wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 07:30 AM EDT

PDB ID	:	4DWK
Title	:	Structure of cystein free insulin degrading enzyme with compound bdm41671 ((s)-2-{2-[carboxymethyl-(3-phenyl-propyl)-amino]-acetylamino}-3-(1h-imidazol-4-yl)-propionic acid methyl ester)
Authors	:	Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on	:	2012-02-24
Resolution	:	3.00 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 (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 (i)) were used in the production of this report:

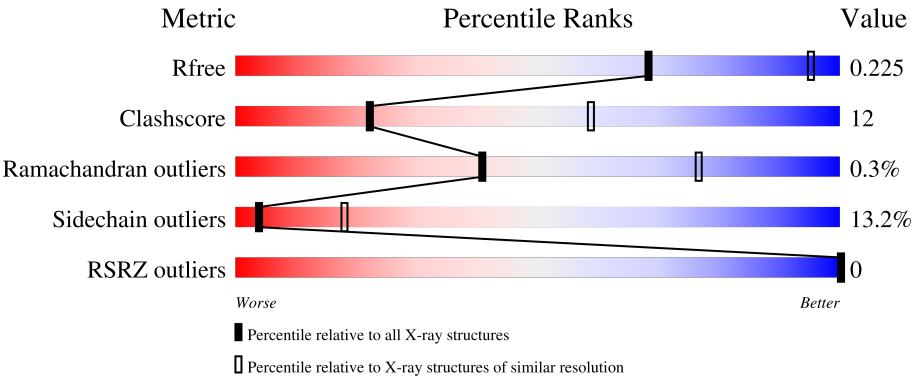
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	990	68% 23% 5% ·
1	B	990	63% 28% 5% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15764 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	955	Total	C	N	O	S	0	0	0
			7802	5026	1310	1443	23			
1	B	955	Total	C	N	O	S	0	0	0
			7796	5023	1309	1442	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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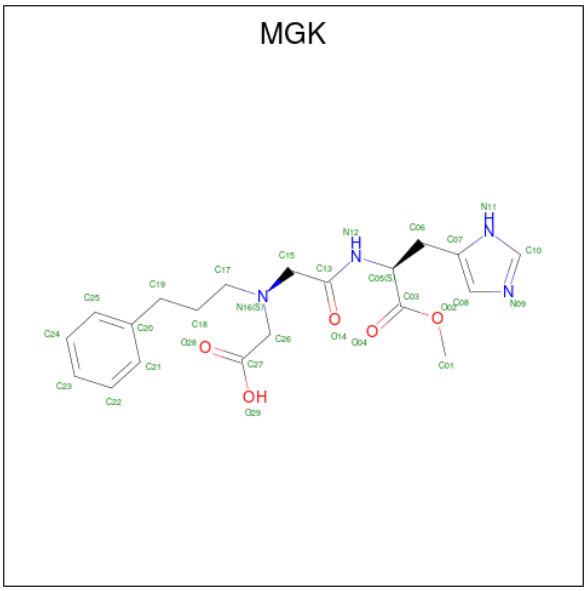
Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is methyl N-(carboxymethyl)-N-(3-phenylpropyl)glycyl-L-histidinate (three-letter code: MGK) (formula: $C_{20}H_{26}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 29 20 4 5	0	0
2	B	1	Total C N O 29 20 4 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is water.

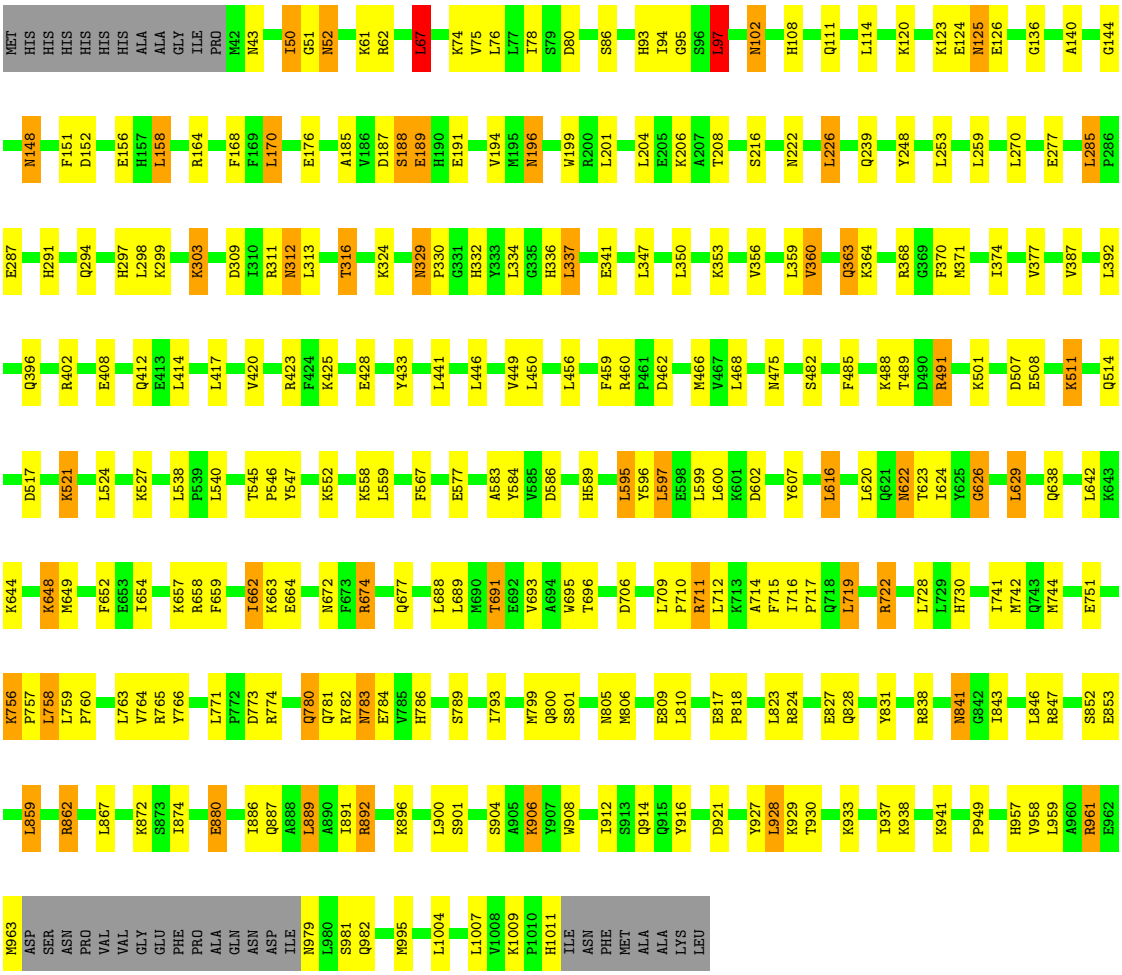
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	67	Total O 67 67	0	0
4	B	39	Total O 39 39	0	0

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.

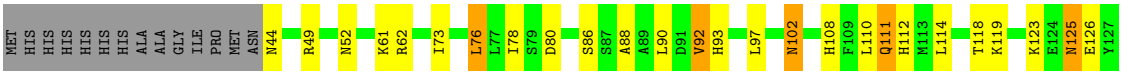
• Molecule 1: Insulin-degrading enzyme

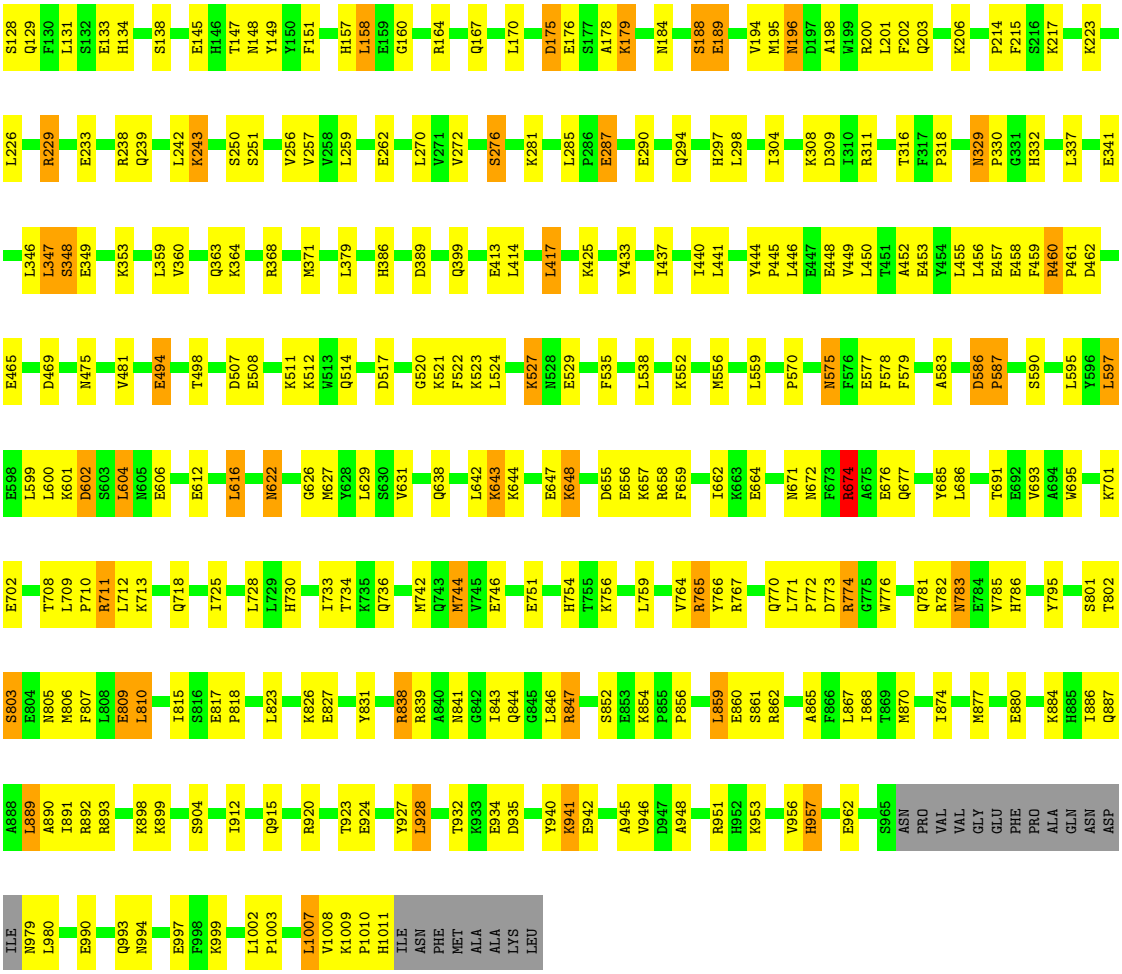
Chain A:



• Molecule 1: Insulin-degrading enzyme

Chain B:




S128 Q129 F130 L131 S132 E133 H134 S138 E145 H146 T147 N148 Y149 Y150 F151 H157 L158 E159 G160 R164 Q167 L170 D175 E176 S177 A178 K179 N184 S188 E189 V194 M195 N196 D197 A198 W199 R200 L201 F202 Q203 K206 P214 F215 S216 K217 K223
L226 R229 E233 R238 Q239 L242 K243 S250 S251 V256 V257 V258 L259 E262 L270 V271 V272 S276 K281 L285 P286 E287 E290 Q294 H297 L298 I304 K308 D309 I310 R311 T316 F317 P318 N329 P330 G331 H332 L337 E341
L346 L347 S348 E349 K353 L359 V360 Q363 K364 R368 M371 L379 H386 D389 Q399 E413 L414 L417 K425 Y433 I437 I440 L441 Y444 P445 L446 E447 E448 V449 L450 T451 A452 E453 Y454 L455 L456 E457 E458 F459 R460 P461 D462
E465 D469 N475 V481 E494 T498 D507 E508 K511 K512 W513 Q514 D517 G520 K521 F522 K523 L524 K527 N528 E529 F535 L538 K552 M556 L559 P570 N575 F576 E577 F578 F579 A583 D586 P587 S590 L595 Y596 L597
E598 L599 L600 K601 D602 S603 L604 N605 E606 E612 L616 N622 G626 M627 Y628 L629 S630 V631 Q638 L642 K643 K644 E647 K648 D655 E656 K657 R658 F659 I662 K663 E664 N671 N672 F673 R674 A675 E676 Q677 Y685 L686 T691 E692 V693 A694 W695 K701
E702 T708 L709 P710 R711 L712 K713 Q718 I725 L728 L729 H730 I733 T734 K735 Q736 M742 Q743 M744 V745 E746 E751 H754 T755 K756 L759 V764 R765 Y766 R767 Q770 L771 P772 D773 R774 G775 W776 Q781 R782 N783 E784 V785 H786 Y795 S801 T802
S803 E804 N805 M806 F807 L808 E809 L810 I815 S816 E817 P818 L823 K826 E827 Y831 R838 R839 A840 N841 G842 I843 Q844 G845 L846 R847 S852 E853 K854 P855 P856 L859 E860 S861 R862 A865 F866 L867 I868 T869 M870 I874 M877 E880 K884 H885 I886 Q887
A888 L889 A890 I891 R892 R893 K898 K899 S904 I912 Q915 R920 T923 E924 Y927 L928 T932 K933 E934 D935 Y940 K941 E942 A945 V946 D947 A948 R951 H952 K953 V956 H957 E962 S965 ASN PRO VAL VAL GLY GLU PHE PRO ALA GLN ASN ASP
ILE N979 L980 E990 Q993 N994 E997 F998 K999 L1002 P1003 L1007 V1008 K1009 P1010 H1011 ILE ASN PHE MET ALA ALA LYS LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	261.51Å 261.51Å 91.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 3.00 49.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.45-3.00) 99.5 (49.42-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.227 0.179 , 0.225	Depositor DCC
R_{free} test set	3628 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MGK, ZN

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	0.93	5/7996 (0.1%)	0.94	12/10817 (0.1%)
1	B	0.91	9/7990 (0.1%)	0.91	10/10810 (0.1%)
All	All	0.92	14/15986 (0.1%)	0.93	22/21627 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CG-CD	9.59	1.66	1.51
1	B	189	GLU	CG-CD	8.38	1.64	1.51
1	A	577	GLU	CG-CD	8.11	1.64	1.51
1	A	189	GLU	CB-CG	8.06	1.67	1.52
1	B	189	GLU	CD-OE1	7.16	1.33	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	GLU	OE1-CD-OE2	-13.54	107.06	123.30
1	A	50	ILE	CB-CA-C	-7.93	95.74	111.60
1	B	847	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	B	674	ARG	NE-CZ-NH1	6.80	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	GLU	CG-CD-OE2	6.75	131.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	979	ASN	Peptide
1	B	455	LEU	Peptide
1	B	979	ASN	Peptide

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	7802	0	7740	172	0
1	B	7796	0	7729	192	0
2	A	29	0	25	2	0
2	B	29	0	25	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	67	0	0	3	0
4	B	39	0	0	3	0
All	All	15764	0	15519	366	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 12.

The worst 5 of 366 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:B:341:GLU:HG2	1:B:347:LEU:HD12	1.34	1.05
1:B:774:ARG:HH11	1:B:774:ARG:HG3	1.24	1.00
1:A:50:ILE:O	1:A:50:ILE:HG22	1.61	0.99
1:A:622:ASN:HD22	1:A:622:ASN:H	1.03	0.96
1:A:622:ASN:H	1:A:622:ASN:ND2	1.62	0.95

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	951/990 (96%)	893 (94%)	55 (6%)	3 (0%)	41 76
1	B	951/990 (96%)	891 (94%)	57 (6%)	3 (0%)	41 76
All	All	1902/1980 (96%)	1784 (94%)	112 (6%)	6 (0%)	41 76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ASP
1	A	961	ARG
1	A	841	ASN
1	B	841	ASN
1	B	1010	PRO

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	848/879 (96%)	741 (87%)	107 (13%)	4 20
1	B	846/879 (96%)	730 (86%)	116 (14%)	3 17
All	All	1694/1758 (96%)	1471 (87%)	223 (13%)	4 18

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	ASN
1	B	1009	LYS
1	B	446	LEU
1	B	993	GLN
1	B	838	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	821	ASN
1	B	841	ASN
1	A	783	ASN
1	A	780	GLN
1	B	883	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\|>2$
2	MGK	B	1101	-	26,30,30	1.70	2 (7%)	32,38,38	1.74	6 (18%)
2	MGK	A	1101	-	26,30,30	1.60	2 (7%)	32,38,38	1.70	7 (21%)

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
2	MGK	B	1101	-	-	14/28/28/28	0/2/2/2
2	MGK	A	1101	-	-	16/28/28/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MGK	O02-C03	6.65	1.49	1.33
2	A	1101	MGK	O02-C03	6.47	1.49	1.33
2	B	1101	MGK	C26-N16	2.61	1.52	1.47
2	A	1101	MGK	C26-N16	2.15	1.51	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	MGK	O02-C03-C05	4.57	123.21	111.52
2	A	1101	MGK	O02-C03-C05	4.45	122.90	111.52
2	B	1101	MGK	C01-O02-C03	4.24	125.52	115.94
2	A	1101	MGK	C01-O02-C03	4.16	125.35	115.94
2	B	1101	MGK	C05-N12-C13	3.23	129.97	121.65

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MGK	C17-C18-C19-C20
2	A	1101	MGK	C03-C05-C06-C07
2	A	1101	MGK	C05-C06-C07-N11
2	B	1101	MGK	C13-C15-N16-C26
2	B	1101	MGK	N16-C26-C27-O29

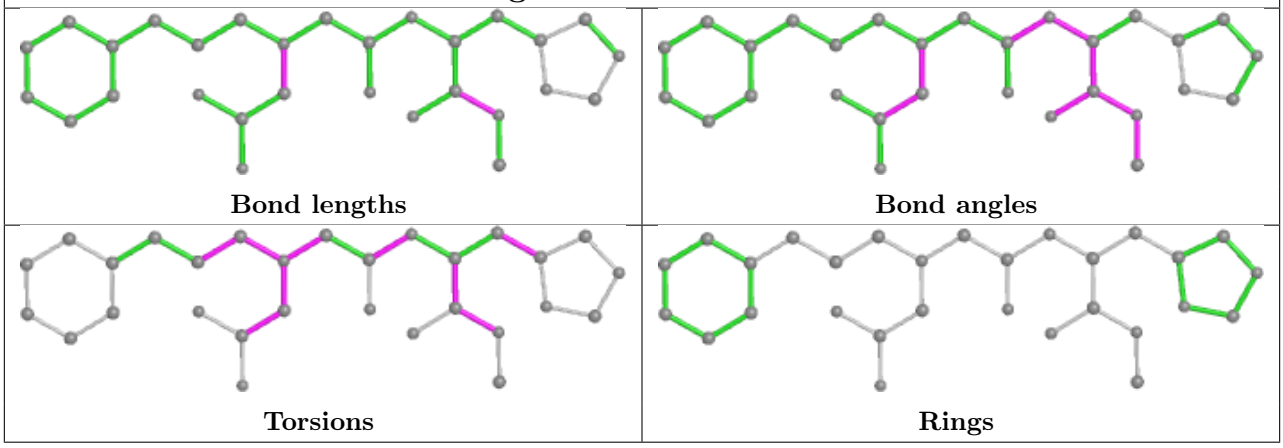
There are no ring outliers.

2 monomers are involved in 6 short contacts:

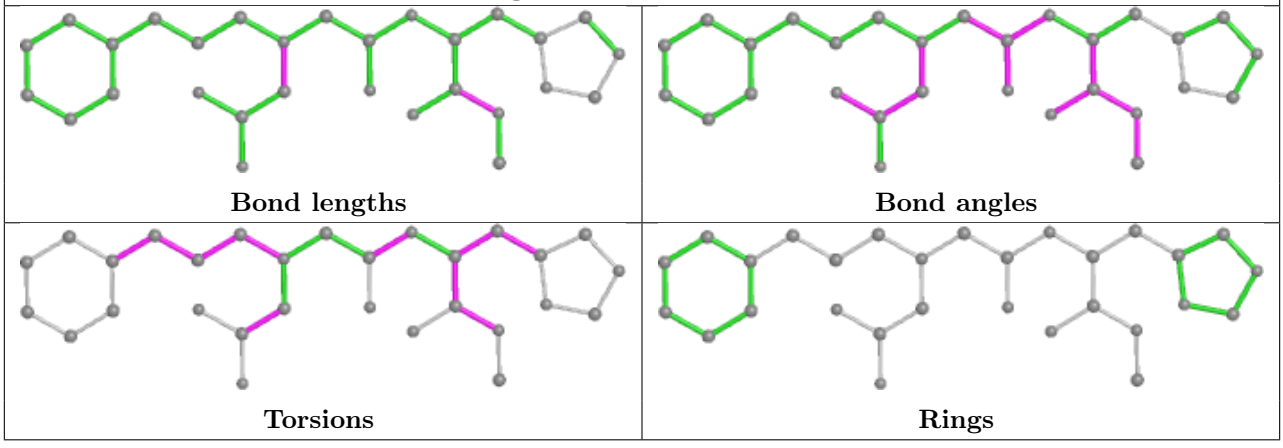
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	MGK	4	0
2	A	1101	MGK	2	0

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 MGK B 1101



Ligand MGK A 1101



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	955/990 (96%)	-0.59	0	100	100	19, 34, 50, 77	0
1	B	955/990 (96%)	-0.53	0	100	100	24, 38, 55, 75	0
All	All	1910/1980 (96%)	-0.56	0	100	100	19, 36, 52, 77	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no 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.

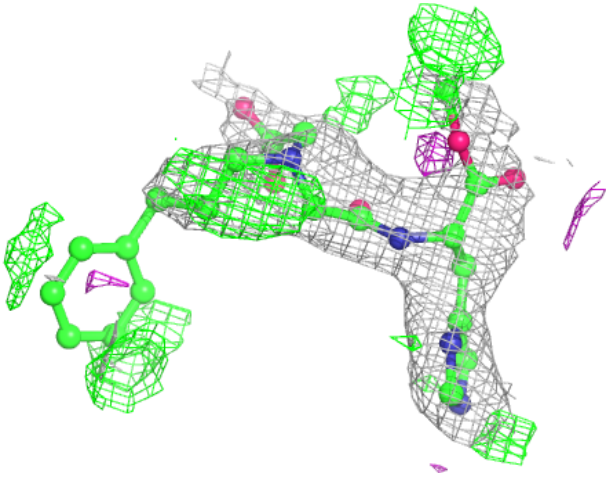
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MGK	B	1101	29/29	0.76	0.32	73,81,100,101	0
3	ZN	B	1102	1/1	0.87	0.21	2,2,2,2	0
2	MGK	A	1101	29/29	0.88	0.24	61,78,92,92	0
3	ZN	A	1102	1/1	0.95	0.23	2,2,2,2	0

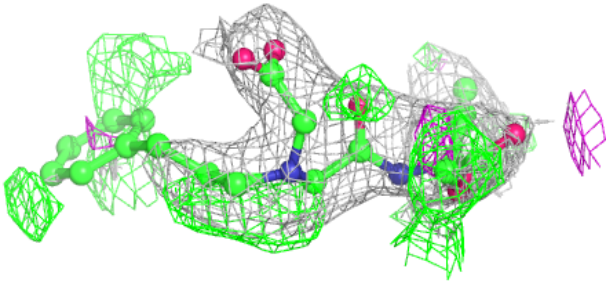
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 MGK B 1101:

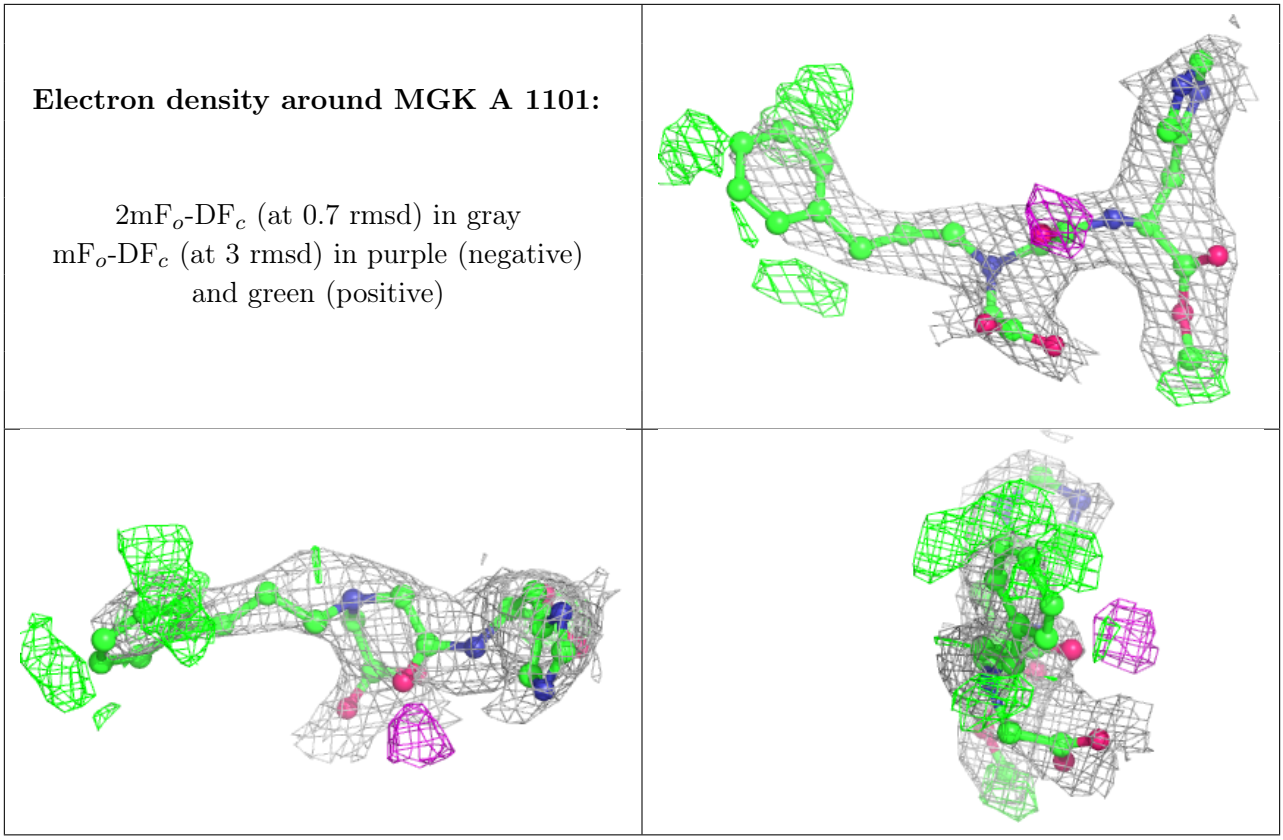
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around MGK A 1101:

$2mF_o$-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.