



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:37 am BST

PDB ID : 6HU3
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with a triazole hydroxamate inhibitor
Authors : Shaik, T.B.; Marek, M.; Romier, C.
Deposited on : 2018-10-05
Resolution : 1.66 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

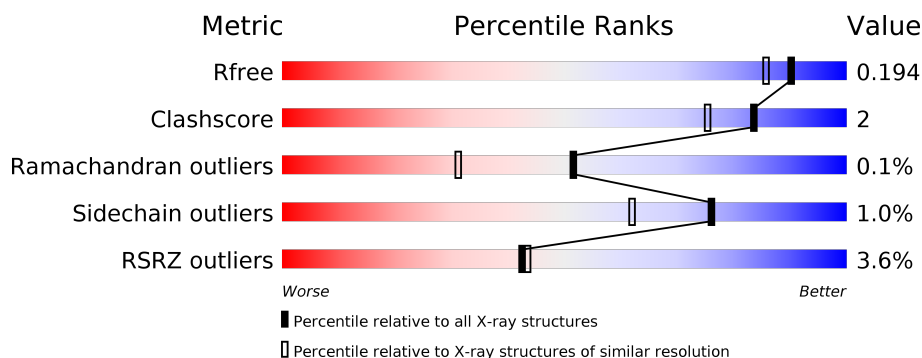
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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>4%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	447	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> </div> </div>
1	C	447	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> </div> </div>
1	D	447	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14261 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	401	Total	C	N	O	S	0	5	0
			3241	2097	536	592	16			
1	B	417	Total	C	N	O	S	0	5	0
			3357	2168	557	616	16			
1	C	413	Total	C	N	O	S	0	5	0
			3324	2146	552	611	15			
1	D	402	Total	C	N	O	S	0	5	0
			3246	2096	537	597	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

Continued on next page...

Continued from previous page...

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

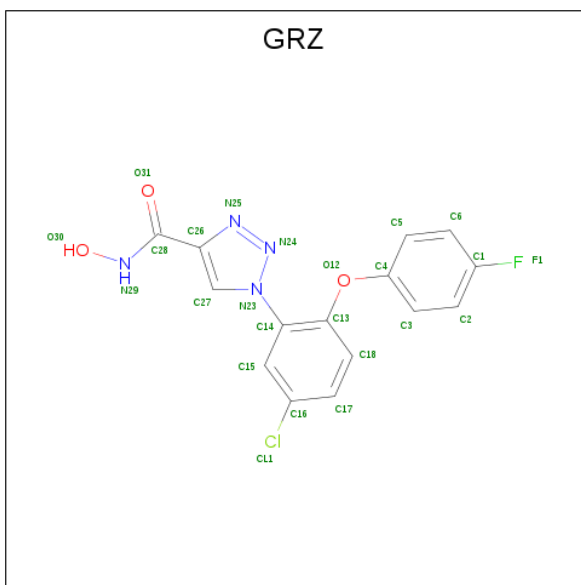
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

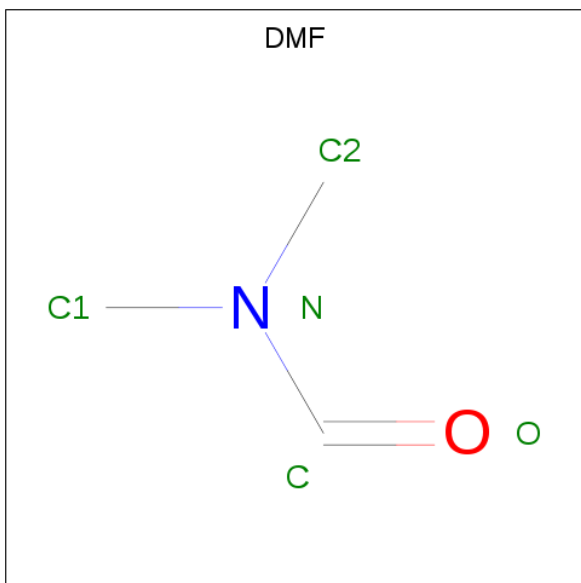
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is 1-[5-chloranyl-2-(4-fluoranylphenoxy)phenyl]- {N}-oxidanyl-1,2,3-triazole-4-carboxamide (three-letter code: GRZ) (formula: C₁₅H₁₀ClFN₄O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 15	Cl 1	F 1	N 4	O 3	0	0
4	B	1	Total 24	C 15	Cl 1	F 1	N 4	O 3	0	0
4	C	1	Total 24	C 15	Cl 1	F 1	N 4	O 3	0	0
4	D	1	Total 24	C 15	Cl 1	F 1	N 4	O 3	0	0

- 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	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	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

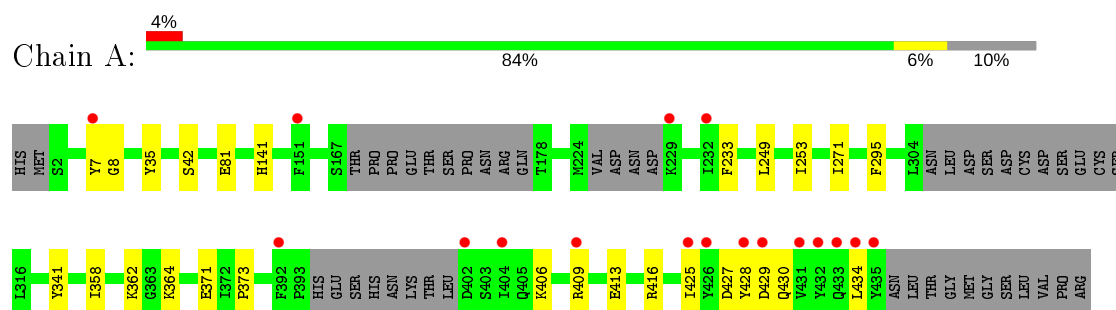
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	187	Total	O	0	0
			187	187		
7	B	240	Total	O	0	0
			240	240		
7	C	226	Total	O	0	0
			226	226		
7	D	197	Total	O	0	0
			197	197		

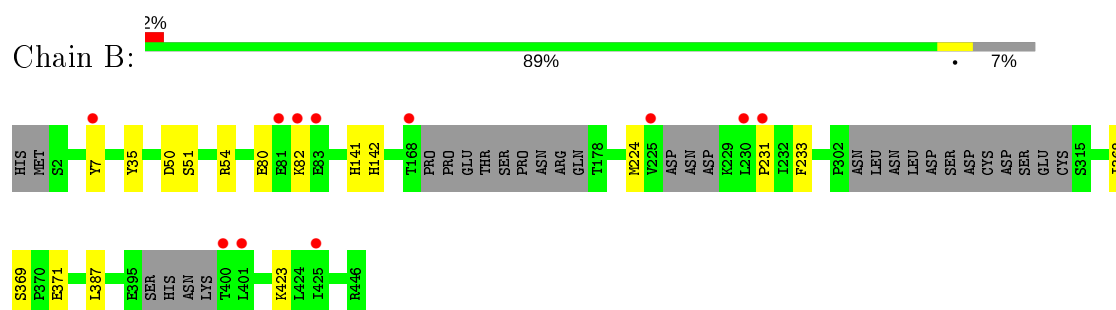
3 Residue-property plots [i](#)

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.

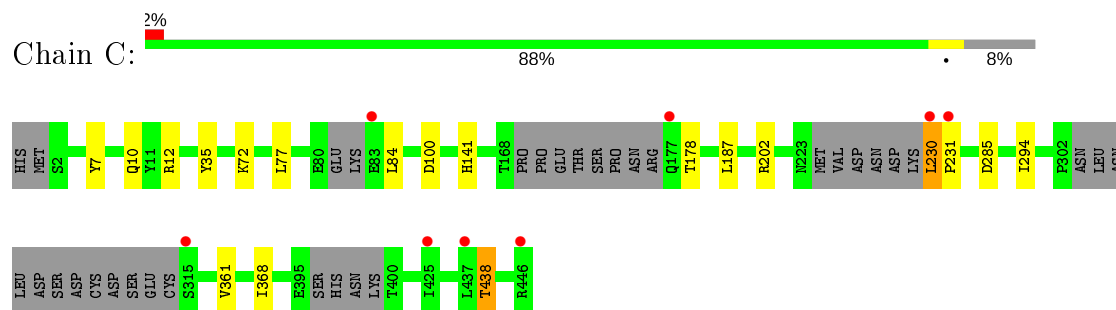
- Molecule 1: Histone deacetylase



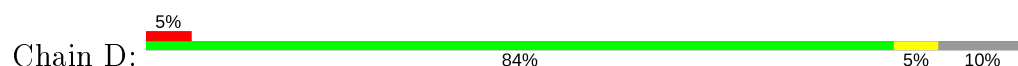
- Molecule 1: Histone deacetylase

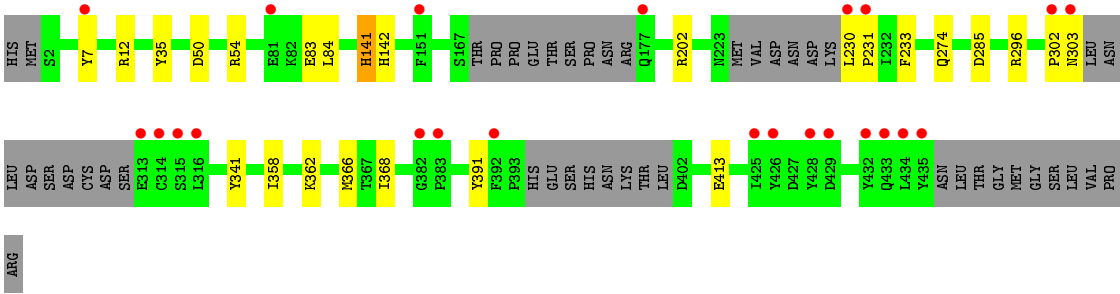


- Molecule 1: Histone deacetylase



- 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	70.64Å 70.43Å 97.92Å 75.48° 78.20° 86.17°	Depositor
Resolution (Å)	48.95 – 1.66 48.95 – 1.65	Depositor EDS
% Data completeness (in resolution range)	92.2 (48.95-1.66) 92.2 (48.95-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.65Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.162 , 0.194 0.162 , 0.194	Depositor DCC
R_{free} test set	9832 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.067 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14261	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, GRZ, 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	0.39	0/3345	0.53	0/4549
1	B	0.43	0/3463	0.58	0/4710
1	C	0.43	0/3429	0.59	2/4665 (0.0%)
1	D	0.40	0/3350	0.56	0/4557
All	All	0.41	0/13587	0.56	2/18481 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	285	ASP	CB-CG-OD2	-5.23	113.60	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	302	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3241	0	3144	17	0
1	B	3357	0	3263	14	0
1	C	3324	0	3220	17	0
1	D	3246	0	3135	14	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
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	24	0	0	1	0
4	B	24	0	0	1	0
4	C	24	0	0	0	0
4	D	24	0	0	2	0
5	A	25	0	35	2	0
5	B	30	0	42	2	0
5	C	25	0	35	8	0
5	D	25	0	35	2	0
6	A	12	0	16	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	187	0	0	2	0
7	B	240	0	0	1	0
7	C	226	0	0	3	0
7	D	197	0	0	1	0
All	All	14261	0	12949	63	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 2.

All (63) 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:341:TYR:OH	4:A:504:GRZ:O31	2.06	0.70
1:D:341:TYR:OH	4:D:504:GRZ:O31	2.08	0.68
1:B:369:SER:OG	1:B:371:GLU:OE1	2.13	0.66
1:A:358:ILE:HG23	1:A:362:LYS:HD2	1.78	0.64
1:A:295:PHE:O	7:A:601:HOH:O	2.14	0.64
1:A:362:LYS:HD3	1:A:364:LYS:HD3	1.81	0.62
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.36	0.61
1:B:7[A]:TYR:CE1	5:B:505:DMF:H13	2.35	0.61
1:C:10:GLN:HB3	5:C:508:DMF:H23	1.83	0.61
1:A:371:GLU:OE2	7:A:602:HOH:O	2.17	0.60
1:B:51:SER:OG	1:B:54:ARG:NE	2.36	0.59
1:B:50:ASP:OD1	1:B:54:ARG:NH1	2.37	0.58
1:D:12:ARG:HE	5:D:506:DMF:H12	1.69	0.57
1:A:413:GLU:HG3	1:A:416:ARG:HH22	1.73	0.54
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.44	0.53
1:A:427:ASP:OD2	1:A:430:GLN:N	2.39	0.53
1:D:7[B]:TYR:OH	1:D:12:ARG:HD2	2.09	0.53
1:C:10:GLN:HG2	5:C:508:DMF:H23	1.91	0.52
1:D:296:ARG:HD2	1:D:391:TYR:OH	2.10	0.52
1:A:406:LYS:HD2	1:A:409:ARG:HH21	1.75	0.51
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.45	0.51
1:D:358:ILE:HG23	1:D:362:LYS:HE3	1.93	0.51
1:C:187:LEU:HD21	1:C:294:ILE:HD12	1.93	0.51
1:C:7[A]:TYR:CD2	5:C:506:DMF:H23	2.47	0.49
1:C:438:THR:O	1:C:438:THR:OG1	2.30	0.49
1:A:81:GLU:N	1:A:81:GLU:OE1	2.35	0.49
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.48	0.48
5:C:508:DMF:H22	7:C:793:HOH:O	2.13	0.48
1:B:54:ARG:NH2	7:B:604:HOH:O	2.46	0.48
1:C:12:ARG:HE	5:C:507:DMF:HC	1.79	0.48
1:A:42:SER:HA	5:A:505:DMF:HC	1.96	0.48
1:D:230:LEU:HD23	1:D:231:PRO:O	2.14	0.47
1:B:80:GLU:HG2	1:B:82:LYS:HE3	1.96	0.47
1:B:80:GLU:OE2	1:B:80:GLU:N	2.48	0.47
1:D:83:GLU:CD	1:D:84:LEU:H	2.19	0.46
1:B:224:MET:HG2	1:B:231:PRO:HB3	1.98	0.45
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.50	0.45
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.52	0.45
1:C:77:LEU:HD13	1:C:84:LEU:HG	1.98	0.45
1:A:7[A]:TYR:CD2	5:A:506:DMF:H23	2.51	0.45
1:D:50:ASP:OD1	1:D:54:ARG:HG3	2.16	0.45
1:D:35:TYR:CD1	1:D:368:ILE:HG23	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD12	1:A:434:LEU:HD11	1.99	0.44
1:C:361:VAL:HG22	5:C:509:DMF:H13	2.00	0.44
1:C:230:LEU:HA	1:C:231:PRO:HD3	1.87	0.43
1:A:7[A]:TYR:CG	1:A:8:GLY:N	2.87	0.43
1:B:7[A]:TYR:CD1	5:B:505:DMF:H13	2.53	0.43
1:D:142:HIS:NE2	4:D:504:GRZ:N29	2.67	0.43
1:B:423:LYS:HD3	1:B:423:LYS:HA	1.82	0.42
1:C:100:ASP:HB2	7:C:781:HOH:O	2.18	0.42
1:C:12:ARG:HE	5:C:507:DMF:C	2.31	0.42
1:A:249:LEU:HD13	1:A:253:ILE:HD13	2.01	0.42
1:A:362:LYS:HB3	1:A:364:LYS:HG3	2.00	0.42
1:C:7[B]:TYR:OH	1:C:12:ARG:HD2	2.20	0.42
1:C:72:LYS:HD3	7:C:735:HOH:O	2.20	0.42
1:A:428:TYR:CG	1:A:428:TYR:O	2.73	0.41
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.51	0.41
1:D:141:HIS:H	1:D:141:HIS:CD2	2.38	0.41
1:B:142:HIS:NE2	4:B:504:GRZ:N29	2.68	0.41
1:C:7[A]:TYR:CE2	5:C:506:DMF:H23	2.54	0.41
1:D:366:MET:O	5:D:505:DMF:H22	2.21	0.41
1:D:274:GLN:HG2	7:D:720:HOH:O	2.21	0.40
1:C:178:THR:HB	1:C:202:ARG:HH21	1.86	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	396/447 (89%)	389 (98%)	6 (2%)	1 (0%)	41	22
1	B	412/447 (92%)	405 (98%)	7 (2%)	0	100	100
1	C	406/447 (91%)	401 (99%)	5 (1%)	0	100	100
1	D	397/447 (89%)	394 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1611/1788 (90%)	1589 (99%)	21 (1%)	1 (0%)	51 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ASP

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	353/392 (90%)	350 (99%)	3 (1%)	81 70
1	B	367/392 (94%)	365 (100%)	2 (0%)	88 81
1	C	363/392 (93%)	360 (99%)	3 (1%)	81 70
1	D	354/392 (90%)	348 (98%)	6 (2%)	60 39
All	All	1437/1568 (92%)	1423 (99%)	14 (1%)	76 62

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	233	PHE
1	A	425	ILE
1	B	141	HIS
1	B	233	PHE
1	C	141	HIS
1	C	230	LEU
1	C	438	THR
1	D	141	HIS
1	D	202	ARG
1	D	233	PHE
1	D	285	ASP
1	D	303	ASN
1	D	413	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 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	C	506	-	4,4,4	0.30	0	4,4,4	0.45	0
6	GOL	A	511	-	5,5,5	0.31	0	5,5,5	0.26	0
5	DMF	A	507	-	4,4,4	0.35	0	4,4,4	0.27	0
5	DMF	B	509	-	4,4,4	0.34	0	4,4,4	0.27	0
6	GOL	C	510	-	5,5,5	0.29	0	5,5,5	0.44	0
6	GOL	D	510	-	5,5,5	0.32	0	5,5,5	0.24	0
5	DMF	B	510	-	4,4,4	0.32	0	4,4,4	0.41	0
4	GRZ	B	504	2	21,26,26	0.46	0	24,36,36	0.78	1 (4%)
5	DMF	D	506	-	4,4,4	0.29	0	4,4,4	0.35	0
5	DMF	C	507	-	4,4,4	0.30	0	4,4,4	0.31	0
5	DMF	D	509	-	4,4,4	0.29	0	4,4,4	0.45	0
4	GRZ	C	504	2	21,26,26	0.43	0	24,36,36	0.74	0
6	GOL	A	510	-	5,5,5	0.26	0	5,5,5	0.44	0
5	DMF	C	505	-	4,4,4	0.30	0	4,4,4	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GRZ	A	504	2	21,26,26	0.44	0	24,36,36	0.68	0
5	DMF	A	505	-	4,4,4	0.33	0	4,4,4	0.18	0
5	DMF	B	508	-	4,4,4	0.29	0	4,4,4	0.40	0
5	DMF	A	508	-	4,4,4	0.34	0	4,4,4	0.36	0
5	DMF	B	505	-	4,4,4	0.24	0	4,4,4	0.41	0
5	DMF	B	507	-	4,4,4	0.33	0	4,4,4	0.45	0
5	DMF	D	507	-	4,4,4	0.34	0	4,4,4	0.35	0
5	DMF	D	508	-	4,4,4	0.33	0	4,4,4	0.37	0
5	DMF	B	506	-	4,4,4	0.33	0	4,4,4	0.42	0
6	GOL	B	511	-	5,5,5	0.21	0	5,5,5	0.61	0
5	DMF	C	508	-	4,4,4	0.43	0	4,4,4	0.60	0
5	DMF	D	505	-	4,4,4	0.30	0	4,4,4	0.44	0
4	GRZ	D	504	2	21,26,26	0.44	0	24,36,36	0.62	0
5	DMF	A	506	-	4,4,4	0.29	0	4,4,4	0.40	0
5	DMF	C	509	-	4,4,4	0.35	0	4,4,4	0.36	0
5	DMF	A	509	-	4,4,4	0.36	0	4,4,4	0.42	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	C	506	-	-	2/2/2/2	-
6	GOL	A	511	-	-	0/4/4/4	-
5	DMF	A	507	-	-	2/2/2/2	-
5	DMF	B	509	-	-	2/2/2/2	-
6	GOL	C	510	-	-	1/4/4/4	-
6	GOL	D	510	-	-	0/4/4/4	-
5	DMF	B	510	-	-	0/2/2/2	-
4	GRZ	B	504	2	-	1/9/14/14	0/3/3/3
5	DMF	D	506	-	-	0/2/2/2	-
5	DMF	C	507	-	-	0/2/2/2	-
5	DMF	D	509	-	-	0/2/2/2	-
4	GRZ	C	504	2	-	1/9/14/14	0/3/3/3
6	GOL	A	510	-	-	2/4/4/4	-
5	DMF	C	505	-	-	0/2/2/2	-
4	GRZ	A	504	2	-	2/9/14/14	0/3/3/3
5	DMF	A	505	-	-	0/2/2/2	-
5	DMF	B	508	-	-	2/2/2/2	-
5	DMF	A	508	-	-	0/2/2/2	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	B	505	-	-	0/2/2/2	-
5	DMF	B	507	-	-	0/2/2/2	-
5	DMF	D	507	-	-	2/2/2/2	-
5	DMF	D	508	-	-	2/2/2/2	-
5	DMF	B	506	-	-	2/2/2/2	-
6	GOL	B	511	-	-	3/4/4/4	-
5	DMF	C	508	-	-	2/2/2/2	-
5	DMF	D	505	-	-	2/2/2/2	-
4	GRZ	D	504	2	-	1/9/14/14	0/3/3/3
5	DMF	A	506	-	-	0/2/2/2	-
5	DMF	C	509	-	-	2/2/2/2	-
5	DMF	A	509	-	-	2/2/2/2	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	GRZ	C13-O12-C4	2.19	123.47	118.00

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	GRZ	C13-C14-N23-N24
5	D	507	DMF	O-C-N-C1
5	D	507	DMF	O-C-N-C2
5	A	509	DMF	O-C-N-C1
5	A	509	DMF	O-C-N-C2
5	C	506	DMF	O-C-N-C2
5	B	508	DMF	O-C-N-C2
5	C	506	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C1
5	B	508	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C2
6	A	510	GOL	O2-C2-C3-O3
5	C	509	DMF	O-C-N-C1
6	A	510	GOL	C1-C2-C3-O3
6	B	511	GOL	C1-C2-C3-O3
5	B	509	DMF	O-C-N-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	509	DMF	O-C-N-C2
5	A	507	DMF	O-C-N-C2
5	B	509	DMF	O-C-N-C1
5	A	507	DMF	O-C-N-C1
6	B	511	GOL	O2-C2-C3-O3
5	D	508	DMF	O-C-N-C1
6	B	511	GOL	O1-C1-C2-C3
5	B	506	DMF	O-C-N-C1
4	B	504	GRZ	C15-C14-N23-C27
4	C	504	GRZ	C15-C14-N23-C27
4	A	504	GRZ	C15-C14-N23-C27
4	D	504	GRZ	C15-C14-N23-C27
5	D	508	DMF	O-C-N-C2
5	B	506	DMF	O-C-N-C2
5	D	505	DMF	O-C-N-C1
6	C	510	GOL	C1-C2-C3-O3
5	D	505	DMF	O-C-N-C2

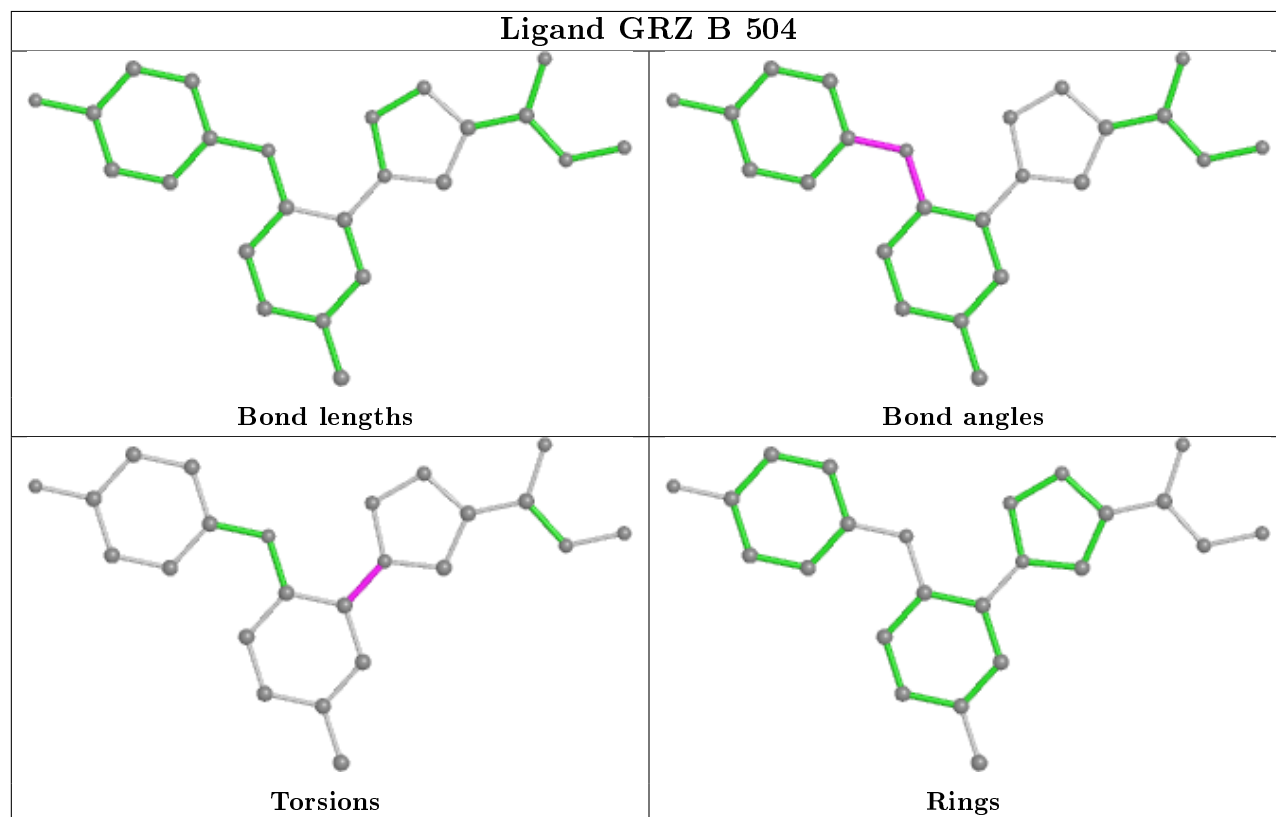
There are no ring outliers.

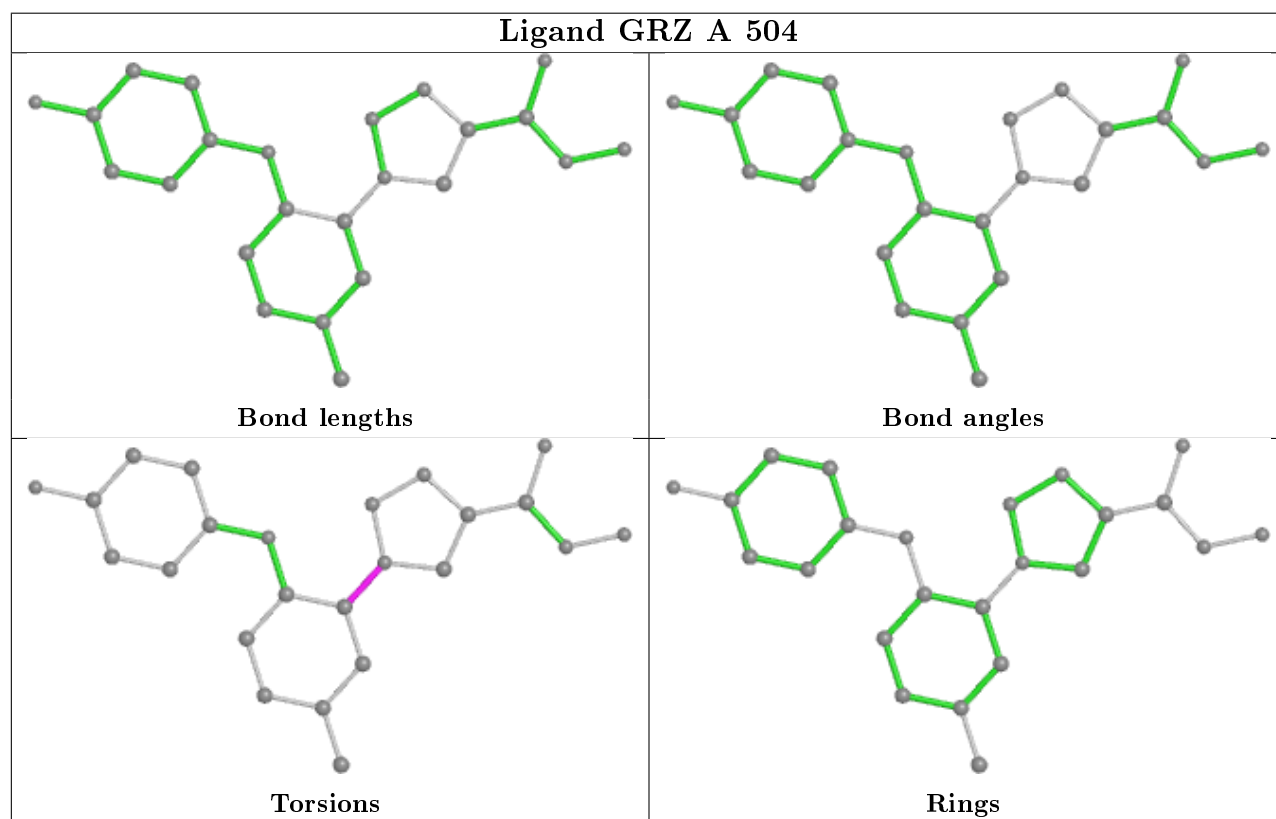
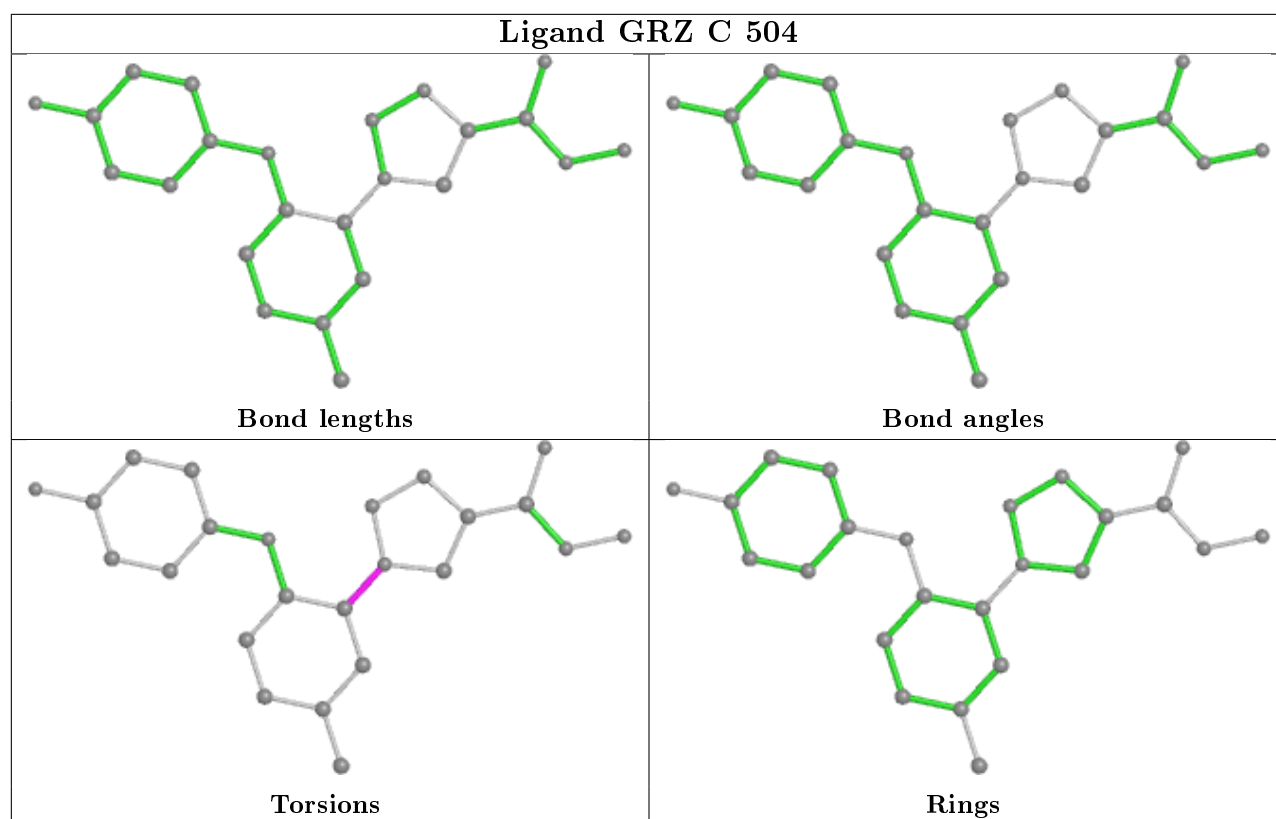
12 monomers are involved in 18 short contacts:

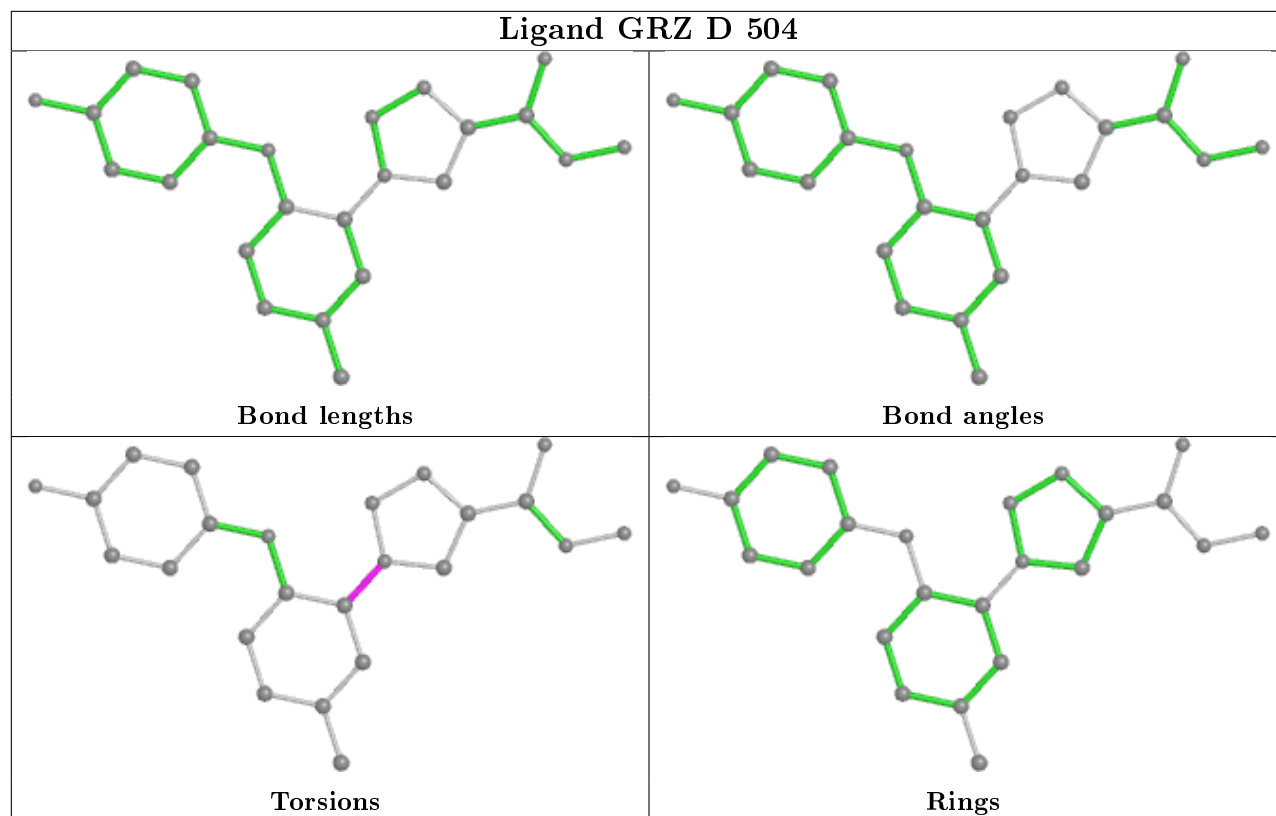
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	506	DMF	2	0
4	B	504	GRZ	1	0
5	D	506	DMF	1	0
5	C	507	DMF	2	0
4	A	504	GRZ	1	0
5	A	505	DMF	1	0
5	B	505	DMF	2	0
5	C	508	DMF	3	0
5	D	505	DMF	1	0
4	D	504	GRZ	2	0
5	A	506	DMF	1	0
5	C	509	DMF	1	0

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 [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	401/447 (89%)	-0.03	17 (4%) 36 35	22, 32, 67, 97	0
1	B	417/447 (93%)	-0.21	11 (2%) 56 56	20, 28, 54, 110	0
1	C	413/447 (92%)	-0.24	8 (1%) 66 69	21, 28, 52, 103	0
1	D	402/447 (89%)	-0.04	23 (5%) 23 23	22, 30, 67, 100	0
All	All	1633/1788 (91%)	-0.13	59 (3%) 42 43	20, 30, 59, 110	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	TYR	10.5
1	A	428	TYR	10.0
1	A	432	TYR	8.8
1	D	230	LEU	8.4
1	A	425	ILE	7.8
1	A	426	TYR	7.5
1	D	426	TYR	7.4
1	C	83	GLU	7.2
1	D	425	ILE	6.7
1	D	428	TYR	6.5
1	A	434	LEU	6.2
1	D	434	LEU	5.8
1	A	435	TYR	5.6
1	A	392	PHE	5.5
1	D	429	ASP	5.0
1	D	392	PHE	4.9
1	B	225	VAL	4.7
1	D	435	TYR	4.7
1	B	81	GLU	4.6
1	D	433	GLN	4.3
1	C	230	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	303	ASN	3.8
1	B	230	LEU	3.7
1	A	232	ILE	3.4
1	D	314	CYS	3.4
1	A	7[A]	TYR	3.3
1	B	425	ILE	3.3
1	A	429	ASP	3.2
1	B	82	LYS	3.1
1	A	431	VAL	3.0
1	B	231	PRO	2.9
1	D	7[A]	TYR	2.9
1	A	402	ASP	2.8
1	D	383	PRO	2.7
1	B	83	GLU	2.7
1	A	409	ARG	2.7
1	B	400	THR	2.7
1	D	313	GLU	2.7
1	D	81	GLU	2.6
1	D	302	PRO	2.6
1	B	401	LEU	2.6
1	D	231	PRO	2.6
1	C	437	LEU	2.5
1	D	177	GLN	2.4
1	D	315	SER	2.4
1	A	229	LYS	2.3
1	B	168	THR	2.3
1	C	315	SER	2.3
1	A	433	GLN	2.3
1	D	151[A]	PHE	2.3
1	C	425	ILE	2.2
1	C	231	PRO	2.2
1	C	446	ARG	2.2
1	D	382	GLY	2.2
1	B	7[A]	TYR	2.2
1	D	316	LEU	2.2
1	C	177	GLN	2.1
1	A	404	ILE	2.1
1	A	151[A]	PHE	2.1

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.

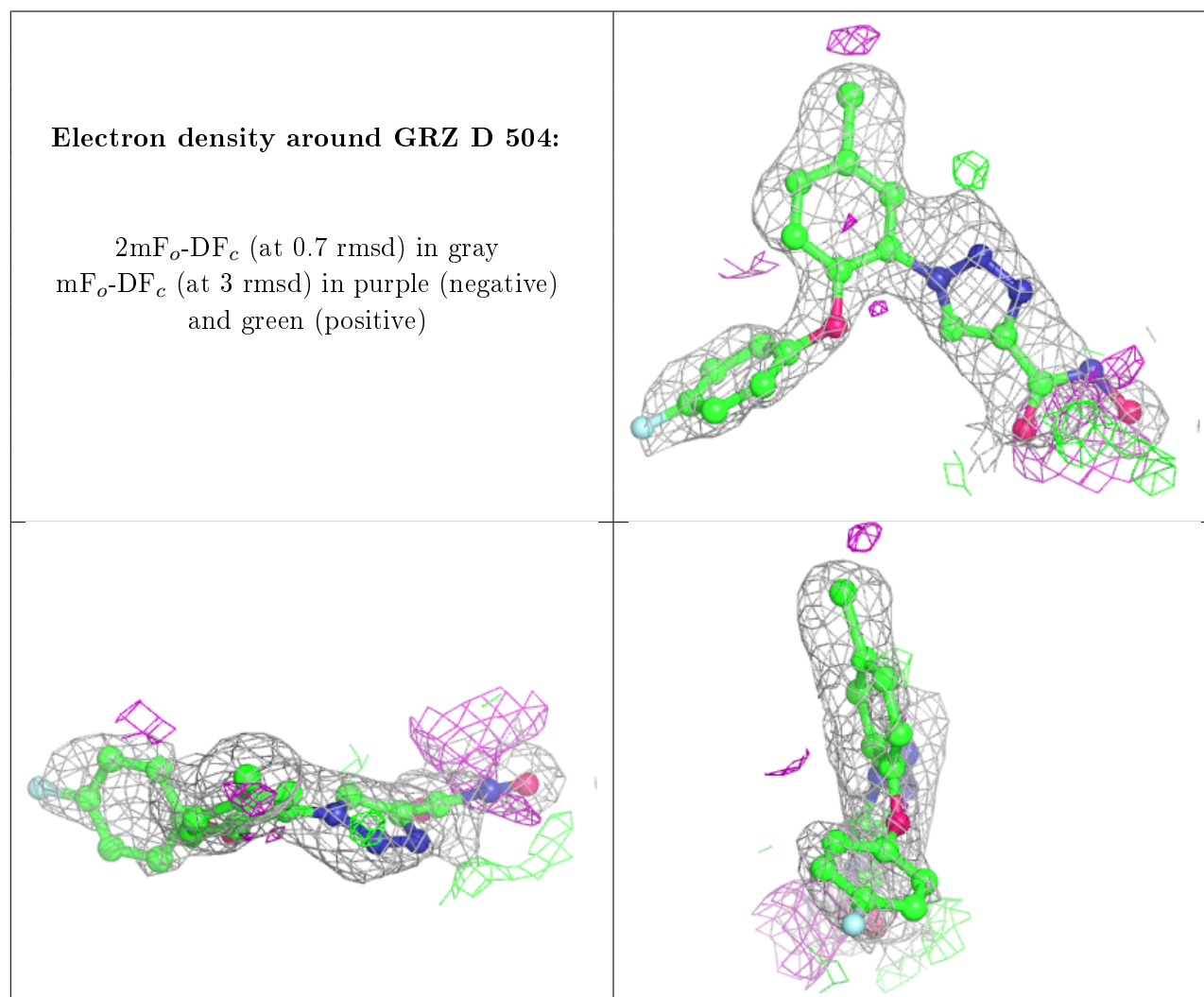
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMF	D	509	5/5	0.72	0.17	60,63,65,69	0
5	DMF	B	510	5/5	0.75	0.26	59,66,69,71	0
6	GOL	A	510	6/6	0.76	0.13	49,52,53,56	0
4	GRZ	D	504	24/24	0.76	0.24	53,69,74,77	0
5	DMF	C	509	5/5	0.76	0.25	52,60,62,63	0
6	GOL	C	510	6/6	0.80	0.14	33,39,43,44	0
5	DMF	C	508	5/5	0.80	0.13	39,44,51,53	0
5	DMF	A	509	5/5	0.80	0.17	61,67,70,71	0
4	GRZ	A	504	24/24	0.81	0.21	43,58,64,68	0
4	GRZ	B	504	24/24	0.82	0.25	31,54,62,64	0
5	DMF	A	505	5/5	0.82	0.17	41,54,60,60	0
5	DMF	D	508	5/5	0.84	0.12	61,62,64,64	0
5	DMF	A	507	5/5	0.86	0.13	40,46,53,54	0
4	GRZ	C	504	24/24	0.86	0.24	33,52,57,59	0
6	GOL	A	511	6/6	0.87	0.10	34,38,40,41	0
5	DMF	C	507	5/5	0.89	0.13	56,59,63,66	0
5	DMF	D	507	5/5	0.89	0.11	54,57,64,64	0
5	DMF	B	508	5/5	0.89	0.13	61,61,66,66	0
6	GOL	B	511	6/6	0.90	0.13	30,40,43,47	0
6	GOL	D	510	6/6	0.90	0.08	31,36,36,36	0
5	DMF	D	506	5/5	0.91	0.15	65,69,73,76	0
5	DMF	D	505	5/5	0.91	0.18	53,61,63,67	0
5	DMF	A	506	5/5	0.92	0.19	61,65,70,72	0
5	DMF	B	509	5/5	0.92	0.12	48,48,51,53	0
5	DMF	B	506	5/5	0.93	0.09	57,61,67,69	0
5	DMF	C	505	5/5	0.93	0.12	40,41,48,52	0
5	DMF	A	508	5/5	0.93	0.09	57,61,63,65	0
5	DMF	B	507	5/5	0.94	0.09	42,43,46,49	0
5	DMF	C	506	5/5	0.95	0.11	52,53,56,57	0
5	DMF	B	505	5/5	0.96	0.09	49,49,53,53	0
2	ZN	A	501	1/1	0.99	0.17	49,49,49,49	0
3	K	D	503	1/1	0.99	0.06	27,27,27,27	0

Continued on next page...

Continued from previous page...

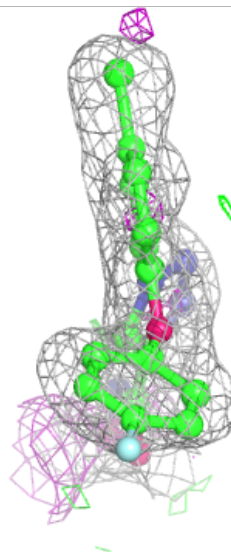
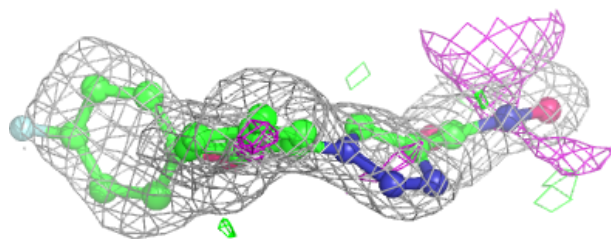
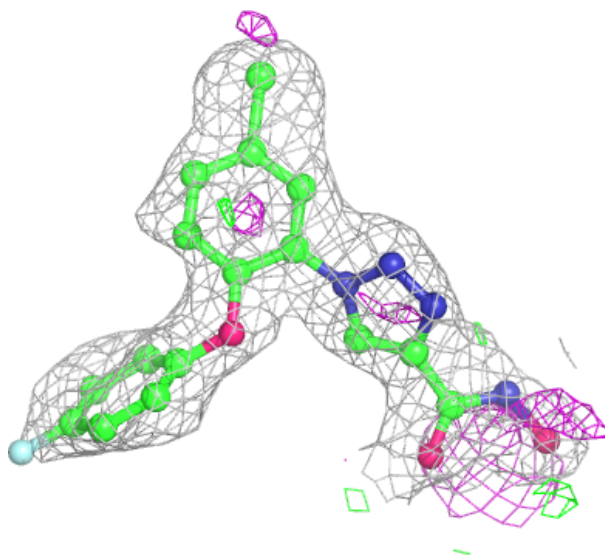
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	A	502	1/1	1.00	0.09	23,23,23,23	0
3	K	B	503	1/1	1.00	0.07	27,27,27,27	0
3	K	B	502	1/1	1.00	0.11	22,22,22,22	0
3	K	A	503	1/1	1.00	0.09	27,27,27,27	0
2	ZN	D	501	1/1	1.00	0.14	47,47,47,47	0
3	K	D	502	1/1	1.00	0.10	23,23,23,23	0
2	ZN	B	501	1/1	1.00	0.17	43,43,43,43	0
3	K	C	503	1/1	1.00	0.08	27,27,27,27	0
3	K	C	502	1/1	1.00	0.11	22,22,22,22	0
2	ZN	C	501	1/1	1.00	0.18	44,44,44,44	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.



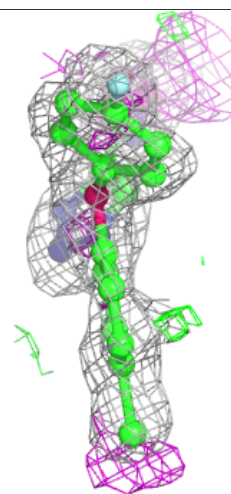
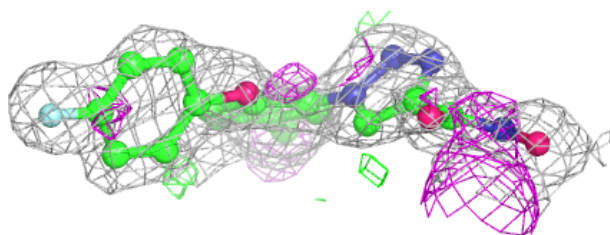
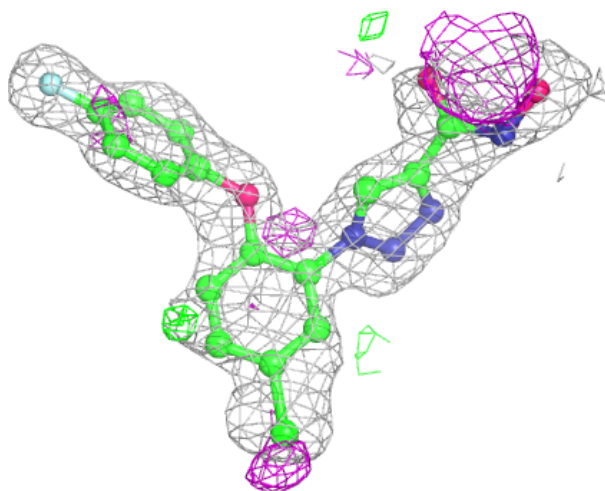
Electron density around GRZ A 504:

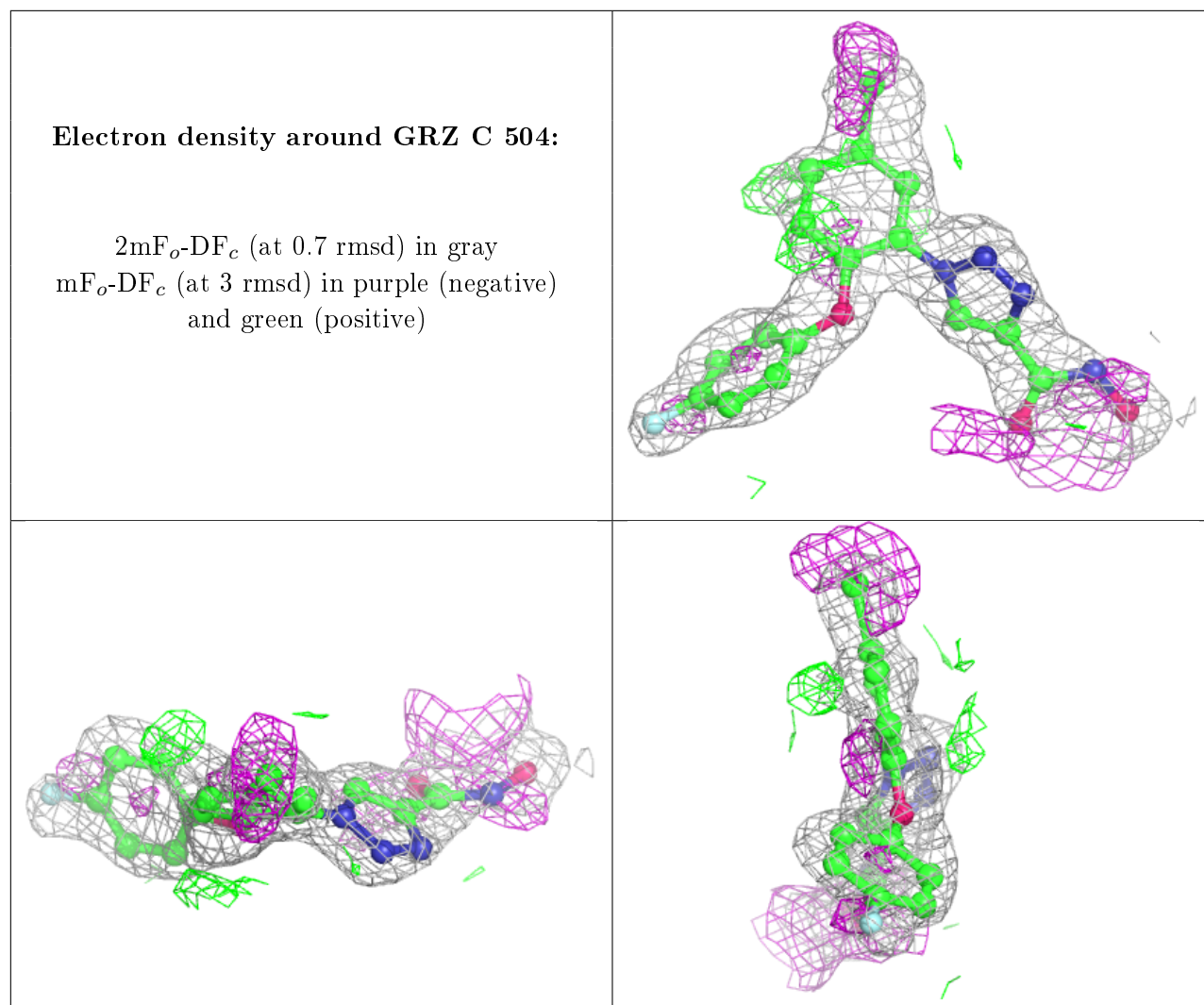
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GRZ B 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 ⓘ

There are no such residues in this entry.