



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2025 – 04:27 pm BST

PDB ID : 9Q9O / pdb_00009q9o
Title : TRIM21 PRYSPRY bound to compound 36
Authors : Luptak, J.
Deposited on : 2025-02-26
Resolution : 2.46 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

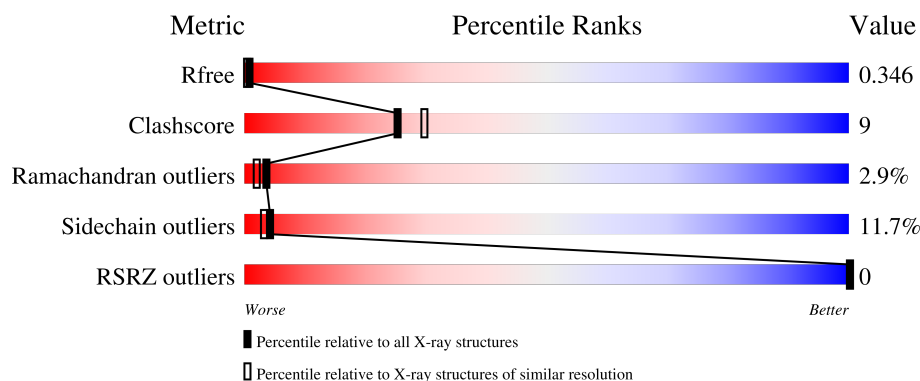
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	198	 67% 21% 5% 8%
1	B	198	 63% 28% 8%
1	C	198	 64% 26% 8%
1	D	198	 61% 27% 5% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11804 atoms, of which 5740 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 E3 ubiquitin-protein ligase TRIM21.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	183	Total	C	H	N	O	S	57	0	0
			2880	948	1403	256	266	7			
1	A	183	Total	C	H	N	O	S	57	0	0
			2880	948	1403	256	266	7			
1	C	183	Total	C	H	N	O	S	57	0	0
			2880	948	1403	256	266	7			
1	D	183	Total	C	H	N	O	S	57	0	0
			2880	948	1403	256	266	7			

There are 36 discrepancies between the modelled and reference sequences:

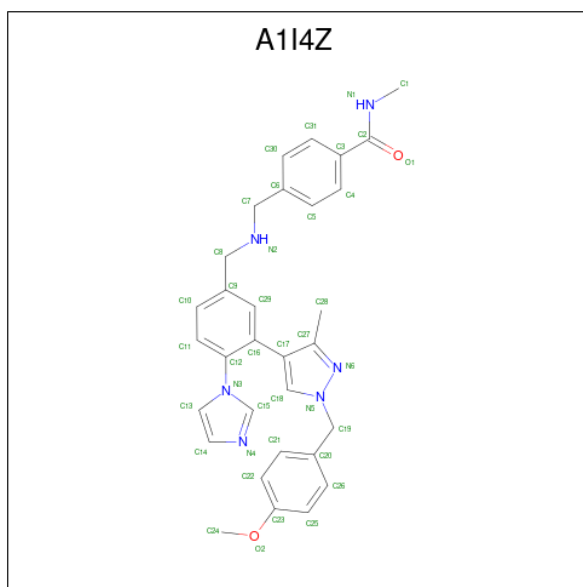
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	initiating methionine	UNP P19474
B	-4	ALA	-	expression tag	UNP P19474
B	-3	HIS	-	expression tag	UNP P19474
B	-2	HIS	-	expression tag	UNP P19474
B	-1	HIS	-	expression tag	UNP P19474
B	0	HIS	-	expression tag	UNP P19474
B	1	HIS	-	expression tag	UNP P19474
B	2	HIS	-	expression tag	UNP P19474
B	3	MET	-	expression tag	UNP P19474
A	-5	MET	-	initiating methionine	UNP P19474
A	-4	ALA	-	expression tag	UNP P19474
A	-3	HIS	-	expression tag	UNP P19474
A	-2	HIS	-	expression tag	UNP P19474
A	-1	HIS	-	expression tag	UNP P19474
A	0	HIS	-	expression tag	UNP P19474
A	1	HIS	-	expression tag	UNP P19474
A	2	HIS	-	expression tag	UNP P19474
A	3	MET	-	expression tag	UNP P19474
C	-5	MET	-	initiating methionine	UNP P19474
C	-4	ALA	-	expression tag	UNP P19474
C	-3	HIS	-	expression tag	UNP P19474

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP P19474
C	-1	HIS	-	expression tag	UNP P19474
C	0	HIS	-	expression tag	UNP P19474
C	1	HIS	-	expression tag	UNP P19474
C	2	HIS	-	expression tag	UNP P19474
C	3	MET	-	expression tag	UNP P19474
D	-5	MET	-	initiating methionine	UNP P19474
D	-4	ALA	-	expression tag	UNP P19474
D	-3	HIS	-	expression tag	UNP P19474
D	-2	HIS	-	expression tag	UNP P19474
D	-1	HIS	-	expression tag	UNP P19474
D	0	HIS	-	expression tag	UNP P19474
D	1	HIS	-	expression tag	UNP P19474
D	2	HIS	-	expression tag	UNP P19474
D	3	MET	-	expression tag	UNP P19474

- Molecule 2 is 4-[[[4-imidazol-1-yl-3-[1-[(4-methoxyphenyl)methyl]-3-methyl-pyrazol-4-yl]phenyl]methylamino]methyl]-N-methyl-benzamide (CCD ID: A1I4Z) (formula: C₃₁H₃₂N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			71	31	32	6	2		
2	A	1	Total	C	H	N	O	0	0
			71	31	32	6	2		
2	C	1	Total	C	H	N	O	0	0
			71	31	32	6	2		

Continued on next page...

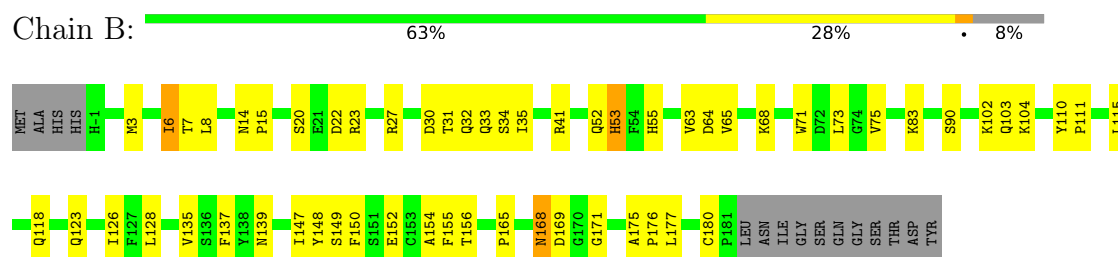
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	0	0
			71	31	32	6	2		

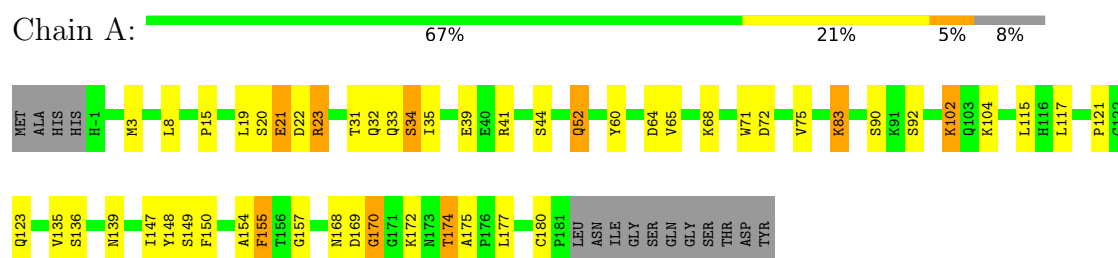
3 Residue-property plots [i](#)

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.

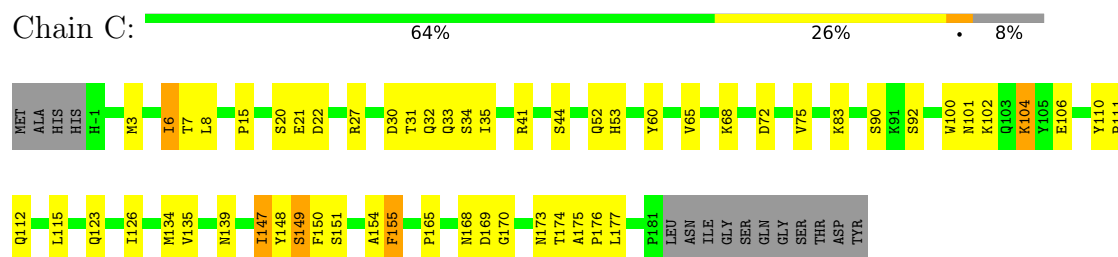
- Molecule 1: E3 ubiquitin-protein ligase TRIM21



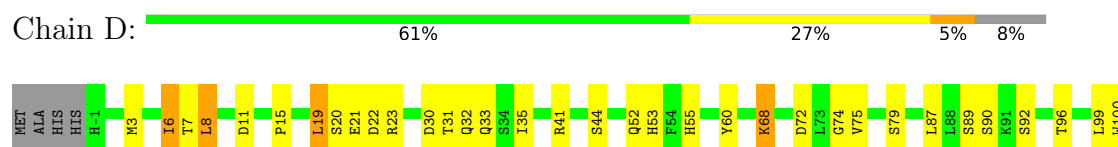
- Molecule 1: E3 ubiquitin-protein ligase TRIM21



- Molecule 1: E3 ubiquitin-protein ligase TRIM21



- Molecule 1: E3 ubiquitin-protein ligase TRIM21



N101	K102	Q103	K104	L115	H116	L117	Q123	V124	M134	V135	S136	N139	D142	H143	G144	S145	L146	I147	Y148	S149	E152	C153	A154	F155	S164	P165	M168	D169	G170	N173	T174	A175	F181	LEU	ASN	ILE	GLY	SER	GLN	GLY	SER	THR	ASP	TYR
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.69Å 74.38Å 90.11Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	50.43 – 2.46 50.43 – 2.46	Depositor EDS
% Data completeness (in resolution range)	83.5 (50.43-2.46) 78.1 (50.43-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.302 , 0.368 0.276 , 0.346	Depositor DCC
R_{free} test set	1243 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	1.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 18.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.063 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4218e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1I4Z

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.20	0/1530	1.42	5/2084 (0.2%)
1	B	1.21	0/1530	1.42	4/2084 (0.2%)
1	C	1.16	1/1530 (0.1%)	1.40	4/2084 (0.2%)
1	D	1.13	0/1530	1.40	3/2084 (0.1%)
All	All	1.18	1/6120 (0.0%)	1.41	16/8336 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	SER	C-O	-5.91	1.17	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	ILE	N-CA-C	-7.68	105.68	111.90
1	D	11	ASP	CA-CB-CG	6.63	119.23	112.60
1	D	30	ASP	CA-CB-CG	6.56	119.16	112.60
1	C	72	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	150	PHE	CA-C-O	-6.38	114.72	121.99
1	B	30	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	155	PHE	CA-CB-CG	6.15	119.95	113.80
1	A	72	ASP	CA-CB-CG	6.09	118.69	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	147	ILE	N-CA-C	-5.53	107.05	111.81
1	A	64	ASP	CA-C-O	-5.38	115.13	121.16
1	C	30	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	150	PHE	CA-C-O	-5.33	115.92	121.99
1	D	124	VAL	CA-C-O	-5.23	114.98	120.27
1	B	137	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	64	ASP	CA-C-O	-5.05	115.50	121.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1477	1403	1394	22	0
1	B	1477	1403	1394	21	1
1	C	1477	1403	1394	27	0
1	D	1477	1403	1394	35	1
2	A	39	32	0	1	0
2	B	39	32	0	1	0
2	C	39	32	0	2	0
2	D	39	32	0	3	0
All	All	6064	5740	5576	110	1

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 (110) 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:148:TYR:CD1	1:A:149:SER:N	2.59	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:VAL:HG12	1:C:177:LEU:CD2	2.22	0.70
1:B:68:LYS:HE3	1:B:175:ALA:O	1.94	0.68
1:C:68:LYS:HE3	1:C:175:ALA:O	1.95	0.65
1:B:7:THR:H	1:B:52:GLN:HE22	1.46	0.63
1:A:34:SER:O	1:A:35:ILE:HG23	1.97	0.63
1:B:148:TYR:CD1	1:B:149:SER:N	2.67	0.62
1:D:148:TYR:CD1	1:D:149:SER:N	2.69	0.61
1:C:65:VAL:HG12	1:C:177:LEU:HD23	1.82	0.61
1:B:7:THR:N	1:B:52:GLN:HE22	1.97	0.61
1:C:7:THR:N	1:C:52:GLN:HE22	2.01	0.58
1:C:148:TYR:CD1	1:C:149:SER:N	2.72	0.57
1:C:68:LYS:NZ	1:C:165:PRO:O	2.37	0.57
1:A:65:VAL:HG23	1:A:65:VAL:O	2.05	0.57
1:A:139:ASN:OD1	1:A:139:ASN:C	2.47	0.57
1:A:20:SER:OG	1:A:22:ASP:OD1	2.22	0.56
1:A:65:VAL:HG12	1:A:177:LEU:CD2	2.35	0.56
1:C:7:THR:H	1:C:52:GLN:HE22	1.53	0.55
1:C:35:ILE:HD12	1:C:41:ARG:CZ	2.36	0.55
1:B:20:SER:OG	1:B:22:ASP:OD1	2.23	0.55
1:C:168:ASN:O	1:C:170:GLY:N	2.40	0.55
1:B:6:ILE:HA	1:B:52:GLN:NE2	2.21	0.54
1:C:173:ASN:O	1:C:173:ASN:CG	2.51	0.54
1:D:19:LEU:HD12	1:D:19:LEU:N	2.23	0.54
1:A:168:ASN:O	1:A:170:GLY:N	2.38	0.53
1:D:168:ASN:ND2	1:D:174:THR:HG22	2.24	0.53
1:A:35:ILE:HD12	1:A:41:ARG:CZ	2.39	0.52
1:C:126:ILE:HD12	1:C:126:ILE:N	2.25	0.52
1:A:21:GLU:OE2	1:A:21:GLU:HA	2.09	0.52
1:A:117:LEU:HD23	1:A:121:PRO:HD3	1.90	0.52
1:C:6:ILE:HA	1:C:52:GLN:NE2	2.24	0.52
1:D:15:PRO:HG3	1:D:41:ARG:HD3	1.91	0.52
1:B:68:LYS:NZ	1:B:165:PRO:O	2.42	0.52
1:A:32:GLN:CG	1:A:33:GLN:H	2.23	0.51
1:A:168:ASN:HD21	1:A:174:THR:HG23	1.76	0.51
1:B:34:SER:O	1:B:35:ILE:HG23	2.11	0.51
1:C:168:ASN:HD21	1:C:174:THR:HG23	1.76	0.50
1:D:19:LEU:N	1:D:19:LEU:CD1	2.75	0.50
1:B:168:ASN:O	1:B:171:GLY:N	2.37	0.50
1:A:68:LYS:HE3	1:A:175:ALA:O	2.11	0.50
1:B:139:ASN:HB2	1:B:147:ILE:HD11	1.94	0.50
1:D:74:GLY:HA3	1:D:96:THR:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:CG	1:A:33:GLN:N	2.75	0.50
1:B:35:ILE:HD12	1:B:41:ARG:CZ	2.43	0.49
1:D:68:LYS:HE3	1:D:175:ALA:O	2.13	0.49
1:D:72:ASP:HB2	1:D:164:SER:HB3	1.94	0.49
1:C:104:LYS:HB3	1:C:104:LYS:NZ	2.27	0.49
1:D:6:ILE:HA	1:D:52:GLN:NE2	2.27	0.49
1:C:32:GLN:HG2	1:C:33:GLN:H	1.78	0.49
2:B:201:A1I4Z:C18	2:B:201:A1I4Z:C15	2.90	0.48
1:D:20:SER:OG	1:D:22:ASP:OD1	2.26	0.48
1:D:35:ILE:HD12	1:D:41:ARG:CZ	2.43	0.48
1:A:22:ASP:O	1:A:23:ARG:HB2	2.12	0.48
1:B:27:ARG:HB3	1:B:176:PRO:HB3	1.94	0.48
1:D:139:ASN:HB2	1:D:147:ILE:HD11	1.96	0.48
1:D:168:ASN:O	1:D:169:ASP:C	2.57	0.47
1:B:139:ASN:C	1:B:139:ASN:OD1	2.55	0.47
1:C:139:ASN:OD1	1:C:139:ASN:C	2.56	0.47
1:D:87:LEU:HD12	2:D:201:A1I4Z:C28	2.44	0.47
1:A:19:LEU:HD12	1:A:19:LEU:N	2.30	0.47
2:D:201:A1I4Z:C18	2:D:201:A1I4Z:C26	2.91	0.47
1:B:15:PRO:HG3	1:B:41:ARG:HD3	1.97	0.46
2:C:201:A1I4Z:C15	2:C:201:A1I4Z:C18	2.93	0.46
1:C:150:PHE:O	1:C:151:SER:HB3	2.15	0.46
1:D:7:THR:N	1:D:52:GLN:HE22	2.12	0.46
1:D:102:LYS:O	1:D:103:GLN:HB2	2.15	0.46
1:A:65:VAL:HG12	1:A:177:LEU:HD23	1.98	0.46
1:D:68:LYS:NZ	1:D:165:PRO:O	2.48	0.46
1:B:65:VAL:HG12	1:B:177:LEU:CD2	2.46	0.46
1:D:168:ASN:OD1	1:D:168:ASN:N	2.49	0.45
1:C:34:SER:O	1:C:35:ILE:HG23	2.16	0.45
1:C:15:PRO:HG3	1:C:41:ARG:HD3	1.98	0.45
1:D:101:ASN:O	1:D:102:LYS:O	2.33	0.45
1:D:8:LEU:HD22	1:D:23:ARG:O	2.17	0.45
1:D:100:TRP:O	1:D:104:LYS:HB2	2.17	0.45
1:D:115:LEU:HB3	1:D:117:LEU:HD13	1.97	0.45
1:D:7:THR:H	1:D:52:GLN:HE22	1.64	0.45
1:C:100:TRP:O	1:C:101:ASN:HB3	2.18	0.44
1:D:87:LEU:CD1	2:D:201:A1I4Z:C28	2.96	0.44
1:A:39:GLU:HA	1:A:83:LYS:HE2	2.00	0.44
1:D:32:GLN:CG	1:D:33:GLN:N	2.81	0.44
1:B:32:GLN:CG	1:B:33:GLN:N	2.82	0.43
2:C:201:A1I4Z:C18	2:C:201:A1I4Z:C26	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASN:HA	1:B:15:PRO:HD3	1.90	0.43
1:D:32:GLN:CG	1:D:33:GLN:H	2.31	0.43
1:B:63:VAL:HG11	1:B:73:LEU:HD21	2.01	0.43
1:D:139:ASN:OD1	1:D:139:ASN:C	2.61	0.43
1:C:27:ARG:HB3	1:C:176:PRO:HB3	2.01	0.43
1:C:110:TYR:HA	1:C:111:PRO:HA	1.88	0.43
1:D:22:ASP:O	1:D:23:ARG:HB2	2.19	0.43
1:B:110:TYR:HA	1:B:111:PRO:HA	1.86	0.42
1:A:35:ILE:HD12	1:A:41:ARG:NH2	2.34	0.42
1:D:53:HIS:ND1	1:D:53:HIS:N	2.67	0.42
1:B:126:ILE:HD12	1:B:126:ILE:N	2.34	0.42
1:C:104:LYS:NZ	1:C:106:GLU:OE2	2.53	0.42
1:C:139:ASN:HB2	1:C:147:ILE:HD11	2.00	0.42
1:A:52:GLN:CD	1:A:52:GLN:H	2.27	0.42
2:A:201:A1I4Z:C15	2:A:201:A1I4Z:C18	2.98	0.42
1:D:52:GLN:OE1	1:D:52:GLN:N	2.41	0.42
1:C:3:MET:HA	1:C:60:TYR:O	2.21	0.41
1:D:165:PRO:O	1:D:173:ASN:ND2	2.54	0.41
1:C:20:SER:OG	1:C:22:ASP:OD1	2.30	0.41
1:D:3:MET:HA	1:D:60:TYR:O	2.20	0.41
1:B:53:HIS:N	1:B:53:HIS:ND1	2.68	0.41
1:C:134:MET:HE3	1:C:134:MET:HB3	1.84	0.41
1:A:3:MET:HA	1:A:60:TYR:O	2.21	0.41
1:A:15:PRO:HG3	1:A:41:ARG:HD3	2.02	0.41
1:D:134:MET:HE3	1:D:134:MET:HB3	1.85	0.40
1:D:99:LEU:HD11	1:D:103:GLN:H	1.86	0.40
1:D:142:ASP:HB3	1:D:145:SER:OG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:THR:O	1:D:79:SER:O[2_545]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/198 (91%)	158 (87%)	17 (9%)	6 (3%)	3	1
1	B	181/198 (91%)	160 (88%)	16 (9%)	5 (3%)	4	2
1	C	181/198 (91%)	162 (90%)	15 (8%)	4 (2%)	5	4
1	D	181/198 (91%)	163 (90%)	12 (7%)	6 (3%)	3	1
All	All	724/792 (91%)	643 (89%)	60 (8%)	21 (3%)	3	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ASP
1	C	169	ASP
1	D	102	LYS
1	B	169	ASP
1	A	102	LYS
1	C	102	LYS
1	C	155	PHE
1	D	169	ASP
1	B	71	TRP
1	B	154	ALA
1	B	155	PHE
1	A	71	TRP
1	A	154	ALA
1	A	155	PHE
1	A	170	GLY
1	C	154	ALA
1	D	152	GLU
1	D	154	ALA
1	B	152	GLU
1	D	155	PHE
1	D	170	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/172 (93%)	140 (88%)	20 (12%)	3	3
1	B	160/172 (93%)	140 (88%)	20 (12%)	3	3
1	C	160/172 (93%)	145 (91%)	15 (9%)	7	7
1	D	160/172 (93%)	140 (88%)	20 (12%)	3	3
All	All	640/688 (93%)	565 (88%)	75 (12%)	4	3

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	MET
1	B	6	ILE
1	B	8	LEU
1	B	23	ARG
1	B	31	THR
1	B	53	HIS
1	B	55	HIS
1	B	75	VAL
1	B	83	LYS
1	B	90	SER
1	B	102	LYS
1	B	103	GLN
1	B	104	LYS
1	B	115	LEU
1	B	118	GLN
1	B	123	GLN
1	B	128	LEU
1	B	135	VAL
1	B	168	ASN
1	B	180	CYS
1	A	8	LEU
1	A	21	GLU
1	A	23	ARG
1	A	31	THR
1	A	34	SER
1	A	44	SER
1	A	52	GLN
1	A	75	VAL
1	A	83	LYS
1	A	90	SER
1	A	92	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	LYS
1	A	104	LYS
1	A	115	LEU
1	A	123	GLN
1	A	135	VAL
1	A	136	SER
1	A	172	LYS
1	A	174	THR
1	A	180	CYS
1	C	6	ILE
1	C	8	LEU
1	C	21	GLU
1	C	31	THR
1	C	44	SER
1	C	53	HIS
1	C	75	VAL
1	C	83	LYS
1	C	90	SER
1	C	92	SER
1	C	104	LYS
1	C	112	GLN
1	C	115	LEU
1	C	123	GLN
1	C	135	VAL
1	D	6	ILE
1	D	8	LEU
1	D	19	LEU
1	D	21	GLU
1	D	31	THR
1	D	44	SER
1	D	55	HIS
1	D	68	LYS
1	D	75	VAL
1	D	89	SER
1	D	90	SER
1	D	92	SER
1	D	104	LYS
1	D	115	LEU
1	D	123	GLN
1	D	135	VAL
1	D	136	SER
1	D	143	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	145	SER
1	D	168	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	HIS
1	A	2	HIS
1	A	25	GLN
1	A	116	HIS
1	D	-1	HIS
1	D	5	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1I4Z	B	201	-	42,43,43	1.10	2 (4%)	52,59,59	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1I4Z	D	201	-	42,43,43	0.79	1 (2%)	52,59,59	0.84	2 (3%)
2	A1I4Z	C	201	-	42,43,43	0.91	2 (4%)	52,59,59	1.04	2 (3%)
2	A1I4Z	A	201	-	42,43,43	1.20	3 (7%)	52,59,59	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1I4Z	B	201	-	-	10/26/26/26	0/5/5/5
2	A1I4Z	D	201	-	-	3/26/26/26	0/5/5/5
2	A1I4Z	C	201	-	-	8/26/26/26	0/5/5/5
2	A1I4Z	A	201	-	-	7/26/26/26	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	A1I4Z	C17-C27	5.05	1.44	1.38
2	A	201	A1I4Z	C12-N3	-4.32	1.40	1.45
2	B	201	A1I4Z	C12-N3	-4.21	1.40	1.45
2	B	201	A1I4Z	C17-C27	4.15	1.43	1.38
2	C	201	A1I4Z	C12-N3	-3.63	1.41	1.45
2	D	201	A1I4Z	C12-N3	-3.32	1.41	1.45
2	C	201	A1I4Z	C17-C27	2.46	1.41	1.38
2	A	201	A1I4Z	C13-N3	-2.38	1.35	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	A1I4Z	C29-C16-C12	2.68	119.45	116.53
2	C	201	A1I4Z	C20-C19-N5	2.63	116.04	112.17
2	D	201	A1I4Z	C19-N5-C18	-2.40	126.13	129.19
2	C	201	A1I4Z	C15-N3-C12	2.34	128.06	125.38

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	A1I4Z	C16-C12-N3-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	201	A1I4Z	C12-C16-C17-C27
2	B	201	A1I4Z	C20-C19-N5-N6
2	A	201	A1I4Z	C12-C16-C17-C27
2	A	201	A1I4Z	C20-C19-N5-N6
2	C	201	A1I4Z	O1-C2-N1-C1
2	C	201	A1I4Z	C3-C2-N1-C1
2	C	201	A1I4Z	C16-C12-N3-C13
2	C	201	A1I4Z	C16-C12-N3-C15
2	C	201	A1I4Z	C12-C16-C17-C27
2	B	201	A1I4Z	C22-C23-O2-C24
2	B	201	A1I4Z	O1-C2-N1-C1
2	B	201	A1I4Z	C25-C23-O2-C24
2	B	201	A1I4Z	C3-C2-N1-C1
2	B	201	A1I4Z	C16-C12-N3-C13
2	D	201	A1I4Z	C16-C12-N3-C15
2	A	201	A1I4Z	C6-C7-N2-C8
2	C	201	A1I4Z	C20-C19-N5-N6
2	B	201	A1I4Z	C20-C19-N5-C18
2	A	201	A1I4Z	C20-C19-N5-C18
2	C	201	A1I4Z	C20-C19-N5-C18
2	A	201	A1I4Z	C25-C23-O2-C24
2	A	201	A1I4Z	C22-C23-O2-C24
2	C	201	A1I4Z	C9-C8-N2-C7
2	B	201	A1I4Z	C9-C8-N2-C7
2	D	201	A1I4Z	C16-C12-N3-C13
2	D	201	A1I4Z	C12-C16-C17-C18
2	A	201	A1I4Z	C11-C12-N3-C15

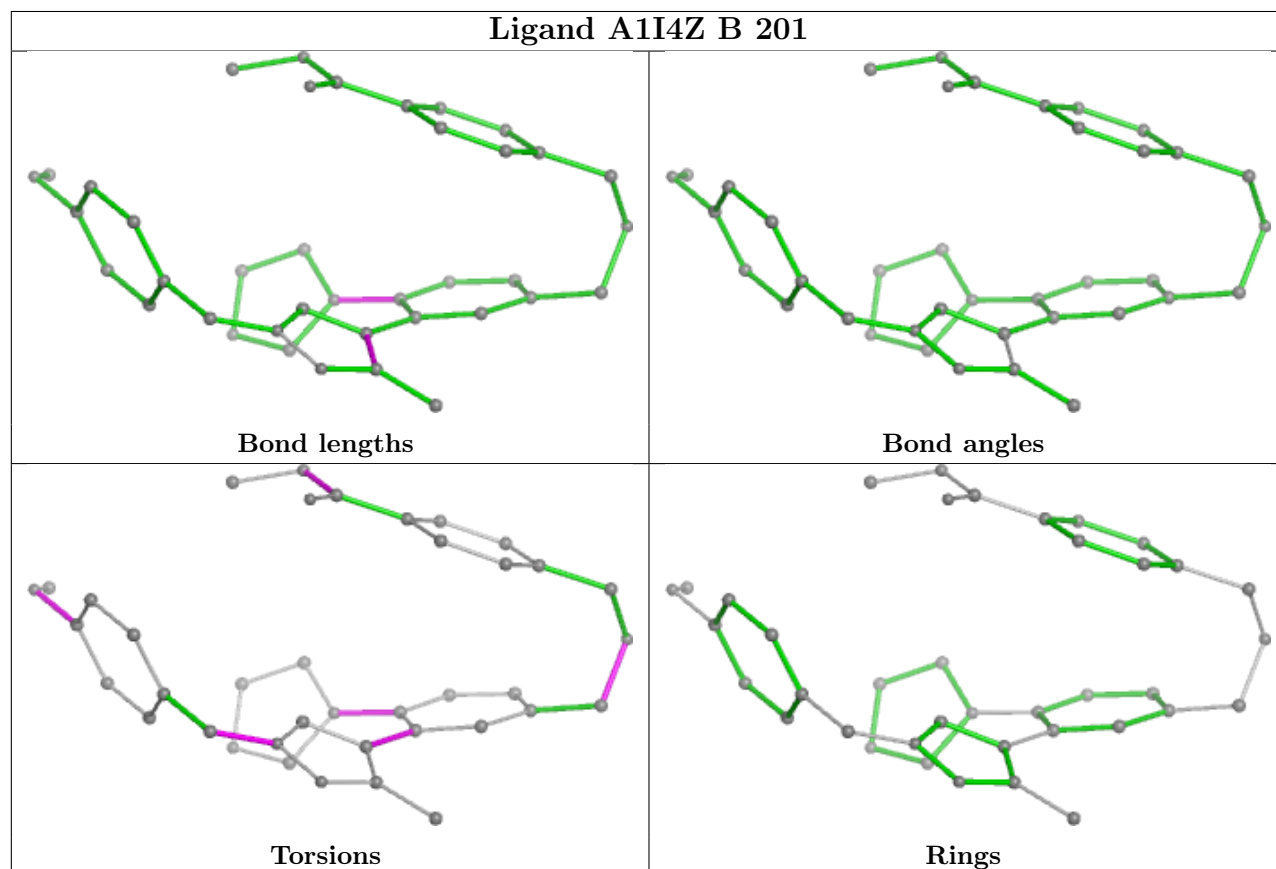
There are no ring outliers.

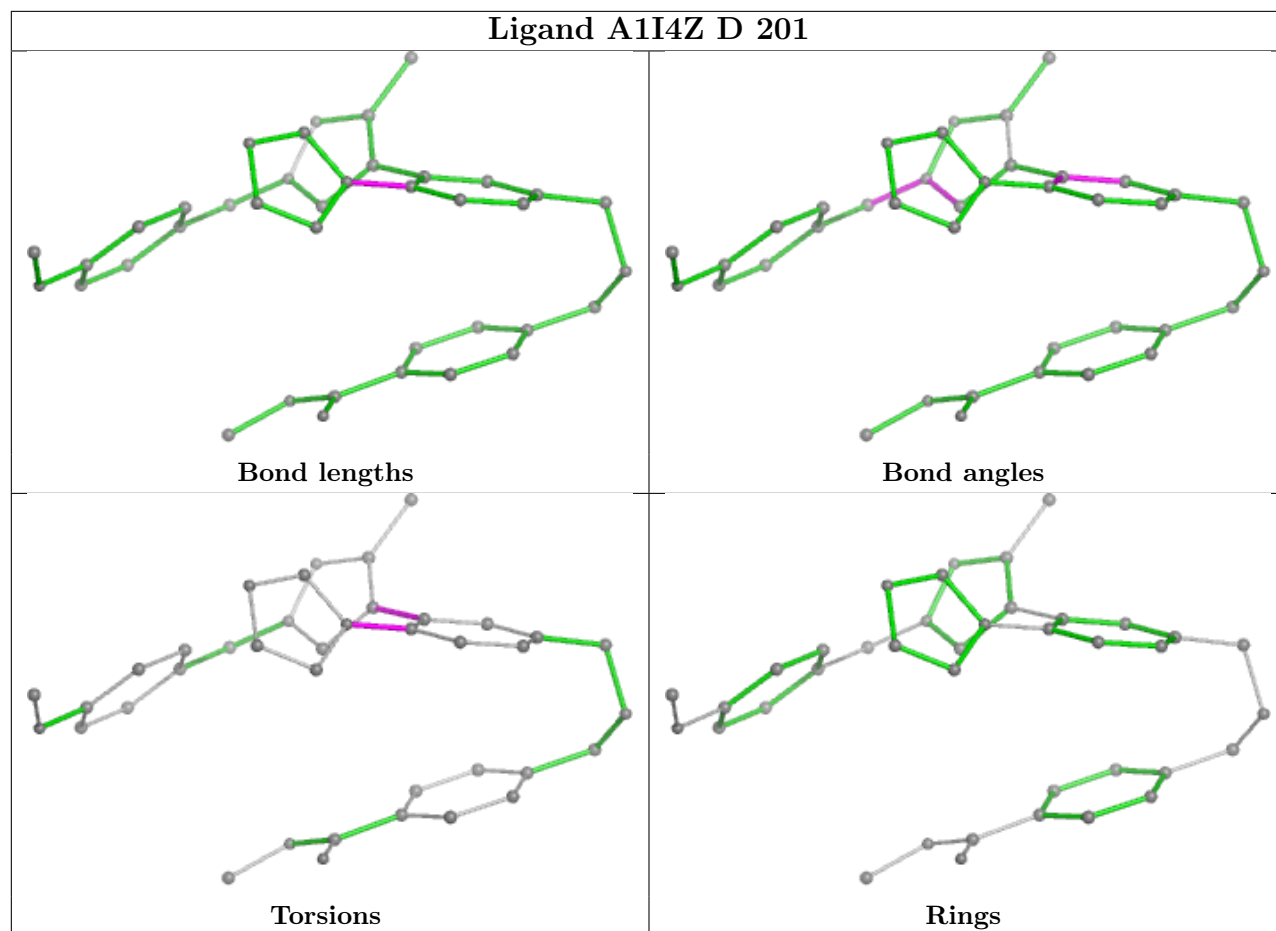
4 monomers are involved in 7 short contacts:

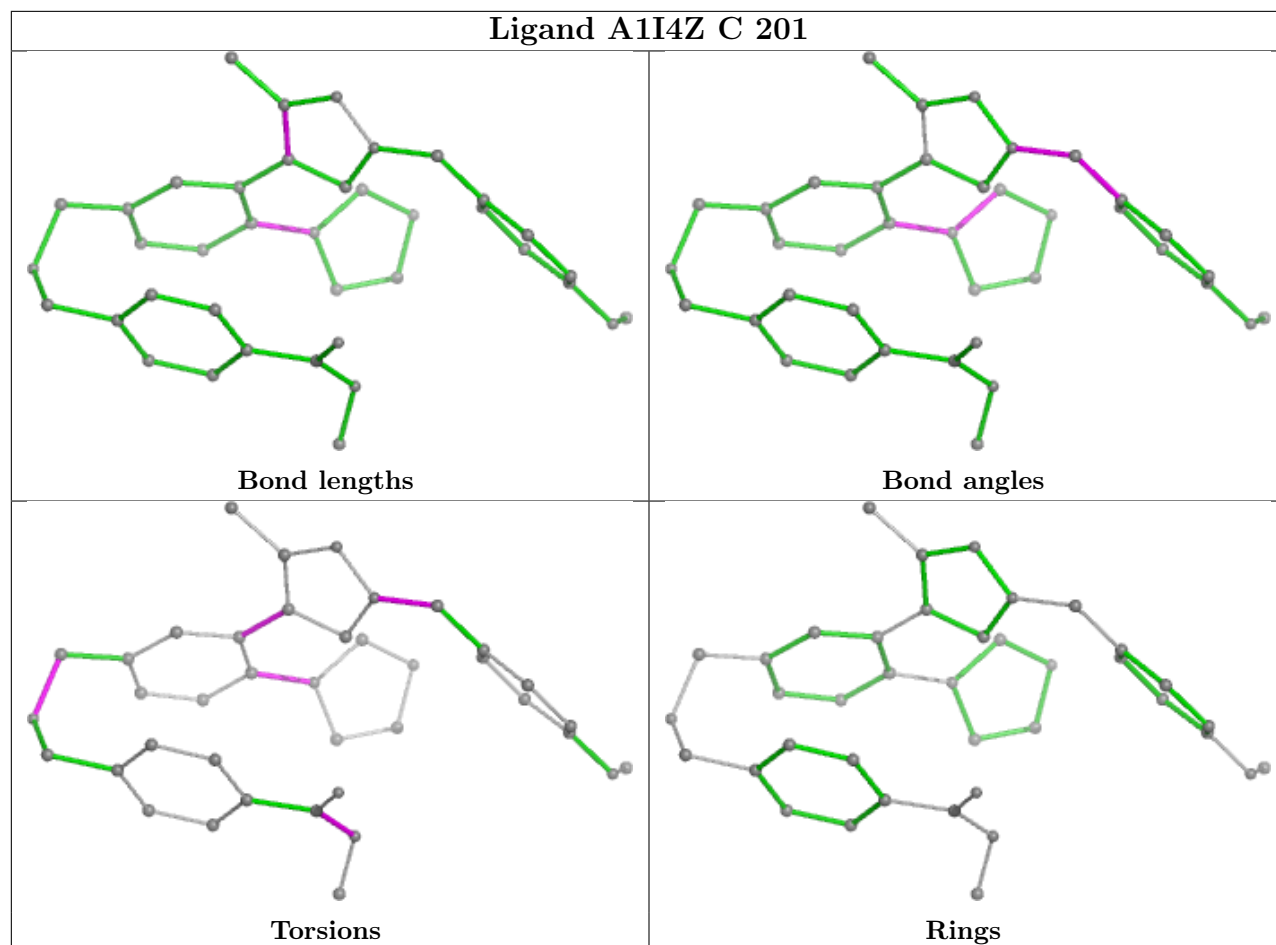
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	A1I4Z	1	0
2	D	201	A1I4Z	3	0
2	C	201	A1I4Z	2	0
2	A	201	A1I4Z	1	0

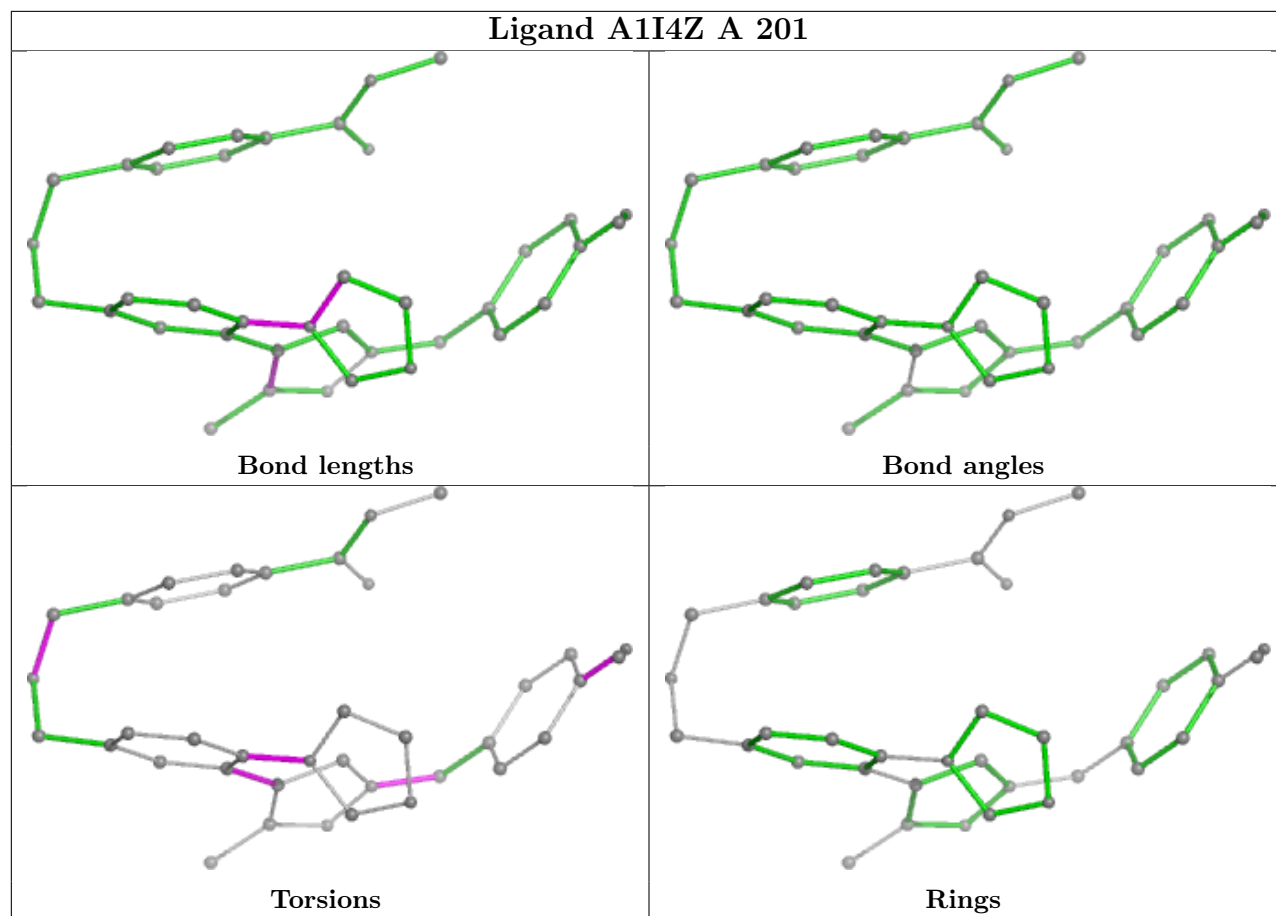
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	183/198 (92%)	-1.57	0 100 100	15, 33, 54, 70	0
1	B	183/198 (92%)	-1.57	0 100 100	16, 34, 58, 88	0
1	C	183/198 (92%)	-1.57	0 100 100	15, 35, 60, 75	0
1	D	183/198 (92%)	-1.55	0 100 100	16, 35, 59, 88	0
All	All	732/792 (92%)	-1.57	0 100 100	15, 34, 58, 88	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

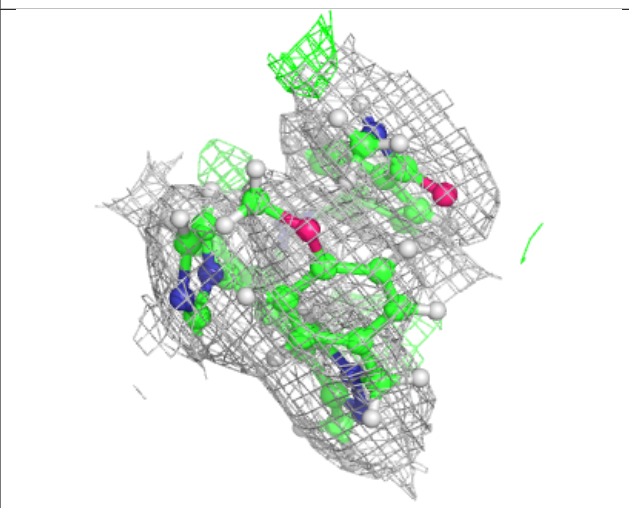
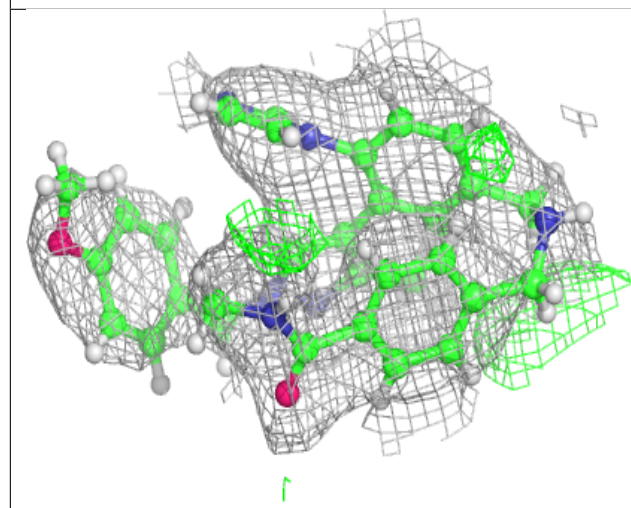
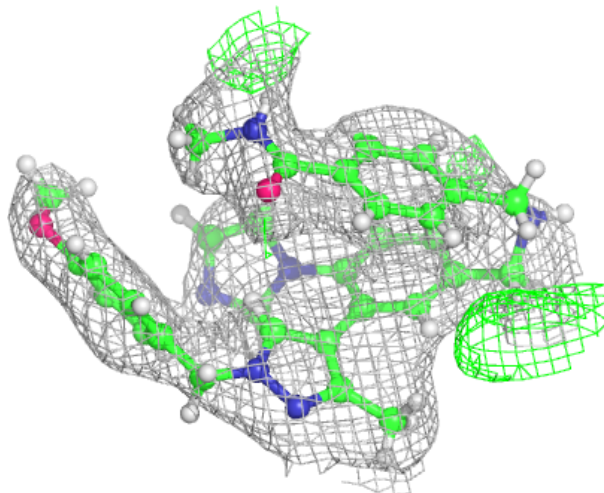
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1I4Z	B	201	39/39	0.99	0.04	18,30,42,43	0
2	A1I4Z	A	201	39/39	0.99	0.03	22,29,40,42	0
2	A1I4Z	C	201	39/39	0.99	0.03	18,23,37,40	0
2	A1I4Z	D	201	39/39	0.99	0.04	24,35,48,66	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.

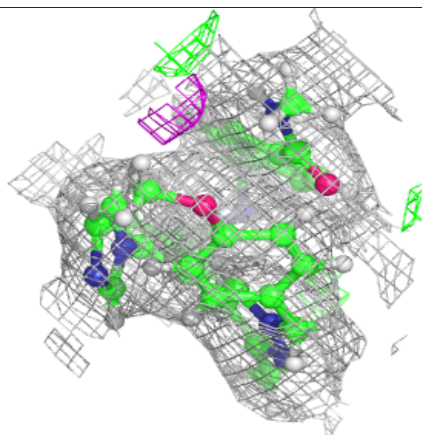
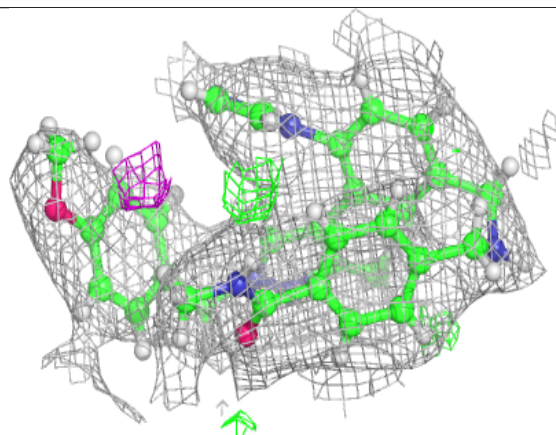
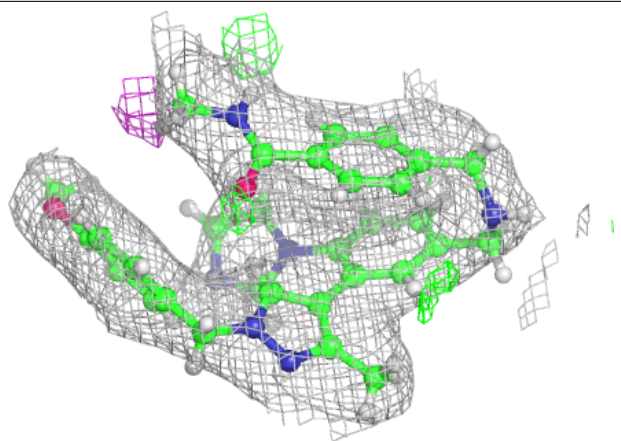
Electron density around A1I4Z B 201:

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



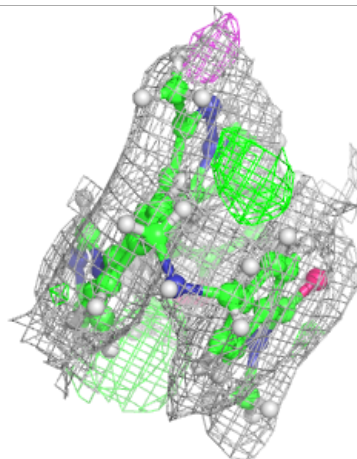
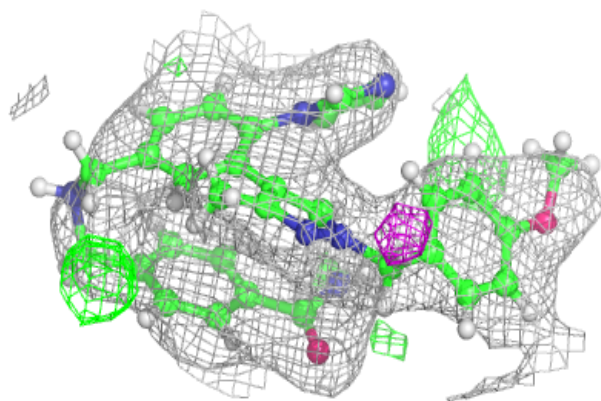
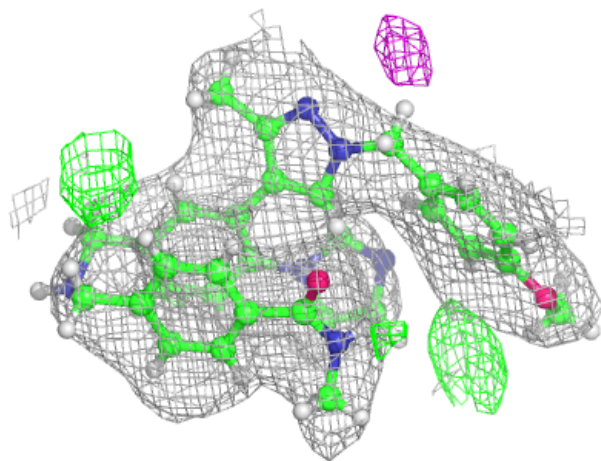
Electron density around A1I4Z A 201:

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



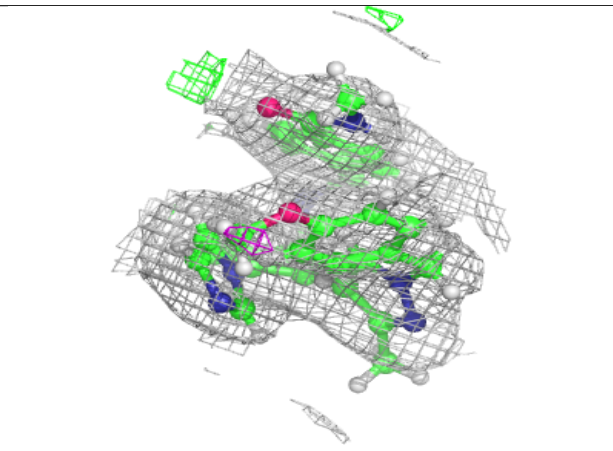
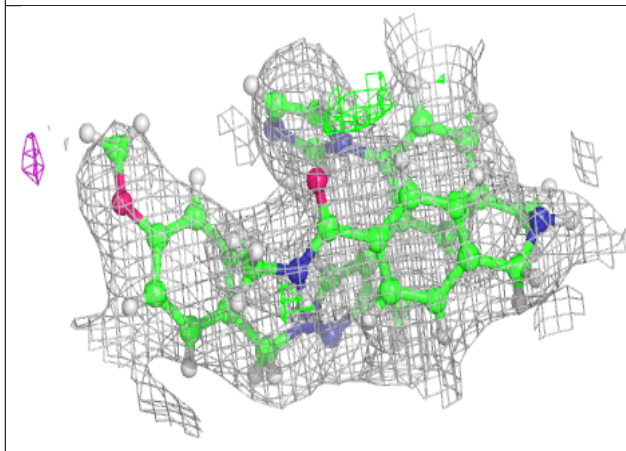
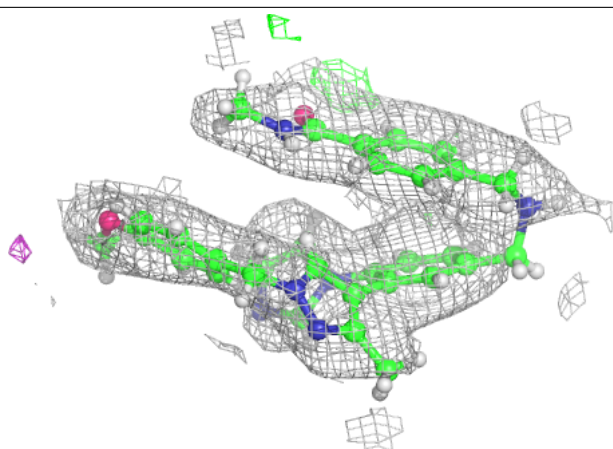
Electron density around A1I4Z C 201:

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



Electron density around A1I4Z D 201:

$2mF_o - DF_c$ (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.