



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:38 am BST

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

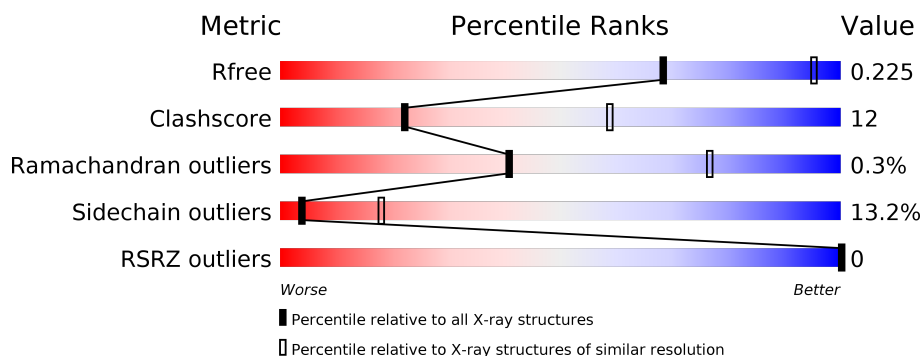
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	
1	B	990	

2 Entry composition

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:

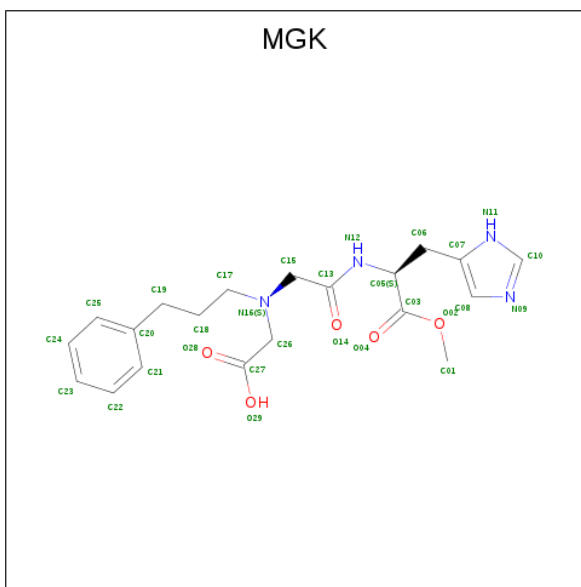
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735
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: C₂₀H₂₆N₄O₅).



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

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

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

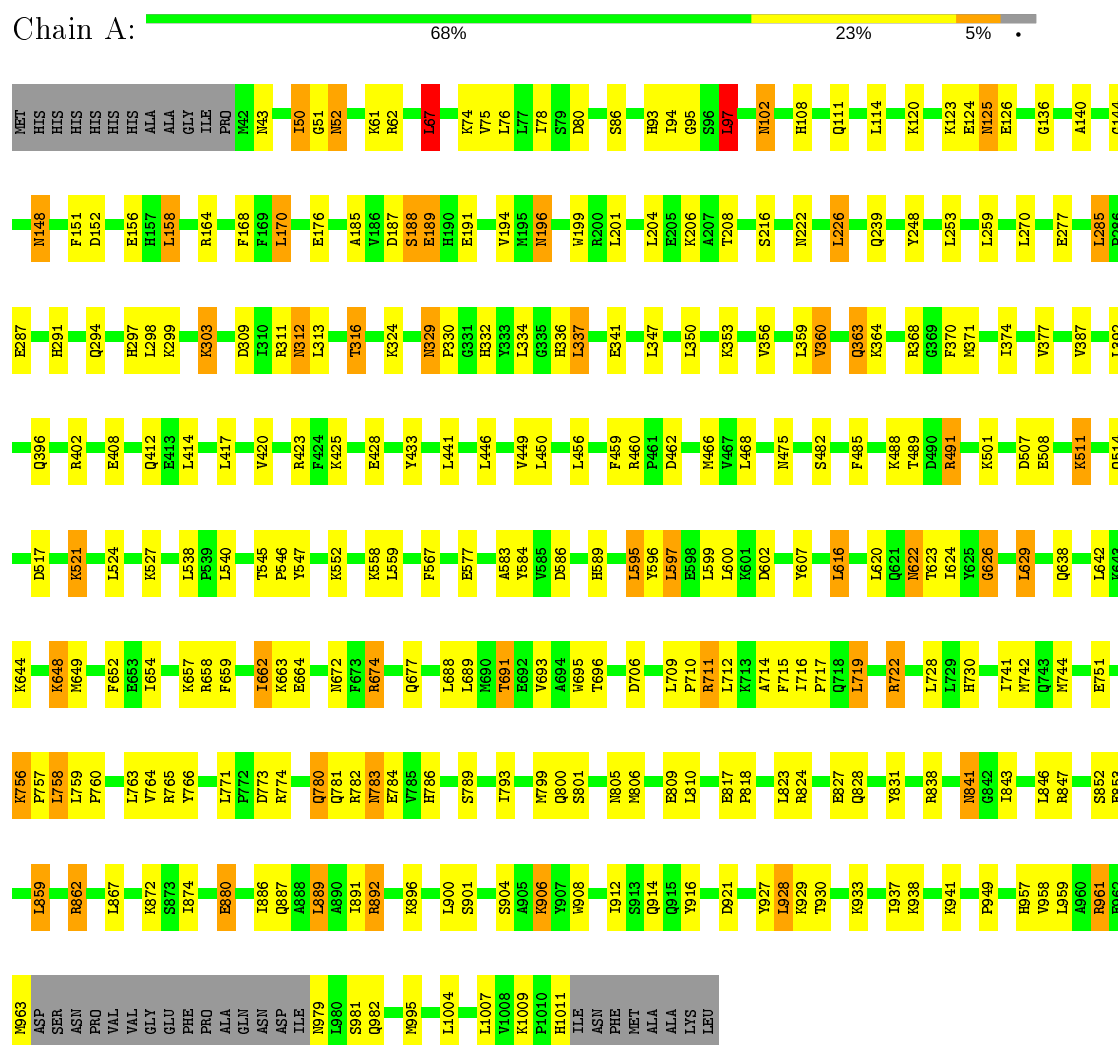
- Molecule 4 is water.

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

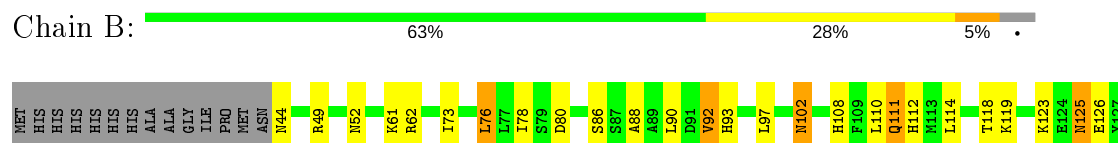
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: Insulin-degrading enzyme



ILE	N979	N980	A888	S803	E702	E598	E465	L226	S128
	L980		L889	E804	T708	L599	L346	L346	Q129
			A890	N805	T708	L600	L347	R229	F130
	E990		I891	N806	L709	D601	S348		L131
			R892	F807	P710	D602	E349	E233	S132
			R893		R711	S603			E133
	Q993			E809	L712	L604	V481	R238	H134
	N994		K898	L810	K713	N605	Q239		
			K899			E506			S138
	E997	F998	K999	I815	Q718		E494	L359	L242
L1002	P1003		S904	E816	I725	E612	T498	K243	H146
			I912	P818		L616	D507	S250	T147
					L728		E508	S251	N148
			Q915	L823	L729	N622	R368		Y149
			R920	K826	H730			V256	F150
	L1007		E927	E827	I733	G626	M371	V257	
	V1008		T923	T734	T734	N627	L379	V258	H157
	K1009		E924	Y831	K735	L629		L259	L158
	P1010				Q736	S630	D517	E262	E159
	H1011		Y827	R838	E751	V631			G160
ILE	ASN		L928	R839	Q742	E620	D389	L270	D175
	PHE			A840	Q743	K521	K521	V271	E176
	MET		T932	N841	M744	F522	F522	V272	S177
	ALA		K933	G842	V745	K523	Q399		A178
	ALA		E934	I843	E746	L642	E413	S276	K179
	LYS		D935	Q944		K644	L414		N184
				G945					
	Y940			R846	E751	K527	K281		L170
	K941		K941	R847	H754	N528	L417		D175
	E942				T755	E529	K425	L285	E176
LEU			A945	S852	K756	D655	F535	E290	S177
			V946	E853		E586	L538	Y433	A178
			D947	K854	L759	K657		I437	K179
			A948	P855		K658			
				P956	V764	F659	K552	Q294	N184
			R951	L859	R765			L440	S188
	H952			E860	V766	K662	M556	H297	E189
	K953			S861	R767	E663	L559	L298	
			V956	R662	Q770	E664		I304	V194
	H957				L771	N671	P570	P445	M195
LEU				A865	P772	N672		L446	N196
				F866	D773	F673	E447	K308	D197
	E962			L867	R774	R674	F576	D309	A198
				I868	G775	A675	E577	V449	R199
	S965			T869	W776	E676	L450	R311	R200
	ASN			M870		Q677	F579	T316	L201
	PRO				Q781			F317	F202
	VAL			I874	R782	V685	A583	P318	Q203
	VAL				N783	L686			K206
	GLY			M877	E784		D586	N829	
LEU	GLU				V785	T691	P587	P330	P214
	PHE			E880	H786	E692	E458	G331	P215
	PRO					V693	F459	H332	S216
	ALA			K384	Y795	A694	R460	L337	K217
	GLN			H885		K695	P461		
	ASN			Q887	S801	T696	D462		K223
	ASP				T802	K701		E341	

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

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(°)	Ideal(°)
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(°)	Ideal(°)
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:HG3	1:B:774:ARG:HH11	1.24	1.00
1:A:50:ILE:O	1:A:50:ILE:HG22	1.61	0.99
1:A:622:ASN:H	1:A:622:ASN:HD22	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	A	929	LYS
1	B	229	ARG
1	B	884	LYS
1	A	957	HIS
1	B	111	GLN

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

Mol	Chain	Res	Type
1	A	841	ASN
1	B	125	ASN
1	B	841	ASN
1	A	887	GLN
1	B	93	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 carbohydrates 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	A	1101	-	23,30,30	1.64	2 (8%)	29,38,38	2.06	6 (20%)
2	MGK	B	1101	-	23,30,30	1.74	2 (8%)	29,38,38	1.99	7 (24%)

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	A	1101	-	-	14/26/28/28	0/2/2/2
2	MGK	B	1101	-	-	13/26/28/28	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	2.65	1.52	1.47
2	A	1101	MGK	C26-N16	2.13	1.51	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGK	C27-C26-N16	6.72	123.05	113.48
2	B	1101	MGK	C27-C26-N16	5.36	121.11	113.48
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

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

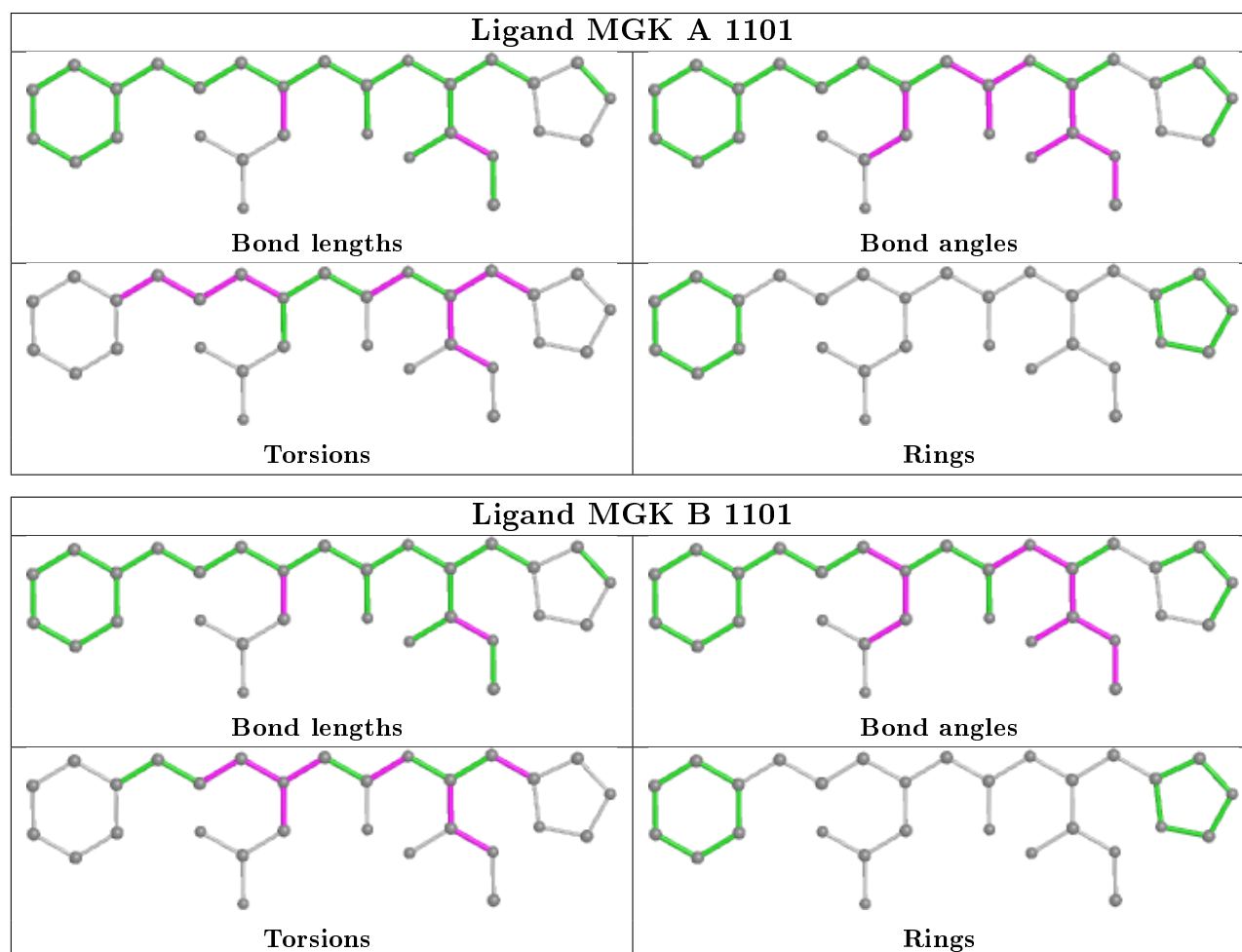
Mol	Chain	Res	Type	Atoms
2	A	1101	MGK	C17-C18-C19-C20
2	A	1101	MGK	C03-C05-C06-C07
2	A	1101	MGK	C05-C06-C07-N11
2	B	1101	MGK	C13-C15-N16-C26
2	B	1101	MGK	C05-C06-C07-N11

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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.

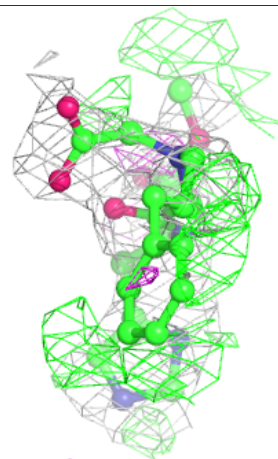
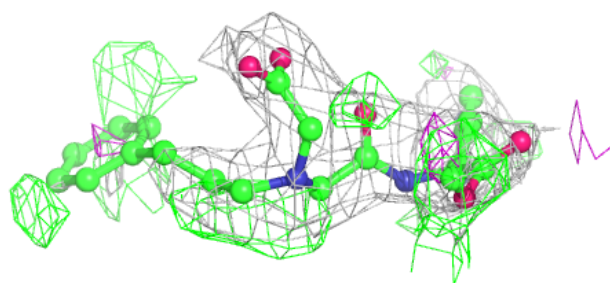
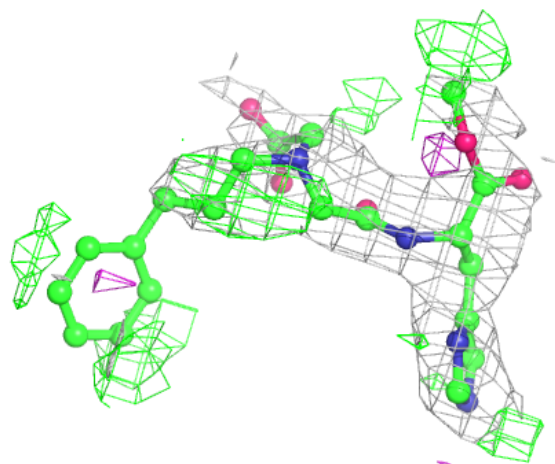
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MGK	B	1101	29/29	0.76	0.32	73,81,100,101	0
3	ZN	B	1102	1/1	0.87	0.21	2,2,2,2	0
2	MGK	A	1101	29/29	0.88	0.24	61,78,92,92	0
3	ZN	A	1102	1/1	0.95	0.23	2,2,2,2	0

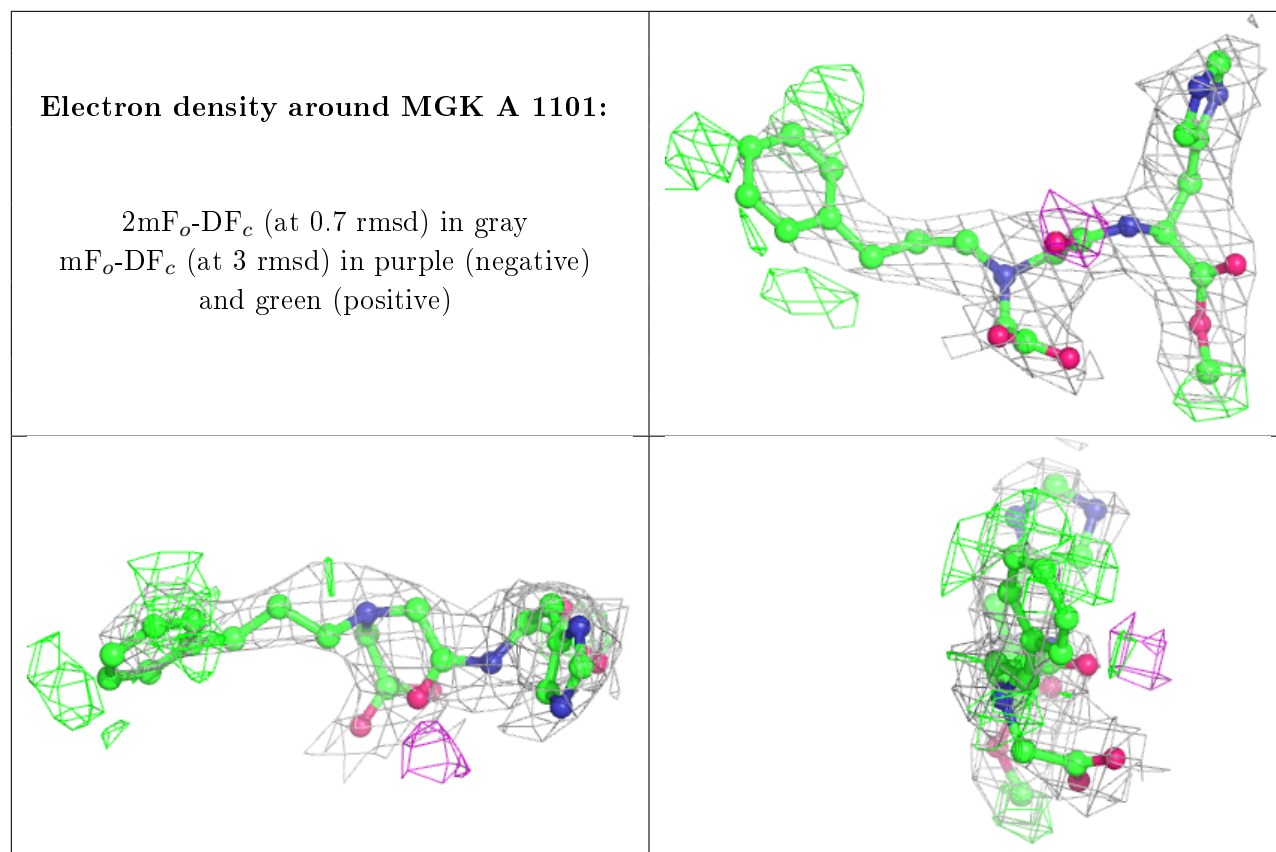
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.