



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:45 am BST

PDB ID : 5UZW
Title : PCY1 G696Insertion Variant in Complex with Follower Peptide and the Covalent Inhibitor ZPP
Authors : Chekan, J.R.; Nair, S.K.
Deposited on : 2017-02-27
Resolution : 2.82 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

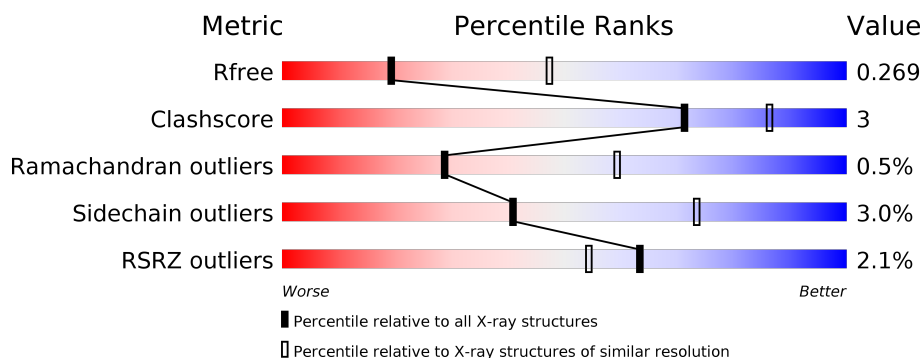
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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.




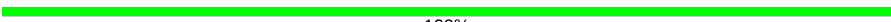
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	751	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	751	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	C	751	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	751	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
2	E	6	<div> <div>17%</div> <div> <div></div> <div>100%</div> </div> </div>
2	F	6	<div> <div></div> <div> <div></div> <div>100%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	6	 83%17%
2	H	6	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22661 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 Peptide cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	3	0
			5540	3542	938	1034	26			
1	B	701	Total	C	N	O	S	0	2	0
			5639	3602	957	1053	27			
1	C	697	Total	C	N	O	S	0	4	0
			5637	3604	959	1048	26			
1	D	685	Total	C	N	O	S	0	3	0
			5531	3534	946	1025	26			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP R4P353
A	-24	SER	-	expression tag	UNP R4P353
A	-23	TYR	-	expression tag	UNP R4P353
A	-22	TYR	-	expression tag	UNP R4P353
A	-21	HIS	-	expression tag	UNP R4P353
A	-20	HIS	-	expression tag	UNP R4P353
A	-19	HIS	-	expression tag	UNP R4P353
A	-18	HIS	-	expression tag	UNP R4P353
A	-17	HIS	-	expression tag	UNP R4P353
A	-16	HIS	-	expression tag	UNP R4P353
A	-15	LEU	-	expression tag	UNP R4P353
A	-14	GLU	-	expression tag	UNP R4P353
A	-13	SER	-	expression tag	UNP R4P353
A	-12	THR	-	expression tag	UNP R4P353
A	-11	SER	-	expression tag	UNP R4P353
A	-10	LEU	-	expression tag	UNP R4P353
A	-9	TYR	-	expression tag	UNP R4P353
A	-8	LYS	-	expression tag	UNP R4P353
A	-7	LYS	-	expression tag	UNP R4P353
A	-6	ALA	-	expression tag	UNP R4P353
A	-5	GLY	-	expression tag	UNP R4P353

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP R4P353
A	-3	GLU	-	expression tag	UNP R4P353
A	-2	PHE	-	expression tag	UNP R4P353
A	-1	ALA	-	expression tag	UNP R4P353
A	0	LEU	-	expression tag	UNP R4P353
A	696	GLY	-	insertion	UNP R4P353
B	-25	MET	-	initiating methionine	UNP R4P353
B	-24	SER	-	expression tag	UNP R4P353
B	-23	TYR	-	expression tag	UNP R4P353
B	-22	TYR	-	expression tag	UNP R4P353
B	-21	HIS	-	expression tag	UNP R4P353
B	-20	HIS	-	expression tag	UNP R4P353
B	-19	HIS	-	expression tag	UNP R4P353
B	-18	HIS	-	expression tag	UNP R4P353
B	-17	HIS	-	expression tag	UNP R4P353
B	-16	HIS	-	expression tag	UNP R4P353
B	-15	LEU	-	expression tag	UNP R4P353
B	-14	GLU	-	expression tag	UNP R4P353
B	-13	SER	-	expression tag	UNP R4P353
B	-12	THR	-	expression tag	UNP R4P353
B	-11	SER	-	expression tag	UNP R4P353
B	-10	LEU	-	expression tag	UNP R4P353
B	-9	TYR	-	expression tag	UNP R4P353
B	-8	LYS	-	expression tag	UNP R4P353
B	-7	LYS	-	expression tag	UNP R4P353
B	-6	ALA	-	expression tag	UNP R4P353
B	-5	GLY	-	expression tag	UNP R4P353
B	-4	SER	-	expression tag	UNP R4P353
B	-3	GLU	-	expression tag	UNP R4P353
B	-2	PHE	-	expression tag	UNP R4P353
B	-1	ALA	-	expression tag	UNP R4P353
B	0	LEU	-	expression tag	UNP R4P353
B	696	GLY	-	insertion	UNP R4P353
C	-25	MET	-	initiating methionine	UNP R4P353
C	-24	SER	-	expression tag	UNP R4P353
C	-23	TYR	-	expression tag	UNP R4P353
C	-22	TYR	-	expression tag	UNP R4P353
C	-21	HIS	-	expression tag	UNP R4P353
C	-20	HIS	-	expression tag	UNP R4P353
C	-19	HIS	-	expression tag	UNP R4P353
C	-18	HIS	-	expression tag	UNP R4P353
C	-17	HIS	-	expression tag	UNP R4P353

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP R4P353
C	-15	LEU	-	expression tag	UNP R4P353
C	-14	GLU	-	expression tag	UNP R4P353
C	-13	SER	-	expression tag	UNP R4P353
C	-12	THR	-	expression tag	UNP R4P353
C	-11	SER	-	expression tag	UNP R4P353
C	-10	LEU	-	expression tag	UNP R4P353
C	-9	TYR	-	expression tag	UNP R4P353
C	-8	LYS	-	expression tag	UNP R4P353
C	-7	LYS	-	expression tag	UNP R4P353
C	-6	ALA	-	expression tag	UNP R4P353
C	-5	GLY	-	expression tag	UNP R4P353
C	-4	SER	-	expression tag	UNP R4P353
C	-3	GLU	-	expression tag	UNP R4P353
C	-2	PHE	-	expression tag	UNP R4P353
C	-1	ALA	-	expression tag	UNP R4P353
C	0	LEU	-	expression tag	UNP R4P353
C	696	GLY	-	insertion	UNP R4P353
D	-25	MET	-	initiating methionine	UNP R4P353
D	-24	SER	-	expression tag	UNP R4P353
D	-23	TYR	-	expression tag	UNP R4P353
D	-22	TYR	-	expression tag	UNP R4P353
D	-21	HIS	-	expression tag	UNP R4P353
D	-20	HIS	-	expression tag	UNP R4P353
D	-19	HIS	-	expression tag	UNP R4P353
D	-18	HIS	-	expression tag	UNP R4P353
D	-17	HIS	-	expression tag	UNP R4P353
D	-16	HIS	-	expression tag	UNP R4P353
D	-15	LEU	-	expression tag	UNP R4P353
D	-14	GLU	-	expression tag	UNP R4P353
D	-13	SER	-	expression tag	UNP R4P353
D	-12	THR	-	expression tag	UNP R4P353
D	-11	SER	-	expression tag	UNP R4P353
D	-10	LEU	-	expression tag	UNP R4P353
D	-9	TYR	-	expression tag	UNP R4P353
D	-8	LYS	-	expression tag	UNP R4P353
D	-7	LYS	-	expression tag	UNP R4P353
D	-6	ALA	-	expression tag	UNP R4P353
D	-5	GLY	-	expression tag	UNP R4P353
D	-4	SER	-	expression tag	UNP R4P353
D	-3	GLU	-	expression tag	UNP R4P353
D	-2	PHE	-	expression tag	UNP R4P353

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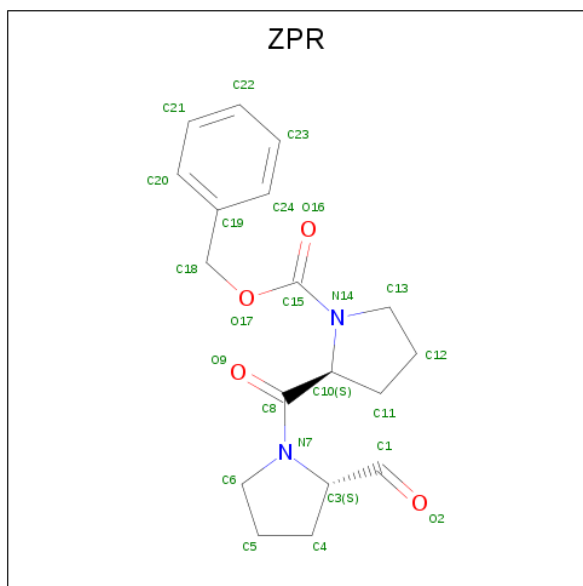
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP R4P353
D	0	LEU	-	expression tag	UNP R4P353
D	696	GLY	-	insertion	UNP R4P353

- Molecule 2 is a protein called Presegetalin A1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	F	6	Total	C	N	O	0	0	0
			39	23	7	9			
2	G	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	H	6	Total	C	N	O	0	0	0
			39	23	7	9			

- Molecule 3 is N-BENZYLOXYCARBONYL-L-PROLYL-L-PROLINAL (three-letter code: ZPR) (formula: C₁₈H₂₂N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	18	2	4		
3	B	1	Total	C	N	O	0	0
			24	18	2	4		
3	C	1	Total	C	N	O	0	0
			24	18	2	4		

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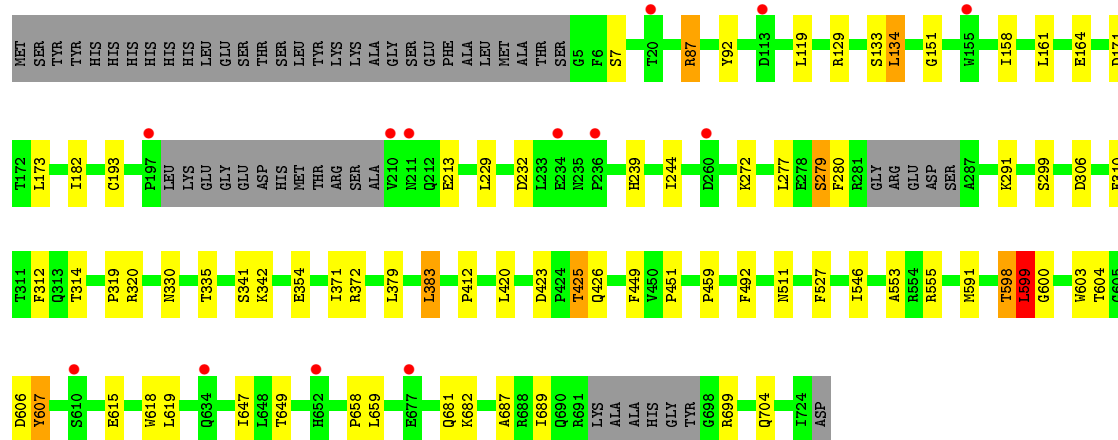
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			24	18	2	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

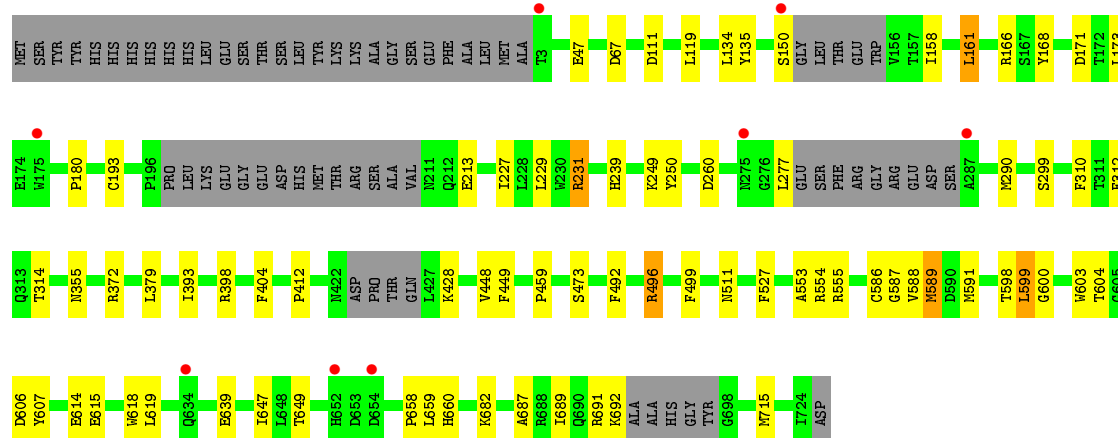
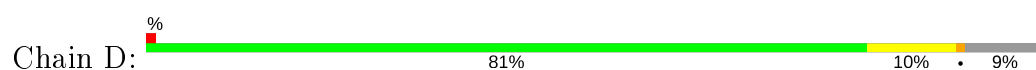
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	15	Total	O	0	0
			15	15		
5	C	15	Total	O	0	0
			15	15		
5	D	21	Total	O	0	0
			21	21		



• Molecule 1: Peptide cyclase 1



• Molecule 2: Presegetalin A1

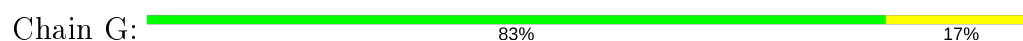


• Molecule 2: Presegetalin A1



There are no outlier residues recorded for this chain.

• Molecule 2: Presegetalin A1





- Molecule 2: Presegetalin A1

Chain H:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.00Å 85.33Å 137.87Å 87.74° 78.53° 89.64°	Depositor
Resolution (Å)	45.70 – 2.82 45.75 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.70-2.82) 98.3 (45.75-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.227 , 0.270 0.229 , 0.269	Depositor DCC
R_{free} test set	3296 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.087 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	22661	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: CA, ZPR

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	0.54	0/5681	0.73	5/7693 (0.1%)
1	B	0.56	0/5782	0.73	6/7829 (0.1%)
1	C	0.57	0/5781	0.73	5/7825 (0.1%)
1	D	0.55	0/5668	0.74	7/7665 (0.1%)
2	E	0.48	0/38	0.47	0/52
2	F	0.54	0/39	0.68	0/52
2	G	0.51	0/38	0.52	0/52
2	H	0.53	0/39	0.57	0/52
All	All	0.55	0/23066	0.73	23/31220 (0.1%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	LEU	CA-CB-CG	10.62	139.74	115.30
1	D	496	ARG	CG-CD-NE	8.20	129.03	111.80
1	C	599	LEU	CA-CB-CG	8.19	134.14	115.30
1	D	496	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	496	ARG	NE-CZ-NH1	6.86	123.73	120.30

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	5540	0	5381	45	1
1	B	5639	0	5487	35	0
1	C	5637	0	5484	35	1
1	D	5531	0	5392	46	1
2	E	38	0	36	0	0
2	F	39	0	36	0	0
2	G	38	0	36	1	0
2	H	39	0	36	0	0
3	A	24	0	21	3	0
3	B	24	0	21	1	0
3	C	24	0	21	1	0
3	D	24	0	21	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	10	0	0	2	1
5	B	15	0	0	1	0
5	C	15	0	0	1	0
5	D	21	0	0	2	0
All	All	22661	0	21972	155	2

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.

The worst 5 of 155 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:555[B]:ARG:HG2	1:D:555[B]:ARG:HH11	1.15	1.09
1:D:555[B]:ARG:HG2	1:D:555[B]:ARG:NH1	1.82	0.89
1:A:213:GLU:HG2	1:A:231:ARG:HG2	1.56	0.87
1:A:61:GLU:OE2	5:A:901:HOH:O	1.92	0.87
1:D:587:GLY:C	1:D:589:MET:HE2	1.97	0.85

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:OG	1:C:291:LYS:O[1_655]	2.06	0.14
1:D:639:GLU:OE2	5:A:902:HOH:O[1_654]	2.16	0.04

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	681/751 (91%)	648 (95%)	31 (5%)	2 (0%)	41	70
1	B	695/751 (92%)	654 (94%)	37 (5%)	4 (1%)	25	54
1	C	693/751 (92%)	655 (94%)	34 (5%)	4 (1%)	25	54
1	D	676/751 (90%)	641 (95%)	31 (5%)	4 (1%)	25	54
2	E	4/6 (67%)	4 (100%)	0	0	100	100
2	F	4/6 (67%)	4 (100%)	0	0	100	100
2	G	4/6 (67%)	4 (100%)	0	0	100	100
2	H	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2761/3028 (91%)	2614 (95%)	133 (5%)	14 (0%)	29	59

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	598	THR
1	A	598	THR
1	C	598	THR
1	D	598	THR
1	B	553	ALA

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	602/652 (92%)	587 (98%)	15 (2%)	47	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	613/652 (94%)	594 (97%)	19 (3%)	40	72
1	C	612/652 (94%)	591 (97%)	21 (3%)	37	69
1	D	600/652 (92%)	583 (97%)	17 (3%)	43	76
2	E	4/4 (100%)	4 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
2	G	4/4 (100%)	4 (100%)	0	100	100
2	H	4/4 (100%)	4 (100%)	0	100	100
All	All	2443/2624 (93%)	2371 (97%)	72 (3%)	41	74

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	655	ARG
1	C	164	GLU
1	D	496	ARG
1	B	682	LYS
1	C	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	HIS
1	D	670	HIS
1	B	670	HIS
1	A	670	HIS
1	B	652	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ZPR	A	801	1	25,26,26	1.47	1 (4%)	31,35,35	2.77	11 (35%)
3	ZPR	D	801	1	25,26,26	1.43	1 (4%)	31,35,35	1.49	7 (22%)
3	ZPR	B	801	1	25,26,26	1.51	1 (4%)	31,35,35	1.89	7 (22%)
3	ZPR	C	801	1	25,26,26	1.40	2 (8%)	31,35,35	1.94	3 (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
3	ZPR	A	801	1	-	13/17/39/39	0/3/3/3
3	ZPR	D	801	1	-	3/17/39/39	0/3/3/3
3	ZPR	B	801	1	-	3/17/39/39	0/3/3/3
3	ZPR	C	801	1	-	3/17/39/39	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	ZPR	O17-C15	6.67	1.47	1.34
3	A	801	ZPR	O17-C15	6.47	1.46	1.34
3	D	801	ZPR	O17-C15	6.16	1.46	1.34
3	C	801	ZPR	O17-C15	5.65	1.45	1.34
3	C	801	ZPR	C3-N7	-2.03	1.46	1.48

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ZPR	O17-C15-N14	8.65	120.55	111.05
3	A	801	ZPR	C11-C10-N14	-7.91	91.28	103.03
3	C	801	ZPR	C4-C3-C1	-6.98	103.10	112.70
3	C	801	ZPR	O17-C15-N14	5.82	117.44	111.05
3	B	801	ZPR	C4-C3-C1	-5.35	105.34	112.70

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

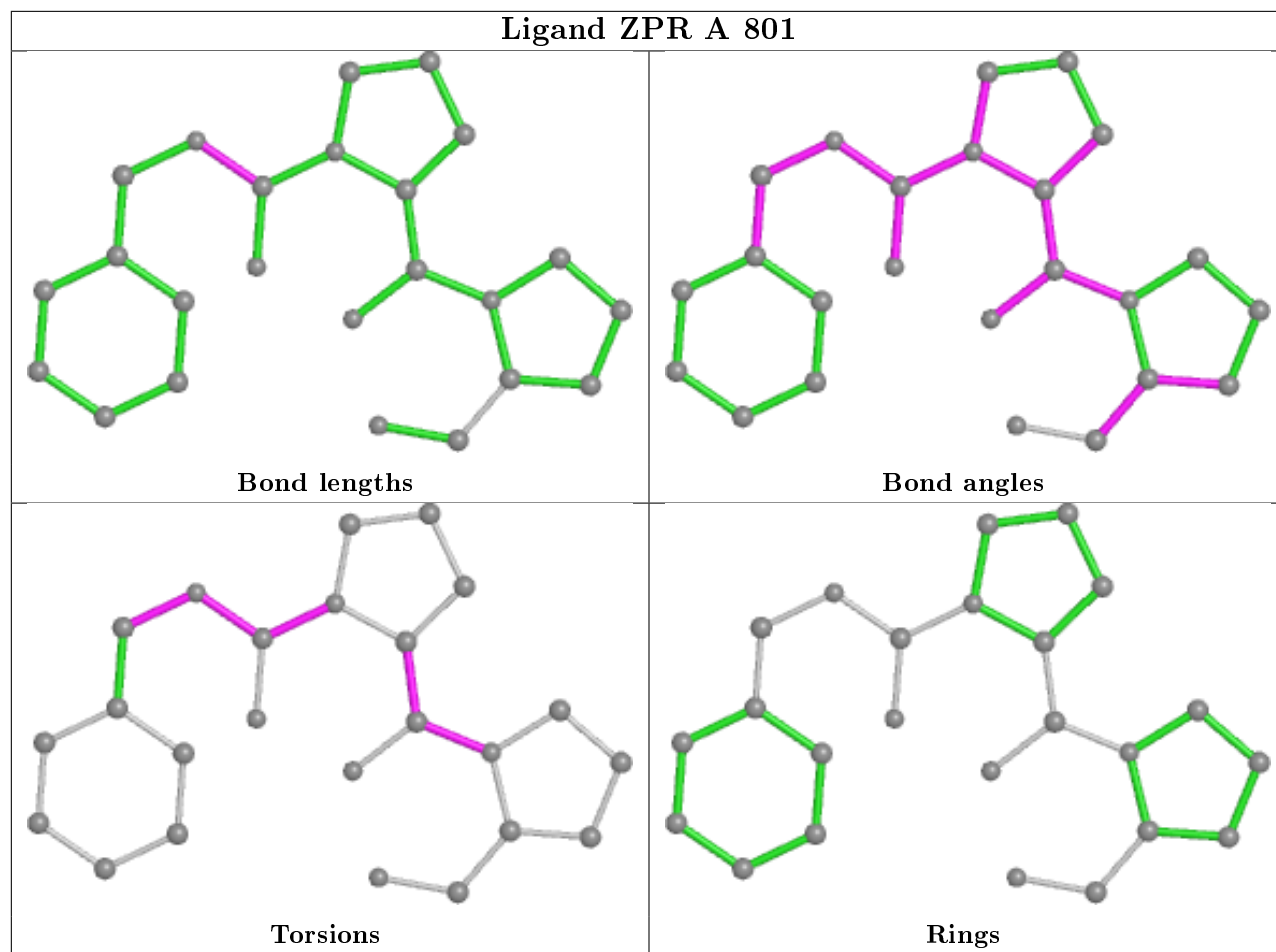
Mol	Chain	Res	Type	Atoms
3	C	801	ZPR	O16-C15-O17-C18
3	C	801	ZPR	N14-C15-O17-C18
3	A	801	ZPR	O16-C15-O17-C18
3	A	801	ZPR	N14-C15-O17-C18
3	A	801	ZPR	O17-C15-N14-C10

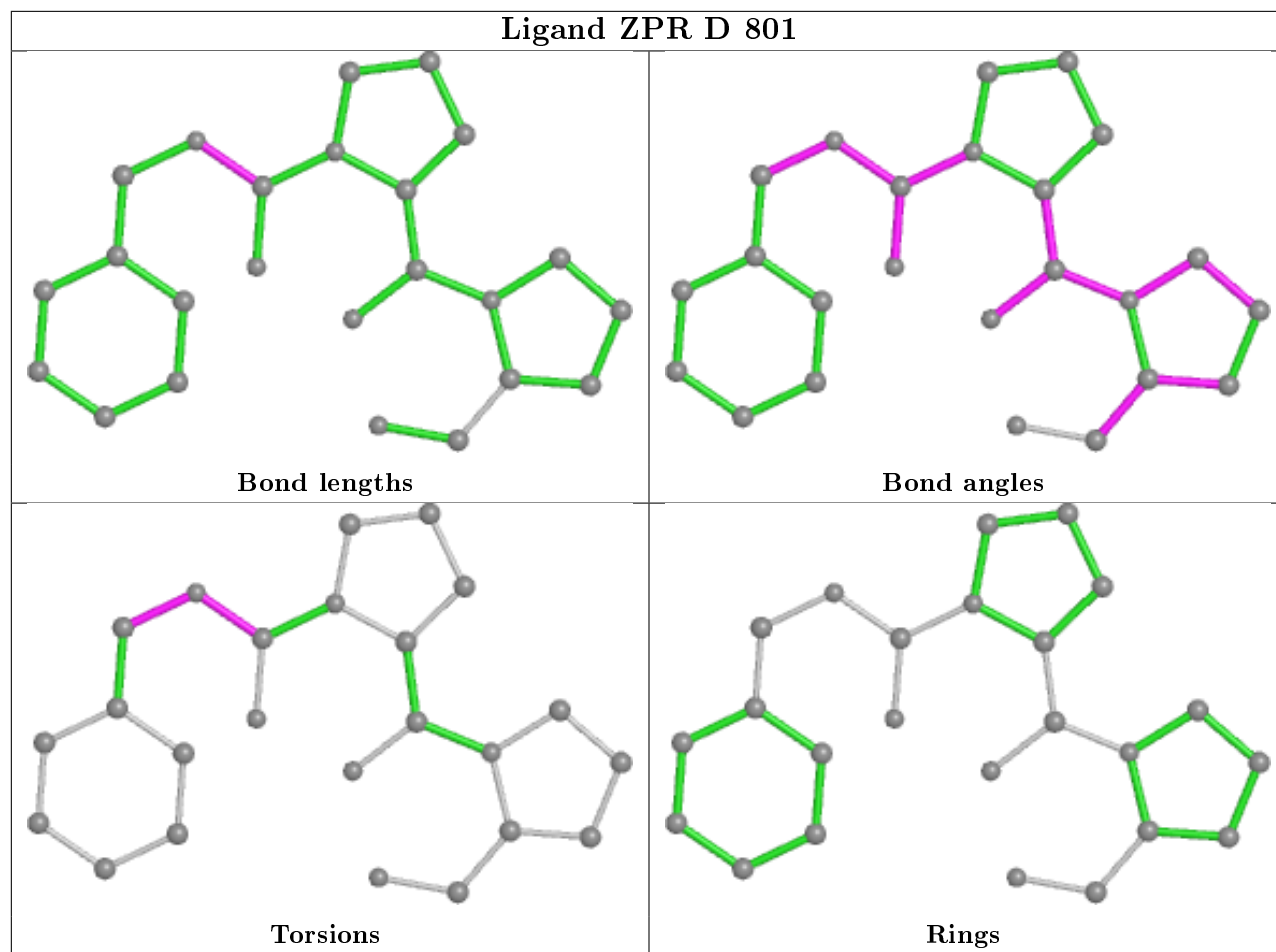
There are no ring outliers.

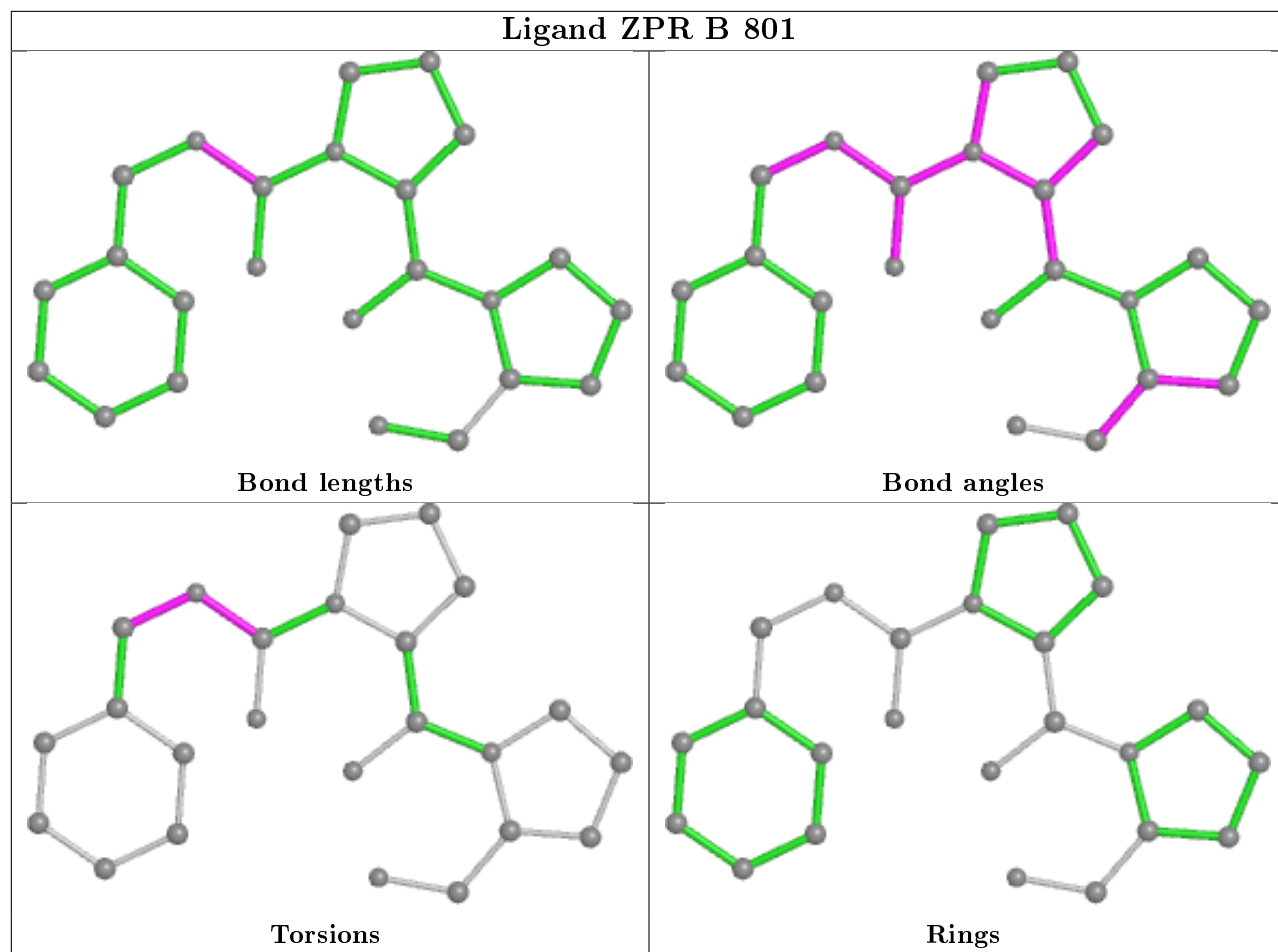
4 monomers are involved in 7 short contacts:

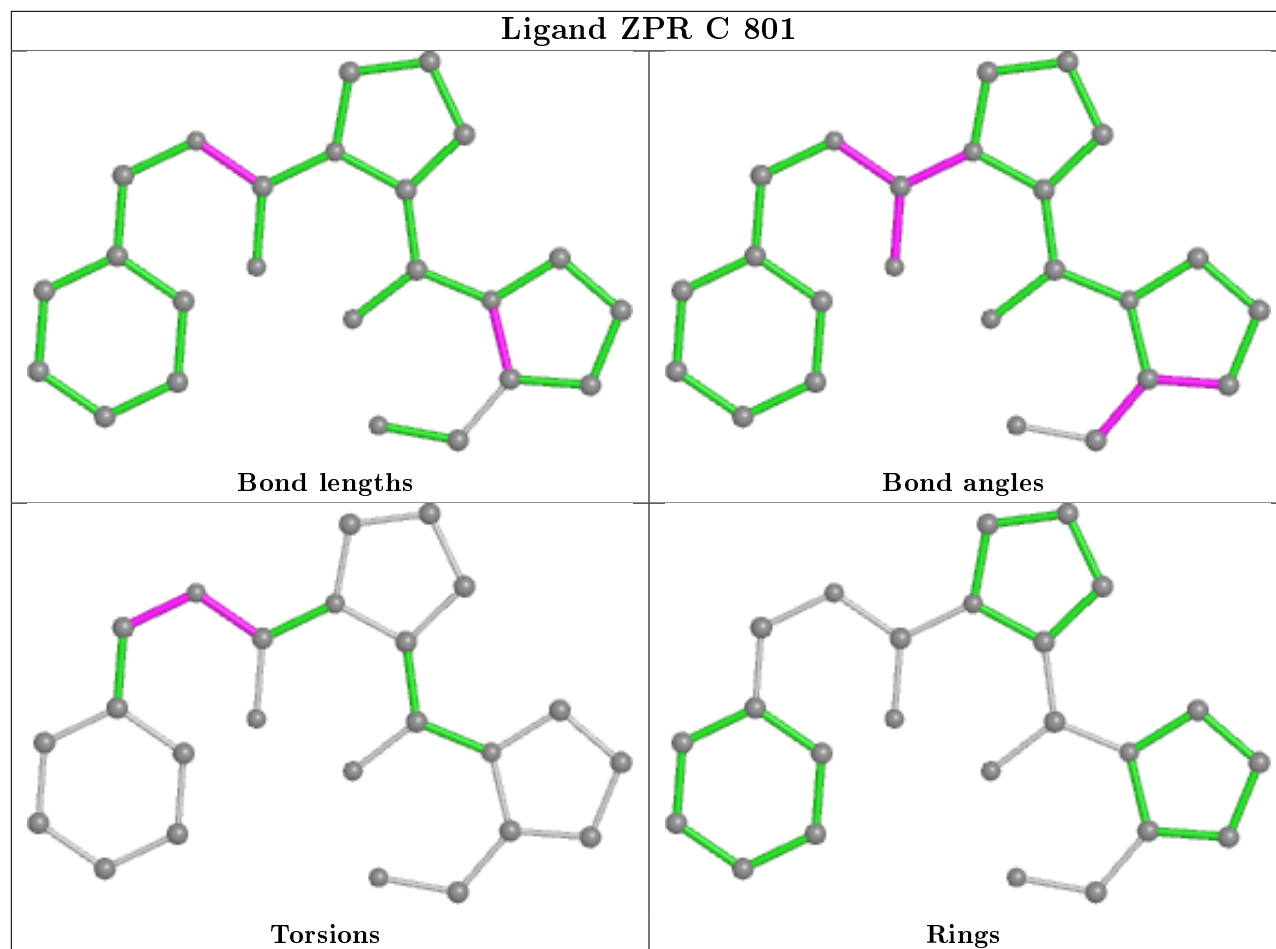
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ZPR	3	0
3	D	801	ZPR	2	0
3	B	801	ZPR	1	0
3	C	801	ZPR	1	0

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, 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	686/751 (91%)	0.15	24 (3%) 44 34	12, 29, 58, 92	0
1	B	701/751 (93%)	0.01	14 (1%) 65 56	11, 26, 50, 97	0
1	C	697/751 (92%)	-0.01	13 (1%) 66 59	9, 25, 54, 80	0
1	D	685/751 (91%)	-0.00	8 (1%) 79 73	10, 26, 49, 81	0
2	E	6/6 (100%)	0.62	1 (16%) 1 1	35, 42, 48, 56	0
2	F	6/6 (100%)	0.46	0 100 100	27, 30, 35, 36	0
2	G	6/6 (100%)	-0.10	0 100 100	26, 29, 35, 37	0
2	H	6/6 (100%)	0.40	0 100 100	27, 33, 40, 45	0
All	All	2793/3028 (92%)	0.04	60 (2%) 63 54	9, 27, 54, 97	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	THR	4.8
1	D	3	THR	4.0
1	A	154	GLU	3.9
1	D	654	ASP	3.9
1	A	234	GLU	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

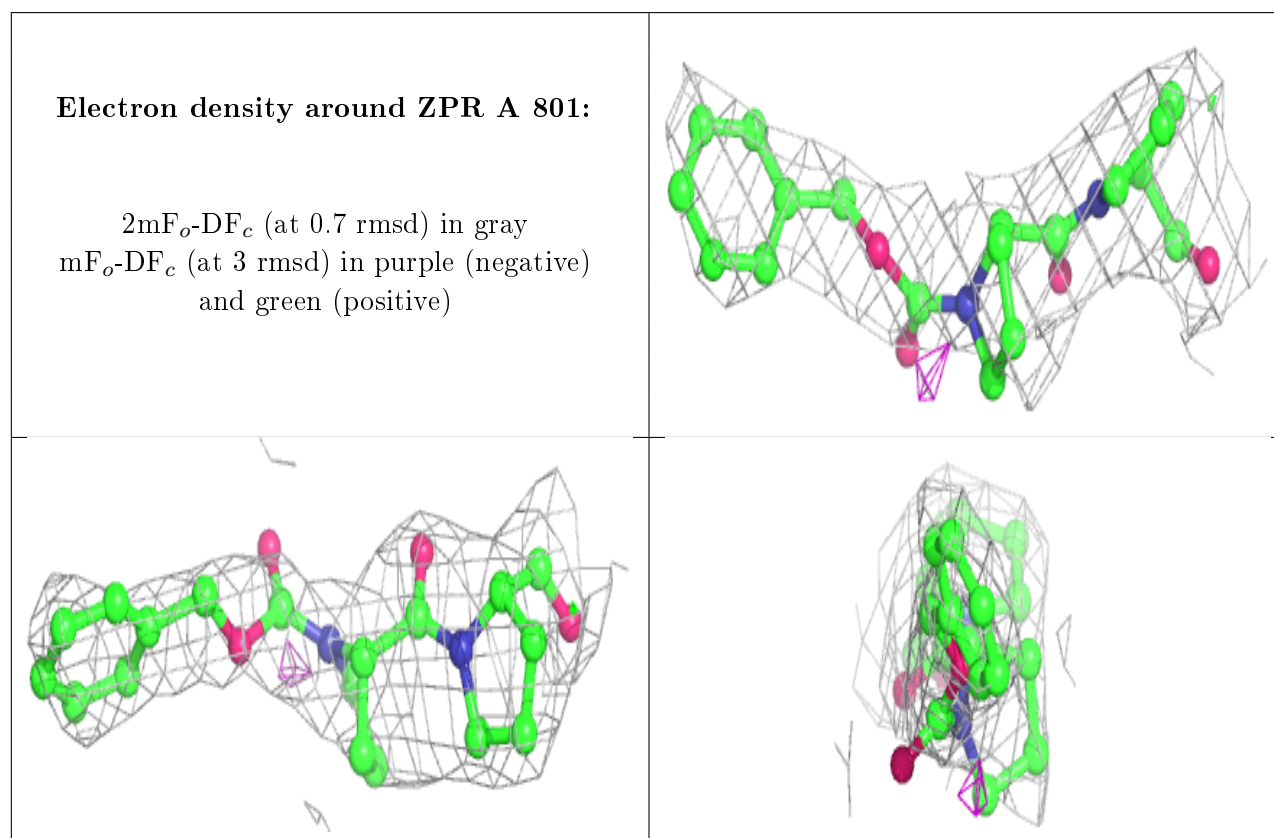
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

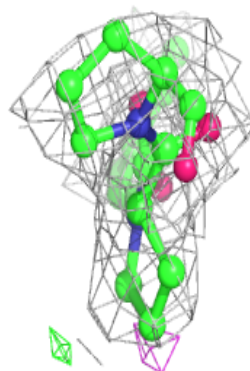
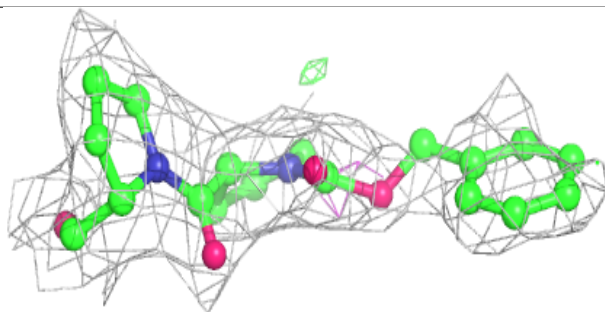
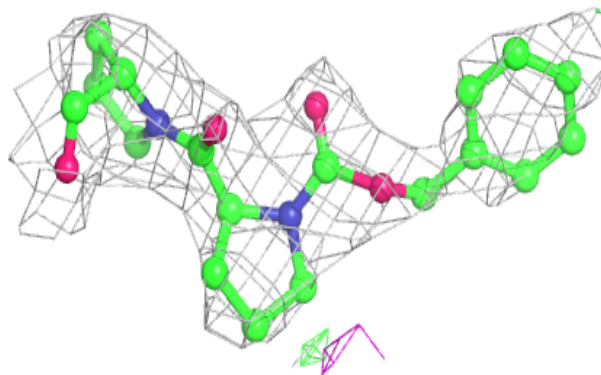
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	A	802	1/1	0.87	0.10	42,42,42,42	0
3	ZPR	A	801	24/24	0.88	0.24	29,40,48,55	0
3	ZPR	B	801	24/24	0.89	0.19	29,32,47,50	0
4	CA	B	803	1/1	0.90	0.13	53,53,53,53	0
3	ZPR	D	801	24/24	0.94	0.17	22,35,38,41	0
4	CA	B	802	1/1	0.96	0.12	39,39,39,39	0
3	ZPR	C	801	24/24	0.96	0.14	25,27,30,32	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.

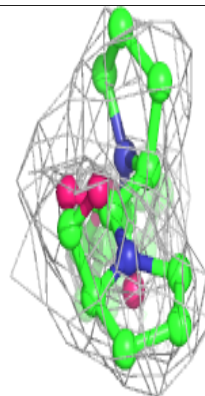
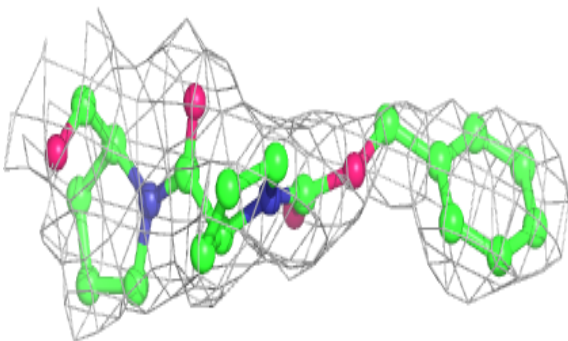
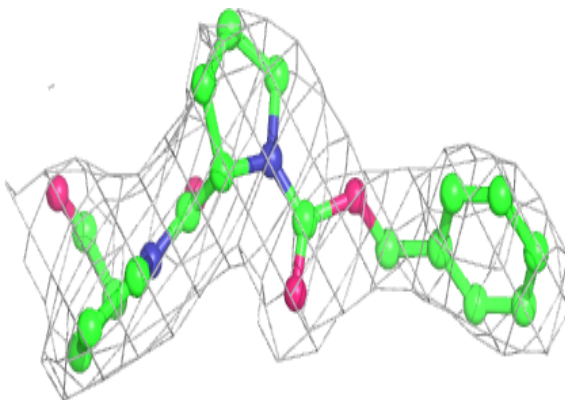


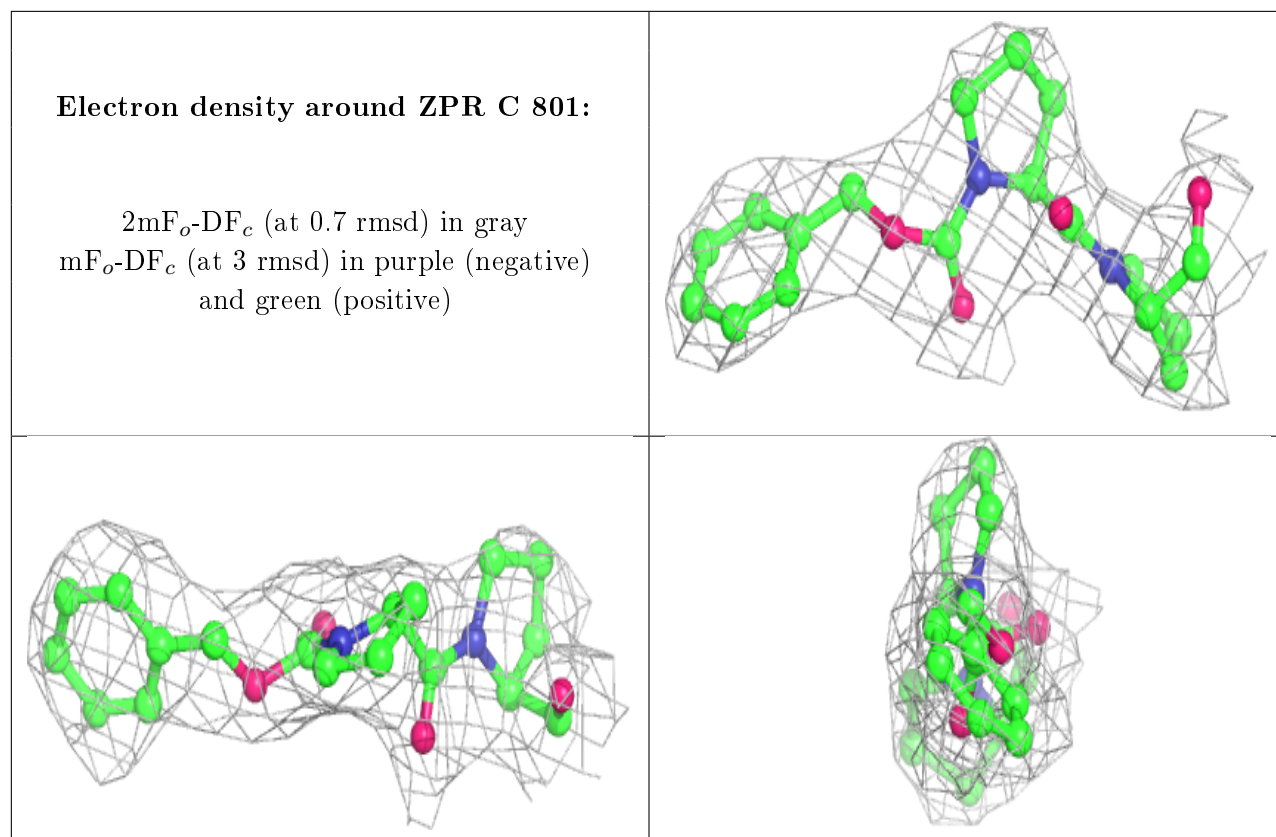
Electron density around ZPR B 801:

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

**Electron density around ZPR D 801:**

$2mF_o-DF_c$ (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.