



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:59 am BST

PDB ID : 4GSC
Title : Structure analysis of insulin degrading enzyme with compound bdm41559 ((s)-2-[2-(carboxymethyl-phenethyl-amino)-acetylamino]-3-(1h-imidazol-4-yl)-propanoic acid methyl ester)
Authors : Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on : 2012-08-27
Resolution : 2.81 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

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

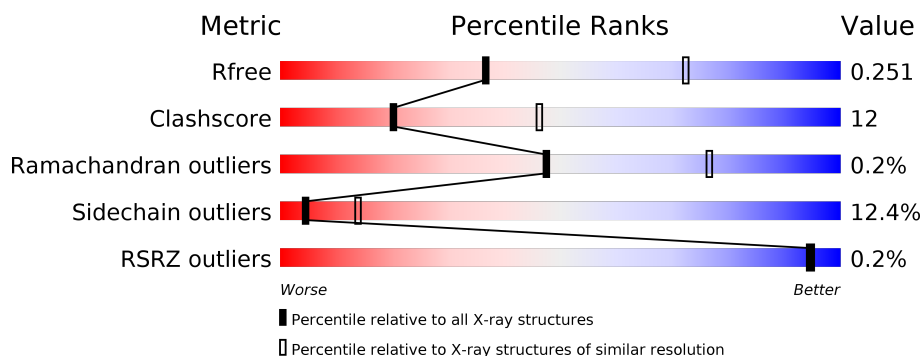
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	 66% 27% . .
1	B	990	 65% 27% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15858 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	958	Total	C	N	O	S	0	0	1
			7818	5035	1315	1445	23			
1	B	956	Total	C	N	O	S	0	0	1
			7802	5026	1312	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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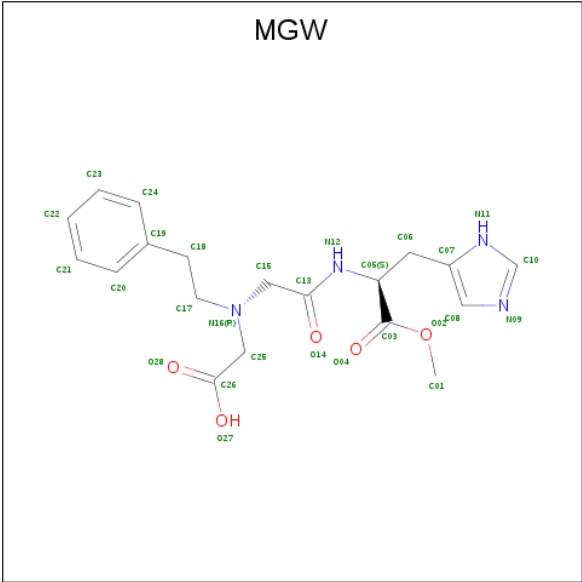
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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	30	MET	-	EXPRESSION TAG	UNP P14735
B	31	HIS	-	EXPRESSION TAG	UNP P14735
B	32	HIS	-	EXPRESSION TAG	UNP P14735
B	33	HIS	-	EXPRESSION TAG	UNP P14735
B	34	HIS	-	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

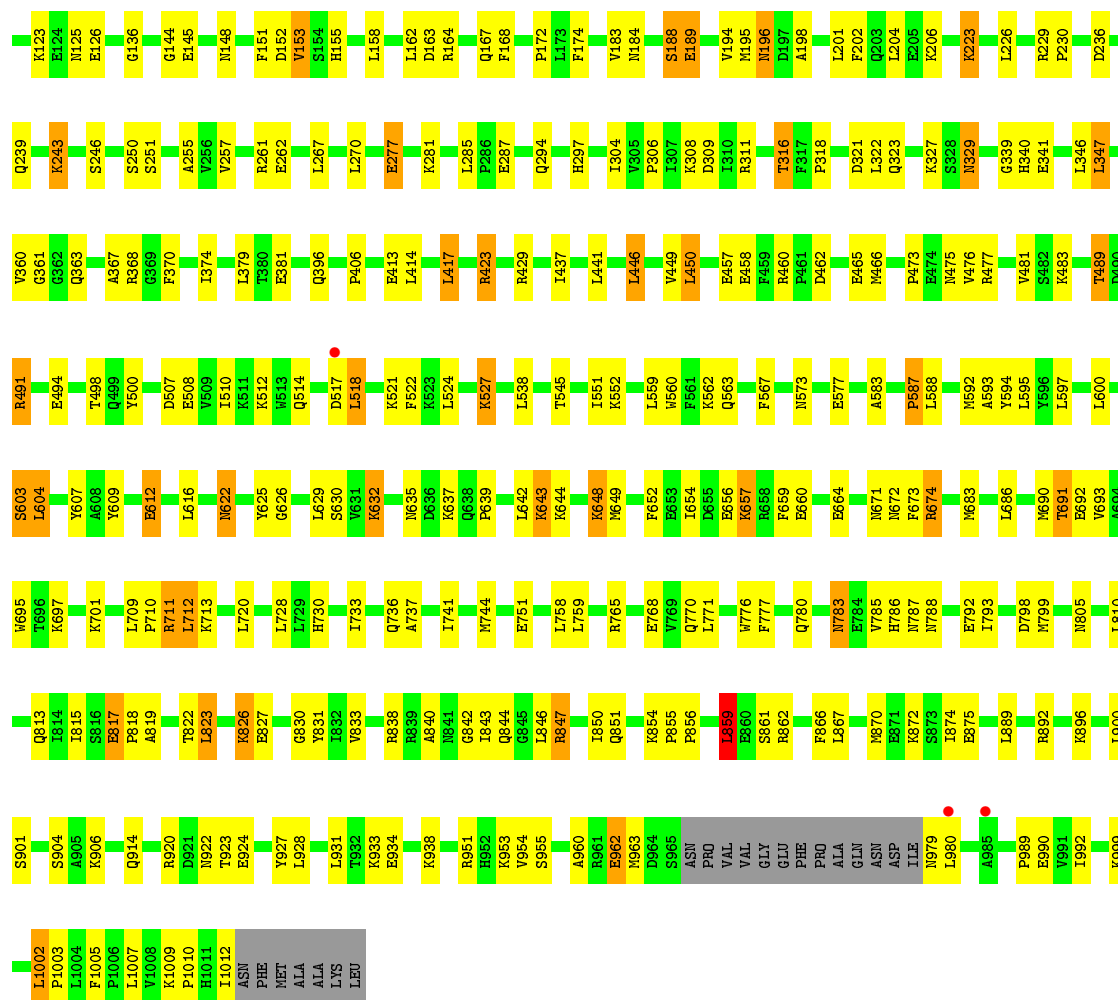
- Molecule 3 is methyl N-(carboxymethyl)-N-(2-phenylethyl)glycyl-L-histidinate (three-letter code: MGW) (formula: C₁₉H₂₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	4	5		
3	B	1	Total	C	N	O	0	0
			28	19	4	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	72	Total	O	0	0
			72	72		



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.76 Å 263.76 Å 91.26 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.81 49.85 – 2.81	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.85-2.81) 89.4 (49.85-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.253 0.196 , 0.251	Depositor DCC
R_{free} test set	3992 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15858	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: ZN, MGW

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	6/8013 (0.1%)	0.94	18/10841 (0.2%)
1	B	0.89	7/7997 (0.1%)	0.89	9/10820 (0.1%)
All	All	0.91	13/16010 (0.1%)	0.92	27/21661 (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	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	GLU	CG-CD	9.95	1.66	1.51
1	A	577	GLU	CG-CD	8.22	1.64	1.51
1	B	189	GLU	CB-CG	6.35	1.64	1.52
1	B	577	GLU	CG-CD	6.04	1.61	1.51
1	B	660	GLU	CG-CD	5.89	1.60	1.51
1	A	189	GLU	CB-CG	5.85	1.63	1.52
1	A	577	GLU	CB-CG	5.73	1.63	1.52
1	A	189	GLU	CG-CD	5.19	1.59	1.51
1	B	287	GLU	CG-CD	5.18	1.59	1.51
1	B	494	GLU	CG-CD	5.18	1.59	1.51
1	A	660	GLU	CG-CD	5.14	1.59	1.51
1	A	596	TYR	CB-CG	-5.06	1.44	1.51
1	B	673	PHE	CE2-CZ	5.01	1.46	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	GLU	OE1-CD-OE2	-8.31	113.32	123.30
1	B	489	THR	CB-CA-C	-7.75	90.66	111.60
1	B	153	VAL	CB-CA-C	6.52	123.79	111.40
1	B	52	ASN	N-CA-C	6.19	127.71	111.00
1	A	75	VAL	CB-CA-C	-6.11	99.78	111.40
1	A	62	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	711	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	A	928	LEU	CA-CB-CG	5.96	129.02	115.30
1	B	92	VAL	CB-CA-C	-5.92	100.15	111.40
1	A	491	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	446	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	655	ASP	N-CA-C	-5.77	95.41	111.00
1	A	586	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	859	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	524	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	797	THR	N-CA-C	5.60	126.12	111.00
1	A	67	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	107	SER	N-CA-CB	5.52	118.78	110.50
1	A	238	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	847	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	674	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	76	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	507	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	524	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	759	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	857	HIS	N-CA-CB	5.07	119.73	110.60
1	A	538	LEU	CB-CG-CD1	5.03	119.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	52	ASN	Peptide

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	7818	0	7749	173	0
1	B	7802	0	7734	216	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	23	6	0
3	B	28	0	22	4	0
4	A	108	0	0	10	0
4	B	72	0	0	6	0
All	All	15858	0	15528	389	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 (389) 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:527:LYS:HB2	1:B:527:LYS:NZ	1.62	1.15
1:A:892:ARG:HD3	4:A:1236:HOH:O	1.52	1.07
1:B:527:LYS:HB2	1:B:527:LYS:HZ3	1.06	1.07
1:A:108:HIS:CE1	1:A:189:GLU:OE1	2.09	1.02
1:A:112:HIS:NE2	1:A:189:GLU:OE1	1.91	1.01
1:A:108:HIS:CE1	1:A:189:GLU:CD	2.40	0.95
1:B:711:ARG:HH21	1:B:711:ARG:HG2	1.34	0.92
1:A:622:ASN:H	1:A:622:ASN:ND2	1.68	0.92
1:B:783:ASN:HD22	1:B:785:VAL:H	1.16	0.91
1:A:189:GLU:HG2	1:A:831:TYR:CE1	2.06	0.91
1:B:527:LYS:NZ	1:B:527:LYS:CB	2.33	0.90
1:B:622:ASN:H	1:B:622:ASN:ND2	1.70	0.90
1:B:309:ASP:H	1:B:672:ASN:HD21	1.21	0.88
1:A:622:ASN:H	1:A:622:ASN:HD22	0.89	0.87
1:B:622:ASN:H	1:B:622:ASN:HD22	0.91	0.87
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.56	0.85
1:A:294:GLN:H	1:A:297:HIS:HD2	1.23	0.85
1:A:341:GLU:HG2	1:A:347:LEU:HD12	1.59	0.85
1:B:622:ASN:N	1:B:622:ASN:HD22	1.73	0.83
1:A:622:ASN:N	1:A:622:ASN:HD22	1.71	0.83
1:A:80:ASP:O	1:A:83:THR:HG22	1.78	0.82
1:B:674:ARG:CG	1:B:674:ARG:HH11	1.93	0.81
1:B:491:ARG:HH11	1:B:491:ARG:HG3	1.45	0.80
1:B:97:LEU:HB2	1:B:144:GLY:O	1.82	0.80
1:A:783:ASN:ND2	1:A:786:HIS:H	1.79	0.80
1:B:196:ASN:ND2	1:B:198:ALA:H	1.78	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:HE1	4:A:1201:HOH:O	1.64	0.79
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.12	0.79
1:A:108:HIS:NE2	1:A:112:HIS:NE2	2.31	0.78
1:A:782:ARG:HH22	1:A:964:ASP:HA	1.49	0.77
1:A:270:LEU:HD22	1:A:274:LEU:HD11	1.64	0.77
1:A:108:HIS:HE1	1:A:189:GLU:CD	1.89	0.76
1:B:783:ASN:ND2	1:B:785:VAL:H	1.85	0.75
1:A:196:ASN:HD22	1:A:199:TRP:HD1	1.32	0.74
1:B:194:VAL:HG12	1:B:195:MET:HG2	1.68	0.74
1:A:112:HIS:CE1	1:A:189:GLU:OE1	2.41	0.74
1:A:722:ARG:HB2	1:A:758:LEU:HD12	1.70	0.73
1:B:309:ASP:H	1:B:672:ASN:ND2	1.86	0.73
1:B:604:LEU:HD21	1:B:648:LYS:HD2	1.71	0.73
3:A:1102:MGW:H206	3:A:1102:MGW:O14	1.88	0.72
1:B:642:LEU:HD23	1:B:642:LEU:C	2.10	0.72
1:A:196:ASN:ND2	1:A:199:TRP:HD1	1.89	0.71
1:B:920:ARG:O	1:B:924:GLU:HG3	1.91	0.71
1:B:603:SER:OG	1:B:648:LYS:HE2	1.91	0.70
1:B:659:PHE:CE1	1:B:712:LEU:HD12	2.27	0.70
1:A:154:SER:HB2	1:A:891:ILE:HD13	1.74	0.70
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.72	0.70
1:B:527:LYS:HZ3	1:B:527:LYS:CB	1.90	0.69
1:A:815:ILE:HG22	1:A:870:MET:HG2	1.75	0.69
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.93	0.69
1:A:512:LYS:O	1:A:512:LYS:HD3	1.93	0.69
1:A:270:LEU:CD2	1:A:274:LEU:HD11	2.22	0.68
1:A:294:GLN:H	1:A:297:HIS:CD2	2.10	0.68
1:A:102:ASN:HD22	1:A:102:ASN:H	1.39	0.68
1:B:491:ARG:HH11	1:B:491:ARG:CG	2.07	0.68
1:B:604:LEU:CD2	1:B:648:LYS:HD2	2.23	0.68
1:B:674:ARG:HH11	1:B:674:ARG:HG2	1.58	0.68
1:B:361:GLY:O	3:B:1102:MGW:N12	2.27	0.67
1:B:642:LEU:HD23	1:B:642:LEU:O	1.93	0.67
1:B:1002:LEU:HB3	1:B:1003:PRO:HD2	1.75	0.67
1:A:270:LEU:HD22	1:A:274:LEU:CD1	2.23	0.67
1:B:527:LYS:HB2	1:B:527:LYS:HZ2	1.60	0.67
1:B:361:GLY:H	3:B:1102:MGW:H106	1.59	0.66
1:B:67:LEU:HD23	1:B:75:VAL:HB	1.77	0.66
1:A:404:GLU:HA	1:A:404:GLU:OE1	1.95	0.66
1:B:196:ASN:HD22	1:B:198:ALA:H	1.43	0.66
1:B:629:LEU:HD23	1:B:630:SER:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:OE1	3:A:1102:MGW:H10	1.96	0.66
1:B:204:LEU:CD2	1:B:304:ILE:HD13	2.26	0.66
1:B:77:LEU:HD22	1:B:267:LEU:HB3	1.78	0.66
1:A:927:TYR:O	1:A:930:THR:HB	1.96	0.65
1:B:294:GLN:H	1:B:297:HIS:CD2	2.14	0.65
1:A:213:HIS:ND1	1:A:214:PRO:HD2	2.12	0.65
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.44	0.65
1:A:843:ILE:HG22	1:A:844:GLN:N	2.12	0.64
1:B:671:ASN:OD1	1:B:701:LYS:HD3	1.97	0.64
1:A:547:TYR:CE2	1:A:919:ASP:HB2	2.32	0.64
1:B:339:GLY:O	3:B:1102:MGW:H08	1.97	0.64
1:A:654:ILE:HG22	1:A:655:ASP:N	2.13	0.64
1:B:339:GLY:HA3	3:B:1102:MGW:H206	1.78	0.64
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.80	0.64
1:B:294:GLN:H	1:B:297:HIS:HD2	1.43	0.64
1:B:102:ASN:H	1:B:102:ASN:HD22	1.44	0.63
1:A:658:ARG:NH2	4:A:1254:HOH:O	2.30	0.63
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.46	0.63
1:B:559:LEU:HD12	1:B:560:TRP:N	2.13	0.63
1:B:625:TYR:CZ	1:B:765:ARG:HD2	2.33	0.63
1:B:45:PRO:HA	4:B:1258:HOH:O	1.98	0.63
1:B:316:THR:HB	1:B:374:ILE:HG22	1.81	0.62
1:B:711:ARG:HD2	4:B:1217:HOH:O	1.97	0.62
1:B:588:LEU:O	1:B:592:MET:HG3	1.98	0.62
1:A:134:HIS:O	1:A:154:SER:HB3	1.99	0.62
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.35	0.62
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.81	0.61
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.98	0.61
1:A:843:ILE:HG22	1:A:844:GLN:H	1.64	0.61
1:A:656:GLU:HG2	1:A:709:LEU:CD2	2.30	0.61
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.81	0.61
1:A:783:ASN:HD21	1:A:786:HIS:H	1.45	0.60
1:A:204:LEU:O	1:A:204:LEU:HG	2.00	0.60
1:B:329:ASN:C	1:B:329:ASN:HD22	2.04	0.60
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.84	0.60
1:B:423:ARG:CG	1:B:423:ARG:HH11	2.15	0.59
1:B:856:PRO:HA	1:B:859:LEU:HD22	1.82	0.59
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.84	0.59
1:B:793:ILE:O	1:B:847:ARG:HA	2.02	0.59
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.35	0.59
1:B:654:ILE:HD12	1:B:713:LYS:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:TRP:CD1	1:B:953:LYS:HD3	2.37	0.59
1:B:196:ASN:HD22	1:B:198:ALA:N	2.01	0.58
1:B:783:ASN:ND2	1:B:786:HIS:H	2.00	0.58
1:B:396:GLN:HG2	1:B:517:ASP:O	2.04	0.58
1:A:512:LYS:HD3	1:A:512:LYS:C	2.24	0.58
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.69	0.58
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.84	0.58
1:B:510:ILE:O	1:B:514:GLN:HG3	2.03	0.58
1:B:711:ARG:CD	4:B:1217:HOH:O	2.51	0.58
1:B:783:ASN:C	1:B:783:ASN:HD22	2.07	0.58
1:A:222:ASN:O	1:A:226:LEU:HB2	2.04	0.57
1:B:329:ASN:HD21	1:B:363:GLN:HE22	1.52	0.57
1:B:674:ARG:HH11	1:B:674:ARG:HG3	1.68	0.57
1:A:281:LYS:HG3	4:A:1214:HOH:O	2.05	0.57
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.87	0.57
1:A:155:HIS:ND1	1:A:261:ARG:HD2	2.19	0.57
1:A:406:PRO:HG2	1:A:461:PRO:HB3	1.85	0.57
1:A:270:LEU:O	1:A:274:LEU:HD12	2.05	0.57
1:B:527:LYS:HZ2	1:B:527:LYS:CB	2.12	0.56
1:B:874:ILE:O	1:B:933:LYS:HE3	2.04	0.56
1:A:317:PHE:N	1:A:317:PHE:CD1	2.74	0.56
1:B:108:HIS:HE1	1:B:189:GLU:CD	2.01	0.56
1:A:921:ASP:O	1:A:925:VAL:HG23	2.06	0.56
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.40	0.56
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.87	0.56
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.41	0.56
1:A:125:ASN:HD22	1:A:125:ASN:H	1.53	0.56
1:B:473:PRO:O	1:B:476:VAL:HG12	2.06	0.56
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.09	0.56
1:A:446:LEU:O	1:A:449:VAL:HG13	2.05	0.56
1:A:656:GLU:HG2	1:A:709:LEU:HD22	1.88	0.56
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.40	0.56
1:A:671:ASN:O	1:A:674:ARG:HG2	2.05	0.55
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.42	0.55
1:B:145:GLU:OE1	1:B:367:ALA:HA	2.06	0.55
1:A:243:LYS:HD3	4:A:1252:HOH:O	2.07	0.55
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.88	0.55
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.07	0.55
1:A:765:ARG:NH1	1:A:912:ILE:O	2.40	0.55
1:A:760:PRO:HA	1:A:763:LEU:HD12	1.89	0.54
1:B:361:GLY:HA2	1:B:374:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:GLN:OE1	1:B:892:ARG:NH2	2.41	0.54
1:A:730:HIS:HD2	1:A:904:SER:OG	1.90	0.54
1:A:602:ASP:OD2	1:A:658:ARG:NH1	2.40	0.53
1:A:245:HIS:O	1:A:249:TYR:HB2	2.08	0.53
1:B:819:ALA:HA	1:B:866:PHE:CZ	2.43	0.53
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.44	0.53
1:A:997:GLU:HG3	1:A:1000:ARG:HH12	1.73	0.53
1:B:204:LEU:HD23	1:B:304:ILE:HD13	1.91	0.53
1:B:674:ARG:CG	1:B:674:ARG:NH1	2.62	0.53
1:A:311:ARG:HA	1:A:481:VAL:O	2.08	0.53
1:A:682:ALA:HA	1:A:956:VAL:HG11	1.89	0.53
1:A:784:GLU:O	1:A:961:ARG:HG3	2.09	0.52
1:B:805:ASN:HD22	1:B:844:GLN:NE2	2.06	0.52
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.55	0.52
1:A:200:ARG:CZ	1:A:307:ILE:HD11	2.38	0.52
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.43	0.52
1:B:642:LEU:C	1:B:642:LEU:CD2	2.76	0.52
1:A:722:ARG:CB	1:A:758:LEU:HD12	2.39	0.52
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.55	0.52
1:B:196:ASN:ND2	1:B:198:ALA:N	2.53	0.52
1:A:151:PHE:C	1:A:151:PHE:CD1	2.82	0.52
1:A:309:ASP:O	1:A:668:ARG:HD2	2.10	0.52
1:A:547:TYR:HB3	1:A:548:PRO:HD2	1.91	0.52
1:A:856:PRO:O	1:A:857:HIS:C	2.47	0.51
1:A:576:PHE:N	1:A:576:PHE:CD1	2.78	0.51
1:A:824:ARG:O	1:A:828:GLN:HA	2.10	0.51
1:B:110:LEU:HD23	1:B:110:LEU:C	2.31	0.51
1:B:697:LYS:O	1:B:701:LYS:HB2	2.10	0.51
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.45	0.51
1:B:196:ASN:HD22	1:B:196:ASN:C	2.14	0.51
1:B:77:LEU:HD22	1:B:267:LEU:CB	2.40	0.51
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.72	0.51
1:A:793:ILE:O	1:A:847:ARG:HA	2.11	0.51
1:B:648:LYS:O	1:B:652:PHE:HB2	2.11	0.51
1:B:172:PRO:HG2	1:B:174:PHE:CE1	2.46	0.51
1:A:880:GLU:CB	1:B:457:GLU:HG2	2.40	0.51
1:B:277:GLU:H	1:B:277:GLU:CD	2.14	0.51
1:A:189:GLU:HG2	1:A:831:TYR:CD1	2.46	0.51
1:B:162:LEU:HD23	1:B:270:LEU:CD2	2.41	0.51
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.93	0.50
1:B:184:ASN:ND2	1:B:223:LYS:NZ	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:VAL:HG21	1:B:437:ILE:HG22	1.92	0.50
1:B:559:LEU:C	1:B:559:LEU:HD12	2.32	0.50
1:B:567:PHE:CE1	1:B:900:LEU:HA	2.47	0.50
1:A:88:ALA:HA	1:A:257:VAL:O	2.12	0.50
1:B:838:ARG:HB2	1:B:847:ARG:HG2	1.93	0.50
1:B:119:LYS:HB2	1:B:119:LYS:HZ2	1.77	0.50
1:B:476:VAL:HG22	1:B:477:ARG:H	1.77	0.50
1:B:787:ASN:OD1	1:B:962:GLU:HG2	2.12	0.50
1:B:843:ILE:HG22	1:B:844:GLN:H	1.76	0.50
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.94	0.49
1:A:829:LEU:O	1:A:852:SER:HB2	2.12	0.49
1:B:476:VAL:HG22	1:B:477:ARG:N	2.27	0.49
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.46	0.49
1:B:622:ASN:N	1:B:622:ASN:ND2	2.42	0.49
1:B:819:ALA:O	1:B:823:LEU:HB2	2.12	0.49
1:B:815:ILE:HA	1:B:870:MET:HE2	1.93	0.49
1:A:248:TYR:O	1:A:250:SER:N	2.43	0.49
1:A:49:ARG:O	1:A:67:LEU:HB2	2.13	0.49
1:A:408:GLU:HG3	1:A:459:PHE:CD2	2.48	0.48
1:A:843:ILE:CG2	1:A:844:GLN:H	2.26	0.48
1:A:368:ARG:HD2	4:A:1250:HOH:O	2.13	0.48
1:A:654:ILE:CG2	1:A:655:ASP:N	2.76	0.48
1:A:880:GLU:O	1:A:881:ALA:C	2.51	0.48
1:A:982:GLN:OE1	1:A:982:GLN:HA	2.13	0.48
1:B:656:GLU:O	1:B:659:PHE:HB3	2.11	0.48
1:B:80:ASP:O	1:B:83:THR:HG22	2.13	0.48
1:B:367:ALA:HB3	1:B:370:PHE:CE2	2.48	0.48
1:B:843:ILE:HG22	1:B:844:GLN:N	2.28	0.48
1:B:155:HIS:CE1	1:B:261:ARG:NH1	2.82	0.48
1:A:961:ARG:HD2	1:A:962:GLU:OE1	2.14	0.48
1:A:342:GLY:O	1:A:345:SER:HB3	2.13	0.48
1:B:657:LYS:HA	1:B:657:LYS:HE3	1.95	0.48
1:A:597:LEU:O	1:A:601:LYS:HG3	2.13	0.48
1:A:961:ARG:NH2	4:A:1231:HOH:O	2.44	0.48
1:A:1001:GLY:O	1:A:1002:LEU:HD23	2.14	0.47
1:B:822:THR:O	1:B:827:GLU:HG3	2.14	0.47
1:A:815:ILE:CG2	1:A:870:MET:HG2	2.44	0.47
1:B:709:LEU:HB3	1:B:710:PRO:CD	2.44	0.47
1:A:374:ILE:C	1:A:375:ILE:HG13	2.33	0.47
1:B:491:ARG:HB2	1:B:500:TYR:O	2.14	0.47
1:B:311:ARG:NH1	1:B:379:LEU:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.97	0.47
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.97	0.47
1:A:298:LEU:HD13	1:A:475:ASN:HB2	1.97	0.47
1:B:818:PRO:HD2	4:B:1201:HOH:O	2.14	0.47
1:A:427:LYS:HE2	1:A:898:LYS:HD2	1.96	0.47
1:A:562:LYS:HG2	1:A:563:GLN:O	2.14	0.47
1:B:308:LYS:HE2	1:B:672:ASN:HB3	1.96	0.47
1:A:843:ILE:CG2	1:A:844:GLN:N	2.78	0.47
1:A:765:ARG:HH11	1:A:914:GLN:HG3	1.80	0.47
1:B:691:THR:O	1:B:999:LYS:CE	2.63	0.47
1:B:817:GLU:N	1:B:818:PRO:HD2	2.29	0.47
1:A:770:GLN:HE21	1:A:1003:PRO:HB2	1.80	0.46
1:A:197:ASP:HA	1:A:200:ARG:HD3	1.98	0.46
1:A:489:THR:HB	1:A:500:TYR:O	2.15	0.46
1:A:559:LEU:C	1:A:559:LEU:HD12	2.35	0.46
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.51	0.46
1:B:236:ASP:OD1	1:B:236:ASP:C	2.53	0.46
1:B:243:LYS:HA	1:B:243:LYS:HD3	1.63	0.46
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.30	0.46
1:B:691:THR:O	1:B:999:LYS:HE2	2.14	0.46
1:A:474:GLU:OE2	1:A:514:GLN:NE2	2.48	0.46
1:A:834:PHE:HE2	1:A:847:ARG:HE	1.63	0.46
1:A:834:PHE:HE2	1:A:847:ARG:NE	2.13	0.46
1:A:196:ASN:ND2	1:A:199:TRP:CD1	2.75	0.46
1:B:413:GLU:OE2	1:B:527:LYS:HD3	2.15	0.46
1:A:65:ARG:HB2	1:A:264:LEU:HD13	1.98	0.46
1:B:417:LEU:HD12	1:B:417:LEU:HA	1.71	0.46
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.46	0.46
1:B:311:ARG:HB2	1:B:379:LEU:HB2	1.98	0.46
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.97	0.46
1:B:674:ARG:HG3	1:B:674:ARG:NH1	2.29	0.46
1:B:818:PRO:HG2	1:B:870:MET:HE2	1.98	0.46
1:B:306:PRO:HG3	1:B:481:VAL:HG12	1.97	0.46
1:B:600:LEU:HD21	1:B:649:MET:HB3	1.98	0.46
1:B:819:ALA:HA	1:B:866:PHE:CE1	2.51	0.46
1:A:360:VAL:HA	3:A:1102:MGW:N09	2.30	0.45
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.81	0.45
1:B:329:ASN:O	1:B:329:ASN:ND2	2.48	0.45
1:A:389:ASP:O	1:A:393:HIS:HD2	2.00	0.45
1:A:920:ARG:HD2	4:A:1249:HOH:O	2.16	0.45
1:B:751:GLU:HG2	1:B:751:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD12	1:A:302:TYR:N	2.31	0.45
1:A:770:GLN:HA	1:A:1005:PHE:CE1	2.51	0.45
1:B:85:LYS:HA	1:B:153:VAL:O	2.16	0.45
1:B:954:VAL:HG12	1:B:955:SER:N	2.31	0.45
1:B:74:LYS:O	1:B:255:ALA:HA	2.17	0.45
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.34	0.45
1:B:573:ASN:OD1	1:B:632:LYS:HB3	2.16	0.45
1:A:242:LEU:O	1:A:246:SER:HB2	2.16	0.45
1:A:308:LYS:HD3	1:A:672:ASN:HB3	1.98	0.45
1:A:815:ILE:HG22	1:A:870:MET:CG	2.43	0.45
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.98	0.45
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.99	0.45
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.16	0.45
1:A:856:PRO:HB2	1:A:957:HIS:CD2	2.52	0.45
1:A:768:GLU:OE1	4:A:1275:HOH:O	2.21	0.45
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.99	0.45
1:B:830:GLY:HA3	1:B:851:GLN:O	2.17	0.45
1:A:319:ILE:HD12	1:A:322:LEU:HD11	1.99	0.44
1:A:361:GLY:H	3:A:1102:MGW:H08	1.82	0.44
1:B:777:PHE:HB3	1:B:992:ILE:HD11	1.99	0.44
1:B:737:ALA:O	1:B:741:ILE:HG13	2.17	0.44
1:B:67:LEU:CD2	1:B:75:VAL:HB	2.44	0.44
1:B:294:GLN:O	1:B:297:HIS:N	2.47	0.44
1:A:932:THR:O	1:A:933:LYS:C	2.56	0.44
1:B:97:LEU:HA	1:B:97:LEU:HD12	1.85	0.44
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.53	0.44
1:A:934:GLU:OE1	1:B:52:ASN:O	2.35	0.44
1:B:770:GLN:HG2	1:B:1003:PRO:HG2	1.99	0.44
1:A:106:LEU:O	1:A:106:LEU:HG	2.18	0.44
1:B:551:ILE:H	1:B:551:ILE:HG13	1.73	0.44
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.82	0.43
1:B:450:LEU:HA	1:B:450:LEU:HD12	1.65	0.43
1:B:491:ARG:NH1	4:B:1231:HOH:O	2.52	0.43
1:A:688:LEU:HD13	1:A:696:THR:HG22	2.00	0.43
1:B:867:LEU:HD12	1:B:867:LEU:HA	1.84	0.43
1:B:649:MET:HE3	1:B:649:MET:HB3	1.68	0.43
1:B:236:ASP:HB3	1:B:239:GLN:HG3	2.00	0.43
1:B:896:LYS:HA	1:B:896:LYS:HE2	2.00	0.43
1:A:801:SER:O	1:A:802:THR:C	2.57	0.43
1:B:720:LEU:HD23	1:B:720:LEU:HA	1.81	0.43
1:A:188:SER:HB3	1:A:831:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:ARG:O	1:B:844:GLN:HA	2.19	0.43
1:B:788:ASN:O	1:B:960:ALA:HA	2.18	0.43
1:A:71:ASN:HB2	1:A:251:SER:OG	2.19	0.43
1:A:189:GLU:CG	1:A:831:TYR:CE1	2.89	0.43
1:B:600:LEU:HD12	1:B:600:LEU:HA	1.76	0.43
1:B:686:LEU:HA	1:B:686:LEU:HD12	1.79	0.43
1:B:922:ASN:HD22	1:B:922:ASN:N	2.15	0.43
1:B:489:THR:OG1	1:B:489:THR:O	2.33	0.43
1:B:683:MET:HA	1:B:792:GLU:OE2	2.18	0.43
1:B:690:MET:O	1:B:768:GLU:HG3	2.19	0.43
1:B:776:TRP:CD2	1:B:989:PRO:HB3	2.54	0.43
1:A:558:LYS:HB2	1:A:726:GLU:HG3	2.01	0.42
1:B:711:ARG:CG	1:B:711:ARG:HH21	2.18	0.42
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.54	0.42
1:B:643:LYS:HB2	1:B:744:MET:SD	2.59	0.42
1:B:833:VAL:HG22	1:B:850:ILE:HG12	2.01	0.42
1:A:794:TYR:CE1	1:A:845:GLY:HA3	2.54	0.42
1:B:250:SER:HB2	1:B:281:LYS:HB2	2.01	0.42
1:B:340:HIS:CD2	1:B:609:TYR:HE2	2.37	0.42
1:B:799:MET:HB3	1:B:799:MET:HE3	1.95	0.42
1:A:776:TRP:CZ3	1:A:987:PRO:O	2.73	0.42
1:A:910:GLU:OE2	1:A:910:GLU:HA	2.20	0.42
1:B:102:ASN:H	1:B:102:ASN:ND2	2.13	0.42
1:B:329:ASN:C	1:B:329:ASN:ND2	2.72	0.42
1:A:309:ASP:H	1:A:672:ASN:ND2	2.17	0.42
1:A:350:LEU:CB	1:A:356:VAL:HG22	2.50	0.42
1:A:444:TYR:CD1	1:A:452:ALA:HB1	2.54	0.42
1:B:163:ASP:O	1:B:164:ARG:C	2.57	0.42
1:B:593:ALA:O	1:B:594:TYR:C	2.57	0.42
1:B:960:ALA:HB3	1:B:963:MET:HG3	2.02	0.42
1:A:776:TRP:HZ3	1:A:987:PRO:O	2.03	0.42
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.63	0.42
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.50	0.42
1:A:505:ILE:HB	1:A:510:ILE:CD1	2.50	0.42
1:A:915:GLN:O	1:A:1011:HIS:HB2	2.19	0.42
1:B:318:PRO:HD2	1:B:475:ASN:O	2.20	0.42
1:B:826:LYS:HE3	1:B:826:LYS:HB2	1.75	0.41
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.88	0.41
1:A:125:ASN:HD22	1:A:125:ASN:N	2.18	0.41
1:B:483:LYS:HD2	1:B:483:LYS:HA	1.82	0.41
3:A:1102:MGW:H125	3:A:1102:MGW:H118	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:SER:O	1:B:281:LYS:NZ	2.45	0.41
1:B:659:PHE:HE1	1:B:712:LEU:HD12	1.80	0.41
1:A:646:ILE:HG13	1:A:745:VAL:HG22	2.02	0.41
1:B:136:GLY:HA3	1:B:152:ASP:O	2.19	0.41
1:B:709:LEU:HB3	1:B:710:PRO:HD3	2.02	0.41
1:A:237:VAL:O	1:A:238:ARG:C	2.58	0.41
1:A:123:LYS:O	1:A:124:GLU:C	2.59	0.41
1:A:444:TYR:CE1	1:A:452:ALA:HB1	2.56	0.41
1:B:609:TYR:O	1:B:612:GLU:HB3	2.20	0.41
1:B:818:PRO:HG2	1:B:870:MET:CE	2.51	0.41
1:A:108:HIS:CE1	1:A:112:HIS:NE2	2.89	0.41
1:A:309:ASP:H	1:A:672:ASN:HD21	1.69	0.41
1:A:676:GLU:HA	1:A:676:GLU:OE1	2.20	0.41
1:A:829:LEU:O	1:A:852:SER:CB	2.69	0.41
1:B:188:SER:HB3	1:B:831:TYR:HB2	2.03	0.41
1:A:887:GLN:O	1:A:890:ALA:HB3	2.20	0.41
1:A:140:ALA:HA	1:A:148:ASN:O	2.21	0.41
1:A:449:VAL:HG23	1:A:450:LEU:HD13	2.03	0.41
1:B:730:HIS:HD2	1:B:904:SER:OG	2.04	0.41
3:A:1102:MGW:O14	3:A:1102:MGW:C06	2.66	0.40
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.21	0.40
1:A:765:ARG:HD3	4:A:1255:HOH:O	2.19	0.40
1:B:491:ARG:NH1	1:B:491:ARG:CG	2.75	0.40
1:B:562:LYS:HG3	1:B:563:GLN:N	2.37	0.40
1:B:770:GLN:HB2	1:B:1005:PHE:CD1	2.57	0.40
1:A:852:SER:OG	1:A:853:GLU:N	2.54	0.40
1:B:262:GLU:HB2	1:B:267:LEU:CD2	2.52	0.40
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.25	0.40
1:B:1012:ILE:N	4:B:1250:HOH:O	2.55	0.40
1:B:321:ASP:OD2	1:B:322:LEU:N	2.54	0.40
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.56	0.40
1:B:817:GLU:N	1:B:818:PRO:CD	2.84	0.40
1:B:840:ALA:C	1:B:842:GLY:H	2.25	0.40
1:B:96:SER:C	1:B:98:SER:H	2.23	0.40
1:A:638:GLN:N	1:A:639:PRO:CD	2.85	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	954/990 (96%)	890 (93%)	61 (6%)	3 (0%)	41	70
1	B	952/990 (96%)	876 (92%)	75 (8%)	1 (0%)	51	80
All	All	1906/1980 (96%)	1766 (93%)	136 (7%)	4 (0%)	47	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1010	PRO
1	A	636	ASP
1	A	1010	PRO
1	A	103	ILE

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	849/879 (97%)	745 (88%)	104 (12%)	5	14
1	B	847/879 (96%)	741 (88%)	106 (12%)	4	14
All	All	1696/1758 (96%)	1486 (88%)	210 (12%)	4	14

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	61	LYS

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Mol	Chain	Res	Type
1	A	67	LEU
1	A	74	LYS
1	A	76	LEU
1	A	96	SER
1	A	97	LEU
1	A	102	ASN
1	A	107	SER
1	A	119	LYS
1	A	120	LYS
1	A	125	ASN
1	A	139	ASN
1	A	154	SER
1	A	158	LEU
1	A	171	SER
1	A	183	VAL
1	A	188	SER
1	A	192	LYS
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	227	GLU
1	A	261	ARG
1	A	270	LEU
1	A	274	LEU
1	A	282	ASN
1	A	285	LEU
1	A	287	GLU
1	A	316	THR
1	A	317	PHE
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	353	LYS
1	A	360	VAL
1	A	364	LYS
1	A	404	GLU
1	A	414	LEU
1	A	417	LEU
1	A	446	LEU
1	A	450	LEU
1	A	466	MET
1	A	468	LEU

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Mol	Chain	Res	Type
1	A	474	GLU
1	A	494	GLU
1	A	508	GLU
1	A	511	LYS
1	A	512	LYS
1	A	521	LYS
1	A	524	LEU
1	A	527	LYS
1	A	556	MET
1	A	575	ASN
1	A	577	GLU
1	A	595	LEU
1	A	597	LEU
1	A	602	ASP
1	A	603	SER
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	643	LYS
1	A	644	LYS
1	A	648	LYS
1	A	656	GLU
1	A	657	LYS
1	A	674	ARG
1	A	691	THR
1	A	712	LEU
1	A	713	LYS
1	A	722	ARG
1	A	728	LEU
1	A	736	GLN
1	A	756	LYS
1	A	771	LEU
1	A	774	ARG
1	A	798	ASP
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	838	ARG
1	A	846	LEU
1	A	847	ARG
1	A	859	LEU

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Mol	Chain	Res	Type
1	A	867	LEU
1	A	872	LYS
1	A	873	SER
1	A	884	LYS
1	A	889	LEU
1	A	892	ARG
1	A	906	LYS
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	937	ILE
1	A	938	LYS
1	A	957	HIS
1	A	980	LEU
1	A	990	GLU
1	A	993	GLN
1	A	996	THR
1	A	1007	LEU
1	B	49	ARG
1	B	52	ASN
1	B	61	LYS
1	B	67	LEU
1	B	74	LYS
1	B	87	SER
1	B	92	VAL
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	119	LYS
1	B	120	LYS
1	B	125	ASN
1	B	148	ASN
1	B	158	LEU
1	B	183	VAL
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	223	LYS
1	B	226	LEU
1	B	243	LYS
1	B	277	GLU
1	B	285	LEU

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Mol	Chain	Res	Type
1	B	316	THR
1	B	323	GLN
1	B	327	LYS
1	B	329	ASN
1	B	347	LEU
1	B	360	VAL
1	B	381	GLU
1	B	406	PRO
1	B	414	LEU
1	B	417	LEU
1	B	423	ARG
1	B	429	ARG
1	B	446	LEU
1	B	450	LEU
1	B	458	GLU
1	B	465	GLU
1	B	466	MET
1	B	491	ARG
1	B	498	THR
1	B	507	ASP
1	B	508	GLU
1	B	512	LYS
1	B	518	LEU
1	B	521	LYS
1	B	527	LYS
1	B	538	LEU
1	B	545	THR
1	B	587	PRO
1	B	595	LEU
1	B	597	LEU
1	B	603	SER
1	B	604	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	632	LYS
1	B	635	ASN
1	B	637	LYS
1	B	639	PRO
1	B	643	LYS
1	B	648	LYS
1	B	657	LYS

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Mol	Chain	Res	Type
1	B	674	ARG
1	B	691	THR
1	B	711	ARG
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	780	GLN
1	B	783	ASN
1	B	798	ASP
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	826	LYS
1	B	846	LEU
1	B	847	ARG
1	B	854	LYS
1	B	859	LEU
1	B	861	SER
1	B	872	LYS
1	B	875	GLU
1	B	889	LEU
1	B	901	SER
1	B	906	LYS
1	B	914	GLN
1	B	923	THR
1	B	928	LEU
1	B	934	GLU
1	B	938	LYS
1	B	951	ARG
1	B	962	GLU
1	B	979	ASN
1	B	980	LEU
1	B	990	GLU
1	B	1002	LEU
1	B	1007	LEU
1	B	1009	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	148	ASN
1	A	184	ASN
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	386	HIS
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	502	GLN
1	A	515	ASN
1	A	575	ASN
1	A	622	ASN
1	A	672	ASN
1	A	718	GLN
1	A	730	HIS
1	A	770	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	957	HIS
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	148	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	297	HIS
1	B	300	GLN
1	B	329	ASN
1	B	336	HIS
1	B	363	GLN
1	B	386	HIS

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Mol	Chain	Res	Type
1	B	475	ASN
1	B	502	GLN
1	B	575	ASN
1	B	589	HIS
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	736	GLN
1	B	743	GLN
1	B	783	ASN
1	B	805	ASN
1	B	828	GLN
1	B	841	ASN
1	B	887	GLN
1	B	922	ASN
1	B	979	ASN

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
3	MGW	A	1102	-	22,29,29	1.58	1 (4%)	28,37,37	1.89	9 (32%)
3	MGW	B	1102	-	22,29,29	1.59	2 (9%)	28,37,37	2.04	6 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGW	A	1102	-	-	15/25/27/27	0/2/2/2
3	MGW	B	1102	-	-	8/25/27/27	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	MGW	O02-C03	6.03	1.47	1.33
3	A	1102	MGW	O02-C03	6.01	1.47	1.33
3	B	1102	MGW	C05-N12	2.01	1.50	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	MGW	C05-N12-C13	6.38	138.06	121.65
3	B	1102	MGW	C03-C05-N12	4.49	121.10	110.72
3	A	1102	MGW	O02-C03-C05	4.18	122.22	111.52
3	B	1102	MGW	C01-O02-C03	3.94	124.85	115.94
3	A	1102	MGW	C01-O02-C03	3.60	124.08	115.94
3	A	1102	MGW	C05-N12-C13	3.47	130.57	121.65
3	A	1102	MGW	O02-C03-O04	-3.36	117.26	123.84
3	B	1102	MGW	C06-C05-C03	3.28	118.51	110.37
3	B	1102	MGW	O02-C03-C05	3.12	119.51	111.52
3	A	1102	MGW	C26-C25-N16	2.80	117.47	113.48
3	A	1102	MGW	C08-N09-C10	2.71	110.01	105.78
3	A	1102	MGW	C17-C18-C19	2.69	119.85	112.16
3	A	1102	MGW	C25-N16-C15	-2.44	106.79	112.02
3	A	1102	MGW	C25-N16-C17	2.43	116.42	111.29
3	B	1102	MGW	C08-N09-C10	2.17	109.17	105.78

There are no chirality outliers.

All (23) torsion outliers are listed below:

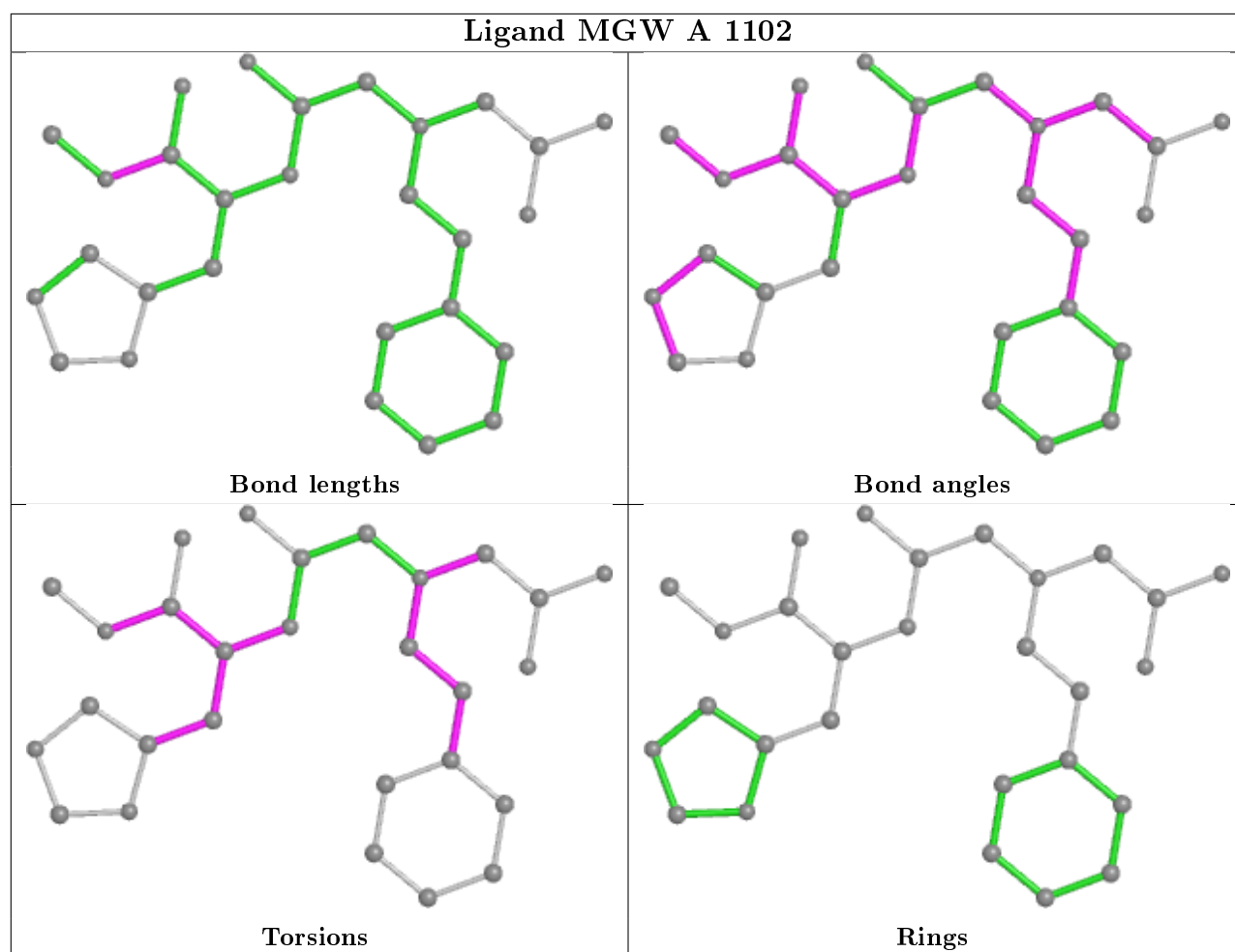
Mol	Chain	Res	Type	Atoms
3	A	1102	MGW	C06-C05-N12-C13
3	B	1102	MGW	N12-C05-C06-C07
3	A	1102	MGW	O04-C03-O02-C01
3	B	1102	MGW	O04-C03-O02-C01
3	A	1102	MGW	C05-C03-O02-C01
3	A	1102	MGW	C18-C17-N16-C25
3	B	1102	MGW	C05-C03-O02-C01
3	B	1102	MGW	C03-C05-N12-C13
3	A	1102	MGW	N16-C17-C18-C19
3	B	1102	MGW	N16-C17-C18-C19
3	B	1102	MGW	C26-C25-N16-C15
3	B	1102	MGW	C26-C25-N16-C17
3	A	1102	MGW	C17-C18-C19-C20
3	A	1102	MGW	C17-C18-C19-C24
3	A	1102	MGW	C03-C05-C06-C07
3	A	1102	MGW	C05-C06-C07-N11
3	B	1102	MGW	C05-C06-C07-N11
3	A	1102	MGW	C05-C06-C07-C08
3	A	1102	MGW	C18-C17-N16-C15
3	A	1102	MGW	C26-C25-N16-C17
3	A	1102	MGW	C26-C25-N16-C15
3	A	1102	MGW	O02-C03-C05-C06
3	A	1102	MGW	O04-C03-C05-C06

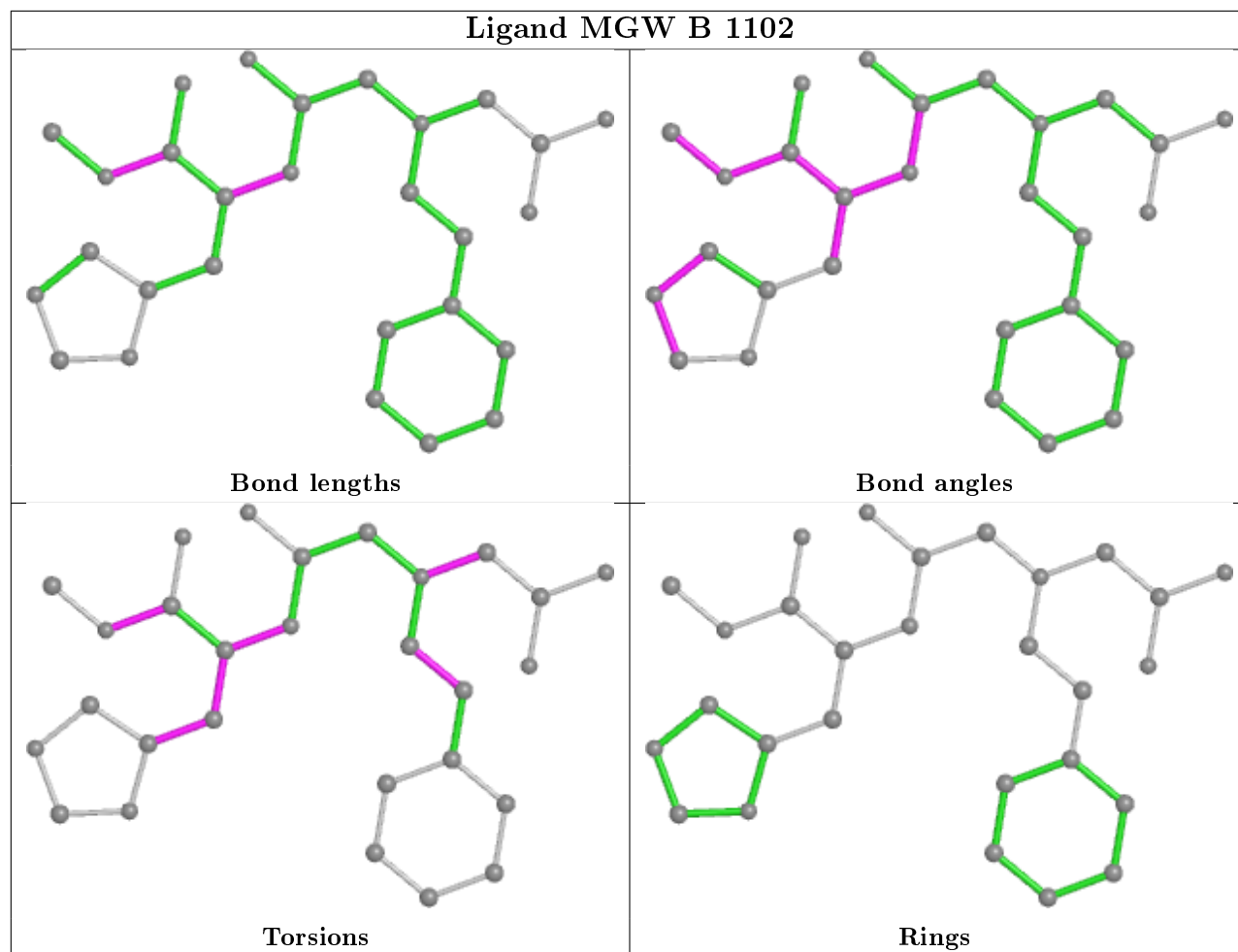
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	MGW	6	0
3	B	1102	MGW	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	958/990 (96%)	-0.35	0 100 100	25, 41, 58, 88	0
1	B	956/990 (96%)	-0.25	3 (0%) 94 93	32, 47, 65, 82	0
All	All	1914/1980 (96%)	-0.30	3 (0%) 95 94	25, 44, 62, 88	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	ASP	2.2
1	B	980	LEU	2.1
1	B	985	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MGW	B	1102	28/28	0.79	0.29	79,87,102,102	0
3	MGW	A	1102	28/28	0.83	0.29	64,80,86,87	0

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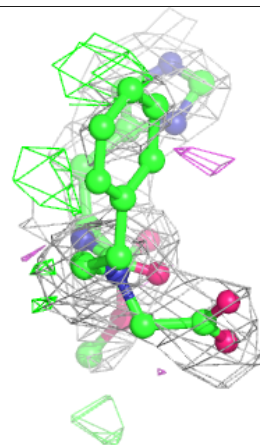
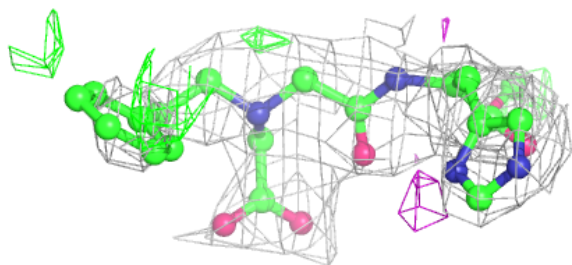
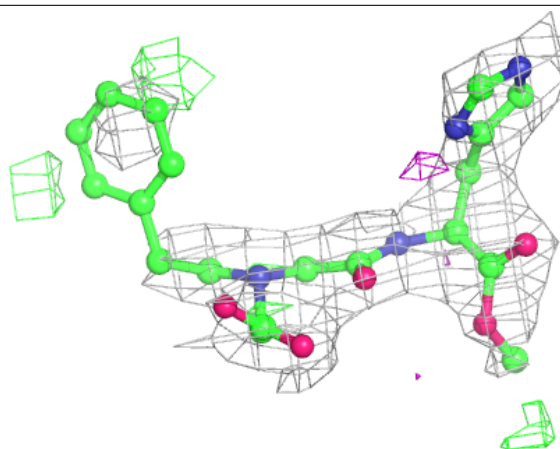
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	1101	1/1	0.87	0.18	2,2,2,2	0
2	ZN	B	1101	1/1	0.89	0.15	2,2,2,2	0

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.

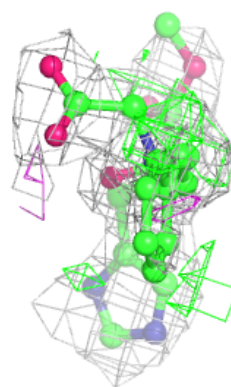
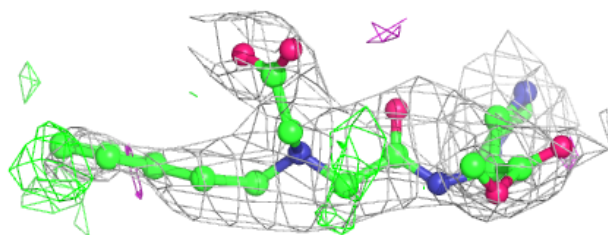
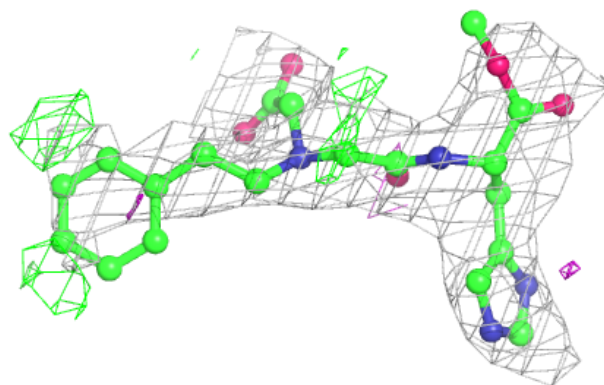
Electron density around MGW B 1102:

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 MGW A 1102:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.