



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:05 pm BST

PDB ID : 2Q2Y
Title : Crystal Structure of KSP in complex with Inhibitor 1
Authors : Yan, Y.
Deposited on : 2007-05-29
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

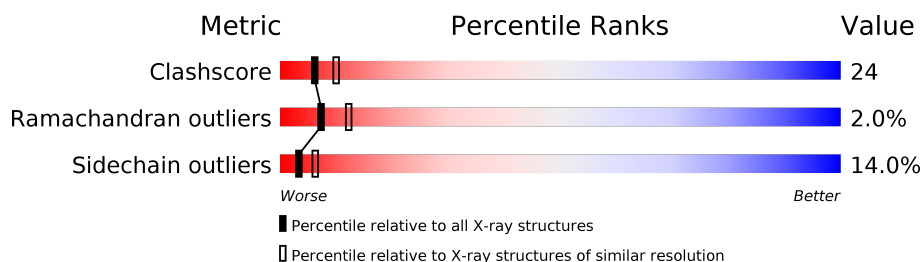
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5559 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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			
1	B	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

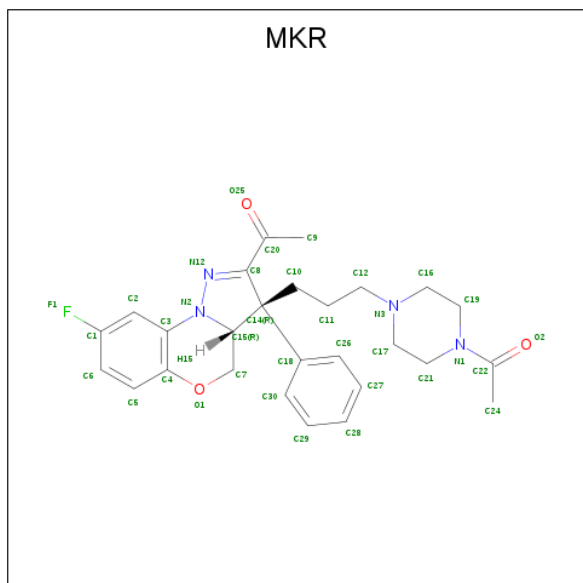
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 1-{(3R,3AR)-3-[3-(4-ACETYLPYPERAZIN-1-YL)PROPYL]-8-FLUORO-3-PHENYL-3A,4-DIHYDRO-3H-PYRAZOLO[5,1-C][1,4]BENZOXAZIN-2-YL}ETHANONE (three-letter code: MKR) (formula: C₂₇H₃₁FN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
4	B	1	Total	C	F	N	O	0	0
			35	27	1	4	3		

- Molecule 5 is water.

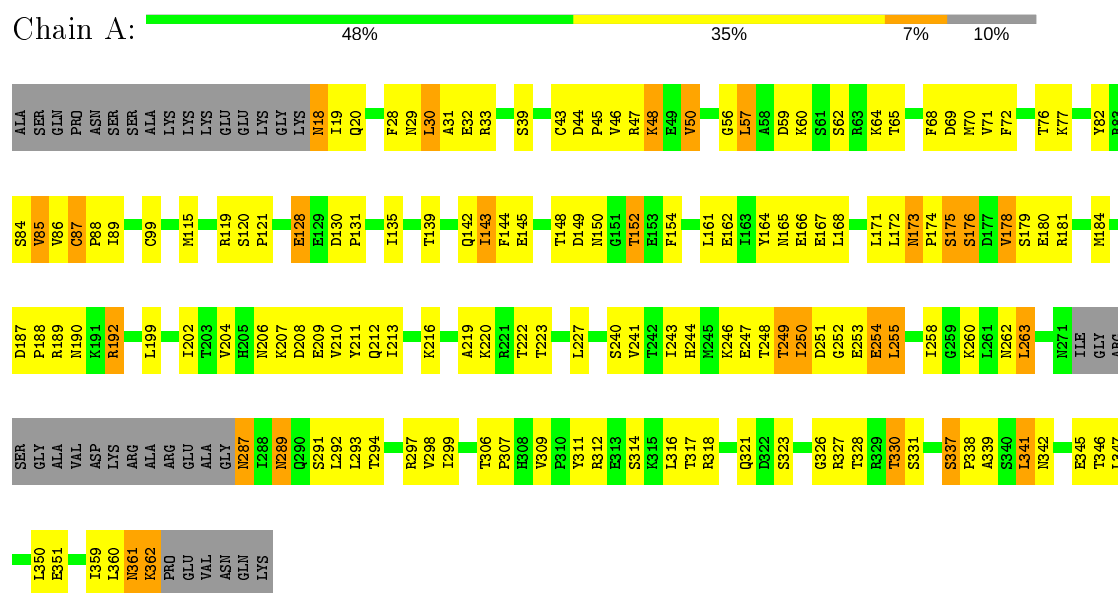
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total	O	0	0
			126	126		
5	B	119	Total	O	0	0
			119	119		

3 Residue-property plots

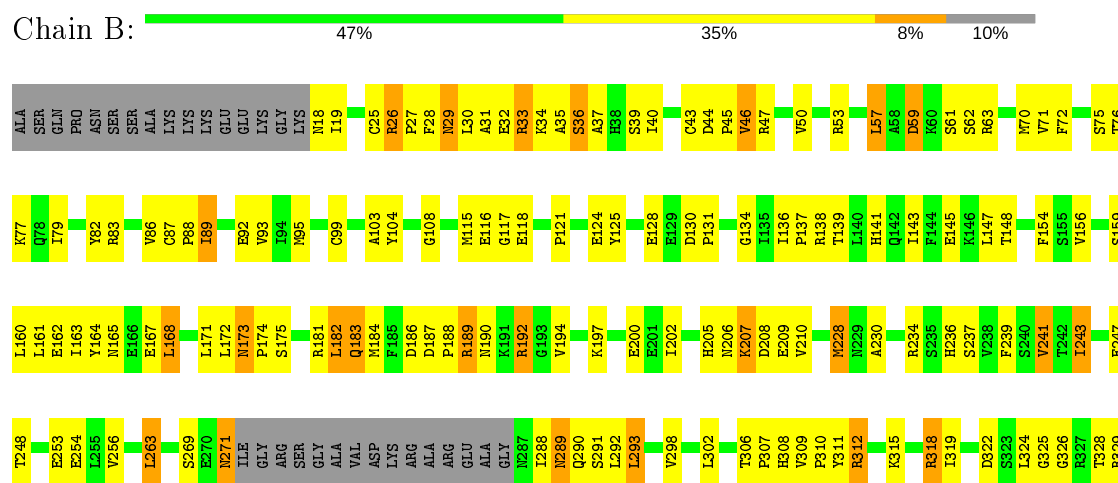
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Kinesin-like protein KIF11



- Molecule 1: Kinesin-like protein KIF11





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.86 Å 79.80 Å 159.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (39.90-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	BUSTER-TNT 1.9.2	Depositor
R, R_{free}	0.190 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5559	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

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: MG, MKR, ADP

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	0.61	0/2632	0.82	2/3559 (0.1%)
1	B	0.62	0/2632	0.79	0/3559
All	All	0.62	0/5264	0.81	2/7118 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	A	263	LEU	CA-CB-CG	-5.47	102.72	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	A	2594	0	2618	113	0
1	B	2594	0	2617	146	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	35	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	35	0	31	2	0
5	A	126	0	0	3	0
5	B	119	0	0	12	0
All	All	5559	0	5321	260	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 24.

All (260) 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:B:190:ASN:HB2	1:B:192:ARG:HH12	1.06	1.13
1:A:167:GLU:HG2	1:A:181:ARG:HE	1.16	1.04
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.37	1.03
1:B:312:ARG:HB3	1:B:312:ARG:HH11	1.29	0.96
1:B:143:ILE:HD13	1:B:243:ILE:HD11	1.46	0.95
1:B:190:ASN:HB2	1:B:192:ARG:NH1	1.87	0.89
1:B:173:ASN:HD21	1:B:175:SER:HB2	1.39	0.88
1:A:204:VAL:HG22	1:A:213:ILE:CD1	2.06	0.85
1:B:318:ARG:HG2	1:B:318:ARG:HH11	1.42	0.85
1:B:43:CYS:O	1:B:45:PRO:HD3	1.80	0.81
1:A:250:ILE:HD13	1:A:250:ILE:H	1.47	0.79
1:A:251:ASP:HB2	1:A:253:GLU:HG3	1.66	0.78
1:A:247:GLU:OE2	1:A:255:LEU:HD23	1.83	0.77
1:A:204:VAL:HG22	1:A:213:ILE:HD12	1.67	0.76
1:B:181:ARG:HH11	1:B:181:ARG:HG2	1.51	0.75
1:A:187:ASP:OD2	1:A:188:PRO:HD2	1.86	0.75
1:B:190:ASN:CB	1:B:192:ARG:HH12	1.95	0.74
1:B:315:LYS:O	1:B:319:ILE:HG13	1.87	0.74
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.68	0.74
1:A:247:GLU:O	1:A:254:GLU:HA	1.89	0.73
1:B:26:ARG:NH1	1:B:337:SER:HB2	2.04	0.72
1:A:167:GLU:HG2	1:A:181:ARG:NE	1.99	0.72
1:B:183:GLN:NE2	1:B:197:LYS:HD3	2.03	0.72
1:B:189:ARG:HD3	5:B:685:HOH:O	1.89	0.72
1:A:162:GLU:HG3	1:A:171:LEU:CD2	2.18	0.71
1:A:62:SER:HB2	5:A:660:HOH:O	1.91	0.70
1:B:139:THR:O	1:B:143:ILE:HG13	1.92	0.70
1:B:183:GLN:HE22	1:B:197:LYS:HD3	1.56	0.69
1:A:152:THR:HG23	1:A:247:GLU:HA	1.73	0.69
1:B:192:ARG:HG2	1:B:192:ARG:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:OG	1:A:342:ASN:ND2	2.26	0.68
1:A:85:VAL:O	1:A:89:ILE:HD12	1.93	0.68
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.75	0.67
1:B:318:ARG:HG2	1:B:318:ARG:NH1	2.03	0.67
1:A:341:LEU:H	1:A:341:LEU:HD13	1.59	0.66
1:B:28:PHE:HB3	1:B:32:GLU:HB2	1.77	0.66
1:A:152:THR:HG23	1:A:247:GLU:CA	2.26	0.66
1:A:30:LEU:HA	1:A:33:ARG:HB2	1.78	0.65
1:A:346:THR:HG22	1:A:350:LEU:HD12	1.77	0.65
1:A:287:ASN:N	1:A:287:ASN:HD22	1.95	0.65
1:B:351:GLU:O	1:B:355:ARG:HG3	1.97	0.64
1:A:341:LEU:H	1:A:341:LEU:CD1	2.11	0.64
1:A:43:CYS:O	1:A:45:PRO:HD3	1.98	0.64
1:B:186:ASP:O	1:B:188:PRO:HD3	1.97	0.64
1:A:44:ASP:OD2	1:A:47:ARG:HB2	1.98	0.64
1:B:325:GLY:H	1:B:361:ASN:ND2	1.97	0.63
1:A:176:SER:HB2	1:A:180:GLU:OE1	1.99	0.63
1:A:323:SER:O	1:A:330:THR:HG21	1.98	0.63
1:A:115:MET:CE	1:A:263:LEU:HB3	2.29	0.62
1:A:32:GLU:HA	5:A:705:HOH:O	1.98	0.62
1:B:290:GLN:NE2	1:B:290:GLN:HA	2.14	0.62
1:A:327:ARG:O	1:A:362:LYS:HE2	2.00	0.62
1:B:173:ASN:HD21	1:B:175:SER:CB	2.10	0.62
1:B:206:ASN:OD1	1:B:208:ASP:HB2	2.01	0.61
1:B:30:LEU:HA	1:B:33:ARG:CG	2.31	0.60
1:B:145:GLU:O	1:B:148:THR:HG22	2.01	0.60
1:A:167:GLU:CG	1:A:181:ARG:HE	2.04	0.60
1:B:128:GLU:OE2	1:B:207:LYS:NZ	2.32	0.60
1:B:26:ARG:HH12	1:B:337:SER:HB2	1.65	0.60
1:B:25:CYS:HB2	1:B:43:CYS:SG	2.41	0.60
1:B:172:LEU:O	1:B:174:PRO:HD3	2.02	0.60
1:A:119:ARG:HD2	4:A:604:MKR:C29	2.31	0.59
1:A:178:VAL:HG13	1:A:220:LYS:HE2	1.83	0.59
1:A:48:LYS:HA	1:A:71:VAL:HG22	1.84	0.59
1:B:18:ASN:HB3	1:B:360:LEU:HA	1.85	0.59
1:A:119:ARG:HD2	4:A:604:MKR:C30	2.32	0.59
1:B:329:ARG:HG2	1:B:329:ARG:HH11	1.68	0.58
1:B:161:LEU:HD11	1:B:168:LEU:HB3	1.84	0.58
1:B:47:ARG:HG3	1:B:47:ARG:O	2.04	0.58
1:A:70:MET:HE1	1:A:84:SER:HB3	1.85	0.58
1:B:253:GLU:HG2	1:B:254:GLU:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASP:OD1	1:B:46:VAL:HG23	2.03	0.58
1:A:341:LEU:N	1:A:341:LEU:CD1	2.67	0.57
1:B:19:ILE:HD12	1:B:359:ILE:HB	1.87	0.57
1:B:271:ASN:HD22	1:B:271:ASN:C	2.08	0.57
1:B:35:ALA:HB2	5:B:683:HOH:O	2.03	0.57
1:B:318:ARG:CG	1:B:318:ARG:HH11	2.17	0.57
1:B:325:GLY:H	1:B:361:ASN:HD21	1.52	0.56
1:A:50:VAL:CG1	1:A:68:PHE:HE1	2.18	0.56
1:B:160:LEU:HB3	1:B:172:LEU:HG	1.88	0.56
1:B:298:VAL:HG13	1:B:309:VAL:CG1	2.36	0.56
1:B:312:ARG:HB3	1:B:312:ARG:NH1	2.10	0.56
1:B:164:TYR:CE1	1:B:228:MET:HG2	2.41	0.55
1:B:173:ASN:HD22	1:B:173:ASN:C	2.10	0.55
1:A:29:ASN:OD1	1:A:31:ALA:HB3	2.06	0.55
1:B:121:PRO:O	1:B:124:GLU:HG3	2.07	0.55
1:B:40:ILE:HD12	1:B:343:LEU:HD23	1.88	0.55
1:B:28:PHE:CD2	1:B:37:ALA:HB3	2.42	0.55
1:B:57:LEU:O	1:B:61:SER:HB3	2.07	0.55
1:B:156:VAL:HG13	1:B:241:VAL:HG23	1.89	0.54
1:A:312:ARG:HA	1:A:318:ARG:CG	2.38	0.54
1:B:173:ASN:ND2	1:B:175:SER:H	2.06	0.54
1:B:89:ILE:O	1:B:93:VAL:HG23	2.08	0.54
1:B:99:CYS:SG	1:B:329:ARG:HB3	2.48	0.53
1:A:306:THR:CG2	1:A:307:PRO:HD2	2.38	0.53
1:A:178:VAL:HG21	1:A:223:THR:OG1	2.09	0.53
1:A:248:THR:HG22	1:A:248:THR:O	2.08	0.53
1:B:173:ASN:HD22	1:B:175:SER:N	2.07	0.53
1:A:311:TYR:CD1	1:A:321:GLN:HB2	2.43	0.52
1:B:173:ASN:ND2	1:B:175:SER:N	2.57	0.52
1:B:134:GLY:O	1:B:137:PRO:HD2	2.08	0.52
1:B:192:ARG:HG3	5:B:649:HOH:O	2.08	0.52
1:B:173:ASN:HD22	1:B:175:SER:H	1.57	0.52
1:B:57:LEU:HD13	1:B:59:ASP:HB2	1.92	0.52
1:A:173:ASN:ND2	1:A:175:SER:H	2.08	0.51
1:A:184:MET:CE	1:A:318:ARG:NE	2.74	0.51
1:A:144:PHE:O	1:A:148:THR:HB	2.11	0.51
1:B:30:LEU:HA	1:B:33:ARG:HD3	1.92	0.51
1:A:207:LYS:C	1:A:209:GLU:H	2.14	0.51
1:B:341:LEU:HD23	1:B:341:LEU:H	1.76	0.51
1:A:72:PHE:CD1	1:A:76:THR:HG21	2.44	0.51
1:B:171:LEU:N	1:B:171:LEU:HD22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLY:C	1:B:118:GLU:HG3	2.30	0.51
1:B:143:ILE:HD13	1:B:243:ILE:CD1	2.29	0.51
1:B:326:GLY:O	1:B:362:LYS:N	2.36	0.51
1:B:346:THR:HG22	1:B:350:LEU:HD22	1.91	0.51
1:A:154:PHE:HA	1:A:244:HIS:O	2.11	0.50
1:B:289:ASN:HA	5:B:692:HOH:O	2.11	0.50
1:A:248:THR:HA	1:A:253:GLU:O	2.11	0.50
1:B:205:HIS:HB2	1:B:209:GLU:OE1	2.10	0.50
1:A:29:ASN:O	1:A:32:GLU:N	2.40	0.50
1:B:181:ARG:HG2	1:B:181:ARG:NH1	2.25	0.50
1:A:317:THR:O	1:A:321:GLN:HB3	2.12	0.49
1:A:306:THR:HG23	1:A:307:PRO:HD2	1.94	0.49
1:B:40:ILE:CD1	1:B:343:LEU:HD23	2.41	0.49
1:A:28:PHE:HD2	1:A:32:GLU:CB	2.24	0.49
1:B:29:ASN:OD1	1:B:32:GLU:HG3	2.13	0.49
1:A:326:GLY:O	1:A:361:ASN:HB2	2.12	0.49
1:A:192:ARG:HG3	1:A:192:ARG:O	2.13	0.49
1:A:70:MET:HE1	1:A:72:PHE:HZ	1.78	0.49
1:A:152:THR:HG23	1:A:247:GLU:HB2	1.95	0.48
1:A:115:MET:HE1	1:A:263:LEU:HB3	1.95	0.48
1:A:289:ASN:HD22	1:A:292:LEU:H	1.60	0.48
1:A:82:TYR:HB2	5:A:612:HOH:O	2.13	0.48
1:B:79:ILE:HG13	1:B:83:ARG:HD2	1.94	0.48
1:B:57:LEU:HD13	1:B:59:ASP:CB	2.43	0.48
1:B:18:ASN:CB	1:B:360:LEU:HA	2.44	0.48
1:A:45:PRO:HA	1:A:71:VAL:HG23	1.95	0.48
1:A:254:GLU:OE2	1:A:254:GLU:O	2.31	0.48
1:A:56:GLY:O	1:A:57:LEU:O	2.31	0.48
1:B:171:LEU:CD2	1:B:171:LEU:N	2.77	0.48
1:B:79:ILE:O	1:B:83:ARG:HG3	2.14	0.48
1:A:128:GLU:OE1	1:A:207:LYS:HD3	2.14	0.47
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.14	0.47
1:A:294:THR:O	1:A:298:VAL:HG23	2.14	0.47
1:A:18:ASN:HB3	1:A:360:LEU:HA	1.96	0.47
1:B:162:GLU:HG3	1:B:237:SER:HA	1.96	0.47
1:B:116:GLU:HG2	4:B:605:MKR:C5	2.44	0.47
1:B:28:PHE:CE2	1:B:37:ALA:HB1	2.49	0.47
1:B:312:ARG:HB2	5:B:664:HOH:O	2.14	0.47
1:B:30:LEU:HA	1:B:33:ARG:HG3	1.97	0.47
1:B:28:PHE:CE2	1:B:37:ALA:CB	2.98	0.47
1:B:172:LEU:HB3	1:B:202:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:VAL:O	1:B:256:VAL:HG23	2.15	0.47
1:A:120:SER:HA	1:A:121:PRO:HD3	1.62	0.46
1:B:172:LEU:HB2	5:B:607:HOH:O	2.15	0.46
1:A:192:ARG:O	1:A:321:GLN:NE2	2.49	0.46
1:A:28:PHE:HD2	1:A:32:GLU:HB3	1.79	0.46
1:A:70:MET:HE1	1:A:72:PHE:CZ	2.51	0.46
1:B:308:HIS:HA	5:B:710:HOH:O	2.14	0.46
1:A:172:LEU:HB3	1:A:202:ILE:HD13	1.98	0.46
1:B:28:PHE:CD2	1:B:37:ALA:CB	2.98	0.46
1:B:298:VAL:HG13	1:B:309:VAL:HG12	1.98	0.46
1:A:20:GLN:O	1:A:331:SER:HA	2.16	0.46
1:B:115:MET:HB3	1:B:115:MET:HE2	1.72	0.46
1:B:156:VAL:CG1	1:B:241:VAL:HG23	2.46	0.46
1:A:338:PRO:HD2	1:A:339:ALA:H	1.82	0.45
1:A:50:VAL:CG1	1:A:68:PHE:CE1	2.99	0.45
1:B:192:ARG:HD2	5:B:649:HOH:O	2.16	0.45
1:B:205:HIS:HD2	1:B:209:GLU:OE2	2.00	0.45
1:B:248:THR:HA	1:B:253:GLU:O	2.17	0.45
1:B:72:PHE:HD1	1:B:76:THR:HG21	1.80	0.45
1:B:147:LEU:HB3	1:B:154:PHE:CD2	2.52	0.45
1:B:72:PHE:HB3	1:B:76:THR:OG1	2.16	0.45
1:B:138:ARG:HA	5:B:709:HOH:O	2.16	0.45
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.99	0.45
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.82	0.45
4:A:604:MKR:H30	4:A:604:MKR:H102	1.85	0.45
1:B:289:ASN:HB3	1:B:292:LEU:HB3	1.98	0.45
1:A:219:ALA:O	1:A:222:THR:HB	2.17	0.45
1:B:136:ILE:HD13	1:B:239:PHE:CG	2.52	0.45
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.97	0.45
1:A:298:VAL:HG13	1:A:309:VAL:CG1	2.47	0.45
1:B:182:LEU:HB3	1:B:197:LYS:O	2.17	0.45
1:B:309:VAL:HB	1:B:311:TYR:CE2	2.52	0.45
1:B:25:CYS:CB	1:B:43:CYS:SG	3.06	0.44
1:A:250:ILE:N	1:A:250:ILE:HD13	2.23	0.44
1:A:328:THR:HG22	1:A:330:THR:HG22	2.00	0.44
1:A:33:ARG:HD3	1:A:33:ARG:HA	1.77	0.44
1:B:288:ILE:HD12	1:B:293:LEU:HD23	1.98	0.44
1:A:249:THR:O	1:A:252:GLY:N	2.45	0.44
1:A:89:ILE:HG23	1:A:99:CYS:CB	2.47	0.44
1:A:291:SER:HB3	1:A:316:LEU:HB3	2.00	0.44
1:B:269:SER:HA	1:B:292:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:THR:CG2	1:B:307:PRO:CD	2.96	0.44
1:A:29:ASN:O	1:A:31:ALA:N	2.51	0.44
1:A:210:VAL:O	1:A:213:ILE:N	2.48	0.44
1:A:294:THR:HG22	1:A:317:THR:HG21	2.00	0.43
1:B:104:TYR:C	1:B:104:TYR:CD1	2.91	0.43
1:B:18:ASN:ND2	1:B:360:LEU:HD12	2.33	0.43
1:A:152:THR:HG23	1:A:247:GLU:CB	2.47	0.43
1:A:263:LEU:HA	1:A:263:LEU:HD23	1.64	0.43
1:B:77:LYS:HB3	5:B:658:HOH:O	2.18	0.43
1:B:28:PHE:HA	1:B:32:GLU:OE2	2.18	0.43
1:B:29:ASN:H	1:B:29:ASN:ND2	2.15	0.43
1:A:347:LEU:O	1:A:351:GLU:HB2	2.19	0.43
1:B:160:LEU:HG	1:B:171:LEU:HB2	2.01	0.43
1:B:322:ASP:O	1:B:328:THR:HB	2.19	0.43
1:B:362:LYS:HG2	5:B:688:HOH:O	2.18	0.43
1:A:164:TYR:C	1:A:164:TYR:CD1	2.92	0.43
1:A:69:ASP:O	1:A:70:MET:HG3	2.19	0.43
1:A:338:PRO:CD	1:A:339:ALA:H	2.32	0.42
1:B:103:ALA:HB2	1:B:115:MET:CG	2.49	0.42
1:B:173:ASN:HD22	1:B:174:PRO:N	2.17	0.42
1:B:306:THR:CG2	1:B:307:PRO:HD2	2.48	0.42
1:B:130:ASP:HA	1:B:131:PRO:HD2	1.61	0.42
1:A:287:ASN:ND2	1:A:287:ASN:N	2.66	0.42
1:B:187:ASP:HA	1:B:188:PRO:HD2	1.80	0.42
1:B:30:LEU:HA	1:B:33:ARG:CD	2.50	0.42
1:B:92:GLU:HA	1:B:95:MET:CE	2.49	0.42
1:B:28:PHE:HB3	1:B:32:GLU:CB	2.48	0.42
1:A:247:GLU:HG2	1:A:248:THR:N	2.35	0.42
1:A:291:SER:HA	1:A:314:SER:HB2	2.02	0.42
1:A:184:MET:HE3	1:A:318:ARG:NE	2.35	0.42
1:B:70:MET:O	1:B:71:VAL:HG12	2.20	0.42
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.84	0.42
1:A:361:ASN:ND2	1:A:362:LYS:N	2.68	0.42
1:B:40:ILE:CD1	1:B:340:SER:HA	2.50	0.42
1:A:56:GLY:O	1:A:60:LYS:O	2.37	0.42
1:B:116:GLU:HG2	4:B:605:MKR:C4	2.50	0.42
1:A:139:THR:O	1:A:143:ILE:HG13	2.20	0.41
1:B:200:GLU:OE1	1:B:200:GLU:HA	2.19	0.41
1:B:29:ASN:C	1:B:31:ALA:N	2.73	0.41
1:B:108:GLY:N	3:B:602:ADP:O1B	2.34	0.41
1:A:130:ASP:HA	1:A:131:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:O	1:A:258:ILE:HA	2.19	0.41
1:A:361:ASN:C	1:A:361:ASN:HD22	2.24	0.41
1:B:163:ILE:HA	1:B:167:GLU:O	2.20	0.41
1:A:206:ASN:O	1:A:209:GLU:HB3	2.20	0.41
1:B:115:MET:CE	1:B:263:LEU:HB3	2.51	0.41
1:B:160:LEU:CB	1:B:172:LEU:HG	2.50	0.41
1:A:240:SER:OG	1:A:262:ASN:ND2	2.53	0.41
1:B:19:ILE:HD12	1:B:359:ILE:CB	2.51	0.41
1:B:29:ASN:O	1:B:33:ARG:HG2	2.21	0.41
1:B:53:ARG:HE	1:B:63:ARG:HH12	1.67	0.41
1:B:115:MET:O	1:B:136:ILE:HG13	2.21	0.41
1:B:28:PHE:N	1:B:28:PHE:CD1	2.89	0.41
1:A:77:LYS:HD2	1:A:77:LYS:HA	1.81	0.41
1:B:181:ARG:CG	1:B:181:ARG:NH1	2.84	0.41
1:A:165:ASN:O	1:A:166:GLU:HB2	2.20	0.41
1:A:246:LYS:O	1:A:246:LYS:HG2	2.20	0.41
1:A:345:GLU:HA	1:A:345:GLU:OE2	2.21	0.41
1:B:141:HIS:HB3	5:B:709:HOH:O	2.20	0.41
1:B:230:ALA:HB3	1:B:234:ARG:HD3	2.03	0.41
1:A:87:CYS:HB3	1:A:88:PRO:CD	2.50	0.40
1:B:236:HIS:NE2	1:B:289:ASN:ND2	2.64	0.40
1:B:288:ILE:HD12	1:B:293:LEU:CD2	2.51	0.40
1:B:183:GLN:HE21	1:B:183:GLN:HB2	1.51	0.40
1:B:82:TYR:CD2	1:B:86:VAL:HB	2.57	0.40
1:B:306:THR:HG22	1:B:307:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

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	326/367 (89%)	300 (92%)	17 (5%)	9 (3%)	5 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	326/367 (89%)	305 (94%)	17 (5%)	4 (1%)	13	24
All	All	652/734 (89%)	605 (93%)	34 (5%)	13 (2%)	7	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	189	ARG
1	A	30	LEU
1	A	149	ASP
1	A	150	ASN
1	A	208	ASP
1	A	211	TYR
1	B	36	SER
1	A	178	VAL
1	B	27	PRO
1	B	189	ARG
1	A	143	ILE
1	B	310	PRO

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	293/321 (91%)	254 (87%)	39 (13%)	4	7
1	B	293/321 (91%)	250 (85%)	43 (15%)	3	5
All	All	586/642 (91%)	504 (86%)	82 (14%)	3	6

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	19	ILE
1	A	39	SER

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Mol	Chain	Res	Type
1	A	46	VAL
1	A	48	LYS
1	A	50	VAL
1	A	59	ASP
1	A	64	LYS
1	A	65	THR
1	A	85	VAL
1	A	87	CYS
1	A	128	GLU
1	A	145	GLU
1	A	152	THR
1	A	161	LEU
1	A	168	LEU
1	A	173	ASN
1	A	175	SER
1	A	176	SER
1	A	179	SER
1	A	190	ASN
1	A	192	ARG
1	A	199	LEU
1	A	212	GLN
1	A	216	LYS
1	A	227	LEU
1	A	241	VAL
1	A	249	THR
1	A	250	ILE
1	A	254	GLU
1	A	255	LEU
1	A	287	ASN
1	A	289	ASN
1	A	293	LEU
1	A	330	THR
1	A	337	SER
1	A	341	LEU
1	A	361	ASN
1	A	362	LYS
1	B	26	ARG
1	B	29	ASN
1	B	33	ARG
1	B	34	LYS
1	B	36	SER
1	B	39	SER

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Mol	Chain	Res	Type
1	B	46	VAL
1	B	50	VAL
1	B	57	LEU
1	B	59	ASP
1	B	62	SER
1	B	75	SER
1	B	89	ILE
1	B	125	TYR
1	B	159	SER
1	B	165	ASN
1	B	168	LEU
1	B	173	ASN
1	B	182	LEU
1	B	183	GLN
1	B	184	MET
1	B	192	ARG
1	B	194	VAL
1	B	207	LYS
1	B	210	VAL
1	B	228	MET
1	B	241	VAL
1	B	243	ILE
1	B	247	GLU
1	B	263	LEU
1	B	271	ASN
1	B	289	ASN
1	B	291	SER
1	B	293	LEU
1	B	302	LEU
1	B	312	ARG
1	B	318	ARG
1	B	324	LEU
1	B	337	SER
1	B	343	LEU
1	B	350	LEU
1	B	355	ARG
1	B	361	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	190	ASN
1	A	229	ASN
1	A	262	ASN
1	A	289	ASN
1	A	321	GLN
1	A	342	ASN
1	A	361	ASN
1	B	18	ASN
1	B	20	GLN
1	B	141	HIS
1	B	142	GLN
1	B	173	ASN
1	B	183	GLN
1	B	190	ASN
1	B	205	HIS
1	B	212	GLN
1	B	262	ASN
1	B	271	ASN
1	B	289	ASN
1	B	290	GLN
1	B	361	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 carbohydrates 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
4	MKR	A	604	-	36,39,39	2.11	10 (27%)	45,57,57	2.51	23 (51%)
4	MKR	B	605	-	36,39,39	2.94	16 (44%)	45,57,57	2.80	21 (46%)
3	ADP	B	602	2	24,29,29	1.91	4 (16%)	29,45,45	1.22	1 (3%)
3	ADP	A	601	2	24,29,29	2.19	4 (16%)	29,45,45	1.26	3 (10%)

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
4	MKR	A	604	-	-	6/21/60/60	0/5/5/5
4	MKR	B	605	-	-	3/21/60/60	0/5/5/5
3	ADP	B	602	2	-	3/12/32/32	0/3/3/3
3	ADP	A	601	2	-	0/12/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ADP	O4'-C1'	8.64	1.53	1.41
4	B	605	MKR	C15-N2	-8.01	1.39	1.49
4	B	605	MKR	N2-N12	-7.53	1.24	1.38
3	B	602	ADP	O4'-C1'	6.81	1.50	1.41
4	A	604	MKR	N2-N12	-6.33	1.26	1.38
4	B	605	MKR	C19-N1	5.22	1.56	1.47
4	B	605	MKR	C27-C26	4.46	1.48	1.38
4	B	605	MKR	C26-C18	4.41	1.46	1.39
4	A	604	MKR	C19-N1	4.32	1.54	1.47
4	B	605	MKR	C21-N1	4.27	1.54	1.47
4	A	604	MKR	C2-C1	4.14	1.44	1.37
4	B	605	MKR	C14-C18	4.03	1.60	1.52
4	B	605	MKR	C9-C20	3.61	1.57	1.50
4	A	604	MKR	C21-N1	3.46	1.53	1.47
4	A	604	MKR	C2-C3	3.45	1.45	1.39
3	A	601	ADP	C2-N3	3.36	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	MKR	C6-C1	3.31	1.43	1.37
4	A	604	MKR	C29-C30	3.27	1.45	1.38
3	A	601	ADP	C2-N1	3.09	1.39	1.33
3	A	601	ADP	O3'-C3'	3.04	1.50	1.43
3	B	602	ADP	C2'-C1'	-3.02	1.49	1.53
4	B	605	MKR	C2-C1	2.94	1.42	1.37
3	B	602	ADP	C4-N3	2.91	1.39	1.35
4	B	605	MKR	C28-C27	2.67	1.45	1.38
4	A	604	MKR	C6-C5	2.55	1.43	1.38
4	A	604	MKR	C26-C18	2.43	1.43	1.39
4	B	605	MKR	F1-C1	-2.40	1.30	1.36
4	B	605	MKR	C29-C28	2.37	1.44	1.38
4	B	605	MKR	C2-C3	2.27	1.43	1.39
4	B	605	MKR	C20-C8	2.20	1.53	1.48
4	B	605	MKR	C29-C30	2.10	1.43	1.38
3	B	602	ADP	PB-O2B	-2.08	1.46	1.54
4	A	604	MKR	C15-N2	-2.06	1.46	1.49
4	A	604	MKR	C20-C8	2.05	1.53	1.48

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	MKR	C24-C22-N1	-7.94	109.02	118.26
4	A	604	MKR	C24-C22-N1	-6.32	110.90	118.26
4	B	605	MKR	C12-N3-C17	5.65	125.68	111.23
4	A	604	MKR	C12-N3-C17	5.20	124.54	111.23
4	B	605	MKR	C9-C20-C8	4.67	123.57	119.08
4	A	604	MKR	C19-C16-N3	-4.60	101.20	110.64
4	B	605	MKR	C28-C27-C26	-4.57	113.23	120.19
4	B	605	MKR	C7-C15-C14	-4.45	111.90	118.30
4	A	604	MKR	C27-C26-C18	4.44	125.42	120.76
4	A	604	MKR	C28-C27-C26	-4.12	113.92	120.19
4	A	604	MKR	C21-N1-C19	4.07	120.47	112.62
4	B	605	MKR	C10-C11-C12	3.97	120.59	112.78
4	B	605	MKR	C27-C26-C18	3.93	124.88	120.76
4	B	605	MKR	O25-C20-C8	-3.75	113.19	119.28
4	B	605	MKR	C19-C16-N3	-3.69	103.07	110.64
4	B	605	MKR	C21-C17-N3	-3.69	103.07	110.64
4	A	604	MKR	C17-N3-C16	3.65	117.05	108.83
4	A	604	MKR	C11-C10-C14	3.64	121.91	115.80
3	A	601	ADP	O3'-C3'-C4'	-3.25	101.66	111.05
4	B	605	MKR	C16-C19-N1	-3.25	103.48	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	MKR	F1-C1-C6	-3.24	113.03	118.54
4	A	604	MKR	C5-C6-C1	3.11	121.58	118.36
4	B	605	MKR	C5-C4-C3	3.11	125.92	120.06
4	B	605	MKR	C21-N1-C19	3.10	118.58	112.62
4	B	605	MKR	C30-C18-C14	3.01	126.58	120.93
4	A	604	MKR	C5-C4-C3	2.82	125.37	120.06
4	A	604	MKR	C7-O1-C4	2.69	120.91	115.30
4	A	604	MKR	C3-C2-C1	-2.66	113.24	117.66
4	B	605	MKR	C10-C14-C15	-2.63	105.12	113.88
4	B	605	MKR	C26-C18-C14	-2.61	116.04	120.93
4	A	604	MKR	C6-C5-C4	-2.60	115.10	120.06
3	A	601	ADP	O2'-C2'-C1'	-2.60	101.26	110.85
4	B	605	MKR	C17-N3-C16	2.53	114.53	108.83
4	A	604	MKR	C14-C8-C20	2.46	130.19	124.14
4	A	604	MKR	C19-N1-C22	-2.43	116.50	122.95
4	B	605	MKR	C6-C5-C4	-2.42	115.45	120.06
4	A	604	MKR	C9-C20-C8	-2.35	116.83	119.08
4	A	604	MKR	C26-C18-C14	-2.34	116.54	120.93
3	A	601	ADP	O4'-C1'-C2'	2.33	110.33	106.93
4	A	604	MKR	C4-C3-N2	-2.33	115.62	118.39
3	B	602	ADP	O3B-PB-O2B	2.24	116.20	107.64
4	A	604	MKR	C12-N3-C16	2.22	116.92	111.23
4	B	605	MKR	C3-C2-C1	-2.18	114.04	117.66
4	A	604	MKR	O1-C7-C15	2.17	116.73	111.34
4	A	604	MKR	C29-C28-C27	2.15	123.92	119.93
4	B	605	MKR	C6-C1-C2	2.06	125.97	123.29
4	A	604	MKR	C30-C18-C14	2.04	124.76	120.93
4	A	604	MKR	C7-C15-C14	-2.04	115.37	118.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	MKR	C11-C10-C14-C8
4	A	604	MKR	C11-C10-C14-C15
4	A	604	MKR	C24-C22-N1-C19
4	A	604	MKR	O2-C22-N1-C19
3	B	602	ADP	C5'-O5'-PA-O1A
3	B	602	ADP	C5'-O5'-PA-O2A
4	B	605	MKR	C11-C12-N3-C17
4	A	604	MKR	C11-C12-N3-C16
4	B	605	MKR	C11-C12-N3-C16

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Mol	Chain	Res	Type	Atoms
4	B	605	MKR	C10-C11-C12-N3
4	A	604	MKR	C14-C10-C11-C12
3	B	602	ADP	C5'-O5'-PA-O3A

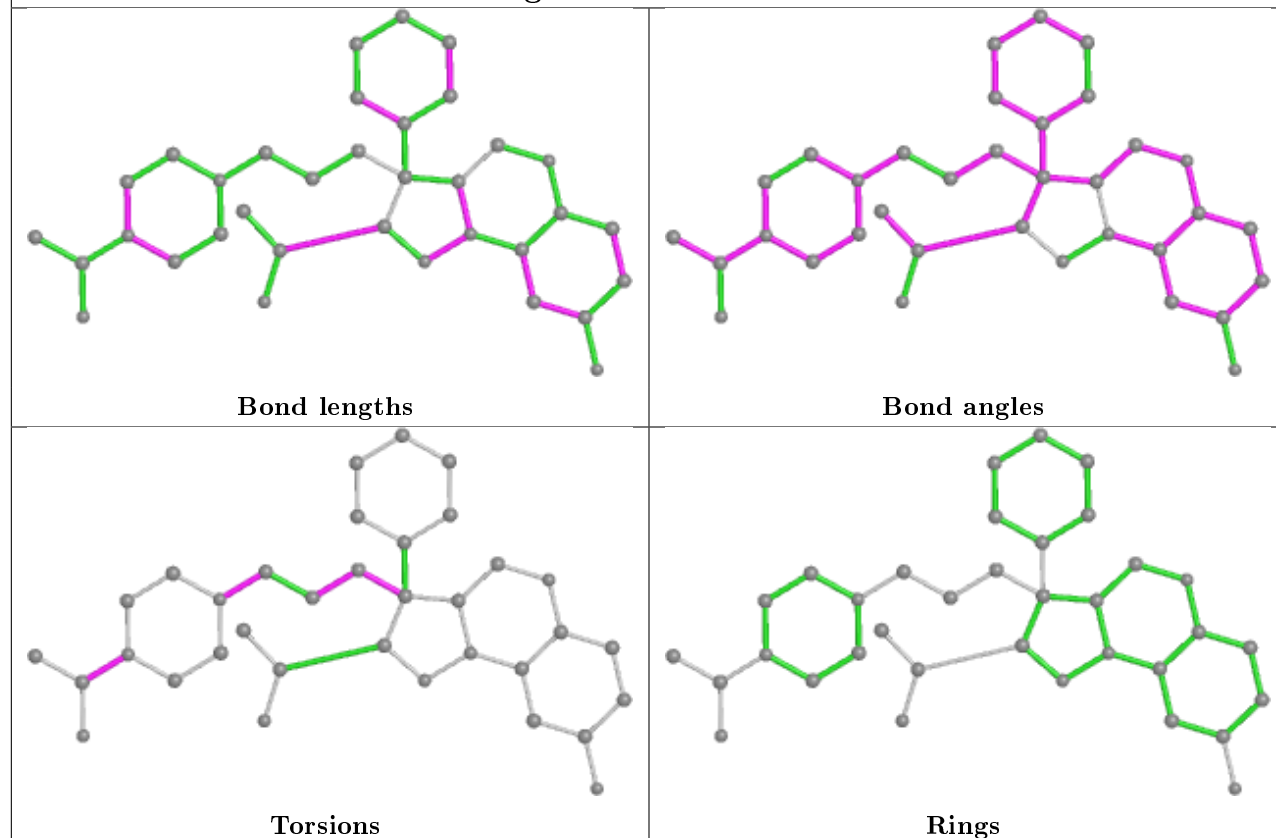
There are no ring outliers.

3 monomers are involved in 6 short contacts:

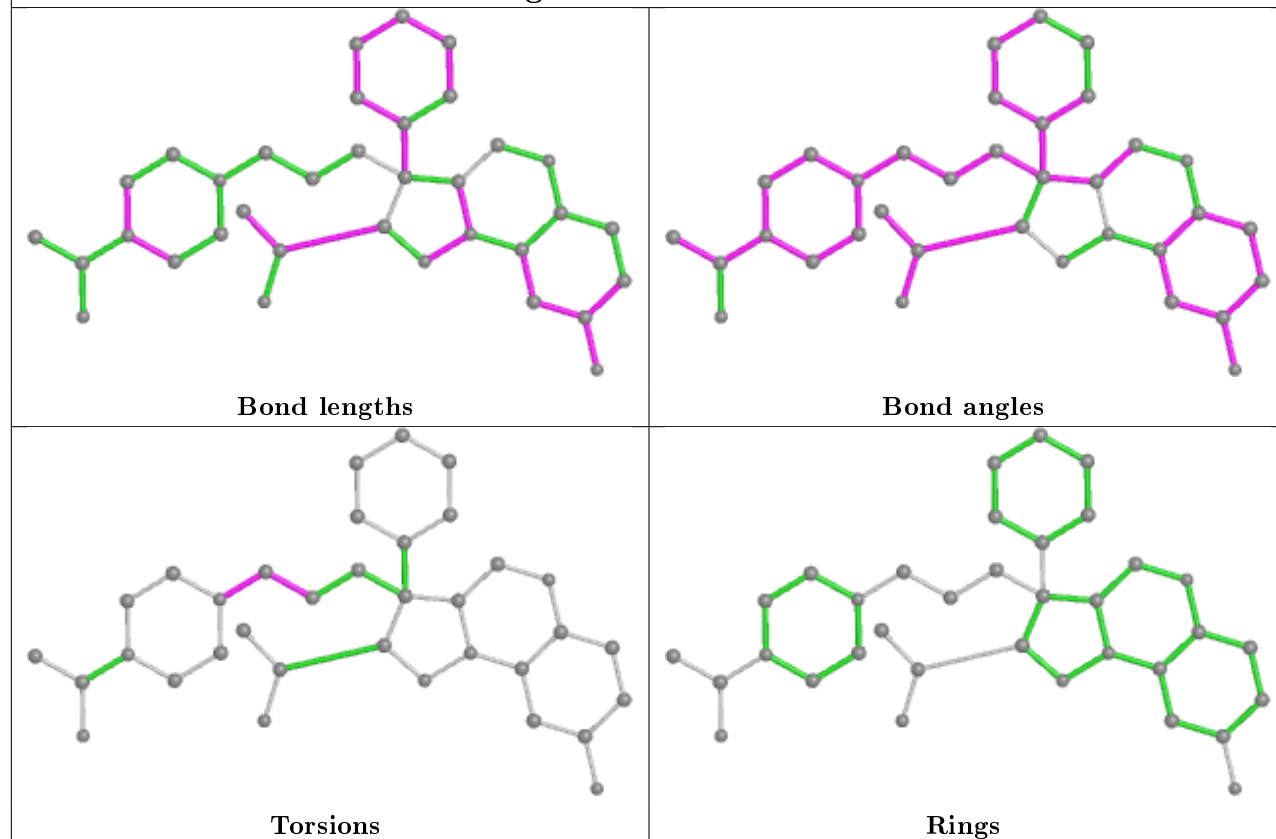
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	MKR	3	0
4	B	605	MKR	2	0
3	B	602	ADP	1	0

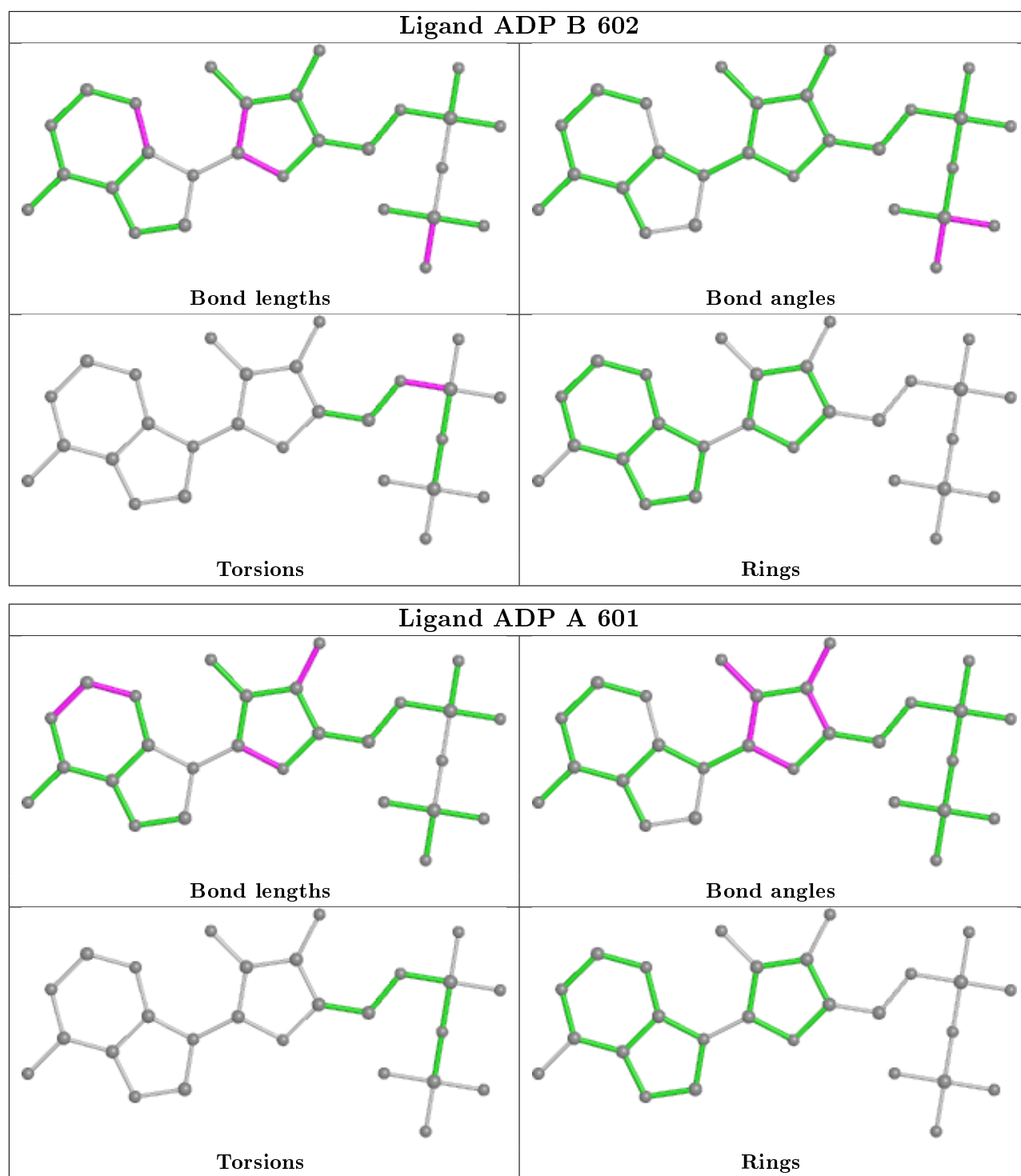
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand MKR A 604



Ligand MKR B 605





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.