



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:27 AM UTC

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

This is a 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

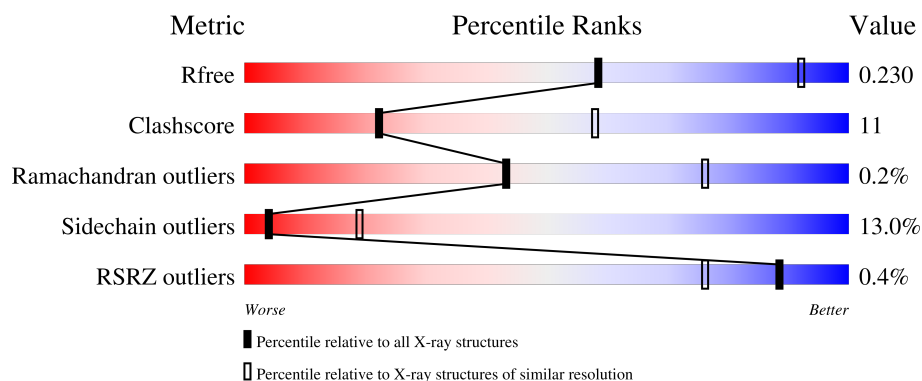
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	
1	B	990	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15726 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	954	Total	C	N	O	S	0	0	0
			7795	5022	1310	1441	22			
1	B	954	Total	C	N	O	S	0	0	0
			7795	5022	1310	1441	22			

There are 52 discrepancies between the modelled and reference sequences:

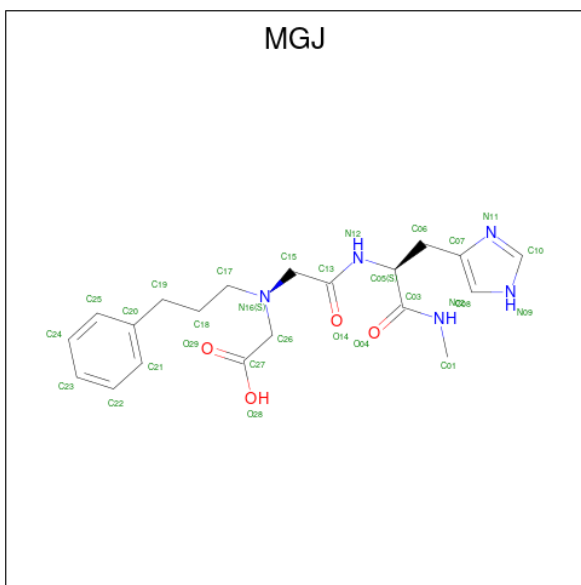
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is N-(carboxymethyl)-N-(3-phenylpropyl)glycyl-N-methyl-L-histidinamide (CCD ID: MGJ) (formula: $C_{20}H_{27}N_5O_4$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

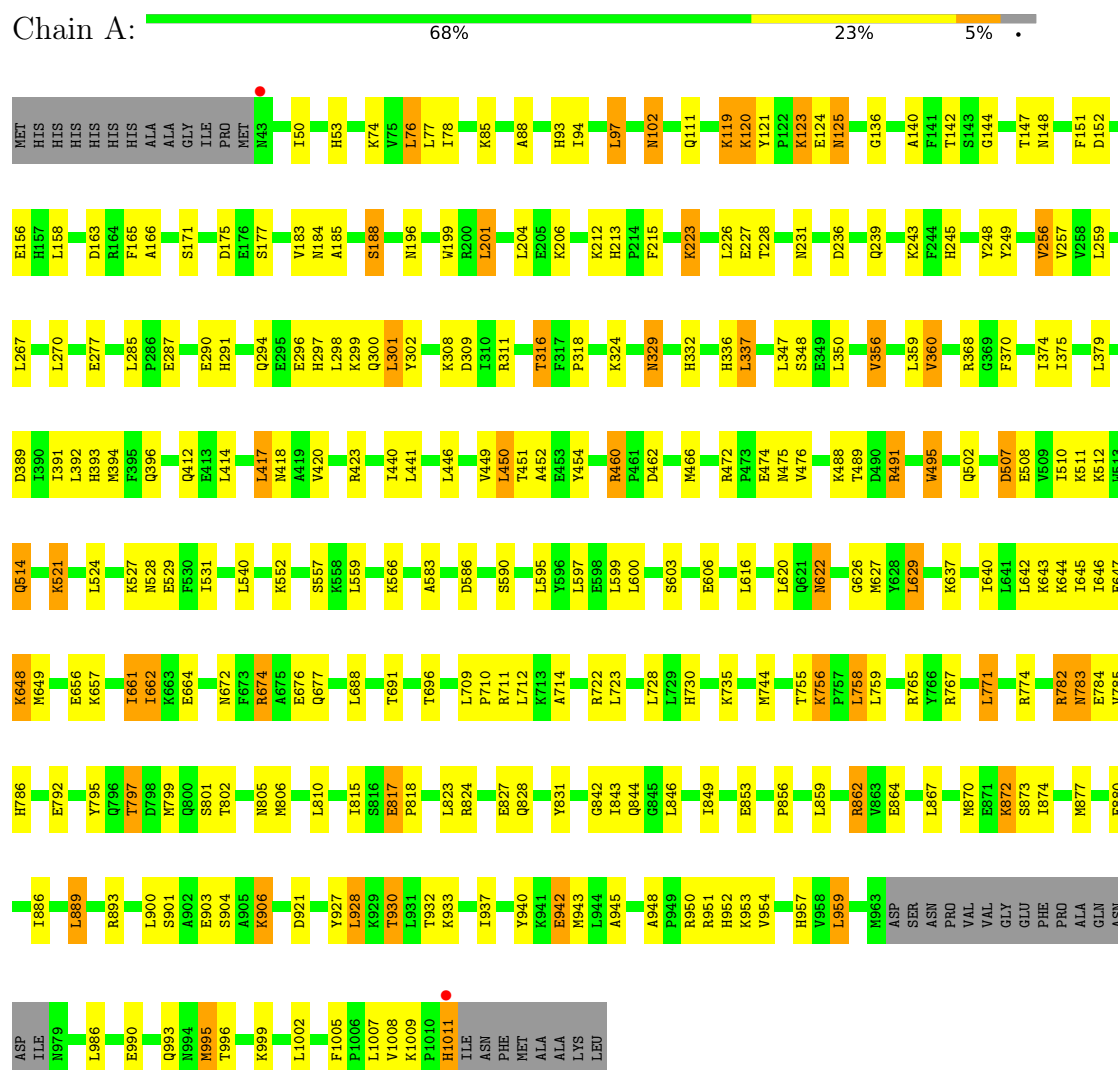
- Molecule 4 is water.

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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Insulin-degrading enzyme



• Molecule 1: Insulin-degrading enzyme





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 50.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.99) 99.8 (50.00-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.178 , 0.235 (Not available) , 0.230	Depositor DCC
R_{free} test set	3679 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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: ZN, MGJ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.07	1/7990 (0.0%)	1.15	16/10810 (0.1%)
1	B	1.02	7/7990 (0.1%)	1.17	32/10810 (0.3%)
All	All	1.05	8/15980 (0.1%)	1.16	48/21620 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CG-CD	7.71	1.75	1.52
1	B	680	GLN	CA-CB	6.82	1.64	1.53
1	A	640	ILE	CA-CB	6.17	1.61	1.54
1	B	316	THR	CA-CB	6.08	1.64	1.53
1	B	229	ARG	CD-NE	5.63	1.54	1.46
1	B	575	ASN	CA-C	-5.18	1.46	1.52
1	B	764	VAL	CA-CB	5.08	1.60	1.54
1	B	504	ALA	CA-CB	-5.04	1.45	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	942	GLU	N-CA-C	7.59	119.19	111.07
1	A	256	VAL	CB-CA-C	-7.29	99.75	110.62
1	B	505	ILE	N-CA-C	-7.08	102.54	108.63
1	B	100	PRO	CA-C-N	7.04	127.64	119.47
1	B	100	PRO	C-N-CA	7.04	127.64	119.47
1	B	576	PHE	CB-CA-C	-6.81	101.33	110.79
1	B	962	GLU	N-CA-C	6.62	121.44	113.23
1	A	507	ASP	N-CA-C	6.48	119.17	111.33
1	B	751	GLU	N-CA-C	6.33	118.18	111.28
1	B	92	VAL	CB-CA-C	-6.26	102.33	110.84
1	A	661	ILE	CB-CA-C	-6.13	103.99	112.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	ASN	N-CA-C	6.10	117.77	110.44
1	B	896	LYS	CA-C-N	5.94	126.28	119.93
1	B	896	LYS	C-N-CA	5.94	126.28	119.93
1	A	329	ASN	CA-C-N	5.74	124.94	118.97
1	A	329	ASN	C-N-CA	5.74	124.94	118.97
1	A	557	SER	N-CA-C	5.71	117.75	109.07
1	B	197	ASP	N-CA-C	5.65	117.52	111.36
1	B	661	ILE	CB-CA-C	-5.64	104.44	112.22
1	B	316	THR	CB-CA-C	5.63	119.37	109.80
1	A	797	THR	N-CA-C	5.62	122.78	110.80
1	B	873	SER	N-CA-C	5.53	118.83	111.75
1	A	290	GLU	N-CA-C	5.44	117.61	108.96
1	A	714	ALA	N-CA-C	5.42	117.26	111.36
1	B	718	GLN	N-CA-C	-5.41	105.28	111.07
1	B	387	VAL	N-CA-C	5.39	115.59	110.42
1	A	495	TRP	N-CA-C	5.39	116.96	111.14
1	B	304	ILE	CB-CA-C	-5.36	102.25	110.50
1	B	239	GLN	CB-CA-C	5.29	119.84	110.85
1	A	213	HIS	N-CA-C	5.26	116.32	109.64
1	B	855	PRO	CA-C-N	5.25	124.70	119.24
1	B	855	PRO	C-N-CA	5.25	124.70	119.24
1	B	405	GLY	CA-C-N	5.24	125.40	119.90
1	B	405	GLY	C-N-CA	5.24	125.40	119.90
1	B	617	SER	N-CA-C	5.23	117.14	109.24
1	A	586	ASP	N-CA-C	5.21	114.13	108.14
1	B	780	GLN	N-CA-C	5.21	117.93	109.24
1	B	107	SER	N-CA-C	5.15	116.90	111.28
1	B	500	TYR	N-CA-C	5.12	114.89	108.45
1	A	1002	LEU	CA-C-N	-5.11	114.97	120.03
1	A	1002	LEU	C-N-CA	-5.11	114.97	120.03
1	A	627	MET	N-CA-C	5.10	118.05	110.14
1	B	557	SER	N-CA-C	5.10	116.81	108.55
1	B	954	VAL	CB-CA-C	-5.06	102.60	110.69
1	B	638	GLN	CA-C-N	-5.04	113.46	119.05
1	B	638	GLN	C-N-CA	-5.04	113.46	119.05
1	B	513	TRP	N-CA-C	5.03	116.76	111.28
1	B	918	PHE	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7795	0	7730	163	0
1	B	7795	0	7730	165	0
2	A	29	0	26	7	0
2	B	29	0	26	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	0	7	0
4	B	32	0	0	6	0
All	All	15726	0	15512	331	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:CG	1:B:229:ARG:CD	1.75	1.57
2:B:1101:MGJ:H06A	2:B:1101:MGJ:O14	1.42	1.08
2:B:1101:MGJ:O14	2:B:1101:MGJ:H26	1.53	1.05
1:A:491:ARG:HG3	1:A:491:ARG:HH11	0.88	1.01
1:A:491:ARG:HG3	1:A:491:ARG:NH1	1.68	1.00
1:A:756:LYS:NZ	1:A:756:LYS:HB3	1.74	1.00
1:A:756:LYS:HB3	1:A:756:LYS:HZ3	1.22	0.99
1:B:674:ARG:HD2	4:B:1218:HOH:O	1.63	0.98
1:A:491:ARG:HH11	1:A:491:ARG:CG	1.80	0.94
1:B:309:ASP:H	1:B:672:ASN:HD21	1.17	0.91
1:A:688:LEU:HB3	1:A:995:MET:HE1	1.54	0.90
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:H	1:A:102:ASN:HD22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:ASN:HD22	1:B:622:ASN:H	1.23	0.81
1:A:53:HIS:HE1	4:A:1215:HOH:O	1.63	0.80
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.77
1:B:125:ASN:HD22	1:B:125:ASN:H	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:HG3	1:A:674:ARG:HH11	1.51	0.75
1:B:196:ASN:C	1:B:196:ASN:HD22	1.95	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:857:HIS:C	1:B:857:HIS:CD2	2.66	0.73
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.05	0.72
1:B:491:ARG:HH11	1:B:491:ARG:HG3	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:A:815:ILE:HG22	1:A:870:MET:HE2	1.73	0.70
1:B:309:ASP:H	1:B:672:ASN:ND2	1.90	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:688:LEU:CB	1:A:995:MET:HE1	2.22	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:713:LYS:HE2	4:B:1212:HOH:O	1.92	0.68
1:A:674:ARG:HH11	1:A:674:ARG:CG	2.07	0.68
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.75	0.67
1:A:622:ASN:H	1:A:622:ASN:HD22	1.42	0.67
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:B:110:LEU:HD23	1:B:110:LEU:C	2.21	0.65
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:C	1:B:196:ASN:ND2	2.55	0.64
1:B:815:ILE:HA	1:B:870:MET:HE2	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:B:294:GLN:H	1:B:297:HIS:CD2	2.16	0.61
1:B:102:ASN:HD22	1:B:102:ASN:H	1.48	0.61
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.33	0.61
1:A:125:ASN:H	1:A:125:ASN:HD22	1.49	0.60
1:A:674:ARG:HG3	1:A:674:ARG:NH1	2.14	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:A:797:THR:O	1:A:943:MET:HE2	2.01	0.60
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.67	0.59
2:B:1101:MGJ:H17	2:B:1101:MGJ:H25	1.84	0.59
1:B:239:GLN:HG3	1:B:243:LYS:HZ1	1.68	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: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
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:451:THR:HB	1:B:455:LEU:HD12	1.86	0.56
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.86	0.56
1:A:801:SER:O	1:A:802:THR:C	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:311:ARG:HH22	1:A:664:GLU:CD	2.15	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:318:PRO:HD2	1:A:475:ASN:HD22	1.72	0.55
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.89	0.55
1:A:756:LYS:NZ	1:A:756:LYS:CB	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:HD22	1:B:125:ASN:N	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:B:622:ASN:H	1:B:622:ASN:ND2	1.96	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:B:43:ASN:C	1:B:43:ASN:HD22	2.16	0.53
1:A:842:GLY:C	1:A:843:ILE:HD12	2.33	0.53
1:A:806:MET:HE3	1:A:928:LEU:HG	1.89	0.53
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.91	0.53
1:A:78:ILE:O	1:A:259:LEU:HA	2.09	0.52
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.56	0.52
1:A:121:TYR:OH	1:A:163:ASP:OD1	2.27	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:123:LYS:O	1:A:124:GLU:C	2.51	0.51
1:A:792:GLU:HG3	1:A:849:ILE:HG12	1.91	0.51
1:A:799:MET:HE1	4:A:1223:HOH:O	2.10	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:B:52:ASN:O	1:B:53:HIS:C	2.53	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:OE1	1:A:676:GLU:HA	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:566:LYS:HD2	1:A:903:GLU:OE1	2.12	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:76:LEU:HB3	1:A:257:VAL:HG13	1.95	0.49
1:A:491:ARG:NH1	1:A:491:ARG:CG	2.51	0.49
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.95	0.49
1:A:843:ILE:CG2	1:A:844:GLN:N	2.75	0.49
1:B:189:GLU:HG3	1:B:831:TYR:CE2	2.48	0.49
1:A:843:ILE:HD12	1:A:843:ILE:N	2.28	0.49
1:A:227:GLU:O	1:A:228:THR:C	2.55	0.49
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:782:ARG:HG3	1:A:959:LEU:HB2	1.94	0.48
1:A:856:PRO:HB2	1:A:957:HIS:CD2	2.48	0.48
1:B:309:ASP:N	1:B:672:ASN:HD21	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:842:GLY:C	1:B:843:ILE:HD13	2.39	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:B:110:LEU:C	1:B:110:LEU:CD2	2.88	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:73:ILE:HG13	1:B:251:SER:HB2	1.97	0.47
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.95	0.47
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.79	0.47
1:A:646:ILE:O	1:A:647:GLU:C	2.57	0.47
1:B:43:ASN:C	1:B:43:ASN:ND2	2.74	0.47
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.96	0.47
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:771:LEU:HB3	1:B:952:HIS:HB3	1.97	0.46
1:B:843:ILE:HG22	1:B:844:GLN:N	2.29	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:HD22	1:B:622:ASN:N	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:HA	1:A:521:LYS:HD3	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:299:LYS:HG2	1:A:510:ILE:HD11	1.98	0.46
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.81	0.46
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1008:VAL:CG1	1:B:1009:LYS:H	2.29	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
1:A:301:LEU:HD12	1:A:301:LEU:C	2.41	0.45
1:A:360:VAL:HG23	2:A:1101:MGJ:H15	1.99	0.45
2:A:1101:MGJ:H06A	2:A:1101:MGJ:O14	2.16	0.45
1:B:162:LEU:HD23	1:B:270:LEU:CD1	2.47	0.45
1:B:245:HIS:O	1:B:249:TYR:HB2	2.17	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:A:649:MET:HE3	1:A:649:MET:HB2	1.70	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:B:294:GLN:N	1:B:297:HIS:HD2	2.11	0.44
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.64	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:451:THR:O	1:A:452:ALA:C	2.61	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:A:1011:HIS:ND1	1:A:1011:HIS:C	2.75	0.44
1:B:770:GLN:HA	1:B:1005:PHE:CE1	2.53	0.44
1:A:374:ILE:HD12	1:A:374:ILE:C	2.43	0.44
1:B:783:ASN:HD22	1:B:783:ASN:C	2.26	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:151:PHE:CD1	1:A:151:PHE:C	2.96	0.43
1:A:540:LEU:HA	1:A:540:LEU:HD12	1.76	0.43
1:B:307:ILE:O	1:B:483:LYS:NZ	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:387:VAL:HA	1:B:390:ILE:HD12	2.01	0.43
1:B:857:HIS:C	1:B:857:HIS:HD2	2.25	0.43
1:A:136:GLY:HA3	1:A:152:ASP:O	2.18	0.43
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.54	0.43
1:B:349:GLU:OE2	1:B:349:GLU:HA	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:HG3	1:B:491:ARG:NH1	2.28	0.43
1:B:622:ASN:ND2	1:B:622:ASN:N	2.64	0.42
1:A:142:THR:HG23	1:A:147:THR:OG1	2.19	0.42
1:A:722:ARG:C	1:A:758:LEU:HD13	2.44	0.42
1:B:336:HIS:HD2	1:B:337:LEU:HD13	1.84	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:HA	1:A:872:LYS:HD2	1.74	0.42
1:A:449:VAL:HG23	1:A:450:LEU:HD13	2.02	0.42
1:B:629:LEU:HD22	1:B:630:SER:N	2.35	0.42
1:B:744:MET:O	1:B:744:MET:HG2	2.17	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:900:LEU:O	1:A:901:SER:C	2.62	0.42
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.67	0.42
1:A:674:ARG:CG	1:A:674:ARG:NH1	2.74	0.42
1:B:450:LEU:HD12	1:B:450:LEU:HA	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: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: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

Continued on next page...

Continued from previous page...

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:417:LEU:HD12	1:B:417:LEU:HA	1.59	0.41
1:B:574:LEU:HD22	1:B:729:LEU:HD22	2.03	0.41
1:B:725:ILE:HG21	1:B:742:MET:HE1	2.03	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: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:932:THR:O	1:A:933:LYS:C	2.62	0.40
1:B:798:ASP:HB3	1:B:804:GLU:HG2	2.03	0.40
2:B:1101:MGJ:H25	2:B:1101:MGJ:C17	2.51	0.40
1:A:165:PHE:O	1:A:166:ALA:C	2.62	0.40
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.80	0.40
1:A:120:LYS:N	1:A:120:LYS:HD2	2.35	0.40
1:A:375:ILE:CG2	1:A:394:MET:HE2	2.51	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:A:995:MET:HE3	1:A:995:MET:HB3	1.79	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 ⓘ

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	950/990 (96%)	900 (95%)	50 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	950/990 (96%)	901 (95%)	45 (5%)	4 (0%)	30	65
All	All	1900/1980 (96%)	1801 (95%)	95 (5%)	4 (0%)	43	76

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	847/879 (96%)	736 (87%)	111 (13%)	4	19
1	B	847/879 (96%)	737 (87%)	110 (13%)	4	19
All	All	1694/1758 (96%)	1473 (87%)	221 (13%)	4	19

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	76	LEU
1	A	85	LYS
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	119	LYS
1	A	120	LYS
1	A	123	LYS
1	A	125	ASN
1	A	156	GLU
1	A	158	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	VAL
1	A	188	SER
1	A	201	LEU
1	A	212	LYS
1	A	223	LYS
1	A	226	LEU
1	A	243	LYS
1	A	256	VAL
1	A	270	LEU
1	A	277	GLU
1	A	285	LEU
1	A	287	GLU
1	A	296	GLU
1	A	301	LEU
1	A	316	THR
1	A	324	LYS
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	360	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	420	VAL
1	A	423	ARG
1	A	440	ILE
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	514	GLN
1	A	521	LYS
1	A	524	LEU
1	A	527	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	590	SER
1	A	595	LEU
1	A	597	LEU
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	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	744	MET
1	A	756	LYS
1	A	758	LEU
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	862	ARG
1	A	867	LEU
1	A	872	LYS
1	A	873	SER
1	A	886	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	889	LEU
1	A	906	LYS
1	A	928	LEU
1	A	930	THR
1	A	937	ILE
1	A	942	GLU
1	A	950	ARG
1	A	959	LEU
1	A	990	GLU
1	A	993	GLN
1	A	995	MET
1	A	996	THR
1	A	1007	LEU
1	A	1009	LYS
1	A	1011	HIS
1	B	43	ASN
1	B	61	LYS
1	B	63	GLU
1	B	76	LEU
1	B	94	ILE
1	B	97	LEU
1	B	102	ASN
1	B	103	ILE
1	B	111	GLN
1	B	125	ASN
1	B	158	LEU
1	B	159	GLU
1	B	179	LYS
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	237	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	316	THR
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	353	LYS
1	B	356	VAL
1	B	360	VAL
1	B	364	LYS
1	B	378	ASP
1	B	385	LEU
1	B	401	LEU
1	B	412	GLN
1	B	414	LEU
1	B	417	LEU
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	456	LEU
1	B	458	GLU
1	B	488	LYS
1	B	508	GLU
1	B	510	ILE
1	B	512	LYS
1	B	523	LYS
1	B	524	LEU
1	B	531	ILE
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	640	ILE
1	B	642	LEU
1	B	643	LYS
1	B	644	LYS
1	B	657	LYS
1	B	674	ARG
1	B	677	GLN
1	B	691	THR
1	B	697	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	744	MET
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	799	MET
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	825	THR
1	B	838	ARG
1	B	846	LEU
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	937	ILE
1	B	962	GLU
1	B	979	ASN
1	B	990	GLU
1	B	1007	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74)

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	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	332	HIS
1	A	336	HIS
1	A	386	HIS
1	A	393	HIS
1	A	442	HIS
1	A	475	ASN
1	A	502	GLN
1	A	573	ASN
1	A	575	ASN
1	A	621	GLN
1	A	622	ASN
1	A	672	ASN
1	A	677	GLN
1	A	730	HIS
1	A	781	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	857	HIS
1	A	922	ASN
1	A	957	HIS
1	A	979	ASN
1	A	988	GLN
1	B	43	ASN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	148	ASN
1	B	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	190	HIS
1	B	196	ASN
1	B	231	ASN
1	B	239	GLN
1	B	282	ASN
1	B	297	HIS
1	B	329	ASN
1	B	336	HIS
1	B	376	ASN
1	B	386	HIS
1	B	399	GLN
1	B	407	GLN
1	B	475	ASN
1	B	502	GLN
1	B	575	ASN
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	718	GLN
1	B	724	HIS
1	B	730	HIS
1	B	736	GLN
1	B	770	GLN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	851	GLN
1	B	857	HIS
1	B	887	GLN
1	B	922	ASN
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 [i](#)

There are no oligosaccharides 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	MGJ	A	1101	-	30,30,30	3.21	6 (20%)	38,38,38	2.25	18 (47%)
2	MGJ	B	1101	-	30,30,30	2.05	4 (13%)	38,38,38	1.29	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MGJ	A	1101	-	-	10/28/28/28	0/2/2/2
2	MGJ	B	1101	-	-	14/28/28/28	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	MGJ	C22-C21	9.03	1.54	1.38
2	A	1101	MGJ	C24-C25	8.93	1.54	1.38
2	B	1101	MGJ	C03-N02	8.27	1.44	1.33
2	A	1101	MGJ	C25-C20	8.02	1.54	1.38
2	A	1101	MGJ	C23-C22	6.95	1.53	1.38
2	B	1101	MGJ	C13-N12	4.53	1.43	1.34
2	B	1101	MGJ	C15-N16	-2.60	1.41	1.47
2	A	1101	MGJ	C17-N16	2.25	1.52	1.47
2	B	1101	MGJ	C07-N11	-2.14	1.33	1.38
2	A	1101	MGJ	C08-C07	2.06	1.40	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGJ	C23-C22-C21	-6.13	112.68	120.24
2	A	1101	MGJ	C24-C25-C20	-4.45	114.36	120.61
2	A	1101	MGJ	O04-C03-N02	-3.75	116.88	123.13
2	A	1101	MGJ	C05-C03-N02	3.32	121.99	116.99
2	B	1101	MGJ	C15-N16-C17	-3.16	104.29	111.91
2	A	1101	MGJ	C27-C26-N16	3.09	123.55	113.77
2	A	1101	MGJ	C22-C21-C20	3.07	124.93	120.61
2	A	1101	MGJ	C23-C24-C25	3.04	123.99	120.24
2	A	1101	MGJ	C18-C17-N16	3.01	122.40	113.93
2	A	1101	MGJ	C15-C13-N12	2.83	122.66	115.70
2	A	1101	MGJ	O28-C27-C26	2.73	124.15	113.38
2	A	1101	MGJ	O14-C13-C15	-2.65	116.39	121.02
2	A	1101	MGJ	C06-C07-C08	-2.47	124.28	129.33
2	B	1101	MGJ	C06-C05-C03	2.43	116.30	110.57
2	A	1101	MGJ	C06-C07-N11	2.28	128.57	121.74
2	A	1101	MGJ	C05-N12-C13	2.28	127.41	121.68
2	B	1101	MGJ	O04-C03-N02	-2.13	119.58	123.13
2	A	1101	MGJ	C06-C05-N12	2.13	114.70	110.64
2	A	1101	MGJ	C26-N16-C17	2.07	116.90	111.91
2	B	1101	MGJ	C03-C05-N12	-2.07	105.52	111.11
2	A	1101	MGJ	C05-C06-C07	2.04	118.54	113.75
2	A	1101	MGJ	C24-C23-C22	2.00	122.61	119.87

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MGJ	C06-C05-N12-C13
2	A	1101	MGJ	C13-C15-N16-C26
2	A	1101	MGJ	O04-C03-N02-C01
2	A	1101	MGJ	C05-C03-N02-C01
2	B	1101	MGJ	C06-C05-N12-C13
2	B	1101	MGJ	C13-C15-N16-C26
2	B	1101	MGJ	C27-C26-N16-C17
2	B	1101	MGJ	N16-C26-C27-O29
2	B	1101	MGJ	N12-C05-C06-C07
2	B	1101	MGJ	C03-C05-C06-C07
2	B	1101	MGJ	C05-C06-C07-N11
2	B	1101	MGJ	N16-C26-C27-O28
2	A	1101	MGJ	C05-C06-C07-C08
2	B	1101	MGJ	C05-C06-C07-C08

Continued on next page...

Continued from previous page...

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

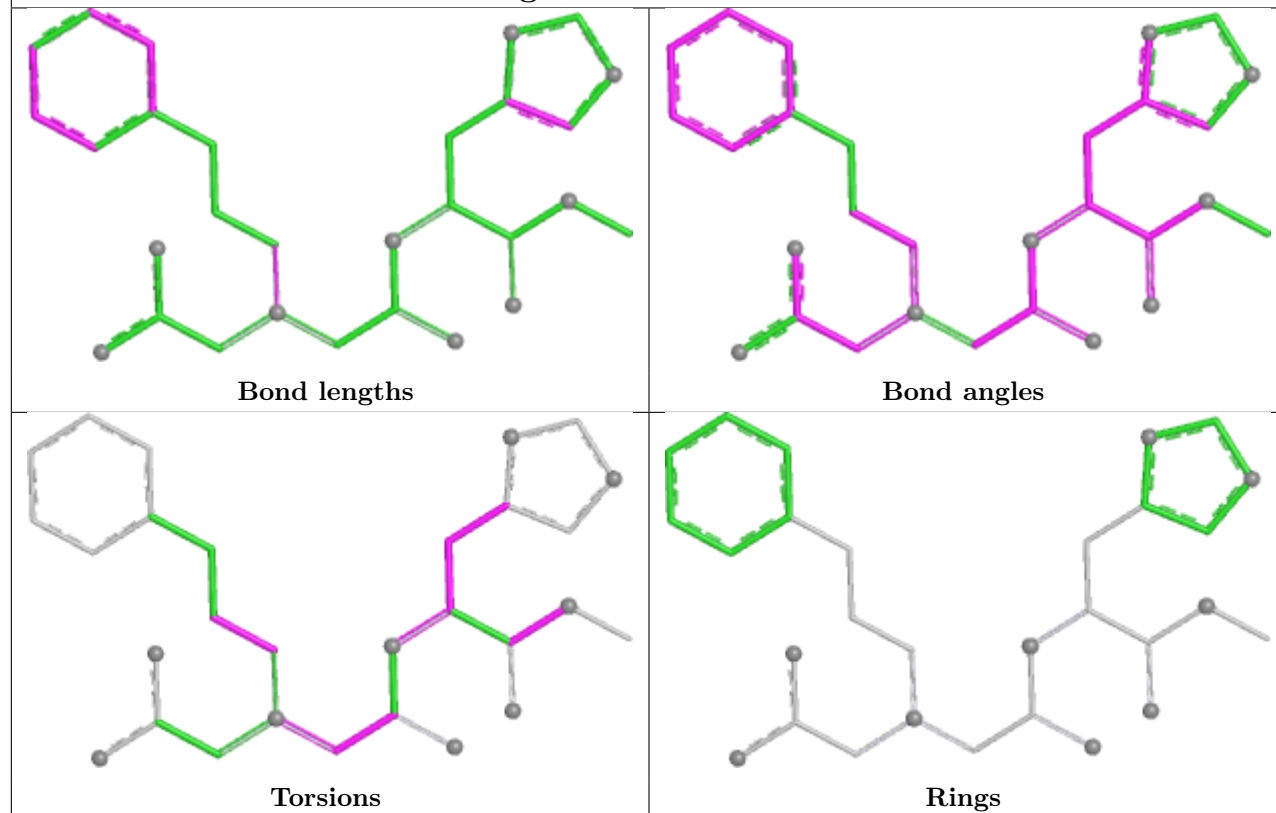
There are no ring outliers.

2 monomers are involved in 13 short contacts:

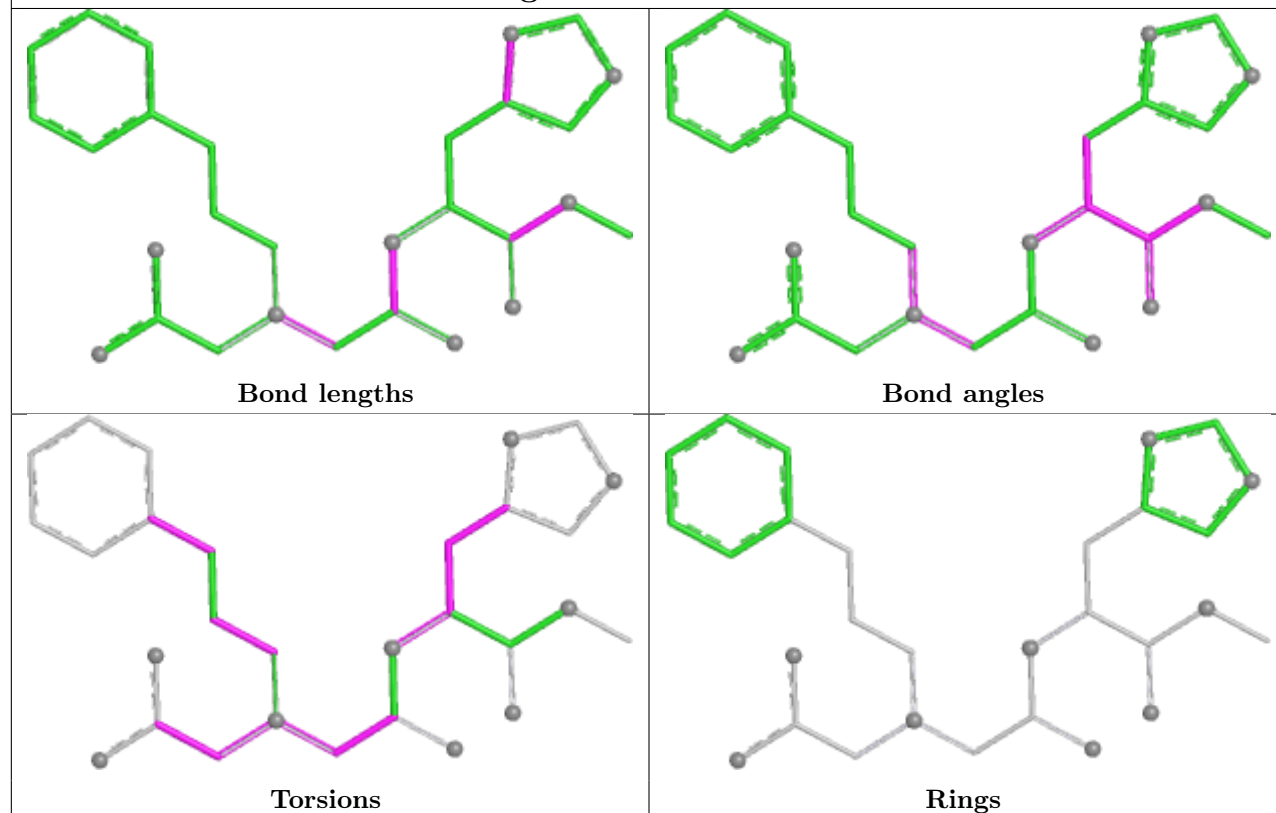
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MGJ	7	0
2	B	1101	MGJ	6	0

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

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	ASN	2.8
1	B	1011	HIS	2.8
1	B	229	ARG	2.3
1	B	857	HIS	2.3
1	B	979	ASN	2.2
1	A	1011	HIS	2.2
1	B	295	GLU	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

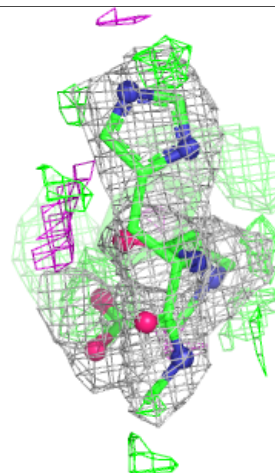
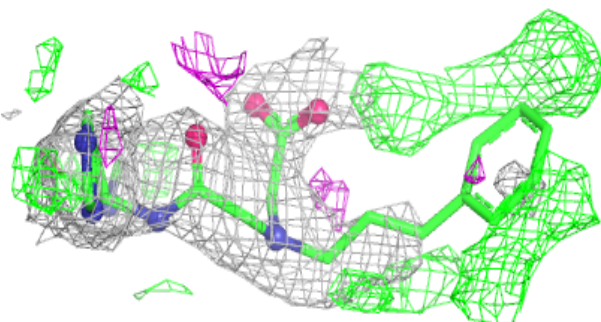
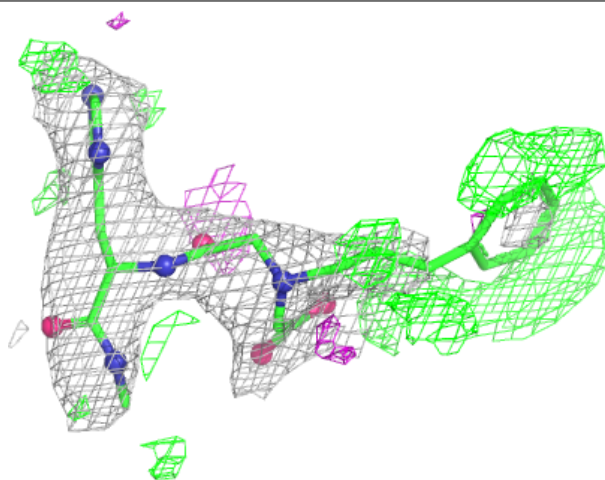
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

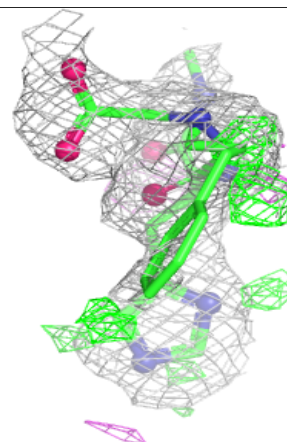
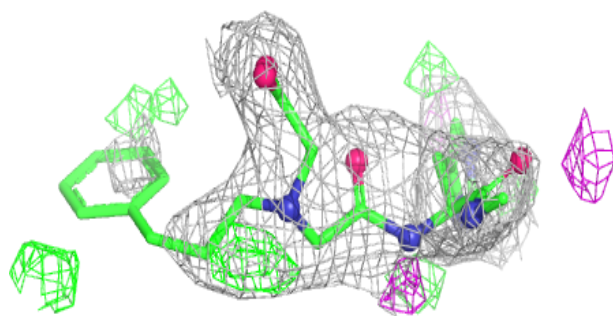
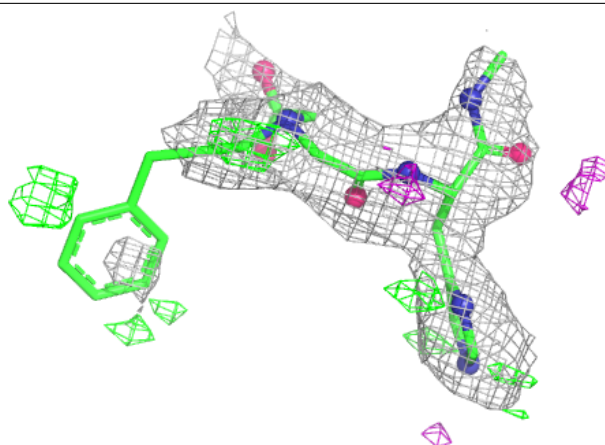
Electron density around MGJ A 1101:

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



Electron density around MGJ B 1101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.