



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:53 AM UTC

PDB ID : 4GSC / pdb_00004gsc
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 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

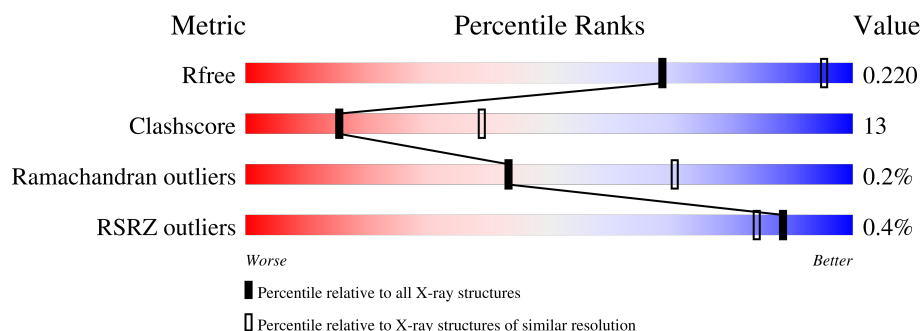
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
RSRZ outliers	180081	4594 (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 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 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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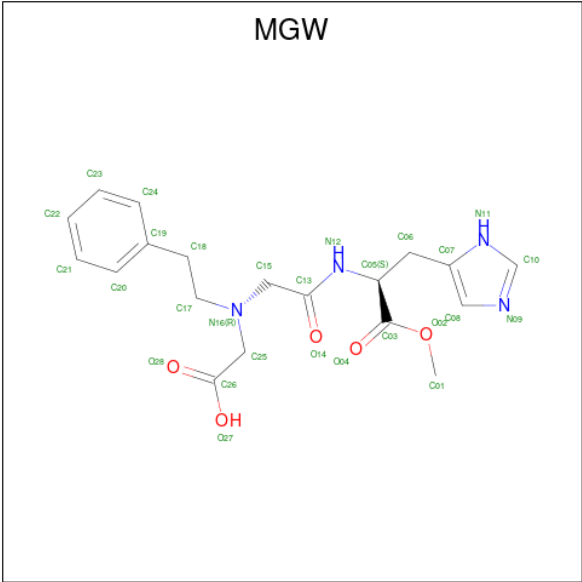
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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is methyl N-(carboxymethyl)-N-(2-phenylethyl)glycyl-L-histidinate (CCD ID: 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		

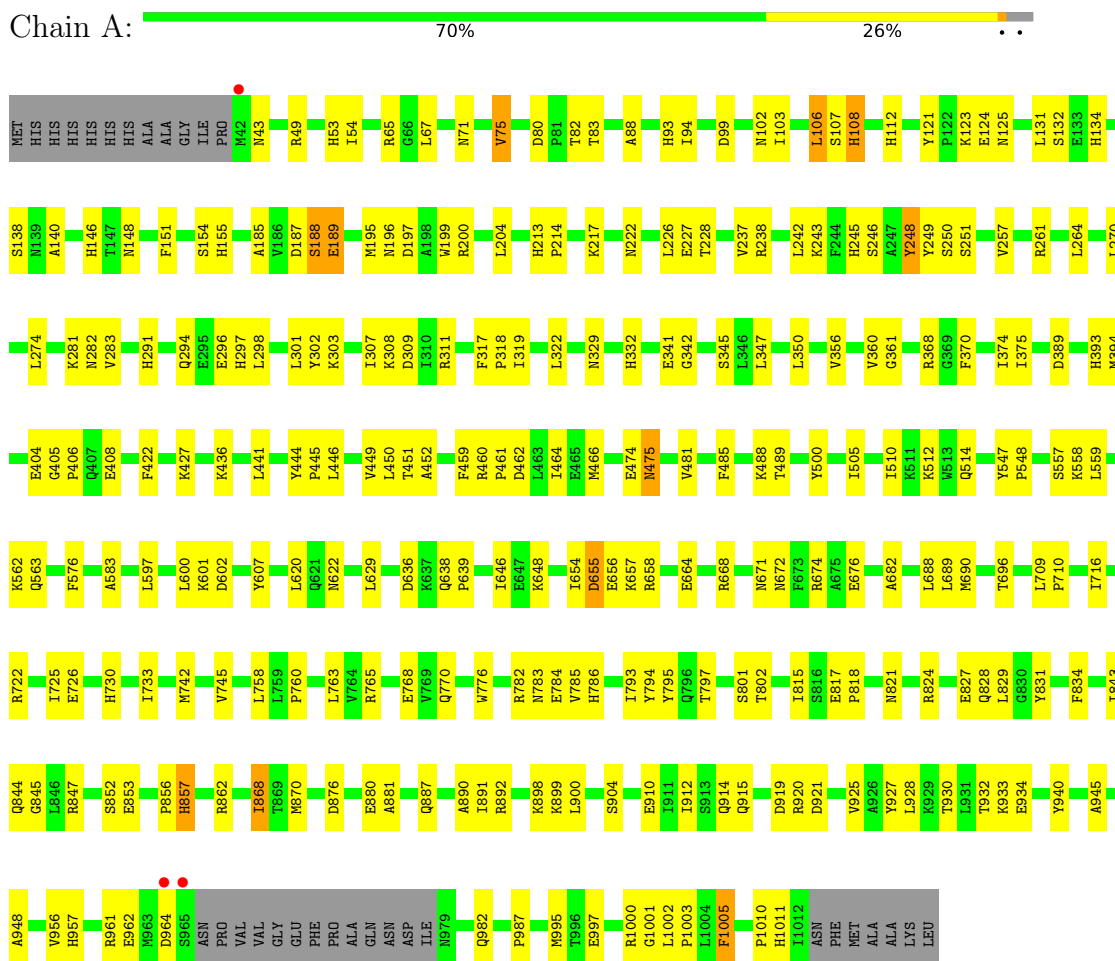
- Molecule 4 is water.

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

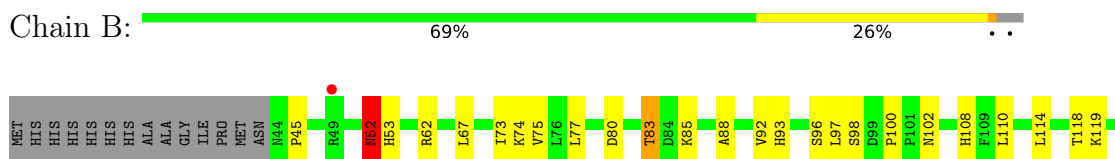
3 Residue-property plots

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



L1002	K123	S246	A367	K527	M649	F777	M870
P1003	E126	S250	R368	T551	F652	M783	I874
L1004	G136	S251	G369	K552	E653	E784	M877
F1005	G144	A255	I374	S557	D655	V785	R892
K1009	E145	V256	L379	K559	E656	H786	R896
P1010	Y150	V257	L396	L559	K657	N787	K896
H1011	F151	R261	Q396	W560	H658	N788	L1012
I1012	D152	E262	E413	F561	F659	E792	L900
ASN	V153	L267	E417	Q563	E664	I793	S904
PHE	S154	L270	R423	F567	M671	H799	I911
MET	H155	V271	L437	N573	M672	R805	Q915
ALA	L162	V272	A438	L574	F673	Q813	R920
LYS	D163	K273	L441	N575	R674	I814	D921
LEU	R164	E277	V449	A583	M683	I815	N922
	Q167	K281	L450	P587	L686	S816	T923
	F168	Q294	T451	L588	M690	E817	E924
	P172	H297	E457	A592	T691	R822	Y927
L173	M184	I304	E458	M593	E692	L823	L931
F174	S188	V305	E459	A593	V693	K826	T932
	E189	P306	F459	Y594	W695	E827	K933
V194	V196	K308	R460	L600	K697	G830	K953
M195	D197	D309	P461	D602	K701	Y831	V954
N196	A198	I310	D462	L604	L709	I832	S955
A199	W199	R311	E473	Y607	P710	V833	A960
R200	R201	T316	E474	A608	R711	R838	R961
L201	F202	F317	N475	Y609	L712	R839	E962
F203	Q203	P318	V476	E612	K713	A840	N963
L204	E205	G321	R477	N622	F715	R841	D964
K206	F218	D322	V481	Y625	L720	G842	S965
	K223	N329	S482	G626	M730	I843	ASN
	R229	G335	K483	M627	A737	Q844	PRO
P230	D236	G339	T489	Y628	I741	I850	VAL
	Q239	H340	R491	L629	M744	Q851	VAL
	K243	E341	Y500	S630	E751	S852	GLY
F244	H245	L346	I510	V631	R765	K854	PHE
		L347	Q514	K632	L641	P855	PRO
		W355	L642	Q638	E768	P856	ALA
		G361	L518	P639	Y768	I859	GLN
		Q362	F522	I640	Q770	R862	ASN
				L643	W776	F866	ASP
				K644		L867	ILE
				K648			N979
							P989
							T992
							K999

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.76Å 263.76Å 91.26Å 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 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.253 (Not available) , 0.220	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 , 39.8	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	0.94	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	1.10	4/8013 (0.0%)	1.23	42/10841 (0.4%)
1	B	1.03	4/7997 (0.1%)	1.21	37/10820 (0.3%)
All	All	1.07	8/16010 (0.0%)	1.22	79/21661 (0.4%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	ALA	CA-CB	-6.30	1.42	1.53
1	B	189	GLU	CG-CD	5.93	1.66	1.52
1	A	82	THR	CA-CB	5.81	1.63	1.53
1	A	464	ILE	CA-CB	-5.57	1.47	1.54
1	A	583	ALA	CA-CB	-5.45	1.45	1.53
1	B	1009	LYS	CA-C	5.15	1.58	1.53
1	B	218	PHE	CA-C	5.05	1.59	1.52
1	A	146	HIS	CA-C	-5.03	1.46	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ASN	N-CA-C	15.03	127.71	111.03
1	A	189	GLU	N-CA-C	-10.88	98.05	111.11
1	B	489	THR	CB-CA-C	-9.47	90.66	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	LYS	N-CA-C	8.79	121.97	111.33
1	A	655	ASP	N-CA-C	-7.88	95.41	108.34
1	B	92	VAL	CB-CA-C	-7.86	100.15	110.84
1	B	153	VAL	CB-CA-C	7.75	123.79	110.38
1	A	475	ASN	N-CA-C	7.74	119.72	110.44
1	A	329	ASN	CA-C-N	7.62	127.16	119.24
1	A	329	ASN	C-N-CA	7.62	127.16	119.24
1	A	1005	PHE	CA-C-N	-7.36	113.15	120.21
1	A	1005	PHE	C-N-CA	-7.36	113.15	120.21
1	A	797	THR	N-CA-C	7.19	126.12	110.80
1	A	948	ALA	CA-C-N	7.13	126.83	119.56
1	A	948	ALA	C-N-CA	7.13	126.83	119.56
1	B	374	ILE	N-CA-C	6.88	120.08	108.86
1	A	108	HIS	N-CA-C	-6.75	103.94	111.71
1	A	75	VAL	CB-CA-C	-6.64	99.78	110.28
1	A	282	ASN	N-CA-C	6.63	120.73	112.24
1	B	451	THR	CB-CA-C	-6.62	98.48	109.99
1	A	868	ILE	N-CA-C	6.50	117.12	110.82
1	A	557	SER	N-CA-C	6.45	118.90	108.32
1	A	857	HIS	N-CA-CB	6.45	119.73	110.06
1	B	53	HIS	N-CA-C	-6.41	98.92	108.99
1	A	436	LYS	N-CA-C	6.29	118.66	111.11
1	A	876	ASP	N-CA-C	6.15	119.89	112.38
1	B	557	SER	N-CA-C	6.15	118.40	108.32
1	B	850	ILE	N-CA-C	5.98	117.37	108.46
1	B	953	LYS	N-CA-C	5.95	118.22	108.52
1	A	795	TYR	N-CA-C	-5.92	97.52	107.99
1	B	654	ILE	N-CA-C	5.88	116.65	108.89
1	B	355	TRP	N-CA-C	5.85	120.59	112.45
1	A	107	SER	N-CA-CB	5.83	118.78	110.16
1	B	460	ARG	CA-C-N	5.80	126.20	119.47
1	B	460	ARG	C-N-CA	5.80	126.20	119.47
1	B	413	GLU	N-CA-C	-5.74	105.03	111.28
1	A	405	GLY	CA-C-N	5.74	125.74	119.89
1	A	405	GLY	C-N-CA	5.74	125.74	119.89
1	B	632	LYS	N-CA-C	5.73	117.89	109.24
1	A	657	LYS	CB-CA-C	-5.72	100.95	110.68
1	B	335	GLY	N-CA-C	-5.70	105.48	112.77
1	B	100	PRO	CA-C-N	5.67	125.35	119.56
1	B	100	PRO	C-N-CA	5.67	125.35	119.56
1	B	840	ALA	N-CA-C	5.66	117.71	108.55
1	B	189	GLU	N-CA-C	-5.62	102.09	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	PHE	N-CA-C	5.56	117.55	108.76
1	B	854	LYS	CA-C-N	5.56	123.66	119.66
1	B	854	LYS	C-N-CA	5.56	123.66	119.66
1	B	911	ILE	N-CA-C	5.56	115.69	110.30
1	A	54	ILE	CB-CA-C	-5.53	105.26	111.23
1	A	332	HIS	N-CA-C	-5.53	104.66	111.40
1	A	785	VAL	N-CA-C	5.52	115.61	110.42
1	A	488	LYS	N-CA-C	5.52	118.80	112.57
1	B	602	ASP	N-CA-C	-5.49	105.38	111.36
1	B	429	ARG	N-CA-C	-5.47	102.88	109.83
1	A	189	GLU	N-CA-CB	5.45	118.05	109.94
1	B	52	ASN	CB-CA-C	-5.41	102.56	110.95
1	B	197	ASP	N-CA-C	5.40	117.92	111.71
1	B	316	THR	CB-CA-C	5.38	118.95	109.80
1	B	244	PHE	N-CA-C	-5.36	105.35	111.14
1	A	43	ASN	N-CA-C	5.35	117.59	110.53
1	B	853	GLU	N-CA-C	-5.35	106.60	113.23
1	A	248	TYR	N-CA-C	5.27	119.81	112.90
1	A	733	ILE	N-CA-C	5.25	115.92	108.42
1	A	821	ASN	N-CA-C	5.22	116.97	111.28
1	A	107	SER	N-CA-C	5.21	117.04	111.36
1	B	915	GLN	N-CA-C	-5.18	107.51	113.88
1	A	121	TYR	CA-C-N	5.17	125.25	119.87
1	A	121	TYR	C-N-CA	5.17	125.25	119.87
1	B	150	TYR	N-CA-C	5.16	116.92	108.76
1	B	607	TYR	N-CA-C	5.16	116.59	111.07
1	A	283	VAL	N-CA-C	5.15	114.57	108.96
1	A	188	SER	N-CA-C	5.12	116.86	111.28
1	A	283	VAL	CB-CA-C	-5.12	104.80	110.68
1	A	716	ILE	N-CA-CB	5.10	114.43	110.45
1	B	458	GLU	N-CA-C	5.08	117.69	109.06
1	A	106	LEU	N-CA-C	5.05	116.79	111.28
1	B	964	ASP	N-CA-C	5.05	115.78	107.20
1	B	83	THR	N-CA-C	5.02	117.51	110.23

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	191	0
1	B	7802	0	7734	229	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	11	0
4	B	72	0	0	6	0
All	All	15858	0	15528	420	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 13.

All (420) 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	1.00
1:B:711:ARG:HH21	1:B:711:ARG:HG2	1.34	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:HD22	1:A:622:ASN:H	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:HD22	1:B:622:ASN:N	1.73	0.83
1:A:622:ASN:HD22	1:A:622:ASN:N	1.71	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:O	1:A:83:THR:HG22	1.78	0.82
1:A:622:ASN:H	1:A:622:ASN:ND2	1.68	0.82
1:B:674:ARG:HH11	1:B:674:ARG:CG	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:A:108:HIS:HE1	1:A:189:GLU:CD	1.89	0.79
1:B:196:ASN:ND2	1:B:198:ALA:H	1.78	0.79
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:466:MET:HE2	1:A:466:MET:O	1.83	0.79
1:A:108:HIS:NE2	1:A:112:HIS:NE2	2.31	0.78
1:B:642:LEU:HD23	1:B:642:LEU:C	2.10	0.77
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: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:O14	3:A:1102:MGW:H206	1.88	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:HD3	1:A:512:LYS:O	1.93	0.69
1:A:270:LEU:CD2	1:A:274:LEU:HD11	2.22	0.68
1:A:196:ASN:HD22	1:A:199:TRP:CD1	2.11	0.68
1:A:294:GLN:H	1:A:297:HIS:CD2	2.10	0.68
1:A:102:ASN:H	1:A:102:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:LEU:HD23	1:B:75:VAL:HB	1.77	0.66
1:B:361:GLY:H	3:B:1102:MGW:H106	1.59	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
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:B:329:ASN:C	1:B:329:ASN:HD22	2.04	0.65
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.44	0.65
1:A:213:HIS:ND1	1:A:214:PRO:HD2	2.12	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:HD22	1:B:102:ASN:H	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:783:ASN:HD22	1:B:783:ASN:C	2.07	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:512:LYS:HD3	1:A:512:LYS:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:HIS:HE1	1:B:189:GLU:CD	2.01	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:B:311:ARG:HH22	1:B:664:GLU:CD	2.09	0.60
1:A:783:ASN:HD21	1:A:786:HIS:H	1.45	0.60
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.84	0.60
1:B:423:ARG:HH11	1:B:423:ARG:CG	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
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:642:LEU:C	1:B:642:LEU:CD2	2.76	0.58
1:B:396:GLN:HG2	1:B:517:ASP:O	2.04	0.58
1:A:204:LEU:HG	1:A:204:LEU:O	2.00	0.58
1:B:423:ARG:HH11	1:B:423:ARG:HG3	1.69	0.58
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.84	0.58
1:A:466:MET:HE2	1:A:466:MET:C	2.29	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: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:151:PHE:CD1	1:A:151:PHE:C	2.82	0.57
1:A:270:LEU:O	1:A:274:LEU:HD12	2.05	0.57
1:B:527:LYS:CB	1:B:527:LYS:HZ2	2.12	0.56
1:A:317:PHE:N	1:A:317:PHE:CD1	2.74	0.56
1:B:874:ILE:O	1:B:933:LYS:HE3	2.04	0.56
1:A:856:PRO:O	1:A:857:HIS:C	2.47	0.56
1:B:110:LEU:HD23	1:B:110:LEU:C	2.31	0.56
1:A:725:ILE:HG21	1:A:742:MET:HE1	1.88	0.56
1:A:921:ASP:O	1:A:925:VAL:HG23	2.06	0.56
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.87	0.56
1:B:196:ASN:HD22	1:B:196:ASN:C	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.40	0.56
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.41	0.56
1:A:125:ASN:H	1:A:125:ASN:HD22	1.53	0.56
1:B:473:PRO:O	1:B:476:VAL:HG12	2.06	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:B:277:GLU:CD	1:B:277:GLU:H	2.14	0.55
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:B:559:LEU:HD12	1:B:559:LEU:C	2.32	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
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:880:GLU:O	1:A:881:ALA:C	2.51	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:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.55	0.53
1:A:784:GLU:O	1:A:961:ARG:HG3	2.09	0.52
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.55	0.52
1:B:805:ASN:HD22	1:B:844:GLN:NE2	2.06	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:A:722:ARG:CB	1:A:758:LEU:HD12	2.39	0.52
1:B:196:ASN:ND2	1:B:198:ALA:N	2.53	0.52
1:B:690:MET:HA	1:B:690:MET:HE2	1.91	0.52
1:A:309:ASP:O	1:A:668:ARG:HD2	2.10	0.52
1:A:374:ILE:C	1:A:375:ILE:HG13	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:TYR:HB3	1:A:548:PRO:HD2	1.91	0.52
1:A:576:PHE:CD1	1:A:576:PHE:N	2.78	0.51
1:A:824:ARG:O	1:A:828:GLN:HA	2.10	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:77:LEU:HD22	1:B:267:LEU:CB	2.40	0.51
1:A:559:LEU:HD12	1:A:559:LEU:C	2.35	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:236:ASP:OD1	1:B:236:ASP:C	2.53	0.51
1:B:648:LYS:O	1:B:652:PHE:HB2	2.11	0.51
1:B:818:PRO:CG	1:B:870:MET:HE1	2.40	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: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
1:B:257:VAL:HG21	1:B:437:ILE:HG22	1.92	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: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:119:LYS:HZ2	1:B:119:LYS:HB2	1.78	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:ND2	1:B:622:ASN:N	2.42	0.49
1:B:819:ALA:O	1:B:823:LEU:HB2	2.12	0.49
1:A:49:ARG:O	1:A:67:LEU:HB2	2.13	0.49
1:A:248:TYR:O	1:A:250:SER:N	2.43	0.49
1:A:932:THR:O	1:A:933:LYS:C	2.56	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:195:MET:HE3	4:A:1231:HOH:O	2.13	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:982:GLN:HA	1:A:982:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASP:O	1:B:83:THR:HG22	2.13	0.48
1:B:656:GLU:O	1:B:659:PHE:HB3	2.11	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:A:99:ASP:O	1:A:217:LYS:NZ	2.44	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:HE3	1:B:657:LYS:HA	1.95	0.48
1:A:597:LEU:O	1:A:601:LYS:HG3	2.13	0.48
1:A:801:SER:O	1:A:802:THR:C	2.57	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:B:491:ARG:HB2	1:B:500:TYR:O	2.14	0.47
1:B:329:ASN:C	1:B:329:ASN:ND2	2.72	0.47
1:B:311:ARG:NH1	1:B:379:LEU:O	2.42	0.47
1:A:298:LEU:HD13	1:A:475:ASN:HB2	1.97	0.47
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: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:765:ARG:HH11	1:A:914:GLN:HG3	1.80	0.47
1:A:843:ILE:CG2	1:A:844:GLN:N	2.78	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:197:ASP:HA	1:A:200:ARG:HD3	1.98	0.46
1:A:770:GLN:HE21	1:A:1003:PRO:HB2	1.80	0.46
1:A:489:THR:HB	1:A:500:TYR:O	2.15	0.46
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.51	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:B:815:ILE:HA	1:B:870:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:237:VAL:O	1:A:238:ARG:C	2.58	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:A:123:LYS:O	1:A:124:GLU:C	2.59	0.46
1:B:163:ASP:O	1:B:164:ARG:C	2.57	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:592:MET:HE3	1:B:715:PHE:CD1	2.51	0.46
1:B:674:ARG:HG3	1:B:674:ARG:NH1	2.29	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:185:ALA:HB2	1:A:828:GLN:HE22	1.81	0.45
1:A:360:VAL:HA	3:A:1102:MGW:N09	2.30	0.45
1:B:329:ASN:ND2	1:B:329:ASN:O	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: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:A:311:ARG:HH22	1:A:664:GLU:CD	2.25	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:B:96:SER:C	1:B:98:SER:H	2.23	0.45
1:B:799:MET:HE3	1:B:799:MET:HB3	1.75	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:B:574:LEU:C	1:B:575:ASN:HD22	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:HD12	1:A:322:LEU:HD11	1.99	0.44
1:A:899:LYS:O	1:A:900:LEU:C	2.60	0.44
1:A:361:GLY:H	3:A:1102:MGW:H08	1.82	0.44
1:A:928:LEU:C	1:A:930:THR:H	2.25	0.44
1:B:777:PHE:HB3	1:B:992:ILE:HD11	1.99	0.44
1:B:67:LEU:CD2	1:B:75:VAL:HB	2.44	0.44
1:B:737:ALA:O	1:B:741:ILE:HG13	2.17	0.44
1:A:827:GLU:CD	1:A:862:ARG:HH11	2.25	0.44
1:B:294:GLN:O	1:B:297:HIS:N	2.47	0.44
1:B:840:ALA:C	1:B:842:GLY:H	2.25	0.44
1:B:97:LEU:HD12	1:B:97:LEU:HA	1.85	0.44
1:B:638:GLN:O	1:B:639:PRO:C	2.60	0.44
1:B:783:ASN:ND2	1:B:783:ASN:C	2.74	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:311:ARG:NH2	1:B:664:GLU:CD	2.75	0.44
1:B:593:ALA:O	1:B:594:TYR:C	2.57	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:HD23	1:A:441:LEU:HA	1.82	0.43
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.65	0.43
1:B:491:ARG:NH1	4:B:1231:HOH:O	2.52	0.43
1:A:607:TYR:C	1:A:607:TYR:CD2	2.96	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:196:ASN:ND2	1:B:196:ASN:C	2.75	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:227:GLU:O	1:A:228:THR:C	2.60	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
1:B:788:ASN:O	1:B:960:ALA:HA	2.18	0.43
1:B:838:ARG:O	1:B:844:GLN:HA	2.19	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:A:868:ILE:C	1:A:870:MET:N	2.74	0.43
1:A:296:GLU:H	1:A:296:GLU:CD	2.24	0.43
1:A:445:PRO:O	1:A:446:LEU:C	2.61	0.43
1:B:600:LEU:HD12	1:B:600:LEU:HA	1.76	0.43
1:B:686:LEU:HD12	1:B:686:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:ASN:N	1:B:922:ASN:HD22	2.15	0.43
1:B:489:THR:O	1:B:489:THR:OG1	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:HH21	1:B:711:ARG:CG	2.18	0.42
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.54	0.42
1:A:451:THR:O	1:A:452:ALA:C	2.62	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:A:776:TRP:CZ3	1:A:987:PRO:O	2.73	0.42
1:A:910:GLU:HA	1:A:910:GLU:OE2	2.20	0.42
1:B:102:ASN:H	1:B:102:ASN:ND2	2.13	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:960:ALA:HB3	1:B:963:MET:HG3	2.02	0.42
1:A:690:MET:HE2	1:A:690:MET:HA	2.01	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:B:199:TRP:O	1:B:200:ARG:C	2.61	0.42
1:B:272:VAL:O	1:B:273:LYS:C	2.62	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:B:877:MET:O	1:B:933:LYS:NZ	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:MET:HE3	1:B:627:MET:HB2	1.94	0.41
1:A:375:ILE:CG2	1:A:394:MET:HE2	2.51	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:OE1	1:A:676:GLU:HA	2.20	0.41
1:A:829:LEU:O	1:A:852:SER:CB	2.69	0.41
1:A:887:GLN:O	1:A:890:ALA:HB3	2.20	0.41
1:B:188:SER:HB3	1:B:831:TYR:HB2	2.03	0.41
1:A:131:LEU:O	1:A:132:SER:C	2.64	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
1:B:818:PRO:HG2	1:B:870:MET:HE1	2.02	0.41
1:B:641:LEU:O	1:B:642:LEU:C	2.61	0.40
1:B:840:ALA:C	1:B:842:GLY:N	2.77	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
3:A:1102:MGW:O14	3:A:1102:MGW:C06	2.66	0.40
1:B:491:ARG:CG	1:B:491:ARG:NH1	2.75	0.40
1:B:562:LYS:HG3	1:B:563:GLN:N	2.37	0.40
1:B:751:GLU:O	1:B:751:GLU:HG2	2.17	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: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:1012:ILE:N	4:B:1250:HOH:O	2.55	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%)	36	64
1	B	952/990 (96%)	876 (92%)	75 (8%)	1 (0%)	48	75
All	All	1906/1980 (96%)	1766 (93%)	136 (7%)	4 (0%)	43	71

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 [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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
3	MGW	B	1102	-	29,29,29	1.57	2 (6%)	36,37,37	2.36	7 (19%)
3	MGW	A	1102	-	29,29,29	1.58	2 (6%)	36,37,37	1.71	8 (22%)

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	B	1102	-	-	12/27/27/27	0/2/2/2
3	MGW	A	1102	-	-	15/27/27/27	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	MGW	O02-C03	5.97	1.47	1.33
3	A	1102	MGW	O02-C03	5.96	1.47	1.33
3	A	1102	MGW	C06-C07	2.38	1.53	1.49
3	B	1102	MGW	C05-N12	2.03	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-C06-C07	7.98	126.78	113.27
3	B	1102	MGW	C05-N12-C13	6.53	138.06	121.68
3	B	1102	MGW	C03-C05-N12	4.53	121.10	110.65
3	A	1102	MGW	O02-C03-C05	4.22	122.22	111.49
3	B	1102	MGW	C01-O02-C03	3.94	124.85	115.92
3	B	1102	MGW	C06-C05-C03	3.64	118.51	110.62
3	A	1102	MGW	C01-O02-C03	3.60	124.08	115.92
3	A	1102	MGW	C05-N12-C13	3.54	130.57	121.68
3	A	1102	MGW	O02-C03-O04	-3.38	117.26	123.85
3	B	1102	MGW	O02-C03-C05	3.15	119.51	111.49
3	A	1102	MGW	C17-C18-C19	2.73	119.85	112.15
3	A	1102	MGW	O27-C26-C25	2.32	122.53	113.38
3	B	1102	MGW	C06-C07-N11	2.16	129.02	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	MGW	C25-N16-C15	-2.07	106.79	111.66
3	A	1102	MGW	C08-N09-C10	2.07	110.01	105.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

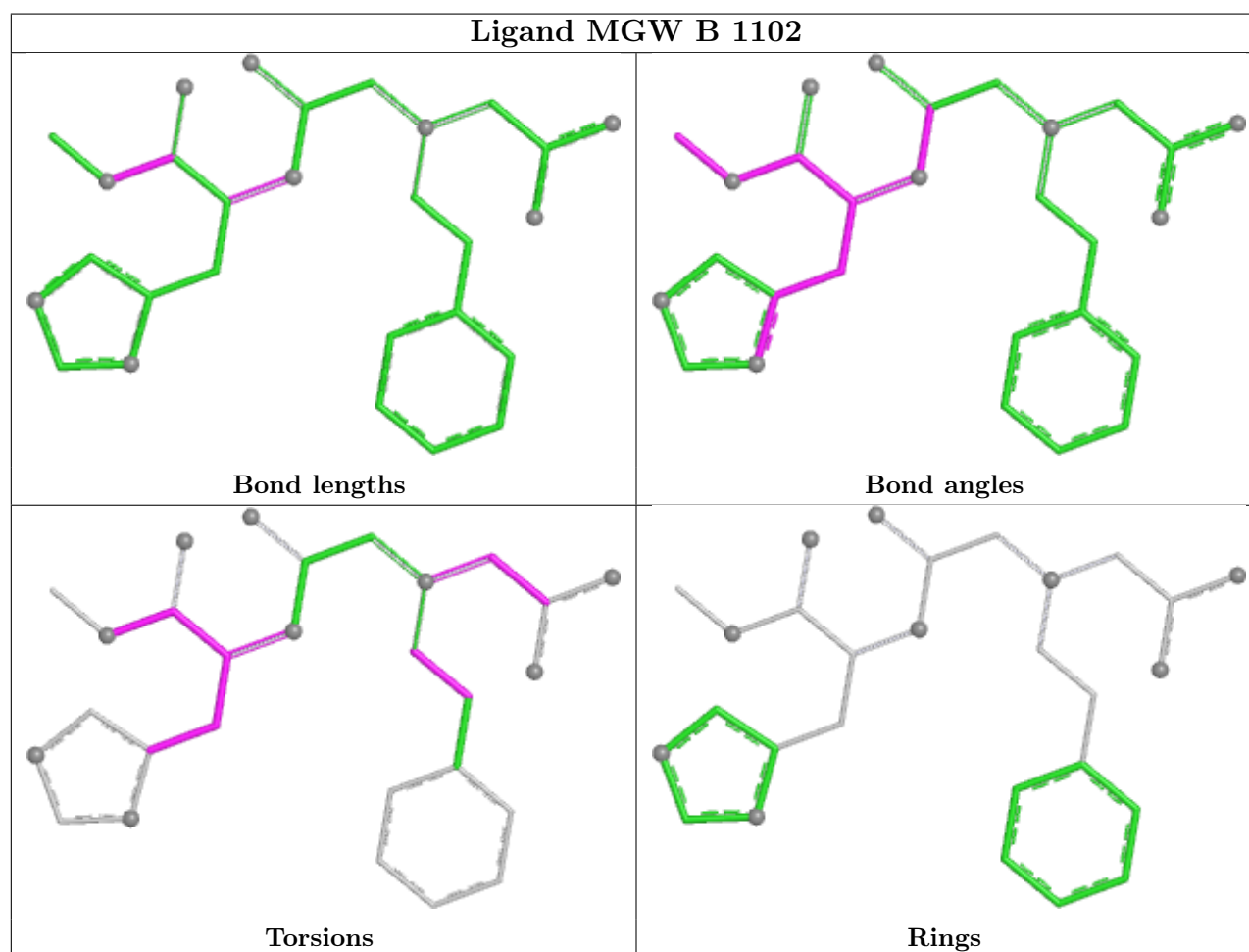
Mol	Chain	Res	Type	Atoms
3	A	1102	MGW	C06-C05-N12-C13
3	B	1102	MGW	N16-C25-C26-O27
3	B	1102	MGW	N16-C25-C26-O28
3	B	1102	MGW	N12-C05-C06-C07
3	A	1102	MGW	O04-C03-O02-C01
3	B	1102	MGW	O04-C03-O02-C01
3	A	1102	MGW	C05-C03-O02-C01
3	A	1102	MGW	C18-C17-N16-C25
3	B	1102	MGW	C05-C03-O02-C01
3	A	1102	MGW	N16-C17-C18-C19
3	B	1102	MGW	C03-C05-N12-C13
3	B	1102	MGW	N16-C17-C18-C19
3	A	1102	MGW	C03-C05-C06-C07
3	A	1102	MGW	C17-C18-C19-C20
3	A	1102	MGW	C17-C18-C19-C24
3	A	1102	MGW	C05-C06-C07-N11
3	B	1102	MGW	C26-C25-N16-C15
3	B	1102	MGW	C26-C25-N16-C17
3	A	1102	MGW	C05-C06-C07-C08
3	A	1102	MGW	N12-C05-C06-C07
3	B	1102	MGW	C05-C06-C07-N11
3	B	1102	MGW	C05-C06-C07-C08
3	A	1102	MGW	C18-C17-N16-C15
3	A	1102	MGW	O02-C03-C05-C06
3	A	1102	MGW	O04-C03-C05-C06
3	A	1102	MGW	C26-C25-N16-C15
3	B	1102	MGW	O04-C03-C05-C06

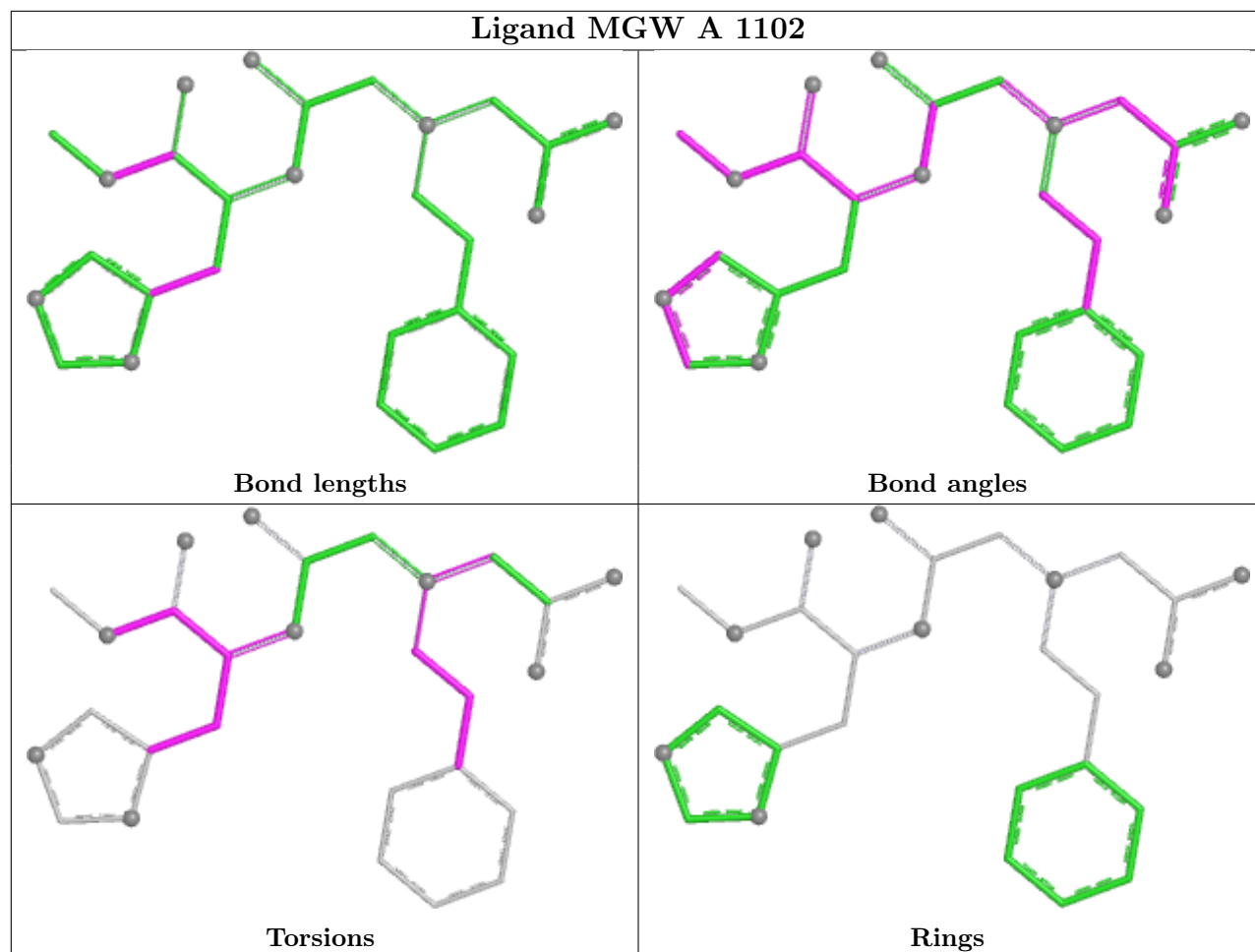
There are no ring outliers.

2 monomers are involved in 10 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.43	3 (0%)	90 86	25, 41, 58, 88	0
1	B	956/990 (96%)	-0.27	4 (0%)	88 84	32, 47, 65, 82	0
All	All	1914/1980 (96%)	-0.35	7 (0%)	88 84	25, 44, 62, 88	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	965	SER	6.0
1	A	965	SER	5.4
1	B	964	ASP	4.0
1	A	964	ASP	3.7
1	A	42	MET	3.1
1	B	49	ARG	2.7
1	B	517	ASP	2.4

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](#)

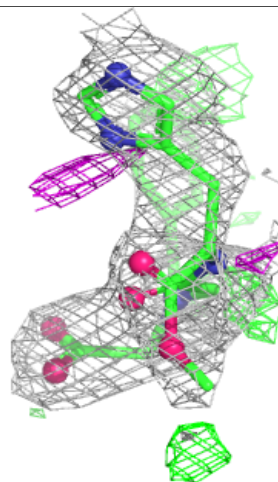
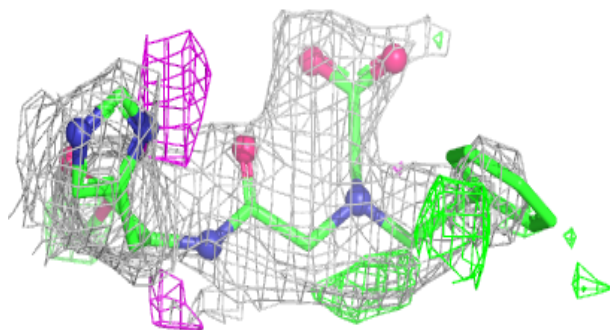
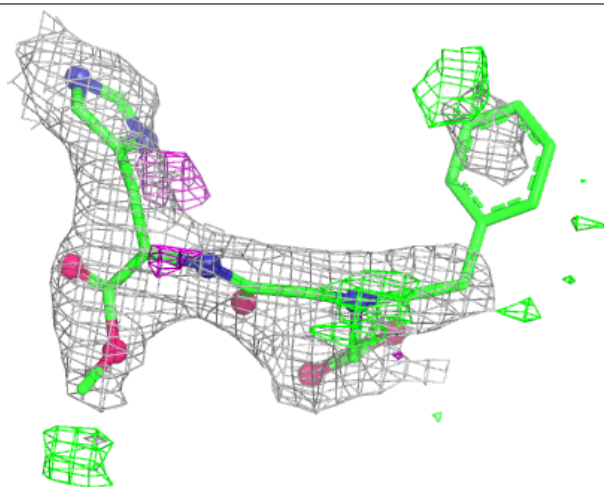
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
3	MGW	B	1102	28/28	0.82	0.24	79,87,102,102	0
3	MGW	A	1102	28/28	0.84	0.22	64,80,86,87	0
2	ZN	A	1101	1/1	0.92	0.39	2,2,2,2	0
2	ZN	B	1101	1/1	0.98	0.37	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.

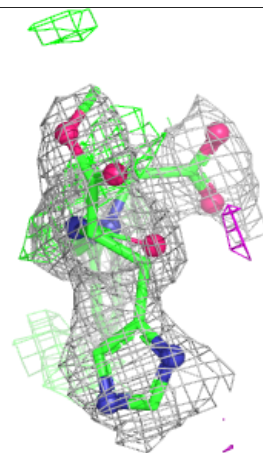
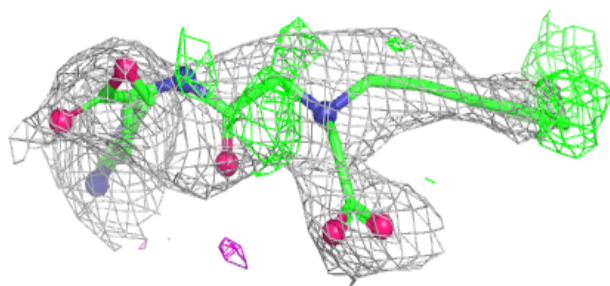
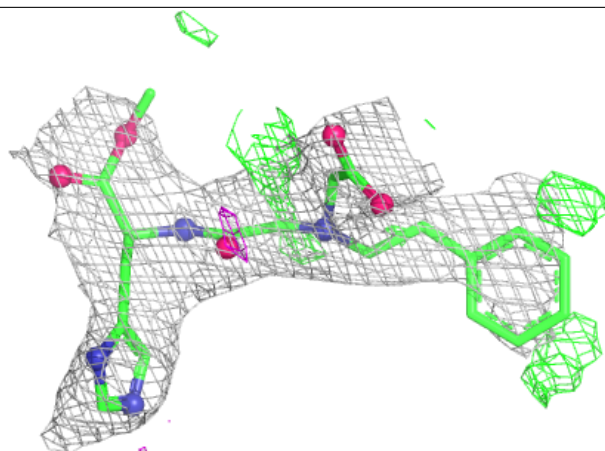
Electron density around MGW B 1102:

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 [i](#)

There are no such residues in this entry.