



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:43 AM UTC

PDB ID : 4DTT / pdb_00004dttt
Title : Crystal structure of human insulin degrading enzyme (ide) in complex with compound 41367
Authors : Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on : 2012-02-21
Resolution : 3.22 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

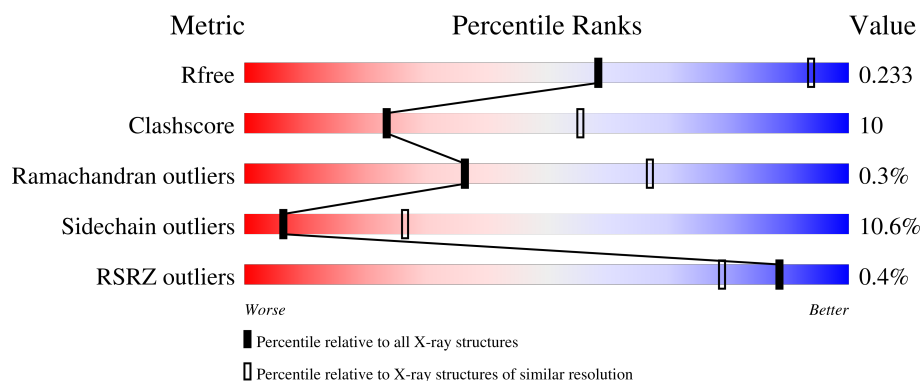
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	% 69% 24% • •
1	B	990	67% 26% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15713 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	956	Total	C	N	O	S	0	0	0
			7768	5008	1306	1432	22			
1	B	954	Total	C	N	O	S	0	0	0
			7758	5002	1304	1430	22			

There are 50 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	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
A	974	ALA	CYS	engineered mutation	UNP P14735

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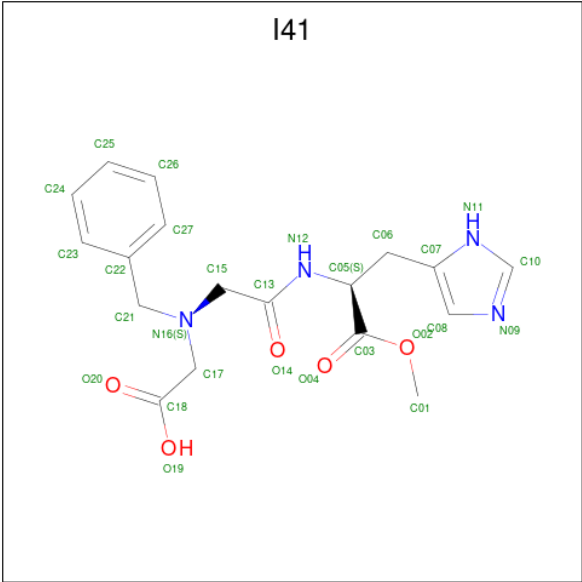
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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression 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	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 2-[[2-[[[(2S)-3-(3H-IMIDAZOL-4-YL)-1-METHOXY-1-OXO-PROPAN-2-YL]AMINO]-2-OXO-ETHYL]-(PHENYLMETHYL)AMINO]ETHANOIC ACID (CCD ID: I41) (formula: C₁₈H₂₂N₄O₅).

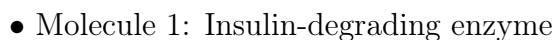


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	18	4	5		
3	A	1	Total	C	N	O	0	0
			27	18	4	5		
3	B	1	Total	C	N	O	0	0
			27	18	4	5		
3	B	1	Total	C	N	O	0	0
			27	18	4	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	30	Total	O	0	0
			30	30		

- Molecule 1: Insulin-degrading enzyme



SER	Q844	G731	G626	K511	M627	E413	N282	D152	MET
ASN	G845	N732	M627	K512	M627	E413	N282	D152	HIS
PRD	I733	I733	M635	M513	M635	D416	L285	H155	HIS
VAL	I850	I741	Q638	Q514	Q638	L417	P286	G160	HIS
VAL	Q851	M742	Q638	M515	Q638	N418	E287		HIS
GLY	S852	Q743	M742	A516	M742	A419	E290	D163	HIS
GLU	E853	M744	M744	K523	M744	Y420	H291	R164	ALA
PHE	K854	Y745	L641	L524	L641	A421			ALA
PRD	L859	E746	I645	I645	I645	F422	Q294	S171	GLY
ALA			I646	K527	I646	R423		P172	GLY
GLN	E864	I750	E647		E647	F424	H297	L173	ILE
ASN				I531		K425	L298	F174	PRO
ASP	L867	T755	E653	E653	E653	E428	K299	D175	MET
ILE		K756	D655	D655	D655		Q300		N43
ASN	M870	Y766	E656	T545	E656	H442	D309	K179	I50
L980						Y443	I310	D180	I50
L986	I874	D773	K657	L550	K657	Y444	R311	R181	G51
I992	E875	R774	R658	I551	R658	P445		N184	N52
Q993	M877					L446	Y314		H53
I994		Q780	K663	T554	K663			N193	P58
H995	E880	H786	E664	A555	E664	L450	F317	E59	E59
	A881	N787	M556	M556	M556	T451	P318	V194	D60
R1000	K884	M788	S669	S557	S669	A452		K61	K61
			L670	K458	L670	E453	Y325	D197	R62
L1004			K671	L559	K671	Y454	Y326	A198	L67
	I891	E792	M672	W560	M672		K327	W199	
P1010	R892	I793	E676	D564	E676	E458	H336	R200	I73
H1011		Y794	Q677	F459	Q677	F459	L201	F202	
ILE	K896	T797	P678	N573	P678	R460	L337		L77
ASN	P897	D798	H679	F578	H679	I464	L347	E205	D80
PHE	K898	M799	Q680		Q680	E465	S348	K206	
MET	K899					M466	E349		D84
ALA	L900	E809	M683	Y584	M683	V467		N210	
ALA	S901	L810		V585		L468	S352	A88	
LYS				D586		D469	K353	A89	
	Q914	Q813		P587	P587		G354	L90	
	Q915	I814	M680	L588	L588	R472	V355	D91	
		I815					V356	V92	
R920		S816	V693	L587	V693	N475	L359	H93	
T923		E817	A694	E598	A694	V476		I94	
E924		P818	W695	L599	W695		R238		
		A819		L600		A479	Q239	D99	
T932			E689		E689		K364		
	I936	T822	V707	L604	V707	T489	A367	S251	E111
I937	L823	R824	L708	D490	L708	D490	R368		
K938		T825	T708	Y609	T708	R491	G369	K119	
				A610		T492	F370	G260	
		Q828	F710	A611	F710	E493	K371	R261	A135
K941			R711	E612	R711	E494	F372	G136	
E942		I832					V271		
L959			F715	L616	F715	T498	L379	N139	
A960		R838	I716	Q499	I716	Q499	L274	A140	
R961			P717	L620	P717	Y500	I391		
E962						K501	E277	S143	
M963		N841	R722	T623	R722	Q502	K394	N280	
D964		I843	L723	I624	L723	F395	F395	F151	
				Y625		I510	Q396	K281	

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.52Å 263.52Å 90.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.22 50.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.22) 99.4 (50.00-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.175 , 0.242 0.172 , 0.233	Depositor DCC
R_{free} test set	2943 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15713	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: I41, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	1/7963 (0.0%)	1.14	19/10779 (0.2%)
1	B	0.96	2/7953 (0.0%)	1.12	20/10765 (0.2%)
All	All	0.97	3/15916 (0.0%)	1.13	39/21544 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	PHE	CA-C	-5.35	1.48	1.52
1	B	707	VAL	CA-CB	5.07	1.59	1.53
1	A	570	PRO	N-CA	-5.04	1.43	1.47

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLU	N-CA-C	-13.21	97.25	113.50
1	A	962	GLU	N-CA-C	7.91	123.03	111.87
1	B	52	ASN	N-CA-C	7.42	121.69	111.90
1	A	305	VAL	N-CA-C	6.93	114.76	107.76
1	B	534	ASN	N-CA-C	6.67	119.60	108.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7768	0	7674	157	0
1	B	7758	0	7670	157	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	54	0	42	7	0
3	B	54	0	42	8	0
4	A	47	0	0	7	0
4	B	30	0	0	2	0
All	All	15713	0	15428	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD12	1:A:286:PRO:HD2	1.47	0.94
1:A:50:ILE:O	1:A:50:ILE:HG22	1.72	0.90
1:B:309:ASP:H	1:B:672:ASN:HD21	1.18	0.90
1:A:300:GLN:HE21	1:A:502:GLN:HE21	1.15	0.89
1:B:962:GLU:O	1:B:963:MET:HB2	1.73	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	952/990 (96%)	880 (92%)	71 (8%)	1 (0%)	48 78
1	B	950/990 (96%)	867 (91%)	78 (8%)	5 (0%)	24 58
All	All	1902/1980 (96%)	1747 (92%)	149 (8%)	6 (0%)	36 67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	961	ARG
1	B	963	MET
1	B	353	LYS
1	B	1010	PRO
1	A	54	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	837/879 (95%)	750 (90%)	87 (10%)	7	27
1	B	837/879 (95%)	747 (89%)	90 (11%)	6	26
All	All	1674/1758 (95%)	1497 (89%)	177 (11%)	6	26

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	GLU
1	B	733	ILE
1	B	491	ARG
1	B	587	PRO
1	B	797	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	B	332	HIS
1	B	231	ASN
1	B	297	HIS
1	B	386	HIS

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	I41	A	1103	-	28,28,28	2.61	8 (28%)	35,36,36	2.64	17 (48%)
3	I41	B	1103	-	28,28,28	2.57	7 (25%)	35,36,36	1.98	9 (25%)
3	I41	A	1102	2	28,28,28	2.61	8 (28%)	35,36,36	3.05	14 (40%)
3	I41	B	1102	2	28,28,28	2.79	13 (46%)	35,36,36	2.42	12 (34%)

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	I41	A	1103	-	-	9/26/26/26	0/2/2/2
3	I41	B	1103	-	-	17/26/26/26	0/2/2/2
3	I41	A	1102	2	-	11/26/26/26	0/2/2/2
3	I41	B	1102	2	-	9/26/26/26	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	I41	C10-N11	7.33	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	I41	C10-N11	6.92	1.46	1.35
3	B	1103	I41	C10-N11	6.84	1.46	1.35
3	A	1103	I41	O02-C03	6.50	1.49	1.33
3	A	1103	I41	C10-N11	6.39	1.45	1.35

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	I41	C05-C06-C07	7.31	125.65	113.27
3	A	1102	I41	C06-C05-C03	7.30	126.43	110.62
3	B	1102	I41	C05-N12-C13	6.38	137.68	121.68
3	A	1102	I41	C05-N12-C13	6.31	137.50	121.68
3	A	1102	I41	C25-C24-C23	-5.87	113.00	120.24

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	I41	C05-C03-O02-C01
3	A	1102	I41	C03-C05-C06-C07
3	A	1102	I41	N12-C05-C06-C07
3	A	1102	I41	C05-C06-C07-C08
3	A	1102	I41	C05-C06-C07-N11

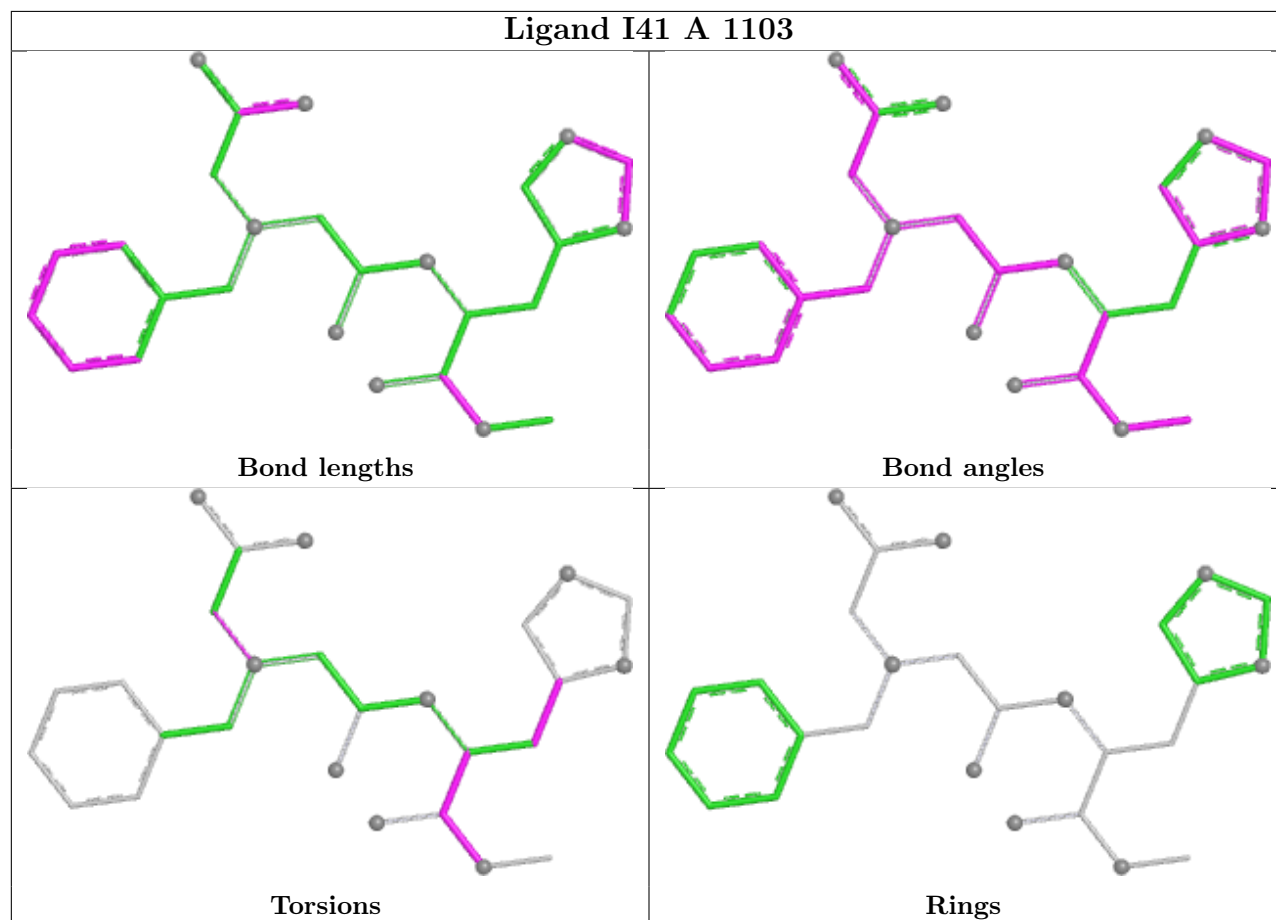
There are no ring outliers.

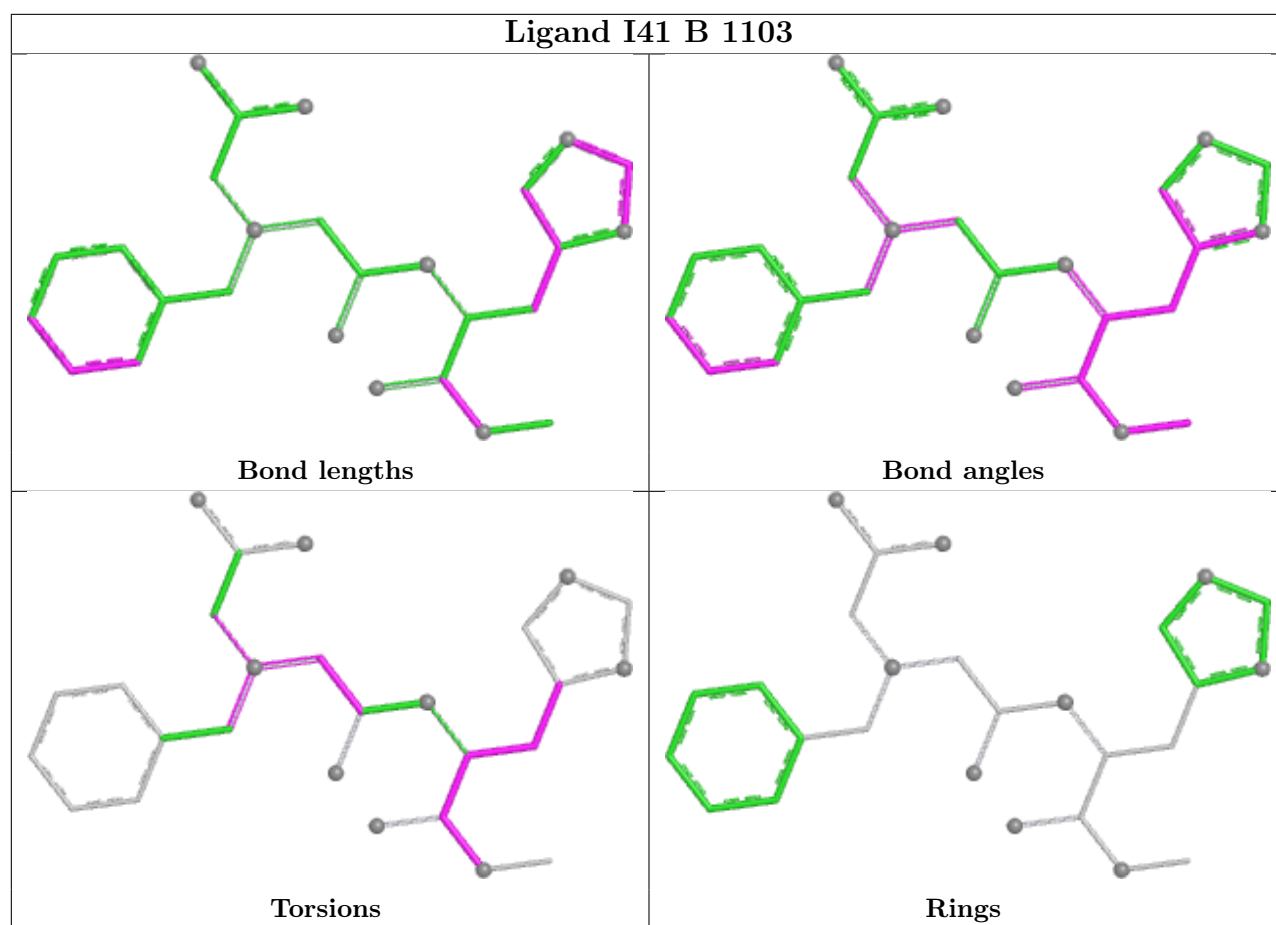
4 monomers are involved in 15 short contacts:

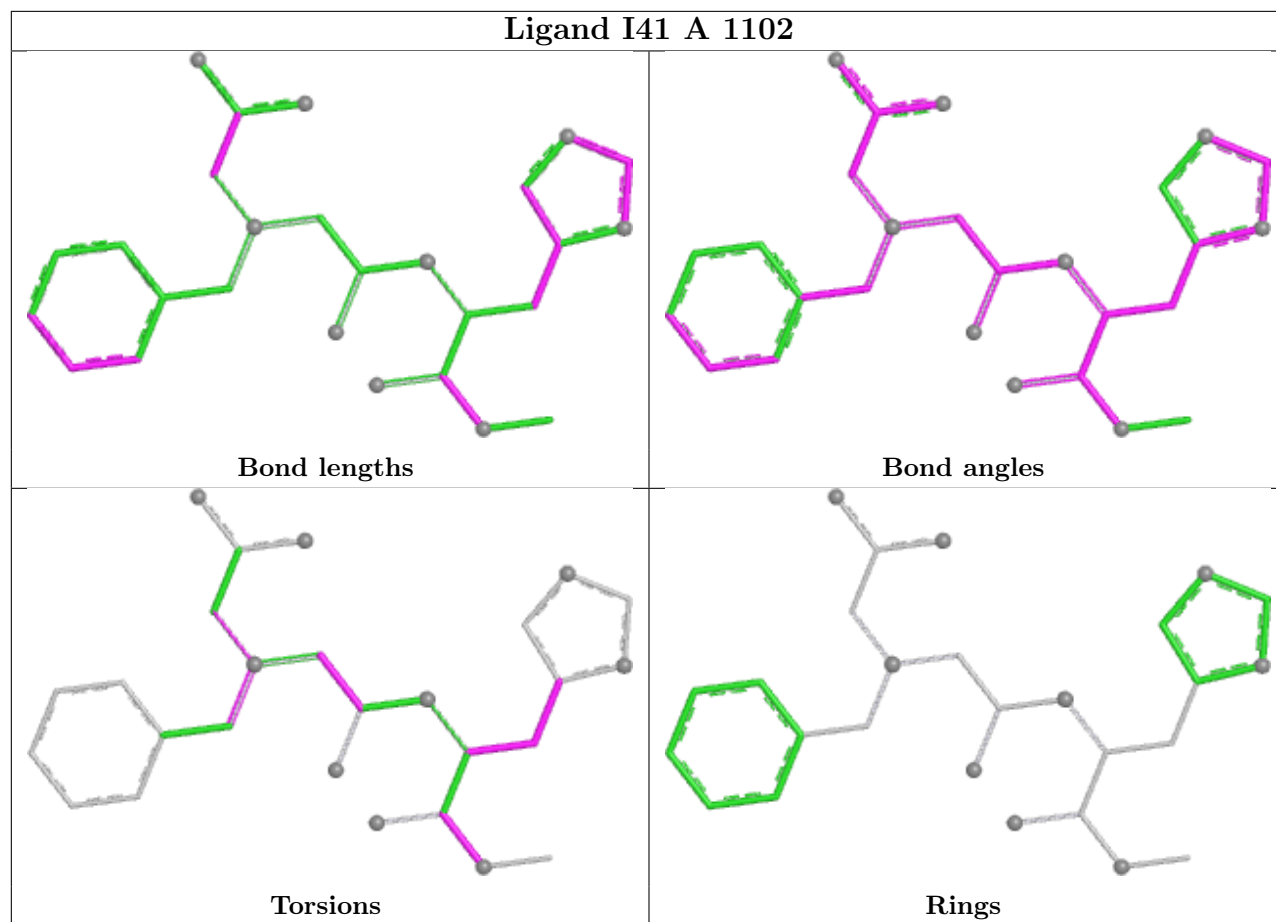
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	I41	6	0
3	B	1103	I41	5	0
3	A	1102	I41	1	0
3	B	1102	I41	3	0

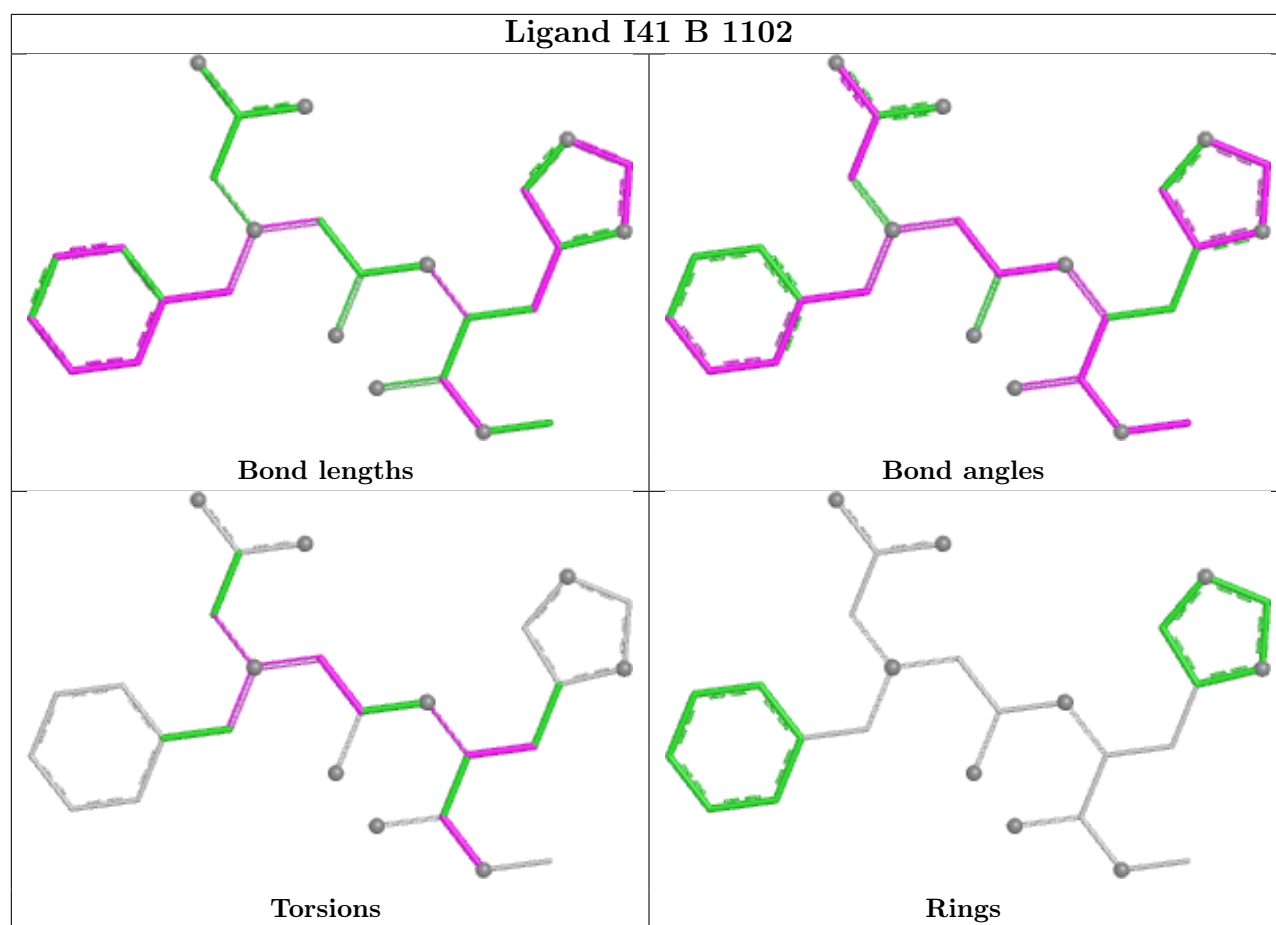
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	956/990 (96%)	-0.63	5 (0%) 87 76	32, 48, 65, 84	0
1	B	954/990 (96%)	-0.50	3 (0%) 90 81	37, 55, 71, 90	0
All	All	1910/1980 (96%)	-0.56	8 (0%) 88 79	32, 52, 69, 90	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	964	ASP	6.5
1	A	964	ASP	5.6
1	A	53	HIS	3.0
1	B	1011	HIS	2.7
1	A	979	ASN	2.5

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](#)

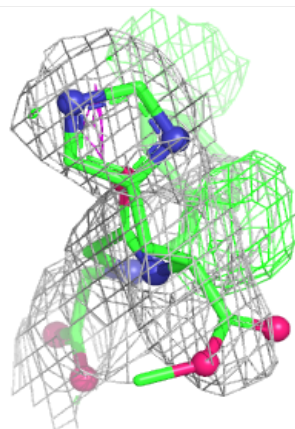
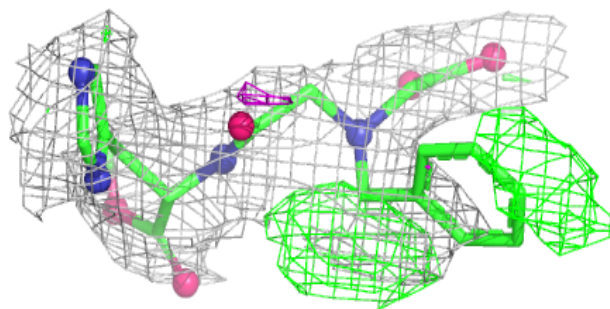
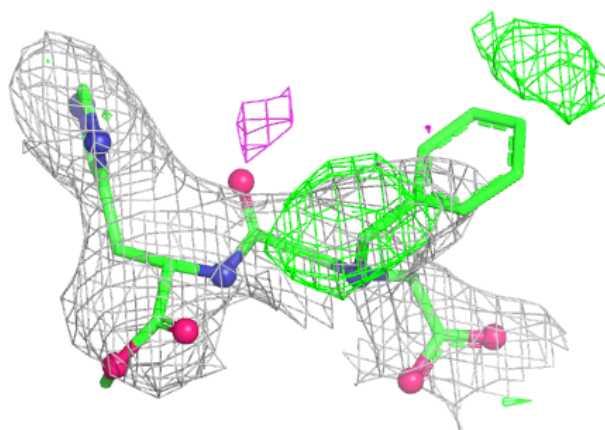
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	I41	B	1103	27/27	0.82	0.22	82,95,106,106	0
3	I41	A	1102	27/27	0.83	0.25	98,107,108,108	0
3	I41	B	1102	27/27	0.86	0.24	98,106,108,110	0
3	I41	A	1103	27/27	0.87	0.22	85,99,109,110	0
2	ZN	B	1101	1/1	0.99	0.02	63,63,63,63	0
2	ZN	A	1101	1/1	1.00	0.02	57,57,57,57	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.

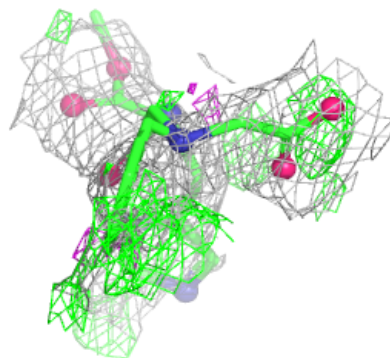
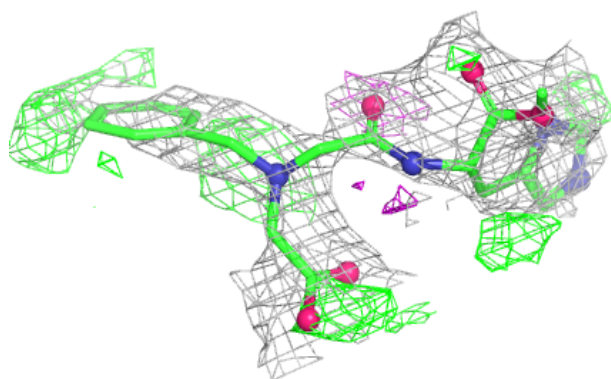
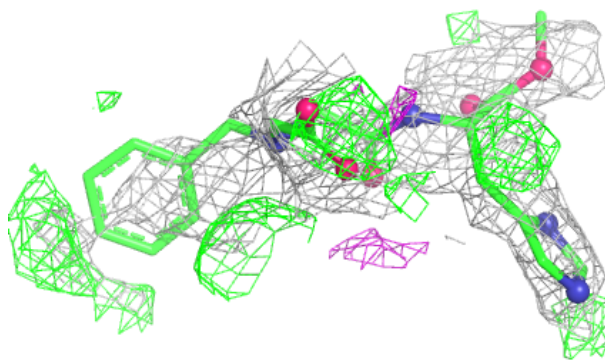
Electron density around I41 B 1103:

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



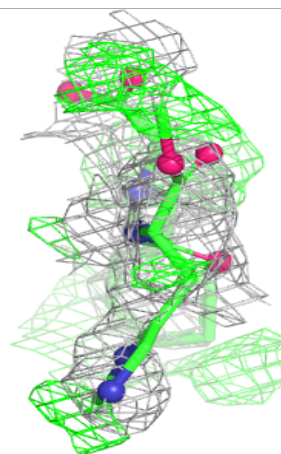
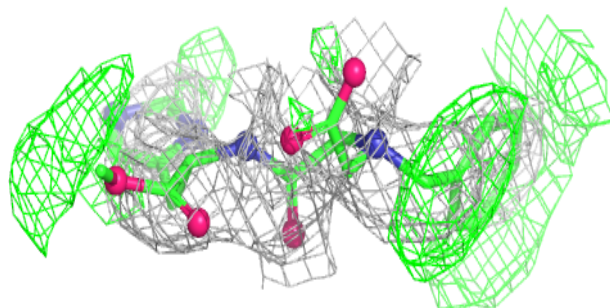
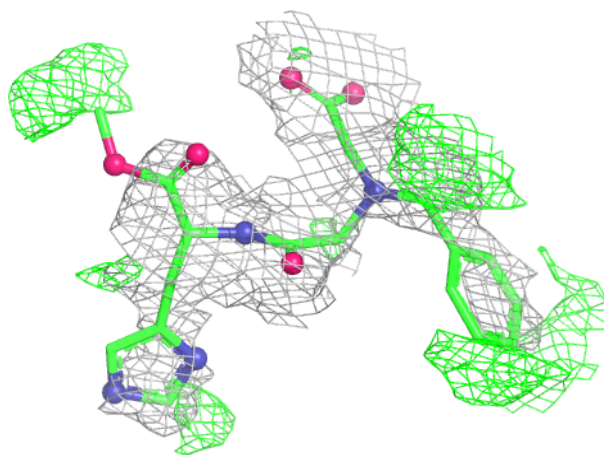
Electron density around I41 A 1102:

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



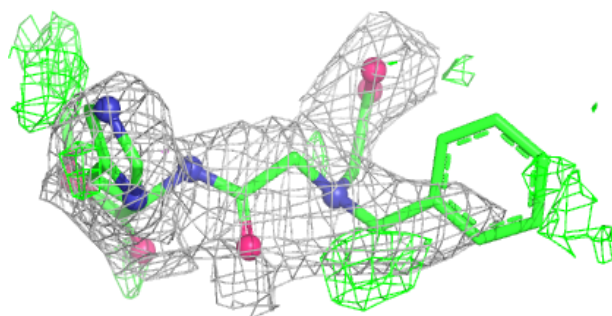
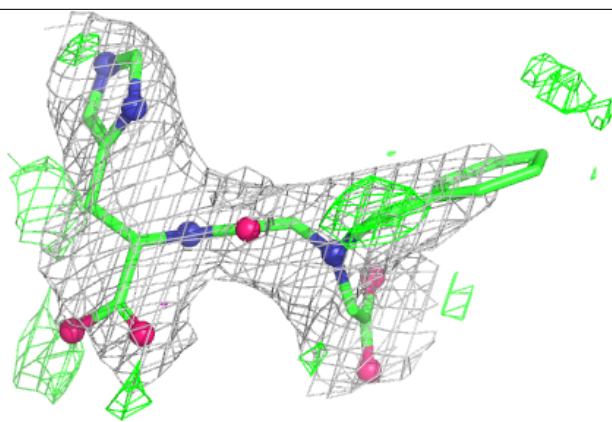
Electron density around I41 B 1102:

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



Electron density around I41 A 1103:

$2mF_o-DF_c$ (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.