



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 05:18 AM BST

PDB ID : 6O8B
Title : Crystal structure of STING CTD in complex with TBK1
Authors : Li, P.; Zhao, B.; Du, F.
Deposited on : 2019-03-09
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

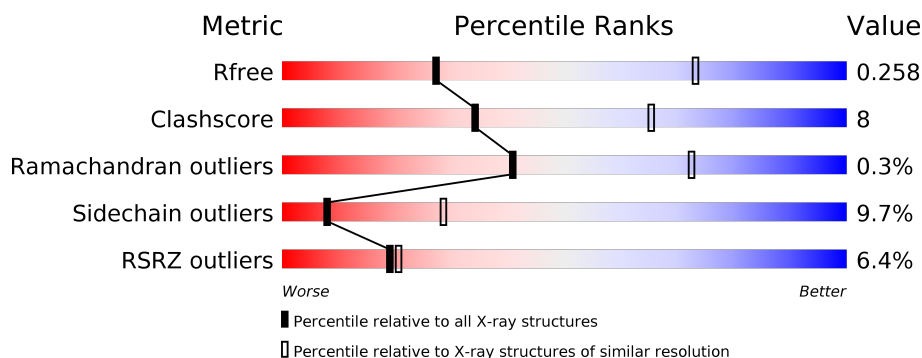
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on 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	D	226	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	E	226	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
2	A	665	<div> <div style="width: 72%;"></div> <div>72%</div> <div style="width: 23%;"></div> <div>23%</div> </div>
2	B	665	<div> <div style="width: 74%;"></div> <div>74%</div> <div style="width: 22%;"></div> <div>22%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10897 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 Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	11	Total	C	N	O	S	0	0	0
			98	64	16	17	1			
1	E	12	Total	C	N	O	S	0	0	0
			106	69	17	18	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	154	SER	-	expression tag	UNP Q86WV6
D	232	ARG	HIS	variant	UNP Q86WV6
D	376	GLU	THR	engineered mutation	UNP Q86WV6
D	378	MET	PHE	engineered mutation	UNP Q86WV6
D	379	TRP	SER	engineered mutation	UNP Q86WV6
E	154	SER	-	expression tag	UNP Q86WV6
E	232	ARG	HIS	variant	UNP Q86WV6
E	376	GLU	THR	engineered mutation	UNP Q86WV6
E	378	MET	PHE	engineered mutation	UNP Q86WV6
E	379	TRP	SER	engineered mutation	UNP Q86WV6

- Molecule 2 is a protein called Serine/threonine-protein kinase TBK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	656	Total	C	N	O	S	0	0	0
			5305	3379	910	991	25			
2	B	657	Total	C	N	O	S	0	0	0
			5320	3389	912	993	26			

There are 26 discrepancies between the modelled and reference sequences:

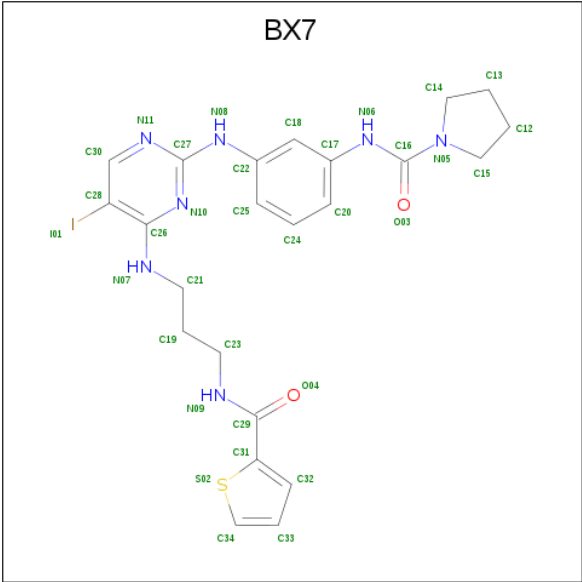
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9UHD2
A	-6	SER	-	expression tag	UNP Q9UHD2

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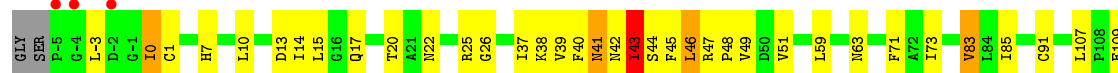
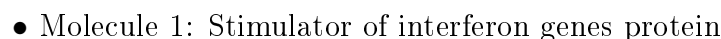
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	PRO	-	expression tag	UNP Q9UHD2
A	-4	GLY	-	expression tag	UNP Q9UHD2
A	-3	LEU	-	expression tag	UNP Q9UHD2
A	-2	ASP	-	expression tag	UNP Q9UHD2
A	-1	GLY	-	expression tag	UNP Q9UHD2
A	0	ILE	-	expression tag	UNP Q9UHD2
A	1	CYS	-	expression tag	UNP Q9UHD2
A	135	ASN	ASP	engineered mutation	UNP Q9UHD2
A	172	GLU	SER	engineered mutation	UNP Q9UHD2
A	388	ASP	ASN	variant	UNP Q9UHD2
A	570	GLN	LYS	variant	UNP Q9UHD2
B	-7	GLY	-	expression tag	UNP Q9UHD2
B	-6	SER	-	expression tag	UNP Q9UHD2
B	-5	PRO	-	expression tag	UNP Q9UHD2
B	-4	GLY	-	expression tag	UNP Q9UHD2
B	-3	LEU	-	expression tag	UNP Q9UHD2
B	-2	ASP	-	expression tag	UNP Q9UHD2
B	-1	GLY	-	expression tag	UNP Q9UHD2
B	0	ILE	-	expression tag	UNP Q9UHD2
B	1	CYS	-	expression tag	UNP Q9UHD2
B	135	ASN	ASP	engineered mutation	UNP Q9UHD2
B	172	GLU	SER	engineered mutation	UNP Q9UHD2
B	388	ASP	ASN	variant	UNP Q9UHD2
B	570	GLN	LYS	variant	UNP Q9UHD2

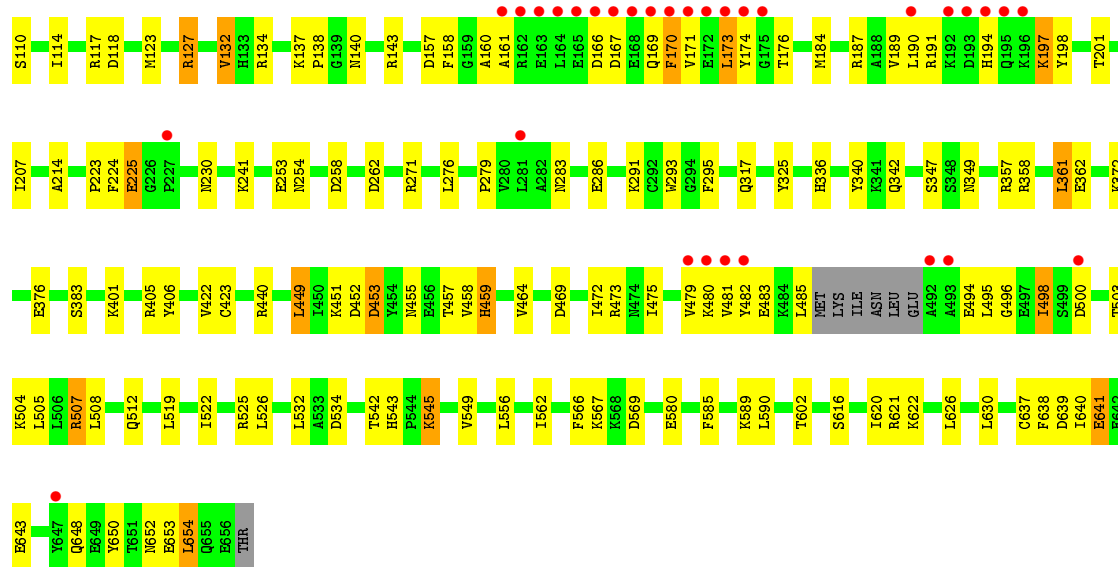
- Molecule 3 is N-(3-{[5-iodo-4-({3-[(thiophen-2-ylcarbonyl)amino]propyl}amino)pyrimidin-2-yl]amino}phenyl)pyrrolidine-1-carboxamide (three-letter code: BX7) (formula: C₂₃H₂₆IN₇O₂S).



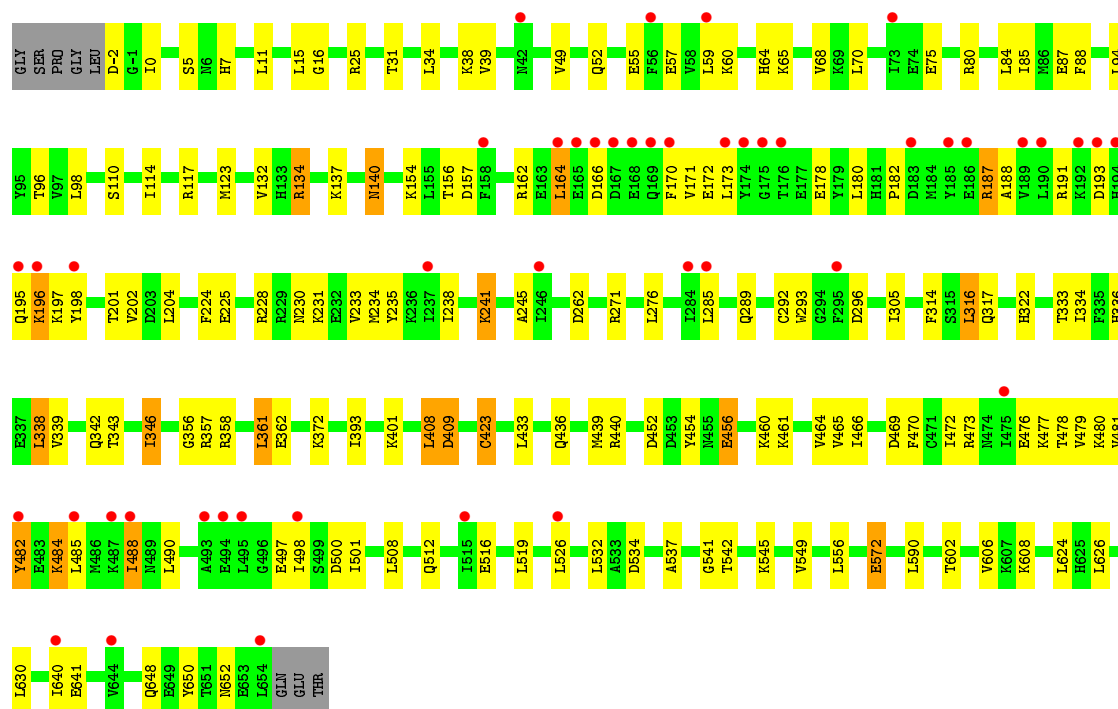
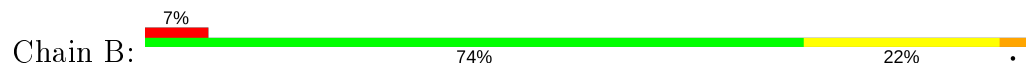
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	S	0	0
			34	23	1	7	2	1		
3	B	1	Total	C	I	N	O	S	0	0
			34	23	1	7	2	1		

- Molecule 1: Stimulator of interferon genes protein





• Molecule 2: Serine/threonine-protein kinase TBK1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	250.69Å 250.69Å 239.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.06 – 3.40 82.06 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (82.06-3.40) 98.4 (82.06-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.243 , 0.258 0.243 , 0.258	Depositor DCC
R_{free} test set	3022 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	117.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10897	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BX7

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	D	0.24	0/101	0.55	0/136
1	E	0.23	0/109	0.43	0/146
2	A	0.25	0/5416	0.43	2/7314 (0.0%)
2	B	0.25	0/5431	0.43	0/7335
All	All	0.25	0/11057	0.43	2/14931 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	LEU	CA-CB-CG	5.83	128.71	115.30
2	A	173	LEU	CA-CB-CG	5.38	127.68	115.30

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	D	98	0	96	2	0
1	E	106	0	105	4	0
2	A	5305	0	5293	88	0
2	B	5320	0	5320	92	0
3	A	34	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	26	5	0
All	All	10897	0	10866	182	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 8.

The worst 5 of 182 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)
2:B:134:ARG:HH12	2:B:172:GLU:HG3	1.42	0.83
2:A:38:LYS:HE3	3:A:701:BX7:H26	1.65	0.78
2:B:241:LYS:NZ	2:B:285:LEU:O	2.17	0.77
2:B:479:VAL:HA	2:B:482:TYR:HB2	1.71	0.72
2:A:357:ARG:NH1	2:B:356:GLY:O	2.23	0.72

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	D	9/226 (4%)	7 (78%)	2 (22%)	0	100	100
1	E	10/226 (4%)	8 (80%)	2 (20%)	0	100	100
2	A	652/665 (98%)	623 (96%)	26 (4%)	3 (0%)	29	61
2	B	655/665 (98%)	627 (96%)	27 (4%)	1 (0%)	47	78
All	All	1326/1782 (74%)	1265 (95%)	57 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	43	ILE

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Mol	Chain	Res	Type
2	A	171	VAL
2	A	224	PHE
2	B	572	GLU

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	D	11/199 (6%)	10 (91%)	1 (9%)	9	32
1	E	12/199 (6%)	10 (83%)	2 (17%)	2	8
2	A	583/592 (98%)	524 (90%)	59 (10%)	7	27
2	B	586/592 (99%)	532 (91%)	54 (9%)	9	31
All	All	1192/1582 (75%)	1076 (90%)	116 (10%)	8	28

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	549	VAL
2	B	31	THR
2	B	500	ASP
2	A	589	LYS
2	A	641	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	254	ASN
2	B	520	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
3	BX7	A	701	-	35,37,37	4.46	15 (42%)	42,49,49	2.18	10 (23%)
3	BX7	B	701	-	35,37,37	4.44	15 (42%)	42,49,49	2.20	8 (19%)

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	BX7	A	701	-	-	4/22/31/31	0/4/4/4
3	BX7	B	701	-	-	5/22/31/31	0/4/4/4

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	BX7	C31-S02	-12.72	1.56	1.72
3	B	701	BX7	C31-S02	-12.54	1.57	1.72
3	B	701	BX7	C26-N07	12.15	1.53	1.34
3	A	701	BX7	C26-N07	12.08	1.53	1.34
3	A	701	BX7	C16-N06	7.51	1.50	1.37

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	BX7	N11-C27-N10	-9.05	117.98	126.55
3	A	701	BX7	N11-C27-N10	-8.93	118.09	126.55
3	B	701	BX7	C33-C34-S02	-6.10	108.03	112.98
3	A	701	BX7	C33-C34-S02	-5.30	108.68	112.98
3	A	701	BX7	C15-N05-C14	-3.45	106.61	111.34

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

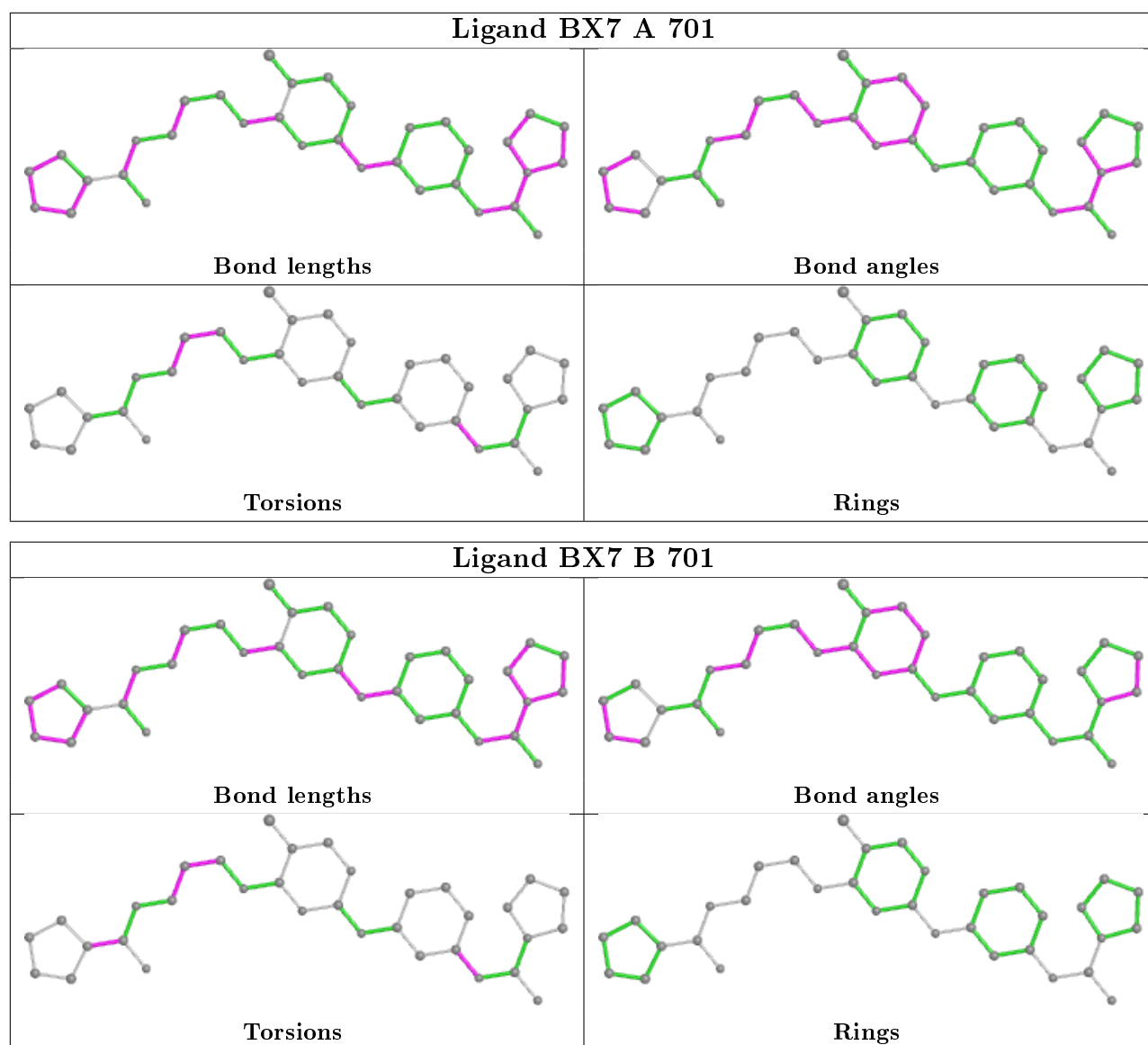
Mol	Chain	Res	Type	Atoms
3	B	701	BX7	O04-C29-C31-C32
3	B	701	BX7	N09-C29-C31-C32
3	A	701	BX7	C21-C19-C23-N09
3	B	701	BX7	C23-C19-C21-N07
3	B	701	BX7	C21-C19-C23-N09

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	BX7	4	0
3	B	701	BX7	5	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	D	11/226 (4%)	1.30	3 (27%) 0 0	158, 172, 188, 195	0
1	E	12/226 (5%)	1.36	3 (25%) 0 0	112, 120, 165, 176	0
2	A	656/665 (98%)	0.49	34 (5%) 27 27	75, 119, 219, 259	0
2	B	657/665 (98%)	0.48	46 (7%) 16 18	91, 132, 225, 268	0
All	All	1336/1782 (74%)	0.50	86 (6%) 19 20	75, 125, 222, 268	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	163	GLU	13.6
2	B	175	GLY	12.2
2	A	162	ARG	11.8
2	A	164	LEU	11.7
2	A	169	GLN	9.0

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](#)

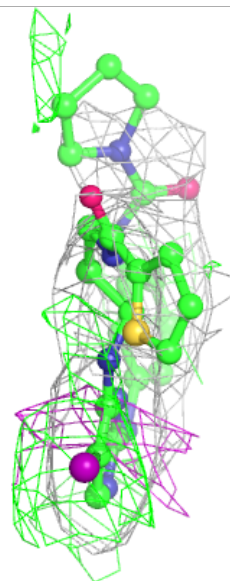
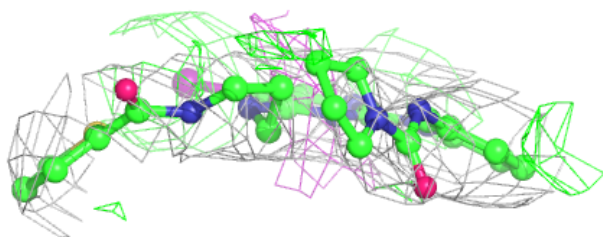
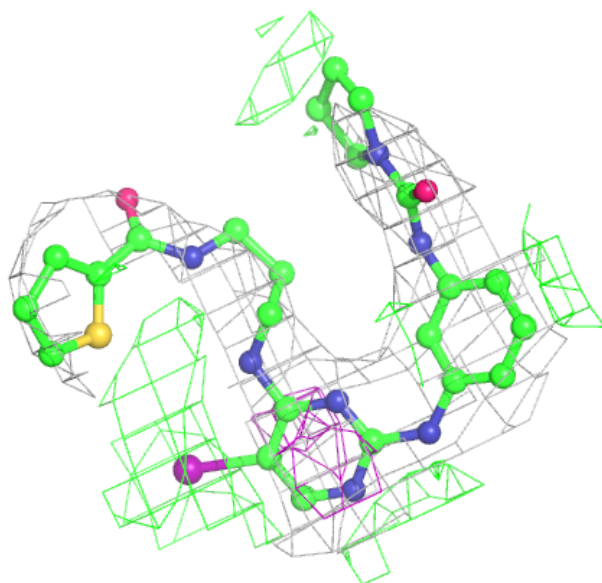
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BX7	B	701	34/34	0.78	0.34	78,123,165,288	0
3	BX7	A	701	34/34	0.85	0.39	46,102,149,210	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.

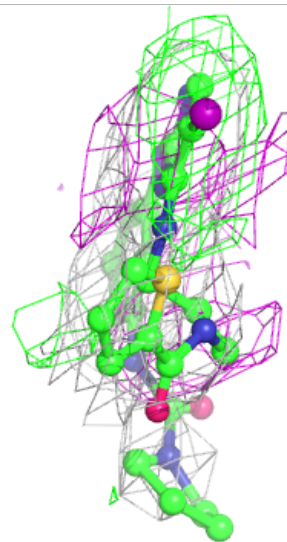
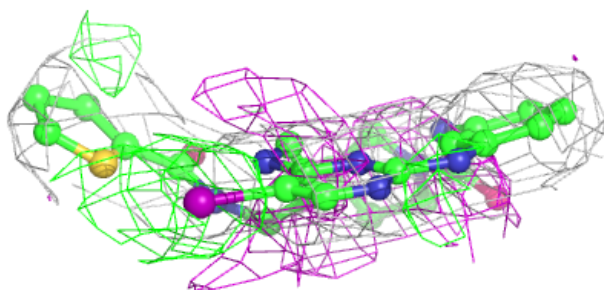
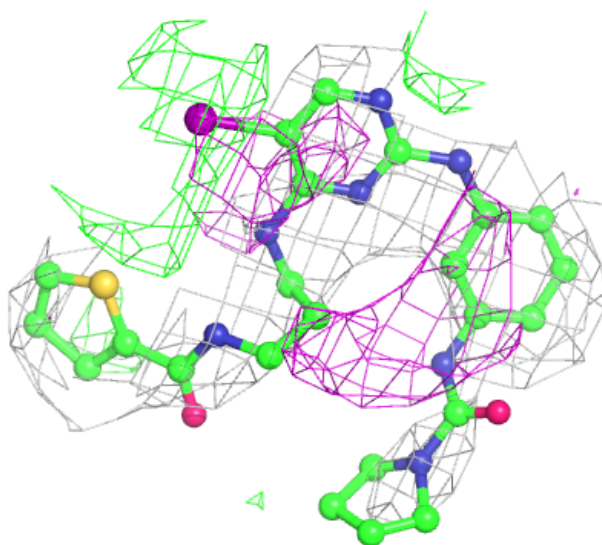
Electron density around BX7 B 701:

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 BX7 A 701:

$2mF_o-DF_c$ (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.