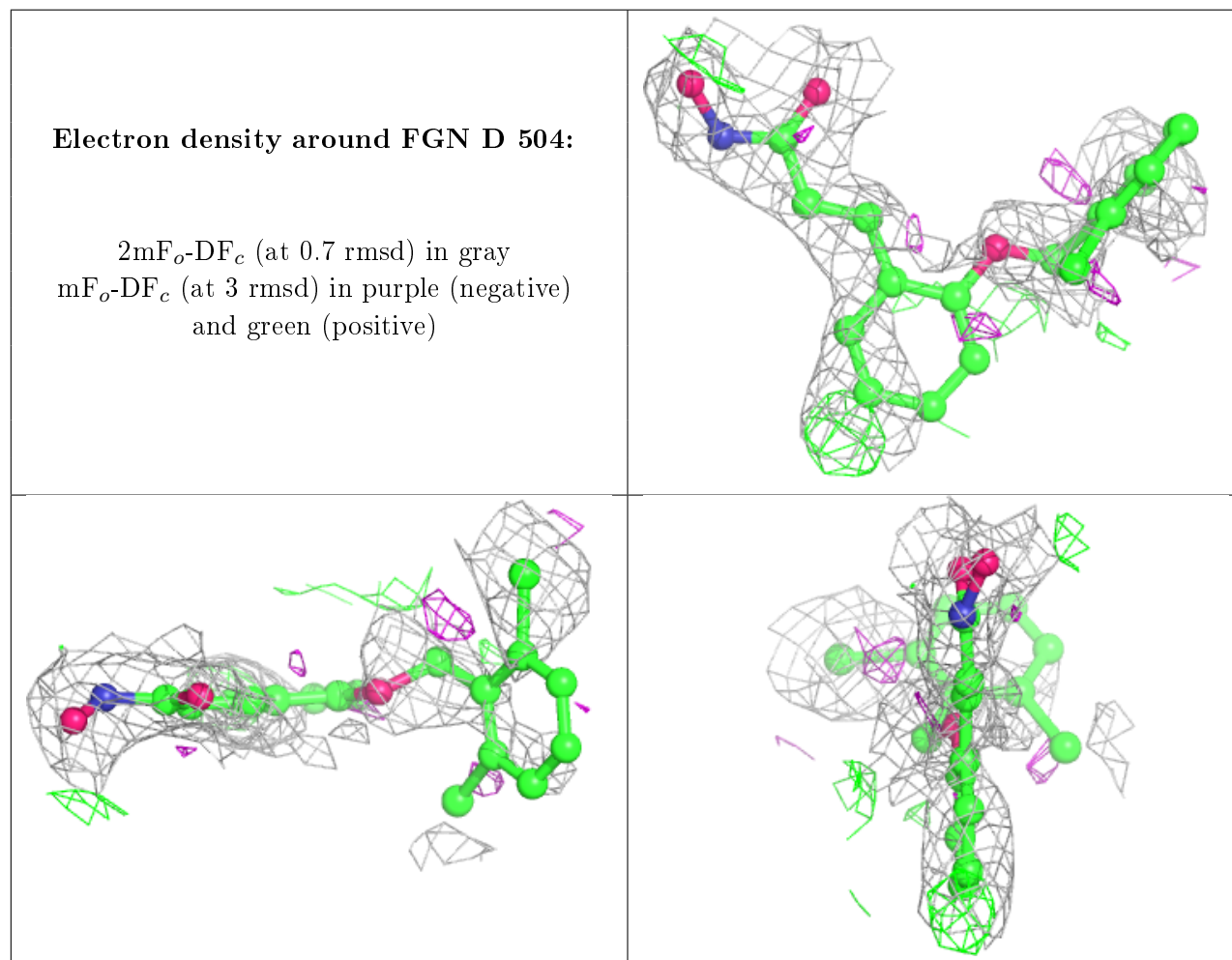
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FGN	D	504	22/22	0.60	0.38	38,91,104,119	0
4	FGN	C	805	22/22	0.63	0.36	41,82,93,102	0
4	FGN	A	504	22/22	0.64	0.33	38,94,106,113	0
4	FGN	B	504	22/22	0.73	0.40	21,81,100,113	0
5	DMF	C	801	5/5	0.81	0.26	57,60,63,64	0
5	DMF	A	506	5/5	0.81	0.19	41,42,53,53	0
6	GOL	A	507	6/6	0.90	0.18	24,33,35,50	0
5	DMF	A	505	5/5	0.92	0.15	45,46,54,58	0
6	GOL	C	806	6/6	0.92	0.12	22,28,31,34	0
6	GOL	D	505	6/6	0.95	0.13	28,31,33,34	0
3	K	B	503	1/1	0.99	0.07	26,26,26,26	0
3	K	D	503	1/1	0.99	0.11	22,22,22,22	0
3	K	A	503	1/1	0.99	0.16	25,25,25,25	0
3	K	C	804	1/1	0.99	0.12	25,25,25,25	0
3	K	D	502	1/1	0.99	0.07	20,20,20,20	0

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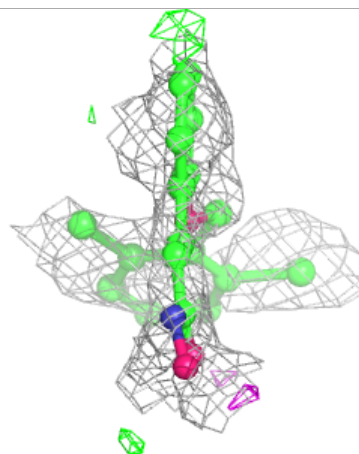
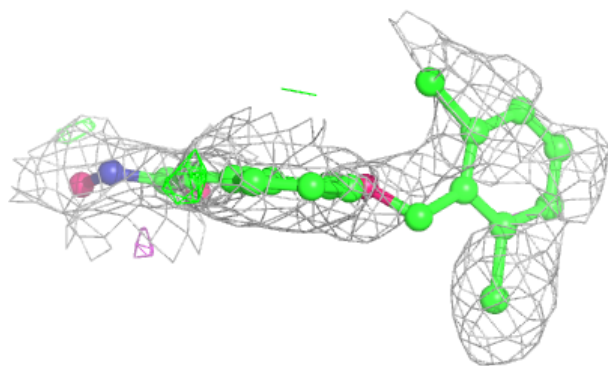
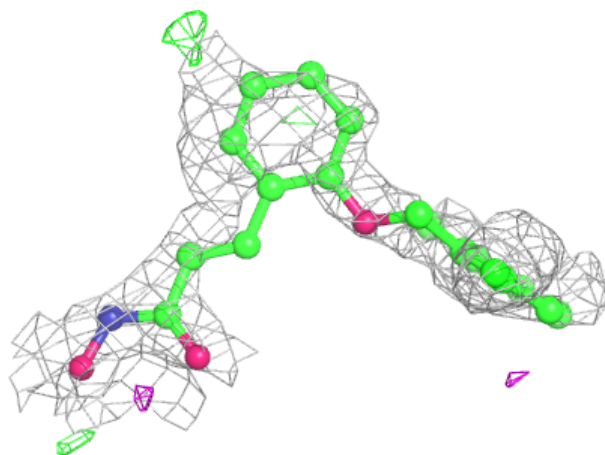
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	501	1/1	0.99	0.06	24,24,24,24	0
3	K	B	502	1/1	0.99	0.09	23,23,23,23	0
3	K	C	803	1/1	0.99	0.07	22,22,22,22	0
3	K	A	502	1/1	0.99	0.06	22,22,22,22	0
2	ZN	D	501	1/1	1.00	0.08	28,28,28,28	0
2	ZN	A	501	1/1	1.00	0.08	26,26,26,26	0
2	ZN	C	802	1/1	1.00	0.06	22,22,22,22	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.



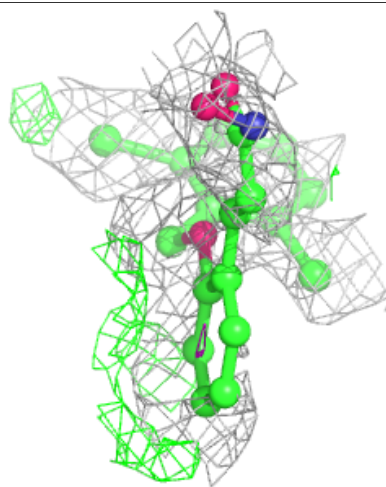
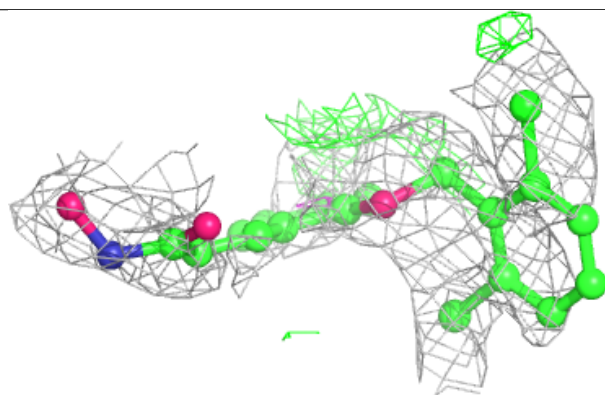
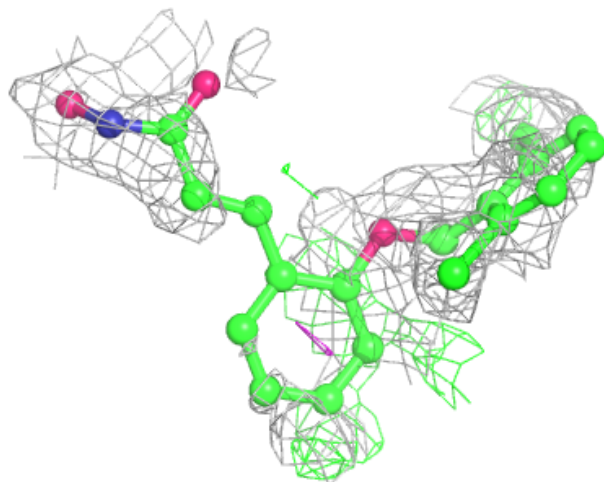
Electron density around FGN C 805:

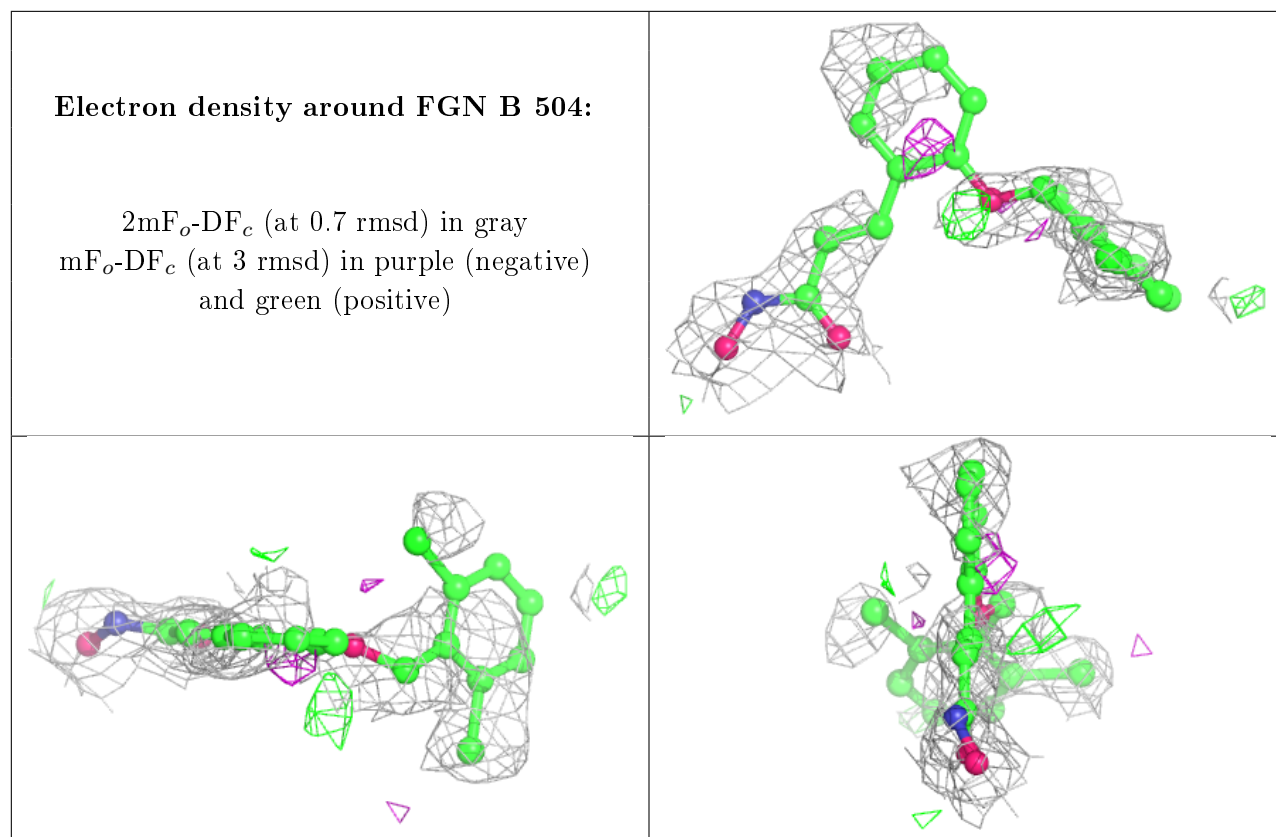
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FGN A 504:

$2mF_o-DF_c$ (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.