



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:23 AM BST

PDB ID : 6O8C
Title : Crystal structure of STING CTT in complex with TBK1
Authors : Li, P.; Zhao, B.; Du, F.
Deposited on : 2019-03-09
Resolution : 3.17 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 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

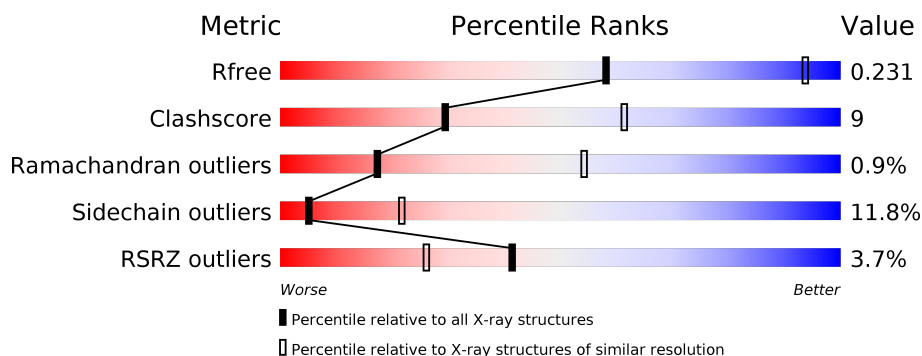
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	A	665	<div> <div>2%</div> <div>69%</div> <div>23%</div> <div>• •</div> </div>
1	B	665	<div> <div>4%</div> <div>69%</div> <div>23%</div> <div>5% •</div> </div>
2	D	39	<div> <div>5%</div> <div>26%</div> <div>8%</div> <div>•</div> <div>64%</div> </div>
2	E	39	<div> <div>10%</div> <div>18%</div> <div>5%</div> <div>5%</div> <div>•</div> <div>69%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10606 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 Serine/threonine-protein kinase TBK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	1	0
			5137	3265	892	955	25			
1	B	643	Total	C	N	O	S	0	0	0
			5193	3299	901	967	26			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9WUN2
A	-6	SER	-	expression tag	UNP Q9WUN2
A	-5	PRO	-	expression tag	UNP Q9WUN2
A	-4	GLY	-	expression tag	UNP Q9WUN2
A	-3	LEU	-	expression tag	UNP Q9WUN2
A	-2	ASP	-	expression tag	UNP Q9WUN2
A	-1	GLY	-	expression tag	UNP Q9WUN2
A	0	ILE	-	expression tag	UNP Q9WUN2
A	1	CYS	-	expression tag	UNP Q9WUN2
A	172	ALA	SER	engineered mutation	UNP Q9WUN2
B	-7	GLY	-	expression tag	UNP Q9WUN2
B	-6	SER	-	expression tag	UNP Q9WUN2
B	-5	PRO	-	expression tag	UNP Q9WUN2
B	-4	GLY	-	expression tag	UNP Q9WUN2
B	-3	LEU	-	expression tag	UNP Q9WUN2
B	-2	ASP	-	expression tag	UNP Q9WUN2
B	-1	GLY	-	expression tag	UNP Q9WUN2
B	0	ILE	-	expression tag	UNP Q9WUN2
B	1	CYS	-	expression tag	UNP Q9WUN2
B	172	ALA	SER	engineered mutation	UNP Q9WUN2

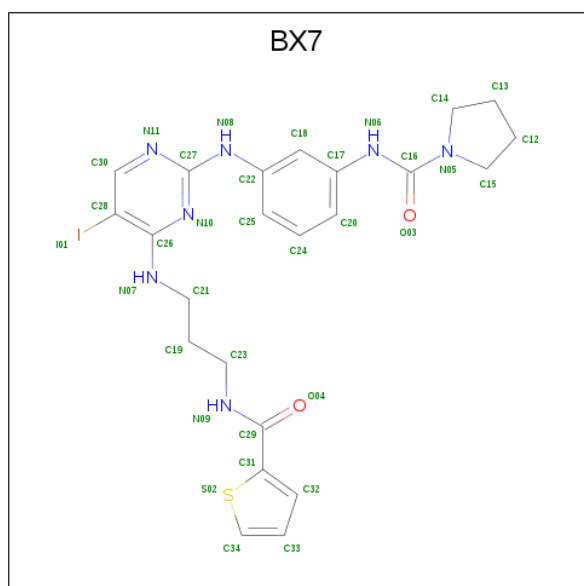
- Molecule 2 is a protein called Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	S	0	0	0
			109	69	18	21	1			
2	E	12	Total	C	N	O	S	0	0	0
			99	64	16	18	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	341	SER	-	expression tag	UNP Q86WV6
D	343	TRP	VAL	engineered mutation	UNP Q86WV6
E	341	SER	-	expression tag	UNP Q86WV6
E	343	TRP	VAL	engineered mutation	UNP Q86WV6

- 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: $C_{23}H_{26}IN_7O_2S$).

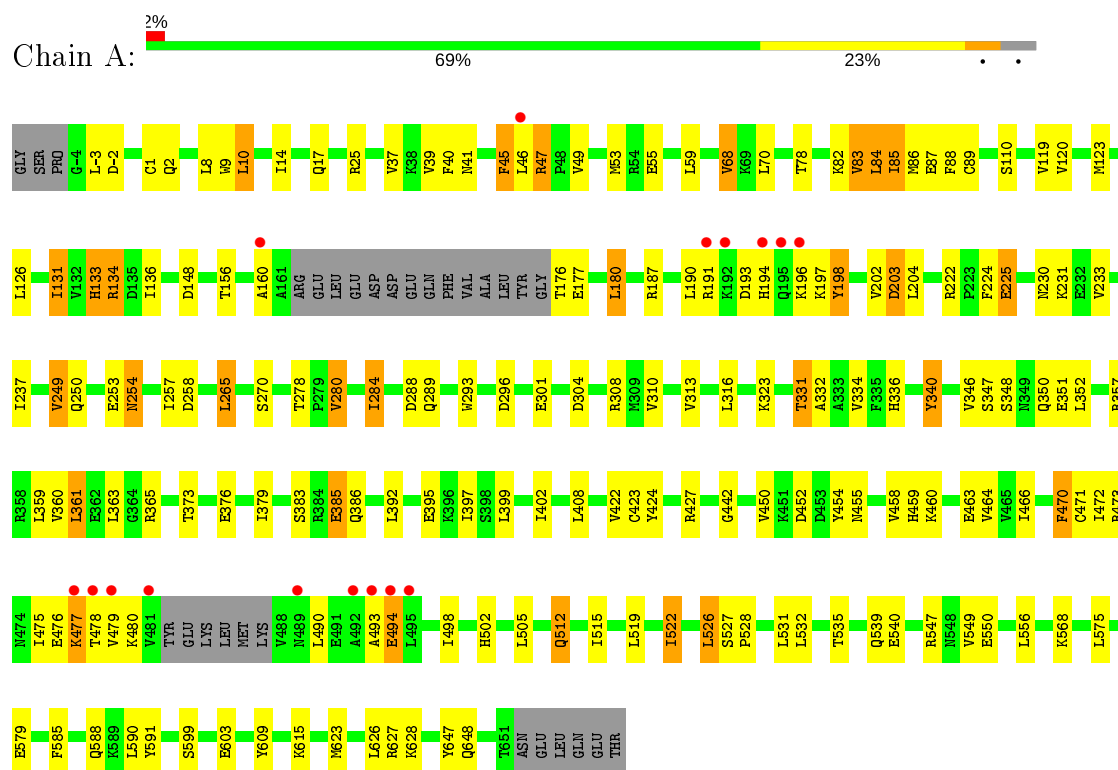


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	S	0	0
			34	23	1	7	2	1		
3	B	1	Total	C	I	N	O	S	0	0
			34	23	1	7	2	1		

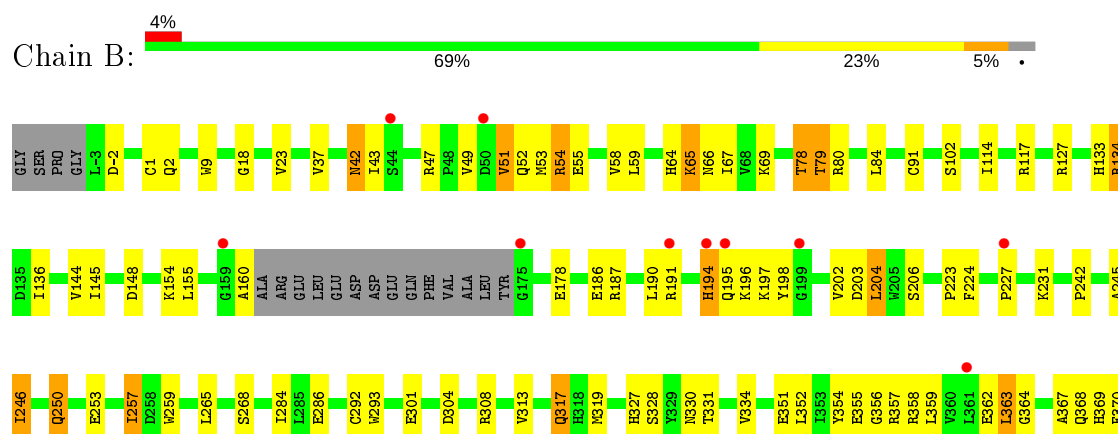
3 Residue-property plots

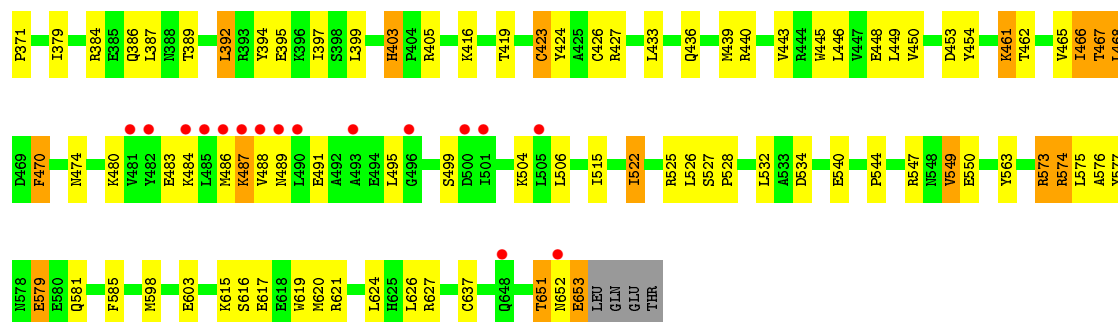
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase TBK1



- Molecule 1: Serine/threonine-protein kinase TBK1





- Molecule 2: Stimulator of interferon genes protein



- Molecule 2: Stimulator of interferon genes protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	249.51Å 249.51Å 243.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.67 – 3.17 81.67 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (81.67-3.17) 99.9 (81.67-3.17)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.213 , 0.231 0.213 , 0.231	Depositor DCC
R_{free} test set	3720 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	95.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.4	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	10606	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: 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	A	0.62	2/5243 (0.0%)	0.65	2/7078 (0.0%)
1	B	0.54	1/5300 (0.0%)	0.59	0/7154
2	D	0.70	0/111	0.76	0/148
2	E	0.59	0/101	0.71	0/135
All	All	0.58	3/10755 (0.0%)	0.62	2/14515 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	CYS	CB-SG	-6.78	1.70	1.82
1	A	89	CYS	CB-SG	-5.92	1.72	1.81
1	B	426	CYS	CB-SG	-5.56	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	46	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ILE	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	5137	0	5130	98	0
1	B	5193	0	5191	101	0
2	D	109	0	109	3	0
2	E	99	0	101	6	0
3	A	34	0	26	2	0
3	B	34	0	26	3	0
All	All	10606	0	10583	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (201) 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:450:VAL:HG22	1:A:627:ARG:HD3	1.70	0.73
1:A:332:ALA:HB1	1:A:361:LEU:HD13	1.73	0.71
1:B:573:ARG:O	1:B:574:ARG:HD2	1.92	0.69
1:B:576:ALA:HB3	1:B:579:GLU:HG2	1.74	0.68
1:A:47:ARG:NH2	1:A:55:GLU:OE1	2.29	0.66
1:A:270:SER:HB3	1:A:323:LYS:HD2	1.76	0.65
1:A:588:GLN:HG2	2:D:368:MET:HB2	1.79	0.65
1:B:286:GLU:HB3	1:B:292:CYS:HB2	1.79	0.65
1:A:532:LEU:HD12	1:A:626:LEU:HD13	1.79	0.64
1:B:204:LEU:HD22	1:B:284:ILE:HD11	1.79	0.64
1:B:134:ARG:HG3	1:B:203:ASP:HA	1.80	0.64
1:B:450:VAL:HG22	1:B:627:ARG:HD3	1.80	0.62
1:B:367:ALA:HA	1:B:370:PHE:CD1	2.35	0.62
1:A:148:ASP:O	1:B:547:ARG:NH1	2.33	0.62
1:A:470:PHE:HE2	1:B:467:THR:HG22	1.65	0.61
1:A:224:PHE:HB3	1:A:250:GLN:HE21	1.65	0.61
1:A:204:LEU:HB3	1:A:284:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HG3	1:A:477:LYS:HD3	1.82	0.61
2:E:369:GLU:HG2	2:E:371:PRO:HD3	1.82	0.61
1:A:547:ARG:NH1	1:B:148:ASP:O	2.33	0.60
1:B:257:ILE:HD11	1:B:259:TRP:CE2	2.36	0.60
1:A:293:TRP:CH2	1:A:301:GLU:HG2	2.36	0.60
1:B:64:HIS:ND1	1:B:65:LYS:O	2.35	0.59
1:A:59:LEU:HD21	1:A:160:ALA:HB2	1.85	0.59
1:B:304:ASP:OD2	1:B:308:ARG:NH1	2.35	0.59
1:B:55:GLU:HG3	1:B:160:ALA:HB3	1.85	0.59
1:A:53:MET:HE1	1:A:82:LYS:HG3	1.84	0.59
1:A:466:ILE:HG13	1:B:466:ILE:HD11	1.84	0.59
1:B:224:PHE:H	1:B:250:GLN:HB2	1.68	0.59
1:A:340:TYR:HD1	1:A:340:TYR:O	1.86	0.58
1:A:265:LEU:HB3	1:A:395:GLU:HB2	1.85	0.58
1:A:288:ASP:OD1	1:A:288:ASP:N	2.37	0.58
1:B:532:LEU:HD12	1:B:626:LEU:HD13	1.85	0.58
1:A:134:ARG:HB3	1:A:203:ASP:HA	1.84	0.58
1:B:433:LEU:HD11	1:B:544:PRO:HD3	1.84	0.58
1:A:40:PHE:HE1	1:A:84:LEU:HD22	1.69	0.57
1:A:68:VAL:HG23	1:A:87:GLU:HG2	1.86	0.56
1:B:419:THR:O	1:B:423:CYS:HB2	2.06	0.56
1:A:304:ASP:OD1	1:A:308:ARG:NH1	2.39	0.56
1:A:180:LEU:HD12	1:A:180:LEU:H	1.71	0.56
1:A:402:ILE:HD13	1:A:591:TYR:CD1	2.40	0.56
1:B:66:ASN:HA	1:B:154:LYS:HA	1.87	0.56
1:B:576:ALA:HB3	1:B:579:GLU:CG	2.36	0.56
1:A:176:THR:OG1	1:A:177:GLU:N	2.36	0.56
1:A:579:GLU:N	1:A:579:GLU:OE2	2.38	0.56
1:B:480:LYS:O	1:B:484:LYS:HB3	2.07	0.55
1:B:470:PHE:O	1:B:474:ASN:HB2	2.07	0.55
1:B:198:TYR:HB3	1:B:202:VAL:HG11	1.89	0.55
1:A:14:ILE:HD11	1:A:17:GLN:HG2	1.90	0.54
1:A:119:VAL:HG12	1:A:123:MET:CE	2.38	0.54
1:A:225:GLU:HG3	1:A:230:ASN:HB2	1.90	0.54
1:A:512:GLN:HA	1:A:515:ILE:HD12	1.90	0.54
1:A:450:VAL:HG12	1:A:526:LEU:HD21	1.89	0.54
1:B:49:VAL:HA	1:B:52:GLN:HB2	1.89	0.53
1:A:254:ASN:ND2	1:A:254:ASN:O	2.37	0.53
1:B:190:LEU:O	1:B:194:HIS:ND1	2.41	0.53
2:E:370:LYS:N	2:E:371:PRO:HD3	2.23	0.53
2:D:370:LYS:N	2:D:371:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HD13	1:A:591:TYR:HD1	1.72	0.53
1:A:454:TYR:HD2	1:A:522:ILE:HD11	1.73	0.53
1:A:383:SER:OG	1:A:385:GLU:HG3	2.08	0.53
1:A:472:ILE:HD11	1:A:505:LEU:HB3	1.90	0.52
1:A:540:GLU:HG3	1:A:615:LYS:HG3	1.91	0.52
1:A:352:LEU:HB3	1:A:359:LEU:HB3	1.92	0.52
1:A:39:VAL:HG22	1:A:83:VAL:HB	1.91	0.52
1:B:403:HIS:CE1	1:B:405:ARG:HG3	2.45	0.51
1:B:368:GLN:HG3	1:B:369:HIS:CE1	2.46	0.51
1:A:480:LYS:HD2	1:A:494:GLU:HB2	1.93	0.51
1:A:585:PHE:CE1	2:D:371:PRO:HB2	2.46	0.51
1:A:599:SER:HB2	1:A:603:GLU:OE2	2.11	0.50
1:B:327:HIS:H	1:B:330:ASN:ND2	2.09	0.50
1:B:67:ILE:HD13	1:B:155:LEU:HB2	1.91	0.50
1:A:224:PHE:CE2	1:A:253:GLU:HG2	2.47	0.50
1:B:51:VAL:HA	1:B:54:ARG:HB2	1.93	0.50
1:A:25:ARG:HD3	1:A:88:PHE:CZ	2.46	0.50
1:A:505:LEU:HD21	1:A:647:TYR:HD2	1.77	0.50
1:A:68:VAL:CG1	1:A:156:THR:HB	2.42	0.49
1:B:392:LEU:HD13	1:B:394:TYR:HD2	1.77	0.49
1:A:120:VAL:HA	1:A:123:MET:HE3	1.94	0.49
1:B:436:GLN:O	1:B:440:ARG:HG3	2.12	0.49
1:A:351:GLU:OE1	1:A:627:ARG:NH2	2.43	0.49
3:A:701:BX7:H13	3:A:701:BX7:N10	2.27	0.49
1:B:358:ARG:NH2	1:B:453:ASP:OD1	2.45	0.49
1:A:85:ILE:HG13	1:A:85:ILE:O	2.13	0.49
1:B:653:GLU:CD	1:B:653:GLU:H	2.15	0.49
1:A:280:VAL:O	1:A:284:ILE:HB	2.13	0.49
1:B:362:GLU:C	1:B:364:GLY:H	2.16	0.49
1:A:476:GLU:HG3	1:A:502:HIS:CD2	2.48	0.48
1:A:547:ARG:NH1	1:A:550:GLU:HG3	2.28	0.48
1:A:1:CYS:SG	2:E:378:PHE:HZ	2.36	0.48
1:A:450:VAL:CG2	1:A:627:ARG:HD3	2.42	0.48
1:B:224:PHE:N	1:B:250:GLN:HB2	2.28	0.48
1:A:237:ILE:HG12	1:A:257:ILE:HG12	1.95	0.48
1:A:293:TRP:HH2	1:A:301:GLU:HG2	1.77	0.48
1:A:475:ILE:O	1:A:480:LYS:HG2	2.13	0.48
1:A:346:VAL:O	1:A:350:GLN:HG3	2.14	0.47
1:A:477:LYS:C	1:A:479:VAL:H	2.16	0.47
1:B:42:ASN:OD1	1:B:42:ASN:N	2.47	0.47
1:B:399:LEU:HD21	1:B:598:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LYS:HG3	1:B:637:CYS:SG	2.54	0.47
1:B:224:PHE:CD2	1:B:253:GLU:HA	2.49	0.47
1:A:490:LEU:HB3	1:A:493:ALA:HB3	1.95	0.47
3:B:701:BX7:N10	3:B:701:BX7:H13	2.30	0.47
2:E:369:GLU:HB3	2:E:370:LYS:H	1.42	0.47
1:A:452:ASP:OD2	1:B:357:ARG:NH2	2.48	0.47
1:B:454:TYR:HD2	1:B:522:ILE:HD11	1.79	0.47
1:B:585:PHE:CE1	2:E:371:PRO:HB2	2.50	0.47
1:A:535:THR:HG22	1:A:539:GLN:NE2	2.29	0.47
1:B:462:THR:HA	1:B:465:VAL:HG12	1.97	0.47
1:B:540:GLU:HG3	1:B:615:LYS:HG3	1.97	0.47
1:A:527:SER:HB2	1:A:528:PRO:HD2	1.97	0.47
1:A:473:ARG:HG3	1:A:477:LYS:CD	2.45	0.46
1:B:257:ILE:HD11	1:B:259:TRP:CZ2	2.50	0.46
1:B:351:GLU:CD	1:B:627:ARG:HH22	2.19	0.46
1:B:525:ARG:O	1:B:532:LEU:HB2	2.15	0.46
1:B:224:PHE:H	1:B:250:GLN:CB	2.26	0.46
1:B:351:GLU:OE1	1:B:627:ARG:NH2	2.42	0.46
1:B:368:GLN:HG3	1:B:369:HIS:ND1	2.31	0.46
1:A:45:PHE:HA	1:A:45:PHE:HD1	1.60	0.46
1:B:223:PRO:HD2	1:B:227:PRO:HA	1.98	0.46
1:B:547:ARG:NH1	1:B:550:GLU:HG3	2.31	0.46
1:A:628:LYS:HB2	1:A:628:LYS:HE3	1.83	0.46
1:B:319:MET:HG3	1:B:439:MET:SD	2.55	0.46
1:B:495:LEU:H	1:B:499:SER:HB2	1.82	0.45
1:A:373:THR:HG21	1:A:379:ILE:HG13	1.99	0.45
1:B:474:ASN:HB3	1:B:651:THR:HG21	1.99	0.45
1:B:317:GLN:HE21	1:B:387:LEU:HD12	1.82	0.45
1:B:446:LEU:O	1:B:450:VAL:HG23	2.17	0.45
1:A:126:LEU:HB3	1:A:131:ILE:O	2.17	0.45
1:A:397:ILE:HD12	1:A:424:TYR:CD2	2.52	0.45
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.82	0.44
1:A:331:THR:O	1:A:334:VAL:HG12	2.17	0.44
1:A:357:ARG:HD2	1:B:448:GLU:HG2	1.98	0.44
1:B:354:TYR:CE2	1:B:355:GLU:HG3	2.52	0.44
1:B:389:THR:HG23	1:B:617:GLU:HG3	1.99	0.44
1:A:134:ARG:NH1	1:A:198:TYR:O	2.47	0.44
1:B:136:ILE:O	1:B:206:SER:HB2	2.18	0.44
1:A:460:LYS:HA	1:A:463:GLU:HB3	1.99	0.44
1:B:223:PRO:HA	1:B:250:GLN:HG3	2.00	0.44
1:B:549:VAL:HG23	1:B:550:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HA	1:B:37:VAL:O	2.17	0.44
1:B:18:GLY:HA3	3:B:701:BX7:C33	2.47	0.44
1:B:186:GLU:O	1:B:190:LEU:HD23	2.17	0.43
1:B:371:PRO:HG2	1:B:379:ILE:HD11	2.00	0.43
1:A:225:GLU:CG	1:A:230:ASN:HB2	2.48	0.43
1:B:47:ARG:NH1	1:B:52:GLN:OE1	2.51	0.43
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.71	0.43
1:A:304:ASP:O	1:A:308:ARG:HG3	2.18	0.43
1:A:316:LEU:HD21	1:A:442:GLY:HA3	1.99	0.43
1:B:114:ILE:HG23	1:B:117:ARG:NH2	2.34	0.43
1:A:70:LEU:HD13	1:A:86:MET:HE3	2.01	0.43
1:B:399:LEU:CD2	1:B:598:MET:HG3	2.49	0.43
1:B:504:LYS:HB2	1:B:504:LYS:HE2	1.85	0.43
1:B:293:TRP:CH2	1:B:301:GLU:HG2	2.53	0.43
1:B:468:LEU:HD23	1:B:468:LEU:HA	1.82	0.43
1:B:242:PRO:HG2	1:B:245:ALA:HB2	2.00	0.42
1:B:527:SER:HB2	1:B:528:PRO:HD2	2.00	0.42
1:B:284:ILE:HA	1:B:284:ILE:HD12	1.76	0.42
1:A:270:SER:CB	1:A:323:LYS:HD2	2.45	0.42
1:B:268:SER:HB3	1:B:427:ARG:HH22	1.84	0.42
1:A:14:ILE:HD11	1:A:17:GLN:CG	2.49	0.42
1:B:198:TYR:HB3	1:B:202:VAL:CG1	2.49	0.42
1:B:399:LEU:H	1:B:399:LEU:HD22	1.85	0.42
1:B:403:HIS:NE2	1:B:405:ARG:HD3	2.35	0.42
3:A:701:BX7:H13	3:A:701:BX7:H17	2.02	0.42
1:B:80:ARG:HD2	1:B:80:ARG:HA	1.81	0.42
1:B:616:SER:O	1:B:620:MET:HB2	2.19	0.42
1:B:246:ILE:HD13	1:B:246:ILE:HA	1.55	0.42
1:B:487:LYS:NZ	1:B:489:ASN:HB2	2.35	0.42
1:A:455:ASN:HA	1:A:458:VAL:HG12	2.01	0.41
1:A:351:GLU:CD	1:A:627:ARG:HH22	2.23	0.41
1:B:79:THR:OG1	1:B:80:ARG:N	2.53	0.41
1:A:408:LEU:HA	1:A:408:LEU:HD23	1.82	0.41
1:A:422:VAL:HG12	1:A:556:LEU:HD13	2.01	0.41
1:B:454:TYR:CD2	1:B:522:ILE:HD11	2.54	0.41
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.91	0.41
1:A:68:VAL:HG13	1:A:156:THR:HB	2.02	0.41
1:A:296:ASP:OD1	1:A:296:ASP:N	2.53	0.41
1:A:470:PHE:CZ	1:B:470:PHE:HB3	2.56	0.41
1:B:331:THR:OG1	1:B:363:LEU:O	2.38	0.41
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HA	1:A:284:ILE:HD12	1.77	0.41
1:B:91:CYS:SG	1:B:145:ILE:HG12	2.61	0.41
1:B:577:TYR:O	1:B:581:GLN:HG2	2.21	0.41
1:A:2:GLN:HB2	1:A:9:TRP:NE1	2.35	0.41
1:B:356:GLY:HA2	1:B:445:TRP:CG	2.56	0.41
1:A:133:HIS:NE2	1:A:136:ILE:HG12	2.36	0.41
1:A:480:LYS:NZ	1:A:498:ILE:HD13	2.36	0.41
1:A:233:VAL:O	1:A:237:ILE:HG13	2.20	0.40
1:A:336:HIS:NE2	1:A:361:LEU:HD12	2.36	0.40
1:B:416:LYS:HG3	1:B:563:TYR:CZ	2.56	0.40
1:A:222:ARG:HB2	1:A:249:VAL:HG12	2.04	0.40
1:B:354:TYR:CZ	1:B:355:GLU:HG3	2.56	0.40
3:B:701:BX7:O04	3:B:701:BX7:N07	2.45	0.40
2:E:369:GLU:HG2	2:E:371:PRO:CD	2.48	0.40
1:B:190:LEU:HD11	1:B:191:ARG:HH11	1.85	0.40
1:B:397:ILE:HD12	1:B:424:TYR:CD2	2.56	0.40
1:B:443:VAL:HG13	1:B:619:TRP:CH2	2.57	0.40
1:A:519:LEU:HD12	1:A:519:LEU:HA	1.91	0.40
1:B:617:GLU:HG2	1:B:621:ARG:NH1	2.36	0.40
1:B:2:GLN:HB2	1:B:9:TRP:NE1	2.37	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	631/665 (95%)	588 (93%)	40 (6%)	3 (0%)	29	66
1	B	639/665 (96%)	605 (95%)	29 (4%)	5 (1%)	19	56
2	D	12/39 (31%)	7 (58%)	4 (33%)	1 (8%)	1	4
2	E	10/39 (26%)	6 (60%)	1 (10%)	3 (30%)	0	0
All	All	1292/1408 (92%)	1206 (93%)	74 (6%)	12 (1%)	17	54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	370	LYS
1	A	494	GLU
1	B	196	LYS
2	E	369	GLU
1	A	289	GLN
1	B	78	THR
1	B	195	GLN
2	E	370	LYS
1	A	348	SER
1	B	491	GLU
2	E	371	PRO
1	B	488	VAL

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	565/590 (96%)	497 (88%)	68 (12%)	5	21
1	B	572/590 (97%)	506 (88%)	66 (12%)	5	23
2	D	13/36 (36%)	12 (92%)	1 (8%)	13	42
2	E	12/36 (33%)	10 (83%)	2 (17%)	2	9
All	All	1162/1252 (93%)	1025 (88%)	137 (12%)	5	22

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	LEU
1	A	-2	ASP
1	A	8	LEU
1	A	10	LEU
1	A	37	VAL
1	A	41	ASN
1	A	45	PHE
1	A	47	ARG

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Mol	Chain	Res	Type
1	A	49	VAL
1	A	68	VAL
1	A	78	THR
1	A	83	VAL
1	A	84	LEU
1	A	85	ILE
1	A	110	SER
1	A	133	HIS
1	A	134	ARG
1	A	180	LEU
1	A	187	ARG
1	A	190	LEU
1	A	191	ARG
1	A	193	ASP
1	A	194	HIS
1	A	196	LYS
1	A	197	LYS
1	A	198	TYR
1	A	202	VAL
1	A	203	ASP
1	A	225	GLU
1	A	231	LYS
1	A	249	VAL
1	A	254	ASN
1	A	258	ASP
1	A	265	LEU
1	A	278	THR
1	A	280	VAL
1	A	284	ILE
1	A	310	VAL
1	A	313	VAL
1	A	331	THR
1	A	340	TYR
1	A	347	SER
1	A	360	VAL
1	A	361	LEU
1	A	363	LEU
1	A	365	ARG
1	A	376	GLU
1	A	385	GLU
1	A	386	GLN
1	A	392	LEU

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Mol	Chain	Res	Type
1	A	399	LEU
1	A	459	HIS
1	A	464	VAL
1	A	470	PHE
1	A	471	CYS
1	A	477	LYS
1	A	478	THR
1	A	512	GLN
1	A	522	ILE
1	A	526	LEU
1	A	531	LEU
1	A	549	VAL
1	A	568	LYS
1	A	575	LEU
1	A	590	LEU
1	A	609	TYR
1	A	623	MET
1	A	648	GLN
1	B	-2	ASP
1	B	1	CYS
1	B	42	ASN
1	B	43	ILE
1	B	51	VAL
1	B	53	MET
1	B	54	ARG
1	B	58	VAL
1	B	59	LEU
1	B	65	LYS
1	B	69	LYS
1	B	78	THR
1	B	79	THR
1	B	84	LEU
1	B	102	SER
1	B	127	ARG
1	B	133	HIS
1	B	134	ARG
1	B	144	VAL
1	B	178	GLU
1	B	187	ARG
1	B	194	HIS
1	B	197	LYS
1	B	204	LEU

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Mol	Chain	Res	Type
1	B	231	LYS
1	B	246	ILE
1	B	250	GLN
1	B	257	ILE
1	B	265	LEU
1	B	313	VAL
1	B	317	GLN
1	B	328	SER
1	B	334	VAL
1	B	352	LEU
1	B	359	LEU
1	B	363	LEU
1	B	384	ARG
1	B	386	GLN
1	B	392	LEU
1	B	395	GLU
1	B	403	HIS
1	B	423	CYS
1	B	449	LEU
1	B	461	LYS
1	B	466	ILE
1	B	467	THR
1	B	468	LEU
1	B	470	PHE
1	B	483	GLU
1	B	486	MET
1	B	487	LYS
1	B	506	LEU
1	B	515	ILE
1	B	522	ILE
1	B	526	LEU
1	B	534	ASP
1	B	549	VAL
1	B	573	ARG
1	B	574	ARG
1	B	575	LEU
1	B	579	GLU
1	B	603	GLU
1	B	624	LEU
1	B	651	THR
1	B	652	ASN
1	B	653	GLU

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Mol	Chain	Res	Type
2	D	377	ASP
2	E	370	LYS
2	E	376	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	41	ASN
1	A	250	GLN
1	A	368	GLN
1	A	539	GLN
1	B	81	HIS
1	B	330	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	701	-	35,37,37	4.96	20 (57%)	42,49,49	2.99	18 (42%)
3	BX7	A	701	-	35,37,37	4.93	20 (57%)	42,49,49	3.22	16 (38%)

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	B	701	-	-	7/22/31/31	0/4/4/4
3	BX7	A	701	-	-	3/22/31/31	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	BX7	C31-S02	-13.56	1.55	1.72
3	A	701	BX7	C31-S02	-13.16	1.56	1.72
3	B	701	BX7	C26-N07	11.65	1.52	1.34
3	A	701	BX7	C26-N07	10.97	1.51	1.34
3	A	701	BX7	C27-N08	9.25	1.55	1.36
3	B	701	BX7	C27-N08	9.03	1.54	1.36
3	B	701	BX7	C16-N06	8.34	1.52	1.37
3	A	701	BX7	C16-N06	8.27	1.52	1.37
3	B	701	BX7	C16-N05	7.59	1.50	1.36
3	A	701	BX7	C16-N05	7.45	1.50	1.36
3	A	701	BX7	C28-I01	7.29	2.26	2.10
3	B	701	BX7	C28-I01	7.09	2.26	2.10
3	A	701	BX7	C22-N08	6.98	1.56	1.40
3	B	701	BX7	C15-N05	6.94	1.62	1.47
3	A	701	BX7	C15-N05	6.74	1.61	1.47
3	B	701	BX7	C33-C32	6.73	1.61	1.39
3	B	701	BX7	C22-N08	6.72	1.55	1.40
3	A	701	BX7	C33-C32	6.42	1.60	1.39
3	A	701	BX7	C29-N09	5.53	1.45	1.33
3	B	701	BX7	C29-N09	5.06	1.44	1.33
3	A	701	BX7	C14-N05	-4.80	1.36	1.47
3	B	701	BX7	C14-N05	-4.61	1.37	1.47
3	A	701	BX7	C27-N11	4.07	1.40	1.34
3	B	701	BX7	C27-N11	3.62	1.39	1.34
3	A	701	BX7	C33-C34	3.61	1.45	1.34
3	B	701	BX7	C33-C34	3.56	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	BX7	C30-C28	3.52	1.44	1.39
3	A	701	BX7	C34-S02	-3.23	1.55	1.71
3	B	701	BX7	C12-C15	-3.16	1.40	1.51
3	B	701	BX7	C34-S02	-3.15	1.55	1.71
3	A	701	BX7	C12-C15	-3.12	1.40	1.51
3	B	701	BX7	C30-C28	2.74	1.43	1.39
3	B	701	BX7	C19-C23	2.70	1.62	1.51
3	B	701	BX7	C13-C14	2.53	1.60	1.51
3	A	701	BX7	C13-C14	2.50	1.60	1.51
3	A	701	BX7	C19-C23	2.35	1.60	1.51
3	A	701	BX7	C21-N07	-2.17	1.41	1.45
3	B	701	BX7	C17-N06	2.13	1.46	1.41
3	A	701	BX7	C18-C17	2.07	1.42	1.39
3	B	701	BX7	C18-C17	2.03	1.42	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	BX7	N11-C27-N10	-10.36	116.74	126.55
3	B	701	BX7	N11-C27-N10	-9.18	117.85	126.55
3	A	701	BX7	C33-C34-S02	-7.23	107.12	112.98
3	A	701	BX7	C25-C22-C18	-7.02	111.32	119.65
3	B	701	BX7	C25-C22-C18	-6.44	112.01	119.65
3	A	701	BX7	C26-C28-I01	6.15	127.40	120.92
3	B	701	BX7	C26-C28-I01	6.14	127.39	120.92
3	A	701	BX7	C24-C25-C22	5.53	126.34	119.72
3	B	701	BX7	C33-C34-S02	-5.31	108.67	112.98
3	A	701	BX7	C15-N05-C14	-5.21	104.19	111.34
3	A	701	BX7	C30-N11-C27	4.75	123.04	115.88
3	A	701	BX7	N07-C26-N10	-4.43	112.84	118.50
3	B	701	BX7	C15-N05-C14	-4.34	105.39	111.34
3	B	701	BX7	N07-C26-N10	-4.32	112.99	118.50
3	B	701	BX7	C30-N11-C27	4.23	122.26	115.88
3	B	701	BX7	C24-C25-C22	4.11	124.65	119.72
3	B	701	BX7	N06-C16-N05	4.10	120.58	115.89
3	B	701	BX7	C24-C20-C17	-3.98	114.96	119.72
3	A	701	BX7	C24-C20-C17	-3.60	115.42	119.72
3	B	701	BX7	C22-C18-C17	3.28	124.62	119.64
3	A	701	BX7	C30-C28-I01	3.06	122.75	118.80
3	B	701	BX7	C21-N07-C26	-3.01	117.85	122.95
3	A	701	BX7	C22-C18-C17	2.90	124.05	119.64
3	B	701	BX7	C19-C21-N07	-2.83	103.88	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	BX7	N08-C27-N11	2.66	124.53	116.28
3	A	701	BX7	C20-C17-C18	2.60	122.74	119.65
3	B	701	BX7	C31-C29-N09	2.45	119.01	115.59
3	B	701	BX7	C30-C28-I01	2.34	121.81	118.80
3	A	701	BX7	N06-C16-N05	2.27	118.48	115.89
3	A	701	BX7	C21-N07-C26	-2.23	119.18	122.95
3	B	701	BX7	O03-C16-N05	-2.22	118.66	121.78
3	A	701	BX7	O04-C29-N09	2.15	126.89	122.61
3	B	701	BX7	N08-C27-N11	2.07	122.72	116.28
3	B	701	BX7	C19-C23-N09	2.05	118.06	112.21

There are no chirality outliers.

All (10) 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	B	701	BX7	C21-C19-C23-N09
3	B	701	BX7	C20-C17-N06-C16
3	B	701	BX7	C18-C17-N06-C16
3	B	701	BX7	C19-C23-N09-C29
3	A	701	BX7	C18-C17-N06-C16
3	A	701	BX7	C20-C17-N06-C16
3	A	701	BX7	C23-C19-C21-N07
3	B	701	BX7	C23-C19-C21-N07

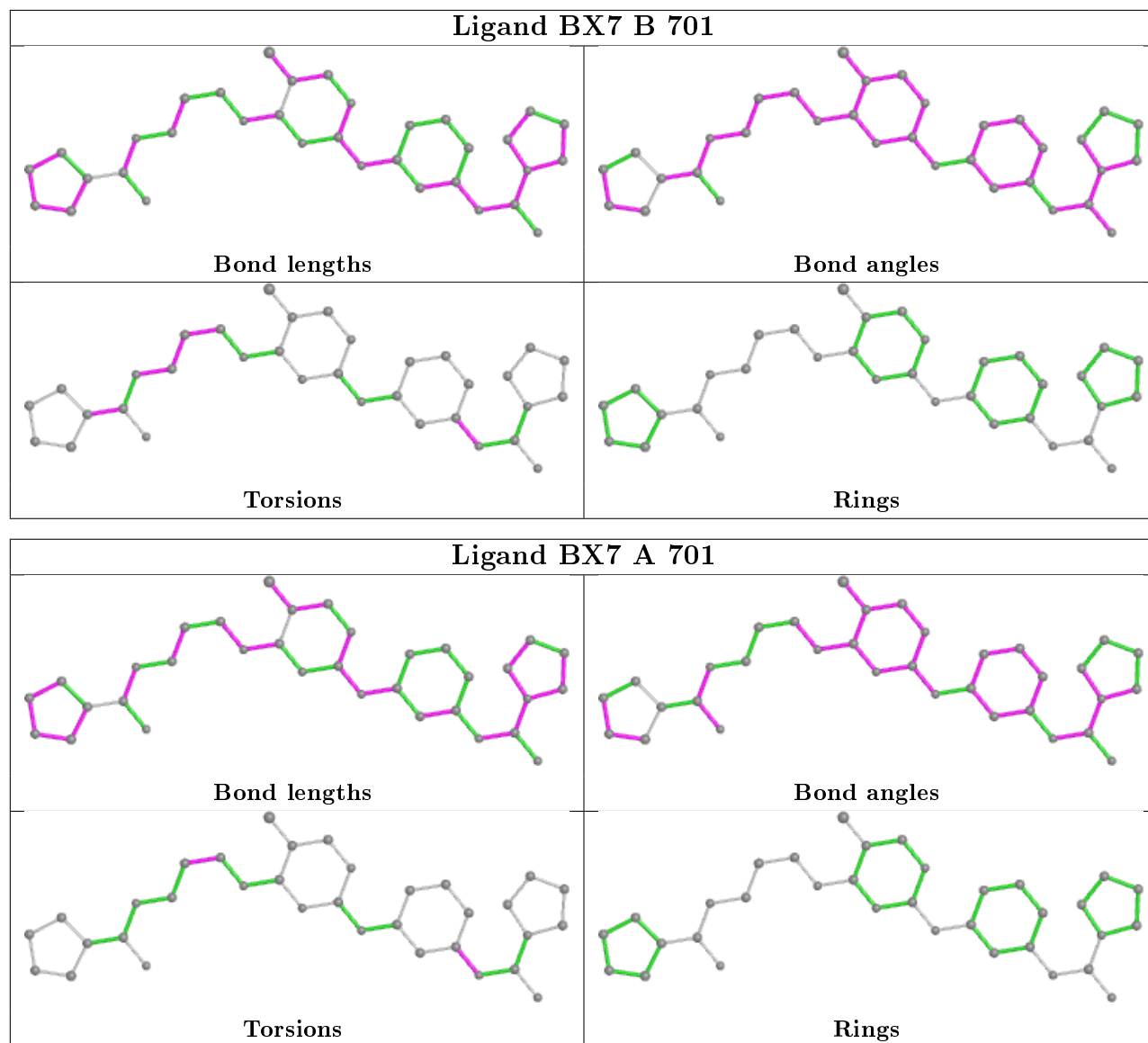
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	BX7	3	0
3	A	701	BX7	2	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

6.1 Protein, DNA and RNA chains

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	636/665 (95%)	0.10	16 (2%) 57 43	60, 90, 161, 217	0
1	B	643/665 (96%)	0.23	26 (4%) 38 24	64, 108, 190, 256	0
2	D	14/39 (35%)	0.74	2 (14%) 2 1	80, 104, 142, 143	0
2	E	12/39 (30%)	1.34	4 (33%) 0 0	88, 112, 150, 158	0
All	All	1305/1408 (92%)	0.18	48 (3%) 41 26	60, 99, 176, 256	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	482	TYR	6.5
1	B	486	MET	5.7
1	B	481	VAL	5.4
2	E	379	SER	5.3
1	A	478	THR	4.7
2	E	368	MET	4.5
1	A	191	ARG	4.4
1	B	194	HIS	4.3
1	A	481	VAL	4.1
1	B	484	LYS	4.0
1	B	485	LEU	3.9
1	B	490	LEU	3.9
1	A	160	ALA	3.9
1	A	495	LEU	3.8
1	A	46	LEU	3.8
1	B	489	ASN	3.7
1	A	493	ALA	3.3
1	B	487	LYS	3.2
1	B	648	GLN	3.1
1	B	500	ASP	3.1
1	B	652	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	369	GLU	3.0
2	D	368	MET	3.0
1	A	192	LYS	2.9
1	B	227	PRO	2.7
1	A	494	GLU	2.6
1	B	195	GLN	2.6
2	D	369	GLU	2.6
1	B	493	ALA	2.5
1	B	175	GLY	2.4
1	B	191	ARG	2.4
1	B	44	SER	2.4
1	B	501	ILE	2.4
1	A	196	LYS	2.4
1	A	194	HIS	2.4
1	A	477	LYS	2.3
1	B	488	VAL	2.3
1	B	159	GLY	2.3
1	B	361	LEU	2.3
1	A	489	ASN	2.3
1	B	199	GLY	2.2
2	E	378	PHE	2.2
1	B	505	LEU	2.2
1	A	492	ALA	2.2
1	A	195	GLN	2.1
1	B	50	ASP	2.1
1	B	496	GLY	2.0
1	A	479	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

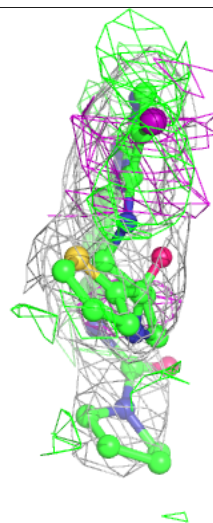
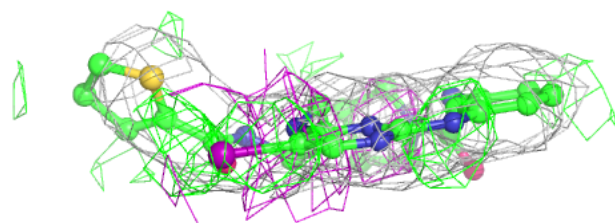
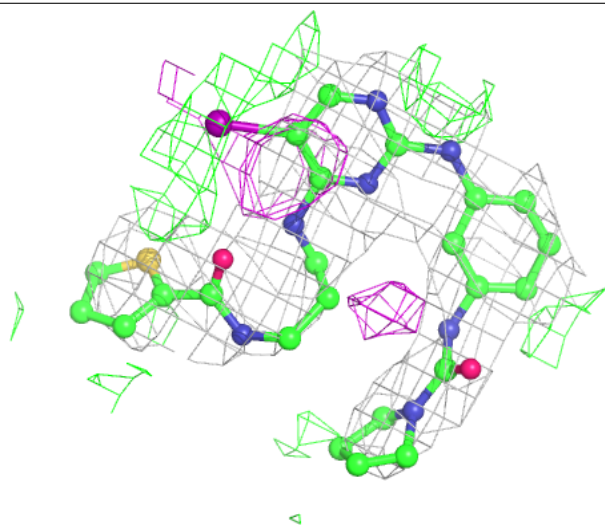
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BX7	B	701	34/34	0.93	0.31	40,106,142,152	0
3	BX7	A	701	34/34	0.93	0.27	34,75,122,129	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.

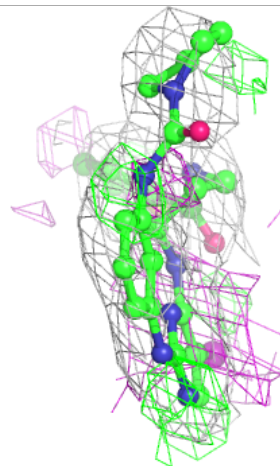
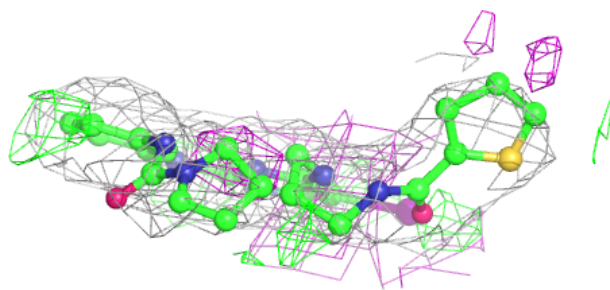
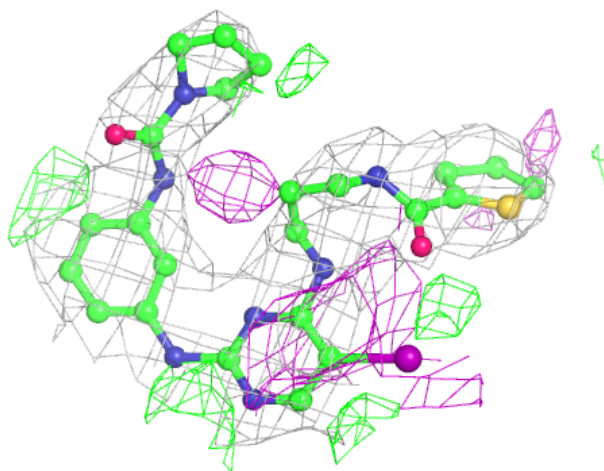
Electron density around BX7 B 701:

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.