Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2023 – 04:08 PM EDT

PDB ID	:	8T55
Title	:	Co-crystal structure of the WD-repeat domain of human WDR91 in complex with MR46654
Authors	:	Ahmad, H.; Zeng, H.; Dong, A.; Li, Y.; Yen, H.; Seitova, A.; Xu, J.; Feng, J.W.; Brown, P.J.; Santhakumar, V.; Ackloo, S.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on	:	2023-06-12
Resolution	:	2.20 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

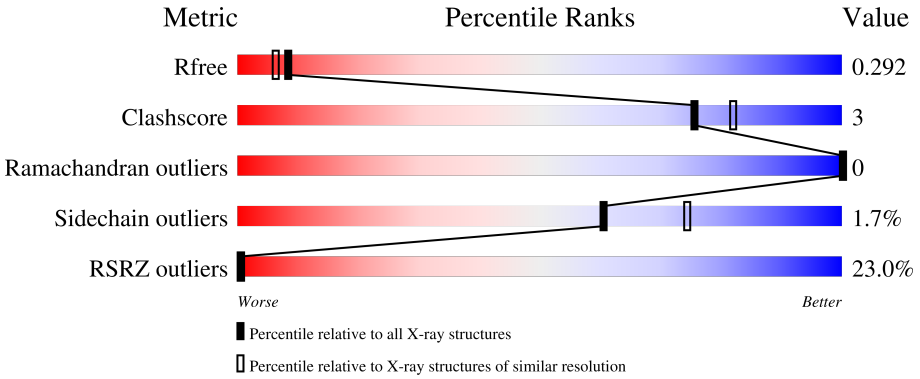
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 >=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 <=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	359	87% 6% 7%
1	B	359	86% 7% 7%
1	C	359	60% 75% 8% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZI3	C	801	-	-	-	X
3	EDO	B	801	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7535 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 WD repeat-containing protein 91.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2529	1592	435	482	20			
1	B	334	Total	C	N	O	S	0	3	0
			2525	1591	432	482	20			
1	C	300	Total	C	N	O	S	0	0	0
			2158	1368	368	405	17			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	MET	-	initiating methionine	UNP A4D1P6
A	375	HIS	-	expression tag	UNP A4D1P6
A	376	HIS	-	expression tag	UNP A4D1P6
A	377	HIS	-	expression tag	UNP A4D1P6
A	378	HIS	-	expression tag	UNP A4D1P6
A	379	HIS	-	expression tag	UNP A4D1P6
A	380	HIS	-	expression tag	UNP A4D1P6
A	381	SER	-	expression tag	UNP A4D1P6
A	382	SER	-	expression tag	UNP A4D1P6
A	383	GLY	-	expression tag	UNP A4D1P6
A	384	ARG	-	expression tag	UNP A4D1P6
A	385	GLU	-	expression tag	UNP A4D1P6
A	386	ASN	-	expression tag	UNP A4D1P6
A	387	LEU	-	expression tag	UNP A4D1P6
A	388	TYR	-	expression tag	UNP A4D1P6
A	389	PHE	-	expression tag	UNP A4D1P6
A	390	GLN	-	expression tag	UNP A4D1P6
A	391	GLY	-	expression tag	UNP A4D1P6
A	?	-	VAL	deletion	UNP A4D1P6
A	?	-	ASP	deletion	UNP A4D1P6
A	?	-	PHE	deletion	UNP A4D1P6
A	?	-	SER	deletion	UNP A4D1P6
A	?	-	ALA	deletion	UNP A4D1P6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP A4D1P6
A	?	-	ASP	deletion	UNP A4D1P6
A	?	-	ILE	deletion	UNP A4D1P6
A	?	-	GLY	deletion	UNP A4D1P6
A	?	-	SER	deletion	UNP A4D1P6
A	?	-	LYS	deletion	UNP A4D1P6
A	?	-	GLY	deletion	UNP A4D1P6
A	?	-	MET	deletion	UNP A4D1P6
A	?	-	ASN	deletion	UNP A4D1P6
A	?	-	GLN	deletion	UNP A4D1P6
B	374	MET	-	initiating methionine	UNP A4D1P6
B	375	HIS	-	expression tag	UNP A4D1P6
B	376	HIS	-	expression tag	UNP A4D1P6
B	377	HIS	-	expression tag	UNP A4D1P6
B	378	HIS	-	expression tag	UNP A4D1P6
B	379	HIS	-	expression tag	UNP A4D1P6
B	380	HIS	-	expression tag	UNP A4D1P6
B	381	SER	-	expression tag	UNP A4D1P6
B	382	SER	-	expression tag	UNP A4D1P6
B	383	GLY	-	expression tag	UNP A4D1P6
B	384	ARG	-	expression tag	UNP A4D1P6
B	385	GLU	-	expression tag	UNP A4D1P6
B	386	ASN	-	expression tag	UNP A4D1P6
B	387	LEU	-	expression tag	UNP A4D1P6
B	388	TYR	-	expression tag	UNP A4D1P6
B	389	PHE	-	expression tag	UNP A4D1P6
B	390	GLN	-	expression tag	UNP A4D1P6
B	391	GLY	-	expression tag	UNP A4D1P6
B	?	-	VAL	deletion	UNP A4D1P6
B	?	-	ASP	deletion	UNP A4D1P6
B	?	-	PHE	deletion	UNP A4D1P6
B	?	-	SER	deletion	UNP A4D1P6
B	?	-	ALA	deletion	UNP A4D1P6
B	?	-	PRO	deletion	UNP A4D1P6
B	?	-	ASP	deletion	UNP A4D1P6
B	?	-	ILE	deletion	UNP A4D1P6
B	?	-	GLY	deletion	UNP A4D1P6
B	?	-	SER	deletion	UNP A4D1P6
B	?	-	LYS	deletion	UNP A4D1P6
B	?	-	GLY	deletion	UNP A4D1P6
B	?	-	MET	deletion	UNP A4D1P6
B	?	-	ASN	deletion	UNP A4D1P6

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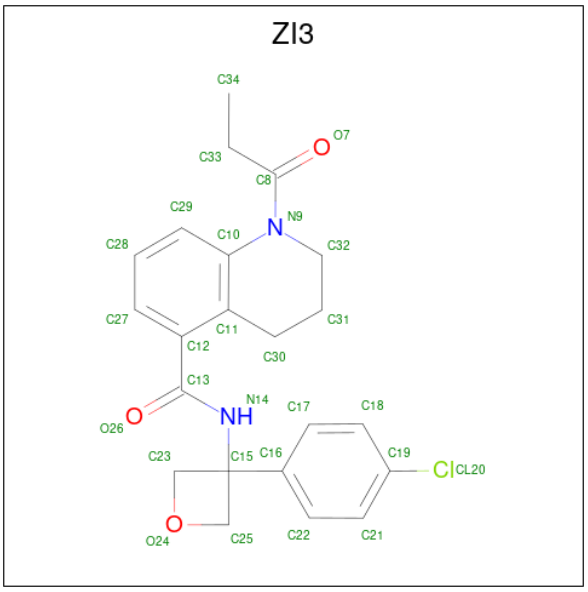
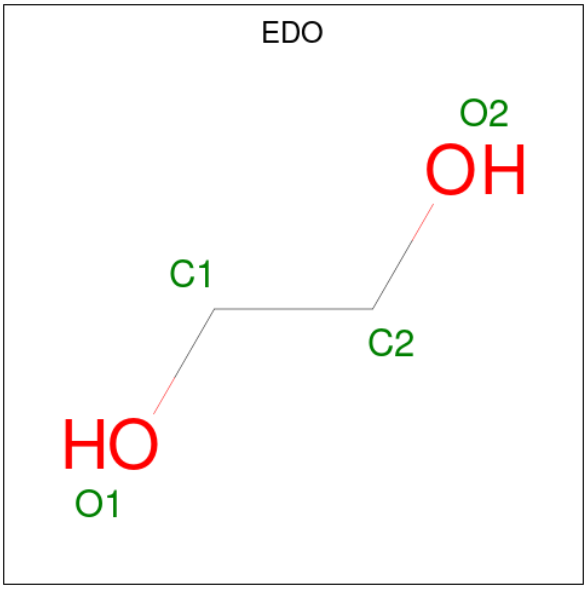
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP A4D1P6
C	374	MET	-	initiating methionine	UNP A4D1P6
C	375	HIS	-	expression tag	UNP A4D1P6
C	376	HIS	-	expression tag	UNP A4D1P6
C	377	HIS	-	expression tag	UNP A4D1P6
C	378	HIS	-	expression tag	UNP A4D1P6
C	379	HIS	-	expression tag	UNP A4D1P6
C	380	HIS	-	expression tag	UNP A4D1P6
C	381	SER	-	expression tag	UNP A4D1P6
C	382	SER	-	expression tag	UNP A4D1P6
C	383	GLY	-	expression tag	UNP A4D1P6
C	384	ARG	-	expression tag	UNP A4D1P6
C	385	GLU	-	expression tag	UNP A4D1P6
C	386	ASN	-	expression tag	UNP A4D1P6
C	387	LEU	-	expression tag	UNP A4D1P6
C	388	TYR	-	expression tag	UNP A4D1P6
C	389	PHE	-	expression tag	UNP A4D1P6
C	390	GLN	-	expression tag	UNP A4D1P6
C	391	GLY	-	expression tag	UNP A4D1P6
C	?	-	VAL	deletion	UNP A4D1P6
C	?	-	ASP	deletion	UNP A4D1P6
C	?	-	PHE	deletion	UNP A4D1P6
C	?	-	SER	deletion	UNP A4D1P6
C	?	-	ALA	deletion	UNP A4D1P6
C	?	-	PRO	deletion	UNP A4D1P6
C	?	-	ASP	deletion	UNP A4D1P6
C	?	-	ILE	deletion	UNP A4D1P6
C	?	-	GLY	deletion	UNP A4D1P6
C	?	-	SER	deletion	UNP A4D1P6
C	?	-	LYS	deletion	UNP A4D1P6
C	?	-	GLY	deletion	UNP A4D1P6
C	?	-	MET	deletion	UNP A4D1P6
C	?	-	ASN	deletion	UNP A4D1P6
C	?	-	GLN	deletion	UNP A4D1P6

- Molecule 2 is N-[3-(4-chlorophenyl)oxetan-3-yl]-1-propanoyl-1,2,3,4-tetrahydroquinoline-5-carboxamide (three-letter code: ZI3) (formula: $C_{22}H_{23}ClN_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	22	1	2	3		
2	B	1	Total	C	Cl	N	O	0	0
			28	22	1	2	3		
2	C	1	Total	C	Cl	N	O	0	0
			28	22	1	2	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

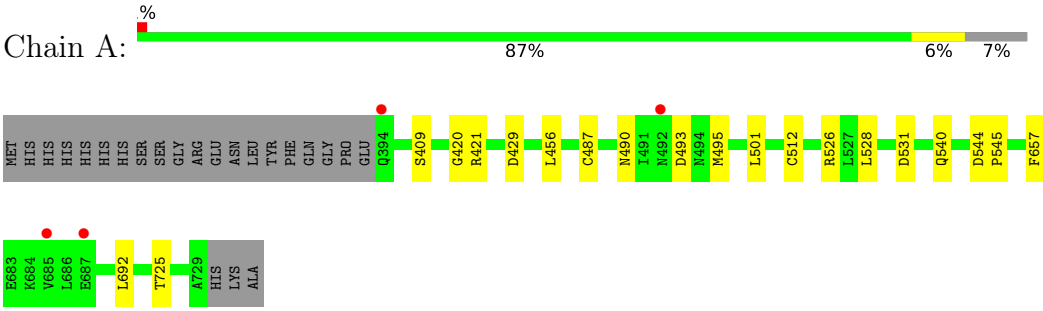
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	118	Total O 119 119	0	1
4	C	5	Total O 5 5	0	0

3 Residue-property plots (i)

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.

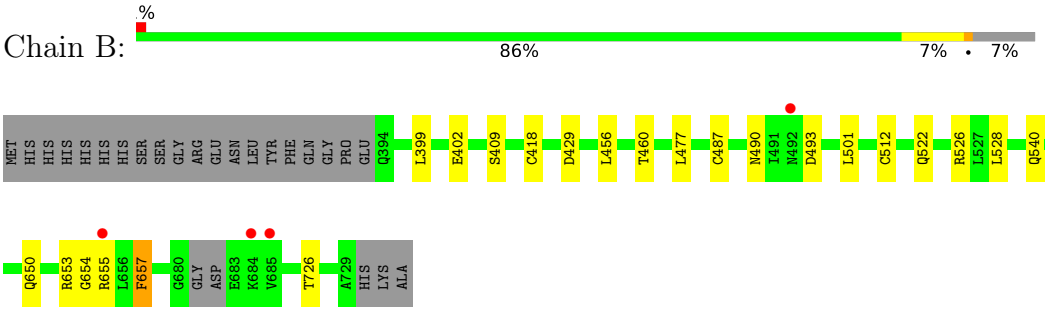
• Molecule 1: WD repeat-containing protein 91

Chain A:



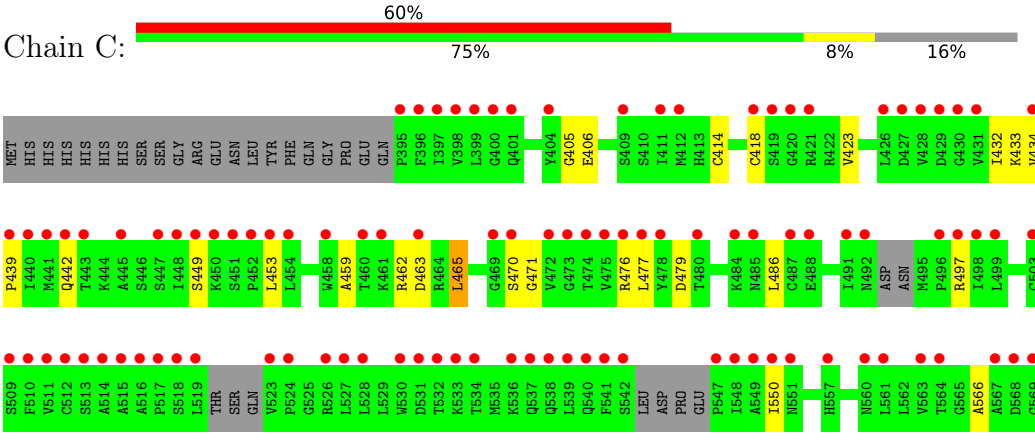
• Molecule 1: WD repeat-containing protein 91

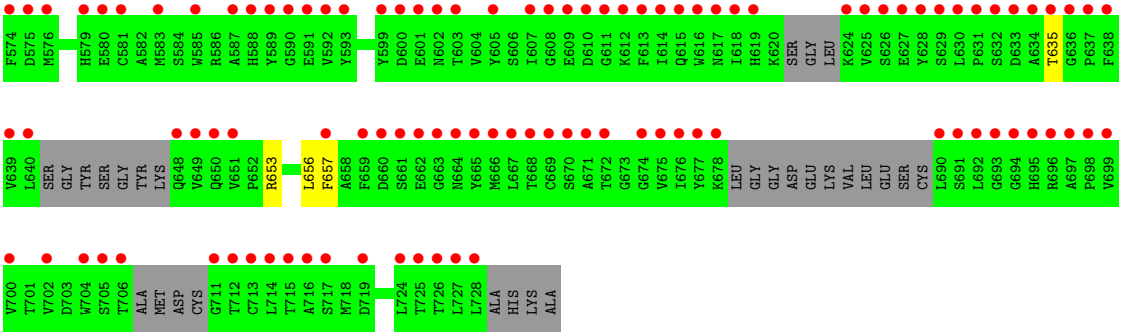
Chain B:



• Molecule 1: WD repeat-containing protein 91

Chain C:




F574 D575 M576 H579 E580 C581 A582 M583 S584 W585 R586 A587 H588 Y589 G590 E591 V592 Y593 Y599 D600 E601 N602 T603 V604 Y605 S606 I607 G608 E609 D610 G611 K612 F613 I614 Q615 W616 N617 I618 H619 K620 SER GLY LEU K624 V625 S626 E627 Y628 S629 L630 P631 S632 D633 A634 T635 G636 P637 F638
V639 L640 SER GLY TYR SER GLY TYR LYS Q648 V649 Q650 V651 P652 R653 L656 F657 A658 F659 D660 S661 E662 G663 N664 Y665 M666 L667 T668 C669 S670 A671 T672 G673 G674 V675 I676 Y677 K678 LEU GLY GLY ASP GLU LYS VAL LEU GLU SER CYS L690 S691 L692 G693 G694 H696 R696 A697 P698 V699
V700 T701 V702 D703 W704 S705 T706 ALA MET ASP CYS G711 T712 C713 L714 T715 A716 S717 M718 D719 L724 T725 T726 L727 L728 ALA HIS LYS ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.70Å 121.62Å 132.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 – 2.20 38.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.78-2.20) 97.8 (38.75-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.245 , 0.288 0.250 , 0.292	Depositor DCC
R_{free} test set	1207 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7535	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 89.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3885e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, ZI3

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	0/2581	0.75	2/3505 (0.1%)
1	B	0.67	0/2577	0.75	0/3501
1	C	0.75	0/2199	0.74	0/2988
All	All	0.70	0/7357	0.75	2/9994 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	487	CYS	CA-CB-SG	5.64	124.15	114.00
1	A	487	CYS	CB-CA-C	-5.57	99.25	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2529	0	2408	10	0
1	B	2525	0	2398	19	0
1	C	2158	0	1954	15	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	6	5	0
4	A	111	0	0	1	0
4	B	119	0	0	0	0
4	C	5	0	0	0	0
All	All	7535	0	6766	43	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 (43) 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:C:418:CYS:SG	1:C:463:ASP:OD1	2.38	0.80
1:B:654:GLY:H	3:B:801:EDO:C1	2.00	0.75
1:B:650:GLN:NE2	3:B:801:EDO:O1	2.28	0.67
1:B:558:ASN:ND2	1:B:560:ASN:OD1	2.23	0.67
1:B:654:GLY:H	3:B:801:EDO:H12	1.61	0.64
1:B:493:ASP:CB	1:B:526:ARG:HH21	2.14	0.61
1:C:438:ASN:HD22	1:C:439:PRO:HA	1.67	0.59
1:B:558:ASN:HD22	1:B:559:GLY:N	2.02	0.57
1:B:654:GLY:H	3:B:801:EDO:H11	1.71	0.55
1:C:438:ASN:ND2	1:C:439:PRO:HA	2.23	0.54
1:B:653:ARG:HB3	3:B:801:EDO:H12	1.92	0.51
1:C:479:ASP:HB2	1:C:486:LEU:HD11	1.93	0.50
1:A:692:LEU:HD22	1:A:725:THR:HG21	1.95	0.48
1:C:459:ALA:HB3	1:C:462:ARG:O	2.13	0.48
1:A:456:LEU:C	1:A:456:LEU:HD23	2.32	0.48
1:A:493:ASP:CB	1:A:526:ARG:HH21	2.27	0.48
1:C:550:ILE:HD13	1:C:566:ALA:HB2	1.95	0.47
1:B:655[B]:ARG:HG2	1:B:657:PHE:O	2.15	0.47
1:B:399:LEU:HD12	1:B:726:THR:HG22	1.98	0.46
1:C:414:CYS:O	1:C:414:CYS:SG	2.73	0.45
1:B:456:LEU:C	1:B:456:LEU:HD23	2.36	0.45
1:B:409:SER:OG	1:B:429:ASP:OD2	2.31	0.45
1:A:501:LEU:HD23	1:A:512:CYS:HB3	1.99	0.44
1:A:531:ASP:OD1	4:A:901:HOH:O	2.21	0.44
1:B:528:LEU:HD22	1:B:540[A]:GLN:HG2	1.99	0.44
1:A:409:SER:OG	1:A:429:ASP:OD2	2.35	0.44
1:B:558:ASN:HD22	1:B:558:ASN:C	2.19	0.44
1:B:477:LEU:HB3	1:B:487:CYS:HB2	2.00	0.44
1:B:501:LEU:HD23	1:B:512:CYS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LEU:HD23	1:A:512:CYS:CB	2.48	0.43
1:C:406:GLU:HB3	1:C:433:LYS:HE3	2.01	0.43
1:C:471:GLY:HA2	1:C:497:ARG:HA	2.01	0.43
1:C:465:LEU:HG	1:C:477:LEU:HD11	2.01	0.42
1:C:449:SER:OG	1:C:476:ARG:NH1	2.51	0.42
1:C:453:LEU:HA	1:C:470:SER:HA	2.01	0.42
1:C:635:THR:HA	1:C:656:LEU:HD13	2.02	0.42
1:B:493:ASP:CB	1:B:526:ARG:NH2	2.81	0.42
1:A:420:GLY:O	1:A:421:ARG:NH1	2.52	0.42
1:A:528:LEU:HD22	1:A:540[A]:GLN:HG2	2.01	0.42
1:B:418:CYS:SG	1:B:460:THR:HA	2.59	0.41
1:A:544:ASP:CG	1:A:545:PRO:HA	2.41	0.41
1:C:423:VAL:O	1:C:434:VAL:HA	2.21	0.40
1:B:522:GLN:HG3	1:C:405:GLY:O	2.22	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	333/359 (93%)	323 (97%)	10 (3%)	0	100	100
1	B	333/359 (93%)	325 (98%)	8 (2%)	0	100	100
1	C	284/359 (79%)	267 (94%)	17 (6%)	0	100	100
All	All	950/1077 (88%)	915 (96%)	35 (4%)	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	263/305 (86%)	260 (99%)	3 (1%)	73 85
1	B	261/305 (86%)	257 (98%)	4 (2%)	65 78
1	C	203/305 (67%)	198 (98%)	5 (2%)	47 60
All	All	727/915 (80%)	715 (98%)	12 (2%)	60 74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	ASN
1	A	495	MET
1	A	657	PHE
1	B	402	GLU
1	B	490	ASN
1	B	558	ASN
1	B	657	PHE
1	C	432	ILE
1	C	442	GLN
1	C	465	LEU
1	C	653	ARG
1	C	657	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	558	ASN
1	C	438	ASN

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)

4 ligands are modelled in this entry.

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	EDO	B	801	-	3,3,3	0.37	0	2,2,2	0.22	0
2	ZI3	A	801	1	27,31,31	3.83	13 (48%)	38,45,45	2.54	8 (21%)
2	ZI3	C	801	1	27,31,31	4.15	17 (62%)	38,45,45	1.70	7 (18%)
2	ZI3	B	802	1	27,31,31	3.75	14 (51%)	38,45,45	2.51	6 (15%)

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	EDO	B	801	-	-	1/1/1/1	-
2	ZI3	A	801	1	-	3/21/39/39	0/4/4/4
2	ZI3	C	801	1	-	6/21/39/39	0/4/4/4
2	ZI3	B	802	1	-	2/21/39/39	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ZI3	C12-C11	11.86	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ZI3	C12-C11	10.90	1.53	1.40
2	B	802	ZI3	C12-C11	10.18	1.52	1.40
2	C	801	ZI3	C8-N9	8.49	1.50	1.36
2	B	802	ZI3	C8-N9	8.38	1.50	1.36
2	A	801	ZI3	C8-N9	8.29	1.49	1.36
2	C	801	ZI3	C22-C16	6.94	1.50	1.39
2	C	801	ZI3	C13-N14	6.84	1.47	1.34
2	A	801	ZI3	C22-C16	6.82	1.50	1.39
2	B	802	ZI3	C22-C16	6.70	1.50	1.39
2	B	802	ZI3	C13-N14	6.22	1.46	1.34
2	A	801	ZI3	C13-N14	6.20	1.46	1.34
2	C	801	ZI3	C29-C10	5.64	1.49	1.39
2	A	801	ZI3	C29-C10	5.45	1.48	1.39
2	C	801	ZI3	C18-C19	5.45	1.48	1.38
2	B	802	ZI3	C29-C10	5.39	1.48	1.39
2	B	802	ZI3	C18-C19	4.44	1.46	1.38
2	A	801	ZI3	C18-C19	4.42	1.46	1.38
2	B	802	ZI3	C28-C29	3.92	1.47	1.38
2	A	801	ZI3	C28-C29	3.76	1.46	1.38
2	C	801	ZI3	C21-C19	3.72	1.45	1.38
2	C	801	ZI3	C28-C29	3.55	1.46	1.38
2	C	801	ZI3	C27-C12	3.47	1.45	1.39
2	B	802	ZI3	C21-C19	3.25	1.44	1.38
2	C	801	ZI3	C30-C11	3.17	1.56	1.51
2	A	801	ZI3	C21-C19	3.05	1.43	1.38
2	A	801	ZI3	C10-N9	2.94	1.46	1.41
2	B	802	ZI3	C10-N9	2.82	1.46	1.41
2	C	801	ZI3	C17-C16	2.74	1.43	1.39
2	B	802	ZI3	C27-C12	2.64	1.44	1.39
2	A	801	ZI3	C27-C12	2.58	1.44	1.39
2	C	801	ZI3	C10-N9	2.57	1.45	1.41
2	C	801	ZI3	C33-C8	2.56	1.55	1.51
2	C	801	ZI3	C28-C27	2.44	1.44	1.38
2	C	801	ZI3	C31-C32	2.25	1.58	1.51
2	B	802	ZI3	C17-C16	2.23	1.42	1.39
2	C	801	ZI3	C18-C17	2.22	1.42	1.38
2	C	801	ZI3	C22-C21	2.21	1.42	1.38
2	B	802	ZI3	C28-C27	2.19	1.43	1.38
2	A	801	ZI3	C28-C27	2.18	1.43	1.38
2	A	801	ZI3	C30-C11	2.16	1.55	1.51
2	A	801	ZI3	C17-C16	2.09	1.42	1.39
2	B	802	ZI3	C30-C11	2.03	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	ZI3	C31-C32	2.01	1.58	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	ZI3	O24-C25-C15	-9.73	87.89	91.63
2	A	801	ZI3	O24-C23-C15	-9.27	88.07	91.63
2	A	801	ZI3	O24-C25-C15	-9.27	88.07	91.63
2	B	802	ZI3	O24-C23-C15	-9.03	88.16	91.63
2	C	801	ZI3	O24-C23-C15	-5.55	89.49	91.63
2	C	801	ZI3	O24-C25-C15	-4.74	89.80	91.63
2	B	802	ZI3	C23-C15-N14	-3.92	104.83	114.57
2	C	801	ZI3	C23-C15-N14	-3.65	105.50	114.57
2	A	801	ZI3	C23-C15-N14	-3.51	105.83	114.57
2	A	801	ZI3	C25-O24-C23	-3.05	88.37	91.11
2	B	802	ZI3	C25-O24-C23	-2.94	88.48	91.11
2	A	801	ZI3	C17-C16-C15	-2.69	116.88	121.08
2	A	801	ZI3	C33-C8-N9	2.66	122.33	117.99
2	B	802	ZI3	C33-C8-N9	2.37	121.85	117.99
2	C	801	ZI3	C25-O24-C23	-2.37	88.98	91.11
2	B	802	ZI3	C17-C16-C15	-2.32	117.47	121.08
2	C	801	ZI3	C34-C33-C8	2.25	116.88	112.72
2	C	801	ZI3	C17-C16-C15	-2.20	117.65	121.08
2	A	801	ZI3	O26-C13-N14	-2.19	118.34	122.60
2	C	801	ZI3	C33-C8-N9	2.09	121.39	117.99
2	A	801	ZI3	O7-C8-N9	-2.06	118.66	121.66

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	ZI3	C34-C33-C8-N9
2	C	801	ZI3	C11-C12-C13-N14
2	C	801	ZI3	C11-C12-C13-O26
2	A	801	ZI3	C23-C15-N14-C13
2	B	802	ZI3	C23-C15-N14-C13
2	C	801	ZI3	C23-C15-N14-C13
3	B	801	EDO	O1-C1-C2-O2
2	C	801	ZI3	N14-C15-C16-C22
2	A	801	ZI3	C11-C12-C13-O26
2	C	801	ZI3	C34-C33-C8-O7
2	A	801	ZI3	C16-C15-N14-C13

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Mol	Chain	Res	Type	Atoms
2	B	802	ZI3	C16-C15-N14-C13

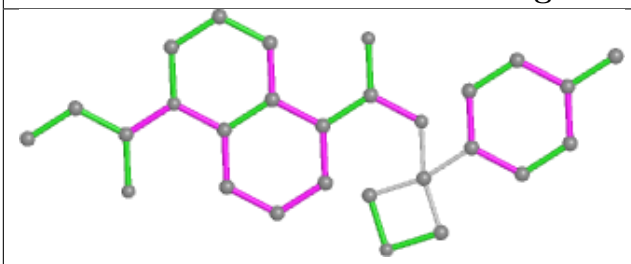
There are no ring outliers.

1 monomer is involved in 5 short contacts:

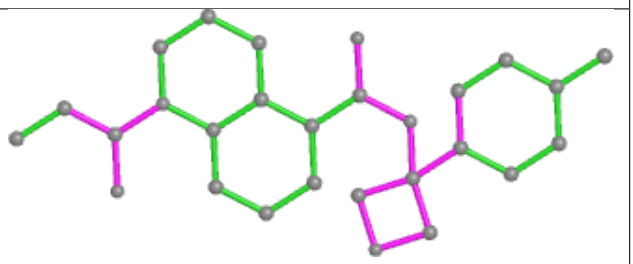
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	EDO	5	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

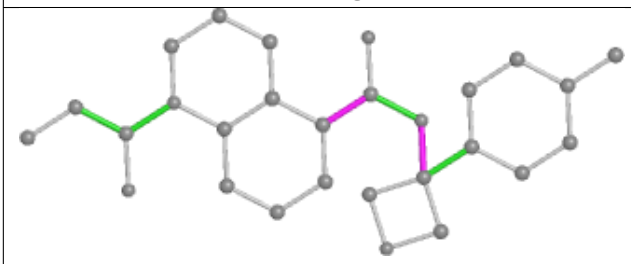
Ligand ZI3 A 801



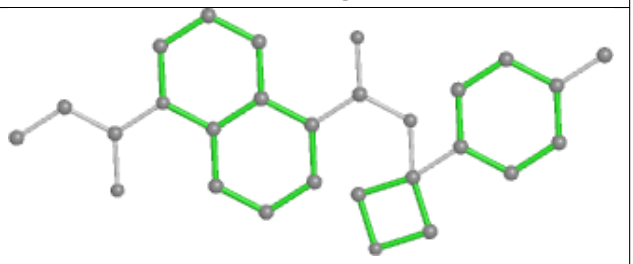
Bond lengths



Bond angles

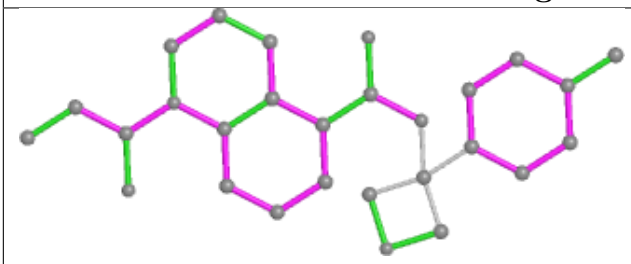


Torsions

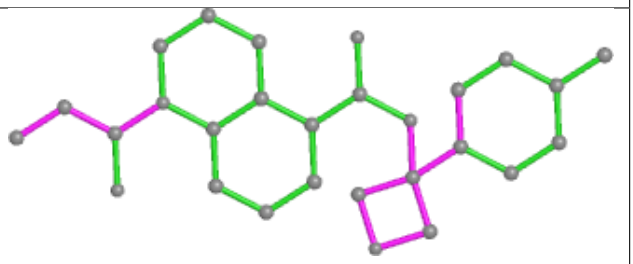


Rings

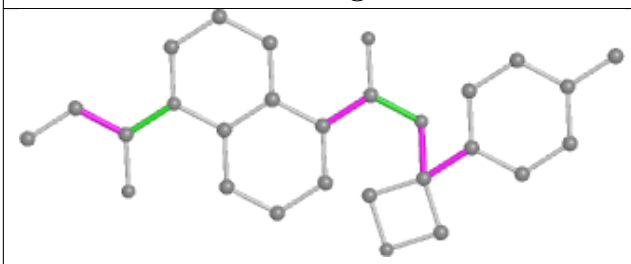
Ligand ZI3 C 801



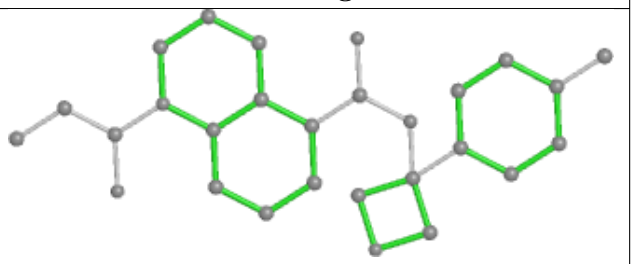
Bond lengths



Bond angles

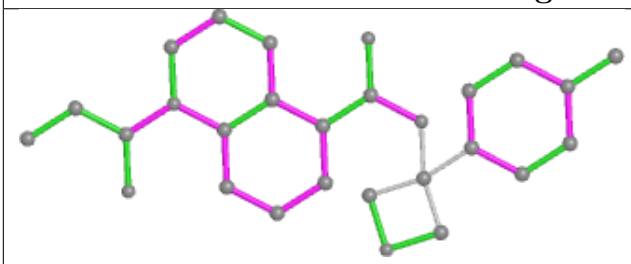


Torsions

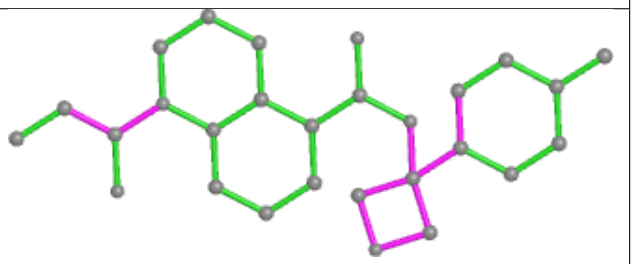


Rings

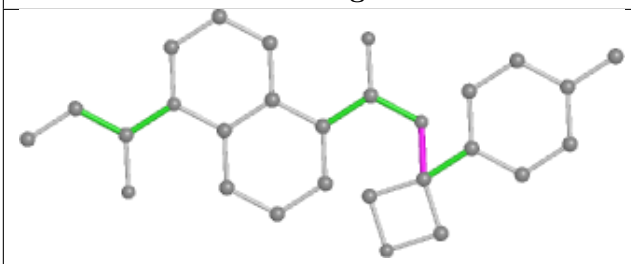
Ligand ZI3 B 802



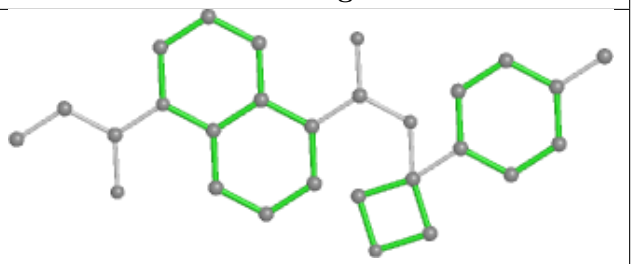
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	334/359 (93%)	0.03	4 (1%) 79 77	31, 45, 76, 102	0
1	B	334/359 (93%)	0.02	4 (1%) 79 77	31, 48, 76, 113	0
1	C	300/359 (83%)	3.60	215 (71%) 0 0	72, 98, 133, 150	0
All	All	968/1077 (89%)	1.13	223 (23%) 0 0	31, 54, 119, 150	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	518	SER	15.0
1	C	523	VAL	14.0
1	C	590	GLY	11.5
1	C	628	TYR	11.3
1	C	516	ALA	10.6
1	C	663	GLY	10.2
1	C	397	ILE	10.2
1	C	625	VAL	10.2
1	C	398	VAL	10.0
1	C	399	LEU	9.8
1	C	669	CYS	9.2
1	C	448	ILE	9.2
1	C	517	PRO	9.1
1	C	396	PHE	8.6
1	C	524	PRO	8.1
1	C	704	TRP	7.9
1	C	395	PRO	7.9
1	C	639	VAL	7.9
1	C	530	TRP	7.7
1	C	726	THR	7.5
1	C	629	SER	7.5
1	C	728	LEU	7.3
1	C	627	GLU	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	615	GLN	7.0
1	C	727	LEU	6.9
1	C	454	LEU	6.8
1	C	690	LEU	6.7
1	C	626	SER	6.7
1	C	665	TYR	6.7
1	C	667	LEU	6.5
1	C	649	VAL	6.5
1	C	630	LEU	6.5
1	C	611	GLY	6.4
1	C	515	ALA	6.4
1	C	661	SER	6.4
1	C	538	GLN	6.3
1	C	599	TYR	6.3
1	C	675	VAL	6.2
1	C	674	GLY	6.2
1	C	534	THR	6.2
1	C	512	CYS	6.2
1	C	452	PRO	6.1
1	C	430	GLY	6.1
1	C	712	THR	6.1
1	C	633	ASP	6.1
1	C	592	VAL	6.1
1	C	640	LEU	6.0
1	C	473	GLY	5.9
1	C	668	THR	5.9
1	C	662	GLU	5.9
1	C	613	PHE	5.9
1	C	670	SER	5.8
1	C	431	VAL	5.8
1	C	676	ILE	5.6
1	C	659	PHE	5.6
1	C	694	GLY	5.6
1	C	677	TYR	5.4
1	C	497	ARG	5.4
1	C	453	LEU	5.4
1	C	571	ILE	5.3
1	C	570	VAL	5.2
1	C	725	THR	5.2
1	A	685	VAL	5.2
1	C	581	CYS	5.1
1	C	616	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	440	ILE	5.1
1	C	636	GLY	5.1
1	C	605	TYR	5.0
1	C	635	THR	5.0
1	C	585	TRP	5.0
1	C	691	SER	4.9
1	C	510	PHE	4.9
1	C	491	ILE	4.9
1	C	713	CYS	4.8
1	C	637	PRO	4.8
1	C	527	LEU	4.8
1	C	477	LEU	4.8
1	C	541	PHE	4.8
1	C	587	ALA	4.7
1	C	400	GLY	4.7
1	C	441	MET	4.7
1	C	449	SER	4.7
1	C	614	ILE	4.7
1	C	610	ASP	4.7
1	C	631	PRO	4.6
1	C	519	LEU	4.6
1	C	603	THR	4.6
1	C	672	THR	4.6
1	C	514	ALA	4.6
1	C	437	PHE	4.6
1	C	698	PRO	4.6
1	C	692	LEU	4.5
1	C	568	ASP	4.5
1	C	573	LEU	4.5
1	C	711	GLY	4.5
1	C	589	TYR	4.5
1	C	600	ASP	4.5
1	C	664	ASN	4.4
1	C	438	ASN	4.4
1	C	509	SER	4.4
1	C	724	LEU	4.3
1	C	705	SER	4.3
1	C	693	GLY	4.3
1	C	588	HIS	4.3
1	C	657	PHE	4.2
1	C	575	ASP	4.2
1	C	419	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	485	ASN	4.2
1	C	451	SER	4.2
1	C	476	ARG	4.2
1	C	478	TYR	4.1
1	C	418	CYS	4.1
1	C	557	HIS	4.0
1	C	618	ILE	4.0
1	C	560	ASN	4.0
1	C	499	LEU	4.0
1	B	685	VAL	4.0
1	C	648	GLN	3.9
1	C	533	LYS	3.9
1	C	632	SER	3.9
1	C	511	VAL	3.9
1	C	593	TYR	3.9
1	C	715	THR	3.9
1	C	532	THR	3.8
1	C	461	LYS	3.8
1	C	470	SER	3.7
1	C	550	ILE	3.7
1	C	601	GLU	3.7
1	C	608	GLY	3.7
1	C	549	ALA	3.7
1	C	551	ASN	3.7
1	C	548	ILE	3.7
1	C	678	LYS	3.6
1	C	537	GLN	3.6
1	C	475	VAL	3.6
1	C	591	GLU	3.5
1	C	401	GLN	3.5
1	C	443	THR	3.5
1	C	706	THR	3.4
1	C	439	PRO	3.4
1	C	472	VAL	3.4
1	C	531	ASP	3.4
1	C	542	SER	3.4
1	C	696	ARG	3.3
1	C	602	ASN	3.3
1	C	666	MET	3.3
1	C	695	HIS	3.3
1	C	450	LYS	3.3
1	C	540	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	638	PHE	3.3
1	C	498	ILE	3.2
1	C	484	LYS	3.2
1	C	492	ASN	3.2
1	C	539	LEU	3.2
1	C	576	MET	3.2
1	C	434	VAL	3.2
1	C	612	LYS	3.2
1	C	442	GLN	3.2
1	C	580	GLU	3.2
1	C	506	ASN	3.2
1	C	607	ILE	3.2
1	C	567	ALA	3.1
1	C	420	GLY	3.1
1	C	409	SER	3.1
1	C	503	CYS	3.1
1	C	697	ALA	3.1
1	C	536	LYS	3.0
1	C	428	VAL	3.0
1	C	561	LEU	3.0
1	C	421	ARG	3.0
1	C	526	ARG	3.0
1	C	435	TRP	3.0
1	C	650	GLN	3.0
1	C	714	LEU	3.0
1	C	634	ALA	3.0
1	C	574	PHE	3.0
1	C	487	CYS	2.9
1	C	717	SER	2.9
1	C	569	GLY	2.9
1	C	508	ALA	2.9
1	C	579	HIS	2.9
1	C	411	ILE	2.8
1	C	480	THR	2.8
1	A	394	GLN	2.8
1	C	617	ASN	2.8
1	C	460	THR	2.8
1	C	412	MET	2.8
1	C	547	PRO	2.8
1	C	624	LYS	2.8
1	C	716	ALA	2.7
1	C	651	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	458	TRP	2.6
1	C	563	VAL	2.6
1	C	513	SER	2.6
1	C	660	ASP	2.6
1	C	436	SER	2.6
1	C	609	GLU	2.5
1	C	699	VAL	2.5
1	C	700	VAL	2.5
1	B	684	LYS	2.5
1	C	447	SER	2.4
1	C	496	PRO	2.4
1	A	492	ASN	2.4
1	C	469	GLY	2.4
1	B	655[A]	ARG	2.4
1	C	619	HIS	2.4
1	C	572	ARG	2.3
1	C	583	MET	2.3
1	C	719	ASP	2.3
1	C	671	ALA	2.3
1	B	492	ASN	2.2
1	A	687	GLU	2.2
1	C	426	LEU	2.2
1	C	427	ASP	2.2
1	C	445	ALA	2.2
1	C	702	VAL	2.1
1	C	528	LEU	2.1
1	C	404	TYR	2.1
1	C	564	THR	2.1
1	C	429	ASP	2.1
1	C	463	ASP	2.1
1	C	474	THR	2.1
1	C	488	GLU	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

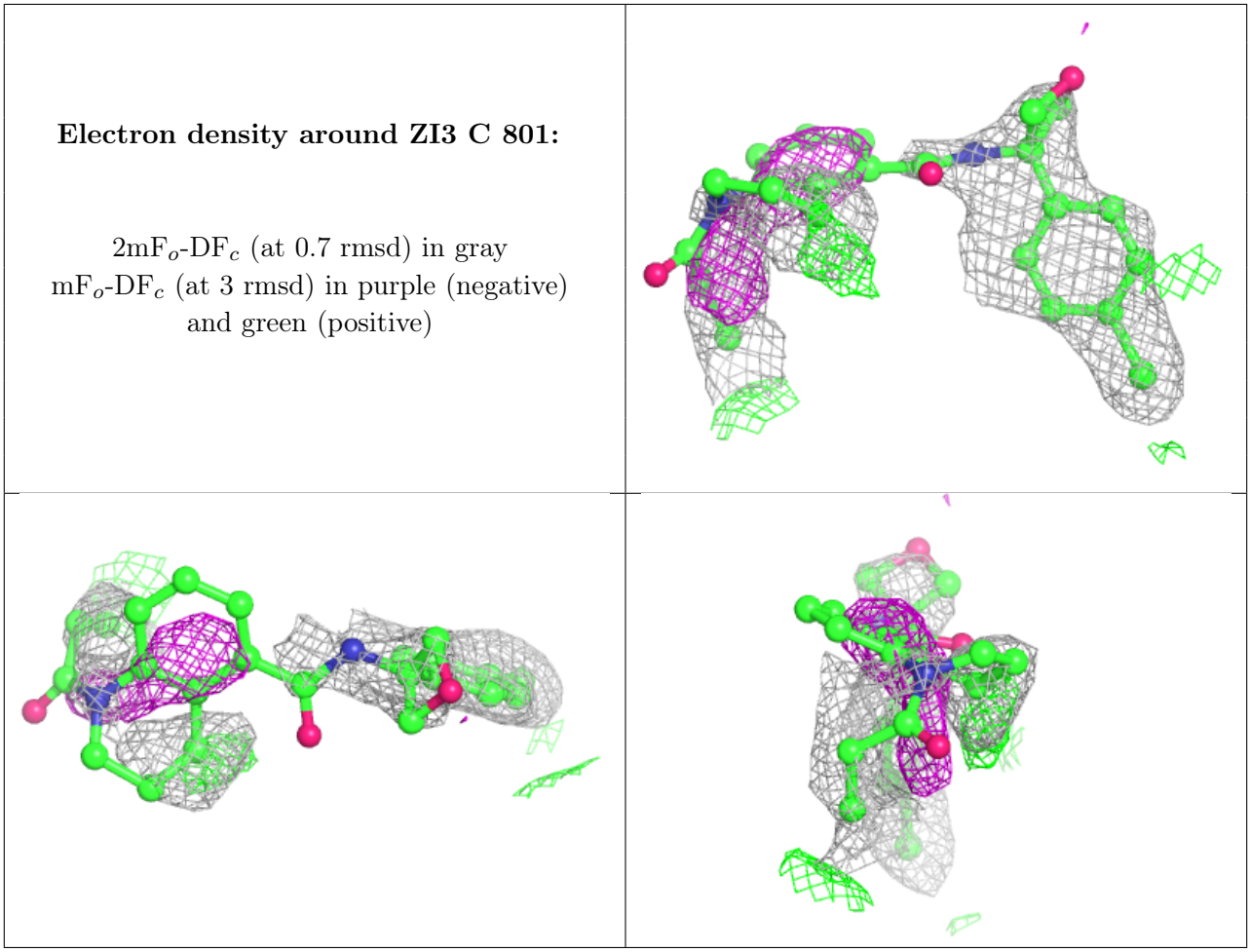
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ZI3	C	801	28/28	0.55	0.46	90,105,112,112	0
3	EDO	B	801	4/4	0.72	0.35	56,61,61,67	0
2	ZI3	A	801	28/28	0.96	0.15	54,61,69,71	0
2	ZI3	B	802	28/28	0.96	0.13	58,64,72,73	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.

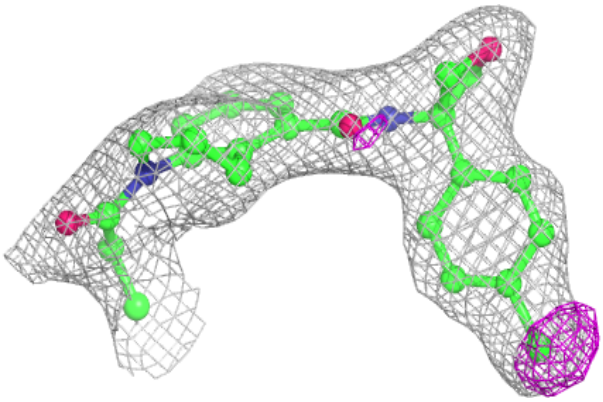
Electron density around ZI3 C 801:

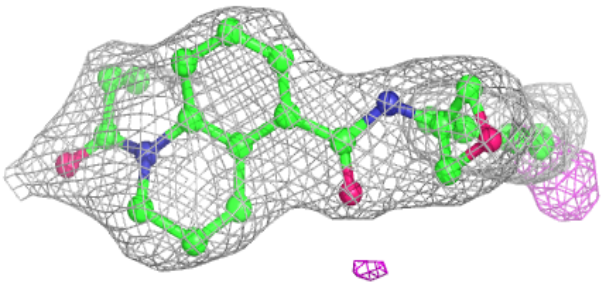
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

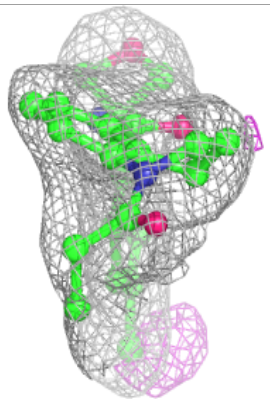


Electron density around ZI3 A 801:

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

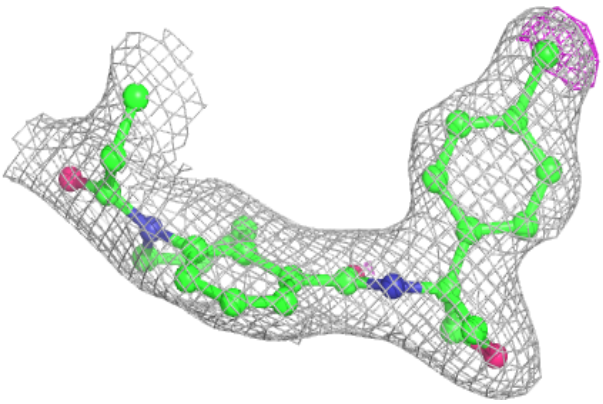


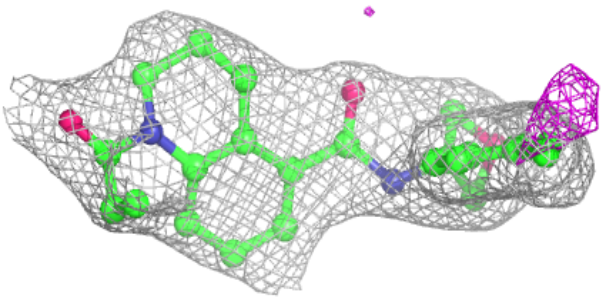


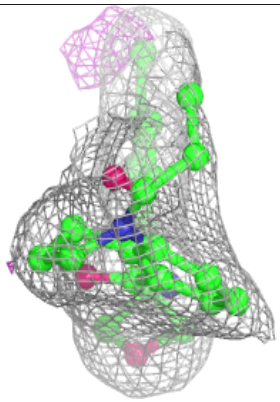


Electron density around ZI3 B 802:

$2mF_o$-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.