



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 09:10 AM EDT

PDB ID : 4DTT  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

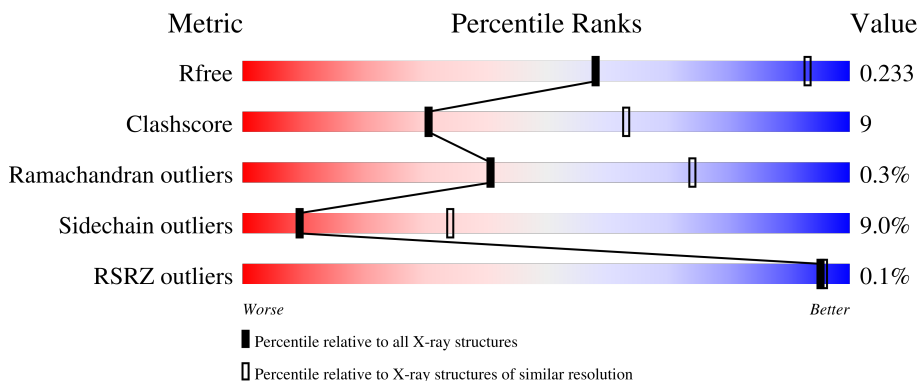
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (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  $\geq 3$ , 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	 73% 21% . .
1	B	990	 71% 23% . .

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	956	7768	5008	1306	1432	22	0	0	0
1	B	954	7758	5002	1304	1430	22	0	0	0

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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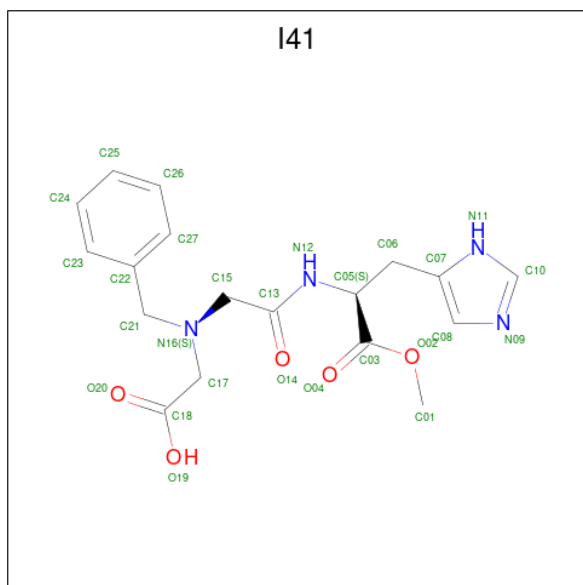
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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression 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 (three-letter code: 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 (three-letter code: I41) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O<sub>5</sub>).



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

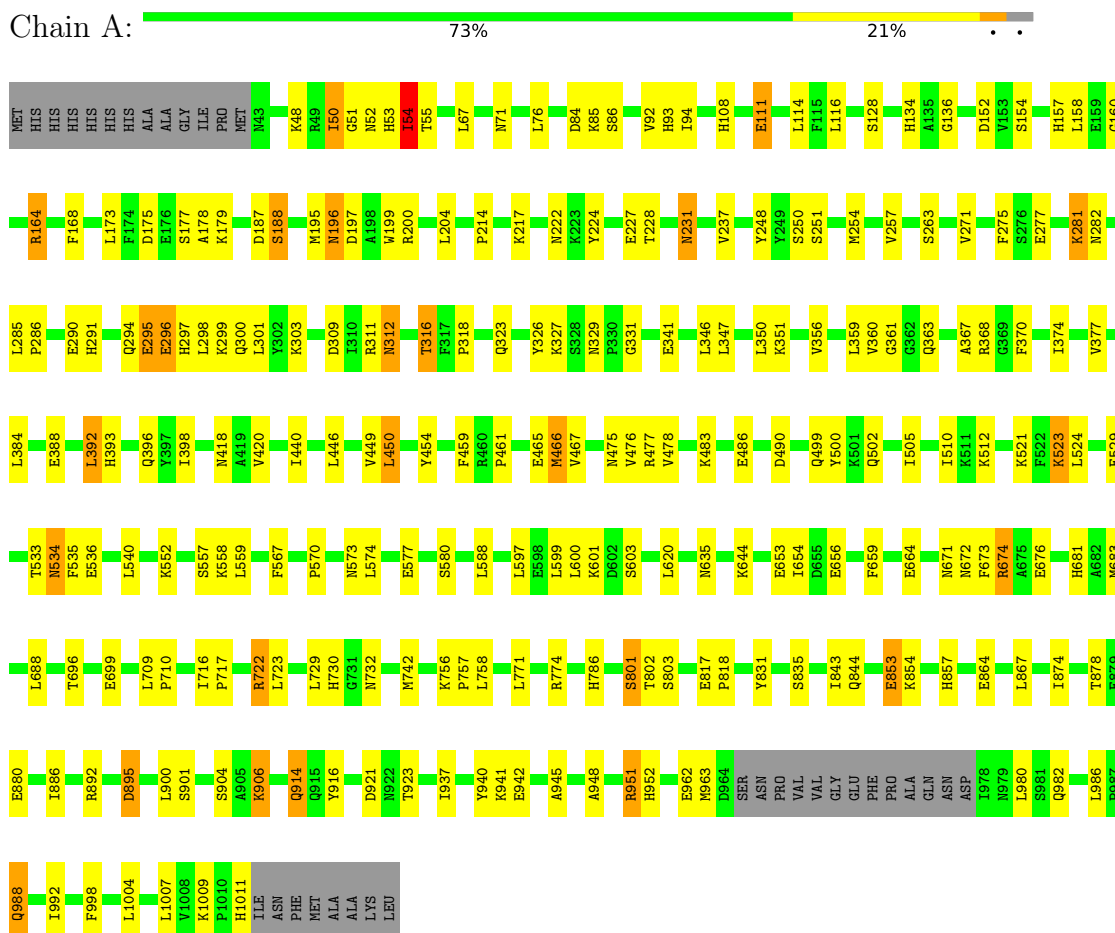
- Molecule 4 is water.

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

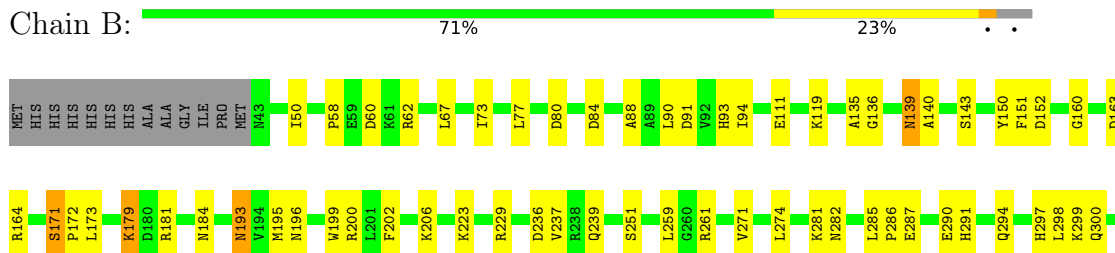
### 3 Residue-property plots

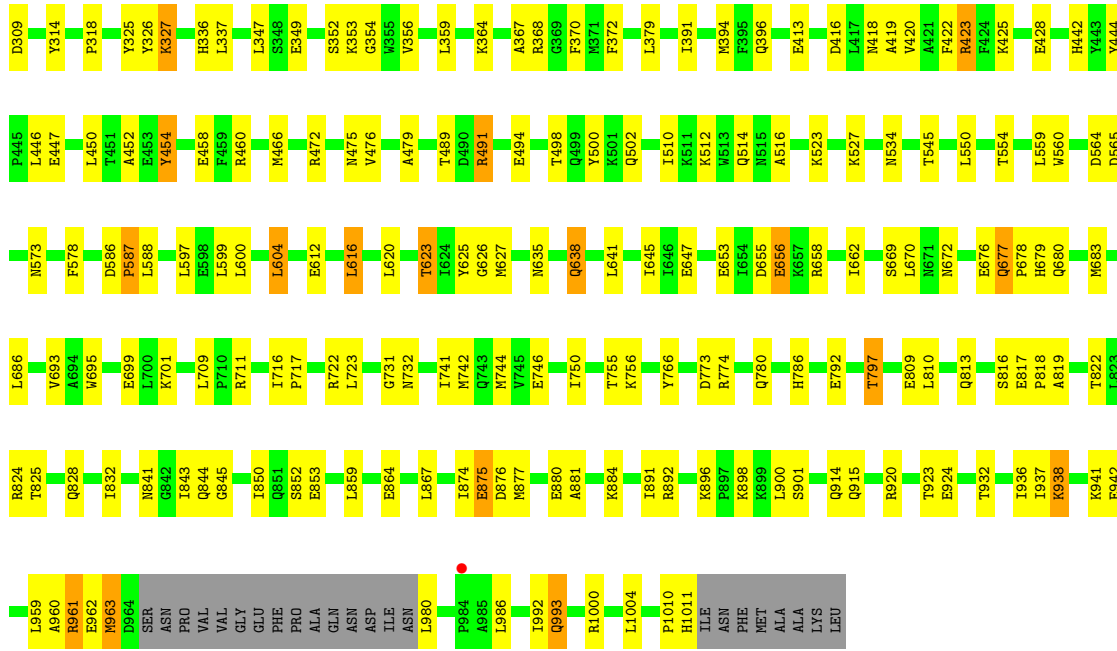
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.52Å 263.52Å 90.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.22 49.80 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.22) 99.2 (49.80-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 3.19Å)	Xtrriage
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 <sup>2</sup> )	60.1	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.82	4/7963 (0.1%)	0.83	7/10779 (0.1%)
1	B	0.80	3/7953 (0.0%)	0.80	0/10765
All	All	0.81	7/15916 (0.0%)	0.82	7/21544 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	656	GLU	CG-CD	5.93	1.60	1.51
1	B	447	GLU	CB-CG	5.64	1.62	1.52
1	A	676	GLU	CG-CD	5.14	1.59	1.51
1	B	699	GLU	CG-CD	5.14	1.59	1.51
1	A	853	GLU	CG-CD	5.12	1.59	1.51
1	A	577	GLU	CG-CD	5.08	1.59	1.51
1	A	880	GLU	CG-CD	5.07	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	895	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	94	ILE	CB-CA-C	-5.47	100.65	111.60
1	A	674	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	173	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	A	296	GLU	N-CA-C	-5.09	97.25	111.00
1	A	477	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	142	0
1	B	7758	0	7670	140	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	286	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 9.

All (286) 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
1:B:797:THR:HG22	1:B:845:GLY:HA2	1.55	0.88
1:B:635:ASN:HD21	1:B:732:ASN:HD22	1.23	0.86
1:B:139:ASN:HD22	1:B:140:ALA:H	1.27	0.83
1:B:962:GLU:O	1:B:963:MET:CB	2.30	0.79
1:A:857:HIS:HD2	4:A:1206:HOH:O	1.66	0.79
1:B:959:LEU:HD22	1:B:963:MET:CE	2.13	0.78
1:B:364:LYS:HG3	3:B:1103:I41:H24	1.64	0.77
1:A:671:ASN:O	1:A:674:ARG:HG2	1.85	0.77
1:B:797:THR:CG2	1:B:845:GLY:HA2	2.14	0.76
1:A:164:ARG:HG3	1:A:164:ARG:HH11	1.51	0.76
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.68	0.75
1:B:810:LEU:HD23	1:B:936:ILE:HD11	1.67	0.75
1:A:309:ASP:H	1:A:672:ASN:HD21	1.35	0.75
1:A:196:ASN:HD21	1:A:199:TRP:HD1	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.68	0.74
1:B:960:ALA:O	1:B:962:GLU:N	2.21	0.74
1:A:51:GLY:O	1:A:52:ASN:ND2	2.21	0.73
1:A:360:VAL:HA	3:A:1103:I41:H10	1.69	0.73
3:A:1103:I41:H062	3:A:1103:I41:H013	1.71	0.72
1:A:722:ARG:HB2	1:A:758:LEU:HD23	1.73	0.71
1:A:164:ARG:HH11	1:A:164:ARG:CG	2.04	0.70
1:A:696:THR:OG1	1:A:699:GLU:HG3	1.90	0.70
1:B:352:SER:C	1:B:354:GLY:H	1.95	0.69
1:A:285:LEU:HD12	1:A:286:PRO:CD	2.22	0.69
1:B:50:ILE:O	1:B:50:ILE:HG13	1.92	0.69
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.74	0.69
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.74	0.69
1:A:756:LYS:HB3	1:A:757:PRO:CD	2.23	0.68
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.75	0.68
1:A:523:LYS:HD3	4:A:1201:HOH:O	1.93	0.68
1:A:311:ARG:HD3	1:A:384:LEU:HD22	1.77	0.67
1:A:196:ASN:ND2	1:A:199:TRP:HD1	1.91	0.67
1:B:327:LYS:HD3	1:B:327:LYS:H	1.61	0.65
1:A:309:ASP:H	1:A:672:ASN:ND2	1.94	0.65
1:B:938:LYS:NZ	1:B:938:LYS:HB3	2.12	0.64
1:A:730:HIS:HD2	1:A:904:SER:OG	1.80	0.64
1:A:224:TYR:HA	1:A:228:THR:HB	1.80	0.64
1:B:676:GLU:HA	1:B:676:GLU:OE1	1.97	0.64
1:A:300:GLN:HE21	1:A:502:GLN:NE2	1.93	0.64
1:A:50:ILE:O	1:A:50:ILE:CG2	2.41	0.64
1:B:139:ASN:HD22	1:B:140:ALA:N	1.94	0.64
1:B:423:ARG:HD3	4:B:1222:HOH:O	1.98	0.63
1:B:309:ASP:H	1:B:672:ASN:ND2	1.92	0.63
1:A:53:HIS:O	1:A:53:HIS:CD2	2.52	0.63
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.79	0.62
1:A:327:LYS:HB2	4:A:1213:HOH:O	1.99	0.61
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.01	0.61
1:A:295:GLU:O	1:A:295:GLU:HG2	2.01	0.60
1:B:139:ASN:HD21	3:B:1102:I41:C17	2.15	0.60
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.83	0.60
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.37	0.59
1:A:85:LYS:HE3	1:A:895:ASP:OD2	2.01	0.59
1:B:564:ASP:HB2	1:B:731:GLY:HA2	1.85	0.59
1:B:773:ASP:O	1:B:774:ARG:HB2	2.02	0.59
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:O	3:B:1103:I41:H10	2.03	0.58
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.38	0.57
1:B:864:GLU:HG3	1:B:986:LEU:HD21	1.85	0.57
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.86	0.57
1:B:193:ASN:HB3	1:B:199:TRP:CD1	2.39	0.57
1:B:693:VAL:HB	1:B:766:TYR:CE2	2.40	0.57
1:B:367:ALA:HB3	1:B:370:PHE:CE2	2.39	0.56
1:A:300:GLN:NE2	1:A:502:GLN:HE21	1.93	0.56
1:A:1007:LEU:HD12	1:B:1000:ARG:HG2	1.86	0.56
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.52	0.56
1:A:393:HIS:HA	1:A:396:GLN:HG3	1.87	0.56
1:A:843:ILE:HG22	1:A:844:GLN:N	2.20	0.55
1:B:960:ALA:C	1:B:962:GLU:N	2.58	0.55
1:B:722:ARG:HE	1:B:756:LYS:HB2	1.72	0.55
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.41	0.55
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.41	0.54
1:B:616:LEU:CD1	1:B:638:GLN:HG3	2.37	0.54
1:B:139:ASN:HD21	3:B:1102:I41:H172	1.72	0.54
1:B:683:MET:HA	1:B:792:GLU:OE1	2.07	0.54
1:B:418:ASN:HB3	1:B:454:TYR:O	2.08	0.54
1:B:325:TYR:HA	1:B:327:LYS:HE2	1.88	0.53
1:A:446:LEU:O	1:A:449:VAL:HG22	2.08	0.53
1:B:573:ASN:HD21	1:B:901:SER:HA	1.72	0.53
1:A:341:GLU:HG2	1:A:347:LEU:CD2	2.39	0.53
1:B:294:GLN:H	1:B:297:HIS:HD2	1.57	0.53
1:A:53:HIS:O	1:A:53:HIS:CG	2.62	0.53
1:B:391:ILE:O	1:B:394:MET:HB2	2.09	0.53
1:B:980:LEU:N	4:B:1202:HOH:O	2.40	0.53
1:A:573:ASN:HD21	1:A:901:SER:HB3	1.73	0.53
1:B:597:LEU:HD11	1:B:627:MET:HG2	1.90	0.52
1:B:67:LEU:HD21	1:B:77:LEU:HD11	1.92	0.52
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.10	0.51
1:B:635:ASN:ND2	1:B:732:ASN:HD22	2.02	0.51
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.91	0.51
1:A:250:SER:HB2	1:A:281:LYS:HB2	1.93	0.51
1:B:600:LEU:HD23	1:B:620:LEU:HD21	1.91	0.51
1:A:114:LEU:HD13	1:A:168:PHE:O	2.11	0.51
1:A:857:HIS:CD2	4:A:1206:HOH:O	2.50	0.51
1:A:937:ILE:HG22	1:A:941:LYS:HD2	1.92	0.51
1:B:139:ASN:ND2	1:B:140:ALA:H	2.03	0.51
1:B:962:GLU:O	1:B:963:MET:CG	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:O	3:A:1103:I41:H10	2.10	0.51
1:A:567:PHE:CE1	1:A:900:LEU:HA	2.46	0.51
1:B:195:MET:HB2	1:B:786:HIS:CE1	2.46	0.51
1:B:352:SER:C	1:B:354:GLY:N	2.60	0.51
1:B:550:LEU:HB2	1:B:560:TRP:CZ3	2.45	0.51
1:A:535:PHE:HB3	1:A:570:PRO:HG3	1.94	0.50
1:B:850:ILE:HG21	1:B:859:LEU:HD22	1.92	0.50
3:B:1103:I41:C06	3:B:1103:I41:H013	2.42	0.50
1:B:259:LEU:HD23	1:B:259:LEU:C	2.32	0.50
1:B:300:GLN:HE21	1:B:502:GLN:HE21	1.59	0.50
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.60	0.50
1:B:416:ASP:O	1:B:419:ALA:HB3	2.12	0.50
1:A:299:LYS:O	1:A:505:ILE:HG13	2.11	0.50
1:A:573:ASN:HD21	1:A:901:SER:CB	2.25	0.50
1:B:196:ASN:C	1:B:196:ASN:OD1	2.50	0.50
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.46	0.49
1:B:416:ASP:O	1:B:420:VAL:HG23	2.11	0.49
1:A:323:GLN:O	1:A:326:TYR:HB3	2.12	0.49
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.93	0.49
1:B:163:ASP:HA	1:B:274:LEU:HD13	1.95	0.49
1:A:982:GLN:HG3	4:A:1203:HOH:O	2.11	0.49
1:B:623:THR:HB	1:B:625:TYR:H	1.77	0.49
1:B:327:LYS:H	1:B:327:LYS:CD	2.24	0.49
1:A:601:LYS:HD3	1:A:620:LEU:O	2.13	0.49
1:B:635:ASN:ND2	1:B:732:ASN:HB3	2.28	0.49
1:B:816:SER:O	1:B:819:ALA:HB3	2.13	0.49
1:B:824:ARG:O	1:B:828:GLN:HA	2.12	0.49
1:B:960:ALA:C	1:B:962:GLU:H	2.15	0.49
1:A:459:PHE:CE2	1:A:461:PRO:HD3	2.48	0.49
1:A:534:ASN:C	1:A:534:ASN:OD1	2.49	0.49
1:A:164:ARG:CG	1:A:164:ARG:NH1	2.68	0.49
1:A:864:GLU:HG3	1:A:986:LEU:HD21	1.94	0.48
1:A:299:LYS:HD2	1:A:510:ILE:HD12	1.95	0.48
1:A:84:ASP:HB2	1:A:895:ASP:OD1	2.13	0.48
1:A:92:VAL:HG22	1:A:254:MET:HG2	1.95	0.48
1:A:86:SER:HB3	1:A:158:LEU:HD13	1.94	0.48
1:A:196:ASN:ND2	1:A:199:TRP:CD1	2.79	0.48
1:B:960:ALA:O	1:B:961:ARG:C	2.52	0.48
1:B:655:ASP:HB3	1:B:658:ARG:HG2	1.95	0.48
1:A:341:GLU:HG2	1:A:347:LEU:HD22	1.96	0.48
1:B:294:GLN:H	1:B:297:HIS:CD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:SER:HB3	1:B:859:LEU:HD11	1.96	0.48
1:A:914:GLN:HA	1:A:916:TYR:CE1	2.49	0.48
1:B:959:LEU:HD22	1:B:963:MET:HE3	1.93	0.48
1:A:529:GLU:OE1	1:A:529:GLU:HA	2.12	0.47
1:B:336:HIS:HD2	1:B:337:LEU:HD23	1.78	0.47
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.96	0.47
1:B:425:LYS:NZ	1:B:425:LYS:HB3	2.29	0.47
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.96	0.47
1:B:578:PHE:O	1:B:626:GLY:HA3	2.13	0.47
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.95	0.47
1:A:392:LEU:O	1:A:396:GLN:HG3	2.14	0.47
1:B:236:ASP:OD1	1:B:236:ASP:C	2.53	0.47
1:B:510:ILE:O	1:B:514:GLN:HG3	2.13	0.47
1:A:301:LEU:HA	1:A:478:VAL:O	2.15	0.47
1:A:316:THR:HG23	1:A:374:ILE:HG22	1.95	0.47
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.50	0.47
3:B:1103:I41:H013	3:B:1103:I41:H062	1.97	0.47
1:A:722:ARG:HB2	1:A:758:LEU:CD2	2.45	0.47
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.96	0.47
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.46	0.47
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.12	0.47
1:B:349:GLU:HA	1:B:349:GLU:OE1	2.15	0.47
1:B:58:PRO:HG2	1:B:423:ARG:HD2	1.96	0.46
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.97	0.46
1:A:175:ASP:OD2	1:A:177:SER:HB3	2.15	0.46
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.76	0.46
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.97	0.46
1:A:108:HIS:O	1:A:111:GLU:HB3	2.15	0.46
1:A:160:GLY:O	1:A:164:ARG:HG3	2.15	0.46
1:A:295:GLU:HA	1:A:298:LEU:HB2	1.97	0.46
1:A:709:LEU:N	1:A:710:PRO:HD2	2.31	0.46
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.98	0.46
1:A:298:LEU:HD13	1:A:475:ASN:HA	1.97	0.46
1:B:635:ASN:HD21	1:B:732:ASN:ND2	2.01	0.46
1:A:312:ASN:HB3	1:A:377:VAL:O	2.16	0.46
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.51	0.46
1:B:962:GLU:O	1:B:963:MET:HG3	2.16	0.46
1:A:71:ASN:HB2	1:A:251:SER:OG	2.16	0.46
1:A:134:HIS:CD2	1:A:157:HIS:CE1	3.04	0.46
1:A:716:ILE:CB	1:A:717:PRO:HD3	2.42	0.46
1:B:364:LYS:HB3	1:B:372:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:THR:HB	1:B:500:TYR:O	2.16	0.46
1:B:135:ALA:HA	1:B:892:ARG:NH1	2.32	0.45
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.17	0.45
1:B:460:ARG:HG3	1:B:460:ARG:HH11	1.81	0.45
1:A:367:ALA:HB3	1:A:370:PHE:CE2	2.51	0.45
1:A:599:LEU:HD13	1:A:654:ILE:HG23	1.99	0.45
1:B:491:ARG:HE	1:B:491:ARG:HB2	1.47	0.45
1:A:801:SER:O	1:A:802:THR:C	2.55	0.45
1:B:285:LEU:HA	1:B:286:PRO:HD3	1.84	0.45
1:B:314:TYR:HB2	1:B:479:ALA:HB3	1.98	0.45
1:B:867:LEU:HD23	1:B:867:LEU:HA	1.89	0.45
1:B:326:TYR:CD1	1:B:444:TYR:HE1	2.35	0.45
1:A:298:LEU:HD21	1:A:318:PRO:HG3	1.99	0.44
1:A:656:GLU:O	1:A:659:PHE:HB3	2.16	0.44
1:A:843:ILE:HG22	1:A:844:GLN:H	1.82	0.44
1:B:139:ASN:HD21	3:B:1102:I41:H171	1.79	0.44
1:A:599:LEU:HD23	1:A:599:LEU:HA	1.76	0.44
1:B:460:ARG:HG3	1:B:460:ARG:NH1	2.33	0.44
1:A:299:LYS:HD2	1:A:510:ILE:CD1	2.48	0.44
1:A:295:GLU:O	1:A:295:GLU:CG	2.64	0.44
1:B:309:ASP:N	1:B:672:ASN:HD21	2.01	0.44
1:A:71:ASN:O	1:A:251:SER:OG	2.35	0.44
1:A:347:LEU:HD13	1:A:359:LEU:CB	2.47	0.43
1:B:181:ARG:O	1:B:184:ASN:HB2	2.18	0.43
1:A:136:GLY:CA	1:A:152:ASP:O	2.66	0.43
1:A:523:LYS:CD	4:A:1201:HOH:O	2.60	0.43
1:B:90:LEU:HD23	1:B:91:ASP:N	2.32	0.43
1:B:472:ARG:HG2	1:B:472:ARG:HH11	1.83	0.43
1:A:231:ASN:HD22	1:A:231:ASN:HA	1.57	0.43
1:B:559:LEU:HD22	1:B:742:MET:HG2	1.99	0.43
1:A:248:TYR:C	1:A:250:SER:H	2.22	0.43
3:A:1102:I41:C01	4:A:1231:HOH:O	2.66	0.43
1:A:346:LEU:HD11	1:A:350:LEU:HD11	2.01	0.43
1:A:992:ILE:HG12	1:A:998:PHE:CD1	2.53	0.43
1:B:920:ARG:O	1:B:924:GLU:HB2	2.19	0.43
1:A:580:SER:HB2	1:A:723:LEU:HD23	2.00	0.43
1:B:77:LEU:HD21	1:B:271:VAL:HG21	2.00	0.43
1:B:139:ASN:HB3	1:B:150:TYR:CE1	2.54	0.43
1:B:635:ASN:HD22	1:B:732:ASN:HB3	1.81	0.43
1:B:677:GLN:HE21	1:B:679:HIS:HE1	1.66	0.43
1:A:214:PRO:O	1:A:217:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH2	1:B:498:THR:HA	2.34	0.43
1:A:204:LEU:HG	1:A:204:LEU:O	2.18	0.43
1:A:294:GLN:HB2	1:A:297:HIS:HD2	1.84	0.43
1:A:867:LEU:HD23	1:A:867:LEU:HA	1.87	0.43
1:B:396:GLN:HG2	1:B:516:ALA:HB1	2.00	0.43
1:A:988:GLN:HE21	1:A:988:GLN:C	2.22	0.43
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.54	0.43
1:B:959:LEU:HB3	1:B:963:MET:HE2	2.00	0.42
1:B:843:ILE:HG22	1:B:844:GLN:N	2.33	0.42
1:B:852:SER:OG	1:B:853:GLU:N	2.52	0.42
1:B:874:ILE:O	1:B:875:GLU:C	2.58	0.42
1:A:294:GLN:O	1:A:295:GLU:HB3	2.20	0.42
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.53	0.42
1:B:352:SER:O	1:B:354:GLY:N	2.52	0.42
1:B:573:ASN:ND2	1:B:901:SER:HA	2.35	0.42
1:B:298:LEU:HD21	1:B:318:PRO:HG3	2.01	0.42
1:B:774:ARG:HG2	1:B:774:ARG:HH11	1.84	0.42
1:A:227:GLU:O	1:A:228:THR:C	2.57	0.42
1:A:466:MET:HE1	1:A:467:VAL:HA	2.02	0.42
1:B:136:GLY:HA3	1:B:152:ASP:O	2.20	0.42
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.83	0.42
1:A:360:VAL:HA	3:A:1103:I41:C10	2.46	0.42
1:B:179:LYS:HD2	1:B:237:VAL:HG12	2.01	0.42
1:B:938:LYS:HB3	1:B:938:LYS:HZ2	1.84	0.42
1:A:179:LYS:HD2	1:A:237:VAL:HB	2.00	0.42
1:A:350:LEU:CB	1:A:356:VAL:HG22	2.50	0.42
1:B:318:PRO:HD2	1:B:475:ASN:O	2.19	0.42
1:A:54:ILE:H	1:A:54:ILE:HG12	1.52	0.42
3:A:1103:I41:H062	3:A:1103:I41:C01	2.47	0.42
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.20	0.42
1:B:422:PHE:HB2	1:B:454:TYR:CD1	2.55	0.42
1:B:686:LEU:HD12	1:B:686:LEU:HA	1.90	0.41
1:B:993:GLN:HE21	1:B:993:GLN:HB2	1.73	0.41
1:B:160:GLY:O	1:B:164:ARG:HG3	2.20	0.41
1:B:604:LEU:HD23	1:B:604:LEU:HA	1.87	0.41
1:B:891:ILE:HD13	1:B:891:ILE:HA	1.97	0.41
1:A:483:LYS:HD2	1:A:483:LYS:HA	1.88	0.41
1:A:843:ILE:CG2	1:A:844:GLN:N	2.83	0.41
1:B:641:LEU:HG	1:B:645:ILE:HD11	2.00	0.41
1:A:197:ASP:HA	1:A:200:ARG:HD3	2.01	0.41
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HB3	1:A:257:VAL:HG13	2.02	0.41
1:A:178:ALA:O	1:A:179:LYS:C	2.59	0.41
1:A:341:GLU:HG2	1:A:347:LEU:HD23	2.03	0.41
1:A:361:GLY:O	3:A:1103:I41:O14	2.39	0.41
1:A:490:ASP:OD1	1:A:490:ASP:C	2.58	0.41
1:A:557:SER:HB2	1:A:742:MET:CE	2.51	0.41
1:A:1004:LEU:HD12	1:B:1004:LEU:HD12	2.03	0.41
1:B:73:ILE:HG13	1:B:251:SER:HB2	2.02	0.41
1:B:813:GLN:OE1	1:B:892:ARG:NH2	2.54	0.41
1:B:881:ALA:O	1:B:884:LYS:HB2	2.20	0.41
1:B:171:SER:HA	1:B:172:PRO:HD3	1.86	0.41
1:A:271:VAL:O	1:A:275:PHE:HB2	2.21	0.40
1:B:723:LEU:HD12	1:B:755:THR:HG21	2.03	0.40
1:A:600:LEU:HD23	1:A:620:LEU:HD21	2.02	0.40
1:A:418:ASN:HB3	1:A:454:TYR:O	2.20	0.40
1:A:730:HIS:CD2	1:A:904:SER:OG	2.67	0.40
1:A:673:PHE:CE2	1:A:681:HIS:HD2	2.39	0.40
3:B:1103:I41:C27	3:B:1103:I41:H171	2.47	0.40
1:A:134:HIS:O	1:A:154:SER:HB3	2.22	0.40
1:A:303:LYS:O	1:A:500:TYR:HA	2.22	0.40
1:B:93:HIS:HB2	1:B:442:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	952/990 (96%)	880 (92%)	71 (8%)	1 (0%)	51 83
1	B	950/990 (96%)	867 (91%)	78 (8%)	5 (0%)	29 66
All	All	1902/1980 (96%)	1747 (92%)	149 (8%)	6 (0%)	41 74

All (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
1	B	992	ILE

### 5.3.2 Protein sidechains [i](#)

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%)	769 (92%)	68 (8%)	11 41
1	B	837/879 (95%)	755 (90%)	82 (10%)	8 30
All	All	1674/1758 (95%)	1524 (91%)	150 (9%)	9 34

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	54	ILE
1	A	55	THR
1	A	67	LEU
1	A	111	GLU
1	A	116	LEU
1	A	128	SER
1	A	164	ARG
1	A	188	SER
1	A	196	ASN
1	A	231	ASN
1	A	263	SER
1	A	277	GLU
1	A	281	LYS
1	A	282	ASN
1	A	290	GLU
1	A	295	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	296	GLU
1	A	312	ASN
1	A	316	THR
1	A	329	ASN
1	A	351	LYS
1	A	388	GLU
1	A	392	LEU
1	A	398	ILE
1	A	420	VAL
1	A	440	ILE
1	A	450	LEU
1	A	465	GLU
1	A	466	MET
1	A	476	VAL
1	A	486	GLU
1	A	499	GLN
1	A	512	LYS
1	A	521	LYS
1	A	523	LYS
1	A	524	LEU
1	A	533	THR
1	A	534	ASN
1	A	536	GLU
1	A	540	LEU
1	A	558	LYS
1	A	588	LEU
1	A	603	SER
1	A	644	LYS
1	A	653	GLU
1	A	683	MET
1	A	722	ARG
1	A	774	ARG
1	A	801	SER
1	A	803	SER
1	A	835	SER
1	A	853	GLU
1	A	854	LYS
1	A	878	THR
1	A	886	ILE
1	A	892	ARG
1	A	906	LYS
1	A	914	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	923	THR
1	A	942	GLU
1	A	951	ARG
1	A	962	GLU
1	A	963	MET
1	A	980	LEU
1	A	988	GLN
1	A	1009	LYS
1	A	1011	HIS
1	B	60	ASP
1	B	84	ASP
1	B	94	ILE
1	B	111	GLU
1	B	119	LYS
1	B	139	ASN
1	B	143	SER
1	B	171	SER
1	B	173	LEU
1	B	179	LYS
1	B	193	ASN
1	B	229	ARG
1	B	239	GLN
1	B	261	ARG
1	B	281	LYS
1	B	282	ASN
1	B	287	GLU
1	B	290	GLU
1	B	299	LYS
1	B	327	LYS
1	B	347	LEU
1	B	356	VAL
1	B	379	LEU
1	B	423	ARG
1	B	446	LEU
1	B	450	LEU
1	B	454	TYR
1	B	458	GLU
1	B	466	MET
1	B	476	VAL
1	B	491	ARG
1	B	494	GLU
1	B	512	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	523	LYS
1	B	534	ASN
1	B	545	THR
1	B	554	THR
1	B	565	ASP
1	B	586	ASP
1	B	587	PRO
1	B	588	LEU
1	B	604	LEU
1	B	612	GLU
1	B	616	LEU
1	B	623	THR
1	B	638	GLN
1	B	647	GLU
1	B	653	GLU
1	B	669	SER
1	B	677	GLN
1	B	678	PRO
1	B	680	GLN
1	B	701	LYS
1	B	711	ARG
1	B	741	ILE
1	B	744	MET
1	B	746	GLU
1	B	750	ILE
1	B	780	GLN
1	B	797	THR
1	B	809	GLU
1	B	822	THR
1	B	825	THR
1	B	832	ILE
1	B	841	ASN
1	B	875	GLU
1	B	876	ASP
1	B	877	MET
1	B	880	GLU
1	B	896	LYS
1	B	898	LYS
1	B	900	LEU
1	B	914	GLN
1	B	915	GLN
1	B	923	THR

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Mol	Chain	Res	Type
1	B	932	THR
1	B	937	ILE
1	B	938	LYS
1	B	941	LYS
1	B	942	GLU
1	B	993	GLN
1	B	1011	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	93	HIS
1	A	129	GLN
1	A	134	HIS
1	A	157	HIS
1	A	184	ASN
1	A	231	ASN
1	A	297	HIS
1	A	300	GLN
1	A	312	ASN
1	A	332	HIS
1	A	407	GLN
1	A	573	ASN
1	A	635	ASN
1	A	672	ASN
1	A	730	HIS
1	A	914	GLN
1	A	988	GLN
1	B	93	HIS
1	B	139	ASN
1	B	184	ASN
1	B	297	HIS
1	B	300	GLN
1	B	336	HIS
1	B	363	GLN
1	B	386	HIS
1	B	635	ASN
1	B	672	ASN
1	B	677	GLN
1	B	730	HIS
1	B	780	GLN

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Mol	Chain	Res	Type
1	B	786	HIS
1	B	914	GLN
1	B	922	ASN
1	B	993	GLN

### 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 monosaccharides 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	1102	2	24,28,28	1.99	3 (12%)	30,36,36	2.73	11 (36%)
3	I41	B	1103	-	24,28,28	1.98	3 (12%)	30,36,36	1.89	7 (23%)
3	I41	B	1102	2	24,28,28	2.30	7 (29%)	30,36,36	2.41	10 (33%)
3	I41	A	1103	-	24,28,28	2.14	6 (25%)	30,36,36	2.64	15 (50%)

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	1102	2	-	11/26/26/26	0/2/2/2
3	I41	B	1103	-	-	14/26/26/26	0/2/2/2
3	I41	B	1102	2	-	9/26/26/26	0/2/2/2
3	I41	A	1103	-	-	8/26/26/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	I41	O02-C03	6.57	1.49	1.33
3	B	1102	I41	O02-C03	6.28	1.48	1.33
3	B	1103	I41	O02-C03	5.97	1.47	1.33
3	A	1102	I41	O02-C03	5.81	1.47	1.33
3	B	1102	I41	C24-C23	5.02	1.49	1.38
3	B	1103	I41	C24-C23	4.62	1.48	1.38
3	A	1103	I41	C24-C23	4.54	1.48	1.38
3	A	1102	I41	C24-C23	4.34	1.48	1.38
3	B	1103	I41	C25-C24	4.14	1.49	1.38
3	B	1102	I41	C25-C24	3.97	1.48	1.38
3	A	1103	I41	C25-C24	3.75	1.48	1.38
3	A	1102	I41	C25-C24	3.69	1.47	1.38
3	B	1102	I41	C05-N12	2.60	1.51	1.45
3	A	1103	I41	C26-C25	2.45	1.44	1.38
3	B	1102	I41	C21-N16	2.22	1.51	1.47
3	B	1102	I41	C21-C22	2.20	1.55	1.51
3	B	1102	I41	C15-N16	2.16	1.51	1.47
3	A	1103	I41	C26-C27	2.09	1.43	1.38
3	A	1103	I41	O20-C18	2.00	1.28	1.22

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	I41	C06-C05-C03	6.46	126.43	110.37
3	B	1102	I41	C05-N12-C13	6.23	137.68	121.65
3	A	1102	I41	C05-N12-C13	6.16	137.50	121.65
3	A	1103	I41	C22-C21-N16	6.08	124.92	113.12
3	A	1103	I41	C13-C15-N16	-5.70	100.14	113.36
3	A	1103	I41	O02-C03-C05	5.10	124.56	111.52
3	B	1103	I41	O02-C03-C05	4.94	124.17	111.52
3	A	1102	I41	C21-N16-C15	-4.89	101.55	112.02
3	A	1102	I41	C25-C24-C23	-4.72	113.00	120.19
3	B	1102	I41	C13-C15-N16	4.45	123.68	113.36
3	B	1102	I41	C25-C24-C23	-4.39	113.51	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	I41	O02-C03-C05	4.36	122.69	111.52
3	A	1103	I41	O02-C03-O04	-4.34	115.34	123.84
3	A	1102	I41	C22-C21-N16	4.16	121.21	113.12
3	A	1102	I41	O02-C03-C05	4.13	122.07	111.52
3	B	1103	I41	C01-O02-C03	4.08	125.17	115.94
3	B	1102	I41	C01-O02-C03	3.95	124.86	115.94
3	B	1103	I41	C17-N16-C15	-3.57	103.48	111.54
3	B	1102	I41	C22-C21-N16	3.56	120.04	113.12
3	A	1102	I41	O02-C03-O04	-3.54	116.92	123.84
3	A	1103	I41	C01-O02-C03	3.37	123.56	115.94
3	A	1103	I41	O14-C13-C15	-3.36	115.20	121.08
3	B	1102	I41	O02-C03-O04	-3.22	117.54	123.84
3	A	1103	I41	C25-C24-C23	-3.21	115.30	120.19
3	B	1103	I41	O02-C03-O04	-3.20	117.58	123.84
3	A	1102	I41	C18-C17-N16	2.97	123.32	113.63
3	A	1102	I41	C13-C15-N16	2.85	119.97	113.36
3	A	1103	I41	C21-N16-C17	2.76	117.93	112.02
3	B	1102	I41	C24-C23-C22	2.66	124.70	120.63
3	A	1103	I41	C15-C13-N12	2.60	121.17	115.31
3	B	1103	I41	C21-N16-C17	2.59	117.56	112.02
3	A	1103	I41	C24-C23-C22	2.53	124.51	120.63
3	B	1103	I41	C25-C24-C23	-2.51	116.37	120.19
3	A	1103	I41	C21-C22-C27	2.45	125.37	120.77
3	A	1102	I41	O19-C18-O20	-2.43	117.24	123.30
3	B	1103	I41	C03-C05-N12	-2.39	105.20	110.72
3	A	1103	I41	C21-C22-C23	-2.32	116.40	120.77
3	A	1102	I41	O14-C13-N12	2.29	126.81	122.95
3	A	1103	I41	O19-C18-C17	2.28	122.43	113.45
3	A	1103	I41	C18-C17-N16	2.24	120.94	113.63
3	A	1103	I41	C21-N16-C15	2.16	116.64	112.02
3	B	1102	I41	C21-N16-C15	2.02	116.33	112.02
3	B	1102	I41	O19-C18-C17	2.01	121.37	113.45

There are no chirality outliers.

All (42) 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

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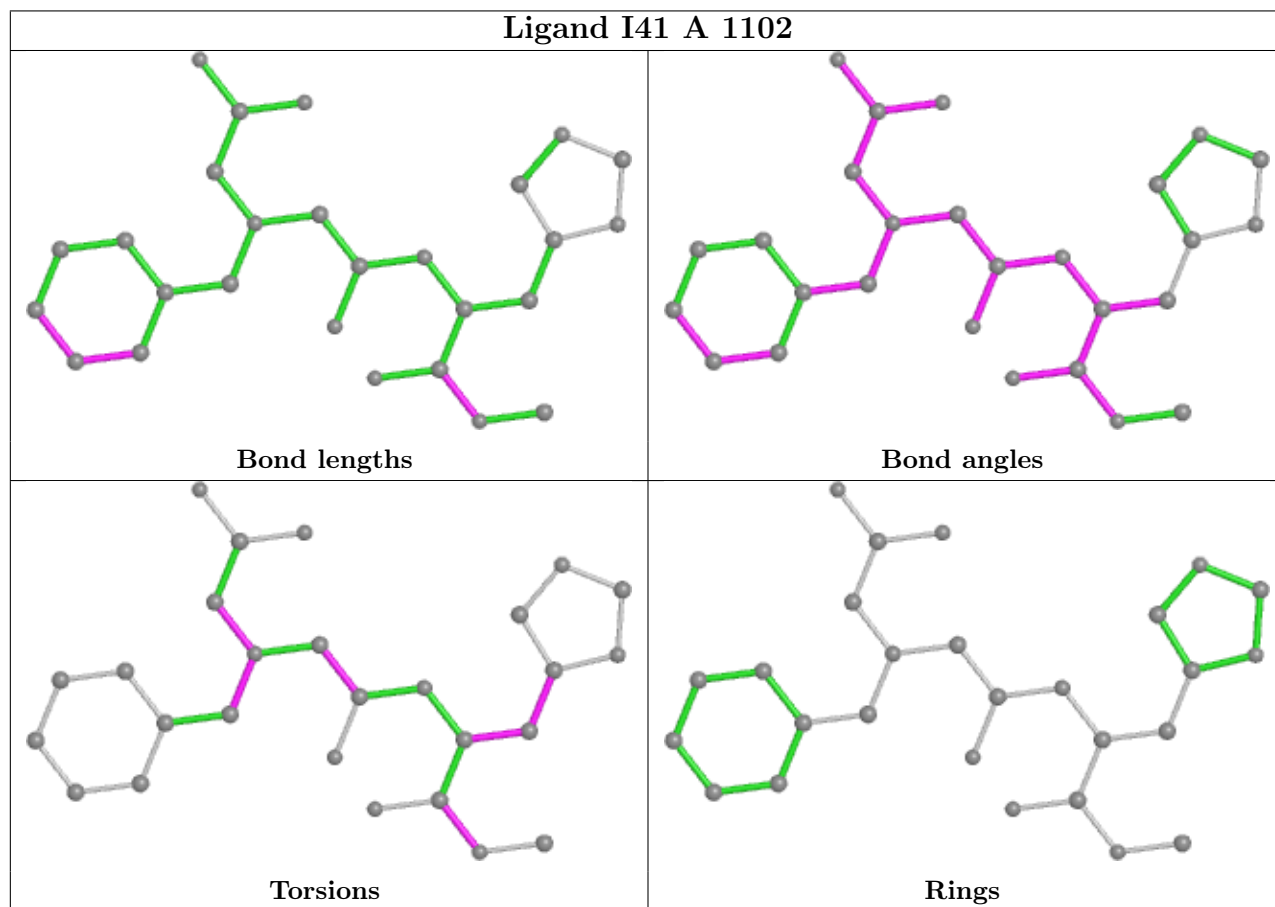
Mol	Chain	Res	Type	Atoms
3	A	1103	I41	C05-C06-C07-N11
3	B	1102	I41	C13-C15-N16-C17
3	B	1103	I41	C13-C15-N16-C21
3	B	1103	I41	C22-C21-N16-C17
3	B	1103	I41	O04-C03-O02-C01
3	A	1103	I41	O04-C03-O02-C01
3	A	1103	I41	C05-C03-O02-C01
3	B	1102	I41	C06-C05-N12-C13
3	B	1103	I41	C05-C03-O02-C01
3	A	1102	I41	O04-C03-O02-C01
3	B	1102	I41	C05-C03-O02-C01
3	B	1102	I41	O04-C03-O02-C01
3	A	1103	I41	C18-C17-N16-C15
3	B	1102	I41	C22-C21-N16-C15
3	B	1103	I41	C22-C21-N16-C15
3	B	1102	I41	O14-C13-C15-N16
3	B	1102	I41	N12-C13-C15-N16
3	B	1103	I41	O02-C03-C05-N12
3	A	1103	I41	O02-C03-C05-C06
3	A	1103	I41	O02-C03-C05-N12
3	A	1102	I41	C18-C17-N16-C21
3	B	1103	I41	O02-C03-C05-C06
3	B	1103	I41	O04-C03-C05-C06
3	A	1103	I41	O04-C03-C05-N12
3	B	1102	I41	C03-C05-C06-C07
3	A	1102	I41	C22-C21-N16-C17
3	B	1103	I41	O04-C03-C05-N12
3	B	1103	I41	C18-C17-N16-C21
3	A	1102	I41	N12-C13-C15-N16
3	A	1103	I41	O04-C03-C05-C06
3	A	1102	I41	O14-C13-C15-N16
3	B	1103	I41	C18-C17-N16-C15
3	B	1102	I41	C18-C17-N16-C21
3	B	1103	I41	N12-C13-C15-N16
3	B	1103	I41	O14-C13-C15-N16
3	A	1102	I41	C22-C21-N16-C15
3	B	1103	I41	C03-C05-C06-C07

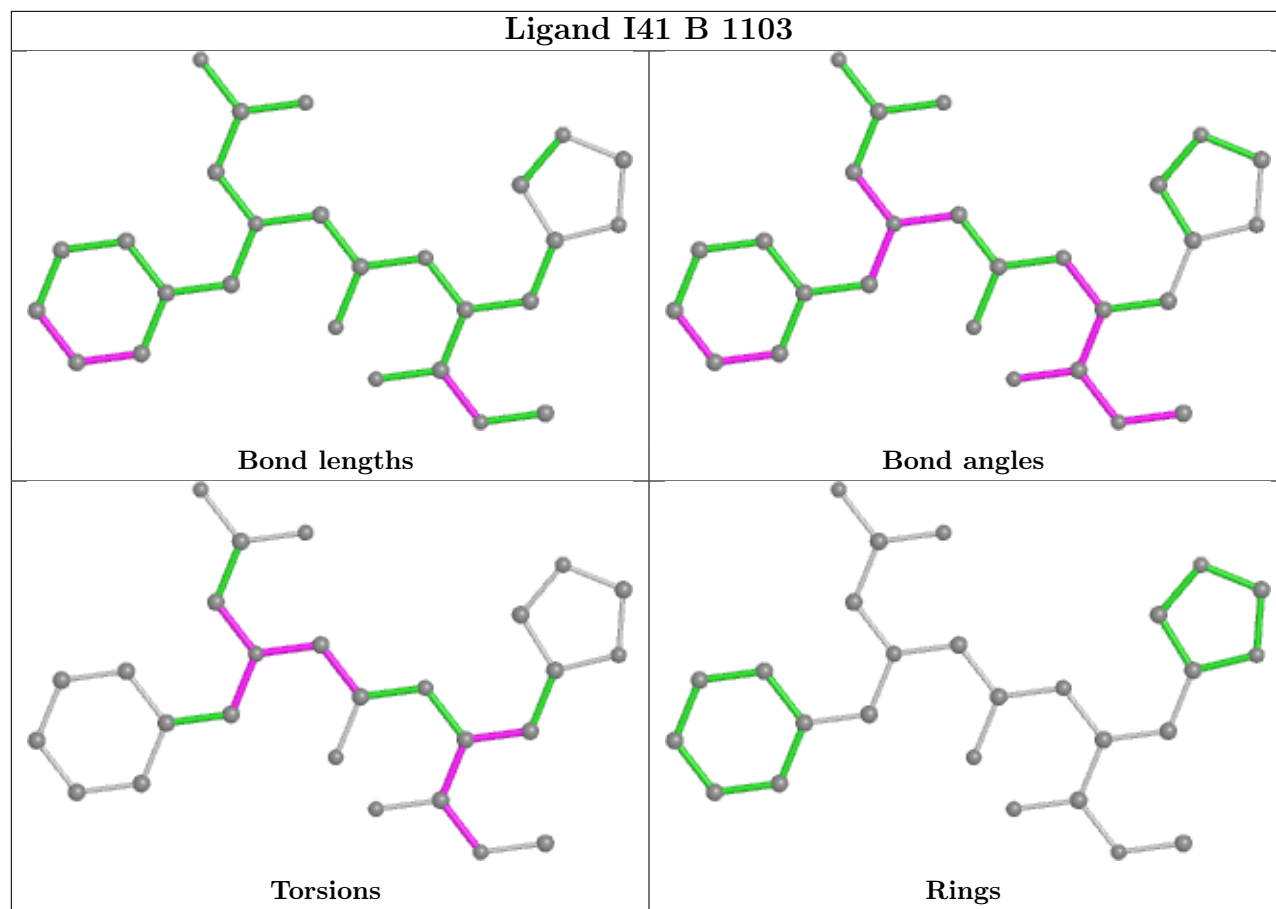
There are no ring outliers.

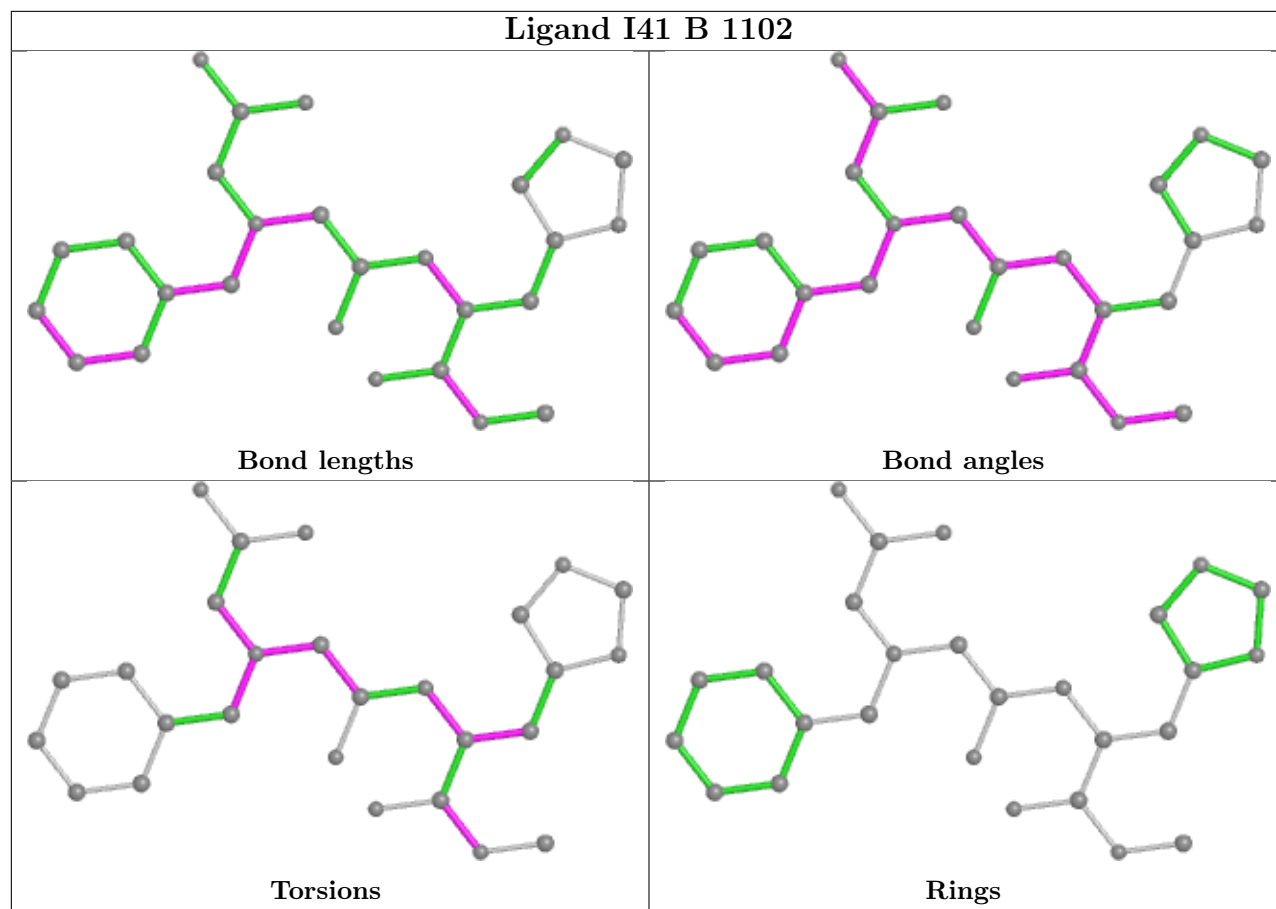
4 monomers are involved in 15 short contacts:

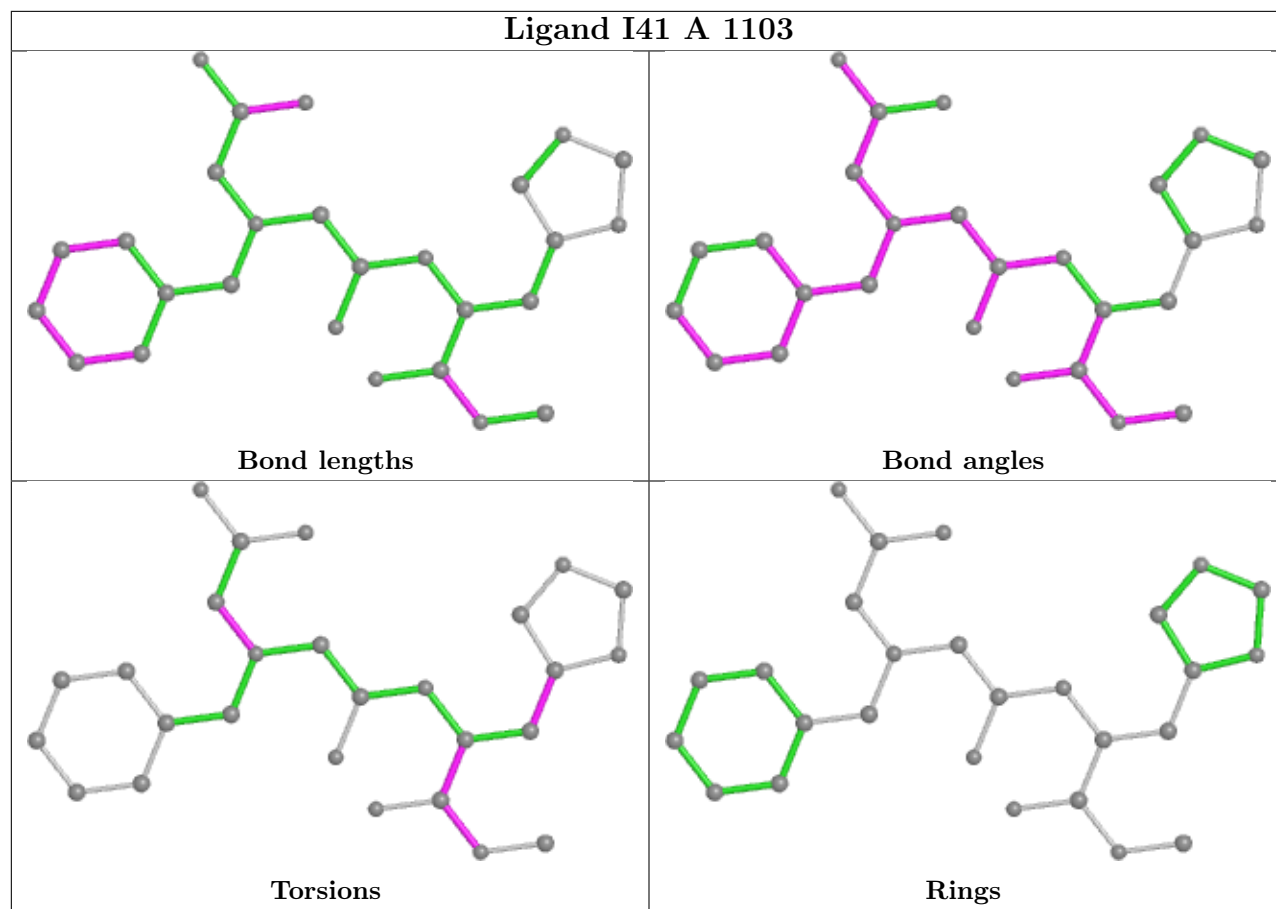
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	I41	1	0
3	B	1103	I41	5	0
3	B	1102	I41	3	0
3	A	1103	I41	6	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	956/990 (96%)	-0.27	0 <b>100</b>   <b>100</b>	32, 48, 65, 84	0
1	B	954/990 (96%)	-0.20	1 (0%) <b>95</b>   <b>96</b>	37, 55, 71, 90	0
All	All	1910/1980 (96%)	-0.24	1 (0%) <b>95</b>   <b>96</b>	32, 52, 69, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	984	PRO	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 monosaccharides 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, 95<sup>th</sup> 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.

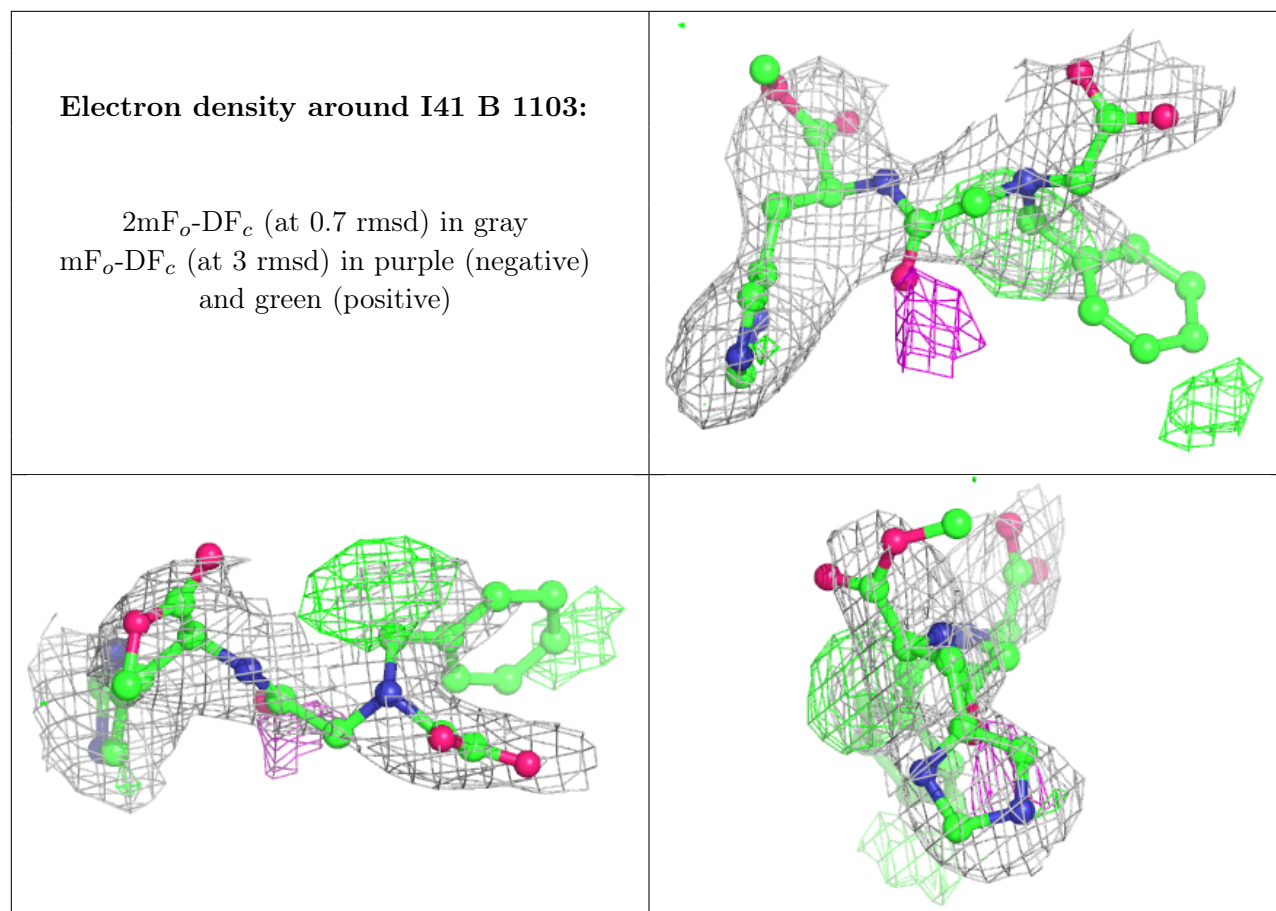
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	I41	B	1103	27/27	0.77	0.37	82,95,106,106	0
3	I41	A	1103	27/27	0.79	0.36	85,99,109,110	0
3	I41	A	1102	27/27	0.82	0.34	98,107,108,108	0
3	I41	B	1102	27/27	0.85	0.31	98,106,108,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	1101	1/1	0.99	0.13	57,57,57,57	0
2	ZN	B	1101	1/1	0.99	0.12	63,63,63,63	0

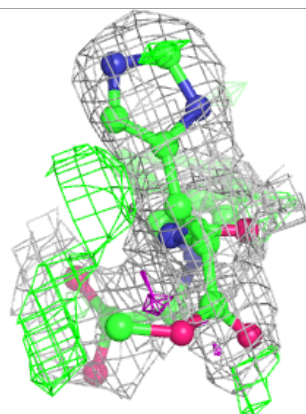
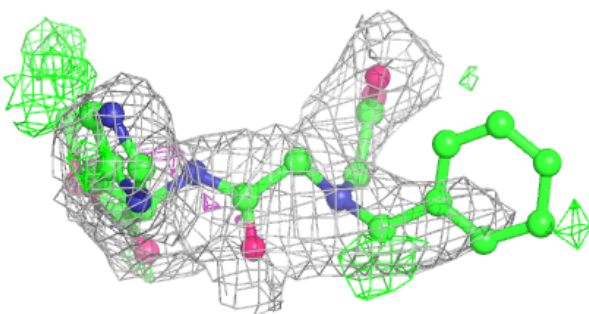
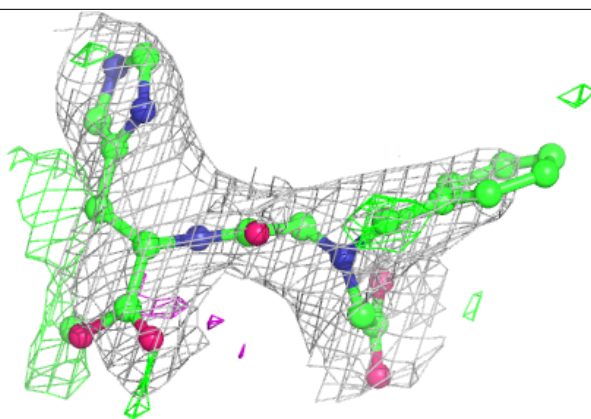
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



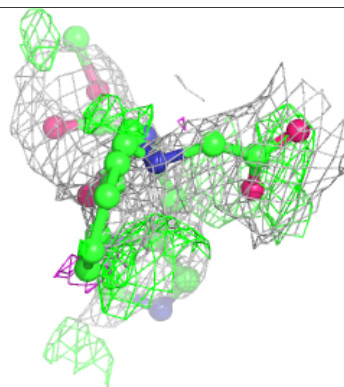
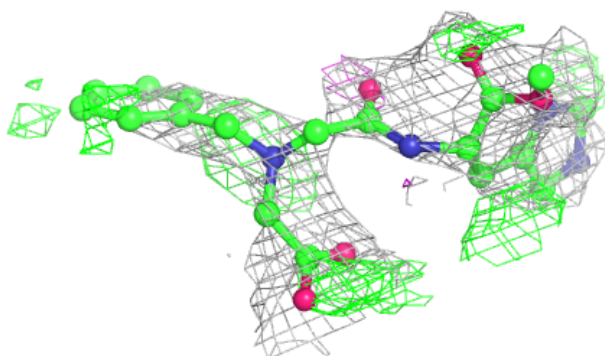
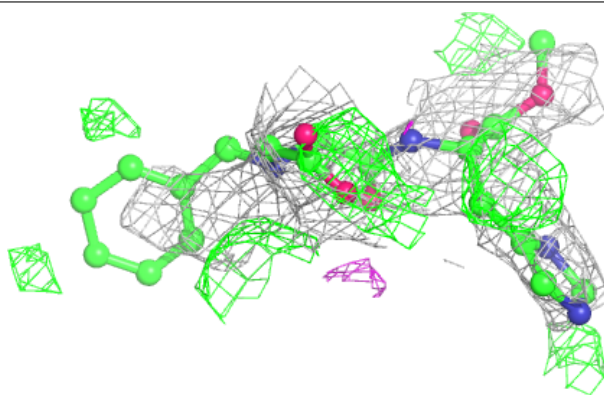


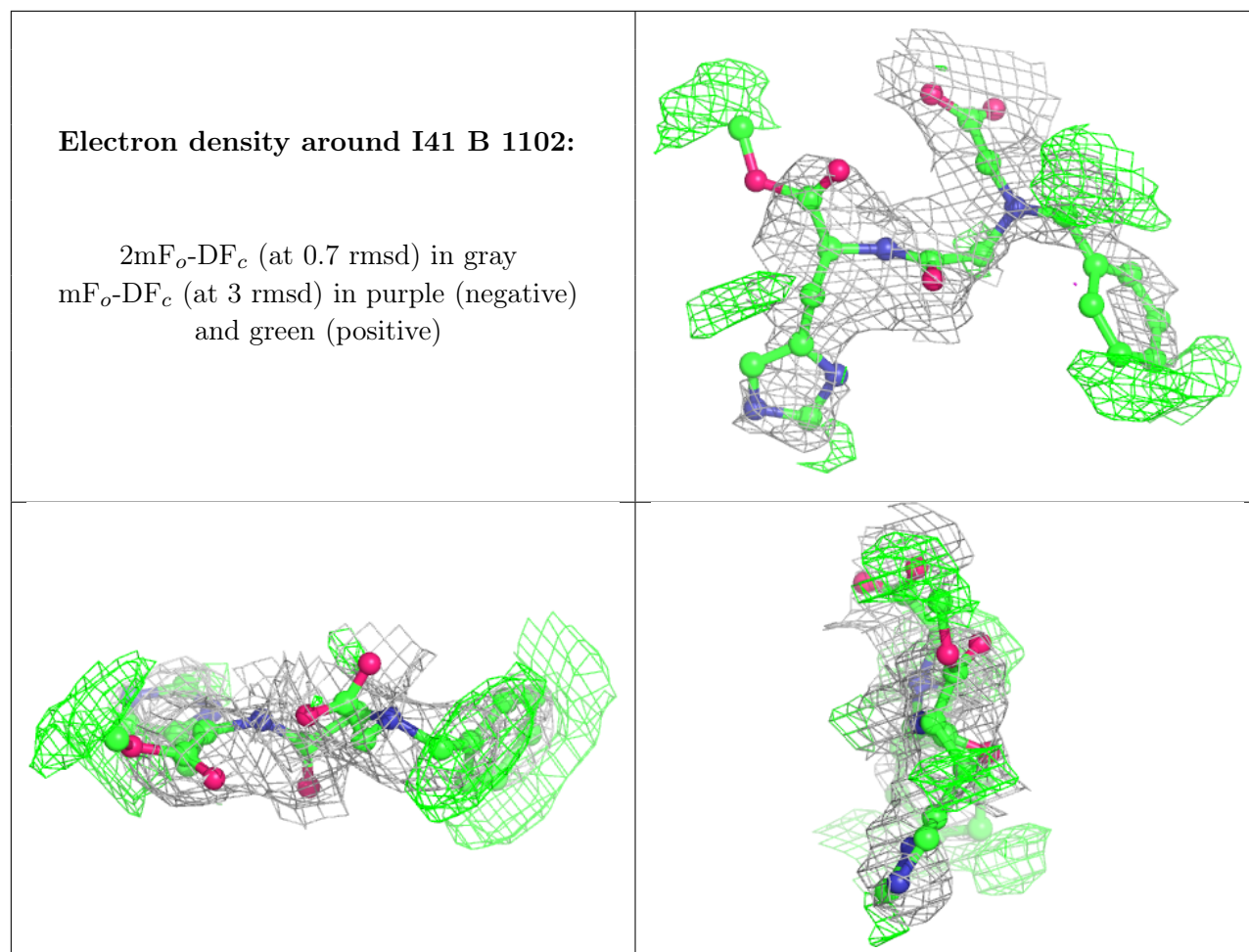
**Electron density around I41 A 1103:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.