wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2026 – 10:26 AM UTC

PDB ID	:	4GS8 / pdb_00004gs8
Title	:	Structure analysis of cysteine free insulin degrading enzyme (ide) with compound bdm43079 [{[(s)-2-(1h-imidazol-4-yl)-1-methylcarbamoyl-ethylcarbamoyl]-methyl}-(3-phenyl-propyl)-amino]-acetic acid
Authors	:	Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on	:	2012-08-27
Resolution	:	2.99 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:

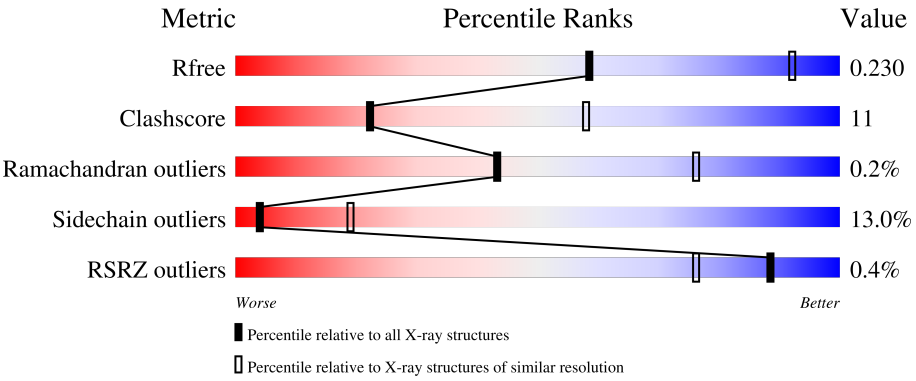
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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	% 68% 23% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15726 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	954	Total	C	N	O	S	0	0	0
			7795	5022	1310	1441	22			
1	B	954	Total	C	N	O	S	0	0	0
			7795	5022	1310	1441	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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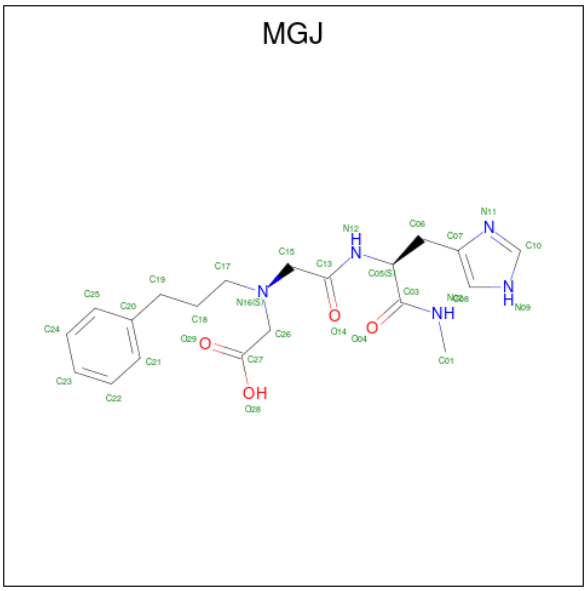
Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	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 N-(carboxymethyl)-N-(3-phenylpropyl)glycyl-N-methyl-L-histidinamide (CCD ID: MGJ) (formula: $C_{20}H_{27}N_5O_4$).



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

- Molecule 3 is ZINC ION (CCD ID: 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.

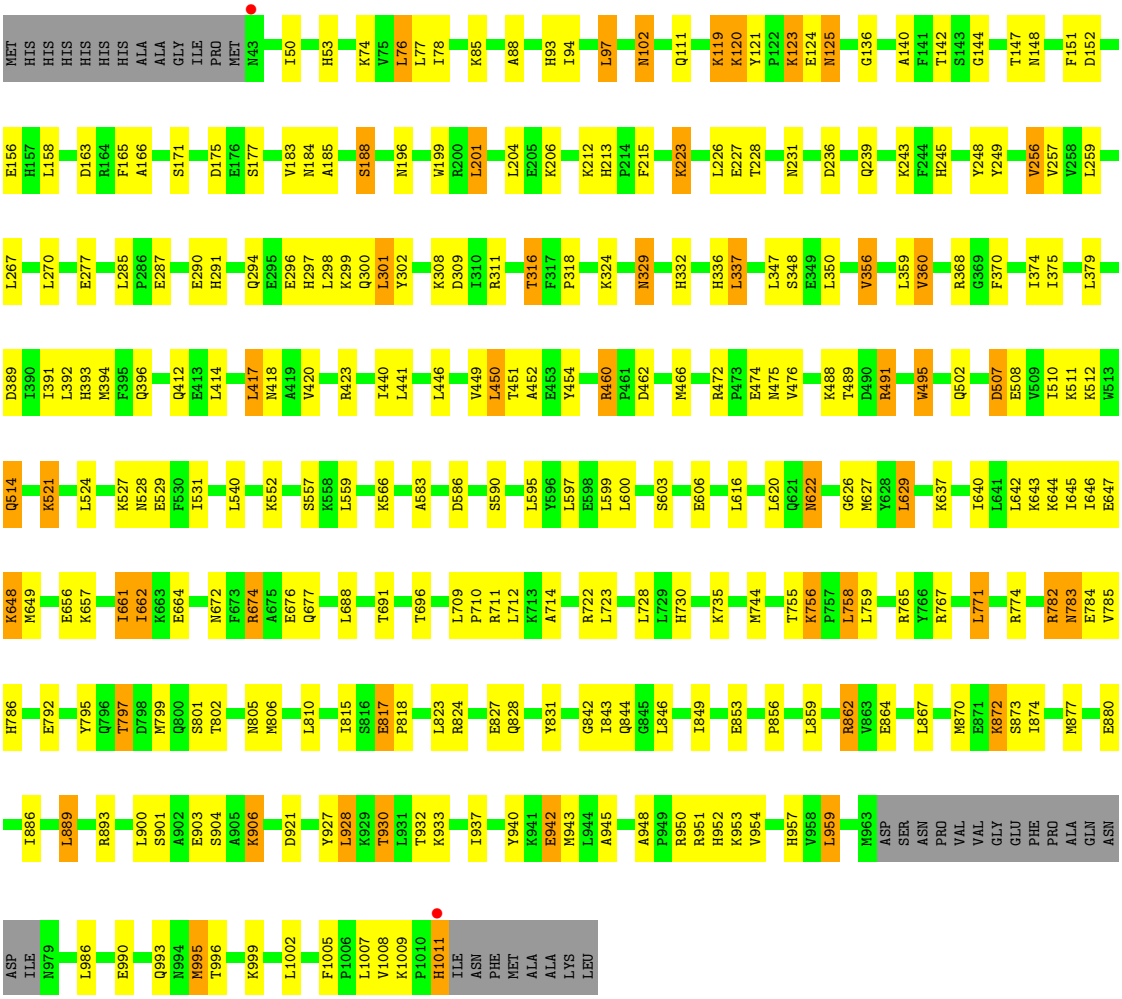
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	32	Total O 32 32	0	0

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.

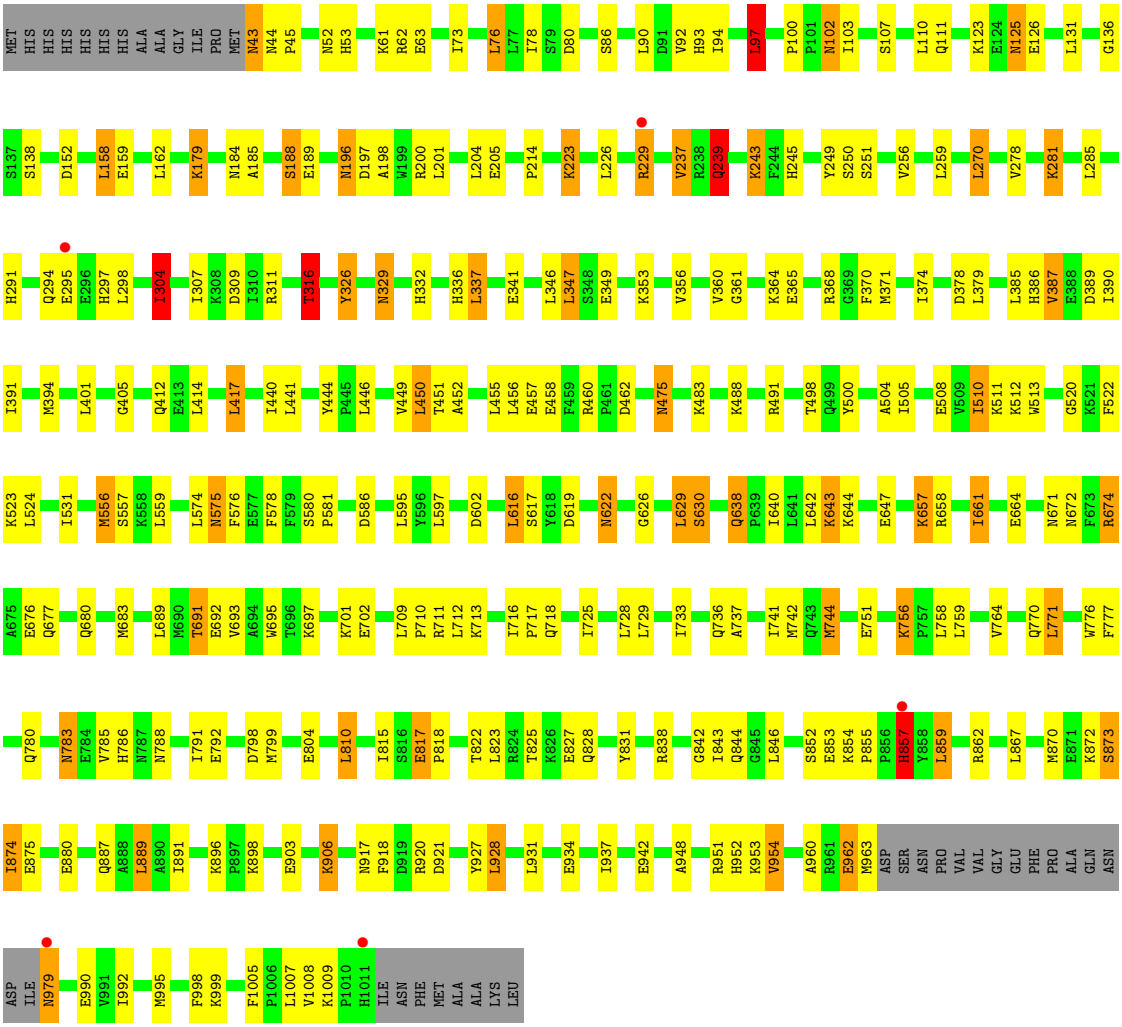
• Molecule 1: Insulin-degrading enzyme

Chain A:



• Molecule 1: Insulin-degrading enzyme

Chain B:


MET HIS HIS HIS HIS HIS ALA ALA GLY ILE PRO MET M43 N44 P45 N52 H53 K61 R62 E63 I73 L76 L77 I78 S79 D80 S86 L90 D91 V92 H93 I94 L97 P100 P101 N102 I103 S107 L110 Q111 K123 E124 N125 E126 L131 G136
S137 S138 D152 L158 E159 L162 K179 N184 A185 S188 E189 N196 D197 A198 W199 R200 L201 L204 E205 P214 K223 L226 R229 V237 R238 Q239 K243 F244 H245 Y249 S250 S251 V256 L259 L270 V278 K281 L285
H291 Q294 E295 E296 H297 L298 I304 I307 K308 D309 I310 R311 T316 Y326 N329 H332 H336 L337 E341 L346 L347 S348 E349 K353 V356 V360 G361 K364 E365 R368 G369 F370 M371 I374 D378 L379 L385 H386 V387 E388 D389 I390
I391 M394 L401 G405 Q412 E413 L414 L417 I440 L441 Y444 P445 L446 V449 L450 T451 A452 L455 L456 E457 E458 F459 R460 P461 D462 N475 K483 K488 R491 T498 Q499 Y500 A504 I505 E508 V509 I510 K511 K512 W513 G520 K521 F522
K523 L524 I531 M556 S557 K558 L559 L574 N575 F576 E577 F578 F579 S580 P581 D586 L595 Y596 L597 D602 L616 S617 Y618 D619 N622 G626 L629 S630 Q638 P639 I640 L641 L642 K643 K644 E647 K657 R658 I661 E664 N671 N672 F673 R674
A675 E676 Q677 Q680 M683 L689 M690 T691 E692 V693 A694 W695 T696 K697 K701 E702 L709 P710 R711 L712 K713 I716 P717 Q718 I725 L728 L729 I733 Q736 A737 I741 M742 Q743 M744 E751 K756 P757 L758 L759 V764 Q770 L771 W776 F777
Q780 N783 E784 V785 H786 N787 N788 I791 E792 D798 M799 E804 L810 I815 S816 E817 P818 T822 L823 R824 T825 K826 E827 Q828 Y831 R838 G842 I843 Q844 G845 L846 S852 E853 K854 P855 P856 R857 Y858 L859 R862 L867 M870 E871 K872 S873
I874 E875 E880 Q887 A888 L889 A890 I891 K896 P897 K898 E903 K906 N917 F918 D919 R920 D921 Y927 L928 L931 E934 I937 E942 A948 R951 H952 K953 Y954 A960 R961 E962 M963 ASP SER ASN PRO VAL VAL GLY GLU PHE PRO ALA GLN ASN
ASP ILE N979 E990 V991 I992 M995 F998 K999 F1005 P1006 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	263.55Å 263.55Å 91.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.99 50.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.99) 99.8 (50.00-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.178 , 0.235 (Not available) , 0.230	Depositor DCC
R_{free} test set	3679 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15726	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: ZN, MGJ

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	1.07	1/7990 (0.0%)	1.15	16/10810 (0.1%)
1	B	1.02	7/7990 (0.1%)	1.17	32/10810 (0.3%)
All	All	1.05	8/15980 (0.1%)	1.16	48/21620 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CG-CD	7.71	1.75	1.52
1	B	680	GLN	CA-CB	6.82	1.64	1.53
1	A	640	ILE	CA-CB	6.17	1.61	1.54
1	B	316	THR	CA-CB	6.08	1.64	1.53
1	B	229	ARG	CD-NE	5.63	1.54	1.46

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	942	GLU	N-CA-C	7.59	119.19	111.07
1	A	256	VAL	CB-CA-C	-7.29	99.75	110.62
1	B	505	ILE	N-CA-C	-7.08	102.54	108.63
1	B	100	PRO	CA-C-N	7.04	127.64	119.47
1	B	100	PRO	C-N-CA	7.04	127.64	119.47

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	7795	0	7730	163	0
1	B	7795	0	7730	165	0
2	A	29	0	26	7	0
2	B	29	0	26	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	0	7	0
4	B	32	0	0	6	0
All	All	15726	0	15512	331	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 11.

The worst 5 of 331 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:229:ARG:CG	1:B:229:ARG:CD	1.75	1.57
2:B:1101:MGJ:H06A	2:B:1101:MGJ:O14	1.42	1.08
2:B:1101:MGJ:O14	2:B:1101:MGJ:H26	1.53	1.05
1:A:491:ARG:HG3	1:A:491:ARG:HH11	0.88	1.01
1:A:491:ARG:HG3	1:A:491:ARG:NH1	1.68	1.00

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	950/990 (96%)	900 (95%)	50 (5%)	0	100 100
1	B	950/990 (96%)	901 (95%)	45 (5%)	4 (0%)	30 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1900/1980 (96%)	1801 (95%)	95 (5%)	4 (0%)	43 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	857	HIS
1	B	97	LEU
1	B	326	TYR
1	B	520	GLY

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	847/879 (96%)	736 (87%)	111 (13%)	4 19
1	B	847/879 (96%)	737 (87%)	110 (13%)	4 19
All	All	1694/1758 (96%)	1473 (87%)	221 (13%)	4 19

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	ILE
1	B	356	VAL
1	B	990	GLU
1	B	838	ARG
1	B	111	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	605	ASN
1	B	887	GLN
1	B	672	ASN
1	B	783	ASN

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Mol	Chain	Res	Type
1	A	677	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	MGJ	A	1101	-	30,30,30	3.21	6 (20%)	38,38,38	2.25	18 (47%)
2	MGJ	B	1101	-	30,30,30	2.05	4 (13%)	38,38,38	1.29	4 (10%)

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	MGJ	A	1101	-	-	10/28/28/28	0/2/2/2
2	MGJ	B	1101	-	-	14/28/28/28	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	MGJ	C22-C21	9.03	1.54	1.38
2	A	1101	MGJ	C24-C25	8.93	1.54	1.38
2	B	1101	MGJ	C03-N02	8.27	1.44	1.33
2	A	1101	MGJ	C25-C20	8.02	1.54	1.38
2	A	1101	MGJ	C23-C22	6.95	1.53	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	MGJ	C23-C22-C21	-6.13	112.68	120.24
2	A	1101	MGJ	C24-C25-C20	-4.45	114.36	120.61
2	A	1101	MGJ	O04-C03-N02	-3.75	116.88	123.13
2	A	1101	MGJ	C05-C03-N02	3.32	121.99	116.99
2	B	1101	MGJ	C15-N16-C17	-3.16	104.29	111.91

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MGJ	C06-C05-N12-C13
2	A	1101	MGJ	C13-C15-N16-C26
2	A	1101	MGJ	O04-C03-N02-C01
2	A	1101	MGJ	C05-C03-N02-C01
2	B	1101	MGJ	C06-C05-N12-C13

There are no ring outliers.

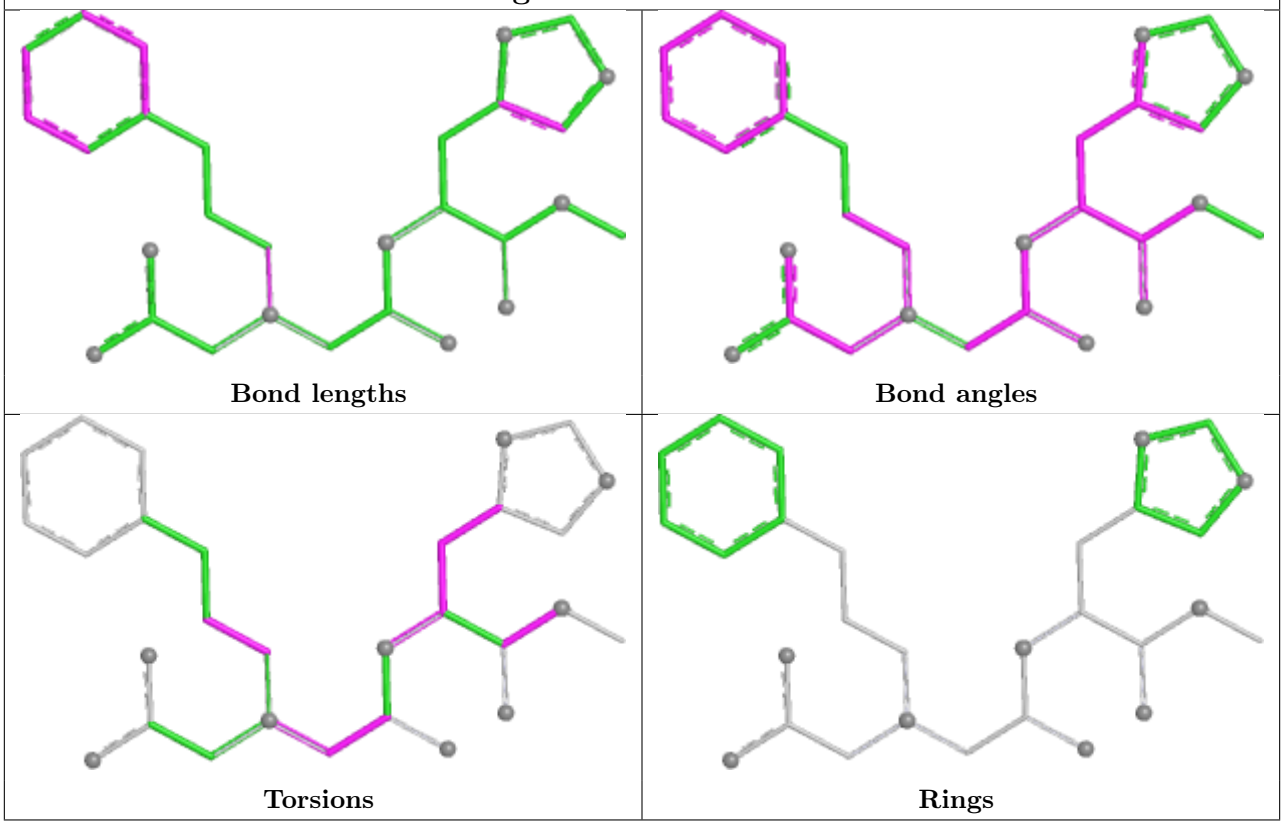
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MGJ	7	0
2	B	1101	MGJ	6	0

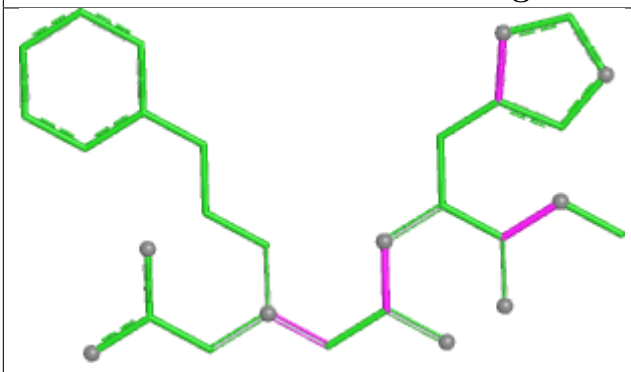
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

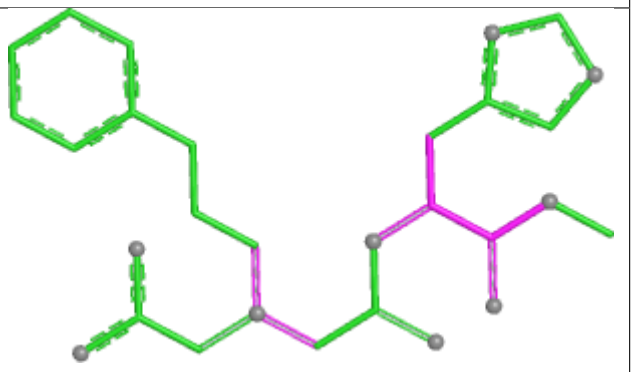
Ligand MGJ A 1101



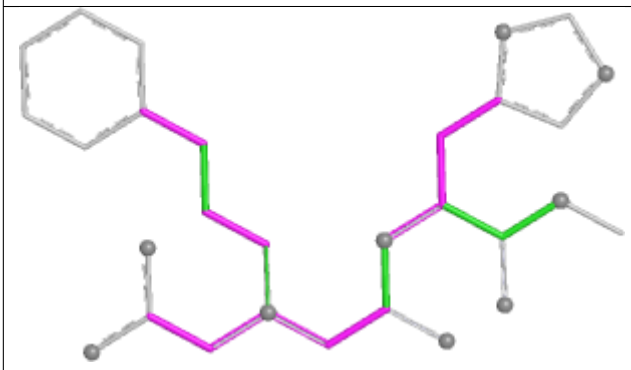
Ligand MGJ B 1101



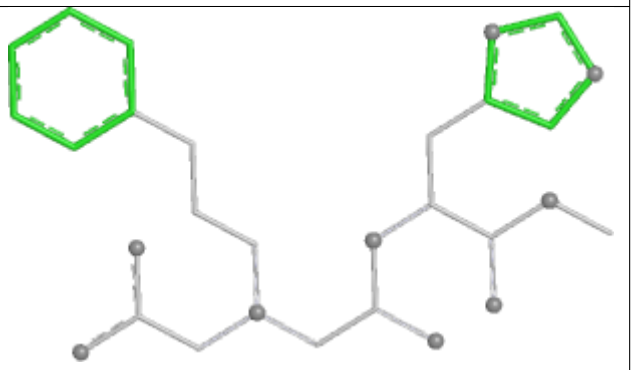
Bond lengths



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	954/990 (96%)	-0.64	2 (0%)	91	83	22, 36, 52, 71	0
1	B	954/990 (96%)	-0.50	5 (0%)	87	72	25, 41, 56, 77	0
All	All	1908/1980 (96%)	-0.57	7 (0%)	88	76	22, 39, 54, 77	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	ASN	2.8
1	B	1011	HIS	2.8
1	B	229	ARG	2.3
1	B	857	HIS	2.3
1	B	979	ASN	2.2

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 oligosaccharides in this entry.

6.4 Ligands

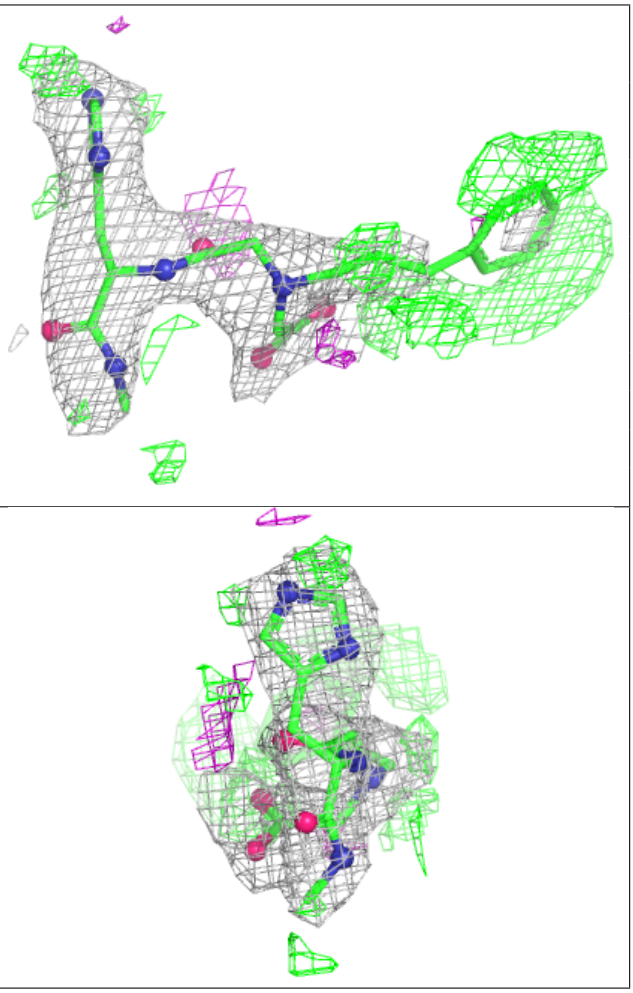
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

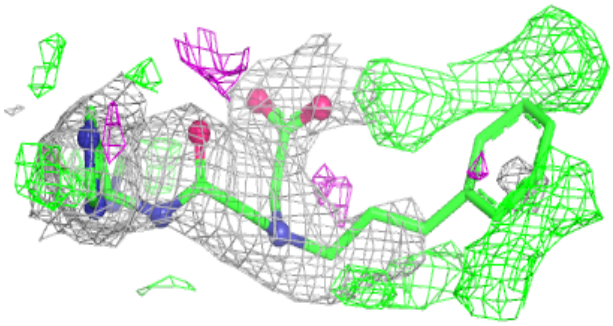
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MGJ	A	1101	29/29	0.78	0.30	68,81,98,98	0
2	MGJ	B	1101	29/29	0.86	0.21	69,76,100,100	0
3	ZN	A	1102	1/1	1.00	0.02	41,41,41,41	0
3	ZN	B	1102	1/1	1.00	0.03	40,40,40,40	0

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 MGJ A 1101:

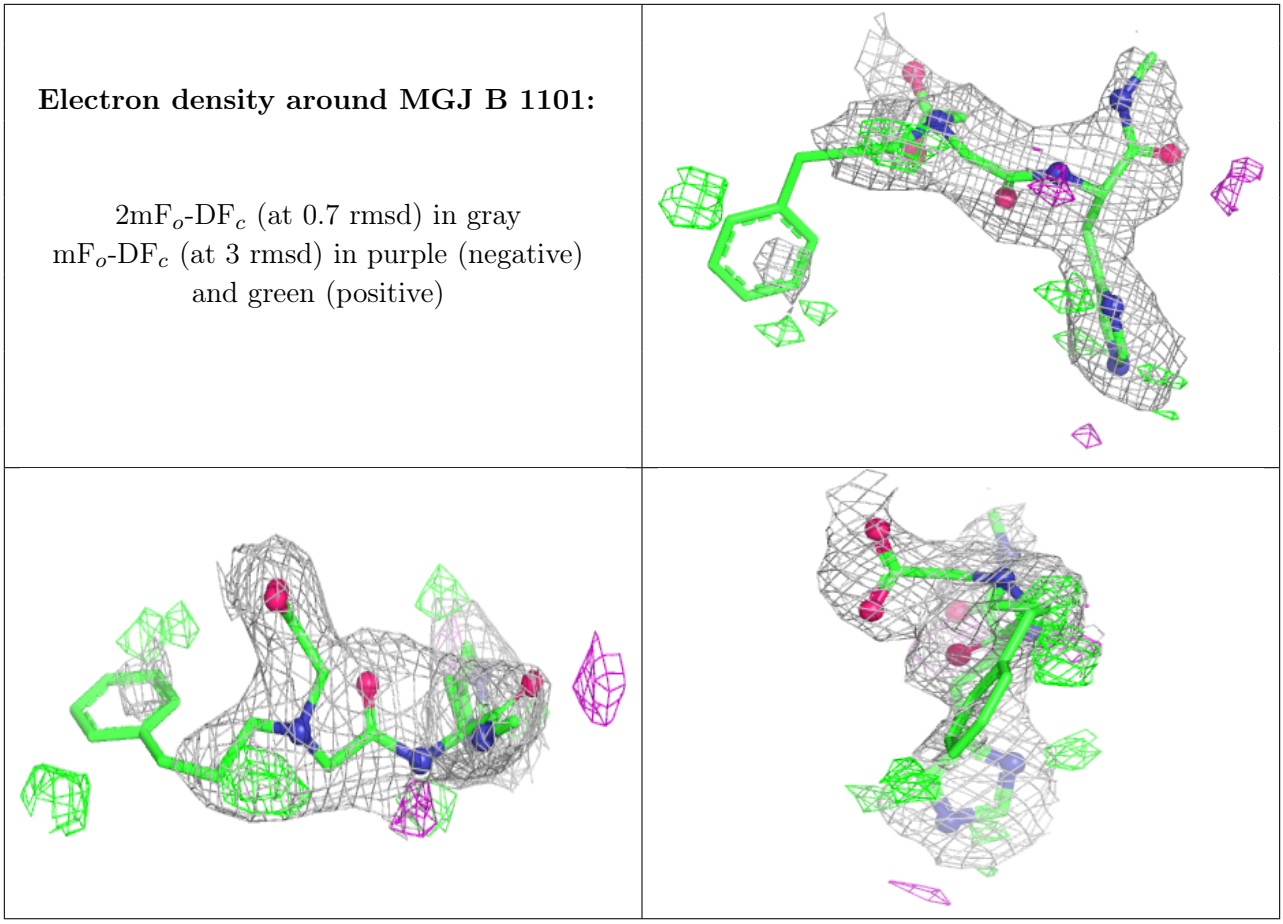
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around MGJ 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.