



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 07:44 pm BST

PDB ID : 4GS8
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 ⓘ 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

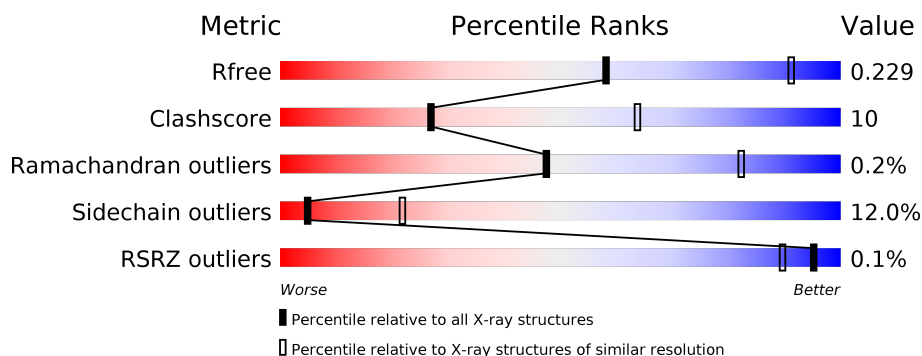
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	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 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:

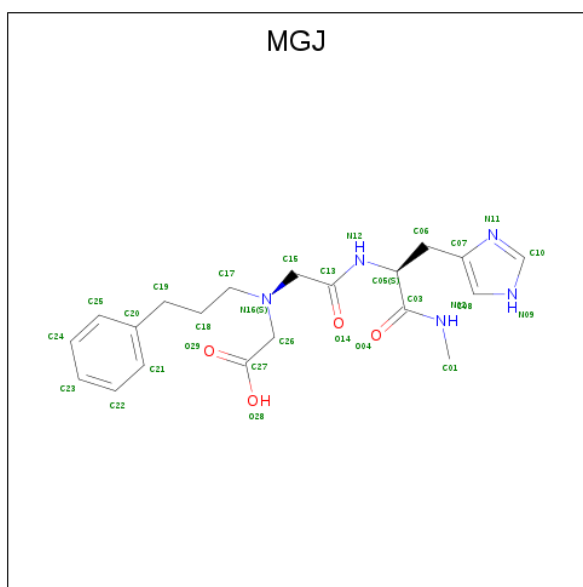
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735
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 (three-letter code: MGJ) (formula: C₂₀H₂₇N₅O₄).



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

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

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

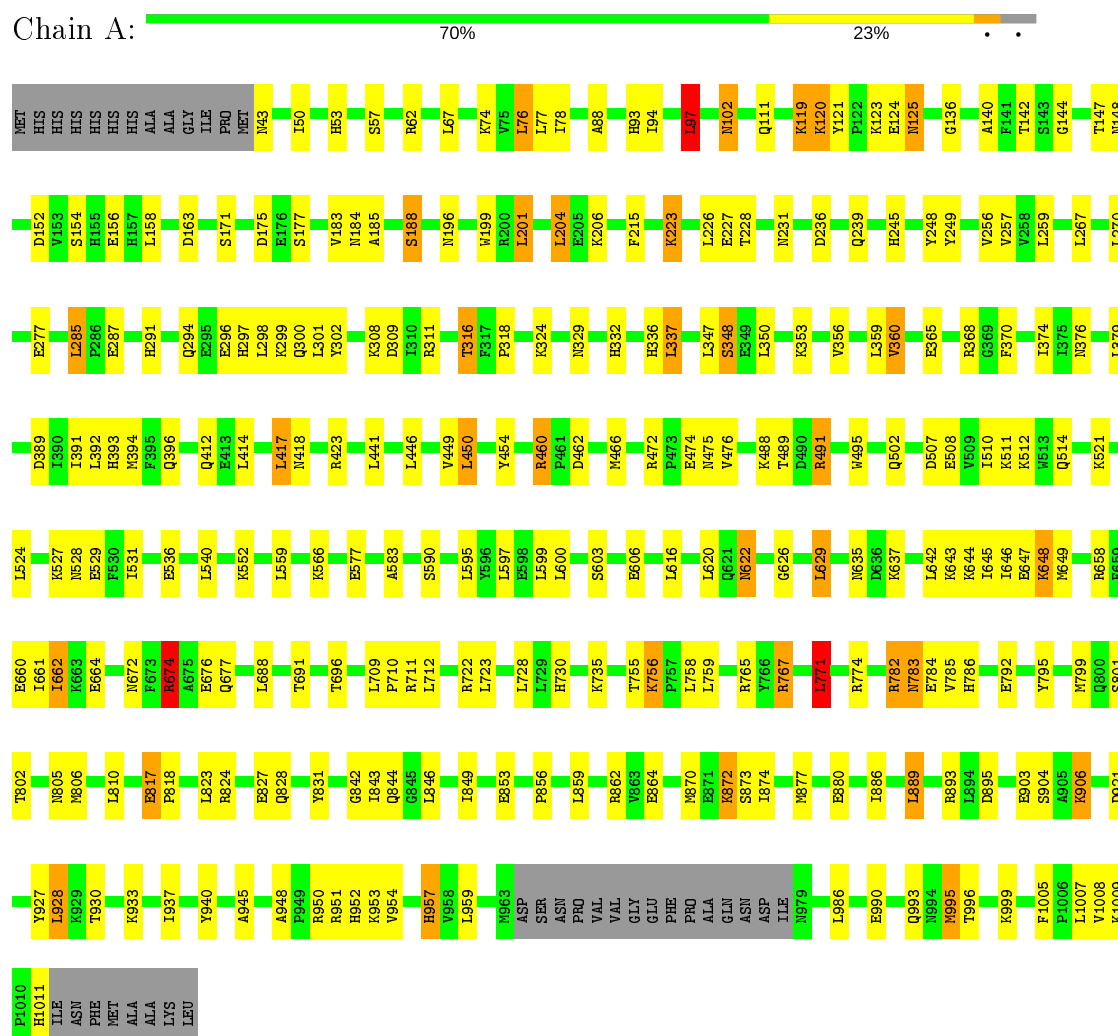
- Molecule 4 is water.

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

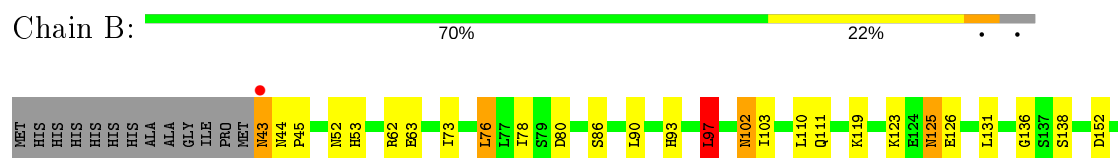
3 Residue-property plots

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



Y954	G842	K713	L595	L417	E295	L158
R957	I843	I716	Y596	L477	E296	E159
	Q844	P717	L597	R423	H297	L162
A960	G845	L728	D602	I440	I304	K179
R962	L846	L729	L616	L441	D309	M184
R963	R847	I733	D619	Y444	I310	A185
ASP	S852	Q736	N622	L446	R311	S188
SER	E853	A737	G626	V449	T316	E189
ASN	K854	I741	L629	L450	Y326	M196
PRO	K855	M742	S630	T451	N329	D197
VAL	R857	M744	Q638	A452	H332	A198
VAL	R858	K756	L642	L455	E341	R199
GLY	L859	P757	L643	L456	H336	R200
GLU	L860	L758	K644	E457	L337	L201
PHE	R862	L759	K645	E458	E341	L204
PRO	L867	Q770	K646	F459	E341	E205
ALA	M870	L771	E647	P461	L346	P214
GLN	M871	L772	E648	D462	L347	K223
ASN	M872	P777	R657	M466	S348	L226
ASP	L880	F777	R658	N475	E349	L226
ILE	Q887	M783	I661	N475	K353	R229
N979	K888	P784	E664	K488	V356	V237
E990	L889	W785	S669	R491	G361	R235
Y991	A890	M787	L670	T498	K364	Q239
Q993	I891	N788	N671	I510	E365	K243
N994	Q897	I791	M672	K511	R368	F244
N995	L898	E792	P673	K512	G369	E245
F998	A899	D798	A675	G520	R369	Y249
K999	I891	M799	E676	F522	F370	S250
F1005	K898	E804	Q677	K523	M371	S251
P1006	E903	L810	M683	L524	I374	V256
L1007	E904	I815	L689	M556	D378	L259
V1008	Y927	S816	M690	T691	L379	L270
K1009	L928	E817	E692	V693	H366	V278
P1010	L931	P818	V693	A694	V387	V278
H1011	E934	T822	W695	W695	E388	K281
ILE	E942	L823	K701	E702	D389	L285
ASN	E943	Q828	E702	L709	I390	P286
ASN	E944	Q828	E702	P710	I391	P286
PHE	E945	Q828	E702	R711	M394	E287
MET	E946	Q828	E702	R712	Q412	H291
ALA	E947	Q828	E702	R713	E413	H291
ALA	E948	Q828	E702	R714	L414	Q294
LYS	E949	Q828	E702	R715		
LEU	E950	Q828	E702	R716		
	E951	Q828	E702	R717		
	E952	Q828	E702	R718		
	E953	Q828	E702	R719		
	E954	Q828	E702	R720		
	E955	Q828	E702	R721		
	E956	Q828	E702	R722		
	E957	Q828	E702	R723		
	E958	Q828	E702	R724		
	E959	Q828	E702	R725		
	E960	Q828	E702	R726		
	E961	Q828	E702	R727		
	E962	Q828	E702	R728		
	E963	Q828	E702	R729		
	E964	Q828	E702	R730		
	E965	Q828	E702	R731		
	E966	Q828	E702	R732		
	E967	Q828	E702	R733		
	E968	Q828	E702	R734		
	E969	Q828	E702	R735		
	E970	Q828	E702	R736		
	E971	Q828	E702	R737		
	E972	Q828	E702	R738		
	E973	Q828	E702	R739		
	E974	Q828	E702	R740		
	E975	Q828	E702	R741		
	E976	Q828	E702	R742		
	E977	Q828	E702	R743		
	E978	Q828	E702	R744		
	E979	Q828	E702	R745		
	E980	Q828	E702	R746		
	E981	Q828	E702	R747		
	E982	Q828	E702	R748		
	E983	Q828	E702	R749		
	E984	Q828	E702	R750		
	E985	Q828	E702	R751		
	E986	Q828	E702	R752		
	E987	Q828	E702	R753		
	E988	Q828	E702	R754		
	E989	Q828	E702	R755		
	E990	Q828	E702	R756		
	E991	Q828	E702	R757		
	E992	Q828	E702	R758		
	E993	Q828	E702	R759		
	E994	Q828	E702	R760		
	E995	Q828	E702	R761		
	E996	Q828	E702	R762		
	E997	Q828	E702	R763		
	E998	Q828	E702	R764		
	E999	Q828	E702	R765		
	E1000	Q828	E702	R766		
	E1001	Q828	E702	R767		
	E1002	Q828	E702	R768		
	E1003	Q828	E702	R769		
	E1004	Q828	E702	R770		
	E1005	Q828	E702	R771		
	E1006	Q828	E702	R772		
	E1007	Q828	E702	R773		
	E1008	Q828	E702	R774		
	E1009	Q828	E702	R775		
	E1010	Q828	E702	R776		
	E1011	Q828	E702	R777		
	E1012	Q828	E702	R778		
	E1013	Q828	E702	R779		
	E1014	Q828	E702	R780		
	E1015	Q828	E702	R781		
	E1016	Q828	E702	R782		
	E1017	Q828	E702	R783		
	E1018	Q828	E702	R784		
	E1019	Q828	E702	R785		
	E1020	Q828	E702	R786		
	E1021	Q828	E702	R787		
	E1022	Q828	E702	R788		
	E1023	Q828	E702	R789		
	E1024	Q828	E702	R790		
	E1025	Q828	E702	R791		
	E1026	Q828	E702	R792		
	E1027	Q828	E702	R793		
	E1028	Q828	E702	R794		
	E1029	Q828	E702	R795		
	E1030	Q828	E702	R796		
	E1031	Q828	E702	R797		
	E1032	Q828	E702	R798		
	E1033	Q828	E702	R799		
	E1034	Q828	E702	R800		
	E1035	Q828	E702	R801		
	E1036	Q828	E702	R802		
	E1037	Q828	E702	R803		
	E1038	Q828	E702	R804		
	E1039	Q828	E702	R805		
	E1040	Q828	E702	R806		
	E1041	Q828	E702	R807		
	E1042	Q828	E702	R808		
	E1043	Q828	E702	R809		
	E1044	Q828	E702	R810		
	E1045	Q828	E702	R811		
	E1046	Q828	E702	R812		
	E1047	Q828	E702	R813		
	E1048	Q828	E702	R814		
	E1049	Q828	E702	R815		
	E1050	Q828	E702	R816		
	E1051	Q828	E702	R817		
	E1052	Q828	E702	R818		
	E1053	Q828	E702	R819		
	E1054	Q828	E702	R820		
	E1055	Q828	E702	R821		
	E1056	Q828	E702	R822		
	E1057	Q828	E702	R823		
	E1058	Q828	E702	R824		
	E1059	Q828	E702	R825		
	E1060	Q828	E702	R826		
	E1061	Q828	E702	R827		
	E1062	Q828	E702	R828		
	E1063	Q828	E702	R829		
	E1064	Q828	E702	R830		
	E1065	Q828	E702	R831		
	E1066	Q828	E702	R832		
	E1067	Q828	E702	R833		
	E1068	Q828	E702	R834		
	E1069	Q828	E702	R835		
	E1070	Q828	E702	R836		
	E1071	Q828	E702	R837		
	E1072	Q828	E702	R838		
	E1073	Q828	E702	R839		
	E1074	Q828	E702	R840		
	E1075	Q828	E702	R841		
	E1076	Q828	E702	R842		
	E1077	Q828	E702	R843		
	E1078	Q828	E702	R844		
	E1079	Q828	E702	R845		
	E1080	Q828	E702	R846		
	E1081	Q828	E702	R847		
	E1082	Q828	E702	R848		
	E1083	Q828	E702	R849		
	E1084	Q828	E702	R850		
	E1085	Q828	E702	R851		
	E1086	Q828	E702	R852		
	E1087	Q828	E702	R853		
	E1088	Q828	E702	R854		
	E1089	Q828	E702	R855		
	E1090	Q828	E702	R856		
	E1091	Q828	E702	R857		
	E1092	Q828	E702	R858		
	E1093	Q828	E702	R859		
	E1094	Q828	E702	R860		
	E1095	Q828	E702	R861		
	E1096	Q828	E702	R862		
	E1097	Q828	E702	R863		
	E1098	Q828	E702	R864		
	E1099	Q828	E702	R865		
	E1100	Q828	E702	R866		
	E1101	Q828	E702	R867		
	E1102	Q828	E702	R868		
	E1103	Q828	E702	R869		
	E1104	Q828	E702	R870		
	E1105	Q828	E702	R871		
	E1106	Q828	E702	R872		
	E1107	Q828	E702	R873		
	E1108	Q828	E702	R874		
	E1109	Q828	E702	R875		
	E1110	Q828	E702	R876		
	E1111	Q828	E702	R877		
	E1112	Q828	E702	R878		
	E1113	Q828	E702	R879		
	E1114	Q828	E702	R880		
	E1115	Q828	E702	R881		
	E1116	Q828	E702	R882		
	E1117	Q828	E702	R883		
	E1118	Q828	E702	R884		
	E1119	Q828	E702	R885		
	E1120	Q828	E702	R886		
	E1121	Q828	E702	R887		
	E1122	Q828	E702	R888		
	E1123	Q828	E702	R889		
	E1124	Q828	E702	R890		
	E1125	Q828	E702	R891		
	E1126	Q828	E702	R892		
	E1127	Q828	E702	R893		
	E1128	Q828	E702	R894		
	E1129	Q828	E702	R895		
	E1130	Q828	E702	R896		
	E1131	Q828	E702	R897		
	E1132	Q828	E702	R898		
	E1133	Q828	E702	R899		
	E1134	Q828</				

4 Data and refinement statistics

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 49.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.99) 99.8 (49.81-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.178 , 0.235 0.176 , 0.229	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)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

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: MGJ, 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	0.92	4/7990 (0.1%)	0.89	10/10810 (0.1%)
1	B	0.88	6/7990 (0.1%)	0.88	3/10810 (0.0%)
All	All	0.90	10/15980 (0.1%)	0.88	13/21620 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CG-CD	9.45	1.75	1.51
1	A	536	GLU	CG-CD	6.00	1.60	1.51
1	A	660	GLU	CG-CD	5.87	1.60	1.51
1	B	577	GLU	CG-CD	5.73	1.60	1.51
1	B	243	LYS	CD-CE	5.71	1.65	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	847	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	895	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	62	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	285	LEU	CA-CB-CG	6.44	130.10	115.30
1	A	256	VAL	CB-CA-C	-6.13	99.75	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7795	0	7730	155	0
1	B	7795	0	7730	160	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	318	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 10.

The worst 5 of 318 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:O14	2:B:1101:MGJ:H06A	1.42	1.08
2:B:1101:MGJ:O14	2:B:1101:MGJ:H26	1.53	1.05
1:A:756:LYS:HB3	1:A:756:LYS:NZ	1.74	1.02
1:A:491:ARG:HG3	1:A:491:ARG:HH11	0.88	1.01

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%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1900/1980 (96%)	1801 (95%)	95 (5%)	4 (0%)	47 82

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 ⓘ

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%)	746 (88%)	101 (12%)	5 22
1	B	847/879 (96%)	745 (88%)	102 (12%)	5 22
All	All	1694/1758 (96%)	1491 (88%)	203 (12%)	5 22

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	937	ILE
1	B	196	ASN
1	B	873	SER
1	A	990	GLU
1	B	76	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	857	HIS
1	B	102	ASN
1	B	841	ASN
1	B	43	ASN

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Mol	Chain	Res	Type
1	B	125	ASN

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 carbohydrates 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	-	23,30,30	3.07	5 (21%)	29,38,38	2.56	12 (41%)
2	MGJ	B	1101	-	23,30,30	2.21	4 (17%)	29,38,38	1.39	6 (20%)

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	-	-	9/26/28/28	0/2/2/2
2	MGJ	B	1101	-	-	13/26/28/28	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MGJ	C03-N02	8.26	1.44	1.33
2	A	1101	MGJ	C25-C20	7.37	1.54	1.38
2	A	1101	MGJ	C22-C21	7.33	1.54	1.38
2	A	1101	MGJ	C24-C25	7.25	1.54	1.38
2	A	1101	MGJ	C23-C22	5.84	1.53	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGJ	C27-C26-N16	7.07	123.55	113.48
2	A	1101	MGJ	C23-C22-C21	-4.93	112.68	120.19
2	A	1101	MGJ	C24-C25-C20	-4.09	114.36	120.63
2	A	1101	MGJ	O04-C03-N02	-3.75	116.88	123.09
2	A	1101	MGJ	C18-C17-N16	3.39	122.40	113.84

There are no chirality outliers.

5 of 22 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	A	1101	MGJ	C05-C06-C07-C08

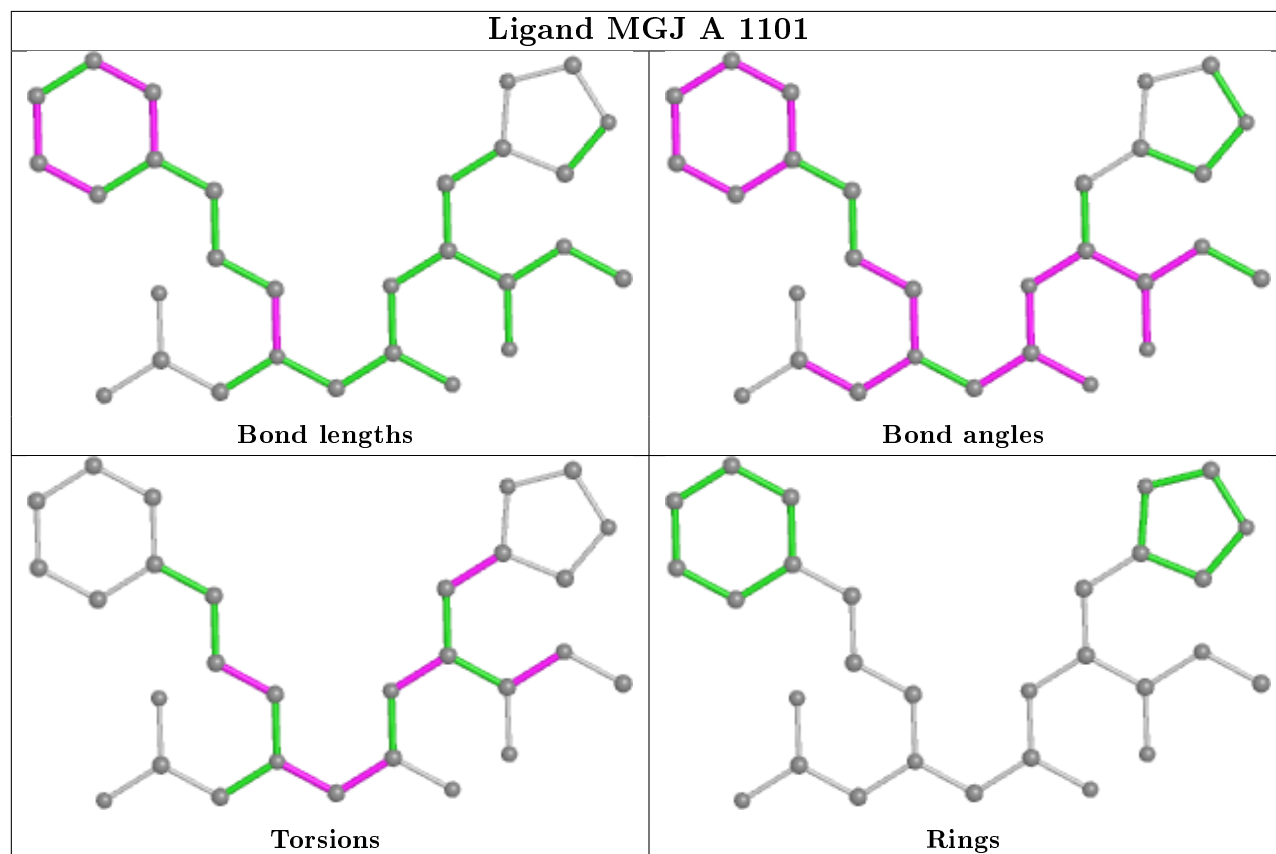
There are no ring outliers.

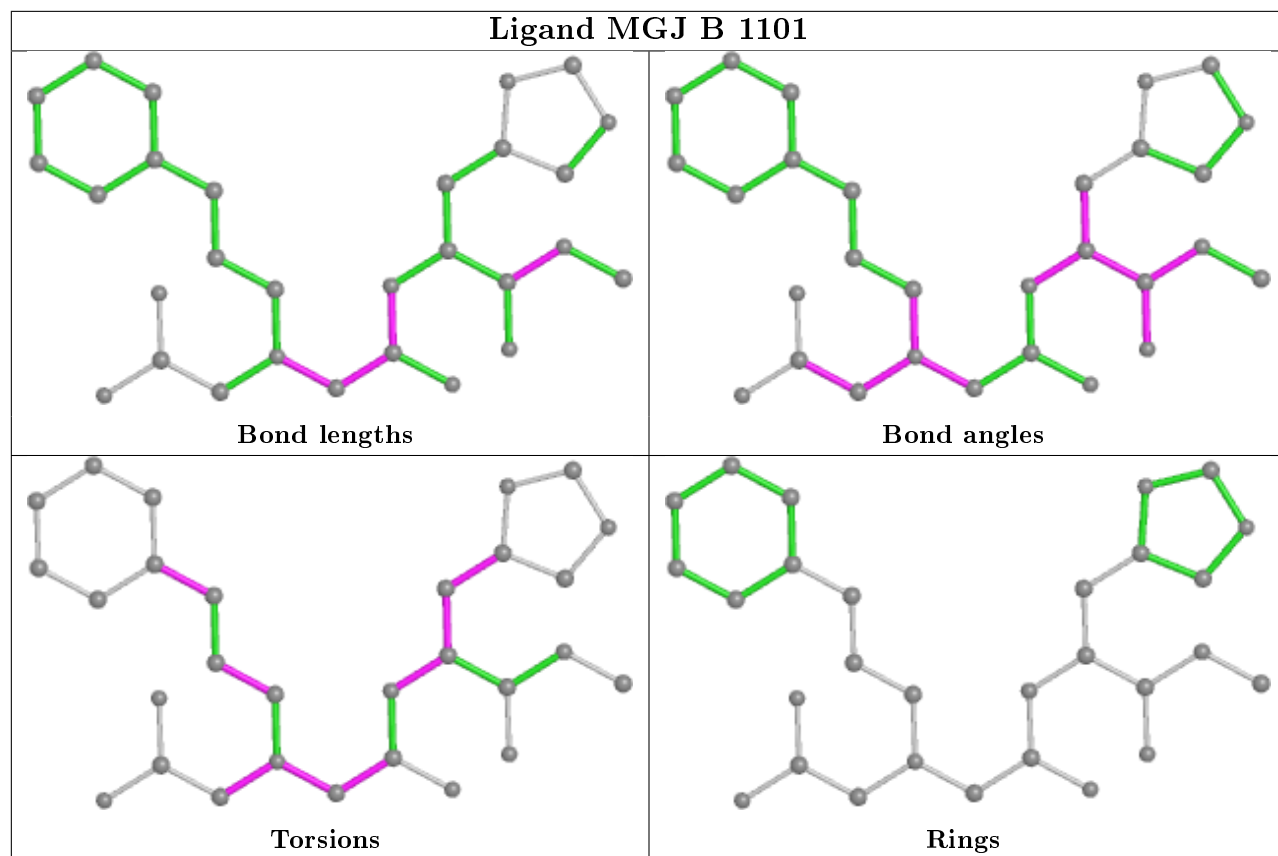
2 monomers are involved in 13 short contacts:

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 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 ⓘ

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	954/990 (96%)	-0.40	0 100 100	22, 36, 52, 71	0
1	B	954/990 (96%)	-0.34	1 (0%) 95 89	25, 41, 56, 77	0
All	All	1908/1980 (96%)	-0.37	1 (0%) 95 89	22, 39, 54, 77	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	ASN	3.2

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 carbohydrates in this entry.

6.4 Ligands ⓘ

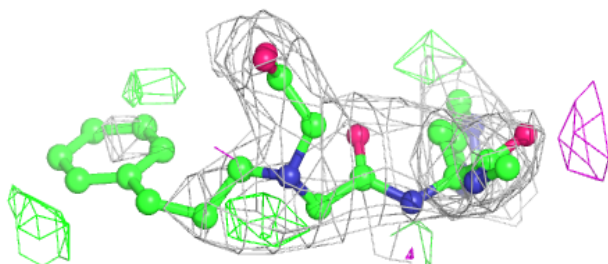
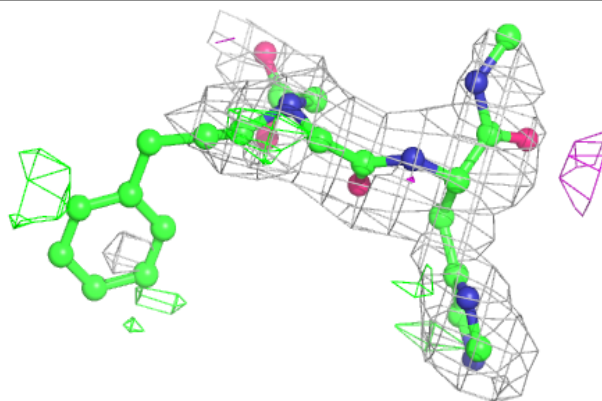
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	MGJ	B	1101	29/29	0.83	0.27	69,76,100,100	0
2	MGJ	A	1101	29/29	0.84	0.28	68,81,98,98	0
3	ZN	B	1102	1/1	0.99	0.15	40,40,40,40	0
3	ZN	A	1102	1/1	1.00	0.14	41,41,41,41	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.

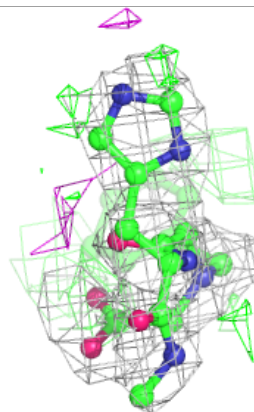
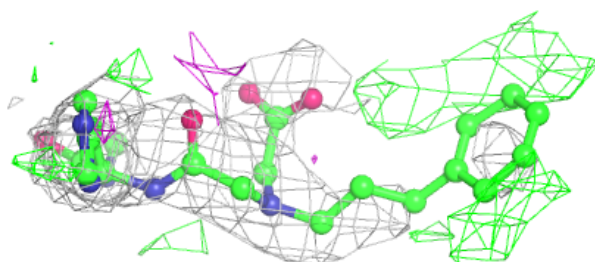
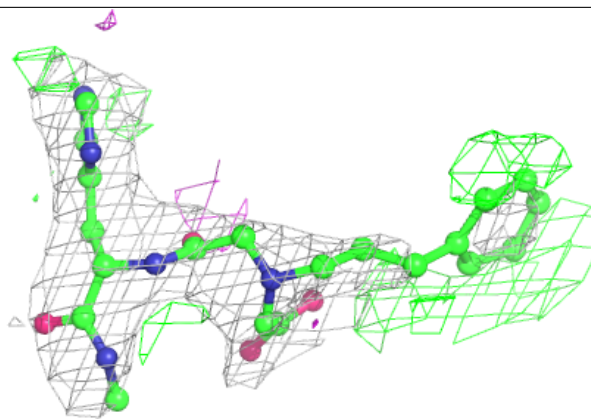
Electron density around MGJ B 1101:

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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.