



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:28 am BST

PDB ID : 6DUG
Title : Crystal structure of HIV-1 reverse transcriptase K101P mutant in complex with non-nucleoside inhibitor 25a
Authors : Yang, Y.; Nguyen, L.A.; Smithline, Z.B.; Steitz, T.A.
Deposited on : 2018-06-20
Resolution : 2.23 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 : 2.11
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) : 2.11

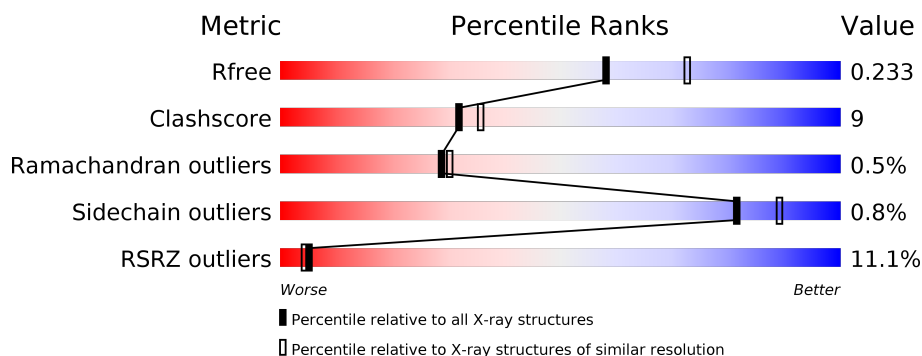
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	557	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
2	B	428	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	506	-	-	-	X
6	EDO	A	608	-	-	-	X
6	EDO	A	613	-	-	-	X
6	EDO	A	616	-	-	-	X
6	EDO	B	516	-	-	-	X
6	EDO	B	517	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8531 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 p66 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	2	0
			4532	2935	752	837	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	101	PRO	LYS	engineered mutation	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

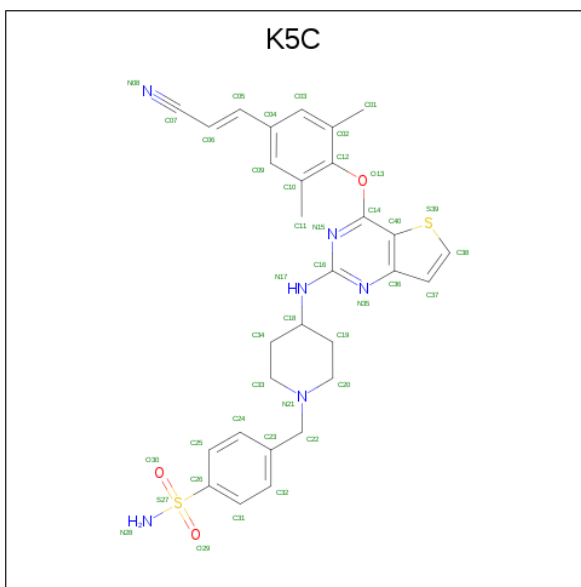
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	1	0
			3421	2229	566	619	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-({4-[(4-{4-[(E)-2-cyanoethenyl]-2,6-dimethylphenoxy}thieno[3,2-d]pyrimidin-2-yl)amino]piperidin-1-yl)methyl)benzene-1-sulfonamide (three-letter code: K5C) (formula: C₂₉H₃₀N₆O₃S₂) (labeled as "Ligand of Interest" by author).

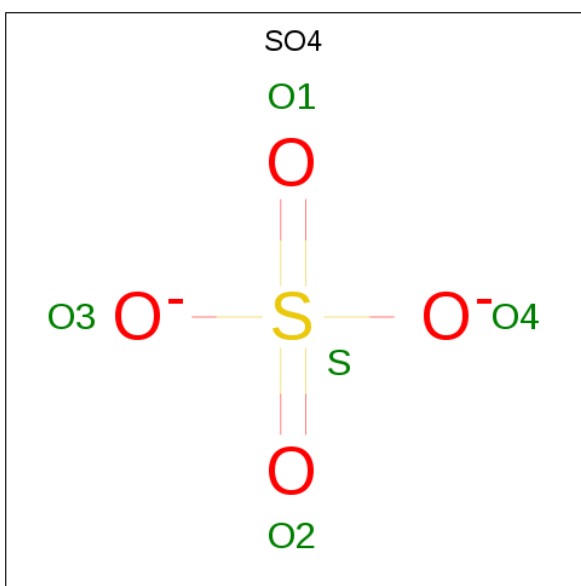


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			40	29	6	3	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

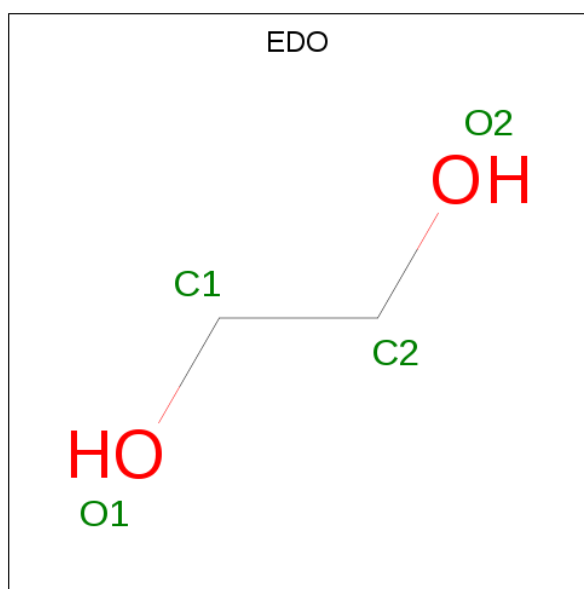
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



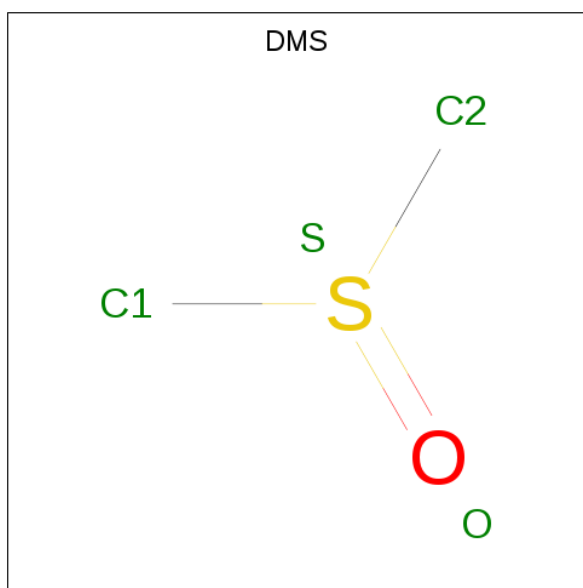
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 8	C 4	O 4	0	1
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			4	2	1	1		

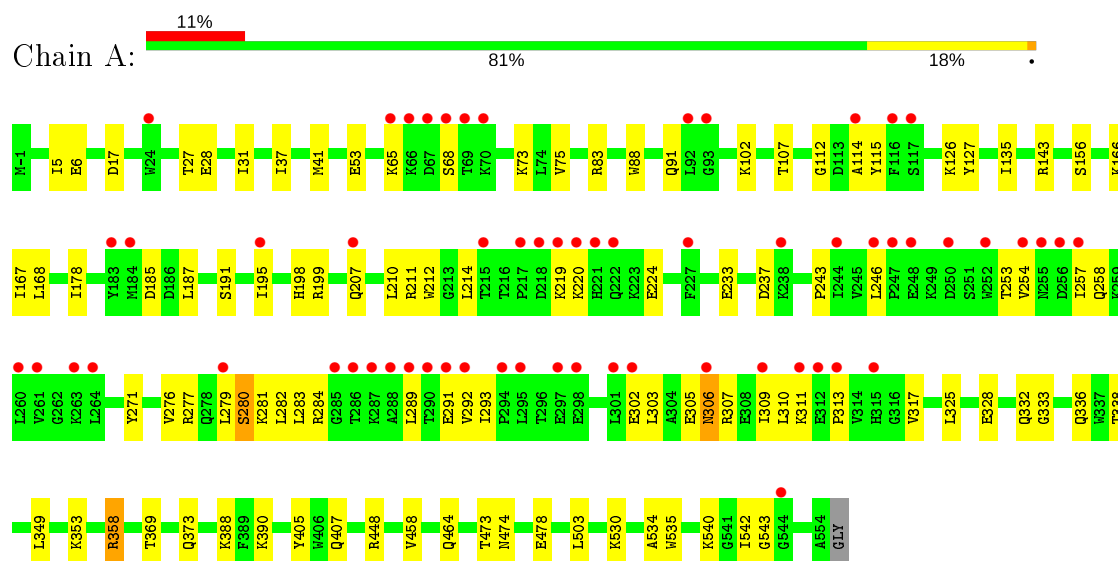
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	225	Total	O	0	0
			225	225		
8	B	163	Total	O	0	0
			163	163		

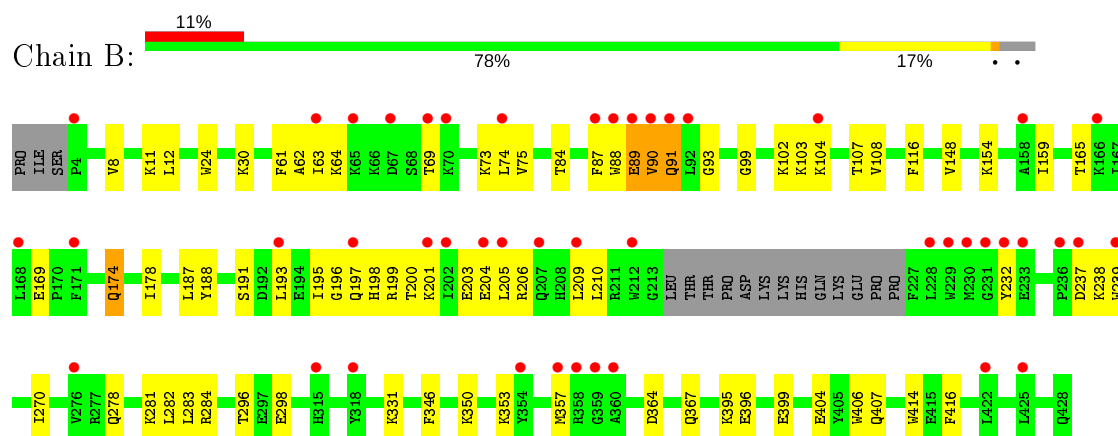
3 Residue-property plots [i](#)

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 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: p66 RT



• Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.04Å 73.30Å 109.31Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	55.00 – 2.23 107.72 – 2.23	Depositor EDS
% Data completeness (in resolution range)	97.7 (55.00-2.23) 97.7 (107.72-2.23)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.185 , 0.233 0.185 , 0.233	Depositor DCC
R_{free} test set	3059 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8531	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: MG, DMS, K5C, EDO, SO4

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	0.28	0/4653	0.47	0/6329
2	B	0.27	0/3520	0.50	0/4780
All	All	0.27	0/8173	0.48	0/11109

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4532	0	4574	82	0
2	B	3421	0	3447	63	0
3	A	40	0	0	0	0
4	A	1	0	0	0	0
5	A	20	0	0	0	0
5	B	25	0	0	0	0
6	A	56	0	84	9	0
6	B	44	0	66	4	0
7	B	4	0	6	1	0
8	A	225	0	0	4	0
8	B	163	0	0	3	0
All	All	8531	0	8177	145	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 (145) 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:27:THR:O	1:A:31:ILE:CD1	2.23	0.87
1:A:27:THR:O	1:A:31:ILE:HD12	1.75	0.86
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.46	0.81
1:A:178:ILE:HD12	1:A:178:ILE:O	1.85	0.77
1:A:31:ILE:HD12	1:A:31:ILE:H	1.49	0.77
1:A:212:TRP:HB2	1:A:214:LEU:HD11	1.68	0.75
1:A:73:LYS:HD3	1:A:75:VAL:HG23	1.68	0.74
2:B:395:LYS:NZ	8:B:601:HOH:O	2.21	0.73
1:A:353:LYS:HG2	6:A:610:EDO:H22	1.69	0.73
1:A:178:ILE:HD12	1:A:178:ILE:C	2.11	0.70
2:B:8:VAL:HG21	2:B:159:ILE:HG12	1.73	0.70
1:A:271:TYR:OH	1:A:313:PRO:HA	1.93	0.67
1:A:276:VAL:O	1:A:280:SER:HB2	1.94	0.67
2:B:87:PHE:HB3	2:B:89:GLU:HG2	1.77	0.67
2:B:108:VAL:HG22	2:B:232:TYR:HB3	1.76	0.67
2:B:30:LYS:NZ	2:B:404:GLU:OE1	2.27	0.66
1:A:535:TRP:H	6:A:615[A]:EDO:H21	1.62	0.64
2:B:11:LYS:NZ	8:B:602:HOH:O	2.30	0.64
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.14	0.63
1:A:31:ILE:HD12	1:A:31:ILE:N	2.15	0.62
1:A:530:LYS:NZ	6:A:616:EDO:O2	2.34	0.60
1:A:306:ASN:O	1:A:309:ILE:N	2.30	0.60
2:B:395:LYS:HE2	2:B:399:GLU:OE2	2.01	0.60
2:B:278:GLN:NE2	8:B:606:HOH:O	2.35	0.59
1:A:91:GLN:N	1:A:91:GLN:OE1	2.36	0.59
1:A:307:ARG:NH2	1:A:311:LYS:HA	2.18	0.58
2:B:174:GLN:HE22	2:B:201:LYS:NZ	2.01	0.58
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.28	0.58
2:B:239:TRP:HB3	2:B:350:LYS:HE2	1.86	0.57
1:A:191:SER:OG	1:A:198:HIS:ND1	2.28	0.57
2:B:201:LYS:HA	2:B:204:GLU:HB2	1.87	0.56
2:B:64:LYS:HZ1	2:B:69:THR:C	2.08	0.56
2:B:91:GLN:HB3	2:B:93:GLY:H	1.69	0.56
1:A:31:ILE:CD1	1:A:31:ILE:H	2.18	0.55
1:A:281:LYS:O	1:A:283:LEU:N	2.40	0.55
2:B:193:LEU:HD13	2:B:197:GLN:HB2	1.88	0.55
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LYS:HD3	2:B:12:LEU:H	1.71	0.54
1:A:112:GLY:HA2	1:A:185:ASP:OD2	2.07	0.54
1:A:219:LYS:NZ	1:A:220:LYS:O	2.41	0.54
2:B:89:GLU:O	2:B:90:VAL:HG12	2.08	0.54
1:A:254:VAL:O	1:A:258:GLN:HG2	2.08	0.54
1:A:277:ARG:NH1	6:A:614:EDO:O1	2.40	0.54
6:A:617:EDO:H22	2:B:396:GLU:HB3	1.89	0.54
1:A:107:THR:HG23	1:A:198:HIS:NE2	2.22	0.54
2:B:200:THR:O	2:B:204:GLU:N	2.36	0.54
1:A:27:THR:O	1:A:31:ILE:HD13	2.05	0.53
2:B:206:ARG:O	2:B:210:LEU:HD12	2.08	0.53
2:B:24:TRP:CD2	6:B:511:EDO:H11	2.43	0.53
2:B:205:LEU:O	2:B:209:LEU:HG	2.09	0.53
1:A:178:ILE:CD1	1:A:178:ILE:C	2.77	0.53
1:A:388:LYS:H	1:A:388:LYS:HD2	1.74	0.53
1:A:102:LYS:HD3	1:A:237:ASP:HA	1.91	0.52
2:B:63:ILE:HD12	2:B:406:TRP:O	2.10	0.52
2:B:61:PHE:CE2	2:B:63:ILE:HD11	2.45	0.52
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.40	0.52
1:A:281:LYS:HD2	1:A:284:ARG:CZ	2.41	0.51
1:A:6:GLU:OE1	1:A:166:LYS:NZ	2.43	0.51
2:B:165:THR:O	2:B:169:GLU:HG2	2.09	0.51
1:A:254:VAL:HB	1:A:289:LEU:HA	1.93	0.51
2:B:30:LYS:HG2	2:B:62:ALA:HB3	1.94	0.50
1:A:27:THR:C	1:A:31:ILE:CD1	2.80	0.50
2:B:191:SER:OG	2:B:198:HIS:ND1	2.35	0.50
1:A:473:THR:HB	6:A:609:EDO:H11	1.92	0.50
1:A:281:LYS:C	1:A:283:LEU:H	2.15	0.49
1:A:333:GLY:O	1:A:336:GLN:HG2	2.11	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.48	0.49
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.94	0.49
2:B:281:LYS:O	2:B:284:ARG:HG2	2.13	0.49
1:A:277:ARG:NH2	8:A:718:HOH:O	2.45	0.49
2:B:197:GLN:O	2:B:200:THR:OG1	2.28	0.49
2:B:99:GLY:O	2:B:103:LYS:HG2	2.12	0.49
2:B:61:PHE:HE2	2:B:63:ILE:HD11	1.77	0.49
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.95	0.48
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.47	0.48
1:A:212:TRP:HB2	1:A:214:LEU:CD1	2.40	0.48
1:A:257:ILE:HG23	1:A:279:LEU:HD13	1.95	0.48
1:A:302:GLU:HA	1:A:305:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:O	1:A:83:ARG:HD3	2.14	0.48
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.95	0.48
2:B:84:THR:HB	2:B:154:LYS:HE2	1.96	0.47
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.96	0.47
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.97	0.47
1:A:114:ALA:HB1	1:A:214:LEU:HD23	1.97	0.46
1:A:207:GLN:HG2	1:A:211:ARG:HH22	1.81	0.46
2:B:203:GLU:HA	2:B:206:ARG:HB3	1.97	0.46
2:B:11:LYS:CD	2:B:12:LEU:H	2.28	0.46
1:A:27:THR:C	1:A:31:ILE:HD13	2.36	0.46
2:B:298:GLU:N	2:B:298:GLU:OE2	2.39	0.45
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.24	0.45
2:B:210:LEU:HD12	2:B:210:LEU:H	1.81	0.45
1:A:458[A]:VAL:HG23	1:A:464:GLN:HG2	1.98	0.45
2:B:174:GLN:HE22	2:B:201:LYS:HZ2	1.64	0.45
1:A:28:GLU:HA	1:A:31:ILE:HD13	1.99	0.45
6:A:619:EDO:H11	7:B:501:DMS:H22	1.99	0.45
1:A:474:ASN:H	6:A:609:EDO:H12	1.81	0.44
1:A:358:ARG:NH1	8:A:718:HOH:O	2.46	0.44
1:A:332:GLN:OE1	1:A:338:THR:HG23	2.18	0.44
1:A:325:LEU:O	1:A:388:LYS:HD2	2.17	0.44
1:A:281:LYS:HD2	1:A:284:ARG:NH2	2.32	0.44
2:B:237:ASP:HB2	2:B:238:LYS:NZ	2.33	0.44
2:B:353:LYS:H	6:B:512:EDO:H22	1.83	0.43
2:B:99:GLY:HA2	2:B:102:LYS:NZ	2.34	0.43
1:A:37:ILE:O	1:A:41:MET:HG3	2.18	0.43
1:A:5:ILE:HG12	1:A:167:ILE:HD11	1.99	0.43
2:B:116:PHE:HA	2:B:148:VAL:HG21	2.00	0.43
1:A:369:THR:O	1:A:373:GLN:HG2	2.18	0.43
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.48	0.43
1:A:233:GLU:OE2	1:A:243:PRO:HD3	2.19	0.43
2:B:63:ILE:HA	2:B:63:ILE:HD13	1.82	0.43
1:A:88:TRP:CZ2	6:B:516:EDO:H12	2.54	0.43
1:A:115:TYR:OH	1:A:156:SER:HB3	2.19	0.43
1:A:143:ARG:NE	8:A:717:HOH:O	2.45	0.43
2:B:107:THR:HA	2:B:232:TYR:O	2.19	0.42
1:A:73:LYS:HE2	8:A:909:HOH:O	2.19	0.42
2:B:108:VAL:HA	2:B:187:LEU:O	2.18	0.42
1:A:246:LEU:HD13	1:A:310:LEU:HD22	2.01	0.42
1:A:303:LEU:O	1:A:306:ASN:HB2	2.19	0.42
1:A:328:GLU:HG3	1:A:390:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:O	1:A:478:GLU:HG3	2.19	0.42
1:A:534:ALA:HA	6:A:615[A]:EDO:H21	2.01	0.42
2:B:196:GLY:O	2:B:200:THR:HG23	2.20	0.42
2:B:281:LYS:O	2:B:281:LYS:HG3	2.19	0.42
1:A:195:ILE:O	1:A:199:ARG:HG3	2.20	0.42
2:B:108:VAL:HG12	2:B:188:TYR:CD2	2.54	0.42
1:A:281:LYS:C	1:A:283:LEU:N	2.74	0.42
2:B:74:LEU:HD12	2:B:75:VAL:H	1.85	0.42
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.78	0.42
1:A:53:GLU:HG2	1:A:53:GLU:H	1.67	0.41
2:B:353:LYS:O	6:B:512:EDO:H11	2.20	0.41
2:B:238:LYS:HE2	2:B:238:LYS:N	2.34	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.95	0.41
1:A:281:LYS:HG3	1:A:284:ARG:NE	2.35	0.41
2:B:357:MET:HB2	2:B:367:GLN:HG2	2.02	0.41
1:A:224:GLU:CD	1:A:224:GLU:H	2.24	0.41
1:A:253:THR:HG22	1:A:292:VAL:HG12	2.03	0.41
2:B:104:LYS:HA	2:B:237:ASP:OD1	2.21	0.41
1:A:178:ILE:HG22	1:A:191:SER:HB3	2.03	0.41
1:A:291:GLU:HB3	1:A:293:ILE:HD11	2.02	0.41
1:A:543:GLY:HA3	2:B:283:LEU:O	2.20	0.41
2:B:64:LYS:O	2:B:407:GLN:HG2	2.20	0.41
1:A:28:GLU:HG3	1:A:135:ILE:HD12	2.02	0.40
1:A:65:LYS:HB3	1:A:65:LYS:HE2	1.88	0.40
2:B:88:TRP:HB3	2:B:91:GLN:O	2.21	0.40
1:A:168:LEU:HD11	1:A:187:LEU:HD11	2.03	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	556/557 (100%)	541 (97%)	12 (2%)	3 (0%)	29	30
2	B	409/428 (96%)	391 (96%)	16 (4%)	2 (0%)	29	30
All	All	965/985 (98%)	932 (97%)	28 (3%)	5 (0%)	29	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	LEU
2	B	89	GLU
1	A	68	SER
1	A	306	ASN
2	B	90	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	496/495 (100%)	493 (99%)	3 (1%)	86	92
2	B	375/390 (96%)	371 (99%)	4 (1%)	73	84
All	All	871/885 (98%)	864 (99%)	7 (1%)	81	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	SER
1	A	358	ARG
1	A	448	ARG
2	B	73	LYS
2	B	91	GLN
2	B	174	GLN
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	$\# Z > 2$
6	EDO	A	618	-	3,3,3	0.45	0	2,2,2	0.32	0
5	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	B	507	-	3,3,3	0.45	0	2,2,2	0.32	0
5	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	A	617	-	3,3,3	0.45	0	2,2,2	0.31	0
6	EDO	B	514	-	3,3,3	0.45	0	2,2,2	0.29	0
6	EDO	A	616	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	A	615[B]	-	3,3,3	0.45	0	2,2,2	0.35	0
5	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.05	0
3	K5C	A	601	-	42,44,44	1.62	3 (7%)	51,63,63	2.33	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	615[A]	-	3,3,3	0.46	0	2,2,2	0.26	0
6	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.28	0
6	EDO	B	515	-	3,3,3	0.45	0	2,2,2	0.34	0
6	EDO	A	614	-	3,3,3	0.46	0	2,2,2	0.33	0
5	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.04	0
6	EDO	A	607	-	3,3,3	0.46	0	2,2,2	0.33	0
5	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.31	0
6	EDO	A	619	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	B	513	-	3,3,3	0.44	0	2,2,2	0.31	0
6	EDO	B	512	-	3,3,3	0.45	0	2,2,2	0.32	0
6	EDO	B	517	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	B	516	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	B	508	-	3,3,3	0.48	0	2,2,2	0.28	0
6	EDO	A	613	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	A	608	-	3,3,3	0.45	0	2,2,2	0.34	0
6	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	B	509	-	3,3,3	0.45	0	2,2,2	0.35	0
7	DMS	B	501	-	3,3,3	0.62	0	3,3,3	0.48	0
6	EDO	B	511	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	B	510	-	3,3,3	0.45	0	2,2,2	0.34	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
6	EDO	A	618	-	-	0/1/1/1	-
6	EDO	A	607	-	-	1/1/1/1	-
6	EDO	A	617	-	-	0/1/1/1	-
6	EDO	B	514	-	-	0/1/1/1	-
6	EDO	A	616	-	-	0/1/1/1	-
6	EDO	A	615[B]	-	-	0/1/1/1	-
3	K5C	A	601	-	-	2/21/32/32	0/5/5/5
6	EDO	A	615[A]	-	-	0/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-
6	EDO	B	515	-	-	0/1/1/1	-
6	EDO	A	614	-	-	0/1/1/1	-
6	EDO	B	507	-	-	0/1/1/1	-
6	EDO	A	612	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	619	-	-	1/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-
6	EDO	B	512	-	-	0/1/1/1	-
6	EDO	B	517	-	-	1/1/1/1	-
6	EDO	A	611	-	-	0/1/1/1	-
6	EDO	B	516	-	-	0/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	A	613	-	-	1/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	B	509	-	-	1/1/1/1	-
6	EDO	B	511	-	-	1/1/1/1	-
6	EDO	B	510	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	K5C	C16-N17	7.41	1.44	1.34
3	A	601	K5C	C14-N15	2.94	1.36	1.31
3	A	601	K5C	S27-N28	2.81	1.66	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5C	C31-C26-C25	-6.10	111.94	120.44
3	A	601	K5C	C22-N21-C20	-5.77	98.21	111.06
3	A	601	K5C	C32-C31-C26	5.72	125.37	119.45
3	A	601	K5C	C24-C25-C26	4.82	124.44	119.45
3	A	601	K5C	C34-C18-N17	-3.83	104.63	110.60
3	A	601	K5C	C16-N17-C18	-3.70	118.07	124.31
3	A	601	K5C	O29-S27-C26	3.54	111.30	107.35
3	A	601	K5C	C31-C26-S27	3.41	124.68	119.73
3	A	601	K5C	O13-C14-C40	3.30	121.07	115.69
3	A	601	K5C	O30-S27-O29	-3.09	113.69	118.76
3	A	601	K5C	C34-C18-C19	2.84	115.75	110.82
3	A	601	K5C	C09-C04-C03	-2.80	115.32	119.12
3	A	601	K5C	O13-C12-C02	2.56	123.92	118.35
3	A	601	K5C	C25-C26-S27	2.52	123.39	119.73
3	A	601	K5C	C01-C02-C03	2.29	123.72	119.49
3	A	601	K5C	N17-C16-N35	-2.26	113.79	117.18
3	A	601	K5C	C37-C36-C40	2.11	112.16	110.62
3	A	601	K5C	C22-C23-C32	2.09	124.69	120.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

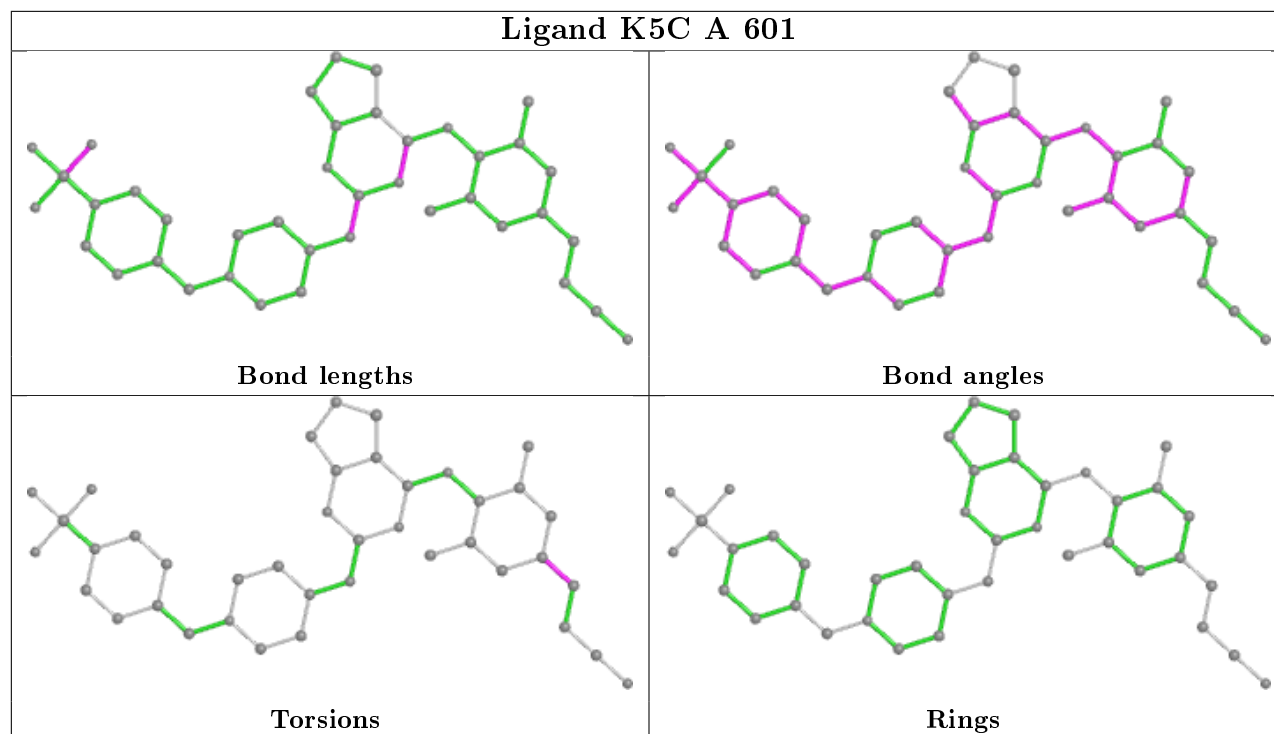
Mol	Chain	Res	Type	Atoms
3	A	601	K5C	C03-C04-C05-C06
3	A	601	K5C	C09-C04-C05-C06
6	A	607	EDO	O1-C1-C2-O2
6	A	612	EDO	O1-C1-C2-O2
6	A	619	EDO	O1-C1-C2-O2
6	B	517	EDO	O1-C1-C2-O2
6	B	511	EDO	O1-C1-C2-O2
6	A	613	EDO	O1-C1-C2-O2
6	B	509	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	617	EDO	1	0
6	A	616	EDO	1	0
6	A	615[A]	EDO	2	0
6	A	610	EDO	1	0
6	A	614	EDO	1	0
6	A	619	EDO	1	0
6	B	512	EDO	2	0
6	B	516	EDO	1	0
6	A	609	EDO	2	0
7	B	501	DMS	1	0
6	B	511	EDO	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 ⓘ

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	556/557 (99%)	0.83	61 (10%) 5 4	48, 82, 165, 235	0
2	B	412/428 (96%)	0.82	46 (11%) 5 4	46, 77, 160, 251	0
All	All	968/985 (98%)	0.83	107 (11%) 5 4	46, 80, 163, 251	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	18.3
1	A	286	THR	11.7
1	A	290	THR	11.7
2	B	358	ARG	9.5
1	A	66	LYS	9.5
1	A	68	SER	8.7
2	B	232	TYR	7.5
1	A	221	HIS	7.1
1	A	289	LEU	6.6
1	A	257	ILE	6.5
1	A	252	TRP	6.3
1	A	292	VAL	6.2
2	B	239	TRP	6.2
2	B	357	MET	5.8
2	B	90	VAL	5.8
1	A	256	ASP	5.5
1	A	288	ALA	5.3
2	B	359	GLY	5.2
2	B	88	TRP	4.8
1	A	69	THR	4.8
2	B	89	GLU	4.7
2	B	4	PRO	4.7
1	A	218	ASP	4.6
2	B	202	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	4.3
2	B	197	GLN	4.2
1	A	279	LEU	4.2
1	A	215	THR	4.1
2	B	229	TRP	4.0
2	B	91	GLN	4.0
1	A	246	LEU	4.0
2	B	231	GLY	4.0
1	A	92	LEU	4.0
1	A	227	PHE	4.0
2	B	318	TYR	3.9
2	B	168	LEU	3.8
1	A	285	GLY	3.7
1	A	65	LYS	3.6
2	B	230	MET	3.5
1	A	313	PRO	3.4
2	B	65	LYS	3.4
1	A	260	LEU	3.3
1	A	254	VAL	3.3
2	B	212	TRP	3.3
2	B	360	ALA	3.3
1	A	219	LYS	3.3
2	B	228	LEU	3.3
1	A	294	PRO	3.2
2	B	315	HIS	3.2
2	B	70	LYS	3.1
2	B	237	ASP	3.0
1	A	291	GLU	3.0
1	A	309	ILE	3.0
1	A	244	ILE	3.0
2	B	63	ILE	3.0
1	A	183	TYR	2.9
2	B	92	LEU	2.9
1	A	220	LYS	2.9
1	A	295	LEU	2.9
2	B	209	LEU	2.9
1	A	247	PRO	2.9
2	B	205	LEU	2.8
2	B	425	LEU	2.8
2	B	236	PRO	2.8
2	B	193	LEU	2.8
2	B	69	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	166	LYS	2.7
2	B	104	LYS	2.7
1	A	93	GLY	2.7
1	A	222	GLN	2.7
1	A	250	ASP	2.6
2	B	74	LEU	2.6
1	A	298	GLU	2.6
1	A	301	LEU	2.5
2	B	171	PHE	2.5
1	A	311	LYS	2.5
1	A	195	ILE	2.5
2	B	87	PHE	2.5
2	B	276	VAL	2.5
2	B	204	GLU	2.4
1	A	315	HIS	2.4
1	A	312	GLU	2.3
2	B	233	GLU	2.3
2	B	201	LYS	2.2
1	A	302	GLU	2.2
1	A	217	PRO	2.2
2	B	422	LEU	2.2
1	A	184	MET	2.2
1	A	238	LYS	2.2
2	B	354	TYR	2.2
2	B	158	ALA	2.2
1	A	297	GLU	2.2
1	A	114	ALA	2.2
1	A	70	LYS	2.1
1	A	207	GLN	2.1
1	A	116	PHE	2.1
1	A	263	LYS	2.1
1	A	544	GLY	2.1
2	B	67	ASP	2.1
1	A	264	LEU	2.1
1	A	287	LYS	2.0
1	A	306	ASN	2.0
1	A	117	SER	2.0
1	A	255	ASN	2.0
1	A	248	GLU	2.0
1	A	261	VAL	2.0
2	B	207	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

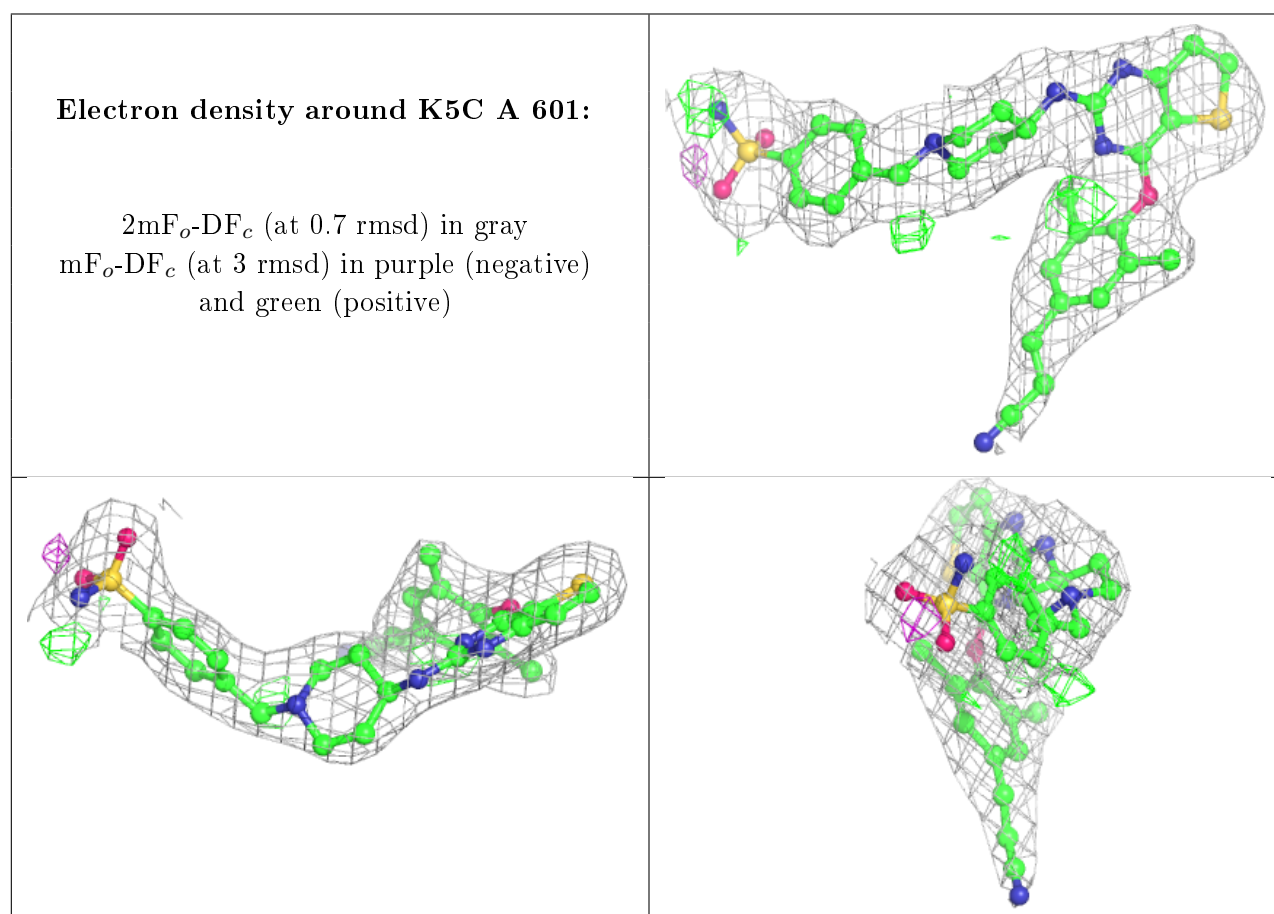
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	B	512	4/4	0.29	0.36	118,122,124,126	0
6	EDO	A	610	4/4	0.51	0.27	100,103,106,107	0
4	MG	A	602	1/1	0.53	0.26	104,104,104,104	0
6	EDO	A	613	4/4	0.53	0.55	101,103,108,113	0
6	EDO	B	516	4/4	0.54	0.63	105,108,109,111	0
6	EDO	A	607	4/4	0.56	0.27	108,109,114,116	0
6	EDO	B	510	4/4	0.60	0.33	103,108,113,113	0
6	EDO	A	608	4/4	0.62	0.53	88,89,92,97	0
6	EDO	A	617	4/4	0.64	0.39	105,105,107,111	0
6	EDO	B	507	4/4	0.67	0.28	107,107,108,109	0
6	EDO	A	614	4/4	0.69	0.19	116,118,118,119	0
6	EDO	A	618	4/4	0.72	0.20	92,94,95,97	0
6	EDO	B	517	4/4	0.72	0.58	107,114,119,121	0
6	EDO	A	612	4/4	0.75	0.20	76,79,83,86	0
6	EDO	A	616	4/4	0.76	0.58	106,109,109,112	0
5	SO4	B	506	5/5	0.76	0.64	192,193,195,195	0
5	SO4	B	505	5/5	0.77	0.26	169,169,170,172	0
6	EDO	B	514	4/4	0.79	0.27	108,109,111,114	0
6	EDO	B	515	4/4	0.81	0.31	87,99,102,106	0
6	EDO	A	609	4/4	0.82	0.19	86,91,95,96	0
6	EDO	B	508	4/4	0.82	0.25	62,68,76,76	0
6	EDO	B	511	4/4	0.83	0.30	75,75,83,93	0
5	SO4	B	503	5/5	0.84	0.53	185,185,187,187	0
6	EDO	A	615[B]	4/4	0.86	0.26	53,63,69,72	4
6	EDO	A	619	4/4	0.86	0.56	141,142,143,144	0
6	EDO	A	615[A]	4/4	0.86	0.26	56,62,69,70	4
6	EDO	B	513	4/4	0.89	0.20	93,96,96,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	B	502	5/5	0.90	0.20	142,144,145,149	0
6	EDO	A	611	4/4	0.90	0.21	67,69,76,76	0
5	SO4	A	605	5/5	0.90	0.15	138,139,140,141	0
5	SO4	A	606	5/5	0.91	0.26	111,111,115,126	0
7	DMS	B	501	4/4	0.92	0.31	82,84,88,94	0
5	SO4	A	603	5/5	0.93	0.14	130,131,133,135	0
5	SO4	A	604	5/5	0.93	0.13	127,129,131,138	0
6	EDO	B	509	4/4	0.93	0.32	79,82,88,99	0
5	SO4	B	504	5/5	0.94	0.44	186,187,189,189	0
3	K5C	A	601	40/40	0.94	0.18	61,75,106,111	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.