



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:51 AM UTC

PDB ID : 4DTT / pdb_00004dtt
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

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

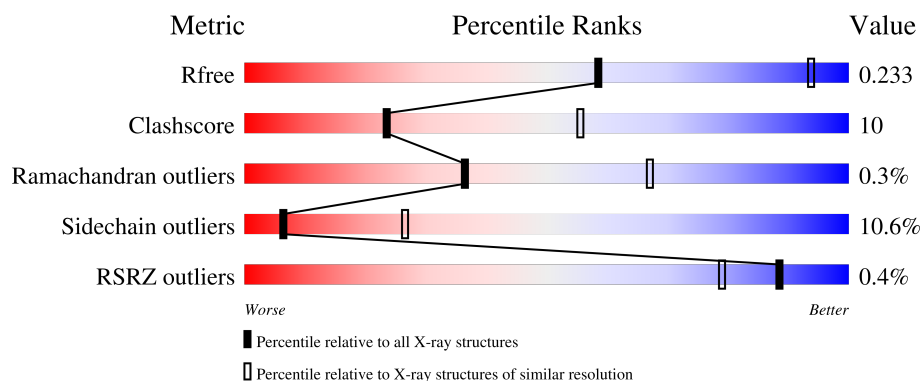
1 Overall quality at a glance

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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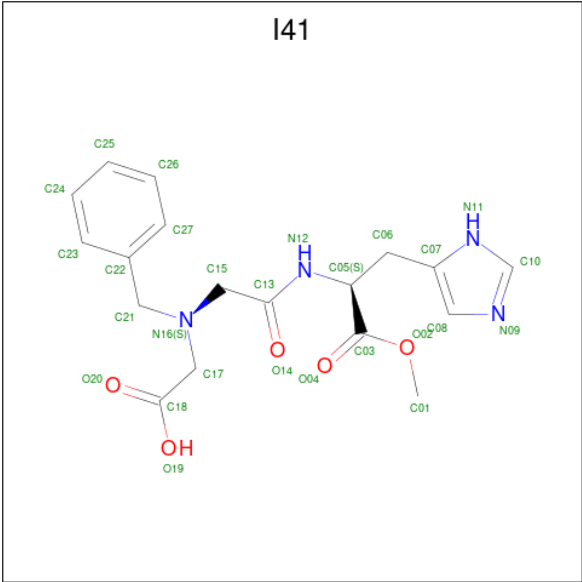
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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression 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		

SER	ASN	PRO	VAL	VAL	GLY	GLU	PHE	PRO	ALA	GLN	ASN	ASP	ILE	ASN	L980	L986	I992	Q993	N994	M995	R1000	L1004	P1010	H1011	ILE	ASN	PHE	MET	ALA	ALA	LYS	LEU												
Q844	G845	I850	Q851	Q853	S852	E853	K854	L859	E864	L867	M870	I874	E875	D876	M877	E880	A881	K884	I891	R892	K896	P897	K898	K899	L900	S901	Q914	Q915	R920	T923	E924	T932	I936	I937	K938	K941	E942	L959	A960	R961	E962	M963	D964	
G626	M627	N635	Q638	L641	I645	E646	E647	E653	I654	D655	E656	K657	R658	I662	K663	E664	S669	L670	R671	N672	E676	Q677	P678	H679	M680	L686	M690	V693	A694	W695	E699	V707	T708	L709	F710	R711	F715	I716	P717	R722	L723			
G731	N732	I733	I741	M742	Q743	R744	V745	E746	I750	T755	K756	Y766	D773	R774	Q780	H786	N787	N788	E792	I793	Y794	T797	D798	M799	Q680	M683	L686	M690	V693	E598	L599	L600	L604	Y609	A610	A611	E612	L616	L620	T623	I624	Y625		
K511	K512	W513	Q514	N515	A516	K523	L524	K527	I531	N534	T545	L550	I551	T554	A555	M556	S557	K558	L559	W560	D564	N573	F578	Y584	V585	D586	P587	L588	L597	E598	L599	L600	L604	Y609	A610	A611	E612	L616	L620	T623	I624	Y625		
E413	D416	L417	N418	A419	A420	F422	R423	F424	K425	E428	H442	Y443	Y444	P445	L446	L450	T451	A452	S453	Y454	E458	F459	R460	I464	E465	M466	V467	D469	R472	N475	V476	A479	T489	D490	R491	T492	E493	E494	T498	Q499	Y500	K501	Q502	I510
N282	L285	P286	E287	E290	H291	Q294	H297	L298	K299	Q300	D309	I310	R311	Y314	F317	P318	Y325	Y326	K327	H336	L337	L347	S348	E349	S352	K353	G354	V355	V356	L359	K364	A367	R368	G369	F370	M371	F372	L379	I391	M394	F395	Q396		
D152	H155	G160	D163	R164	S171	P172	L173	F174	D175	K179	D180	R181	N184	N193	V194	M195	N196	D197	A198	W199	R200	L201	F202	E205	K206	N210	K223	Q232	D236	V237	R238	Q239	S251	L259	G260	R261	V271	L274	E277	N280	K281			
MET	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	GLY	ILE	PRO	MET	N43	I50	G51	N52	H53	P58	E59	D60	K61	R62	L67	I73	L77	D80	D84	A88	A89	L90	D91	V92	H93	I94	D99	E111	K119	A135	G136	N139	A140	S143	Y150	F151

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

5.1 Standard geometry

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

All (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
1	B	500	TYR	N-CA-C	6.55	116.92	108.34
1	B	155	HIS	N-CA-C	6.13	120.31	112.34
1	A	495	TRP	N-CA-C	5.98	117.88	111.36
1	B	854	LYS	CA-C-N	5.93	126.49	120.38
1	B	854	LYS	C-N-CA	5.93	126.49	120.38
1	A	94	ILE	N-CA-C	-5.84	100.64	108.35
1	A	57	SER	CA-C-N	-5.83	114.89	120.83
1	A	57	SER	C-N-CA	-5.83	114.89	120.83
1	A	94	ILE	CB-CA-C	-5.76	100.65	111.30
1	A	222	ASN	N-CA-C	5.73	115.67	108.45
1	B	197	ASP	N-CA-C	5.71	118.28	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	VAL	CB-CA-C	-5.66	103.23	110.98
1	A	353	LYS	N-CA-C	-5.56	106.08	112.92
1	B	99	ASP	CA-C-N	-5.38	115.73	119.66
1	B	99	ASP	C-N-CA	-5.38	115.73	119.66
1	A	370	PHE	N-CA-C	5.36	117.40	108.99
1	A	988	GLN	CB-CA-C	5.34	116.29	110.15
1	A	773	ASP	CB-CA-C	-5.33	100.87	109.72
1	B	557	SER	N-CA-C	5.31	116.48	108.46
1	B	551	ILE	N-CA-C	5.28	118.06	112.83
1	A	296	GLU	CB-CA-C	5.26	118.86	109.29
1	B	715	PHE	N-CA-C	5.23	116.67	111.07
1	A	568	PHE	N-CA-C	5.22	118.65	111.54
1	B	420	VAL	CB-CA-C	-5.21	105.38	111.94
1	B	896	LYS	CA-C-N	5.20	125.45	119.83
1	B	896	LYS	C-N-CA	5.20	125.45	119.83
1	B	699	GLU	N-CA-C	-5.15	105.56	111.07
1	A	948	ALA	CA-C-N	5.10	124.55	119.24
1	A	948	ALA	C-N-CA	5.10	124.55	119.24
1	B	210	ASN	CA-C-N	-5.09	114.54	120.04
1	B	210	ASN	C-N-CA	-5.09	114.54	120.04
1	B	654	ILE	N-CA-C	5.08	116.57	109.55
1	A	771	LEU	CA-C-N	5.07	125.34	119.92
1	A	771	LEU	C-N-CA	5.07	125.34	119.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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:A:557:SER:HB2	1:A:742:MET:HE2	1.65	0.78
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
1:B:352:SER:C	1:B:354:GLY:H	1.95	0.74
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:559:LEU:HB2	1:B:742:MET:HE2	1.79	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:B:960:ALA:C	1:B:962:GLU:N	2.58	0.59
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:A:196:ASN:HD21	1:A:199:TRP:CD1	2.19	0.58
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.51	0.58
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:B:815:ILE:HG22	1:B:870:MET:HE2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:352:SER:C	1:B:354:GLY:N	2.60	0.56
1:A:843:ILE:HG22	1:A:844:GLN:N	2.20	0.55
1:A:466:MET:HE2	1:A:467:VAL:HA	1.89	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:B:259:LEU:HD23	1:B:259:LEU:C	2.32	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:960:ALA:C	1:B:962:GLU:H	2.15	0.54
1:A:534:ASN:C	1:A:534:ASN:OD1	2.49	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:196:ASN:C	1:B:196:ASN:OD1	2.50	0.53
1:B:557:SER:HB2	1:B:742:MET:HE3	1.91	0.53
1:B:294:GLN:H	1:B:297:HIS:HD2	1.57	0.53
1:B:960:ALA:O	1:B:961:ARG:C	2.52	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:236:ASP:OD1	1:B:236:ASP:C	2.53	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:556:MET:HE3	1:B:750:ILE:HD11	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:A:801:SER:O	1:A:802:THR:C	2.55	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:A:459:PHE:CE2	1:A:461:PRO:HD3	2.48	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:A:248:TYR:C	1:A:250:SER:H	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:988:GLN:HE21	1:A:988:GLN:C	2.22	0.47
1:B:874:ILE:O	1:B:875:GLU:C	2.58	0.47
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.63	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: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:227:GLU:O	1:A:228:THR:C	2.57	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:815:ILE:HG22	1:A:870:MET:HE2	1.97	0.46
1:B:959:LEU:HD22	1:B:963:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:489:THR:HB	1:B:500:TYR:O	2.16	0.46
1:A:178:ALA:O	1:A:179:LYS:C	2.59	0.45
1:A:490:ASP:OD1	1:A:490:ASP:C	2.58	0.45
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: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:B:311:ARG:HH22	1:B:664:GLU:CD	2.26	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:B:280:ASN:C	1:B:282:ASN:H	2.25	0.44
1:B:959:LEU:HB3	1:B:963:MET:HE2	1.99	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:359:LEU:C	1:A:359:LEU:HD23	2.43	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:B:467:VAL:C	1:B:469:ASP:H	2.25	0.44
1:B:584:TYR:O	1:B:585:VAL:C	2.59	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:294:GLN:C	1:A:296:GLU:H	2.26	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:B:938:LYS:HB3	1:B:938:LYS:HZ2	1.83	0.43
1:A:231:ASN:HD22	1:A:231:ASN:HA	1.57	0.43
1:B:174:PHE:O	1:B:175:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:LEU:HD22	1:B:742:MET:HG2	1.99	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:467:VAL:C	1:B:469:ASP:N	2.77	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:B:798:ASP:CG	1:B:799:MET:H	2.27	0.43
1:A:214:PRO:O	1:A:217:LYS:HD2	2.18	0.43
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:B:359:LEU:C	1:B:359:LEU:HD23	2.44	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:B:291:HIS:CD2	1:B:370:PHE:HB2	2.54	0.43
1:A:113:MET:HE3	1:A:113:MET:HB3	1.87	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:A:248:TYR:C	1:A:250:SER:N	2.78	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:A:378:ASP:OD1	1:A:378:ASP:C	2.63	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:374:ILE:HD12	1:A:374:ILE:C	2.44	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:237:VAL:O	1:A:238:ARG:C	2.60	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:A:151:PHE:CD1	1:A:151:PHE:C	2.97	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:52:ASN:CG	1:B:52:ASN:O	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:HD2	1:B:475:ASN:O	2.19	0.42
1:B:690:MET:HE2	1:B:794:TYR:HE2	1.84	0.42
1:A:54:ILE:H	1:A:54:ILE:HG12	1.52	0.42
1:A:584:TYR:O	1:A:585:VAL:C	2.62	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:A:526:THR:O	1:A:527:LYS:C	2.63	0.41
1:B:993:GLN:HE21	1:B:993:GLN:HB2	1.73	0.41
1:A:925:VAL:O	1:A:926:ALA:C	2.63	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:110:LEU:C	1:A:110:LEU:HD23	2.45	0.41
1:A:197:ASP:HA	1:A:200:ARG:HD3	2.01	0.41
1:B:280:ASN:C	1:B:282:ASN:N	2.78	0.41
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.92	0.41
1:A:76:LEU:HB3	1:A:257:VAL:HG13	2.02	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: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:609:TYR:O	1:B:610:ALA:C	2.64	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:387:VAL:O	1:A:388:GLU:C	2.62	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%)	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

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%)	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

All (177) 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	114	LEU
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	239	GLN
1	A	273	LYS
1	A	277	GLU
1	A	281	LYS
1	A	282	ASN
1	A	290	GLU
1	A	295	GLU
1	A	296	GLU
1	A	301	LEU
1	A	308	LYS
1	A	312	ASN
1	A	313	LEU
1	A	316	THR
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	498	THR
1	A	499	GLN
1	A	512	LYS
1	A	518	LEU
1	A	521	LYS
1	A	523	LYS

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Mol	Chain	Res	Type
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	562	LYS
1	A	588	LEU
1	A	603	SER
1	A	624	ILE
1	A	642	LEU
1	A	644	LYS
1	A	653	GLU
1	A	662	ILE
1	A	683	MET
1	A	702	GLU
1	A	713	LYS
1	A	719	LEU
1	A	722	ARG
1	A	723	LEU
1	A	734	THR
1	A	774	ARG
1	A	803	SER
1	A	849	ILE
1	A	853	GLU
1	A	854	LYS
1	A	863	VAL
1	A	878	THR
1	A	886	ILE
1	A	900	LEU
1	A	906	LYS
1	A	914	GLN
1	A	915	GLN
1	A	922	ASN
1	A	923	THR
1	A	937	ILE
1	A	942	GLU
1	A	946	VAL
1	A	954	VAL
1	A	962	GLU
1	A	963	MET
1	A	980	LEU

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Mol	Chain	Res	Type
1	A	988	GLN
1	A	1009	LYS
1	A	1011	HIS
1	B	60	ASP
1	B	67	LEU
1	B	84	ASP
1	B	94	ILE
1	B	111	GLU
1	B	119	LYS
1	B	143	SER
1	B	171	SER
1	B	173	LEU
1	B	179	LYS
1	B	193	ASN
1	B	205	GLU
1	B	232	GLN
1	B	239	GLN
1	B	261	ARG
1	B	277	GLU
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	425	LYS
1	B	446	LEU
1	B	450	LEU
1	B	458	GLU
1	B	464	ILE
1	B	466	MET
1	B	476	VAL
1	B	491	ARG
1	B	492	THR
1	B	494	GLU
1	B	512	LYS
1	B	523	LYS
1	B	524	LEU
1	B	531	ILE

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Mol	Chain	Res	Type
1	B	534	ASN
1	B	545	THR
1	B	554	THR
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	647	GLU
1	B	653	GLU
1	B	669	SER
1	B	677	GLN
1	B	678	PRO
1	B	680	GLN
1	B	711	ARG
1	B	733	ILE
1	B	741	ILE
1	B	744	MET
1	B	746	GLU
1	B	750	ILE
1	B	780	GLN
1	B	788	ASN
1	B	797	THR
1	B	809	GLU
1	B	822	THR
1	B	825	THR
1	B	832	ILE
1	B	838	ARG
1	B	841	ASN
1	B	875	GLU
1	B	876	ASP
1	B	877	MET
1	B	880	GLU
1	B	891	ILE
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	980	LEU
1	B	993	GLN
1	B	995	MET
1	B	1011	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) 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	203	GLN
1	A	231	ASN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	312	ASN
1	A	329	ASN
1	A	332	HIS
1	A	399	GLN
1	A	407	GLN
1	A	573	ASN
1	A	635	ASN
1	A	672	ASN
1	A	724	HIS
1	A	730	HIS
1	A	781	GLN
1	A	914	GLN
1	A	988	GLN
1	B	93	HIS
1	B	129	GLN
1	B	134	HIS
1	B	139	ASN
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	231	ASN
1	B	239	GLN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	312	ASN
1	B	332	HIS
1	B	336	HIS
1	B	386	HIS
1	B	442	HIS
1	B	499	GLN
1	B	672	ASN
1	B	677	GLN
1	B	730	HIS
1	B	732	ASN
1	B	851	GLN
1	B	914	GLN
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 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

All (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
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
3	B	1102	I41	O02-C03	6.22	1.48	1.33
3	B	1102	I41	C24-C23	6.19	1.49	1.38
3	B	1103	I41	O02-C03	5.91	1.47	1.33
3	A	1102	I41	O02-C03	5.75	1.47	1.33
3	B	1103	I41	C24-C23	5.69	1.48	1.38
3	A	1103	I41	C24-C23	5.60	1.48	1.38
3	A	1102	I41	C24-C23	5.35	1.48	1.38
3	B	1103	I41	C25-C24	4.89	1.49	1.38
3	B	1102	I41	C25-C24	4.68	1.48	1.38
3	A	1103	I41	C25-C24	4.42	1.48	1.38
3	A	1102	I41	C25-C24	4.34	1.47	1.38
3	B	1102	I41	C10-N09	3.34	1.46	1.32
3	A	1102	I41	C10-N09	3.25	1.46	1.32
3	B	1103	I41	C10-N09	3.12	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	I41	C10-N09	3.10	1.45	1.32
3	A	1102	I41	C06-C07	2.89	1.54	1.49
3	A	1103	I41	C26-C25	2.84	1.44	1.38
3	B	1103	I41	C08-C07	2.64	1.41	1.35
3	B	1102	I41	C05-N12	2.63	1.51	1.45
3	A	1103	I41	C26-C27	2.58	1.43	1.38
3	B	1102	I41	C06-C07	2.47	1.53	1.49
3	A	1102	I41	C08-C07	2.35	1.40	1.35
3	B	1103	I41	C06-C07	2.33	1.53	1.49
3	B	1102	I41	C08-C07	2.23	1.40	1.35
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	2.19	1.51	1.47
3	B	1102	I41	C23-C22	2.13	1.43	1.38
3	B	1102	I41	C26-C27	2.11	1.42	1.38
3	A	1103	I41	O20-C18	2.05	1.28	1.22
3	A	1102	I41	C17-C18	2.03	1.55	1.51

All (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
3	A	1103	I41	C22-C21-N16	5.75	124.92	113.15
3	A	1103	I41	C13-C15-N16	-5.71	100.14	113.41
3	B	1102	I41	C25-C24-C23	-5.45	113.51	120.24
3	A	1103	I41	O02-C03-C05	5.14	124.56	111.49
3	A	1102	I41	C21-N16-C15	-5.08	101.55	111.77
3	B	1103	I41	O02-C03-C05	4.98	124.17	111.49
3	B	1102	I41	C13-C15-N16	4.42	123.68	113.41
3	B	1102	I41	O02-C03-C05	4.40	122.69	111.49
3	A	1103	I41	O02-C03-O04	-4.37	115.34	123.85
3	A	1103	I41	C08-C07-N11	4.22	110.64	105.65
3	A	1102	I41	O02-C03-C05	4.16	122.07	111.49
3	B	1103	I41	C01-O02-C03	4.08	125.17	115.92
3	A	1103	I41	C25-C24-C23	-4.00	115.30	120.24
3	B	1102	I41	C01-O02-C03	3.94	124.86	115.92
3	A	1102	I41	C22-C21-N16	3.94	121.21	113.15
3	A	1102	I41	N11-C10-N09	-3.56	104.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	I41	O02-C03-O04	-3.56	116.92	123.85
3	B	1103	I41	C05-C06-C07	3.50	119.19	113.27
3	B	1103	I41	C17-N16-C15	-3.49	103.48	111.66
3	B	1102	I41	C22-C21-N16	3.37	120.04	113.15
3	A	1103	I41	C01-O02-C03	3.37	123.56	115.92
3	A	1103	I41	O14-C13-C15	-3.32	115.20	121.02
3	B	1102	I41	O02-C03-O04	-3.24	117.54	123.85
3	B	1103	I41	O02-C03-O04	-3.22	117.58	123.85
3	B	1102	I41	N11-C10-N09	-3.19	105.09	111.00
3	B	1103	I41	C25-C24-C23	-3.14	116.37	120.24
3	A	1103	I41	C21-N16-C17	3.06	117.93	111.77
3	A	1102	I41	C18-C17-N16	3.01	123.32	113.77
3	B	1103	I41	C08-C07-N11	2.92	109.10	105.65
3	B	1102	I41	C24-C23-C22	2.91	124.70	120.61
3	B	1103	I41	C21-N16-C17	2.88	117.56	111.77
3	A	1102	I41	C13-C15-N16	2.82	119.97	113.41
3	A	1103	I41	C24-C23-C22	2.77	124.51	120.61
3	A	1103	I41	C21-C22-C27	2.51	125.37	120.75
3	A	1103	I41	C21-N16-C15	2.42	116.64	111.77
3	A	1102	I41	O19-C18-O20	-2.37	117.24	123.33
3	B	1103	I41	C03-C05-N12	-2.36	105.20	110.65
3	A	1103	I41	C21-C22-C23	-2.36	116.40	120.75
3	A	1102	I41	C06-C07-N11	2.34	129.51	123.22
3	A	1103	I41	N11-C10-N09	-2.30	106.75	111.00
3	A	1103	I41	O19-C18-C17	2.29	122.43	113.38
3	A	1102	I41	O14-C13-N12	2.28	126.81	122.95
3	B	1102	I41	C21-N16-C15	2.27	116.33	111.77
3	A	1103	I41	C18-C17-N16	2.26	120.94	113.77
3	A	1103	I41	C15-C13-N12	2.23	121.17	115.70
3	B	1102	I41	C08-C07-N11	2.18	108.23	105.65
3	B	1102	I41	O19-C18-C17	2.03	121.37	113.38

There are no chirality outliers.

All (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
3	B	1102	I41	C13-C15-N16-C17

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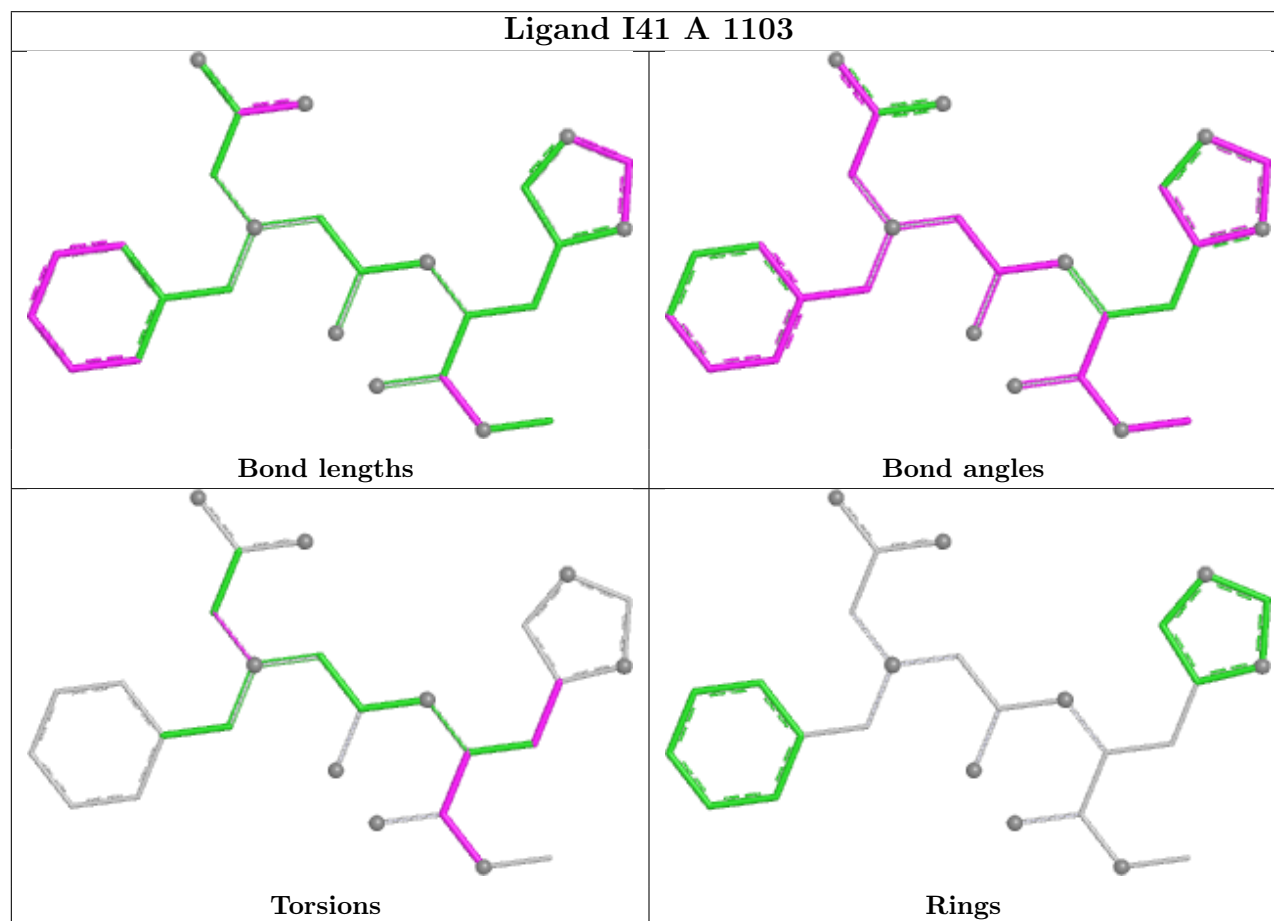
Mol	Chain	Res	Type	Atoms
3	B	1103	I41	N12-C05-C06-C07
3	B	1103	I41	C13-C15-N16-C21
3	B	1103	I41	C22-C21-N16-C17
3	B	1103	I41	O04-C03-O02-C01
3	A	1103	I41	O04-C03-O02-C01
3	A	1103	I41	C05-C03-O02-C01
3	B	1102	I41	C06-C05-N12-C13
3	B	1103	I41	C05-C03-O02-C01
3	A	1102	I41	O04-C03-O02-C01
3	B	1102	I41	C05-C03-O02-C01
3	B	1102	I41	O04-C03-O02-C01
3	A	1103	I41	C18-C17-N16-C15
3	B	1103	I41	C22-C21-N16-C15
3	B	1102	I41	C22-C21-N16-C15
3	B	1102	I41	O14-C13-C15-N16
3	B	1103	I41	O02-C03-C05-N12
3	B	1102	I41	C03-C05-C06-C07
3	A	1102	I41	C22-C21-N16-C17
3	B	1102	I41	N12-C13-C15-N16
3	A	1103	I41	O02-C03-C05-N12
3	A	1102	I41	C18-C17-N16-C21
3	A	1103	I41	O02-C03-C05-C06
3	A	1103	I41	O04-C03-C05-N12
3	B	1103	I41	O04-C03-C05-N12
3	B	1103	I41	O02-C03-C05-C06
3	A	1102	I41	N12-C13-C15-N16
3	B	1103	I41	O04-C03-C05-C06
3	A	1103	I41	O04-C03-C05-C06
3	B	1103	I41	C18-C17-N16-C21
3	A	1102	I41	O14-C13-C15-N16
3	B	1103	I41	O14-C13-C15-N16
3	B	1103	I41	N12-C13-C15-N16
3	B	1102	I41	C18-C17-N16-C21
3	B	1103	I41	C18-C17-N16-C15
3	A	1103	I41	C05-C06-C07-N11
3	A	1103	I41	C05-C06-C07-C08
3	B	1103	I41	C05-C06-C07-N11
3	B	1103	I41	C03-C05-C06-C07
3	B	1103	I41	C05-C06-C07-C08
3	A	1102	I41	C22-C21-N16-C15

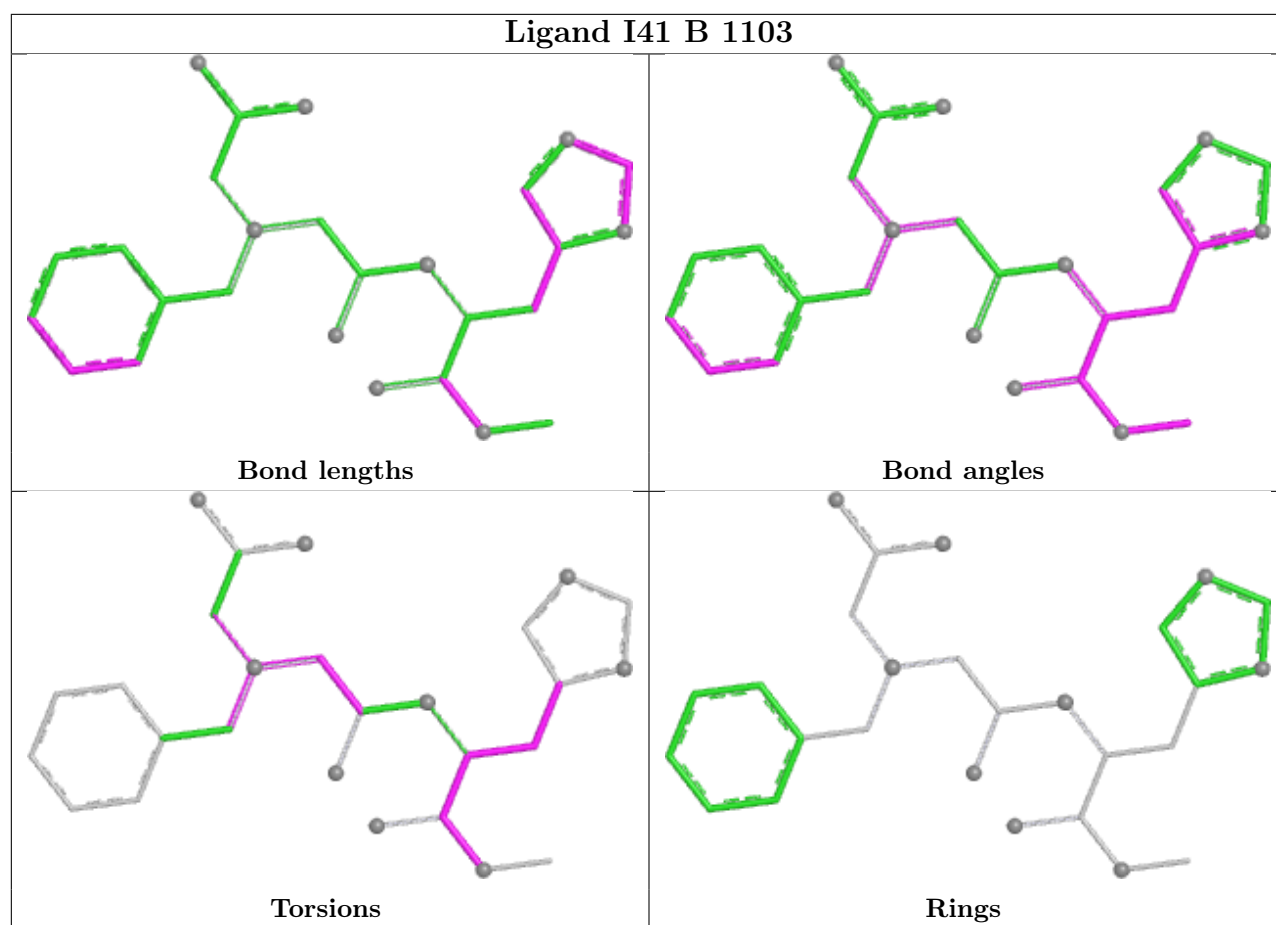
There are no ring outliers.

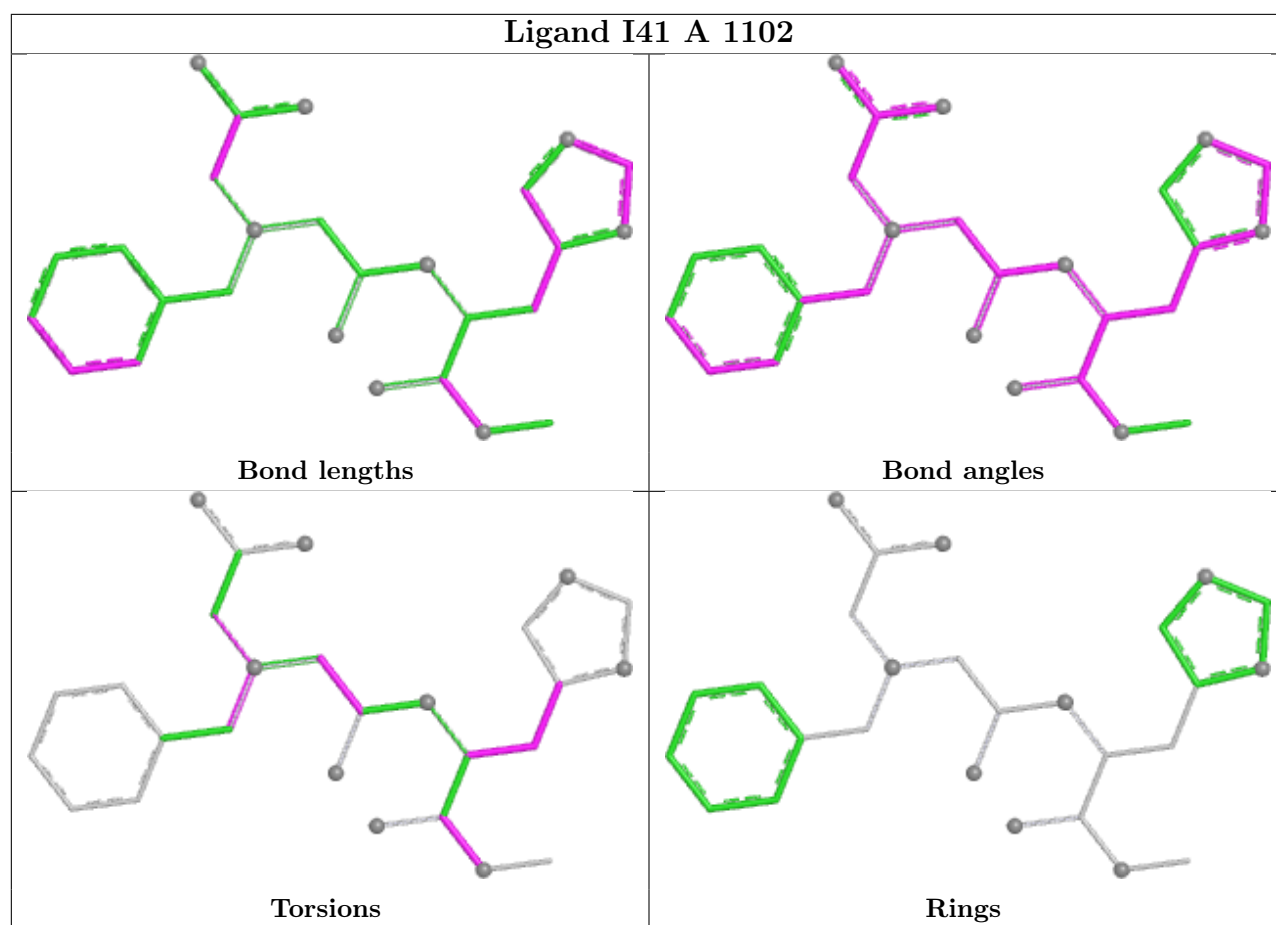
4 monomers are involved in 15 short contacts:

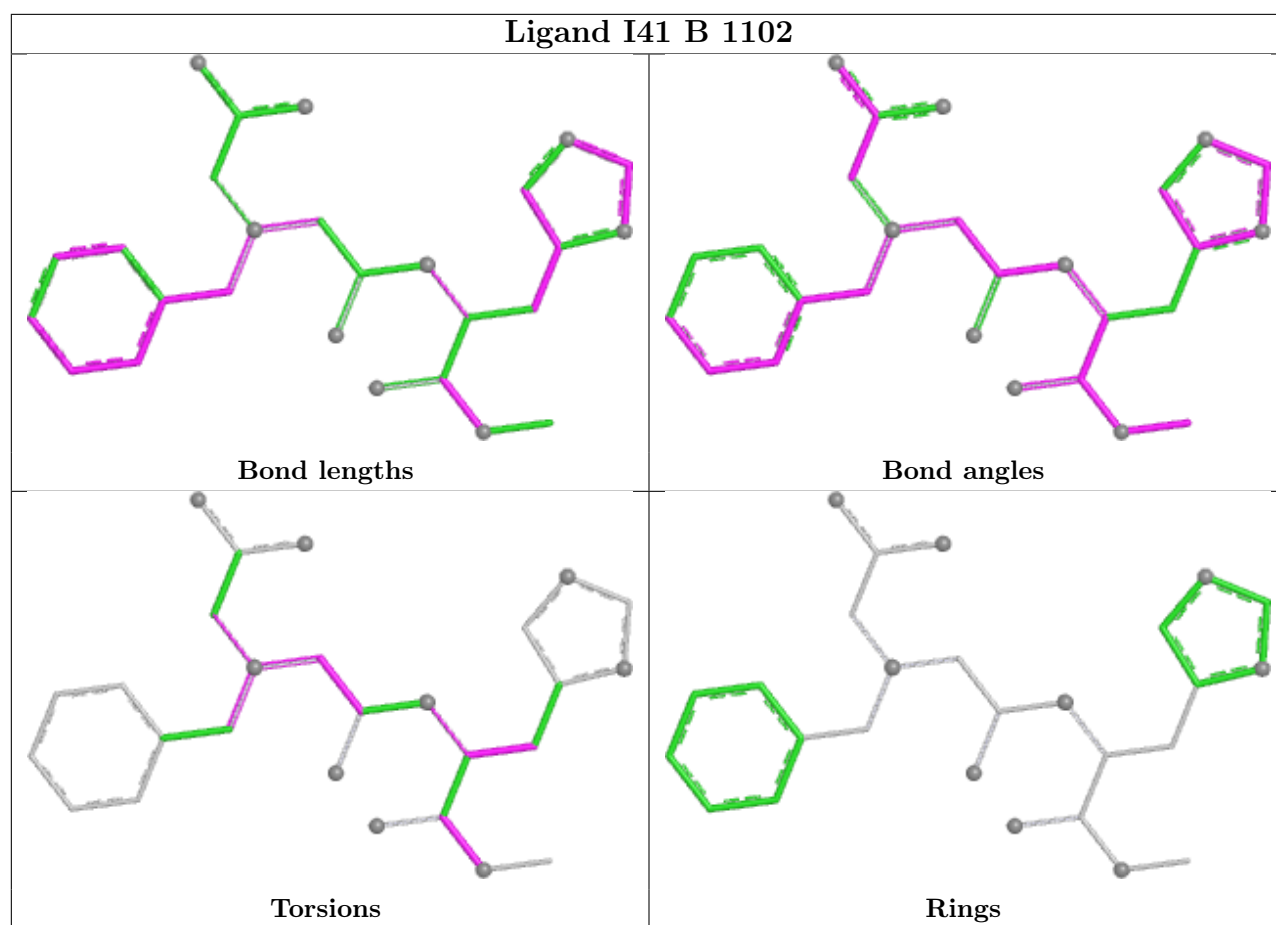
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	I41	6	0
3	B	1103	I41	5	0
3	A	1102	I41	1	0
3	B	1102	I41	3	0

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

All (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
1	A	1011	HIS	2.5
1	A	978	ILE	2.4
1	B	53	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

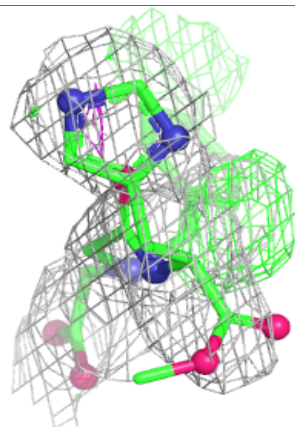
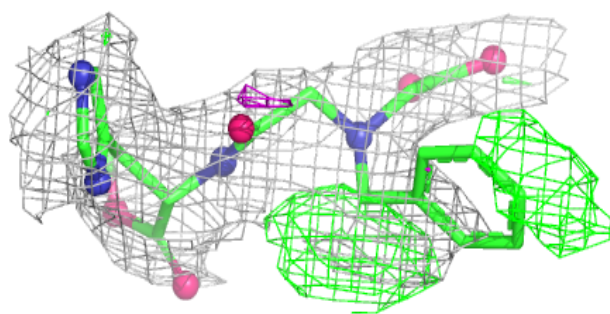
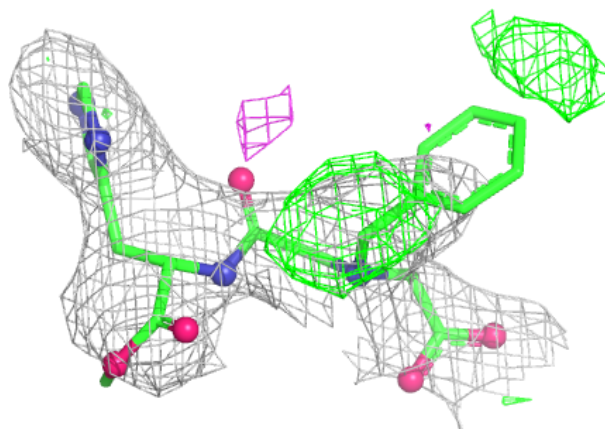
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.

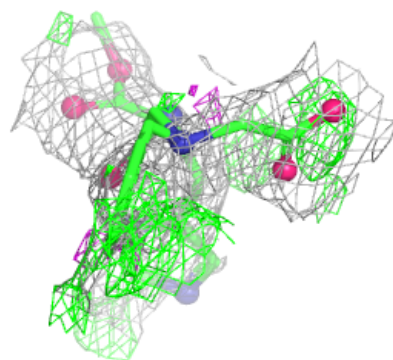
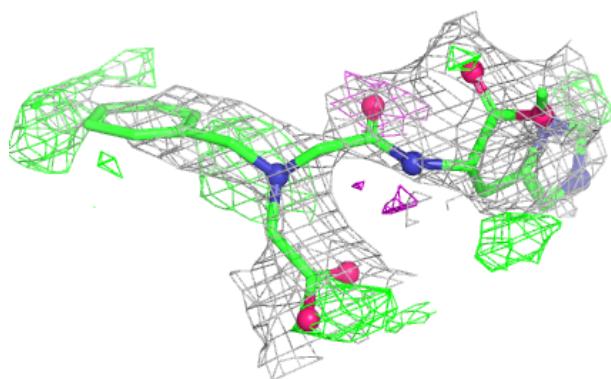
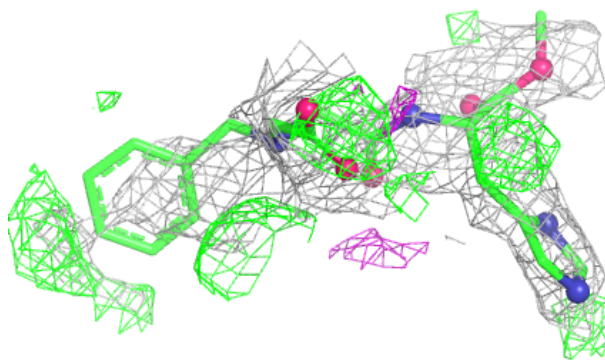
Electron density around I41 B 1103:

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



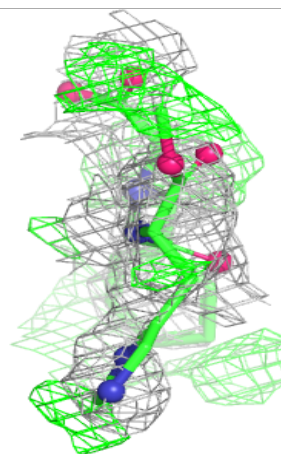
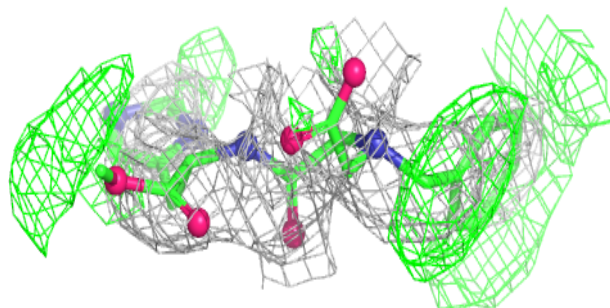
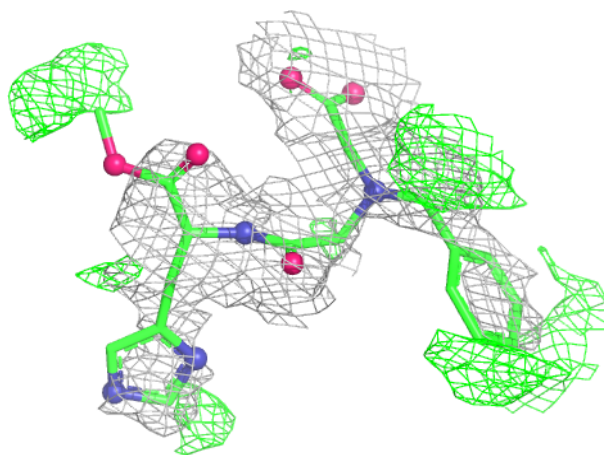
Electron density around I41 A 1102:

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



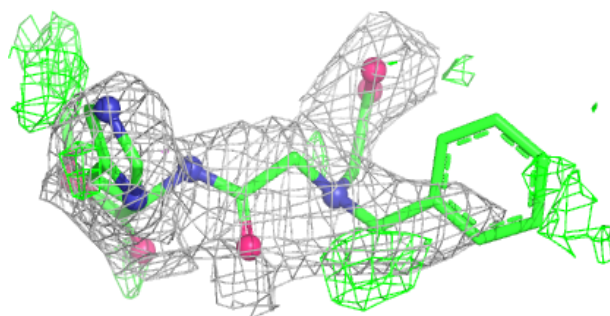
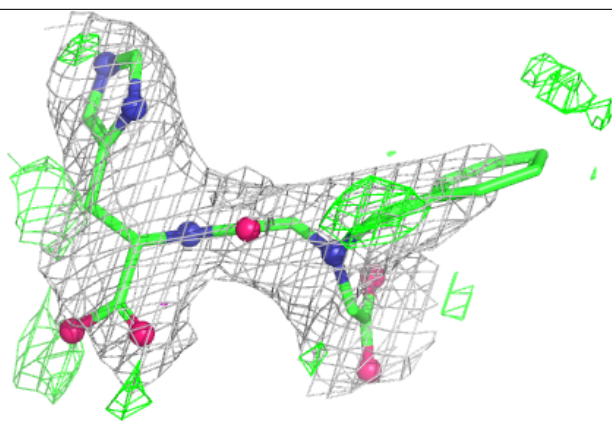
Electron density around I41 B 1102:

$2mF_o-DF_c$ (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.