



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2021 – 03:15 pm BST

PDB ID : 7AB9  
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-656  
Authors : Singh, A.K.; Blaazer, A.R.; Zara, L.; de Esch, I.J.P.; Leurs, R.; Brown, D.G.  
Deposited on : 2020-09-07  
Resolution : 2.19 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

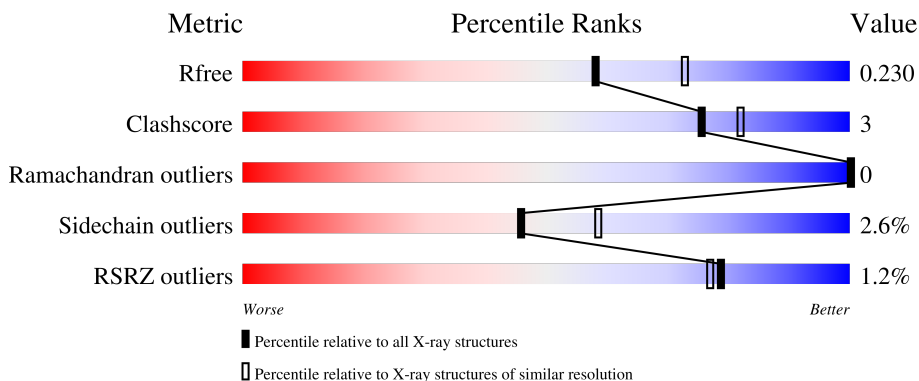
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	364	 2% 83% 7% • 9%
1	B	364	 % 81% 8% 11%
1	C	364	 % 81% 7% • 11%
1	D	364	 % 82% 7% 11%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11323 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
			Total	C	N	O	S			
1	A	330	2669	1690	455	510	14	0	0	0
1	B	324	2622	1659	448	501	14	0	0	0
1	C	324	2622	1659	448	501	14	0	0	0
1	D	324	2622	1659	448	501	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	HIS	-	expression tag	UNP Q08499
A	78	MET	-	expression tag	UNP Q08499
B	75	GLY	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	HIS	-	expression tag	UNP Q08499
B	78	MET	-	expression tag	UNP Q08499
C	75	GLY	-	expression tag	UNP Q08499
C	76	SER	-	expression tag	UNP Q08499
C	77	HIS	-	expression tag	UNP Q08499
C	78	MET	-	expression tag	UNP Q08499
D	75	GLY	-	expression tag	UNP Q08499
D	76	SER	-	expression tag	UNP Q08499
D	77	HIS	-	expression tag	UNP Q08499
D	78	MET	-	expression tag	UNP Q08499

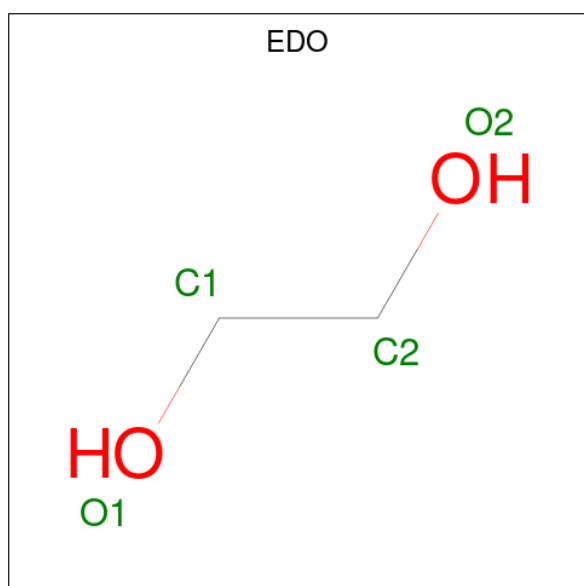
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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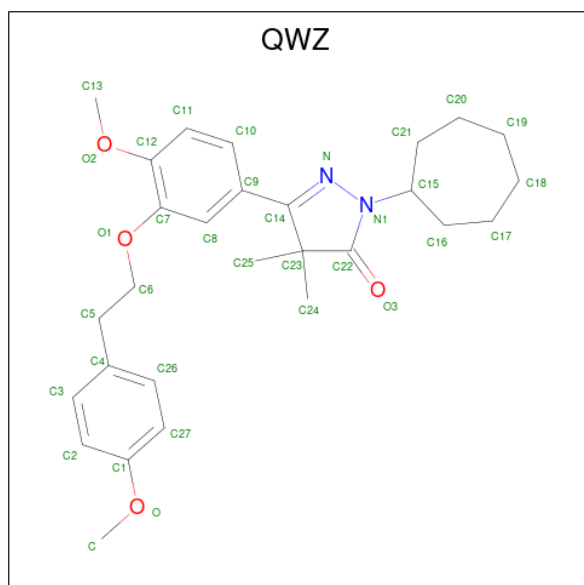
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0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

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

- Molecule 5 is 1-cycloheptyl-3-{4-methoxy-3-[2-(4-methoxyphenyl)ethoxy]phenyl}-4,4-dimethyl-4,5-dihydro-1H-pyrazol-5-one (three-letter code: QWZ) (formula: C<sub>28</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



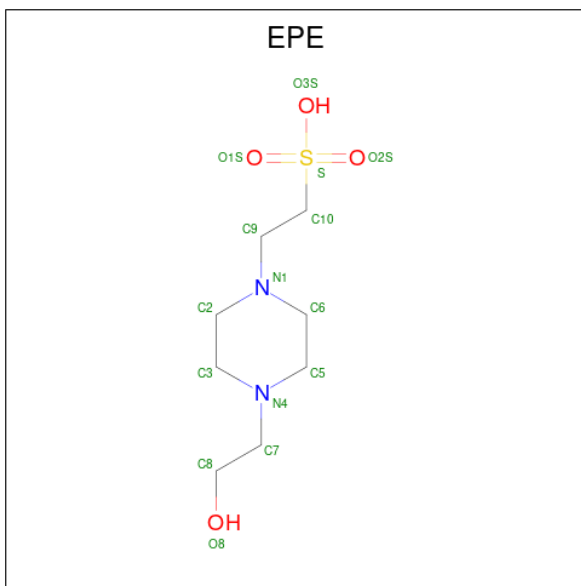
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			34	28	2	4		
5	B	1	Total	C	N	O	0	0
			34	28	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			34	28	2	4		
5	D	1	Total	C	N	O	0	0
			34	28	2	4		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

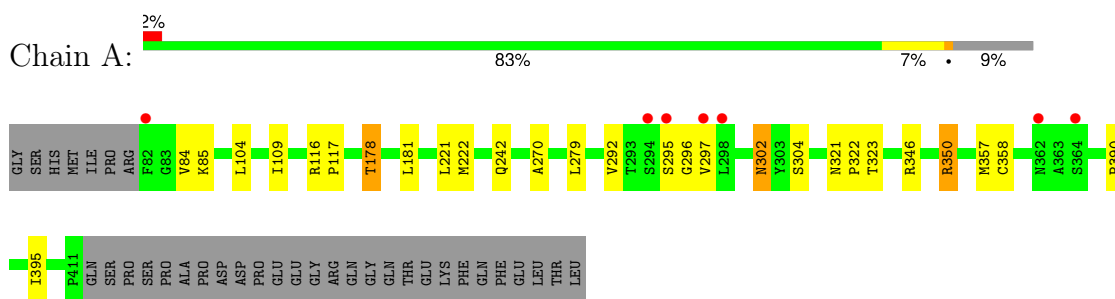
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	135	Total	O	0	0
			135	135		
7	B	113	Total	O	0	0
			113	113		
7	C	92	Total	O	0	0
			92	92		
7	D	150	Total	O	0	0
			150	150		

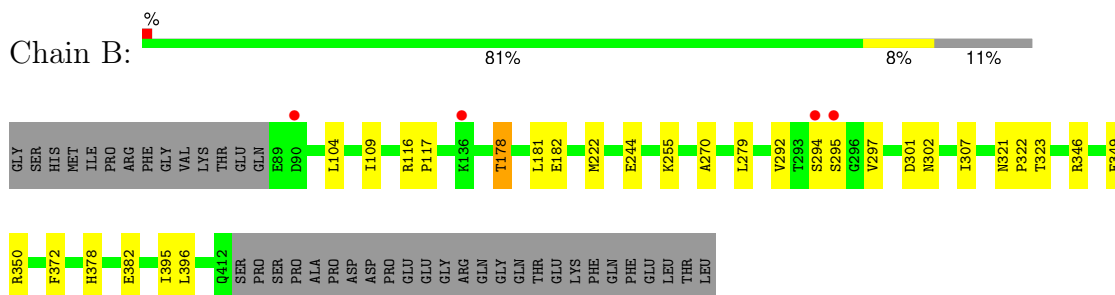
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

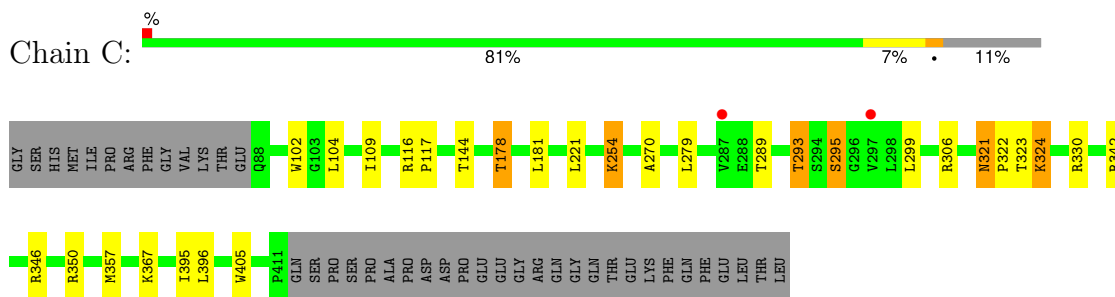
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



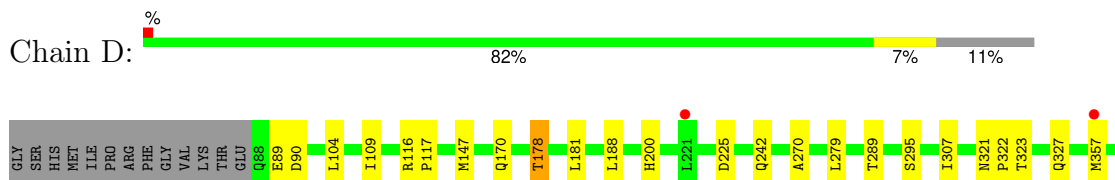
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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



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





K367	GLN
I395	SER
P411	PRO
	SER
	PRO
	ALA
	PRO
	ASP
	ASP
	PRO
	GLU
	GLU
	GLY
	ARG
	GLN
	GLY
	GLN
	THR
	GLU
	LYS
	PHE
	GLN
	PHE
	GLU
	LEU
	THR
	LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.17Å 111.80Å 160.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.69 – 2.19 91.69 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (91.69-2.19) 100.0 (91.69-2.19)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.185 , 0.223 0.192 , 0.230	Depositor DCC
$R_{free}$ test set	4722 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	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	0.96	EDS
Total number of atoms	11323	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: ZN, EPE, MG, QWZ, EDO

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	0.68	0/2724	0.74	0/3700
1	B	0.68	0/2676	0.76	1/3636 (0.0%)
1	C	0.72	2/2676 (0.1%)	0.75	0/3636
1	D	0.68	0/2676	0.73	0/3636
All	All	0.69	2/10752 (0.0%)	0.75	1/14608 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	321	ASN	C-N	8.35	1.50	1.34
1	C	324	LYS	C-N	8.18	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ASP	CB-CA-C	-5.56	99.28	110.40

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	2669	0	2625	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2622	0	2578	19	0
1	C	2622	0	2578	22	0
1	D	2622	0	2578	13	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
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	40	0	60	1	0
4	B	20	0	30	2	0
4	C	20	0	30	0	0
4	D	44	0	66	1	0
5	A	34	0	0	2	0
5	B	34	0	0	1	0
5	C	34	0	0	2	0
5	D	34	0	0	1	0
6	C	15	0	18	0	0
6	D	15	0	17	0	0
7	A	135	0	0	0	0
7	B	113	0	0	1	0
7	C	92	0	0	1	0
7	D	150	0	0	0	0
All	All	11323	0	10580	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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:222:MET:HE1	1:B:222:MET:SD	2.13	0.89
1:A:222:MET:CE	1:B:222:MET:SD	2.64	0.86
1:A:302:ASN:ND2	1:A:302:ASN:H	1.86	0.73
1:C:321:ASN:HB2	7:C:665:HOH:O	1.90	0.71
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.72	0.71
5:A:512:QWZ:C8	5:A:512:QWZ:C5	2.78	0.62
1:A:302:ASN:H	1:A:302:ASN:HD22	1.47	0.61
1:C:321:ASN:CB	1:C:322:PRO:HD3	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ARG:NH1	1:C:306:ARG:HG2	2.19	0.57
1:C:306:ARG:HG2	1:C:306:ARG:HH11	1.69	0.55
1:D:188:LEU:HD23	4:D:511:EDO:H11	1.88	0.55
1:B:292:VAL:HG22	4:B:506:EDO:H22	1.88	0.54
1:C:293:THR:HG23	1:C:295:SER:H	1.73	0.54
1:B:244:GLU:OE1	1:C:254:LYS:HE3	2.10	0.52
1:B:302:ASN:ND2	1:B:302:ASN:H	2.07	0.52
1:C:178:THR:HG22	1:C:181:LEU:HD12	1.91	0.51
1:A:323:THR:HB	1:A:395:ILE:HG23	1.93	0.51
1:C:289:THR:O	1:C:289:THR:HG22	2.11	0.50
1:D:357:MET:SD	5:D:515:QWZ:C26	2.99	0.50
1:A:178:THR:HG22	1:A:181:LEU:HD12	1.93	0.50
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.47	0.50
1:C:346:ARG:O	1:C:350:ARG:HD2	2.11	0.50
1:A:292:VAL:CG1	1:A:296:GLY:HA2	2.43	0.49
1:B:178:THR:HG22	1:B:181:LEU:HD12	1.94	0.49
1:B:323:THR:HB	1:B:395:ILE:HG23	1.93	0.49
1:D:323:THR:HB	1:D:395:ILE:HG23	1.93	0.49
1:D:289:THR:O	1:D:289:THR:HG22	2.13	0.49
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.31	0.49
1:B:349:GLU:HG3	1:D:147:MET:SD	2.52	0.49
1:D:178:THR:HG22	1:D:181:LEU:HD12	1.94	0.48
1:B:104:LEU:HD11	1:B:109:ILE:HD11	1.96	0.47
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.97	0.47
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.97	0.46
1:C:323:THR:HB	1:C:395:ILE:HG23	1.95	0.46
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.96	0.46
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.98	0.46
1:C:102:TRP:CE2	1:C:324:LYS:HE2	2.51	0.46
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.97	0.46
1:C:116:ARG:N	1:C:117:PRO:CD	2.80	0.45
1:D:116:ARG:N	1:D:117:PRO:CD	2.80	0.45
1:B:346:ARG:O	1:B:350:ARG:HD2	2.17	0.45
1:A:116:ARG:N	1:A:117:PRO:CD	2.80	0.45
1:A:357:MET:SD	5:A:512:QWZ:C3	3.05	0.45
1:A:302:ASN:ND2	1:A:302:ASN:N	2.60	0.45
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.98	0.45
1:A:350:ARG:HG2	1:C:144:THR:HG23	1.99	0.45
1:A:358:CYS:SG	4:A:503:EDO:H12	2.57	0.44
1:B:116:ARG:N	1:B:117:PRO:CD	2.81	0.44
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ARG:HH11	1:C:306:ARG:CG	2.31	0.44
1:B:182:GLU:O	1:B:297:VAL:HG11	2.18	0.43
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.99	0.43
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.01	0.43
1:A:270:ALA:HB1	1:A:279:LEU:HD11	2.01	0.43
1:C:321:ASN:HD22	1:C:321:ASN:HA	1.60	0.42
1:B:378:HIS:ND1	7:B:601:HOH:O	2.36	0.42
1:A:346:ARG:O	1:A:350:ARG:HD3	2.20	0.41
1:B:292:VAL:HG22	4:B:506:EDO:C2	2.51	0.41
1:B:307:ILE:HD12	1:B:307:ILE:HA	1.94	0.41
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.03	0.41
1:B:372:PHE:HB2	5:B:508:QWZ:C4	2.51	0.41
1:B:396:LEU:HD12	1:B:396:LEU:HA	1.96	0.40
1:C:357:MET:SD	5:C:509:QWZ:C3	3.09	0.40
1:D:307:ILE:HD12	1:D:307:ILE:HA	1.94	0.40
1:C:396:LEU:HD12	1:C:396:LEU:HA	1.97	0.40
1:C:357:MET:SD	5:C:509:QWZ:C4	3.10	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	328/364 (90%)	322 (98%)	6 (2%)	0	100	100
1	B	322/364 (88%)	315 (98%)	7 (2%)	0	100	100
1	C	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
1	D	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
All	All	1294/1456 (89%)	1269 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/331 (91%)	291 (97%)	10 (3%)	38	49
1	B	296/331 (89%)	291 (98%)	5 (2%)	60	74
1	C	296/331 (89%)	288 (97%)	8 (3%)	44	57
1	D	296/331 (89%)	288 (97%)	8 (3%)	44	57
All	All	1189/1324 (90%)	1158 (97%)	31 (3%)	46	58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	85	LYS
1	A	178	THR
1	A	221	LEU
1	A	295	SER
1	A	297	VAL
1	A	302	ASN
1	A	304	SER
1	A	350	ARG
1	A	390	PRO
1	B	178	THR
1	B	255	LYS
1	B	294	SER
1	B	295	SER
1	B	382	GLU
1	C	178	THR
1	C	221	LEU
1	C	254	LYS
1	C	293	THR
1	C	295	SER
1	C	299	LEU
1	C	342	ARG
1	C	367	LYS
1	D	89	GLU

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Mol	Chain	Res	Type
1	D	90	ASP
1	D	178	THR
1	D	200	HIS
1	D	225	ASP
1	D	295	SER
1	D	327	GLN
1	D	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	B	302	ASN
1	C	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 8 are monoatomic - leaving 37 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	EDO	B	504	-	3,3,3	0.08	0	2,2,2	0.18	0
4	EDO	D	509	-	3,3,3	0.13	0	2,2,2	0.14	0
4	EDO	C	503	-	3,3,3	0.22	0	2,2,2	0.22	0
4	EDO	D	505	-	3,3,3	0.17	0	2,2,2	0.05	0
4	EDO	D	507	-	3,3,3	0.10	0	2,2,2	0.06	0
4	EDO	D	506	-	3,3,3	0.14	0	2,2,2	0.15	0
5	QWZ	A	512	-	36,37,37	0.59	0	44,52,52	1.29	5 (11%)
4	EDO	D	503	-	3,3,3	0.29	0	2,2,2	0.38	0
4	EDO	D	510	-	3,3,3	0.39	0	2,2,2	0.40	0
4	EDO	A	510	-	3,3,3	0.25	0	2,2,2	0.40	0
4	EDO	A	509	-	3,3,3	0.15	0	2,2,2	0.05	0
4	EDO	B	507	-	3,3,3	0.37	0	2,2,2	0.86	0
4	EDO	A	505	-	3,3,3	0.26	0	2,2,2	0.39	0
5	QWZ	D	515	-	36,37,37	0.57	1 (2%)	44,52,52	1.29	4 (9%)
5	QWZ	C	509	-	36,37,37	0.50	0	44,52,52	0.99	1 (2%)
4	EDO	A	511	-	3,3,3	0.33	0	2,2,2	0.22	0
4	EDO	A	507	-	3,3,3	0.16	0	2,2,2	0.11	0
4	EDO	A	506	-	3,3,3	0.12	0	2,2,2	0.18	0
4	EDO	B	503	-	3,3,3	0.17	0	2,2,2	0.06	0
4	EDO	C	504	-	3,3,3	0.09	0	2,2,2	0.34	0
6	EPE	D	513	-	15,15,15	1.69	1 (6%)	18,20,20	1.99	7 (38%)
4	EDO	D	504	-	3,3,3	0.07	0	2,2,2	0.10	0
4	EDO	A	508	-	3,3,3	0.16	0	2,2,2	0.21	0
4	EDO	B	506	-	3,3,3	0.14	0	2,2,2	0.35	0
4	EDO	A	513	-	3,3,3	0.28	0	2,2,2	0.28	0
4	EDO	D	508	-	3,3,3	0.06	0	2,2,2	0.38	0
4	EDO	A	503	-	3,3,3	0.10	0	2,2,2	0.19	0
6	EPE	C	508	-	15,15,15	1.91	1 (6%)	18,20,20	1.26	3 (16%)
4	EDO	C	505	-	3,3,3	0.09	0	2,2,2	0.22	0
4	EDO	C	507	-	3,3,3	0.25	0	2,2,2	0.52	0
4	EDO	C	506	-	3,3,3	0.06	0	2,2,2	0.41	0
4	EDO	B	505	-	3,3,3	0.05	0	2,2,2	0.21	0
4	EDO	D	512	-	3,3,3	0.23	0	2,2,2	0.13	0
4	EDO	A	504	-	3,3,3	0.11	0	2,2,2	0.24	0
4	EDO	D	514	-	3,3,3	0.37	0	2,2,2	0.42	0
4	EDO	D	511	-	3,3,3	0.71	0	2,2,2	0.79	0
5	QWZ	B	508	-	36,37,37	0.58	1 (2%)	44,52,52	1.18	4 (9%)

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	EDO	B	504	-	-	1/1/1/1	-
4	EDO	D	509	-	-	1/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	D	505	-	-	1/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	D	506	-	-	1/1/1/1	-
5	QWZ	A	512	-	-	6/16/47/47	0/4/4/4
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
5	QWZ	D	515	-	-	3/16/47/47	0/4/4/4
5	QWZ	C	509	-	-	3/16/47/47	0/4/4/4
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
6	EPE	D	513	-	-	4/9/19/19	0/1/1/1
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
6	EPE	C	508	-	-	1/9/19/19	0/1/1/1
4	EDO	C	505	-	-	0/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	D	512	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	D	514	-	-	0/1/1/1	-
4	EDO	D	511	-	-	1/1/1/1	-
5	QWZ	B	508	-	-	5/16/47/47	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	508	EPE	C10-S	-6.94	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	513	EPE	C10-S	-5.81	1.69	1.77
5	B	508	QWZ	C15-N1	2.25	1.50	1.47
5	D	515	QWZ	C15-N1	2.14	1.50	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	512	QWZ	C6-C5-C4	4.94	124.86	113.00
5	D	515	QWZ	C6-C5-C4	4.66	124.19	113.00
6	D	513	EPE	O1S-S-C10	4.34	112.14	106.92
6	C	508	EPE	O3S-S-C10	3.88	112.04	105.77
5	B	508	QWZ	C6-C5-C4	3.78	122.09	113.00
5	D	515	QWZ	C15-N1-C22	-3.50	124.89	131.38
6	D	513	EPE	C3-C2-N1	3.45	117.71	110.64
5	B	508	QWZ	O1-C7-C12	3.24	122.41	115.73
5	D	515	QWZ	C6-O1-C7	3.01	125.06	117.69
6	D	513	EPE	O3S-S-C10	2.98	110.58	105.77
5	C	509	QWZ	O1-C7-C12	2.80	121.52	115.73
5	A	512	QWZ	C6-O1-C7	2.75	124.41	117.69
6	D	513	EPE	C2-C3-N4	2.68	116.15	110.64
5	A	512	QWZ	C15-N1-C22	-2.55	126.65	131.38
6	D	513	EPE	C6-N1-C2	2.38	114.18	108.83
6	D	513	EPE	C5-N4-C3	2.37	114.17	108.83
5	B	508	QWZ	C9-C14-N	-2.33	116.18	119.65
5	B	508	QWZ	C10-C9-C14	2.15	124.64	120.66
6	D	513	EPE	C5-C6-N1	-2.13	106.27	110.64
5	D	515	QWZ	O1-C6-C5	2.11	115.22	109.37
5	A	512	QWZ	O1-C7-C12	2.09	120.05	115.73
6	C	508	EPE	O3S-S-O2S	-2.06	106.23	111.27
5	A	512	QWZ	C9-C8-C7	2.05	122.34	119.61
6	C	508	EPE	O1S-S-C10	2.02	109.34	106.92

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	512	QWZ	C4-C5-C6-O1
5	B	508	QWZ	C4-C5-C6-O1
5	A	512	QWZ	C5-C6-O1-C7
4	B	507	EDO	O1-C1-C2-O2
6	C	508	EPE	N4-C7-C8-O8
6	D	513	EPE	C9-C10-S-O3S

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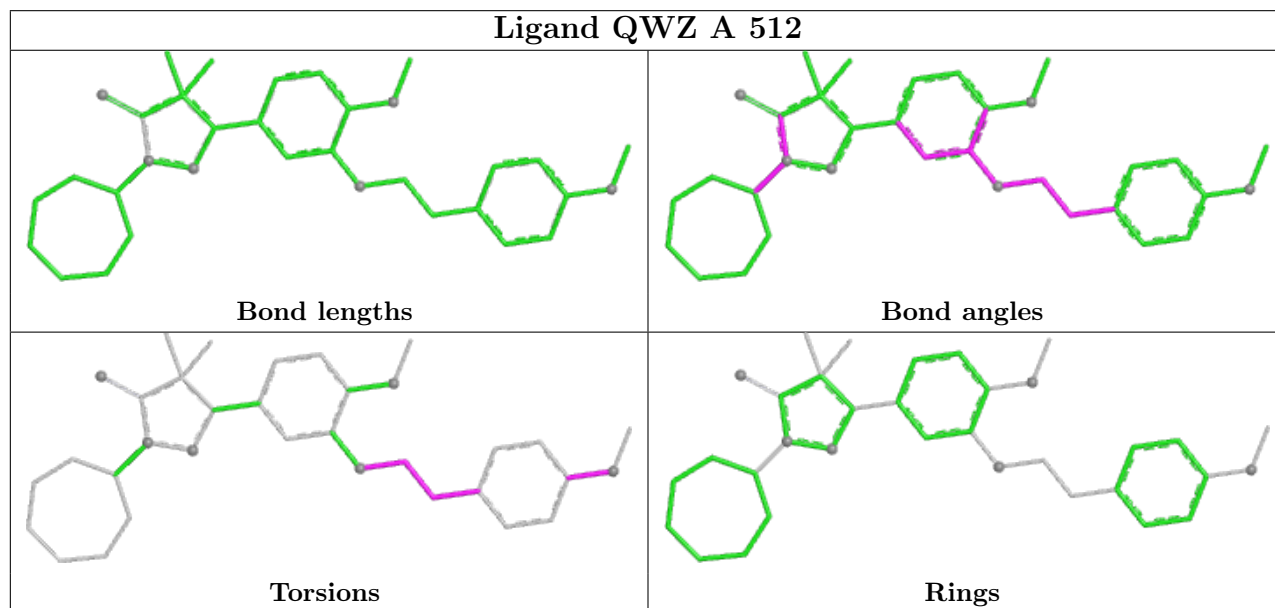
Mol	Chain	Res	Type	Atoms
5	A	512	QWZ	C2-C1-O-C
5	A	512	QWZ	C27-C1-O-C
4	A	508	EDO	O1-C1-C2-O2
4	A	510	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
4	D	511	EDO	O1-C1-C2-O2
4	D	509	EDO	O1-C1-C2-O2
6	D	513	EPE	S-C10-C9-N1
5	D	515	QWZ	C12-C7-O1-C6
5	C	509	QWZ	C12-C7-O1-C6
5	B	508	QWZ	C3-C4-C5-C6
5	A	512	QWZ	C3-C4-C5-C6
5	D	515	QWZ	C5-C6-O1-C7
4	A	506	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
4	D	512	EDO	O1-C1-C2-O2
6	D	513	EPE	C9-C10-S-O1S
6	D	513	EPE	C9-C10-S-O2S
5	D	515	QWZ	C8-C7-O1-C6
5	A	512	QWZ	C26-C4-C5-C6
5	B	508	QWZ	C26-C4-C5-C6
5	C	509	QWZ	C8-C7-O1-C6
4	A	509	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	D	505	EDO	O1-C1-C2-O2
4	D	506	EDO	O1-C1-C2-O2
5	C	509	QWZ	C5-C6-O1-C7
4	A	511	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
5	B	508	QWZ	C27-C1-O-C
4	A	503	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
5	B	508	QWZ	C2-C1-O-C

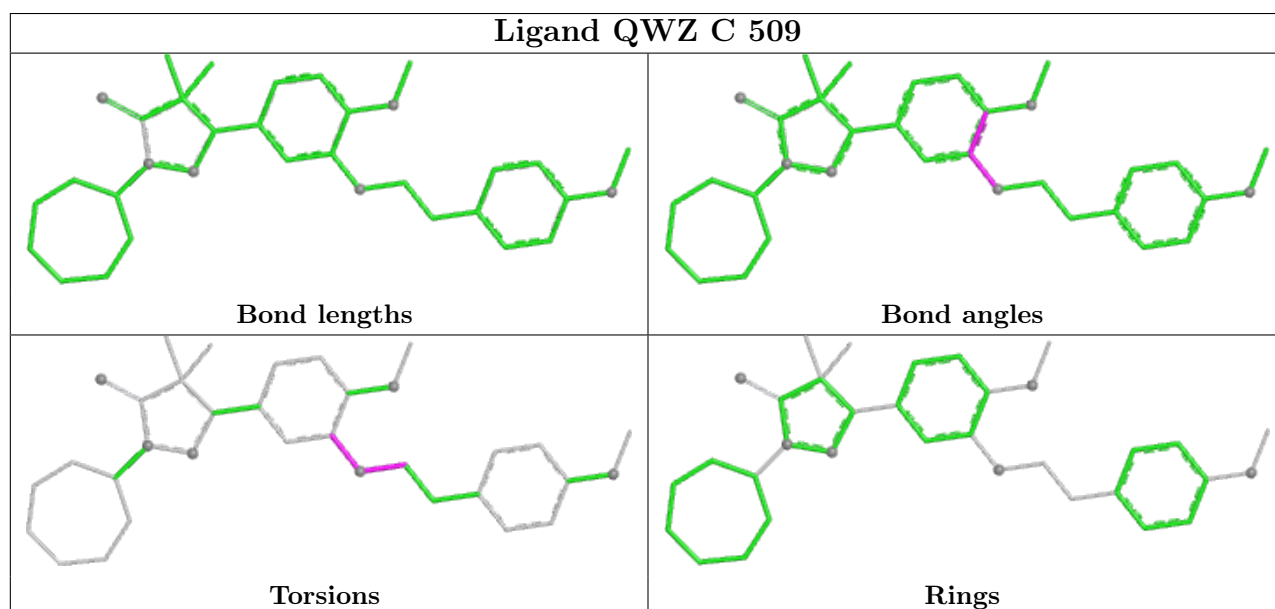
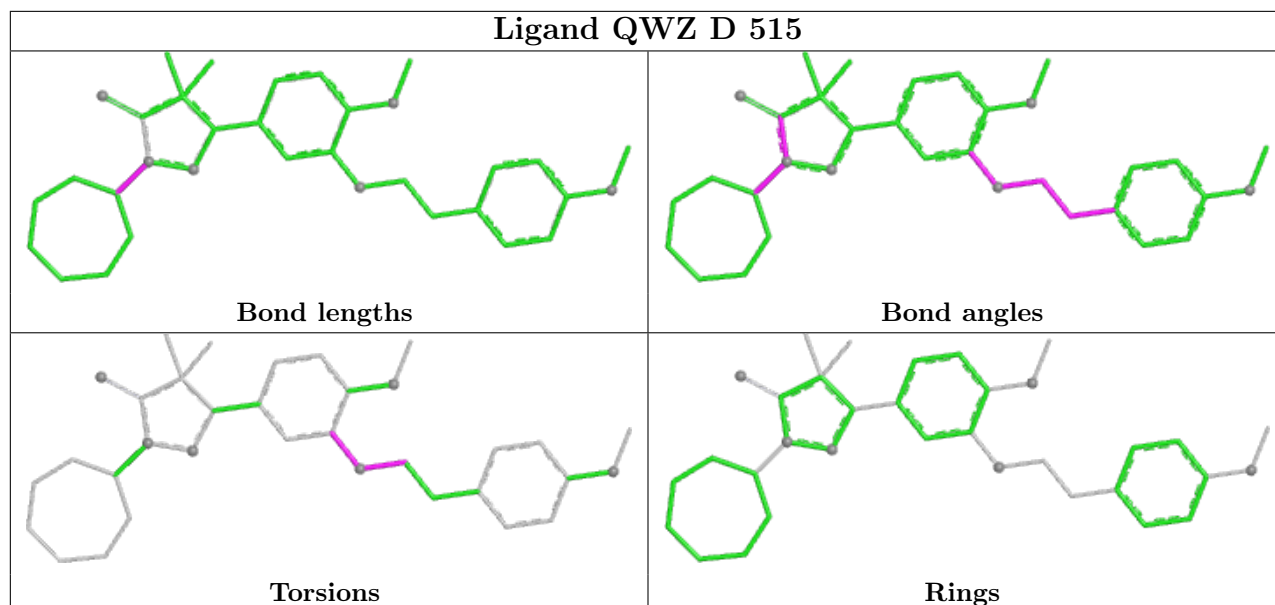
There are no ring outliers.

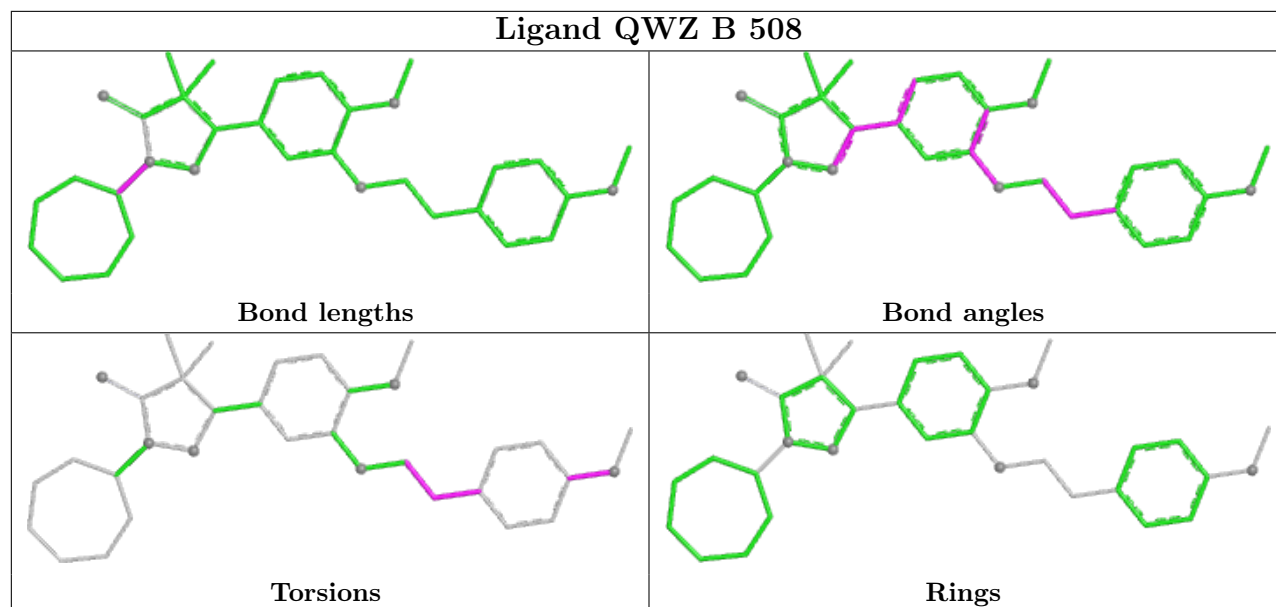
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	512	QWZ	2	0
5	D	515	QWZ	1	0
5	C	509	QWZ	2	0
4	B	506	EDO	2	0
4	A	503	EDO	1	0
4	D	511	EDO	1	0
5	B	508	QWZ	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	330/364 (90%)	0.10	7 (2%) 63 61	28, 45, 82, 119	0
1	B	324/364 (89%)	0.18	4 (1%) 79 77	30, 56, 85, 111	0
1	C	324/364 (89%)	0.09	2 (0%) 89 88	30, 53, 86, 123	0
1	D	324/364 (89%)	0.06	2 (0%) 89 88	27, 41, 76, 100	0
All	All	1302/1456 (89%)	0.11	15 (1%) 79 77	27, 49, 84, 123	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	SER	8.3
1	B	294	SER	3.7
1	A	362	ASN	3.5
1	B	295	SER	3.5
1	A	82	PHE	3.4
1	D	357	MET	3.2
1	C	297	VAL	2.6
1	C	287	VAL	2.5
1	B	90	ASP	2.4
1	D	221	LEU	2.3
1	A	298	LEU	2.3
1	A	364	SER	2.3
1	A	295	SER	2.1
1	B	136	LYS	2.1
1	A	297	VAL	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 monosaccharides 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.

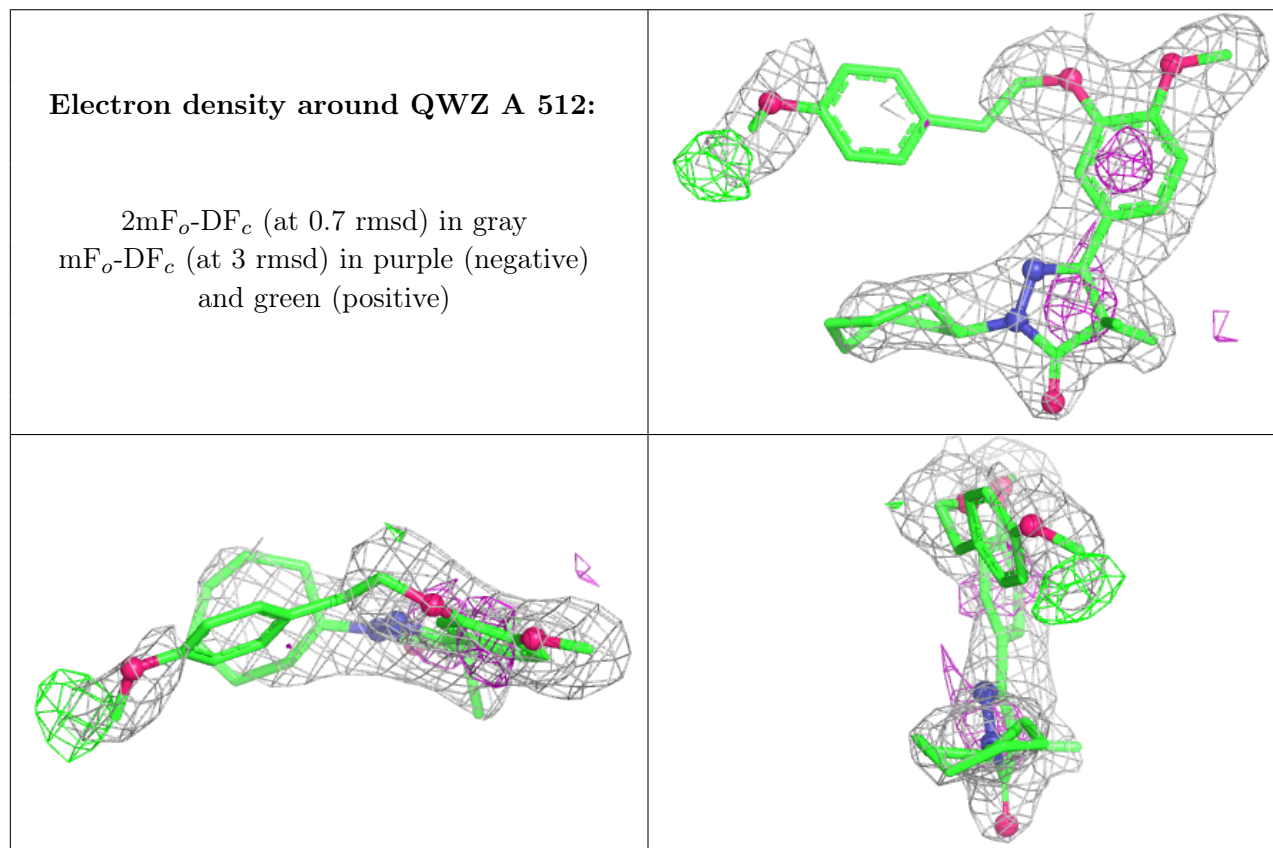
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	506	4/4	0.31	0.20	89,89,94,95	0
4	EDO	A	508	4/4	0.73	0.12	72,73,75,78	0
4	EDO	D	514	4/4	0.77	0.23	56,61,65,66	0
4	EDO	D	510	4/4	0.78	0.20	55,61,64,70	0
5	QWZ	A	512	34/34	0.79	0.35	52,69,137,147	0
4	EDO	B	504	4/4	0.80	0.22	74,78,85,91	0
4	EDO	D	512	4/4	0.80	0.35	69,71,81,83	0
4	EDO	D	509	4/4	0.81	0.21	81,81,82,85	0
4	EDO	A	509	4/4	0.81	0.24	68,80,86,86	0
4	EDO	B	507	4/4	0.81	0.42	55,60,64,68	0
4	EDO	D	504	4/4	0.81	0.14	78,79,79,81	0
4	EDO	D	505	4/4	0.81	0.28	57,61,62,77	0
4	EDO	D	511	4/4	0.83	0.14	46,59,64,67	0
4	EDO	C	504	4/4	0.84	0.15	69,69,71,73	0
5	QWZ	D	515	34/34	0.84	0.25	52,72,131,138	0
4	EDO	A	505	4/4	0.85	0.16	66,67,70,71	0
4	EDO	B	505	4/4	0.86	0.20	74,77,79,85	0
4	EDO	A	507	4/4	0.87	0.14	83,83,85,87	0
4	EDO	A	503	4/4	0.87	0.17	66,66,68,70	0
4	EDO	C	507	4/4	0.87	0.15	63,65,71,72	0
4	EDO	A	510	4/4	0.88	0.13	61,62,64,70	0
5	QWZ	B	508	34/34	0.88	0.20	53,60,115,123	0
4	EDO	C	506	4/4	0.88	0.15	69,69,73,74	0
5	QWZ	C	509	34/34	0.89	0.23	55,69,134,140	0
4	EDO	D	507	4/4	0.89	0.20	61,64,65,78	0
4	EDO	A	504	4/4	0.91	0.12	59,60,60,65	0
4	EDO	A	511	4/4	0.92	0.15	49,50,51,51	0
4	EDO	D	506	4/4	0.93	0.15	46,54,54,58	0
4	EDO	C	503	4/4	0.94	0.16	70,71,72,79	0
4	EDO	D	503	4/4	0.94	0.12	50,51,52,53	0
4	EDO	A	506	4/4	0.94	0.21	52,73,74,75	0
4	EDO	C	505	4/4	0.94	0.11	70,74,75,76	0

*Continued on next page...*

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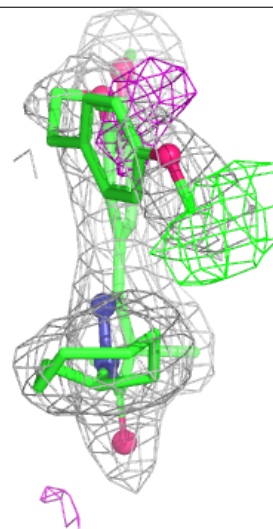
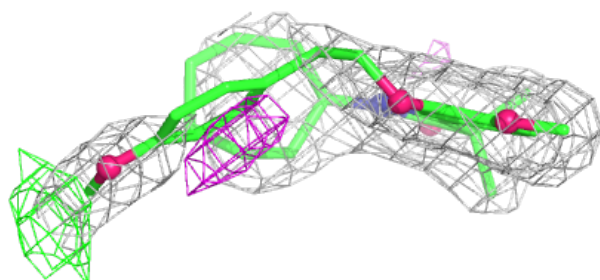
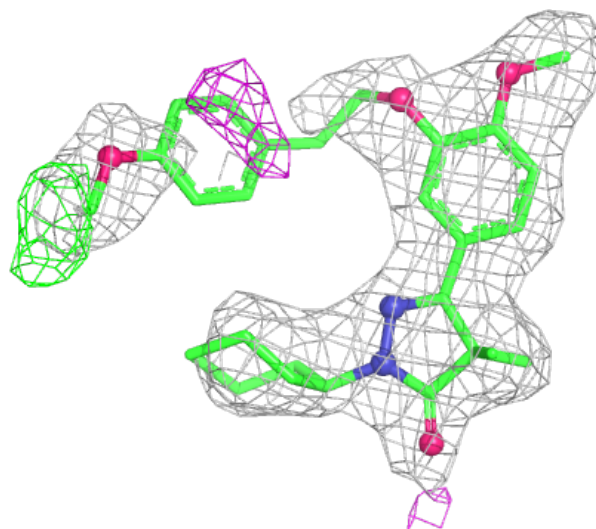
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	A	513	4/4	0.94	0.13	57,59,61,64	0
6	EPE	D	513	15/15	0.94	0.20	47,108,124,125	0
4	EDO	B	503	4/4	0.95	0.13	57,61,64,67	0
4	EDO	D	508	4/4	0.95	0.16	49,54,58,60	0
6	EPE	C	508	15/15	0.97	0.19	60,87,100,101	0
3	MG	D	502	1/1	0.98	0.12	26,26,26,26	0
3	MG	B	502	1/1	0.98	0.15	29,29,29,29	0
3	MG	C	502	1/1	0.99	0.10	27,27,27,27	0
3	MG	A	502	1/1	0.99	0.12	24,24,24,24	0
2	ZN	B	501	1/1	0.99	0.12	43,43,43,43	0
2	ZN	D	501	1/1	1.00	0.12	37,37,37,37	0
2	ZN	A	501	1/1	1.00	0.14	37,37,37,37	0
2	ZN	C	501	1/1	1.00	0.12	42,42,42,42	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.



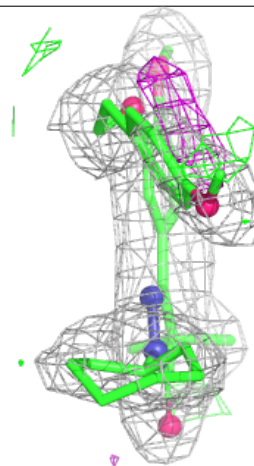
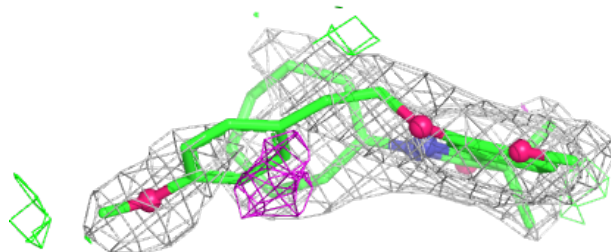
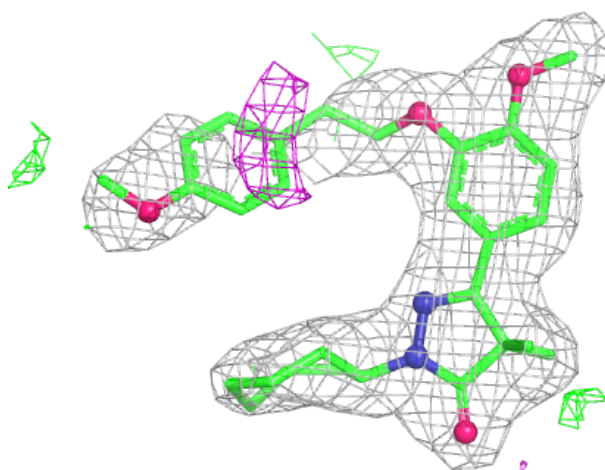
**Electron density around QWZ D 515:**

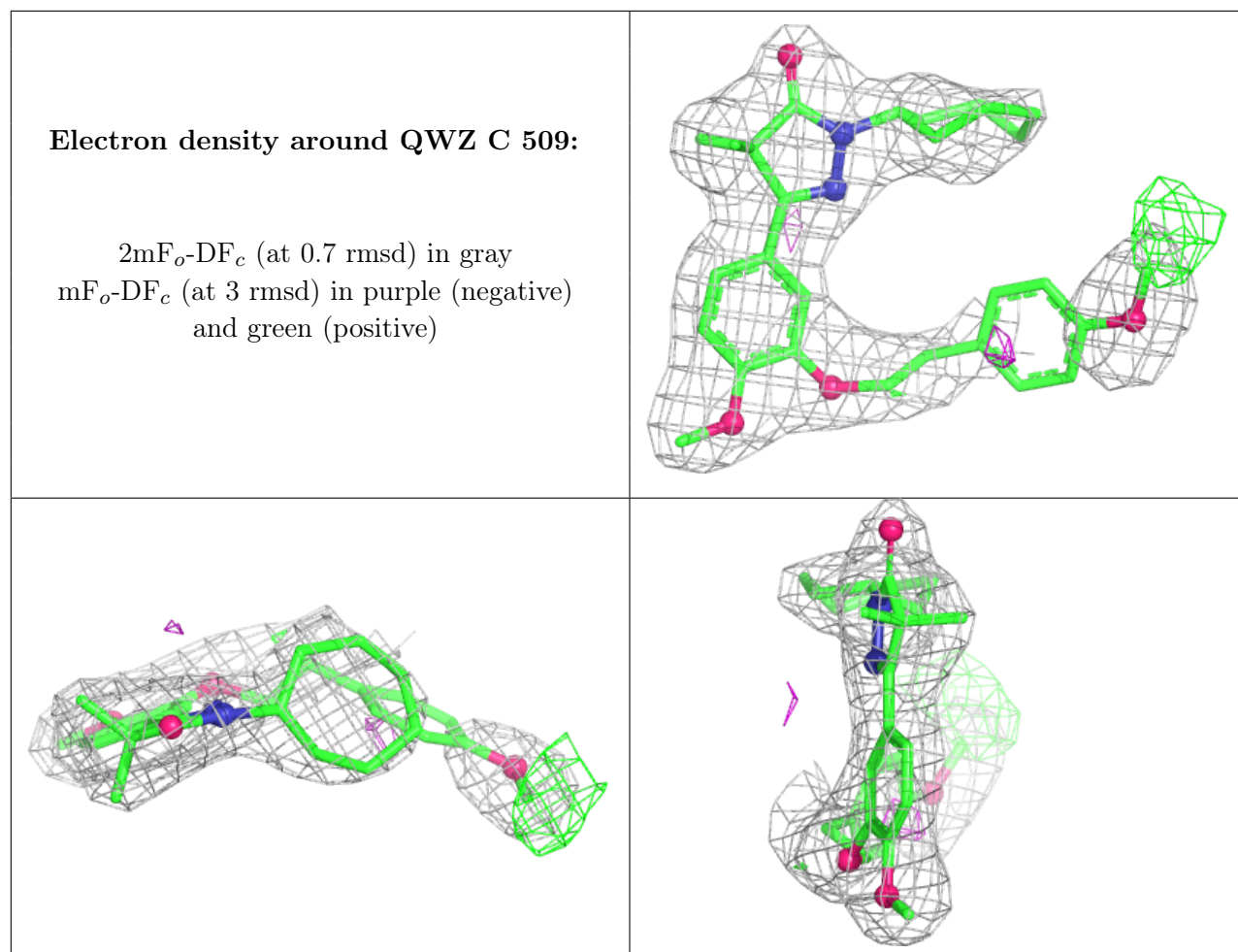
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around QWZ B 508:**

$2mF_o-DF_c$  (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.