



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:10 AM UTC

PDB ID : 4DWK / pdb_00004dwk
Title : Structure of cystein free insulin degrading enzyme with compound bdm41671 ((s)-2-{2-[carboxymethyl-(3-phenyl-propyl)-amino]-acetylamino}-3-(1h-imidazol-4-yl)-propionic acid methyl ester)
Authors : Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on : 2012-02-24
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

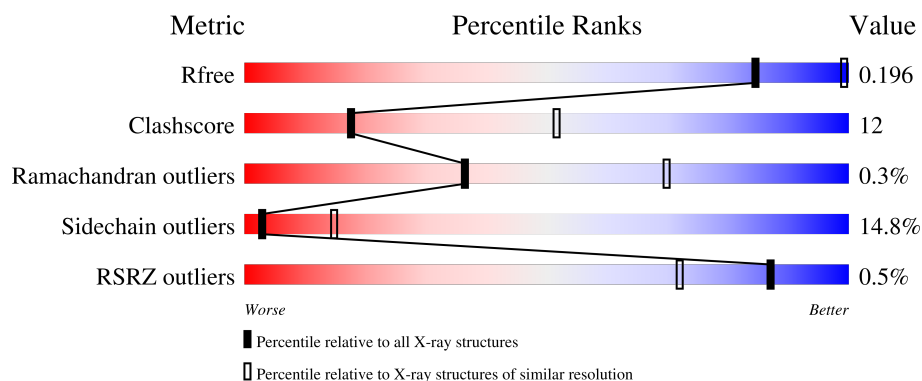
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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 15764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	955	Total	C	N	O	S	0	0	0
			7802	5026	1310	1443	23			
1	B	955	Total	C	N	O	S	0	0	0
			7796	5023	1309	1442	22			

There are 52 discrepancies between the modelled and reference sequences:

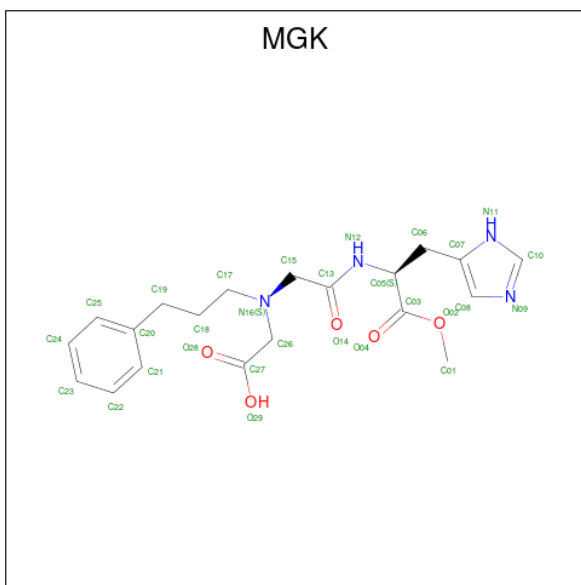
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735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

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

- Molecule 2 is methyl N-(carboxymethyl)-N-(3-phenylpropyl)glycyl-L-histidinate (CCD ID: MGK) (formula: $C_{20}H_{26}N_4O_5$).



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

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

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

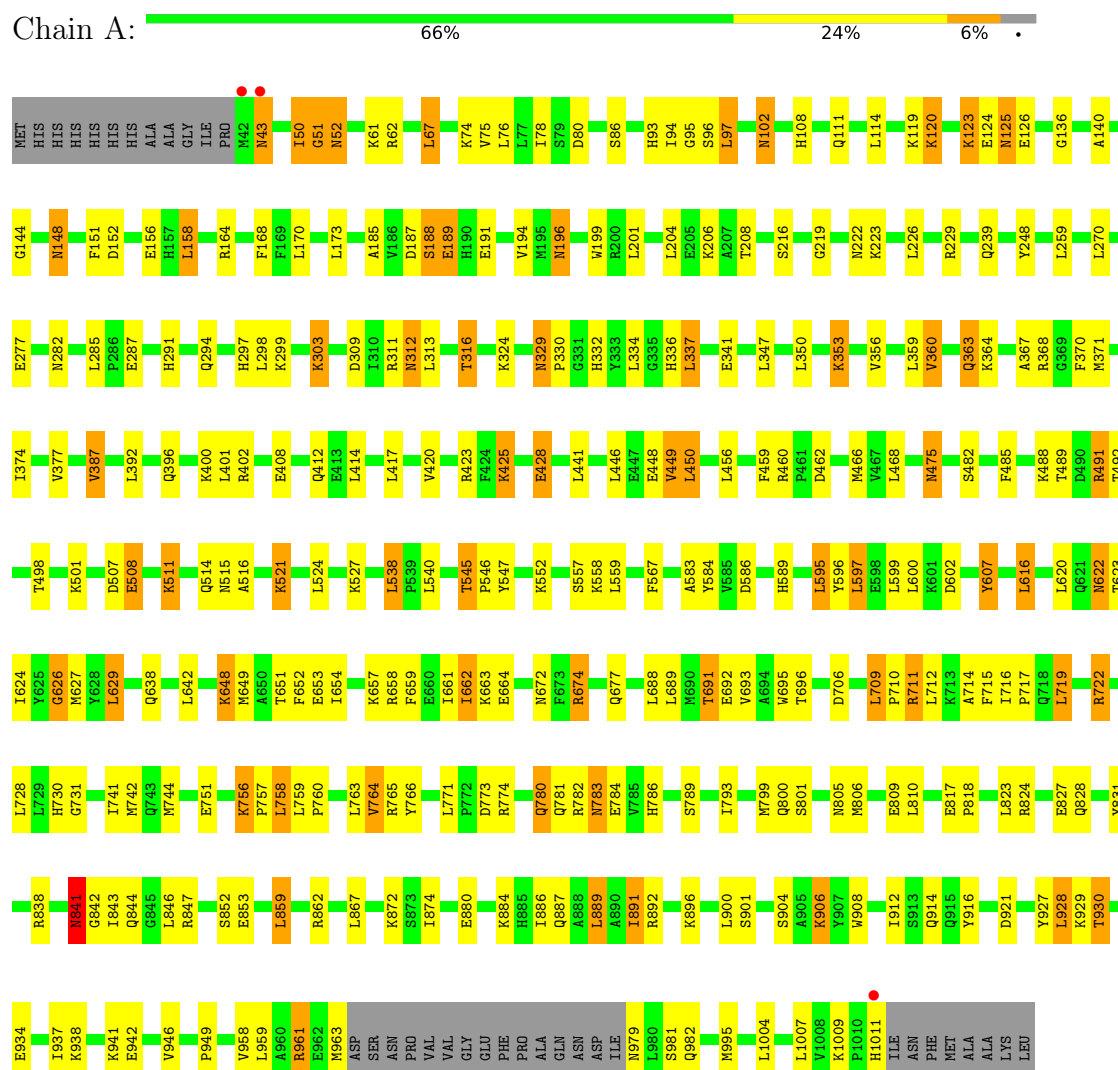
- Molecule 4 is water.

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

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



P1010	K933	I843	E751	H649	P546	P445	D321	S216	N125	MET
H1011	E934	Q844	H754	D655	K552	L446	K329	K217	E126	HIS
ILE	G945	G945	T755	E656	K553	E447	P330	N222	Y127	HIS
ASN	L846	L846	T756	E657	T554	V449	G331	K223	S128	HIS
PHE	R847	R847	K757	R658	K558	L450	H332	L226	Q129	HIS
MET	S852	S852	L758	P659	L559	T451	L337	L226	F130	HIS
ALA	E853	E853	L759	T662	K562	A452	E341	R229	L131	HIS
ALA	K854	K854	V764	E664	P570	L455	L347	E233	S132	ALA
LYS	P855	P855	R765	R671	M575	L456	S348	G234	E133	ALA
LEU	H857	H857	Y766	R672	F578	E457	E349	L235	H134	ILE
	Y858	Y858	R767	R673	F579	E458	S348	E235	S138	PRO
	L859	L859	Q770	E674	F579	R460	E349	R238	E145	ASN
	S860	S860	P772	E675	A583	P461	K353	T147	H146	N44
	S861	S861	D773	E676	D586	D462	K353	T147	T147	N44
	R862	R862	R774	Q677	P587	L463	K353	K243	N148	I50
	H865	H865	G775	Y685	S590	T464	L359	S250	Y149	G51
	F866	F866	W776	L686		E466	V360	S251	Y150	N52
	L867	L867	Q780	R687		N466	Q363	V256	F151	H53
	T868	T868	R781	L688		D469	K364	V257	H157	K61
	M870	M870	R782			N475	K368	V258	L158	R62
	I874	I874	M783	T691	L595		E368	L259	G160	I73
	M877	M877	E784	E692	Y596	V481	M371	E262	R164	L76
	V878	V878	H786	V693	L597	E494	I375	E262	L77	L77
	E880	E880	Y795	W695	E598		I375	L270	Q167	I78
	K884	K884	Y795	K701	L600	T498	L379	V271	L170	D80
	H885	H885	S801	E702	K601	Q499	T380	V272	D175	S86
	T886	T886	T802		D602	Y500	E381	S276	E176	S87
	Q887	Q887	S803	T708	L604	D507	H386	K231	S177	A88
	A888	A888	E804	L709	R605	E508	D389	L285	A178	A89
	L889	L889	N805	P710	E606	V509	D389	P286	L90	L90
	A890	A890	M806	R711	E612	I510	M394	E287	D91	D91
	I891	I891	F807	L712		K511	M394	E287	V92	V92
	R892	R892	L808	K713	L616	K512	Q399	E290	H93	H93
	R893	R893	E809		Q621	Q514	Q405	E290	L97	L97
	K898	K898	L810	Q718	Q621	N515	Q405	E290	S98	S98
	K899	K899	I815	I725	W622	A516	Q412	Q294	M102	M102
	S904	S904	S816	L728	G626	P517	E413	H297	M195	M195
	I912	I912	P818	L729	W627	L518	L414	L298	D197	S107
	Q915	Q915	L823	H730	Y628	G520	L417	A198	A198	H108
	R920	R920	K826	I733	L629	K521	K425	R200	F109	F109
	T923	T923	E827	T734	S630	F522	K425	L201	L110	L110
	E924	E924	Y831	Q736	W631	K523	Y433	P202	Q111	Q111
	Y927	Y927	R838	W742	Q638	L524	Y433	Q203	M113	M113
	L928	L928	R839	W743	L642	K527	L437	R311	L114	L114
	T932	T932	N841	W744	K644	N534	L437	T316	T118	T118
			G842	W746	K647	P535	L440	F317	K119	K119
				E746	E647	L538	L441	P318	K123	K123
					K648		Y444	P320	E124	E124

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	261.51Å 261.51Å 91.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 3.00 49.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.45-3.00) 99.7 (49.45-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.227 (Not available) , 0.196	Depositor DCC
R_{free} test set	3628 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MGK, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.08	5/7996 (0.1%)	1.23	32/10817 (0.3%)
1	B	1.05	8/7990 (0.1%)	1.19	27/10810 (0.2%)
All	All	1.06	13/15986 (0.1%)	1.21	59/21627 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	764	VAL	CA-CB	7.02	1.62	1.54
1	B	570	PRO	CA-C	6.99	1.59	1.52
1	A	367	ALA	CA-CB	-6.32	1.43	1.53
1	A	764	VAL	CA-CB	5.96	1.62	1.53
1	A	189	GLU	CG-CD	5.71	1.66	1.52
1	B	991	VAL	CA-CB	5.44	1.59	1.53
1	B	857	HIS	N-CA	5.31	1.52	1.46
1	B	189	GLU	N-CA	5.28	1.52	1.46
1	A	120	LYS	CA-C	5.21	1.59	1.52
1	B	1010	PRO	CA-C	5.04	1.59	1.52
1	B	189	GLU	CA-CB	5.01	1.61	1.53
1	A	189	GLU	CB-CG	5.00	1.67	1.52
1	B	964	ASP	CA-C	5.00	1.59	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	GLU	N-CA-C	-10.40	99.94	111.28
1	A	50	ILE	CB-CA-C	-9.48	95.74	111.29
1	B	963	MET	N-CA-C	9.19	123.66	109.60
1	A	626	GLY	N-CA-C	-8.79	100.48	112.52
1	A	189	GLU	N-CA-C	-8.52	101.02	111.33
1	A	229	ARG	CA-C-N	-8.13	110.34	119.28
1	A	229	ARG	C-N-CA	-8.13	110.34	119.28
1	A	43	ASN	N-CA-C	7.20	121.30	110.64
1	B	189	GLU	N-CA-CB	7.20	120.70	110.12
1	A	329	ASN	CA-C-N	7.14	127.46	119.32
1	A	329	ASN	C-N-CA	7.14	127.46	119.32
1	B	107	SER	N-CA-C	7.12	119.12	111.36
1	B	197	ASP	N-CA-C	6.93	118.83	111.28
1	B	92	VAL	CB-CA-C	-6.92	101.44	110.84
1	A	731	GLY	N-CA-C	6.72	118.89	110.29
1	B	500	TYR	N-CA-C	6.63	117.33	108.38
1	A	189	GLU	OE1-CD-OE2	-6.60	107.06	122.90
1	A	332	HIS	N-CA-C	-6.60	103.57	111.69
1	B	405	GLY	CA-C-N	6.58	127.62	119.98
1	B	405	GLY	C-N-CA	6.58	127.62	119.98
1	A	557	SER	N-CA-C	6.52	119.06	108.76
1	A	538	LEU	CA-C-N	-6.40	113.69	120.03
1	A	538	LEU	C-N-CA	-6.40	113.69	120.03
1	B	586	ASP	N-CA-C	6.37	113.86	108.13
1	B	962	GLU	N-CA-C	6.24	120.89	113.28
1	A	219	GLY	N-CA-C	6.24	119.73	112.50
1	B	189	GLU	CA-CB-CG	6.23	126.56	114.10
1	B	459	PHE	CA-C-N	-6.02	115.75	123.16
1	B	459	PHE	C-N-CA	-6.02	115.75	123.16
1	A	282	ASN	N-CA-C	6.01	123.61	110.80
1	A	353	LYS	N-CA-C	-5.93	106.09	113.15
1	B	988	GLN	N-CA-C	-5.88	102.24	109.65
1	A	545	THR	CA-C-N	5.83	125.53	119.05
1	A	545	THR	C-N-CA	5.83	125.53	119.05
1	A	189	GLU	CG-CD-OE2	5.83	131.81	118.40
1	B	456	LEU	CB-CA-C	-5.79	99.27	109.62
1	A	627	MET	N-CA-C	5.75	119.33	110.42
1	A	51	GLY	N-CA-C	-5.72	104.59	112.25
1	B	626	GLY	N-CA-C	-5.63	102.38	110.60
1	A	498	THR	CA-C-N	-5.57	114.36	122.65
1	A	498	THR	C-N-CA	-5.57	114.36	122.65
1	A	173	LEU	N-CA-C	5.51	118.21	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	THR	N-CA-C	-5.37	104.35	112.99
1	B	329	ASN	CA-C-N	-5.31	113.27	119.32
1	B	329	ASN	C-N-CA	-5.31	113.27	119.32
1	A	189	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	946	VAL	N-CA-C	5.25	116.61	110.62
1	A	508	GLU	CB-CA-C	5.25	118.78	109.65
1	A	844	GLN	N-CA-C	5.24	116.95	109.14
1	B	108	HIS	N-CA-C	-5.24	105.46	111.07
1	A	475	ASN	N-CA-C	5.22	116.70	110.44
1	B	238	ARG	CA-C-N	-5.16	112.96	120.29
1	B	238	ARG	C-N-CA	-5.16	112.96	120.29
1	B	1009	LYS	CA-C-N	5.13	126.25	119.84
1	B	1009	LYS	C-N-CA	5.13	126.25	119.84
1	B	980	LEU	N-CA-C	5.11	118.35	110.42
1	A	449	VAL	N-CA-C	5.06	116.39	110.62
1	B	621	GLN	N-CA-C	5.03	116.83	109.24
1	B	534	ASN	N-CA-C	5.01	117.07	107.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	979	ASN	Peptide
1	B	455	LEU	Peptide
1	B	979	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7802	0	7740	180	0
1	B	7796	0	7729	205	0
2	A	29	0	25	2	0
2	B	29	0	25	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	67	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	39	0	0	3	0
All	All	15764	0	15519	387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.34	1.05
1:B:774:ARG:HH11	1:B:774:ARG:HG3	1.24	1.00
1:A:50:ILE:O	1:A:50:ILE:HG22	1.61	0.99
1:A:622:ASN:HD22	1:A:622:ASN:H	1.03	0.96
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.33	0.94
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.52	0.91
1:A:622:ASN:H	1:A:622:ASN:ND2	1.62	0.88
1:B:754:HIS:CE1	4:B:1236:HOH:O	2.28	0.85
1:B:622:ASN:HD22	1:B:622:ASN:H	1.25	0.84
1:B:348:SER:OG	1:B:606:GLU:OE2	1.97	0.81
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.62	0.80
1:B:754:HIS:HE1	4:B:1236:HOH:O	1.62	0.79
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.77
2:B:1101:MGK:O14	2:B:1101:MGK:H26A	1.84	0.76
1:A:722:ARG:HB2	1:A:758:LEU:HD12	1.67	0.76
1:B:206:LYS:HG2	1:B:215:PHE:O	1.85	0.76
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.16	0.75
1:B:189:GLU:HG2	1:B:831:TYR:CE1	2.22	0.75
1:A:309:ASP:H	1:A:672:ASN:HD21	1.32	0.75
1:A:491:ARG:HG3	1:A:491:ARG:NH1	1.96	0.75
1:B:774:ARG:HH11	1:B:774:ARG:CG	1.99	0.75
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.87	0.74
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.86	0.74
1:A:730:HIS:HD2	1:A:904:SER:OG	1.71	0.73
1:A:927:TYR:O	1:A:930:THR:HB	1.86	0.73
1:A:50:ILE:O	1:A:50:ILE:CG2	2.33	0.73
1:A:756:LYS:HB2	1:A:757:PRO:CD	2.18	0.73
1:B:309:ASP:H	1:B:672:ASN:HD21	1.37	0.73
1:B:108:HIS:CE1	1:B:189:GLU:OE1	2.21	0.72
1:A:622:ASN:HD22	1:A:622:ASN:N	1.85	0.72
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.72	0.71
1:B:783:ASN:HD22	1:B:785:VAL:H	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PRO:HG3	1:B:466:MET:HE1	1.71	0.71
1:A:102:ASN:H	1:A:102:ASN:HD22	1.39	0.70
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.40	0.70
1:B:994:ASN:HB3	1:B:997:GLU:HB2	1.74	0.70
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.76	0.69
1:A:711:ARG:HG2	1:A:711:ARG:HH21	1.59	0.68
1:B:243:LYS:HB2	1:B:243:LYS:NZ	2.09	0.67
1:B:257:VAL:HG21	1:B:437:ILE:HG22	1.76	0.67
1:A:623:THR:OG1	1:A:626:GLY:O	2.06	0.67
1:B:196:ASN:ND2	1:B:198:ALA:H	1.93	0.67
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.30	0.67
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.43	0.66
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.30	0.66
1:A:783:ASN:ND2	1:A:786:HIS:H	1.95	0.65
1:B:110:LEU:HD23	1:B:110:LEU:C	2.22	0.65
1:A:191:GLU:HA	1:A:194:VAL:HG23	1.79	0.65
1:B:86:SER:HB3	1:B:158:LEU:HG	1.79	0.65
1:A:760:PRO:HA	1:A:763:LEU:HD12	1.77	0.65
1:B:622:ASN:HD22	1:B:622:ASN:N	1.91	0.65
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.32	0.64
1:B:920:ARG:O	1:B:924:GLU:HG3	1.98	0.63
1:A:67:LEU:CD2	1:A:75:VAL:HB	2.29	0.63
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.82	0.62
1:B:575:ASN:HD22	1:B:575:ASN:N	1.96	0.62
1:B:294:GLN:H	1:B:297:HIS:HD2	1.45	0.62
1:B:309:ASP:H	1:B:672:ASN:ND2	1.96	0.62
1:B:311:ARG:NH1	1:B:379:LEU:O	2.30	0.62
1:B:676:GLU:HA	1:B:676:GLU:OE1	1.99	0.62
1:A:294:GLN:H	1:A:297:HIS:CD2	2.16	0.62
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.82	0.61
1:B:112:HIS:CE1	1:B:189:GLU:OE1	2.39	0.61
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.82	0.61
1:B:102:ASN:HD22	1:B:102:ASN:H	1.48	0.61
1:A:545:THR:HB	1:A:546:PRO:HD2	1.82	0.61
1:A:108:HIS:CE1	1:A:189:GLU:OE2	2.50	0.60
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.36	0.60
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.32	0.60
1:B:272:VAL:O	1:B:276:SER:OG	2.20	0.60
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.83	0.60
1:A:62:ARG:HG2	1:A:80:ASP:HB2	1.84	0.59
1:A:491:ARG:HH11	1:A:491:ARG:CG	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:GLN:HB3	1:A:805:ASN:HD21	1.68	0.59
1:B:93:HIS:HD2	1:B:145:GLU:O	1.86	0.59
1:A:303:LYS:HG2	1:A:485:PHE:CE2	2.38	0.58
1:B:693:VAL:HB	1:B:766:TYR:CE2	2.39	0.58
1:A:784:GLU:O	1:A:961:ARG:HG3	2.03	0.58
1:B:962:GLU:OE2	1:B:962:GLU:HA	2.03	0.58
1:A:298:LEU:HD13	1:A:475:ASN:CB	2.33	0.58
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.37	0.58
1:B:262:GLU:CD	1:B:262:GLU:H	2.12	0.58
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.37	0.58
1:A:309:ASP:H	1:A:672:ASN:ND2	2.01	0.58
1:A:136:GLY:CA	1:A:152:ASP:O	2.52	0.57
1:A:316:THR:HB	1:A:374:ILE:HG22	1.86	0.57
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.57
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.70	0.57
1:A:428:GLU:H	1:A:428:GLU:CD	2.12	0.57
1:B:375:ILE:HG22	1:B:394:MET:HE2	1.86	0.57
1:A:341:GLU:OE1	2:A:1101:MGK:H10	2.05	0.57
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.87	0.57
1:B:803:SER:HB2	1:B:927:TYR:OH	2.04	0.57
1:B:941:LYS:HB2	1:B:941:LYS:HZ1	1.69	0.57
1:B:298:LEU:HD13	1:B:475:ASN:HB2	1.86	0.57
1:A:674:ARG:HD3	4:A:1235:HOH:O	2.05	0.57
1:A:715:PHE:CZ	1:A:719:LEU:CD2	2.88	0.57
1:B:134:HIS:CD2	1:B:157:HIS:CD2	2.93	0.57
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.87	0.56
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.40	0.56
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.32	0.56
1:B:765:ARG:NH1	1:B:912:ILE:O	2.39	0.56
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.88	0.56
1:B:108:HIS:HE1	1:B:189:GLU:CD	2.08	0.56
1:B:535:PHE:HB3	1:B:570:PRO:HG3	1.87	0.56
1:A:722:ARG:HA	1:A:756:LYS:O	2.05	0.55
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.72	0.55
1:B:941:LYS:HB2	1:B:941:LYS:NZ	2.20	0.55
1:A:780:GLN:HE22	1:A:959:LEU:HD11	1.72	0.55
1:B:375:ILE:CG2	1:B:394:MET:HE2	2.35	0.55
1:A:599:LEU:HD23	1:A:662:ILE:HD13	1.89	0.55
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.87	0.55
1:B:579:PHE:HE2	1:B:765:ARG:HH22	1.55	0.55
1:A:108:HIS:CE1	1:A:189:GLU:CD	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:HA2	1:A:152:ASP:O	2.07	0.55
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.36	0.55
1:A:196:ASN:C	1:A:196:ASN:ND2	2.64	0.55
1:A:887:GLN:HE21	1:A:891:ILE:HD11	1.72	0.55
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.23	0.54
1:B:196:ASN:C	1:B:196:ASN:HD22	2.15	0.54
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.15	0.54
1:A:425:LYS:NZ	1:A:425:LYS:HB3	2.22	0.54
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.90	0.54
1:B:538:LEU:HD22	1:B:734:THR:HG23	1.90	0.54
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.43	0.54
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.90	0.54
1:B:856:PRO:HA	1:B:859:LEU:HB2	1.90	0.54
1:A:329:ASN:N	1:A:330:PRO:CD	2.71	0.54
1:B:108:HIS:O	1:B:111:GLN:HB3	2.08	0.54
1:A:298:LEU:HD13	1:A:475:ASN:HB2	1.90	0.53
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.88	0.53
1:A:602:ASP:OD2	1:A:658:ARG:NH1	2.42	0.53
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.90	0.53
1:B:685:TYR:HB2	1:B:956:VAL:HG11	1.90	0.53
1:A:482:SER:HB3	1:A:485:PHE:CE1	2.43	0.53
1:B:643:LYS:O	1:B:647:GLU:HB2	2.09	0.53
1:B:783:ASN:ND2	1:B:786:HIS:H	2.07	0.53
1:B:203:GLN:HG3	1:B:203:GLN:O	2.08	0.53
1:B:815:ILE:HG22	1:B:870:MET:HG2	1.91	0.53
1:B:809:GLU:OE2	1:B:839:ARG:NH2	2.39	0.53
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.43	0.53
1:B:807:PHE:HE1	1:B:935:ASP:HB3	1.73	0.53
2:B:1101:MGK:O14	2:B:1101:MGK:C26	2.55	0.53
1:A:97:LEU:HB2	1:A:144:GLY:O	2.09	0.53
1:B:772:PRO:HD3	1:B:1002:LEU:HD21	1.91	0.53
1:A:78:ILE:O	1:A:259:LEU:HA	2.09	0.52
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.39	0.52
1:B:887:GLN:O	1:B:890:ALA:HB3	2.09	0.52
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.91	0.52
1:A:756:LYS:HB2	1:A:757:PRO:HD2	1.92	0.52
1:B:134:HIS:HD2	1:B:157:HIS:CD2	2.28	0.52
1:B:774:ARG:HG3	1:B:774:ARG:NH1	2.04	0.52
1:A:188:SER:HB3	1:A:831:TYR:CB	2.35	0.52
1:A:805:ASN:O	1:A:809:GLU:HG3	2.09	0.52
2:A:1101:MGK:HN12	2:A:1101:MGK:H08	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:ARG:CG	1:B:774:ARG:NH1	2.66	0.52
1:B:196:ASN:ND2	1:B:198:ALA:N	2.57	0.52
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.92	0.52
1:B:575:ASN:N	1:B:575:ASN:ND2	2.57	0.52
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.92	0.51
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.46	0.51
1:A:359:LEU:C	1:A:359:LEU:HD23	2.36	0.51
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.91	0.51
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.92	0.51
1:A:714:ALA:O	1:A:717:PRO:HD2	2.11	0.51
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.09	0.51
1:B:194:VAL:HG12	1:B:195:MET:HG2	1.91	0.51
1:A:511:LYS:HE3	1:A:514:GLN:OE1	2.11	0.51
1:A:595:LEU:HD12	1:A:662:ILE:HG22	1.92	0.51
1:B:298:LEU:HD21	1:B:318:PRO:HG3	1.93	0.51
1:B:843:ILE:HG22	1:B:844:GLN:N	2.25	0.51
1:A:334:LEU:HD22	1:A:468:LEU:HD13	1.93	0.50
1:B:817:GLU:N	1:B:818:PRO:HD2	2.25	0.50
1:A:693:VAL:HB	1:A:766:TYR:CE2	2.45	0.50
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.93	0.50
1:A:806:MET:HE3	1:A:928:LEU:HG	1.93	0.50
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.93	0.50
1:B:803:SER:HB2	1:B:927:TYR:CZ	2.46	0.50
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.47	0.50
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.94	0.50
1:B:229:ARG:NH1	1:B:233:GLU:OE2	2.41	0.50
1:A:196:ASN:HD22	1:A:199:TRP:H	1.60	0.50
1:B:52:ASN:N	1:B:52:ASN:HD22	2.09	0.50
1:B:175:ASP:HB3	1:B:178:ALA:HB3	1.93	0.50
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.46	0.50
1:B:708:THR:OG1	1:B:711:ARG:HB2	2.11	0.50
1:A:86:SER:HB3	1:A:158:LEU:HG	1.94	0.49
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.94	0.49
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.93	0.49
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.76	0.49
1:B:795:TYR:CE2	1:B:953:LYS:HD2	2.48	0.49
1:B:413:GLU:OE2	1:B:527:LYS:HE2	2.12	0.49
1:B:214:PRO:O	1:B:217:LYS:HG3	2.13	0.49
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.20	0.49
1:B:688:LEU:HD13	1:B:995:MET:HE1	1.94	0.49
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.94	0.49
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.48	0.49
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.95	0.49
1:B:196:ASN:ND2	1:B:196:ASN:C	2.71	0.49
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.95	0.48
1:A:312:ASN:HB3	1:A:377:VAL:O	2.13	0.48
1:B:359:LEU:O	2:B:1101:MGK:H10	2.13	0.48
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.95	0.48
1:B:643:LYS:HB2	1:B:744:MET:SD	2.53	0.48
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.95	0.48
1:B:196:ASN:HD22	1:B:198:ALA:N	2.11	0.48
1:B:874:ILE:HA	1:B:877:MET:HG2	1.94	0.48
1:A:123:LYS:O	1:A:124:GLU:C	2.56	0.48
1:A:67:LEU:HD23	1:A:67:LEU:C	2.38	0.48
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.48
1:A:363:GLN:HG3	1:A:371:MET:CE	2.44	0.48
1:A:793:ILE:O	1:A:847:ARG:HA	2.14	0.48
1:B:189:GLU:HG2	1:B:831:TYR:CD1	2.47	0.48
1:B:125:ASN:HD22	1:B:125:ASN:H	1.62	0.48
1:B:655:ASP:HB3	1:B:658:ARG:HB2	1.96	0.48
1:B:688:LEU:CD1	1:B:995:MET:HE1	2.44	0.48
1:B:329:ASN:HD22	1:B:332:HIS:H	1.60	0.47
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.95	0.47
1:A:521:LYS:HD2	1:A:521:LYS:HA	1.58	0.47
1:A:908:TRP:O	1:A:912:ILE:HG12	2.15	0.47
1:B:649:MET:HB2	1:B:649:MET:HE3	1.56	0.47
1:B:686:LEU:HD12	1:B:686:LEU:HA	1.66	0.47
2:B:1101:MGK:H18A	2:B:1101:MGK:H15A	1.75	0.47
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.62	0.47
1:B:243:LYS:HB2	1:B:243:LYS:HZ2	1.80	0.47
1:B:579:PHE:HE2	1:B:765:ARG:NH2	2.11	0.47
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.97	0.47
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.95	0.47
1:B:52:ASN:N	1:B:52:ASN:ND2	2.62	0.47
1:B:600:LEU:O	1:B:604:LEU:HB2	2.14	0.47
1:B:616:LEU:HD21	1:B:638:GLN:HG3	1.97	0.47
1:A:196:ASN:ND2	1:A:199:TRP:H	2.13	0.47
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.48	0.47
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.96	0.47
1:A:756:LYS:CB	1:A:757:PRO:CD	2.88	0.46
1:A:780:GLN:O	1:A:781:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.16	0.46
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.44	0.46
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.97	0.46
1:B:250:SER:HB2	1:B:281:LYS:HB2	1.97	0.46
1:A:782:ARG:NH1	1:A:963:MET:O	2.45	0.46
1:A:709:LEU:O	1:A:710:PRO:C	2.59	0.46
1:B:597:LEU:HD21	1:B:627:MET:HG2	1.97	0.46
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.98	0.46
1:A:392:LEU:O	1:A:396:GLN:HG3	2.15	0.46
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.45	0.46
1:B:671:ASN:OD1	1:B:701:LYS:HD3	2.16	0.46
1:A:196:ASN:C	1:A:196:ASN:HD22	2.24	0.46
1:B:932:THR:OG1	1:B:934:GLU:HB2	2.16	0.46
1:A:102:ASN:HD22	1:A:102:ASN:N	2.06	0.46
1:A:140:ALA:HA	1:A:148:ASN:O	2.16	0.46
1:A:789:SER:HB2	1:A:958:VAL:O	2.16	0.46
1:A:914:GLN:HA	1:A:916:TYR:CE1	2.51	0.46
1:B:809:GLU:OE1	1:B:893:ARG:HD3	2.16	0.46
1:B:329:ASN:O	1:B:330:PRO:C	2.56	0.45
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.98	0.45
1:A:313:LEU:HD22	1:A:387:VAL:HG22	1.98	0.45
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.49	0.45
1:B:815:ILE:HA	1:B:870:MET:HE2	1.97	0.45
1:A:151:PHE:CD1	1:A:151:PHE:C	2.94	0.45
1:B:200:ARG:NH2	1:B:498:THR:HA	2.32	0.45
1:B:861:SER:O	1:B:865:ALA:N	2.48	0.45
1:B:622:ASN:N	1:B:622:ASN:ND2	2.63	0.45
1:B:691:THR:O	1:B:999:LYS:CE	2.65	0.45
1:B:915:GLN:HG2	1:B:1008:VAL:HG11	1.99	0.45
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.63	0.45
1:B:672:ASN:HD22	1:B:672:ASN:HA	1.53	0.45
1:B:801:SER:O	1:B:802:THR:C	2.60	0.45
1:B:838:ARG:HG3	1:B:847:ARG:HD3	1.98	0.45
1:A:773:ASP:O	1:A:774:ARG:HB2	2.17	0.45
1:B:308:LYS:HD3	1:B:672:ASN:HB3	1.98	0.45
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.97	0.45
1:A:706:ASP:O	1:A:711:ARG:HD3	2.15	0.44
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.99	0.44
1:A:756:LYS:CB	1:A:757:PRO:HD3	2.47	0.44
1:B:76:LEU:HD12	1:B:437:ILE:HG21	1.99	0.44
1:B:229:ARG:HA	1:B:229:ARG:HD3	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:PHE:CD2	1:B:725:ILE:HG12	2.52	0.44
1:A:756:LYS:HB2	1:A:757:PRO:HD3	1.97	0.44
1:B:341:GLU:HG2	1:B:347:LEU:CD1	2.25	0.44
1:B:770:GLN:HG2	1:B:1003:PRO:HG2	1.98	0.44
1:B:810:LEU:HG	1:B:928:LEU:HD21	2.00	0.44
1:B:583:ALA:O	1:B:590:SER:HA	2.17	0.44
1:A:206:LYS:HB3	1:A:216:SER:HA	1.98	0.44
1:A:689:LEU:HD21	1:A:995:MET:HG2	1.99	0.44
1:B:826:LYS:HB2	1:B:826:LYS:HE3	1.61	0.44
1:B:349:GLU:OE2	1:B:349:GLU:HA	2.18	0.44
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.48	0.44
1:A:824:ARG:O	1:A:828:GLN:HA	2.18	0.44
1:B:294:GLN:H	1:B:297:HIS:CD2	2.31	0.44
1:A:294:GLN:O	1:A:298:LEU:HG	2.18	0.43
1:A:334:LEU:CD2	1:A:468:LEU:HD13	2.48	0.43
1:B:425:LYS:HB3	1:B:425:LYS:HE3	1.82	0.43
1:B:744:MET:O	1:B:744:MET:HG2	2.17	0.43
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.80	0.43
1:A:583:ALA:HB2	1:A:626:GLY:HA2	1.99	0.43
1:A:691:THR:O	1:A:692:GLU:C	2.61	0.43
1:B:329:ASN:ND2	1:B:332:HIS:CB	2.81	0.43
1:A:886:ILE:HG12	1:A:928:LEU:HD22	2.00	0.43
1:A:1009:LYS:HA	1:A:1009:LYS:HD2	1.80	0.43
1:B:329:ASN:ND2	1:B:332:HIS:HB2	2.33	0.43
1:B:363:GLN:HG3	1:B:371:MET:CE	2.49	0.43
1:B:656:GLU:O	1:B:659:PHE:HB3	2.18	0.43
1:A:136:GLY:HA3	1:A:152:ASP:O	2.19	0.43
1:A:50:ILE:C	1:A:51:GLY:O	2.58	0.43
1:A:51:GLY:HA2	1:A:52:ASN:HA	1.71	0.43
1:A:862:ARG:NH2	1:A:981:SER:O	2.44	0.43
1:B:52:ASN:O	1:B:53:HIS:C	2.59	0.43
1:B:546:PRO:O	1:B:562:LYS:NZ	2.44	0.43
1:B:785:VAL:HG12	1:B:786:HIS:CD2	2.53	0.43
1:A:125:ASN:H	1:A:125:ASN:HD22	1.66	0.43
1:B:93:HIS:CD2	1:B:145:GLU:O	2.70	0.43
1:A:299:LYS:HB2	1:A:299:LYS:HE3	1.88	0.43
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.43
1:A:887:GLN:HE21	1:A:891:ILE:CD1	2.32	0.43
1:B:78:ILE:O	1:B:259:LEU:HA	2.19	0.43
1:B:160:GLY:O	1:B:164:ARG:HG3	2.18	0.43
1:B:962:GLU:OE2	1:B:962:GLU:CA	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.61	0.43
1:B:311:ARG:HB3	1:B:379:LEU:HB2	2.01	0.43
1:A:567:PHE:CE1	1:A:900:LEU:HA	2.53	0.43
1:A:809:GLU:HB3	1:A:889:LEU:HD11	2.01	0.43
1:B:597:LEU:HD23	1:B:622:ASN:N	2.34	0.43
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.84	0.42
1:A:441:LEU:HD23	1:A:441:LEU:HA	1.85	0.42
1:B:129:GLN:O	1:B:133:GLU:HB2	2.18	0.42
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.52	0.42
1:B:631:VAL:HG12	1:B:638:GLN:HG2	2.01	0.42
1:B:674:ARG:HH11	1:B:674:ARG:CG	2.32	0.42
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.48	0.42
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.18	0.42
1:A:596:TYR:OH	1:A:649:MET:HG3	2.19	0.42
1:A:607:TYR:CD2	1:A:607:TYR:C	2.97	0.42
1:A:896:LYS:HB2	1:A:896:LYS:HE2	1.52	0.42
1:B:511:LYS:HD2	1:B:514:GLN:OE1	2.19	0.42
1:B:463:LEU:O	1:B:464:ILE:C	2.62	0.42
1:A:408:GLU:HB2	1:A:459:PHE:CE2	2.55	0.42
1:B:730:HIS:HD2	1:B:904:SER:OG	2.02	0.42
1:A:114:LEU:HD13	1:A:168:PHE:HB3	2.01	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.75	0.42
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.50	0.42
1:A:187:ASP:O	1:A:191:GLU:HG2	2.20	0.42
1:A:400:LYS:O	1:A:401:LEU:C	2.63	0.42
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.01	0.42
1:A:774:ARG:NH1	1:A:774:ARG:HG3	2.34	0.42
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.34	0.42
1:B:243:LYS:HE2	4:B:1206:HOH:O	2.20	0.42
1:A:584:TYR:CE2	1:A:624:ILE:HG22	2.55	0.41
1:A:783:ASN:C	1:A:783:ASN:HD22	2.28	0.41
1:B:691:THR:O	1:B:692:GLU:C	2.63	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.83	0.41
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.85	0.41
1:B:445:PRO:HG2	1:B:448:GLU:HG3	2.01	0.41
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	2.02	0.41
1:A:559:LEU:HD22	1:A:742:MET:HB2	2.02	0.41
1:B:238:ARG:O	1:B:242:LEU:HD12	2.20	0.41
1:B:586:ASP:O	1:B:587:PRO:C	2.62	0.41
1:A:359:LEU:HD23	1:A:360:VAL:N	2.36	0.41
1:A:515:ASN:O	1:A:516:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.56	0.41
1:B:417:LEU:HD12	1:B:417:LEU:HA	1.69	0.41
1:A:547:TYR:HB2	4:A:1202:HOH:O	2.20	0.41
1:B:433:TYR:CE1	1:B:437:ILE:HD11	2.55	0.41
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.55	0.41
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.55	0.41
1:A:941:LYS:O	1:A:949:PRO:HD2	2.21	0.41
1:B:515:ASN:O	1:B:516:ALA:C	2.63	0.41
1:A:94:ILE:HG22	1:A:95:GLY:N	2.35	0.41
1:A:652:PHE:CE2	1:A:654:ILE:HG12	2.55	0.41
1:B:321:ASP:C	1:B:321:ASP:OD2	2.63	0.41
1:A:74:LYS:NZ	4:A:1255:HOH:O	2.53	0.41
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.32	0.41
1:A:540:LEU:HA	1:A:540:LEU:HD12	1.63	0.41
1:A:852:SER:OG	1:A:853:GLU:N	2.54	0.41
1:A:1004:LEU:HD23	1:A:1004:LEU:HA	1.88	0.41
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.55	0.41
1:B:222:ASN:O	1:B:223:LYS:C	2.64	0.41
1:B:465:GLU:O	1:B:469:ASP:HB2	2.20	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.54	0.41
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.21	0.40
1:B:885:HIS:O	1:B:886:ILE:C	2.64	0.40
1:A:204:LEU:O	1:A:208:THR:HG23	2.22	0.40
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.85	0.40
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.57	0.40
1:A:428:GLU:CD	1:A:428:GLU:N	2.78	0.40
1:A:842:GLY:C	1:A:843:ILE:HD13	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	951/990 (96%)	893 (94%)	55 (6%)	3 (0%)	36	70
1	B	951/990 (96%)	891 (94%)	57 (6%)	3 (0%)	36	70
All	All	1902/1980 (96%)	1784 (94%)	112 (6%)	6 (0%)	36	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ASP
1	A	961	ARG
1	A	841	ASN
1	B	841	ASN
1	B	1010	PRO
1	B	520	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/879 (96%)	730 (86%)	118 (14%)	3	17
1	B	846/879 (96%)	714 (84%)	132 (16%)	2	13
All	All	1694/1758 (96%)	1444 (85%)	250 (15%)	3	15

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	52	ASN
1	A	61	LYS
1	A	67	LEU
1	A	76	LEU
1	A	96	SER
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	119	LYS

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Mol	Chain	Res	Type
1	A	120	LYS
1	A	123	LYS
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	188	SER
1	A	196	ASN
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	239	GLN
1	A	270	LEU
1	A	277	GLU
1	A	285	LEU
1	A	287	GLU
1	A	303	LYS
1	A	312	ASN
1	A	316	THR
1	A	324	LYS
1	A	337	LEU
1	A	347	LEU
1	A	353	LYS
1	A	360	VAL
1	A	363	GLN
1	A	364	LYS
1	A	387	VAL
1	A	402	ARG
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	420	VAL
1	A	423	ARG
1	A	425	LYS
1	A	428	GLU
1	A	446	LEU
1	A	448	GLU
1	A	450	LEU
1	A	466	MET
1	A	488	LYS
1	A	489	THR
1	A	491	ARG

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Mol	Chain	Res	Type
1	A	492	THR
1	A	501	LYS
1	A	508	GLU
1	A	511	LYS
1	A	521	LYS
1	A	524	LEU
1	A	527	LYS
1	A	538	LEU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	607	TYR
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	648	LYS
1	A	653	GLU
1	A	657	LYS
1	A	661	ILE
1	A	662	ILE
1	A	663	LYS
1	A	674	ARG
1	A	677	GLN
1	A	691	THR
1	A	709	LEU
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	722	ARG
1	A	728	LEU
1	A	741	ILE
1	A	744	MET
1	A	751	GLU
1	A	756	LYS
1	A	758	LEU
1	A	759	LEU
1	A	764	VAL
1	A	765	ARG
1	A	771	LEU
1	A	780	GLN
1	A	783	ASN

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Mol	Chain	Res	Type
1	A	801	SER
1	A	810	LEU
1	A	823	LEU
1	A	838	ARG
1	A	841	ASN
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	872	LYS
1	A	884	LYS
1	A	889	LEU
1	A	891	ILE
1	A	892	ARG
1	A	901	SER
1	A	906	LYS
1	A	928	LEU
1	A	929	LYS
1	A	930	THR
1	A	934	GLU
1	A	938	LYS
1	A	942	GLU
1	A	982	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	44	ASN
1	B	50	ILE
1	B	52	ASN
1	B	61	LYS
1	B	76	LEU
1	B	92	VAL
1	B	97	LEU
1	B	98	SER
1	B	102	ASN
1	B	110	LEU
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	128	SER
1	B	158	LEU
1	B	167	GLN
1	B	179	LYS
1	B	188	SER

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Mol	Chain	Res	Type
1	B	194	VAL
1	B	196	ASN
1	B	201	LEU
1	B	212	LYS
1	B	226	LEU
1	B	229	ARG
1	B	235	ILE
1	B	243	LYS
1	B	270	LEU
1	B	276	SER
1	B	285	LEU
1	B	287	GLU
1	B	290	GLU
1	B	316	THR
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	353	LYS
1	B	360	VAL
1	B	364	LYS
1	B	381	GLU
1	B	399	GLN
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	458	GLU
1	B	465	GLU
1	B	494	GLU
1	B	507	ASP
1	B	508	GLU
1	B	510	ILE
1	B	512	LYS
1	B	518	LEU
1	B	521	LYS
1	B	523	LYS
1	B	524	LEU
1	B	527	LYS
1	B	534	ASN
1	B	554	THR

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Mol	Chain	Res	Type
1	B	558	LYS
1	B	575	ASN
1	B	587	PRO
1	B	595	LEU
1	B	597	LEU
1	B	601	LYS
1	B	602	ASP
1	B	604	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	643	LYS
1	B	644	LYS
1	B	648	LYS
1	B	657	LYS
1	B	674	ARG
1	B	677	GLN
1	B	687	ARG
1	B	702	GLU
1	B	712	LEU
1	B	713	LYS
1	B	718	GLN
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	744	MET
1	B	746	GLU
1	B	751	GLU
1	B	756	LYS
1	B	758	LEU
1	B	759	LEU
1	B	764	VAL
1	B	765	ARG
1	B	771	LEU
1	B	774	ARG
1	B	780	GLN
1	B	782	ARG
1	B	783	ASN
1	B	803	SER
1	B	806	MET

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Mol	Chain	Res	Type
1	B	809	GLU
1	B	810	LEU
1	B	823	LEU
1	B	838	ARG
1	B	846	LEU
1	B	854	LYS
1	B	859	LEU
1	B	862	ARG
1	B	867	LEU
1	B	868	ILE
1	B	880	GLU
1	B	884	LYS
1	B	886	ILE
1	B	889	LEU
1	B	892	ARG
1	B	898	LYS
1	B	899	LYS
1	B	923	THR
1	B	928	LEU
1	B	941	LYS
1	B	942	GLU
1	B	954	VAL
1	B	962	GLU
1	B	980	LEU
1	B	990	GLU
1	B	993	GLN
1	B	1007	LEU
1	B	1008	VAL
1	B	1009	LYS
1	B	1011	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	502	GLN
1	A	573	ASN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	621	GLN
1	A	622	ASN
1	A	672	ASN
1	A	718	GLN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	786	HIS
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	887	GLN
1	A	922	ASN
1	A	988	GLN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	134	HIS
1	B	148	ASN
1	B	157	HIS
1	B	167	GLN
1	B	184	ASN
1	B	190	HIS
1	B	196	ASN
1	B	231	ASN
1	B	297	HIS
1	B	300	GLN
1	B	329	ASN

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Mol	Chain	Res	Type
1	B	336	HIS
1	B	376	ASN
1	B	386	HIS
1	B	499	GLN
1	B	502	GLN
1	B	534	ASN
1	B	575	ASN
1	B	589	HIS
1	B	622	ASN
1	B	672	ASN
1	B	718	GLN
1	B	730	HIS
1	B	743	GLN
1	B	770	GLN
1	B	780	GLN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	887	GLN
1	B	957	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	MGK	B	1101	-	30,30,30	1.73	4 (13%)	37,38,38	1.72	9 (24%)
2	MGK	A	1101	-	30,30,30	1.61	2 (6%)	37,38,38	1.83	8 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MGK	B	1101	-	-	14/28/28/28	0/2/2/2
2	MGK	A	1101	-	-	17/28/28/28	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MGK	O02-C03	6.58	1.49	1.33
2	A	1101	MGK	O02-C03	6.41	1.49	1.33
2	B	1101	MGK	C26-N16	2.64	1.52	1.47
2	A	1101	MGK	C26-N16	2.17	1.51	1.47
2	B	1101	MGK	C21-C20	2.14	1.43	1.38
2	B	1101	MGK	C08-C07	2.11	1.40	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGK	C05-C06-C07	5.35	122.34	113.27
2	B	1101	MGK	O02-C03-C05	4.61	123.21	111.49
2	A	1101	MGK	O02-C03-C05	4.49	122.90	111.49
2	B	1101	MGK	C01-O02-C03	4.23	125.52	115.92
2	A	1101	MGK	C01-O02-C03	4.16	125.35	115.92
2	B	1101	MGK	C05-N12-C13	3.30	129.97	121.68
2	A	1101	MGK	C27-C26-N16	2.93	123.05	113.77
2	B	1101	MGK	C03-C05-N12	2.82	117.15	110.65
2	A	1101	MGK	C15-C13-N12	2.77	122.50	115.70
2	B	1101	MGK	O02-C03-O04	-2.61	118.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGK	O04-C03-C05	-2.54	116.42	123.94
2	B	1101	MGK	C27-C26-N16	2.32	121.11	113.77
2	A	1101	MGK	O14-C13-N12	-2.13	119.34	122.95
2	B	1101	MGK	C08-C07-N11	2.05	108.08	105.65
2	A	1101	MGK	O29-C27-C26	2.03	121.39	113.38
2	B	1101	MGK	O04-C03-C05	-2.02	117.97	123.94
2	B	1101	MGK	C05-C06-C07	-2.00	109.87	113.27

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MGK	C17-C18-C19-C20
2	A	1101	MGK	N12-C05-C06-C07
2	A	1101	MGK	C03-C05-C06-C07
2	B	1101	MGK	C13-C15-N16-C26
2	B	1101	MGK	N16-C26-C27-O29
2	B	1101	MGK	N16-C26-C27-O28
2	B	1101	MGK	C05-C06-C07-N11
2	B	1101	MGK	C05-C06-C07-C08
2	B	1101	MGK	C05-C03-O02-C01
2	B	1101	MGK	O04-C03-O02-C01
2	A	1101	MGK	C05-C03-O02-C01
2	A	1101	MGK	O14-C13-N12-C05
2	A	1101	MGK	C15-C13-N12-C05
2	A	1101	MGK	O04-C03-O02-C01
2	A	1101	MGK	N16-C26-C27-O29
2	A	1101	MGK	N16-C26-C27-O28
2	B	1101	MGK	C18-C17-N16-C15
2	B	1101	MGK	C27-C26-N16-C17
2	A	1101	MGK	N16-C17-C18-C19
2	B	1101	MGK	N16-C17-C18-C19
2	B	1101	MGK	O14-C13-N12-C05
2	A	1101	MGK	C05-C06-C07-N11
2	A	1101	MGK	C05-C06-C07-C08
2	A	1101	MGK	O02-C03-C05-N12
2	A	1101	MGK	O04-C03-C05-N12
2	B	1101	MGK	C15-C13-N12-C05
2	B	1101	MGK	C18-C17-N16-C26
2	A	1101	MGK	C18-C17-N16-C15
2	A	1101	MGK	C18-C19-C20-C25
2	A	1101	MGK	C18-C19-C20-C21

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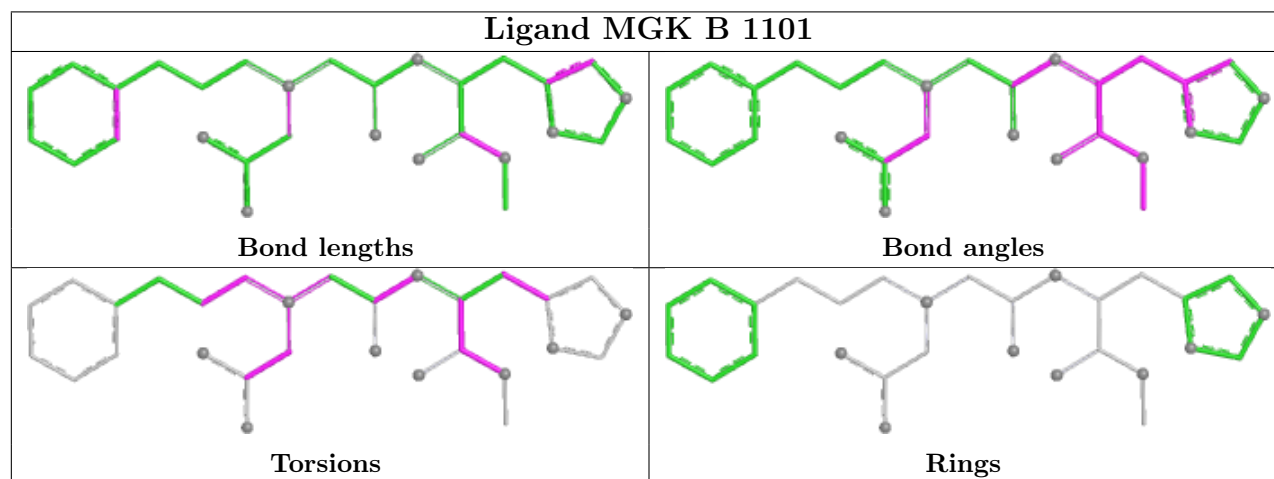
Mol	Chain	Res	Type	Atoms
2	B	1101	MGK	O04-C03-C05-C06

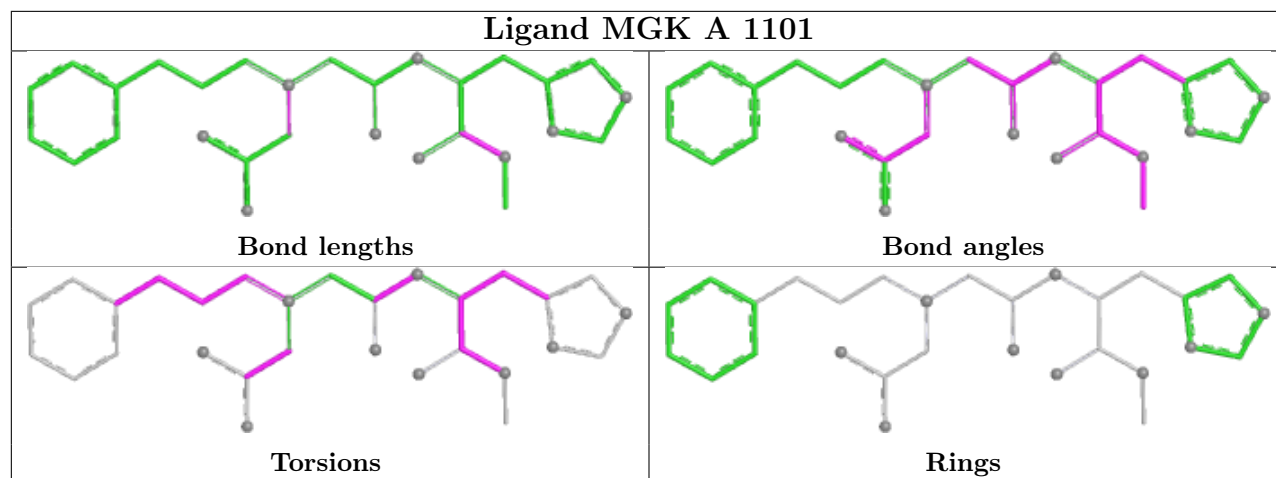
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	MGK	4	0
2	A	1101	MGK	2	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	955/990 (96%)	-0.70	3 (0%)	90 79	19, 34, 50, 77	0
1	B	955/990 (96%)	-0.58	6 (0%)	85 69	24, 38, 55, 75	0
All	All	1910/1980 (96%)	-0.64	9 (0%)	87 72	19, 36, 52, 77	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	965	SER	4.4
1	B	964	ASP	4.2
1	B	1011	HIS	2.8
1	B	52	ASN	2.7
1	A	1011	HIS	2.5
1	A	43	ASN	2.5
1	A	42	MET	2.1
1	B	1010	PRO	2.1
1	B	764	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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,

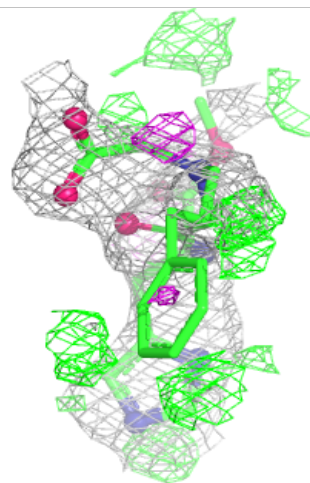
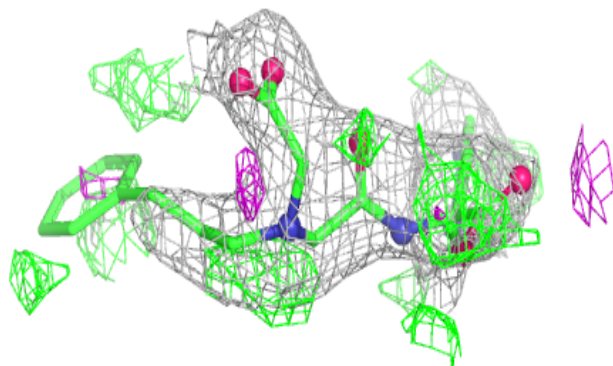
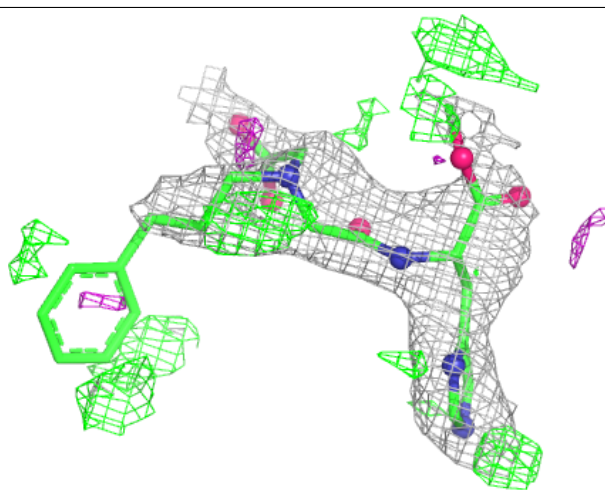
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

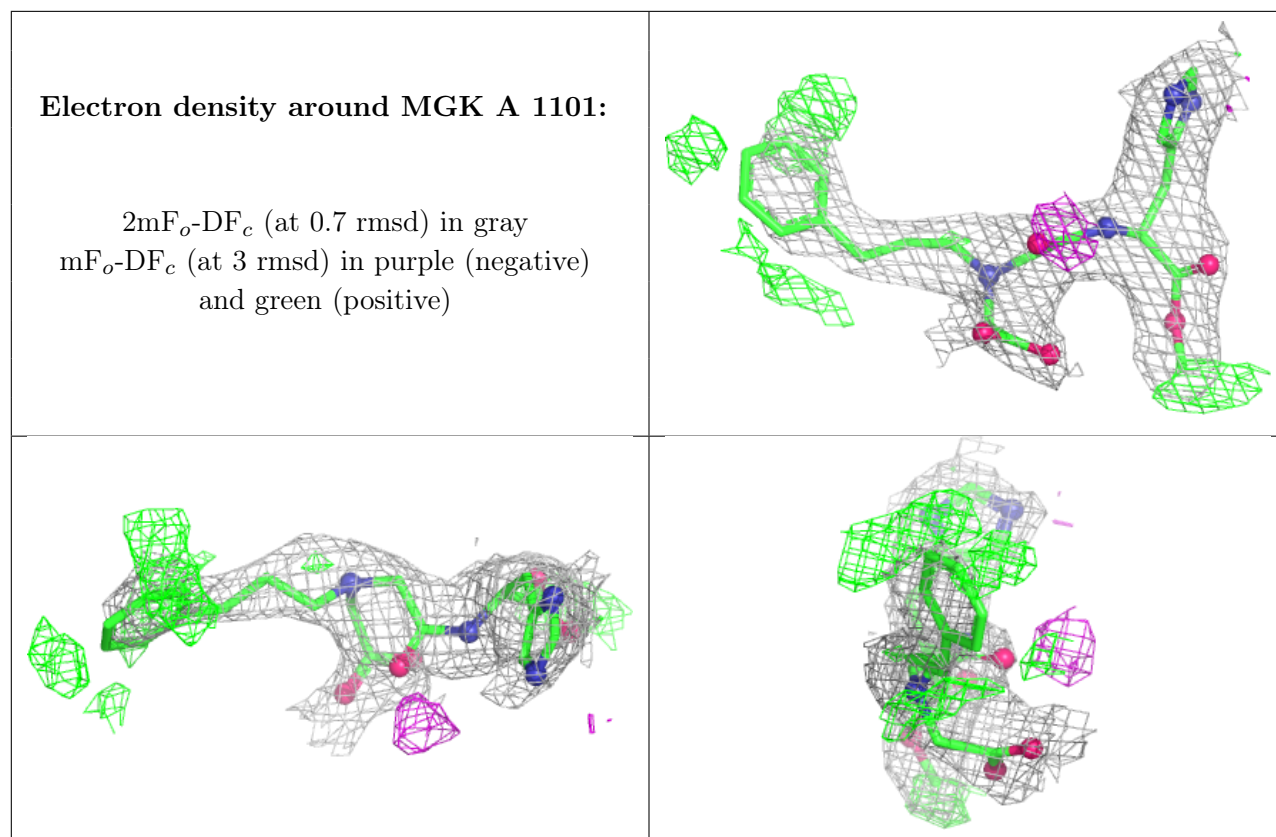
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MGK	B	1101	29/29	0.82	0.27	73,81,100,101	0
2	MGK	A	1101	29/29	0.85	0.22	61,78,92,92	0
3	ZN	A	1102	1/1	0.97	0.37	2,2,2,2	0
3	ZN	B	1102	1/1	0.97	0.38	2,2,2,2	0

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

Electron density around MGK B 1101:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.