



Full wwPDB X-ray Structure Validation 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 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

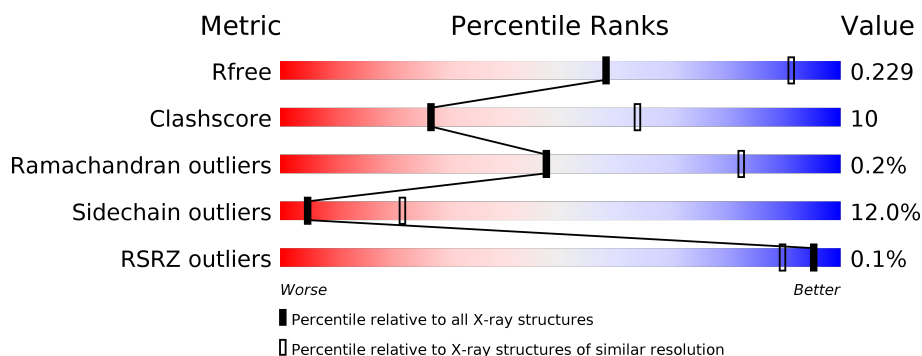
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	 70% 23% . .
1	B	990	 70% 22% . .

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:

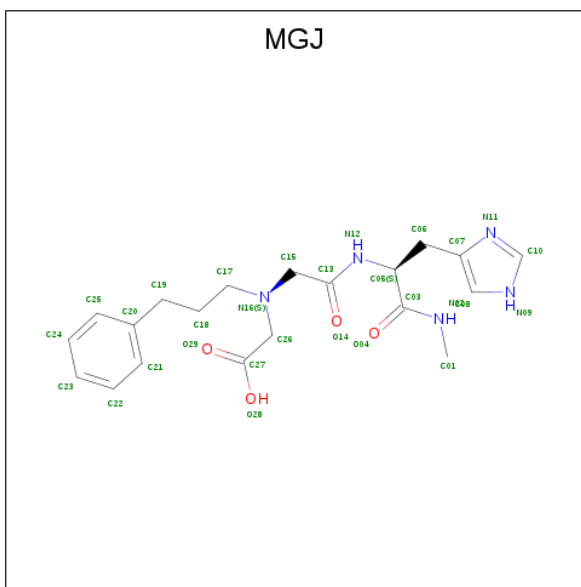
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735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

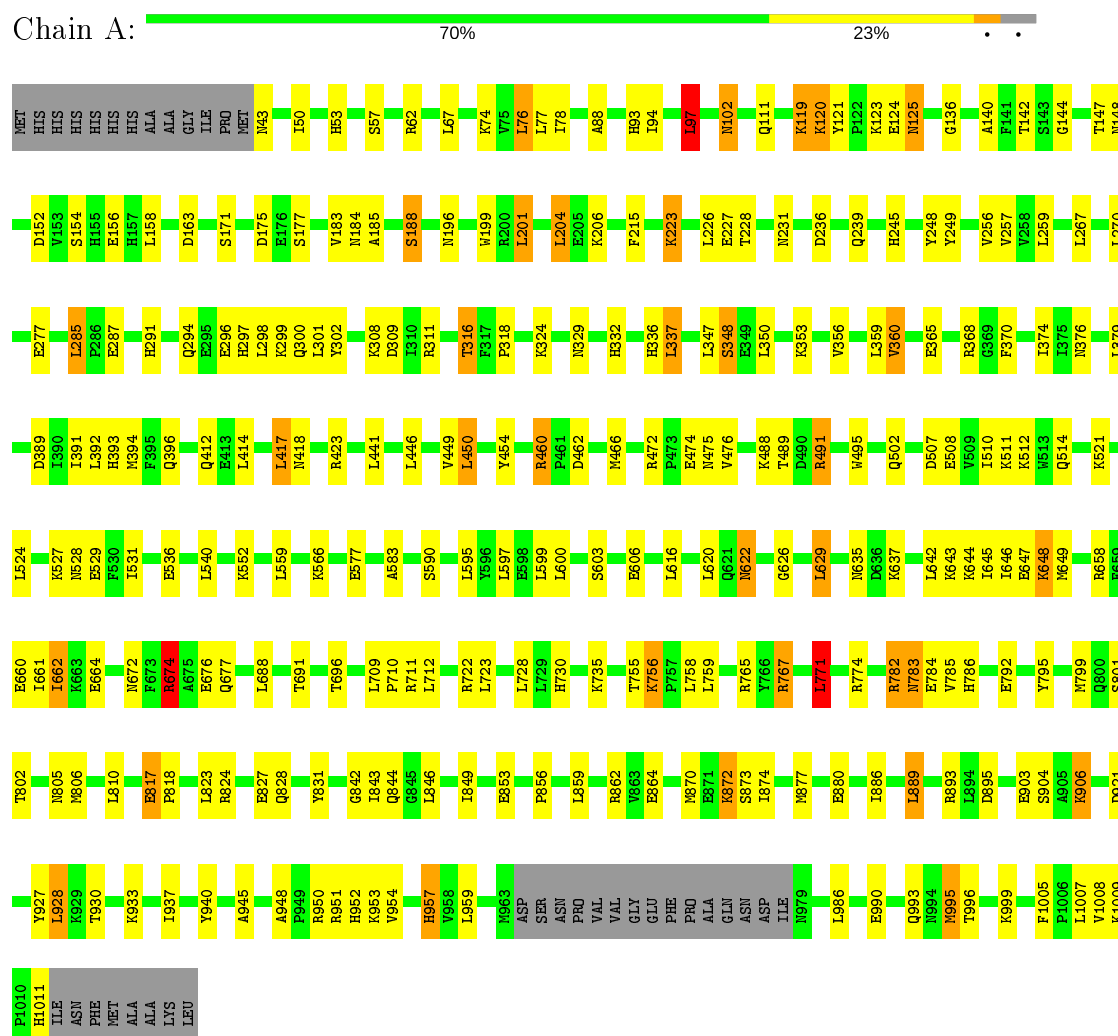
- Molecule 4 is water.

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

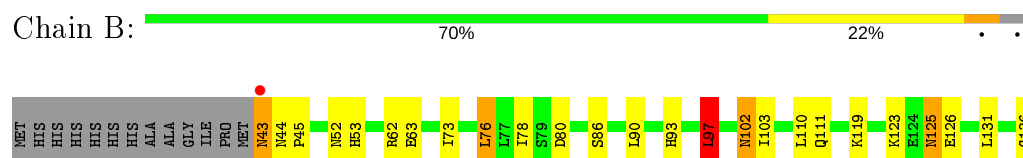
3 Residue-property plots

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
E962	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	K857	M742	S630	T451	N329	D197
VAL	E858	Q743	Q638	A452	H332	A198
VAL	L859	M744	L642	L455	E341	H199
GLY	R862	K756	L643	L456	E347	R200
PHE	E867	P757	K644	E457	H336	L201
ALA	M870	L758	K647	E458	L337	L204
GLN	E871	L759	K648	F459	E341	E205
ASN	K872	Q770	E647	R460	L346	P214
ASP	S873	L771	R657	D462	L347	K223
ILE	I874	F777	R658	M466	S348	L226
N979	E875	F777	I661	N475	E349	L226
E990	E880	N783	E664	K488	K353	R229
Y991	E889	E784	S669	R491	V356	V237
Q993	L889	H785	L670	T498	G361	R235
N994	A890	N787	N671	I510	K364	Q239
N995	I891	E788	M672	K511	E365	K243
F998	E898	I791	P673	K512	R368	F244
K999	I891	D798	A675	G520	G369	E245
F1005	E898	M799	E676	F522	M371	Y249
P1006	N917	E804	Q677	K521	I374	S250
L1007	K898	L810	M683	F523	D378	S251
L1007	E903	I815	L689	L524	L379	V256
V1008	E906	S816	M690	M556	L270	L259
K1009	R906	E817	T691	L559	V278	L270
P1010	N917	P818	E692	L574	H366	V278
H1011	E934	T822	V693	M575	V387	K281
ILE	E942	L823	A694	F576	E368	L285
ASN	E948	Q828	M695	E577	D389	P286
ASN	R951	Y831	K701	F578	I391	E287
PHE	H952	R838	E702	F579	M394	H291
MET	K953		L709	S580	Q412	H291
ALA			P710	P581	E413	Q294
ALA			R711		L414	
LYS						
LEU						

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 [i](#)

5.1 Standard geometry [i](#)

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%)

All (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
1	A	577	GLU	CG-CD	5.49	1.60	1.51
1	A	365	GLU	CG-CD	5.17	1.59	1.51
1	B	673	PHE	CE2-CZ	5.09	1.47	1.37
1	B	287	GLU	CG-CD	5.07	1.59	1.51
1	B	776	TRP	CB-CG	5.07	1.59	1.50

All (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
1	A	771	LEU	CA-CB-CG	5.65	128.31	115.30
1	B	510	ILE	CG1-CB-CG2	-5.62	99.03	111.40
1	A	67	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	674	ARG	NE-CZ-NH1	5.57	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	767	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	423	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	97	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	97	LEU	CA-CB-CG	5.08	126.98	115.30

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.

All (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
1:A:491:ARG:NH1	1:A:491:ARG:HG3	1.68	1.00
1:B:674:ARG:HD2	4:B:1218:HOH:O	1.63	0.98
1:A:491:ARG:CG	1:A:491:ARG:HH11	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HB3	1:A:756:LYS:HZ3	1.34	0.92
1:B:309:ASP:H	1:B:672:ASN:HD21	1.17	0.91
1:B:575:ASN:HD22	1:B:630:SER:HB2	1.37	0.89
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.38	0.87
1:B:777:PHE:HB3	1:B:992:ILE:HD11	1.57	0.87
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.21	0.84
1:B:689:LEU:HD23	1:B:995:MET:HG2	1.59	0.84
1:A:102:ASN:HD22	1:A:102:ASN:H	1.22	0.84
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.08	0.83
1:A:880:GLU:HG2	1:B:457:GLU:HG2	1.58	0.83
1:B:622:ASN:H	1:B:622:ASN:HD22	1.23	0.81
1:A:53:HIS:HE1	4:A:1215:HOH:O	1.63	0.80
1:A:688:LEU:HB3	1:A:995:MET:HE1	1.62	0.80
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.77
1:B:125:ASN:H	1:B:125:ASN:HD22	1.32	0.77
1:B:250:SER:HB2	1:B:281:LYS:HB2	1.65	0.77
1:A:622:ASN:H	1:A:622:ASN:ND2	1.82	0.76
1:A:332:HIS:CD2	2:A:1101:MGJ:H01B	2.22	0.75
1:A:332:HIS:HD2	2:A:1101:MGJ:H01B	1.51	0.75
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.68	0.75
1:A:301:LEU:HD12	1:A:302:TYR:N	2.01	0.75
1:A:674:ARG:HH11	1:A:674:ARG:HG3	1.51	0.75
1:B:602:ASP:OD1	1:B:658:ARG:HD3	1.86	0.74
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.18	0.73
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.20	0.73
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.19	0.73
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.05	0.72
1:B:491:ARG:HG3	1:B:491:ARG:HH11	1.56	0.71
2:B:1101:MGJ:O14	2:B:1101:MGJ:C06	2.30	0.71
1:A:730:HIS:HD2	1:A:904:SER:OG	1.73	0.71
1:B:815:ILE:HA	1:B:870:MET:HE2	1.71	0.70
1:B:309:ASP:H	1:B:672:ASN:ND2	1.90	0.70
1:B:196:ASN:HD22	1:B:196:ASN:C	1.95	0.70
1:B:674:ARG:CD	4:B:1218:HOH:O	2.28	0.70
1:A:417:LEU:HD11	1:A:531:ILE:HD13	1.73	0.69
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.75	0.69
1:B:294:GLN:H	1:B:297:HIS:HD2	1.40	0.68
1:B:857:HIS:CD2	1:B:857:HIS:C	2.66	0.68
1:B:713:LYS:HE2	4:B:1212:HOH:O	1.92	0.68
1:A:674:ARG:CG	1:A:674:ARG:HH11	2.07	0.68
1:A:622:ASN:H	1:A:622:ASN:HD22	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ASN:OD1	1:B:701:LYS:HD3	1.94	0.67
1:A:309:ASP:H	1:A:672:ASN:HD21	1.43	0.66
1:A:119:LYS:HB2	1:A:171:SER:HB3	1.77	0.65
1:A:196:ASN:HD22	1:A:199:TRP:H	1.45	0.65
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.78	0.65
1:A:392:LEU:O	1:A:396:GLN:HG3	1.97	0.65
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.78	0.64
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.79	0.64
1:A:783:ASN:ND2	1:A:786:HIS:H	1.96	0.63
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.33	0.63
1:B:783:ASN:ND2	1:B:786:HIS:H	1.95	0.62
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.29	0.62
1:A:308:LYS:HD3	1:A:672:ASN:HB3	1.81	0.62
1:B:657:LYS:HE3	4:B:1213:HOH:O	1.99	0.62
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.35	0.61
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.81	0.61
1:B:294:GLN:H	1:B:297:HIS:CD2	2.16	0.61
1:B:102:ASN:H	1:B:102:ASN:HD22	1.48	0.61
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.33	0.61
1:B:110:LEU:HD23	1:B:110:LEU:C	2.21	0.61
1:A:125:ASN:HD22	1:A:125:ASN:H	1.49	0.60
1:A:674:ARG:NH1	1:A:674:ARG:HG3	2.14	0.60
1:B:196:ASN:ND2	1:B:196:ASN:C	2.55	0.60
1:B:657:LYS:O	1:B:661:ILE:HG12	2.01	0.60
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.99	0.60
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.67	0.59
2:B:1101:MGJ:H25	2:B:1101:MGJ:H17	1.84	0.59
1:A:783:ASN:ND2	1:A:785:VAL:H	2.01	0.59
1:B:683:MET:HA	1:B:792:GLU:OE2	2.04	0.58
1:B:43:ASN:HB2	4:B:1228:HOH:O	2.02	0.58
1:B:196:ASN:ND2	1:B:198:ALA:H	2.02	0.58
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.85	0.58
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.39	0.58
1:A:722:ARG:HE	1:A:756:LYS:HG3	1.68	0.57
1:A:756:LYS:HB3	1:A:756:LYS:HZ2	1.66	0.57
1:B:204:LEU:HD23	1:B:304:ILE:HD12	1.85	0.57
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.86	0.57
1:B:822:THR:O	1:B:827:GLU:HG3	2.03	0.57
1:B:361:GLY:O	2:B:1101:MGJ:N12	2.36	0.57
1:B:311:ARG:NH1	1:B:379:LEU:O	2.37	0.57
1:B:870:MET:O	1:B:874:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.40	0.57
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.87	0.56
1:B:777:PHE:HB3	1:B:992:ILE:CD1	2.33	0.56
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.86	0.56
1:B:451:THR:HB	1:B:455:LEU:HD12	1.86	0.56
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.88	0.56
1:B:776:TRP:NE1	1:B:953:LYS:HE2	2.21	0.56
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.39	0.56
1:A:927:TYR:O	1:A:930:THR:HB	2.06	0.56
1:B:622:ASN:H	1:B:622:ASN:ND2	1.96	0.56
1:A:782:ARG:HH11	1:A:782:ARG:HG2	1.71	0.55
1:B:1008:VAL:CG1	1:B:1009:LYS:N	2.69	0.55
1:B:992:ILE:HD12	1:B:998:PHE:CD1	2.41	0.55
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.41	0.55
1:B:575:ASN:ND2	1:B:630:SER:HB2	2.16	0.55
1:B:783:ASN:HD22	1:B:785:VAL:H	1.54	0.55
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.89	0.55
1:A:318:PRO:HD2	1:A:475:ASN:HD22	1.72	0.55
1:A:756:LYS:CB	1:A:756:LYS:NZ	2.58	0.55
1:A:332:HIS:HD2	2:A:1101:MGJ:C01	2.20	0.54
1:A:74:LYS:HD2	4:A:1213:HOH:O	2.07	0.54
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.42	0.54
1:B:239:GLN:HG3	1:B:243:LYS:NZ	2.22	0.54
1:A:97:LEU:HB2	1:A:144:GLY:O	2.08	0.54
1:A:795:TYR:HE2	1:A:953:LYS:HD2	1.73	0.54
1:A:309:ASP:H	1:A:672:ASN:ND2	2.06	0.54
1:B:1008:VAL:HG12	1:B:1009:LYS:N	2.23	0.54
1:A:691:THR:O	1:A:999:LYS:HE3	2.07	0.54
1:B:125:ASN:N	1:B:125:ASN:HD22	2.04	0.54
1:B:556:MET:O	1:B:556:MET:HG3	2.06	0.54
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.72	0.54
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.72	0.53
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.89	0.53
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.91	0.53
1:A:121:TYR:OH	1:A:163:ASP:OD1	2.27	0.52
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.56	0.52
1:A:78:ILE:O	1:A:259:LEU:HA	2.09	0.52
1:A:843:ILE:HG22	1:A:844:GLN:N	2.25	0.52
1:B:783:ASN:ND2	1:B:785:VAL:H	2.07	0.52
1:B:777:PHE:CB	1:B:992:ILE:HD11	2.37	0.52
1:A:297:HIS:HE1	4:A:1205:HOH:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:THR:O	1:B:999:LYS:HE3	2.09	0.52
1:B:204:LEU:CD2	1:B:304:ILE:CD1	2.88	0.52
1:A:301:LEU:HD12	1:A:302:TYR:H	1.73	0.52
1:A:389:ASP:O	1:A:393:HIS:HD2	1.92	0.52
1:A:359:LEU:O	2:A:1101:MGJ:H10	2.10	0.52
1:B:110:LEU:HD23	1:B:110:LEU:O	2.10	0.52
1:B:204:LEU:CD2	1:B:304:ILE:HD12	2.40	0.52
1:A:801:SER:O	1:A:802:THR:C	2.47	0.51
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.91	0.51
1:B:196:ASN:ND2	1:B:198:ALA:N	2.57	0.51
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.92	0.51
1:A:391:ILE:O	1:A:394:MET:HB2	2.10	0.51
1:A:792:GLU:HG3	1:A:849:ILE:HG12	1.91	0.51
1:B:510:ILE:HG22	1:B:511:LYS:HD2	1.93	0.51
1:B:86:SER:HB3	1:B:158:LEU:HG	1.93	0.51
1:B:906:LYS:NZ	1:B:921:ASP:OD2	2.43	0.51
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.11	0.50
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.15	0.50
1:A:880:GLU:CG	1:B:457:GLU:CG	2.87	0.50
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.45	0.49
1:A:676:GLU:HA	1:A:676:GLU:OE1	2.11	0.49
1:A:783:ASN:HD22	1:A:785:VAL:H	1.58	0.49
1:A:418:ASN:HB3	1:A:454:TYR:O	2.12	0.49
1:A:102:ASN:HD22	1:A:102:ASN:N	2.01	0.49
1:A:102:ASN:ND2	1:A:102:ASN:H	2.00	0.49
1:A:566:LYS:HD2	1:A:903:GLU:OE1	2.12	0.49
1:A:843:ILE:CG2	1:A:844:GLN:N	2.75	0.49
1:B:76:LEU:HB2	1:B:441:LEU:HD11	1.93	0.49
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.94	0.49
1:A:491:ARG:CG	1:A:491:ARG:NH1	2.51	0.49
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.95	0.49
1:A:76:LEU:HB3	1:A:257:VAL:HG13	1.95	0.49
1:B:189:GLU:HG3	1:B:831:TYR:CE2	2.48	0.49
1:A:843:ILE:N	1:A:843:ILE:HD12	2.28	0.49
1:A:123:LYS:O	1:A:124:GLU:C	2.51	0.48
1:A:298:LEU:HD13	1:A:475:ASN:CB	2.43	0.48
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.95	0.48
1:A:842:GLY:HA3	4:A:1221:HOH:O	2.12	0.48
1:B:843:ILE:HD13	1:B:843:ILE:N	2.26	0.48
1:A:856:PRO:HB2	1:A:957:HIS:CD2	2.48	0.48
1:A:782:ARG:HG3	1:A:959:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:N	1:B:672:ASN:HD21	1.98	0.48
1:A:842:GLY:C	1:A:843:ILE:HD12	2.33	0.48
1:B:43:ASN:C	1:B:43:ASN:HD22	2.16	0.48
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.96	0.48
1:B:674:ARG:NE	4:B:1218:HOH:O	2.44	0.48
1:A:645:ILE:HG22	1:A:649:MET:CE	2.43	0.48
1:B:329:ASN:ND2	1:B:332:HIS:H	2.12	0.48
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.96	0.48
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.95	0.48
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.62	0.48
1:B:189:GLU:HG3	1:B:831:TYR:CD2	2.49	0.48
1:B:887:GLN:NE2	1:B:891:ILE:HD11	2.20	0.47
1:A:77:LEU:HD22	1:A:267:LEU:HB3	1.95	0.47
1:B:578:PHE:O	1:B:626:GLY:HA3	2.13	0.47
1:B:737:ALA:O	1:B:741:ILE:HG12	2.14	0.47
1:B:852:SER:OG	1:B:853:GLU:N	2.47	0.47
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.95	0.47
1:A:870:MET:O	1:A:874:ILE:HG12	2.14	0.47
1:A:723:LEU:HD12	1:A:755:THR:HG21	1.96	0.47
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.14	0.47
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.95	0.47
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.97	0.47
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.79	0.47
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.96	0.47
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.62	0.46
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.97	0.46
1:B:449:VAL:HG23	1:B:450:LEU:HD13	1.97	0.46
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.96	0.46
1:A:348:SER:OG	1:A:606:GLU:OE2	2.28	0.46
1:B:843:ILE:HG22	1:B:844:GLN:N	2.29	0.46
1:B:771:LEU:HB3	1:B:952:HIS:HB3	1.97	0.46
1:A:877:MET:O	1:A:933:LYS:NZ	2.39	0.46
1:B:162:LEU:HD23	1:B:270:LEU:HD13	1.96	0.46
1:B:622:ASN:N	1:B:622:ASN:HD22	2.03	0.46
1:B:179:LYS:HD2	1:B:237:VAL:HG12	1.97	0.46
1:A:184:ASN:ND2	1:A:223:LYS:HE3	2.31	0.46
1:A:521:LYS:HD3	1:A:521:LYS:HA	1.41	0.46
1:B:316:THR:HB	1:B:374:ILE:HG22	1.97	0.46
1:B:643:LYS:O	1:B:647:GLU:HB2	2.16	0.46
1:A:188:SER:HB3	1:A:831:TYR:CB	2.43	0.46
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LYS:HG2	1:A:510:ILE:HD11	1.98	0.46
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.46	0.46
1:B:298:LEU:HD13	1:B:475:ASN:HB2	1.97	0.46
1:B:78:ILE:O	1:B:259:LEU:HA	2.17	0.45
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.52	0.45
1:A:799:MET:HE1	4:A:1223:HOH:O	2.15	0.45
1:B:1008:VAL:CG1	1:B:1009:LYS:H	2.29	0.45
1:B:52:ASN:O	1:B:53:HIS:C	2.53	0.45
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.50	0.45
1:B:326:TYR:CD1	1:B:444:TYR:HE1	2.34	0.45
1:B:204:LEU:HD23	1:B:304:ILE:CD1	2.47	0.45
2:A:1101:MGJ:H06A	2:A:1101:MGJ:O14	2.16	0.45
1:A:360:VAL:HG23	2:A:1101:MGJ:H15	1.99	0.45
1:A:688:LEU:CB	1:A:995:MET:HE1	2.39	0.45
1:B:245:HIS:O	1:B:249:TYR:HB2	2.17	0.45
1:B:162:LEU:HD23	1:B:270:LEU:CD1	2.47	0.45
1:B:391:ILE:O	1:B:394:MET:HB2	2.17	0.45
1:A:245:HIS:O	1:A:249:TYR:HB2	2.17	0.45
1:A:771:LEU:HB3	1:A:952:HIS:HB3	1.98	0.45
1:A:827:GLU:OE2	1:A:862:ARG:NH1	2.50	0.45
1:A:864:GLU:HG3	1:A:986:LEU:HD21	1.99	0.45
1:B:744:MET:O	1:B:744:MET:HG2	2.17	0.44
1:A:231:ASN:HD22	1:A:231:ASN:HA	1.63	0.44
1:B:676:GLU:HA	1:B:676:GLU:OE1	2.18	0.44
1:A:227:GLU:O	1:A:228:THR:C	2.55	0.44
1:B:294:GLN:N	1:B:297:HIS:HD2	2.11	0.44
1:B:196:ASN:HD21	1:B:198:ALA:H	1.66	0.44
1:B:574:LEU:O	1:B:630:SER:HA	2.17	0.44
1:A:332:HIS:CD2	2:A:1101:MGJ:C01	2.98	0.44
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.98	0.44
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.47	0.44
1:A:824:ARG:O	1:A:828:GLN:HA	2.18	0.44
1:B:770:GLN:HA	1:B:1005:PHE:CE1	2.53	0.44
1:B:917:ASN:O	1:B:920:ARG:HB2	2.18	0.44
1:B:942:GLU:O	1:B:948:ALA:HB1	2.18	0.44
1:A:140:ALA:HA	1:A:148:ASN:O	2.18	0.43
1:A:206:LYS:HG2	1:A:215:PHE:O	2.17	0.43
1:B:979:ASN:N	1:B:979:ASN:OD1	2.51	0.43
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.76	0.43
1:A:889:LEU:HD22	1:A:893:ARG:HG2	2.00	0.43
1:A:316:THR:HB	1:A:374:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:VAL:HA	1:B:390:ILE:HD12	2.01	0.43
1:A:136:GLY:HA3	1:A:152:ASP:O	2.18	0.43
1:B:842:GLY:C	1:B:843:ILE:HD13	2.39	0.43
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.54	0.43
1:B:349:GLU:HA	1:B:349:GLU:OE2	2.18	0.43
1:B:619:ASP:O	1:B:629:LEU:HD23	2.18	0.43
1:B:783:ASN:HD21	1:B:786:HIS:H	1.64	0.43
1:B:491:ARG:NH1	1:B:491:ARG:HG3	2.28	0.43
1:B:622:ASN:N	1:B:622:ASN:ND2	2.64	0.42
1:A:142:THR:HG23	1:A:147:THR:OG1	2.19	0.42
1:B:336:HIS:HD2	1:B:337:LEU:HD13	1.84	0.42
1:B:110:LEU:C	1:B:110:LEU:CD2	2.88	0.42
1:A:795:TYR:CE2	1:A:953:LYS:HD2	2.53	0.42
1:B:97:LEU:HD12	1:B:214:PRO:O	2.20	0.42
1:A:528:ASN:O	1:A:531:ILE:HG12	2.20	0.42
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.49	0.42
1:A:872:LYS:HD2	1:A:872:LYS:HA	1.74	0.42
1:A:449:VAL:HG23	1:A:450:LEU:HD13	2.02	0.42
1:A:646:ILE:O	1:A:647:GLU:C	2.57	0.42
1:B:629:LEU:HD22	1:B:630:SER:N	2.35	0.42
1:A:474:GLU:OE2	1:A:514:GLN:NE2	2.45	0.42
1:A:529:GLU:O	1:A:637:LYS:NZ	2.53	0.42
1:A:799:MET:HE3	1:A:799:MET:HB3	1.79	0.42
1:B:43:ASN:C	1:B:43:ASN:ND2	2.74	0.42
1:A:674:ARG:CG	1:A:674:ARG:NH1	2.74	0.42
1:B:450:LEU:HA	1:B:450:LEU:HD12	1.80	0.42
1:B:580:SER:HA	1:B:581:PRO:HD2	1.68	0.42
1:A:843:ILE:CG2	1:A:844:GLN:H	2.32	0.41
1:B:365:GLU:HA	1:B:371:MET:HG2	2.02	0.41
1:A:311:ARG:HD2	1:A:379:LEU:O	2.21	0.41
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.50	0.41
1:A:767:ARG:HD3	1:A:1005:PHE:O	2.19	0.41
1:A:236:ASP:OD2	1:A:239:GLN:HG2	2.19	0.41
1:B:799:MET:HB3	1:B:799:MET:HE3	1.91	0.41
1:A:495:TRP:HA	1:A:495:TRP:CE3	2.56	0.41
1:B:136:GLY:HA3	1:B:152:ASP:O	2.20	0.41
1:A:806:MET:CE	1:A:928:LEU:HG	2.50	0.41
1:B:90:LEU:HG	1:B:256:VAL:HG22	2.02	0.41
1:A:88:ALA:HA	1:A:257:VAL:O	2.21	0.41
1:A:948:ALA:HB3	1:A:951:ARG:HB2	2.02	0.41
1:B:386:HIS:HD2	1:B:389:ASP:OD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD23	4:A:1236:HOH:O	2.21	0.41
1:A:599:LEU:HD23	1:A:662:ILE:HD13	2.02	0.41
1:B:200:ARG:NH2	1:B:498:THR:HA	2.35	0.41
1:B:756:LYS:HB3	1:B:756:LYS:HE2	1.61	0.41
1:A:175:ASP:OD2	1:A:177:SER:HB3	2.21	0.41
1:B:311:ARG:HB3	1:B:379:LEU:HB2	2.03	0.41
1:B:574:LEU:HD22	1:B:729:LEU:HD22	2.03	0.41
1:B:417:LEU:HD12	1:B:417:LEU:HA	1.59	0.41
1:B:810:LEU:HG	1:B:928:LEU:HD21	2.03	0.41
1:A:300:GLN:NE2	1:A:502:GLN:OE1	2.53	0.41
1:A:688:LEU:HD13	1:A:696:THR:HG22	2.03	0.41
1:A:756:LYS:CB	1:A:756:LYS:HZ2	2.30	0.41
1:B:44:ASN:OD1	1:B:45:PRO:HD2	2.21	0.41
1:A:648:LYS:HE3	4:A:1208:HOH:O	2.20	0.40
1:A:645:ILE:HG22	1:A:649:MET:HE3	2.02	0.40
2:B:1101:MGJ:C17	2:B:1101:MGJ:H25	2.51	0.40
1:B:798:ASP:HB3	1:B:804:GLU:HG2	2.03	0.40
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.80	0.40
1:A:120:LYS:HD2	1:A:120:LYS:N	2.35	0.40
1:A:301:LEU:HD12	1:A:301:LEU:C	2.41	0.40
1:A:510:ILE:HG22	1:A:511:LYS:HD2	2.03	0.40
1:A:722:ARG:HA	1:A:756:LYS:O	2.22	0.40
1:B:616:LEU:HD21	1:B:638:GLN:CG	2.51	0.40

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

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	50	ILE
1	A	57	SER
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	119	LYS
1	A	120	LYS
1	A	125	ASN
1	A	154	SER
1	A	156	GLU
1	A	158	LEU
1	A	183	VAL

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Mol	Chain	Res	Type
1	A	188	SER
1	A	201	LEU
1	A	204	LEU
1	A	223	LYS
1	A	226	LEU
1	A	270	LEU
1	A	277	GLU
1	A	285	LEU
1	A	287	GLU
1	A	296	GLU
1	A	316	THR
1	A	324	LYS
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	348	SER
1	A	353	LYS
1	A	360	VAL
1	A	376	ASN
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	446	LEU
1	A	450	LEU
1	A	460	ARG
1	A	466	MET
1	A	476	VAL
1	A	488	LYS
1	A	489	THR
1	A	491	ARG
1	A	507	ASP
1	A	508	GLU
1	A	512	LYS
1	A	524	LEU
1	A	527	LYS
1	A	590	SER
1	A	595	LEU
1	A	597	LEU
1	A	603	SER
1	A	616	LEU
1	A	622	ASN

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	635	ASN
1	A	642	LEU
1	A	643	LYS
1	A	644	LYS
1	A	648	LYS
1	A	658	ARG
1	A	661	ILE
1	A	662	ILE
1	A	674	ARG
1	A	677	GLN
1	A	711	ARG
1	A	712	LEU
1	A	728	LEU
1	A	735	LYS
1	A	756	LYS
1	A	759	LEU
1	A	765	ARG
1	A	771	LEU
1	A	774	ARG
1	A	782	ARG
1	A	783	ASN
1	A	784	GLU
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	846	LEU
1	A	853	GLU
1	A	859	LEU
1	A	872	LYS
1	A	873	SER
1	A	886	ILE
1	A	889	LEU
1	A	906	LYS
1	A	928	LEU
1	A	937	ILE
1	A	950	ARG
1	A	957	HIS
1	A	990	GLU
1	A	993	GLN
1	A	995	MET
1	A	996	THR

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Mol	Chain	Res	Type
1	A	1007	LEU
1	A	1009	LYS
1	A	1011	HIS
1	B	43	ASN
1	B	63	GLU
1	B	76	LEU
1	B	97	LEU
1	B	102	ASN
1	B	103	ILE
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	158	LEU
1	B	159	GLU
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	205	GLU
1	B	223	LYS
1	B	226	LEU
1	B	239	GLN
1	B	243	LYS
1	B	270	LEU
1	B	281	LYS
1	B	285	LEU
1	B	295	GLU
1	B	304	ILE
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	356	VAL
1	B	364	LYS
1	B	378	ASP
1	B	412	GLN
1	B	414	LEU
1	B	417	LEU
1	B	423	ARG
1	B	440	ILE
1	B	446	LEU

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Mol	Chain	Res	Type
1	B	450	LEU
1	B	456	LEU
1	B	458	GLU
1	B	466	MET
1	B	488	LYS
1	B	491	ARG
1	B	512	LYS
1	B	523	LYS
1	B	524	LEU
1	B	556	MET
1	B	595	LEU
1	B	597	LEU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	630	SER
1	B	642	LEU
1	B	643	LYS
1	B	644	LYS
1	B	657	LYS
1	B	669	SER
1	B	674	ARG
1	B	677	GLN
1	B	691	THR
1	B	702	GLU
1	B	711	ARG
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	756	LYS
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	783	ASN
1	B	788	ASN
1	B	791	ILE
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	838	ARG
1	B	846	LEU

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Mol	Chain	Res	Type
1	B	854	LYS
1	B	857	HIS
1	B	859	LEU
1	B	867	LEU
1	B	872	LYS
1	B	873	SER
1	B	874	ILE
1	B	875	GLU
1	B	880	GLU
1	B	889	LEU
1	B	898	LYS
1	B	903	GLU
1	B	906	LYS
1	B	928	LEU
1	B	934	GLU
1	B	951	ARG
1	B	957	HIS
1	B	962	GLU
1	B	990	GLU
1	B	993	GLN
1	B	1007	LEU

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	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	332	HIS
1	A	336	HIS
1	A	393	HIS
1	A	475	ASN

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Mol	Chain	Res	Type
1	A	502	GLN
1	A	573	ASN
1	A	575	ASN
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	857	HIS
1	A	957	HIS
1	A	979	ASN
1	B	43	ASN
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	239	GLN
1	B	294	GLN
1	B	297	HIS
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	622	ASN
1	B	672	ASN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	841	ASN
1	B	857	HIS
1	B	887	GLN
1	B	922	ASN

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Mol	Chain	Res	Type
1	B	979	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

All (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
2	B	1101	MGJ	C13-N12	4.50	1.43	1.34
2	B	1101	MGJ	C15-N16	-2.62	1.41	1.47
2	B	1101	MGJ	C15-C13	-2.39	1.48	1.52
2	A	1101	MGJ	C17-N16	2.22	1.52	1.47

All (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
2	A	1101	MGJ	C05-C03-N02	3.30	121.99	116.99
2	A	1101	MGJ	C15-C13-N12	3.26	122.66	115.31
2	B	1101	MGJ	C15-N16-C17	-3.15	104.29	111.94
2	A	1101	MGJ	C22-C21-C20	2.80	124.93	120.63
2	B	1101	MGJ	C27-C26-N16	2.79	117.46	113.48
2	A	1101	MGJ	O14-C13-C15	-2.68	116.39	121.08
2	A	1101	MGJ	C26-N16-C17	2.66	116.90	111.29
2	A	1101	MGJ	C23-C24-C25	2.49	123.99	120.19
2	B	1101	MGJ	C06-C05-C03	2.33	116.30	110.25
2	B	1101	MGJ	C26-N16-C15	-2.29	107.11	112.02
2	A	1101	MGJ	C05-N12-C13	2.24	127.41	121.65
2	B	1101	MGJ	O04-C03-N02	-2.13	119.58	123.09
2	B	1101	MGJ	C03-C05-N12	-2.07	105.52	111.16

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
2	A	1101	MGJ	C05-C06-C07-N11
2	B	1101	MGJ	C06-C05-N12-C13
2	B	1101	MGJ	C13-C15-N16-C26
2	B	1101	MGJ	N12-C05-C06-C07
2	B	1101	MGJ	C03-C05-C06-C07
2	B	1101	MGJ	C05-C06-C07-C08
2	B	1101	MGJ	C05-C06-C07-N11
2	B	1101	MGJ	C27-C26-N16-C17
2	A	1101	MGJ	N16-C17-C18-C19
2	A	1101	MGJ	O14-C13-C15-N16
2	A	1101	MGJ	N12-C13-C15-N16
2	B	1101	MGJ	C18-C19-C20-C25
2	B	1101	MGJ	N12-C13-C15-N16
2	B	1101	MGJ	C18-C19-C20-C21
2	B	1101	MGJ	N16-C17-C18-C19
2	B	1101	MGJ	C27-C26-N16-C15
2	B	1101	MGJ	O14-C13-C15-N16

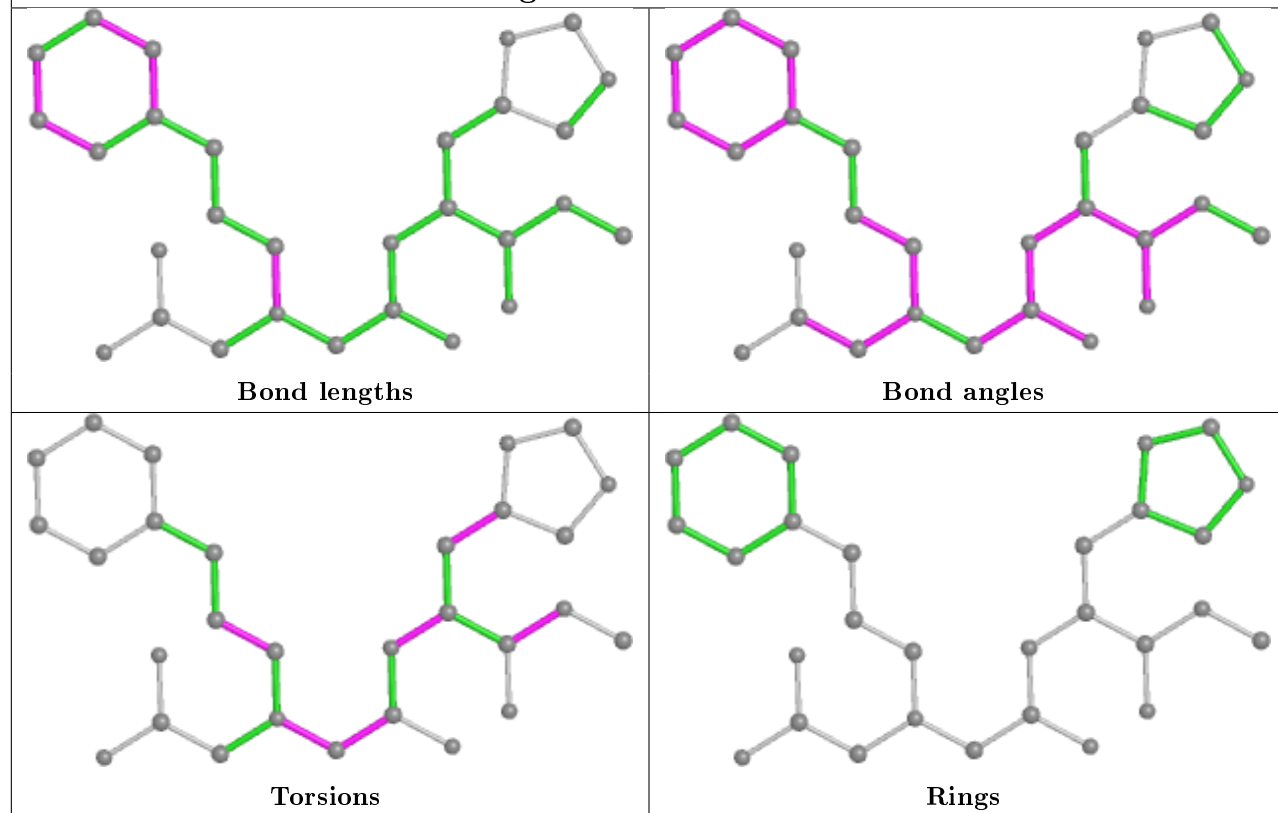
There are no ring outliers.

2 monomers are involved in 13 short contacts:

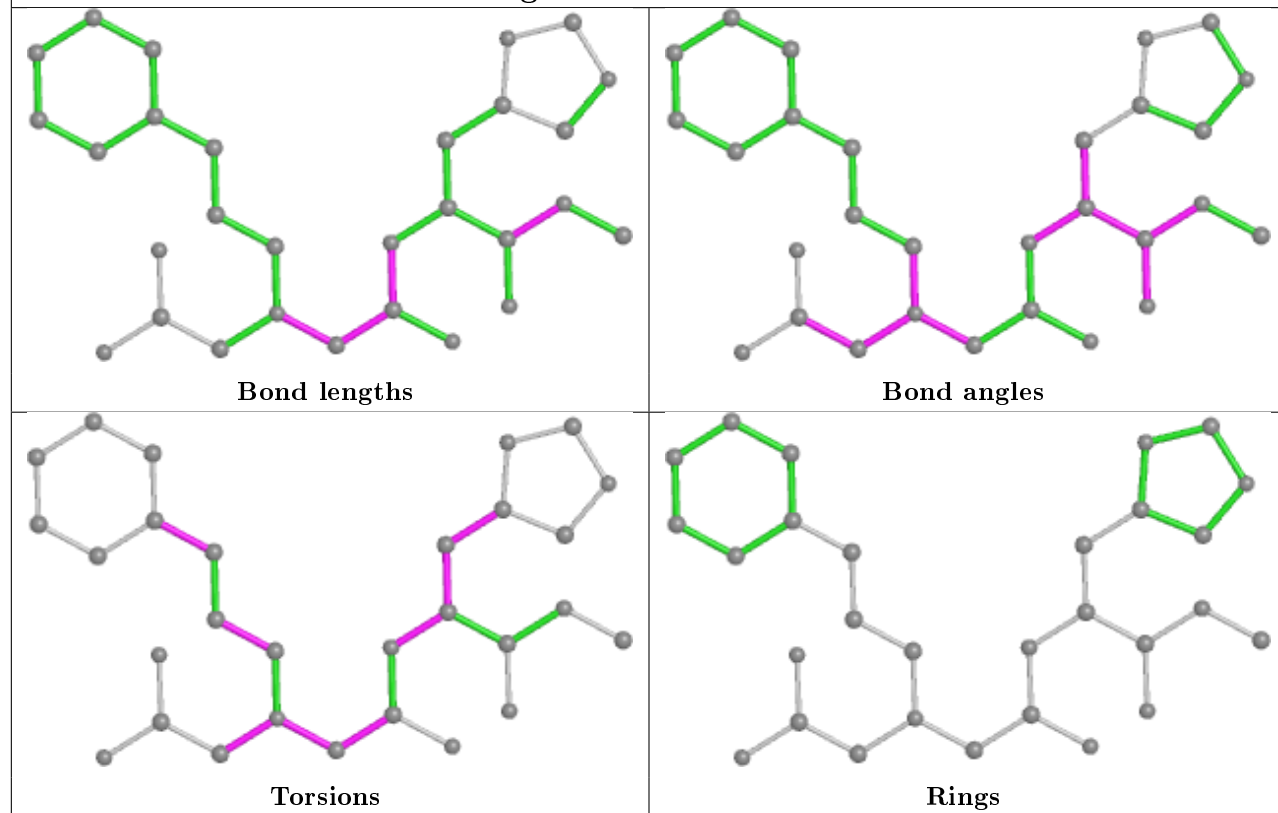
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MGJ	7	0
2	B	1101	MGJ	6	0

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.

Ligand MGJ A 1101



Ligand MGJ B 1101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

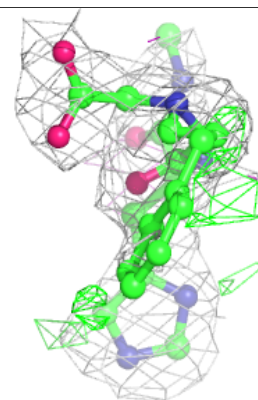
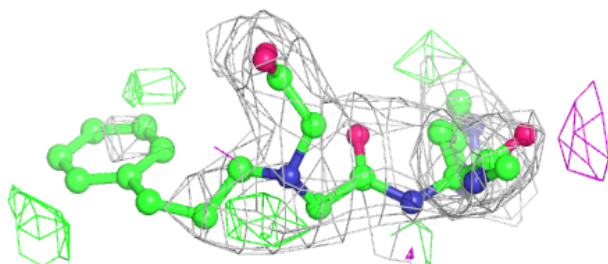
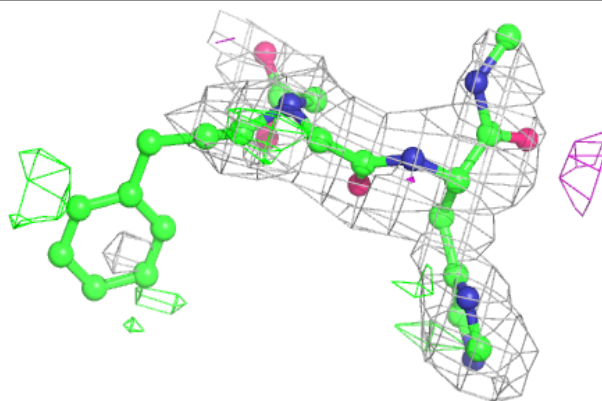
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	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.

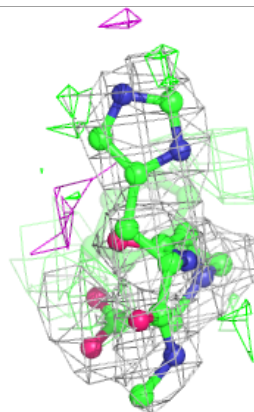
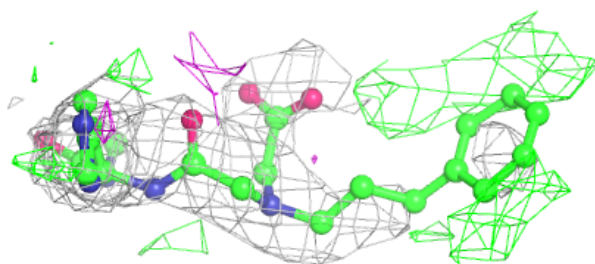
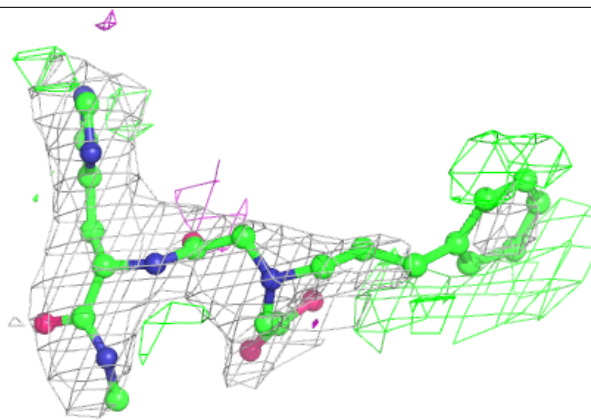
Electron density around MGJ B 1101:

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.