



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 AM UTC

PDB ID : 8T55 / pdb_00008t55
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

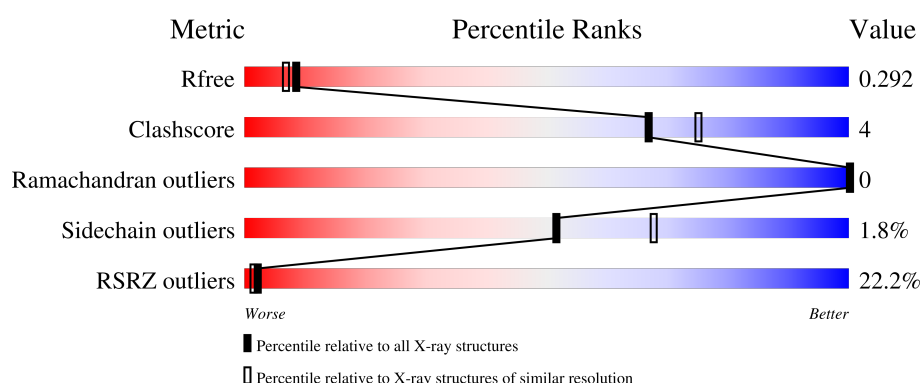
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	359	5% 86% 6% 7%
1	B	359	4% 84% 8% 7%
1	C	359	51% 74% 9% 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
3	EDO	B	801	-	-	X	-

2 Entry composition

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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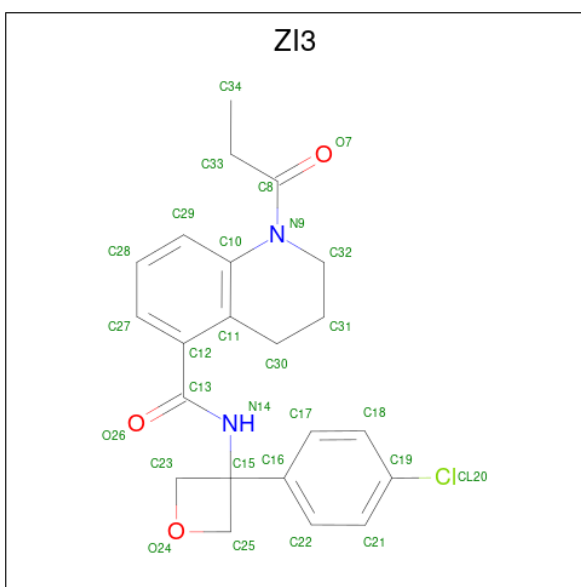
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP A4D1P6
A	?	-	ASP	deletion	UNP A4D1P6
A	?	-	ILE	deletion	UNP A4D1P6
A	?	-	GLY	deletion	UNP A4D1P6
A	?	-	SER	deletion	UNP A4D1P6
A	?	-	LYS	deletion	UNP A4D1P6
A	?	-	GLY	deletion	UNP A4D1P6
A	?	-	MET	deletion	UNP A4D1P6
A	?	-	ASN	deletion	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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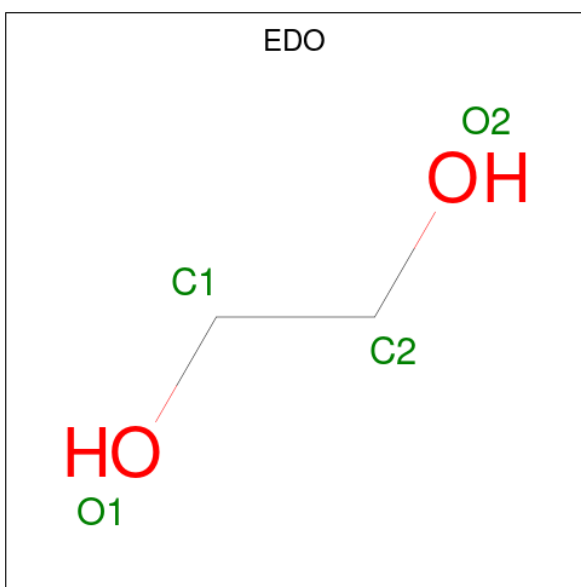
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP A4D1P6
C	374	MET	-	initiating methionine	UNP A4D1P6
C	375	HIS	-	expression tag	UNP A4D1P6
C	376	HIS	-	expression tag	UNP A4D1P6
C	377	HIS	-	expression tag	UNP A4D1P6
C	378	HIS	-	expression tag	UNP A4D1P6
C	379	HIS	-	expression tag	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 (CCD ID: 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		

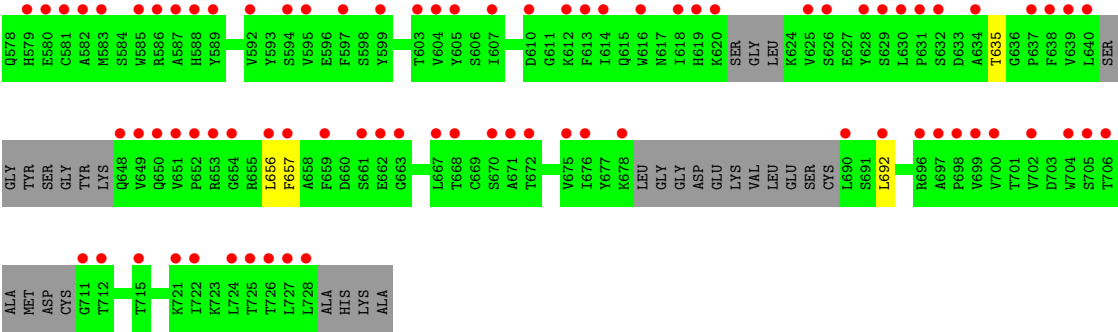
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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 111	O 111	0	0
4	B	118	Total 119	O 119	0	1
4	C	5	Total 5	O 5	0	0



4 Data and refinement statistics

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 38.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.78-2.20) 97.8 (38.78-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.20Å)	Xtrriage
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 (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: ZI3, 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	1.01	0/2581	1.20	1/3505 (0.0%)
1	B	1.00	0/2577	1.21	0/3501
1	C	1.17	0/2199	1.29	0/2988
All	All	1.06	0/7357	1.23	1/9994 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	487	CYS	CB-CA-C	-5.27	99.25	109.68

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	2529	0	2408	12	0
1	B	2525	0	2398	23	0
1	C	2158	0	1954	19	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
3	B	4	0	6	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	52	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 4.

All (52) 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:A:412:MET:HE1	1:A:454:LEU:HA	1.90	0.54
1:C:438:ASN:ND2	1:C:439:PRO:HA	2.23	0.54
1:A:456:LEU:C	1:A:456:LEU:HD23	2.32	0.53
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:B:456:LEU:C	1:B:456:LEU:HD23	2.36	0.50
1:B:583:MET:HE1	1:B:618:ILE:O	2.11	0.49
1:B:558:ASN:HD22	1:B:558:ASN:C	2.19	0.49
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: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:C:412:MET:HE1	1:C:454:LEU:HA	1.96	0.46
1:B:399:LEU:HD12	1:B:726:THR:HG22	1.98	0.46
1:A:544:ASP:CG	1:A:545:PRO:HA	2.41	0.45
1:C:562:LEU:HB3	1:C:576:MET:HE3	1.98	0.45
1:C:414:CYS:O	1:C:414:CYS:SG	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:544:ASP:CG	1:B:545:PRO:HA	2.43	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
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:583:MET:HE1	1:A:618:ILE:O	2.19	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:412:MET:HE1	1:B:454:LEU:HA	2.01	0.42
1:B:418:CYS:SG	1:B:460:THR:HA	2.59	0.41
1:C:456:LEU:C	1:C:456:LEU:HD23	2.46	0.41
1:B:522:GLN:HG3	1:C:405:GLY:C	2.45	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	950/1077 (88%)	915 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	263/305 (86%)	259 (98%)	4 (2%)	57	73
1	B	261/305 (86%)	257 (98%)	4 (2%)	57	73
1	C	203/305 (67%)	198 (98%)	5 (2%)	42	56
All	All	727/915 (80%)	714 (98%)	13 (2%)	51	68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	LEU
1	A	495	MET
1	A	518	SER
1	A	657	PHE
1	B	402	GLU
1	B	456	LEU
1	B	558	ASN
1	B	657	PHE
1	C	432	ILE
1	C	442	GLN
1	C	465	LEU
1	C	657	PHE
1	C	692	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	GLN
1	B	490	ASN
1	B	558	ASN
1	C	438	ASN
1	C	557	HIS

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 oligosaccharides 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	0.15	0
2	ZI3	B	802	1	31,31,31	4.17	17 (54%)	33,45,45	1.39	4 (12%)
2	ZI3	C	801	1	31,31,31	4.32	20 (64%)	33,45,45	1.22	5 (15%)
2	ZI3	A	801	1	31,31,31	4.20	17 (54%)	33,45,45	1.49	6 (18%)

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	B	802	1	-	3/21/39/39	0/4/4/4
2	ZI3	C	801	1	-	7/21/39/39	0/4/4/4
2	ZI3	A	801	1	-	4/21/39/39	0/4/4/4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	ZI3	C25-C15	-9.56	1.45	1.54
2	A	801	ZI3	C25-C15	-9.43	1.45	1.54
2	C	801	ZI3	C8-N9	9.40	1.50	1.36
2	B	802	ZI3	C8-N9	9.26	1.50	1.36
2	A	801	ZI3	C8-N9	9.17	1.49	1.36
2	C	801	ZI3	C25-C15	-9.14	1.45	1.54
2	B	802	ZI3	C23-C15	-8.80	1.45	1.54
2	A	801	ZI3	C23-C15	-8.68	1.46	1.54
2	C	801	ZI3	C23-C15	-7.82	1.46	1.54
2	C	801	ZI3	C12-C11	7.24	1.54	1.40
2	C	801	ZI3	C13-N14	7.21	1.47	1.34
2	A	801	ZI3	C12-C11	6.66	1.53	1.40
2	C	801	ZI3	C22-C16	6.64	1.50	1.39
2	B	802	ZI3	C13-N14	6.56	1.46	1.34
2	A	801	ZI3	C13-N14	6.54	1.46	1.34
2	A	801	ZI3	C22-C16	6.52	1.50	1.39
2	B	802	ZI3	C22-C16	6.40	1.50	1.39
2	B	802	ZI3	C12-C11	6.21	1.52	1.40
2	C	801	ZI3	C29-C10	6.07	1.49	1.39
2	A	801	ZI3	C29-C10	5.87	1.48	1.39
2	B	802	ZI3	C29-C10	5.79	1.48	1.39
2	C	801	ZI3	C18-C19	5.62	1.48	1.38
2	A	801	ZI3	C15-C16	-5.26	1.46	1.53
2	B	802	ZI3	C28-C29	4.83	1.47	1.38
2	B	802	ZI3	C15-C16	-4.70	1.47	1.53
2	A	801	ZI3	C28-C29	4.64	1.46	1.38
2	B	802	ZI3	C18-C19	4.57	1.46	1.38
2	A	801	ZI3	C18-C19	4.55	1.46	1.38
2	C	801	ZI3	C28-C29	4.38	1.46	1.38
2	C	801	ZI3	C15-C16	-4.11	1.48	1.53
2	C	801	ZI3	C21-C19	3.83	1.45	1.38
2	C	801	ZI3	C27-C12	3.61	1.45	1.39
2	B	802	ZI3	C21-C19	3.34	1.44	1.38
2	C	801	ZI3	C30-C11	3.30	1.56	1.51
2	A	801	ZI3	C21-C19	3.13	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ZI3	C28-C27	3.01	1.44	1.38
2	A	801	ZI3	C10-N9	2.98	1.46	1.41
2	B	802	ZI3	C10-N9	2.85	1.46	1.41
2	B	802	ZI3	C27-C12	2.73	1.44	1.39
2	B	802	ZI3	C28-C27	2.70	1.43	1.38
2	A	801	ZI3	C28-C27	2.70	1.43	1.38
2	A	801	ZI3	C27-C12	2.68	1.44	1.39
2	C	801	ZI3	C33-C8	2.64	1.55	1.51
2	C	801	ZI3	C10-N9	2.60	1.45	1.41
2	C	801	ZI3	C17-C16	2.59	1.43	1.39
2	C	801	ZI3	C18-C17	2.47	1.42	1.38
2	C	801	ZI3	C22-C21	2.45	1.42	1.38
2	C	801	ZI3	C31-C32	2.31	1.58	1.51
2	A	801	ZI3	C30-C11	2.25	1.55	1.51
2	B	802	ZI3	C30-C11	2.11	1.54	1.51
2	B	802	ZI3	C17-C16	2.10	1.42	1.39
2	B	802	ZI3	C31-C32	2.06	1.58	1.51
2	A	801	ZI3	C33-C8	2.04	1.54	1.51
2	A	801	ZI3	C31-C32	2.02	1.57	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	ZI3	C11-C10-N9	-3.65	115.50	118.58
2	A	801	ZI3	C25-O24-C23	-3.31	88.37	91.35
2	B	802	ZI3	C25-O24-C23	-3.19	88.48	91.35
2	A	801	ZI3	C11-C10-N9	-3.17	115.90	118.58
2	A	801	ZI3	C17-C16-C15	-2.86	116.88	121.09
2	A	801	ZI3	C30-C11-C10	-2.82	114.29	120.90
2	B	802	ZI3	C30-C11-C10	-2.66	114.67	120.90
2	C	801	ZI3	C25-O24-C23	-2.63	88.98	91.35
2	C	801	ZI3	C11-C10-N9	-2.49	116.48	118.58
2	B	802	ZI3	C17-C16-C15	-2.46	117.47	121.09
2	C	801	ZI3	C34-C33-C8	2.39	116.88	112.69
2	C	801	ZI3	C17-C16-C15	-2.33	117.65	121.09
2	A	801	ZI3	O7-C8-N9	-2.18	118.66	121.70
2	A	801	ZI3	O26-C13-N14	-2.16	118.34	122.59
2	C	801	ZI3	C30-C11-C10	-2.13	115.92	120.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	C	801	ZI3	C34-C33-C8-N9
3	B	801	EDO	O1-C1-C2-O2
2	A	801	ZI3	C16-C15-N14-C13
2	B	802	ZI3	C16-C15-N14-C13
2	C	801	ZI3	N14-C15-C16-C22
2	C	801	ZI3	C34-C33-C8-O7
2	A	801	ZI3	C11-C12-C13-O26
2	B	802	ZI3	C25-C15-C16-C22
2	C	801	ZI3	C23-C15-C16-C22
2	A	801	ZI3	C25-C15-N14-C13

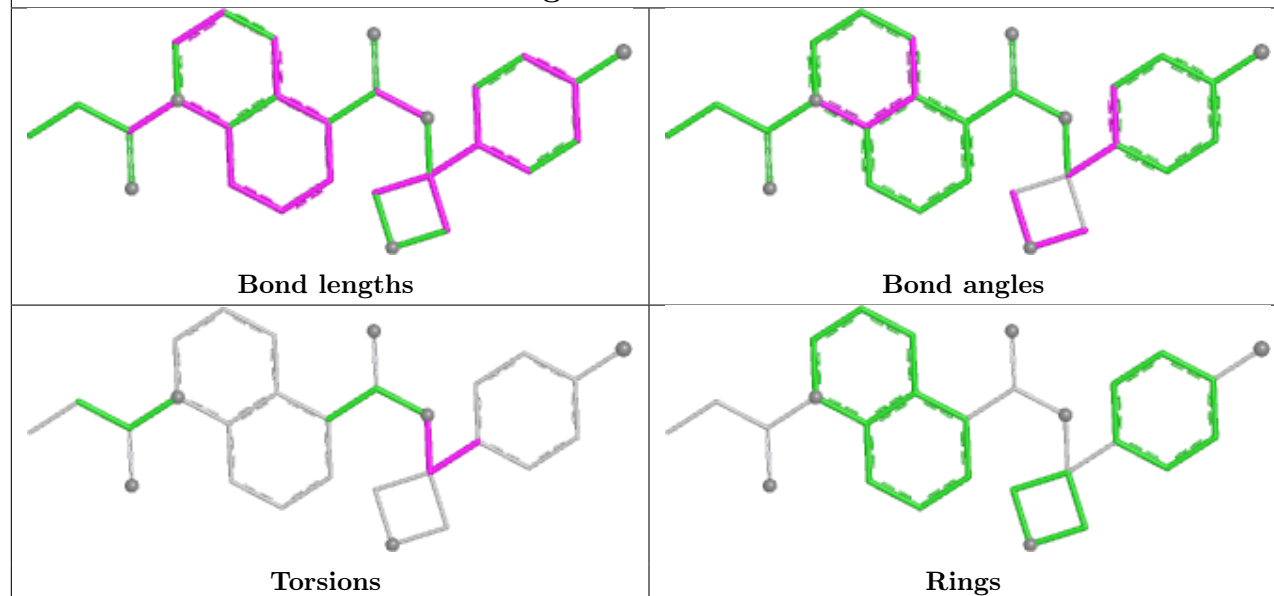
There are no ring outliers.

1 monomer is involved in 5 short contacts:

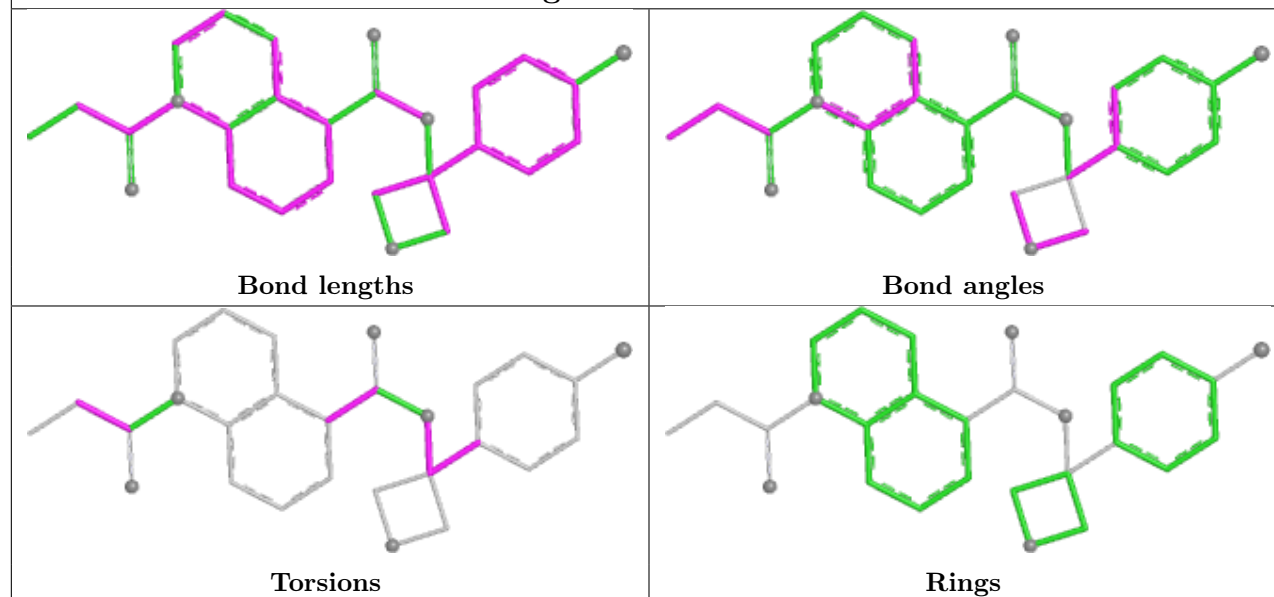
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	EDO	5	0

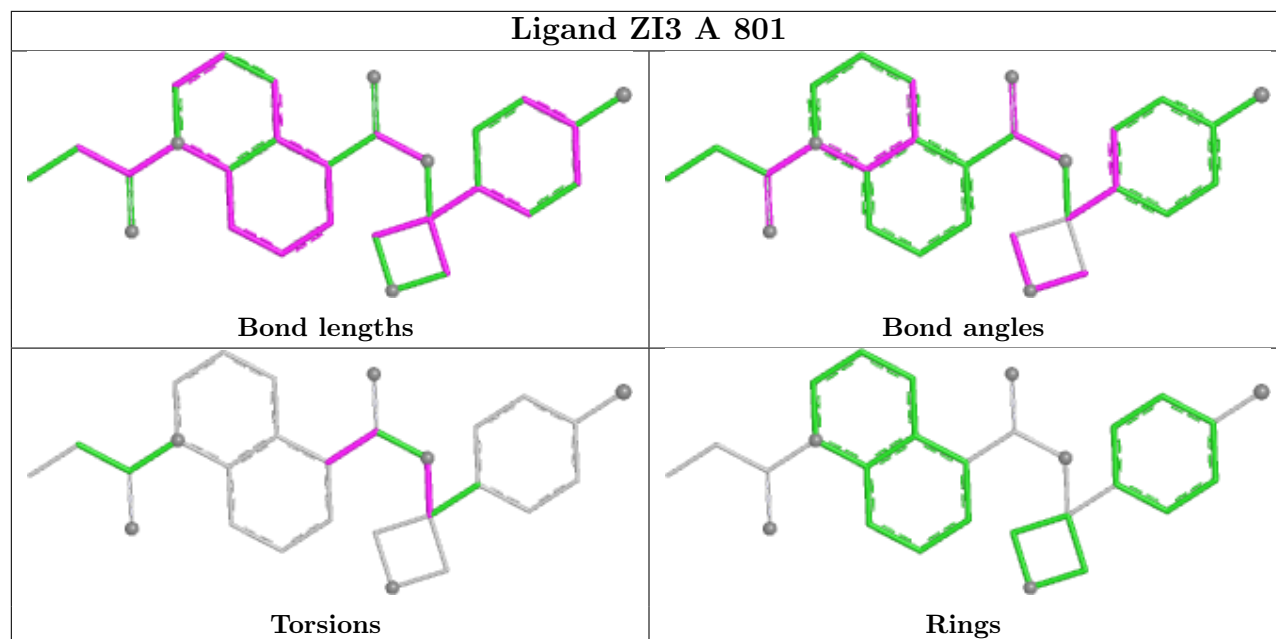
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Ligand ZI3 B 802



Ligand ZI3 C 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	334/359 (93%)	0.21	17 (5%)	33 30	19, 45, 76, 102	3 (0%)
1	B	334/359 (93%)	0.29	15 (4%)	38 35	20, 48, 76, 113	3 (0%)
1	C	300/359 (83%)	2.42	183 (61%)	0 0	72, 98, 133, 150	0
All	All	968/1077 (89%)	0.92	215 (22%)	2 1	19, 54, 119, 150	6 (0%)

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	706	THR	6.2
1	C	448	ILE	6.2
1	C	542	SER	6.1
1	C	519	LEU	5.9
1	C	651	VAL	5.7
1	C	518	SER	5.0
1	C	690	LEU	5.0
1	C	431	VAL	4.9
1	C	547	PRO	4.8
1	C	453	LEU	4.8
1	C	634	ALA	4.8
1	C	620	LYS	4.8
1	C	607	ILE	4.7
1	C	589	TYR	4.6
1	C	477	LEU	4.6
1	C	492	ASN	4.6
1	C	517	PRO	4.6
1	C	499	LEU	4.5
1	C	491	ILE	4.5
1	C	428	VAL	4.4
1	C	489	ILE	4.4
1	C	568	ASP	4.4
1	C	516	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	454	LEU	4.2
1	C	573	LEU	4.2
1	C	524	PRO	4.2
1	C	563	VAL	4.2
1	C	672	THR	4.2
1	A	644	SER	4.1
1	C	422	ARG	4.1
1	C	511	VAL	4.1
1	B	644	SER	4.0
1	C	452	PRO	4.0
1	C	475	VAL	4.0
1	C	440	ILE	4.0
1	C	656	LEU	3.9
1	C	661	SER	3.9
1	C	418	CYS	3.9
1	C	613	PHE	3.9
1	C	618	ILE	3.9
1	C	523	VAL	3.8
1	C	582	ALA	3.8
1	C	548	ILE	3.8
1	C	595	VAL	3.8
1	C	625	VAL	3.8
1	C	465	LEU	3.7
1	C	581	CYS	3.7
1	C	450	LYS	3.7
1	C	510	PHE	3.6
1	C	539	LEU	3.6
1	C	652	PRO	3.6
1	C	649	VAL	3.6
1	C	675	VAL	3.6
1	C	585	TRP	3.6
1	C	727	LEU	3.5
1	C	728	LEU	3.5
1	C	423	VAL	3.5
1	C	671	ALA	3.5
1	C	711	GLY	3.5
1	C	434	VAL	3.5
1	C	484	LYS	3.5
1	C	397	ILE	3.5
1	C	704	TRP	3.5
1	C	398	VAL	3.4
1	B	519	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	586	ARG	3.4
1	B	680	GLY	3.4
1	C	612	LYS	3.4
1	C	557	HIS	3.3
1	C	640	LEU	3.3
1	C	571	ILE	3.3
1	C	700	VAL	3.3
1	C	724	LEU	3.3
1	C	657	PHE	3.3
1	C	468	LEU	3.2
1	C	459	ALA	3.2
1	C	639	VAL	3.2
1	C	653	ARG	3.2
1	A	519	LEU	3.2
1	C	538	GLN	3.2
1	C	599	TYR	3.2
1	A	680	GLY	3.2
1	C	530	TRP	3.2
1	C	498	ILE	3.2
1	C	692	LEU	3.2
1	A	491	ILE	3.2
1	C	495	MET	3.2
1	C	525	GLY	3.1
1	C	614	ILE	3.1
1	C	697	ALA	3.1
1	C	536	LYS	3.1
1	B	643	TYR	3.0
1	C	458	TRP	3.0
1	C	662	GLU	3.0
1	C	650	GLN	3.0
1	C	570	VAL	3.0
1	C	629	SER	3.0
1	B	628	TYR	3.0
1	C	562	LEU	2.9
1	B	686	LEU	2.9
1	C	577	GLN	2.9
1	B	491	ILE	2.9
1	C	411	ILE	2.9
1	C	630	LEU	2.9
1	C	564	THR	2.9
1	C	616	TRP	2.9
1	C	402	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	594	SER	2.8
1	C	628	TYR	2.8
1	C	659	PHE	2.8
1	C	587	ALA	2.8
1	C	597	PHE	2.8
1	C	676	ILE	2.8
1	C	490	ASN	2.8
1	C	560	ASN	2.8
1	C	663	GLY	2.8
1	C	670	SER	2.8
1	C	605	TYR	2.8
1	C	405	GLY	2.8
1	C	396	PHE	2.8
1	C	486	LEU	2.7
1	A	709	ASP	2.7
1	C	610	ASP	2.7
1	C	451	SER	2.7
1	C	583	MET	2.7
1	A	686	LEU	2.7
1	A	687	GLU	2.7
1	C	512	CYS	2.7
1	C	482	ALA	2.7
1	A	685	VAL	2.7
1	C	550	ILE	2.7
1	C	501	LEU	2.7
1	B	645	GLY	2.6
1	C	432	ILE	2.6
1	C	469	GLY	2.6
1	A	628	TYR	2.6
1	C	527	LEU	2.6
1	B	685	VAL	2.6
1	C	722	ILE	2.6
1	B	687	GLU	2.6
1	A	493	ASP	2.6
1	C	575	ASP	2.6
1	C	480	THR	2.5
1	B	448[A]	ILE	2.5
1	C	654	GLY	2.5
1	C	698	PRO	2.5
1	C	712	THR	2.5
1	A	521	SER	2.5
1	C	626	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	709	ASP	2.5
1	C	526	ARG	2.5
1	C	592	VAL	2.5
1	C	699	VAL	2.5
1	C	487	CYS	2.4
1	C	532	THR	2.4
1	C	696	ARG	2.4
1	C	725	THR	2.4
1	C	702	VAL	2.4
1	C	399	LEU	2.4
1	C	619	HIS	2.4
1	A	432	ILE	2.4
1	C	637	PRO	2.4
1	C	447	SER	2.4
1	C	632	SER	2.4
1	C	483	LYS	2.4
1	B	684	LYS	2.3
1	C	678	LYS	2.3
1	C	604	VAL	2.3
1	C	648	GLN	2.3
1	C	502	ALA	2.3
1	C	412	MET	2.3
1	C	668	THR	2.3
1	C	715	THR	2.3
1	C	455	SER	2.3
1	C	705	SER	2.3
1	C	426	LEU	2.3
1	C	496	PRO	2.3
1	C	478	TYR	2.3
1	C	514	ALA	2.3
1	C	534	THR	2.3
1	C	579	HIS	2.3
1	C	638	PHE	2.3
1	C	721	LYS	2.3
1	A	642	GLY	2.3
1	C	553	THR	2.3
1	C	726	THR	2.3
1	C	509	SER	2.3
1	C	533	LYS	2.3
1	C	500	SER	2.2
1	A	490	ASN	2.2
1	C	421	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	ASN	2.2
1	C	588	HIS	2.2
1	C	456	LEU	2.2
1	C	503	CYS	2.2
1	C	437	PHE	2.1
1	B	430	GLY	2.1
1	C	603	THR	2.1
1	C	476	ARG	2.1
1	C	497	ARG	2.1
1	C	561	LEU	2.1
1	C	580	GLU	2.1
1	C	435	TRP	2.1
1	A	684	LYS	2.1
1	C	413	HIS	2.1
1	C	439	PRO	2.1
1	C	508	ALA	2.1
1	C	667	LEU	2.1
1	B	710	CYS	2.0
1	C	549	ALA	2.0
1	A	520	THR	2.0
1	C	425	SER	2.0
1	C	528	LEU	2.0
1	C	395	PRO	2.0
1	C	631	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

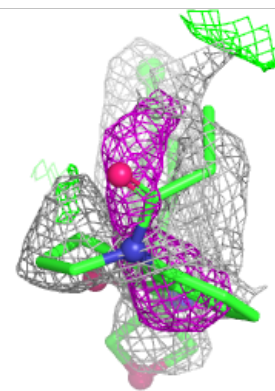
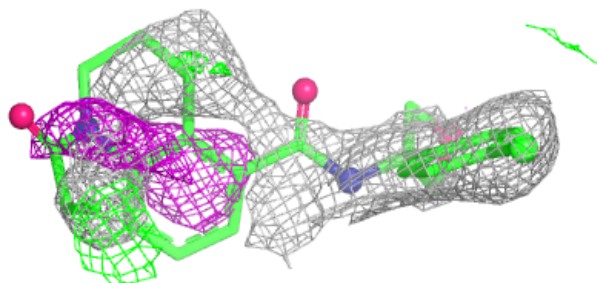
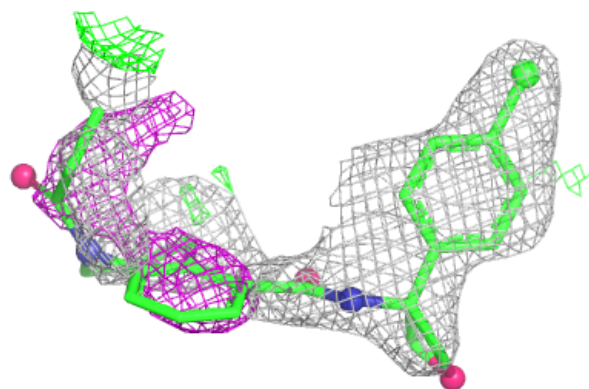
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZI3	C	801	28/28	0.66	0.22	90,105,112,112	0
3	EDO	B	801	4/4	0.87	0.28	56,61,61,67	0
2	ZI3	A	801	28/28	0.90	0.10	54,61,69,71	0
2	ZI3	B	802	28/28	0.90	0.10	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.

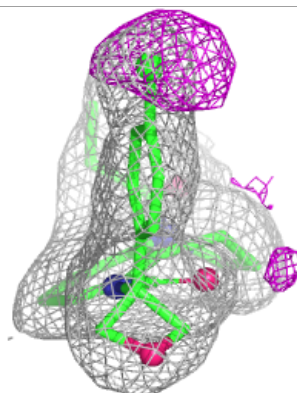
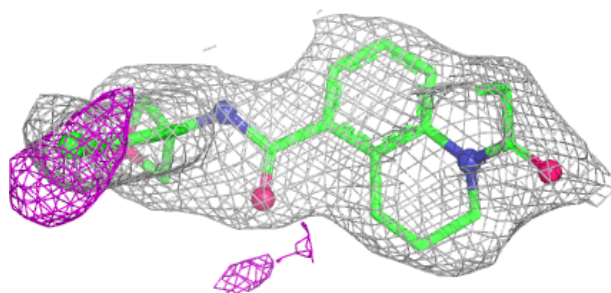
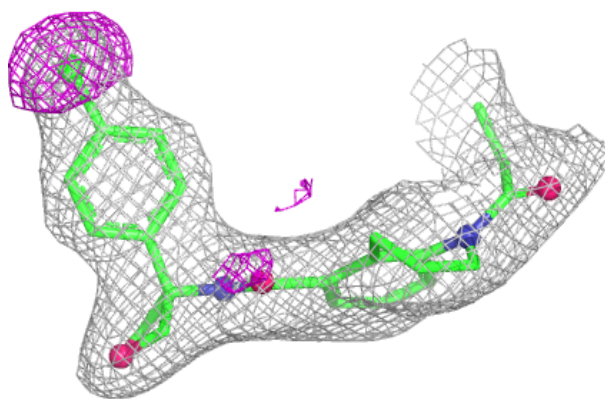
Electron density around ZI3 C 801:

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

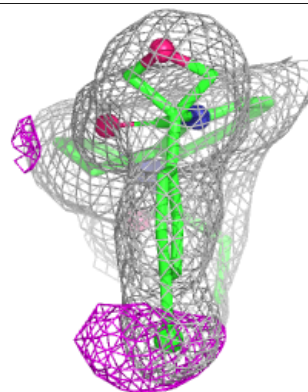
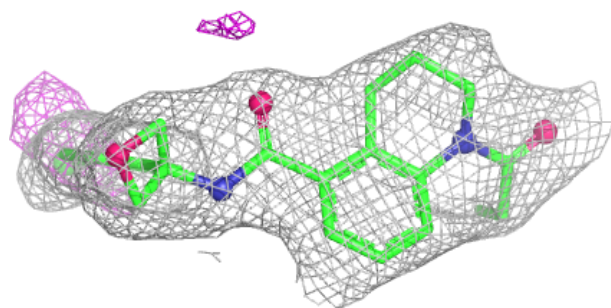
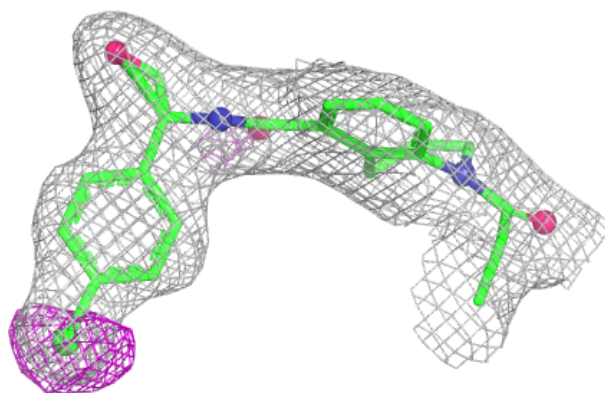


Electron density around ZI3 A 801:

$2mF_o-DF_c$ (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.