



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

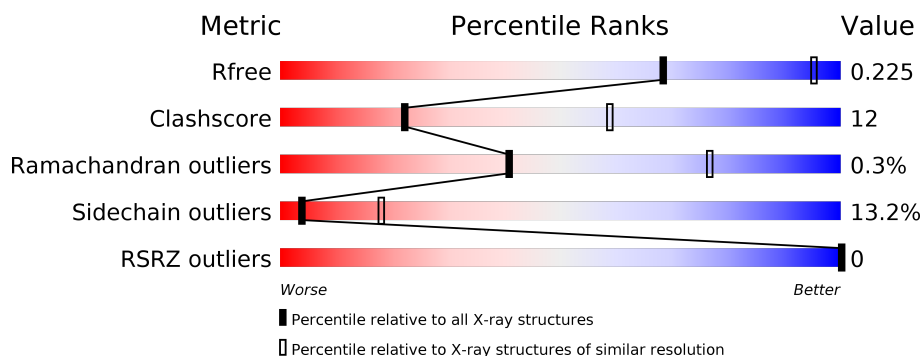
# 1 Overall quality at a glance ⓘ

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  $\geq 3$ , 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:

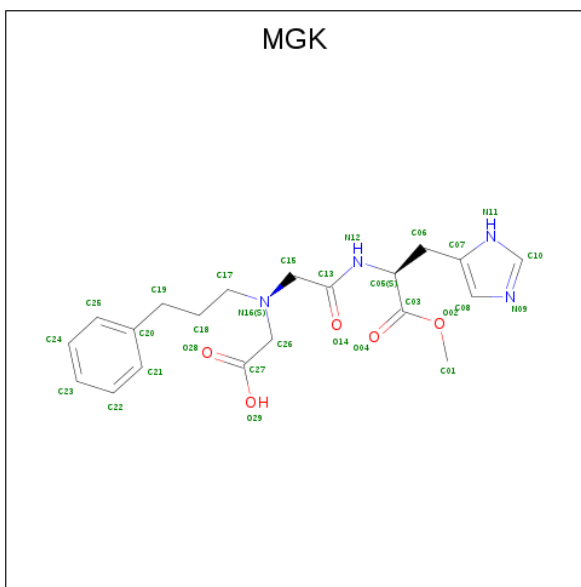
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735
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: C<sub>20</sub>H<sub>26</sub>N<sub>4</sub>O<sub>5</sub>).



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

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

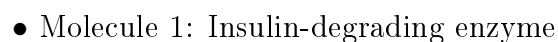
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

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

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:  68% 23% 5% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

All (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
1	B	577	GLU	CG-CD	6.96	1.62	1.51
1	B	287	GLU	CG-CD	6.61	1.61	1.51
1	B	287	GLU	CB-CG	6.04	1.63	1.52
1	B	453	GLU	CB-CG	6.01	1.63	1.52
1	B	189	GLU	CB-CG	5.99	1.63	1.52
1	B	529	GLU	CB-CG	5.67	1.62	1.52
1	A	176	GLU	CG-CD	5.62	1.60	1.51
1	A	880	GLU	CG-CD	5.62	1.60	1.51
1	B	494	GLU	CG-CD	5.01	1.59	1.51

All (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
1	A	189	GLU	CG-CD-OE2	6.75	131.81	118.30
1	A	226	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	67	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	253	LEU	CB-CG-CD1	-6.19	100.47	111.00
1	B	189	GLU	CA-CB-CG	5.98	126.56	113.40
1	A	285	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	456	LEU	CB-CA-C	-5.75	99.27	110.20
1	A	892	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	189	GLU	N-CA-CB	5.61	120.70	110.60
1	B	49	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	97	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	92	VAL	CB-CA-C	-5.25	101.44	111.40
1	B	175	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	243	LYS	CD-CE-NZ	5.22	123.71	111.70
1	A	170	LEU	CA-CB-CG	-5.13	103.49	115.30
1	A	189	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	626	GLY	N-CA-C	-5.05	100.48	113.10
1	B	771	LEU	CA-CB-CG	5.04	126.88	115.30

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

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

All (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
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.33	0.94
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.52	0.91
1:B:754:HIS:CE1	4:B:1236:HOH:O	2.28	0.85
1:B:622:ASN:H	1:B:622:ASN:HD22	1.25	0.84
1:B:348:SER:OG	1:B:606:GLU:OE2	1.97	0.81
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.62	0.80
1:B:754:HIS:HE1	4:B:1236:HOH:O	1.62	0.79
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.77
2:B:1101:MGK:H26A	2:B:1101:MGK:O14	1.84	0.76
1:A:722:ARG:HB2	1:A:758:LEU:HD12	1.67	0.76
1:B:206:LYS:HG2	1:B:215:PHE:O	1.85	0.76
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.16	0.75
1:B:189:GLU:HG2	1:B:831:TYR:CE1	2.22	0.75
1:A:309:ASP:H	1:A:672:ASN:HD21	1.32	0.75
1:A:491:ARG:NH1	1:A:491:ARG:HG3	1.96	0.75
1:B:774:ARG:CG	1:B:774:ARG:HH11	1.99	0.75
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.87	0.74
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.86	0.74
1:A:730:HIS:HD2	1:A:904:SER:OG	1.71	0.73
1:A:927:TYR:O	1:A:930:THR:HB	1.86	0.73
1:A:50:ILE:O	1:A:50:ILE:CG2	2.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HB2	1:A:757:PRO:CD	2.18	0.73
1:B:309:ASP:H	1:B:672:ASN:HD21	1.37	0.73
1:B:108:HIS:CE1	1:B:189:GLU:OE1	2.21	0.72
1:A:622:ASN:N	1:A:622:ASN:HD22	1.85	0.72
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.72	0.71
1:B:783:ASN:HD22	1:B:785:VAL:H	1.36	0.71
1:A:102:ASN:HD22	1:A:102:ASN:H	1.39	0.70
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.40	0.70
1:B:994:ASN:HB3	1:B:997:GLU:HB2	1.74	0.70
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.76	0.69
1:A:711:ARG:HH21	1:A:711:ARG:HG2	1.59	0.68
1:B:243:LYS:NZ	1:B:243:LYS:HB2	2.09	0.67
1:B:257:VAL:HG21	1:B:437:ILE:HG22	1.76	0.67
1:A:623:THR:OG1	1:A:626:GLY:O	2.06	0.67
1:B:196:ASN:ND2	1:B:198:ALA:H	1.93	0.67
1:B:112:HIS:CE1	1:B:189:GLU:OE1	2.39	0.67
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.30	0.67
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.43	0.66
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.30	0.66
1:A:783:ASN:ND2	1:A:786:HIS:H	1.95	0.65
1:A:191:GLU:HA	1:A:194:VAL:HG23	1.79	0.65
1:B:86:SER:HB3	1:B:158:LEU:HG	1.79	0.65
1:A:760:PRO:HA	1:A:763:LEU:HD12	1.77	0.65
1:B:622:ASN:HD22	1:B:622:ASN:N	1.91	0.65
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.32	0.64
1:B:920:ARG:O	1:B:924:GLU:HG3	1.98	0.63
1:A:67:LEU:CD2	1:A:75:VAL:HB	2.29	0.63
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.82	0.62
1:B:575:ASN:N	1:B:575:ASN:HD22	1.96	0.62
1:B:294:GLN:H	1:B:297:HIS:HD2	1.45	0.62
1:B:311:ARG:NH1	1:B:379:LEU:O	2.30	0.62
1:B:309:ASP:H	1:B:672:ASN:ND2	1.96	0.62
1:B:676:GLU:HA	1:B:676:GLU:OE1	1.99	0.62
1:A:294:GLN:H	1:A:297:HIS:CD2	2.16	0.62
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.82	0.61
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.82	0.61
1:B:102:ASN:H	1:B:102:ASN:HD22	1.48	0.61
1:A:545:THR:HB	1:A:546:PRO:HD2	1.82	0.61
1:A:108:HIS:CE1	1:A:189:GLU:OE2	2.50	0.60
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.36	0.60
1:B:110:LEU:HD23	1:B:110:LEU:C	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.32	0.60
1:B:272:VAL:O	1:B:276:SER:OG	2.20	0.60
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.83	0.60
1:A:491:ARG:CG	1:A:491:ARG:HH11	2.10	0.59
1:A:62:ARG:HG2	1:A:80:ASP:HB2	1.84	0.59
1:A:800:GLN:HB3	1:A:805:ASN:HD21	1.68	0.59
1:B:93:HIS:HD2	1:B:145:GLU:O	1.86	0.59
1:A:303:LYS:HG2	1:A:485:PHE:CE2	2.38	0.58
1:B:693:VAL:HB	1:B:766:TYR:CE2	2.39	0.58
1:A:784:GLU:O	1:A:961:ARG:HG3	2.03	0.58
1:B:962:GLU:OE2	1:B:962:GLU:HA	2.03	0.58
1:A:298:LEU:HD13	1:A:475:ASN:CB	2.33	0.58
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.37	0.58
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.37	0.58
1:A:309:ASP:H	1:A:672:ASN:ND2	2.01	0.58
1:A:136:GLY:CA	1:A:152:ASP:O	2.52	0.57
1:A:316:THR:HB	1:A:374:ILE:HG22	1.86	0.57
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.57
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.70	0.57
1:A:341:GLU:OE1	2:A:1101:MGK:H10	2.05	0.57
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.87	0.57
1:B:803:SER:HB2	1:B:927:TYR:OH	2.04	0.57
1:B:298:LEU:HD13	1:B:475:ASN:HB2	1.86	0.57
1:A:674:ARG:HD3	4:A:1235:HOH:O	2.05	0.57
1:A:715:PHE:CZ	1:A:719:LEU:CD2	2.88	0.57
1:B:134:HIS:CD2	1:B:157:HIS:CD2	2.93	0.57
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.87	0.56
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.40	0.56
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.32	0.56
1:B:765:ARG:NH1	1:B:912:ILE:O	2.39	0.56
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.88	0.56
1:B:535:PHE:HB3	1:B:570:PRO:HG3	1.87	0.56
1:A:722:ARG:HA	1:A:756:LYS:O	2.05	0.55
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.72	0.55
1:B:941:LYS:HB2	1:B:941:LYS:NZ	2.20	0.55
1:A:780:GLN:HE22	1:A:959:LEU:HD11	1.72	0.55
1:A:363:GLN:HG3	1:A:371:MET:HE1	1.87	0.55
1:A:599:LEU:HD23	1:A:662:ILE:HD13	1.89	0.55
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.87	0.55
1:B:579:PHE:HE2	1:B:765:ARG:HH22	1.55	0.55
1:A:136:GLY:HA2	1:A:152:ASP:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.36	0.55
1:A:887:GLN:HE21	1:A:891:ILE:HD11	1.72	0.55
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.23	0.54
1:A:425:LYS:NZ	1:A:425:LYS:HB3	2.22	0.54
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.90	0.54
1:B:538:LEU:HD22	1:B:734:THR:HG23	1.90	0.54
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.43	0.54
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.90	0.54
1:B:856:PRO:HA	1:B:859:LEU:HB2	1.90	0.54
1:A:329:ASN:N	1:A:330:PRO:CD	2.71	0.54
1:B:108:HIS:O	1:B:111:GLN:HB3	2.08	0.54
1:A:298:LEU:HD13	1:A:475:ASN:HB2	1.90	0.53
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.88	0.53
1:A:602:ASP:OD2	1:A:658:ARG:NH1	2.42	0.53
1:B:262:GLU:CD	1:B:262:GLU:H	2.12	0.53
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.90	0.53
1:B:685:TYR:HB2	1:B:956:VAL:HG11	1.90	0.53
1:A:482:SER:HB3	1:A:485:PHE:CE1	2.43	0.53
1:B:643:LYS:O	1:B:647:GLU:HB2	2.09	0.53
1:B:783:ASN:ND2	1:B:786:HIS:H	2.07	0.53
1:B:203:GLN:HG3	1:B:203:GLN:O	2.08	0.53
1:B:815:ILE:HG22	1:B:870:MET:HG2	1.91	0.53
1:B:809:GLU:OE2	1:B:839:ARG:NH2	2.39	0.53
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.43	0.53
2:B:1101:MGK:O14	2:B:1101:MGK:C26	2.55	0.53
1:B:807:PHE:HE1	1:B:935:ASP:HB3	1.73	0.53
1:A:97:LEU:HB2	1:A:144:GLY:O	2.09	0.53
1:B:772:PRO:HD3	1:B:1002:LEU:HD21	1.91	0.53
1:A:78:ILE:O	1:A:259:LEU:HA	2.09	0.52
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.39	0.52
1:B:887:GLN:O	1:B:890:ALA:HB3	2.09	0.52
1:A:428:GLU:H	1:A:428:GLU:CD	2.12	0.52
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.91	0.52
1:A:756:LYS:HB2	1:A:757:PRO:HD2	1.92	0.52
1:B:134:HIS:HD2	1:B:157:HIS:CD2	2.28	0.52
1:B:774:ARG:HG3	1:B:774:ARG:NH1	2.04	0.52
2:A:1101:MGK:H08	2:A:1101:MGK:HN12	1.74	0.52
1:A:188:SER:HB3	1:A:831:TYR:CB	2.35	0.52
1:A:805:ASN:O	1:A:809:GLU:HG3	2.09	0.52
1:B:774:ARG:CG	1:B:774:ARG:NH1	2.66	0.52
1:B:196:ASN:ND2	1:B:198:ALA:N	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.92	0.52
1:B:575:ASN:ND2	1:B:575:ASN:N	2.57	0.52
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.92	0.51
1:B:108:HIS:HE1	1:B:189:GLU:CD	2.08	0.51
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.46	0.51
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.91	0.51
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.92	0.51
1:A:714:ALA:O	1:A:717:PRO:HD2	2.11	0.51
1:B:194:VAL:HG12	1:B:195:MET:HG2	1.91	0.51
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.09	0.51
1:A:511:LYS:HE3	1:A:514:GLN:OE1	2.11	0.51
1:A:595:LEU:HD12	1:A:662:ILE:HG22	1.92	0.51
1:B:298:LEU:HD21	1:B:318:PRO:HG3	1.93	0.51
1:B:843:ILE:HG22	1:B:844:GLN:N	2.25	0.51
1:A:334:LEU:HD22	1:A:468:LEU:HD13	1.93	0.50
1:B:817:GLU:N	1:B:818:PRO:HD2	2.25	0.50
1:A:693:VAL:HB	1:A:766:TYR:CE2	2.45	0.50
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.93	0.50
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.93	0.50
1:B:803:SER:HB2	1:B:927:TYR:CZ	2.46	0.50
1:A:108:HIS:CE1	1:A:189:GLU:CD	2.84	0.50
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.47	0.50
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.15	0.50
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.94	0.50
1:A:196:ASN:ND2	1:A:196:ASN:C	2.64	0.50
1:B:229:ARG:NH1	1:B:233:GLU:OE2	2.41	0.50
1:A:196:ASN:HD22	1:A:199:TRP:H	1.60	0.50
1:B:175:ASP:HB3	1:B:178:ALA:HB3	1.93	0.50
1:B:196:ASN:HD22	1:B:196:ASN:C	2.15	0.50
1:B:52:ASN:HD22	1:B:52:ASN:N	2.09	0.50
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.46	0.50
1:B:708:THR:OG1	1:B:711:ARG:HB2	2.11	0.50
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.94	0.49
1:A:86:SER:HB3	1:A:158:LEU:HG	1.94	0.49
1:B:815:ILE:HA	1:B:870:MET:HE2	1.93	0.49
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.93	0.49
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.76	0.49
1:B:795:TYR:CE2	1:B:953:LYS:HD2	2.48	0.49
1:B:413:GLU:OE2	1:B:527:LYS:HE2	2.12	0.49
1:B:214:PRO:O	1:B:217:LYS:HG3	2.13	0.49
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.94	0.49
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.48	0.49
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.95	0.49
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.95	0.48
1:A:312:ASN:HB3	1:A:377:VAL:O	2.13	0.48
1:B:359:LEU:O	2:B:1101:MGK:H10	2.13	0.48
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.95	0.48
1:B:643:LYS:HB2	1:B:744:MET:SD	2.53	0.48
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.95	0.48
1:B:196:ASN:HD22	1:B:198:ALA:N	2.11	0.48
1:B:874:ILE:HA	1:B:877:MET:HG2	1.94	0.48
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.48
1:A:793:ILE:O	1:A:847:ARG:HA	2.14	0.48
1:B:189:GLU:HG2	1:B:831:TYR:CD1	2.47	0.48
1:B:125:ASN:H	1:B:125:ASN:HD22	1.62	0.48
1:B:655:ASP:HB3	1:B:658:ARG:HB2	1.96	0.48
1:B:329:ASN:HD22	1:B:332:HIS:H	1.60	0.47
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.95	0.47
1:A:521:LYS:HD2	1:A:521:LYS:HA	1.58	0.47
1:A:908:TRP:O	1:A:912:ILE:HG12	2.15	0.47
2:B:1101:MGK:H18A	2:B:1101:MGK:H15A	1.75	0.47
1:B:622:ASN:H	1:B:622:ASN:ND2	2.03	0.47
1:B:686:LEU:HA	1:B:686:LEU:HD12	1.66	0.47
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.62	0.47
1:B:243:LYS:HZ2	1:B:243:LYS:HB2	1.80	0.47
1:B:579:PHE:HE2	1:B:765:ARG:NH2	2.11	0.47
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.97	0.47
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.95	0.47
1:B:52:ASN:ND2	1:B:52:ASN:N	2.62	0.47
1:B:600:LEU:O	1:B:604:LEU:HB2	2.14	0.47
1:A:363:GLN:HG3	1:A:371:MET:CE	2.44	0.47
1:B:616:LEU:HD21	1:B:638:GLN:HG3	1.97	0.47
1:A:196:ASN:ND2	1:A:199:TRP:H	2.13	0.47
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.48	0.47
1:A:359:LEU:HD23	1:A:359:LEU:C	2.36	0.47
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.96	0.47
1:A:756:LYS:CB	1:A:757:PRO:CD	2.88	0.46
1:A:780:GLN:O	1:A:781:GLN:HG2	2.16	0.46
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.16	0.46
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.44	0.46
1:B:250:SER:HB2	1:B:281:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.97	0.46
1:A:782:ARG:NH1	1:A:963:MET:O	2.45	0.46
1:B:597:LEU:HD21	1:B:627:MET:HG2	1.97	0.46
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.98	0.46
1:A:392:LEU:O	1:A:396:GLN:HG3	2.15	0.46
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.45	0.46
1:B:671:ASN:OD1	1:B:701:LYS:HD3	2.16	0.46
1:B:932:THR:OG1	1:B:934:GLU:HB2	2.16	0.46
1:A:102:ASN:HD22	1:A:102:ASN:N	2.06	0.46
1:A:140:ALA:HA	1:A:148:ASN:O	2.16	0.46
1:A:914:GLN:HA	1:A:916:TYR:CE1	2.51	0.46
1:A:789:SER:HB2	1:A:958:VAL:O	2.16	0.46
1:B:809:GLU:OE1	1:B:893:ARG:HD3	2.16	0.46
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.98	0.45
1:A:313:LEU:HD22	1:A:387:VAL:HG22	1.98	0.45
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.49	0.45
1:B:200:ARG:NH2	1:B:498:THR:HA	2.32	0.45
1:B:861:SER:O	1:B:865:ALA:N	2.48	0.45
1:B:622:ASN:ND2	1:B:622:ASN:N	2.63	0.45
1:B:691:THR:O	1:B:999:LYS:CE	2.65	0.45
1:B:915:GLN:HG2	1:B:1008:VAL:HG11	1.99	0.45
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.63	0.45
1:B:672:ASN:HA	1:B:672:ASN:HD22	1.53	0.45
1:B:838:ARG:HG3	1:B:847:ARG:HD3	1.98	0.45
1:A:773:ASP:O	1:A:774:ARG:HB2	2.17	0.45
1:B:308:LYS:HD3	1:B:672:ASN:HB3	1.98	0.45
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.97	0.45
1:A:706:ASP:O	1:A:711:ARG:HD3	2.15	0.44
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.99	0.44
1:A:756:LYS:CB	1:A:757:PRO:HD3	2.47	0.44
1:B:229:ARG:HD3	1:B:229:ARG:HA	1.54	0.44
1:B:578:PHE:CD2	1:B:725:ILE:HG12	2.52	0.44
1:B:76:LEU:HD12	1:B:437:ILE:HG21	1.99	0.44
1:A:756:LYS:HB2	1:A:757:PRO:HD3	1.97	0.44
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.20	0.44
1:B:341:GLU:HG2	1:B:347:LEU:CD1	2.25	0.44
1:B:770:GLN:HG2	1:B:1003:PRO:HG2	1.98	0.44
1:B:810:LEU:HG	1:B:928:LEU:HD21	2.00	0.44
1:B:941:LYS:HZ1	1:B:941:LYS:HB2	1.82	0.44
1:B:583:ALA:O	1:B:590:SER:HA	2.17	0.44
1:A:206:LYS:HB3	1:A:216:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:HD21	1:A:995:MET:HG2	1.99	0.44
1:B:196:ASN:ND2	1:B:196:ASN:C	2.71	0.44
1:B:826:LYS:HE3	1:B:826:LYS:HB2	1.61	0.44
1:B:349:GLU:HA	1:B:349:GLU:OE2	2.18	0.44
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.48	0.44
1:A:123:LYS:O	1:A:124:GLU:C	2.56	0.44
1:A:824:ARG:O	1:A:828:GLN:HA	2.18	0.44
1:B:294:GLN:H	1:B:297:HIS:CD2	2.31	0.44
1:A:294:GLN:O	1:A:298:LEU:HG	2.18	0.43
1:A:334:LEU:CD2	1:A:468:LEU:HD13	2.48	0.43
1:B:425:LYS:HB3	1:B:425:LYS:HE3	1.82	0.43
1:B:744:MET:O	1:B:744:MET:HG2	2.17	0.43
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.80	0.43
1:A:583:ALA:HB2	1:A:626:GLY:HA2	1.99	0.43
1:B:329:ASN:ND2	1:B:332:HIS:CB	2.81	0.43
1:A:1009:LYS:HD2	1:A:1009:LYS:HA	1.80	0.43
1:A:886:ILE:HG12	1:A:928:LEU:HD22	2.00	0.43
1:B:329:ASN:ND2	1:B:332:HIS:HB2	2.33	0.43
1:B:363:GLN:HG3	1:B:371:MET:CE	2.49	0.43
1:B:656:GLU:O	1:B:659:PHE:HB3	2.18	0.43
1:A:136:GLY:HA3	1:A:152:ASP:O	2.19	0.43
1:A:67:LEU:C	1:A:67:LEU:HD23	2.38	0.43
1:A:51:GLY:HA2	1:A:52:ASN:HA	1.71	0.43
1:A:862:ARG:NH2	1:A:981:SER:O	2.44	0.43
1:B:785:VAL:HG12	1:B:786:HIS:CD2	2.53	0.43
1:A:125:ASN:HD22	1:A:125:ASN:H	1.66	0.43
1:B:93:HIS:CD2	1:B:145:GLU:O	2.70	0.43
1:A:299:LYS:HB2	1:A:299:LYS:HE3	1.88	0.43
1:A:887:GLN:HE21	1:A:891:ILE:CD1	2.32	0.43
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.43
1:B:160:GLY:O	1:B:164:ARG:HG3	2.18	0.43
1:B:78:ILE:O	1:B:259:LEU:HA	2.19	0.43
1:B:962:GLU:OE2	1:B:962:GLU:CA	2.66	0.43
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.61	0.43
1:B:311:ARG:HB3	1:B:379:LEU:HB2	2.01	0.43
1:A:809:GLU:HB3	1:A:889:LEU:HD11	2.01	0.43
1:A:567:PHE:CE1	1:A:900:LEU:HA	2.53	0.43
1:B:597:LEU:HD23	1:B:622:ASN:N	2.34	0.43
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.84	0.42
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.85	0.42
1:B:129:GLN:O	1:B:133:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.52	0.42
1:B:631:VAL:HG12	1:B:638:GLN:HG2	2.01	0.42
1:B:674:ARG:CG	1:B:674:ARG:HH11	2.32	0.42
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.48	0.42
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.18	0.42
1:A:596:TYR:OH	1:A:649:MET:HG3	2.19	0.42
1:A:896:LYS:HE2	1:A:896:LYS:HB2	1.52	0.42
1:B:511:LYS:HD2	1:B:514:GLN:OE1	2.19	0.42
1:A:408:GLU:HB2	1:A:459:PHE:CE2	2.55	0.42
1:B:730:HIS:HD2	1:B:904:SER:OG	2.02	0.42
1:A:114:LEU:HD13	1:A:168:PHE:HB3	2.01	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.75	0.42
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.50	0.42
1:A:187:ASP:O	1:A:191:GLU:HG2	2.20	0.42
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.01	0.42
1:A:774:ARG:NH1	1:A:774:ARG:HG3	2.34	0.42
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.34	0.42
1:B:243:LYS:HE2	4:B:1206:HOH:O	2.20	0.42
1:A:584:TYR:CE2	1:A:624:ILE:HG22	2.55	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.83	0.41
1:A:709:LEU:O	1:A:710:PRO:C	2.59	0.41
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.85	0.41
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	2.02	0.41
1:B:445:PRO:HG2	1:B:448:GLU:HG3	2.01	0.41
1:A:559:LEU:HD22	1:A:742:MET:HB2	2.02	0.41
1:B:238:ARG:O	1:B:242:LEU:HD12	2.20	0.41
1:A:359:LEU:HD23	1:A:360:VAL:N	2.36	0.41
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.56	0.41
1:B:417:LEU:HA	1:B:417:LEU:HD12	1.69	0.41
1:A:547:TYR:HB2	4:A:1202:HOH:O	2.20	0.41
1:B:433:TYR:CE1	1:B:437:ILE:HD11	2.55	0.41
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.55	0.41
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.55	0.41
1:A:941:LYS:O	1:A:949:PRO:HD2	2.21	0.41
1:A:652:PHE:CE2	1:A:654:ILE:HG12	2.55	0.41
1:A:94:ILE:HG22	1:A:95:GLY:N	2.35	0.41
1:A:1004:LEU:HA	1:A:1004:LEU:HD23	1.88	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.63	0.41
1:B:329:ASN:O	1:B:330:PRO:C	2.56	0.41
1:B:465:GLU:O	1:B:469:ASP:HB2	2.20	0.41
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:NZ	4:A:1255:HOH:O	2.53	0.41
1:A:852:SER:OG	1:A:853:GLU:N	2.54	0.41
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.55	0.41
1:A:196:ASN:C	1:A:196:ASN:HD22	2.24	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.54	0.41
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.21	0.40
1:A:151:PHE:C	1:A:151:PHE:CD1	2.94	0.40
1:A:204:LEU:O	1:A:208:THR:HG23	2.22	0.40
1:B:773:ASP:O	1:B:774:ARG:HB2	2.21	0.40
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.85	0.40
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.57	0.40
1:B:801:SER:O	1:B:802:THR:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

All (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
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	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

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	52	ASN
1	A	61	LYS
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	120	LYS
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	188	SER
1	A	196	ASN
1	A	201	LEU
1	A	226	LEU
1	A	239	GLN
1	A	270	LEU
1	A	277	GLU
1	A	285	LEU
1	A	287	GLU
1	A	303	LYS
1	A	312	ASN
1	A	316	THR
1	A	324	LYS
1	A	329	ASN

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Mol	Chain	Res	Type
1	A	332	HIS
1	A	337	LEU
1	A	347	LEU
1	A	353	LYS
1	A	360	VAL
1	A	363	GLN
1	A	364	LYS
1	A	402	ARG
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	420	VAL
1	A	423	ARG
1	A	433	TYR
1	A	446	LEU
1	A	466	MET
1	A	488	LYS
1	A	489	THR
1	A	491	ARG
1	A	501	LYS
1	A	508	GLU
1	A	511	LYS
1	A	517	ASP
1	A	521	LYS
1	A	524	LEU
1	A	527	LYS
1	A	538	LEU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	607	TYR
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	644	LYS
1	A	648	LYS
1	A	657	LYS
1	A	662	ILE
1	A	663	LYS
1	A	674	ARG
1	A	677	GLN

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Mol	Chain	Res	Type
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	722	ARG
1	A	728	LEU
1	A	741	ILE
1	A	744	MET
1	A	751	GLU
1	A	756	LYS
1	A	758	LEU
1	A	759	LEU
1	A	764	VAL
1	A	765	ARG
1	A	771	LEU
1	A	780	GLN
1	A	783	ASN
1	A	801	SER
1	A	810	LEU
1	A	823	LEU
1	A	838	ARG
1	A	846	LEU
1	A	859	LEU
1	A	862	ARG
1	A	867	LEU
1	A	872	LYS
1	A	889	LEU
1	A	892	ARG
1	A	901	SER
1	A	906	LYS
1	A	928	LEU
1	A	929	LYS
1	A	933	LYS
1	A	938	LYS
1	A	957	HIS
1	A	982	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	44	ASN
1	B	61	LYS
1	B	76	LEU
1	B	92	VAL

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	128	SER
1	B	148	ASN
1	B	158	LEU
1	B	179	LYS
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	229	ARG
1	B	239	GLN
1	B	270	LEU
1	B	276	SER
1	B	285	LEU
1	B	287	GLU
1	B	290	GLU
1	B	316	THR
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	348	SER
1	B	353	LYS
1	B	360	VAL
1	B	364	LYS
1	B	399	GLN
1	B	414	LEU
1	B	417	LEU
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	458	GLU
1	B	460	ARG
1	B	494	GLU
1	B	507	ASP
1	B	508	GLU
1	B	512	LYS
1	B	517	ASP
1	B	521	LYS

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Mol	Chain	Res	Type
1	B	523	LYS
1	B	524	LEU
1	B	527	LYS
1	B	556	MET
1	B	575	ASN
1	B	586	ASP
1	B	587	PRO
1	B	595	LEU
1	B	597	LEU
1	B	601	LYS
1	B	602	ASP
1	B	604	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	643	LYS
1	B	644	LYS
1	B	648	LYS
1	B	657	LYS
1	B	674	ARG
1	B	677	GLN
1	B	702	GLU
1	B	711	ARG
1	B	712	LEU
1	B	713	LYS
1	B	718	GLN
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	744	MET
1	B	746	GLU
1	B	751	GLU
1	B	756	LYS
1	B	759	LEU
1	B	764	VAL
1	B	765	ARG
1	B	774	ARG
1	B	782	ARG
1	B	783	ASN
1	B	803	SER

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Mol	Chain	Res	Type
1	B	806	MET
1	B	809	GLU
1	B	810	LEU
1	B	823	LEU
1	B	838	ARG
1	B	846	LEU
1	B	854	LYS
1	B	859	LEU
1	B	867	LEU
1	B	868	ILE
1	B	880	GLU
1	B	884	LYS
1	B	886	ILE
1	B	889	LEU
1	B	892	ARG
1	B	898	LYS
1	B	899	LYS
1	B	923	THR
1	B	928	LEU
1	B	941	LYS
1	B	942	GLU
1	B	957	HIS
1	B	980	LEU
1	B	990	GLU
1	B	993	GLN
1	B	1007	LEU
1	B	1009	LYS
1	B	1011	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS

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Mol	Chain	Res	Type
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	393	HIS
1	A	407	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	786	HIS
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	887	GLN
1	A	988	GLN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	134	HIS
1	B	148	ASN
1	B	157	HIS
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	232	GLN
1	B	297	HIS
1	B	300	GLN
1	B	329	ASN
1	B	336	HIS
1	B	386	HIS
1	B	475	ASN
1	B	502	GLN
1	B	575	ASN
1	B	589	HIS

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Mol	Chain	Res	Type
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	783	ASN
1	B	805	ASN
1	B	821	ASN
1	B	828	GLN
1	B	841	ASN
1	B	883	GLN
1	B	887	GLN
1	B	922	ASN
1	B	957	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

All (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
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
2	A	1101	MGK	C15-C13-N12	3.19	122.50	115.31
2	B	1101	MGK	C03-C05-N12	2.79	117.15	110.72
2	B	1101	MGK	O02-C03-O04	-2.59	118.77	123.84
2	A	1101	MGK	O04-C03-C05	-2.51	116.42	123.92
2	B	1101	MGK	C26-N16-C17	2.28	116.09	111.29
2	A	1101	MGK	O14-C13-N12	-2.14	119.34	122.95

There are no chirality outliers.

All (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

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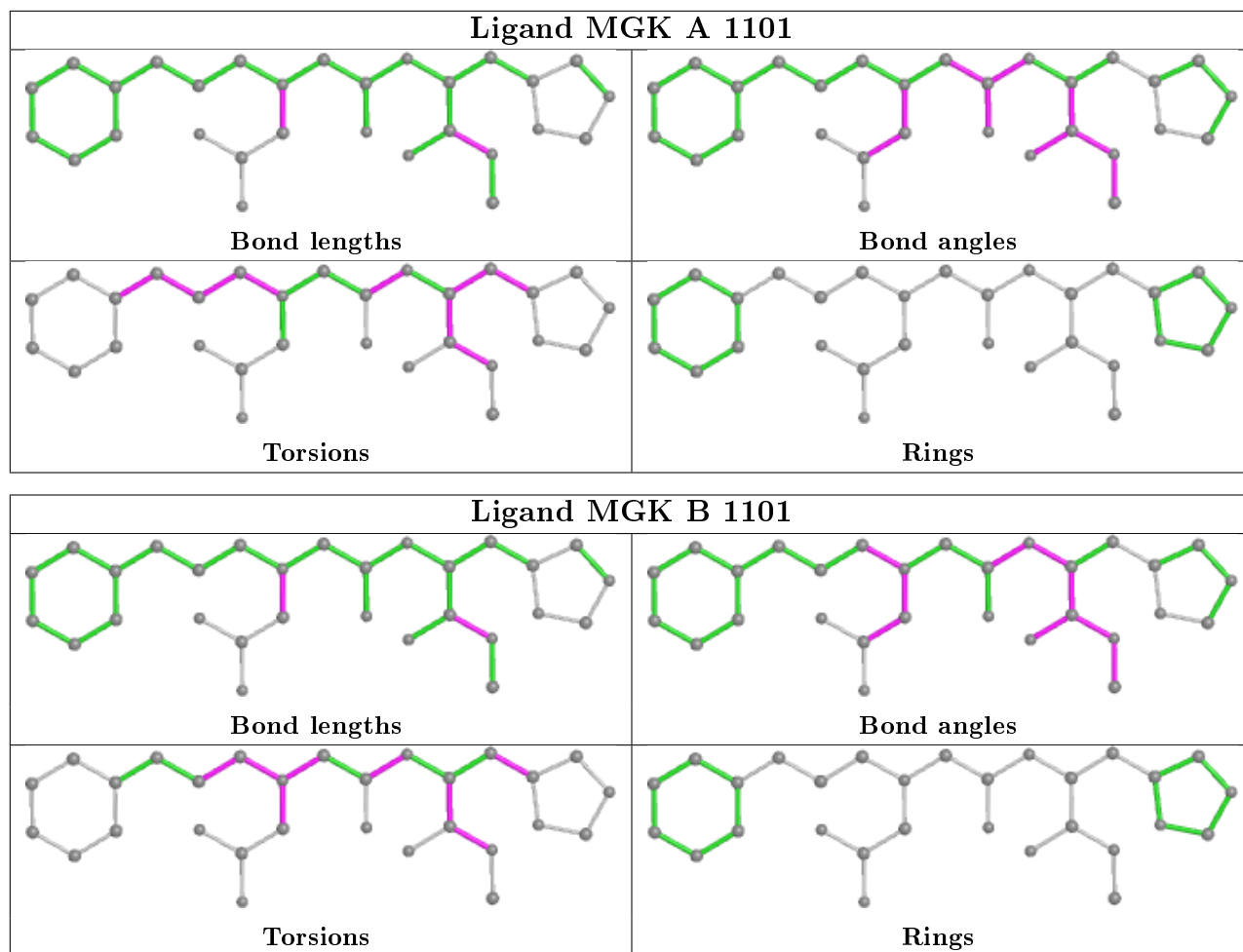
Mol	Chain	Res	Type	Atoms
2	B	1101	MGK	C05-C06-C07-C08
2	B	1101	MGK	C05-C03-O02-C01
2	B	1101	MGK	O04-C03-O02-C01
2	A	1101	MGK	C05-C03-O02-C01
2	A	1101	MGK	O14-C13-N12-C05
2	A	1101	MGK	C15-C13-N12-C05
2	A	1101	MGK	O04-C03-O02-C01
2	B	1101	MGK	C18-C17-N16-C15
2	A	1101	MGK	N16-C17-C18-C19
2	B	1101	MGK	N16-C17-C18-C19
2	B	1101	MGK	C27-C26-N16-C17
2	B	1101	MGK	O14-C13-N12-C05
2	A	1101	MGK	O02-C03-C05-N12
2	A	1101	MGK	O04-C03-C05-N12
2	B	1101	MGK	C15-C13-N12-C05
2	A	1101	MGK	N12-C05-C06-C07
2	B	1101	MGK	C18-C17-N16-C26
2	A	1101	MGK	C18-C17-N16-C15
2	A	1101	MGK	C18-C19-C20-C25
2	A	1101	MGK	C18-C19-C20-C21
2	B	1101	MGK	O04-C03-C05-C06
2	B	1101	MGK	C27-C26-N16-C15

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, 95<sup>th</sup> 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 <sup>2</sup> )	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, 95<sup>th</sup> 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 <sup>2</sup> )	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

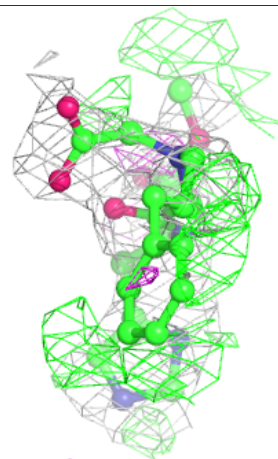
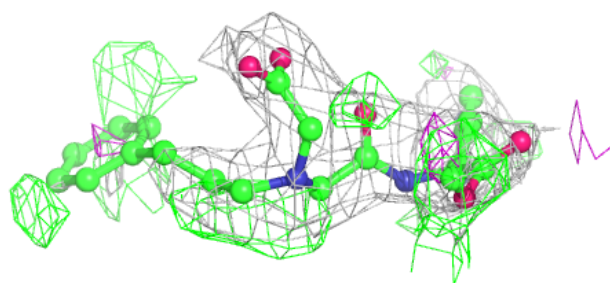
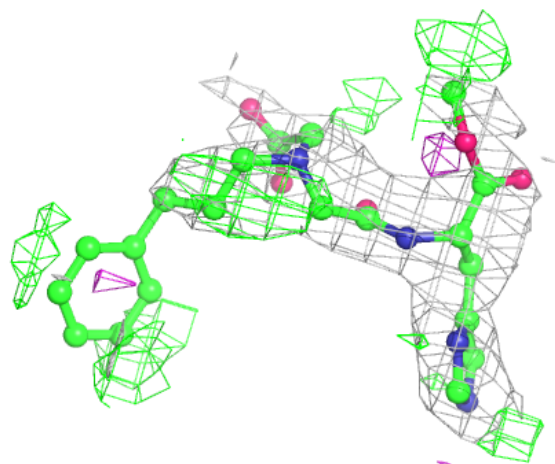
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

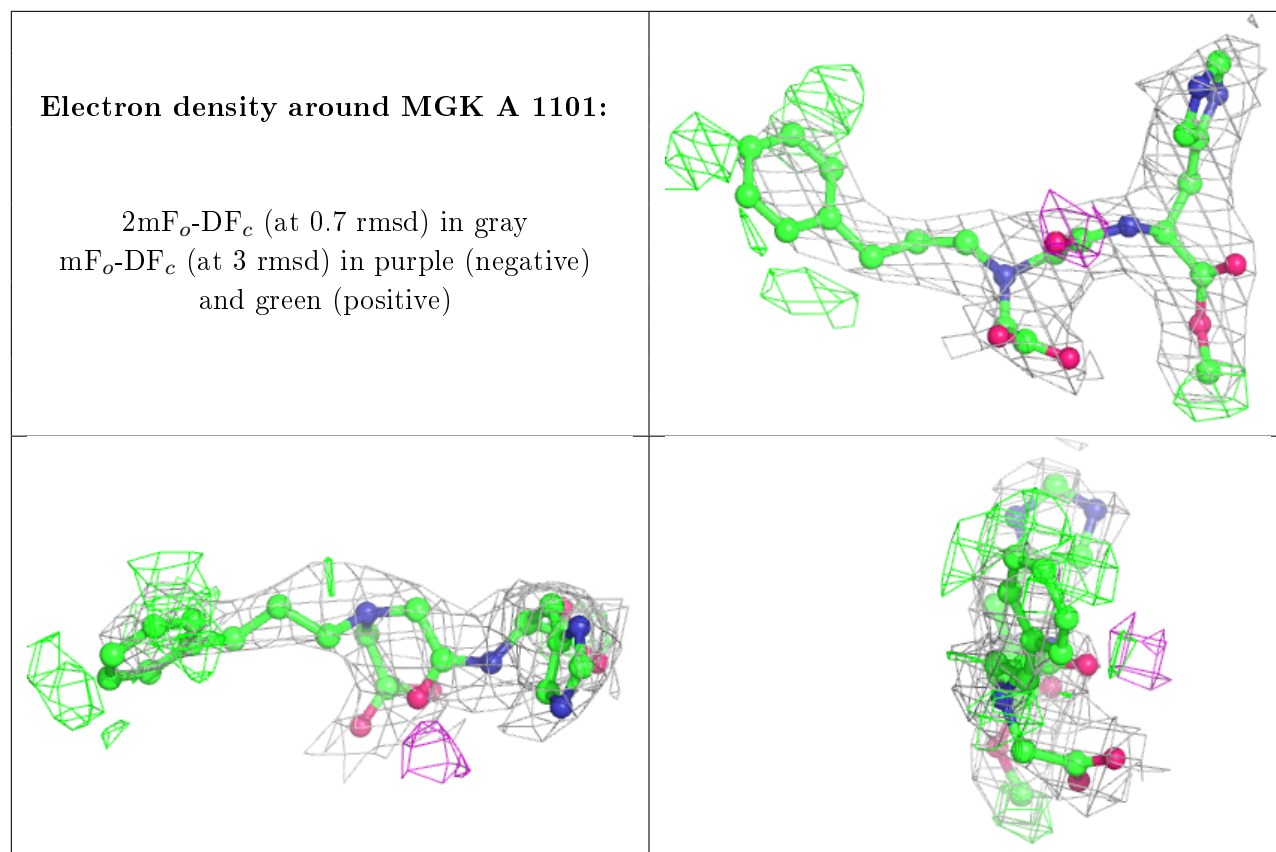


as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**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.