



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 6AQG / pdb_00006aqg
Title : Crystal Structure of Lysyl-tRNA Synthetase from Mycobacterium ulcerans complexed with L-lysine and Cladosporin
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2017-08-19
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

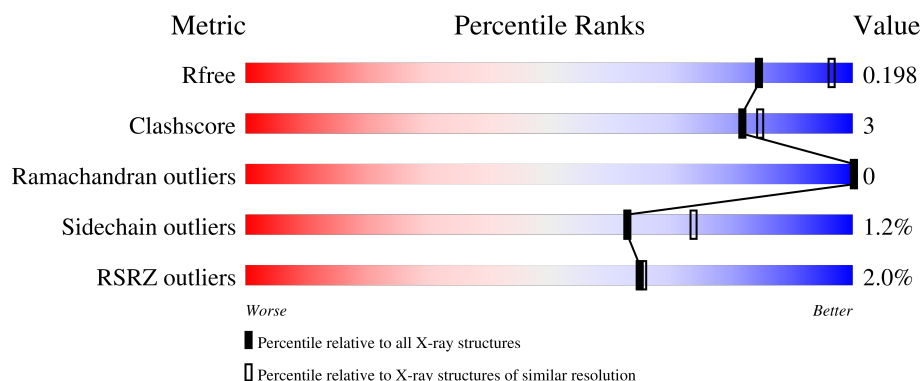
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	0% 90% 6% .
1	B	506	0% 90% 6% .
1	C	506	3% 90% 7% .
1	D	506	3% 89% 7% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16277 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 Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	2	0
			3768	2361	670	721	16			
1	B	487	Total	C	N	O	S	0	1	0
			3766	2357	669	724	16			
1	C	490	Total	C	N	O	S	0	3	0
			3787	2370	673	726	18			
1	D	487	Total	C	N	O	S	0	1	0
			3774	2360	669	728	17			

There are 32 discrepancies between the modelled and reference sequences:

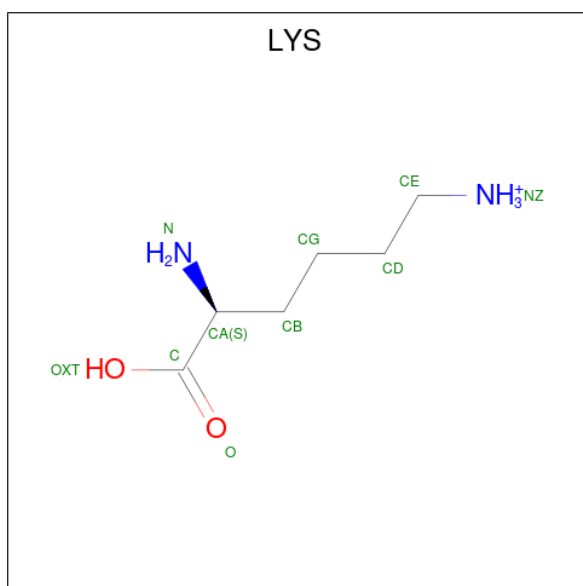
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0PV47
A	-6	ALA	-	expression tag	UNP A0PV47
A	-5	HIS	-	expression tag	UNP A0PV47
A	-4	HIS	-	expression tag	UNP A0PV47
A	-3	HIS	-	expression tag	UNP A0PV47
A	-2	HIS	-	expression tag	UNP A0PV47
A	-1	HIS	-	expression tag	UNP A0PV47
A	0	HIS	-	expression tag	UNP A0PV47
B	-7	MET	-	initiating methionine	UNP A0PV47
B	-6	ALA	-	expression tag	UNP A0PV47
B	-5	HIS	-	expression tag	UNP A0PV47
B	-4	HIS	-	expression tag	UNP A0PV47
B	-3	HIS	-	expression tag	UNP A0PV47
B	-2	HIS	-	expression tag	UNP A0PV47
B	-1	HIS	-	expression tag	UNP A0PV47
B	0	HIS	-	expression tag	UNP A0PV47
C	-7	MET	-	initiating methionine	UNP A0PV47
C	-6	ALA	-	expression tag	UNP A0PV47
C	-5	HIS	-	expression tag	UNP A0PV47
C	-4	HIS	-	expression tag	UNP A0PV47
C	-3	HIS	-	expression tag	UNP A0PV47

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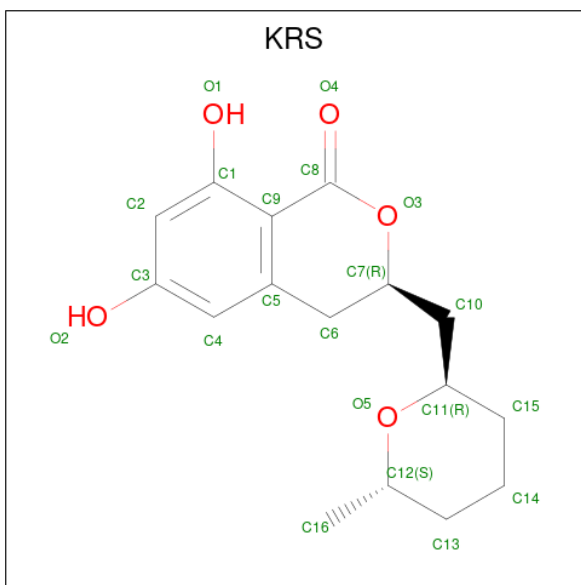
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP A0PV47
C	-1	HIS	-	expression tag	UNP A0PV47
C	0	HIS	-	expression tag	UNP A0PV47
D	-7	MET	-	initiating methionine	UNP A0PV47
D	-6	ALA	-	expression tag	UNP A0PV47
D	-5	HIS	-	expression tag	UNP A0PV47
D	-4	HIS	-	expression tag	UNP A0PV47
D	-3	HIS	-	expression tag	UNP A0PV47
D	-2	HIS	-	expression tag	UNP A0PV47
D	-1	HIS	-	expression tag	UNP A0PV47
D	0	HIS	-	expression tag	UNP A0PV47

- Molecule 2 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



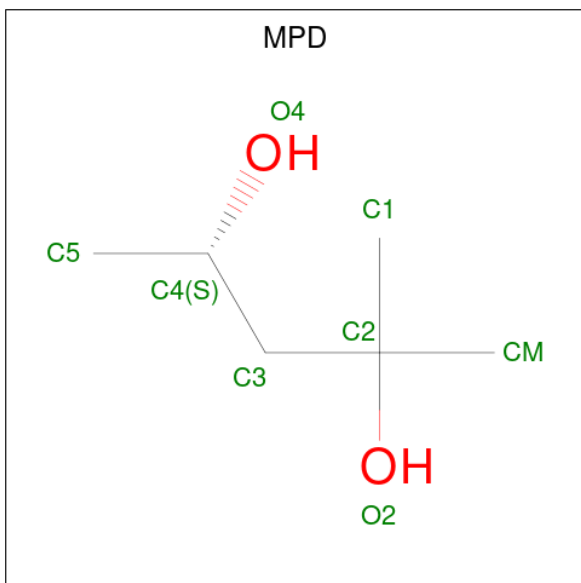
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is cladosporin (CCD ID: KRS) (formula: $C_{16}H_{20}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

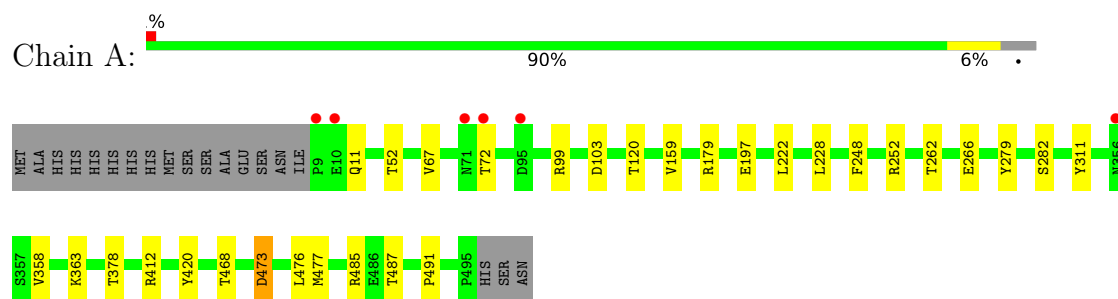
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	278	Total O 280 280	0	2
5	B	274	Total O 274 274	0	0
5	C	210	Total O 210 210	0	0
5	D	220	Total O 222 222	0	2

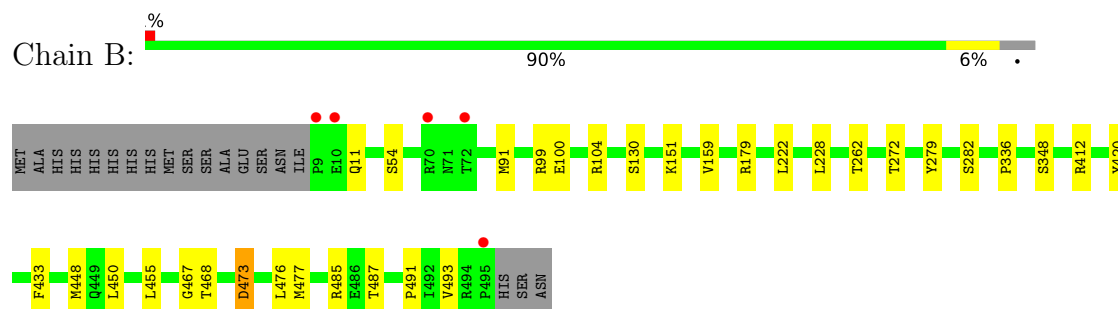
3 Residue-property plots [i](#)

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

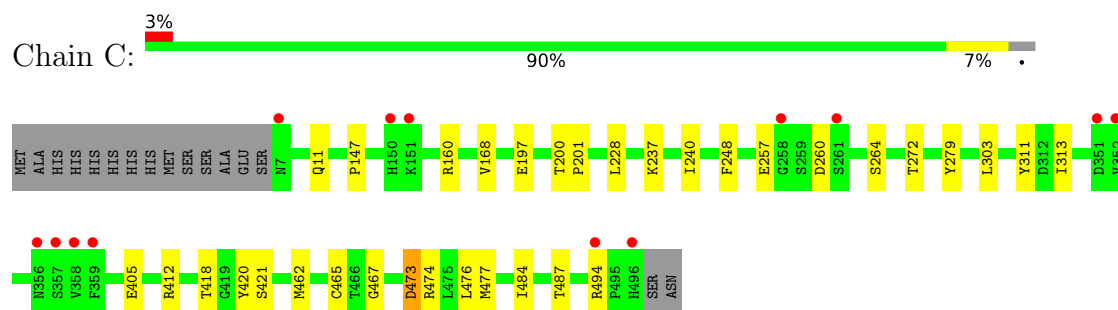
- Molecule 1: Lysine-tRNA ligase



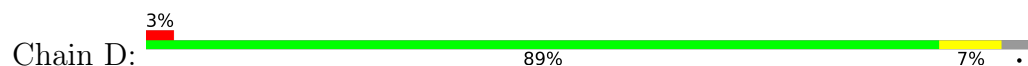
- Molecule 1: Lysine-tRNA ligase

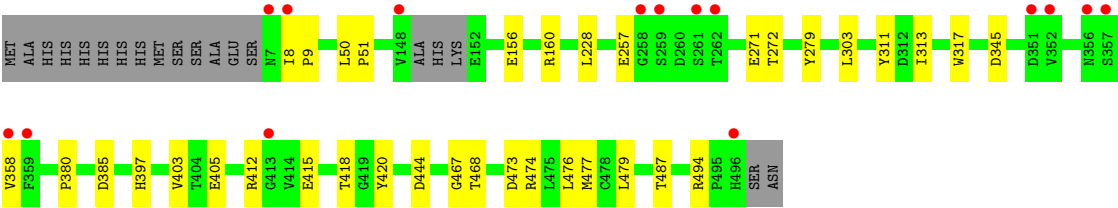


- Molecule 1: Lysine-tRNA ligase



- Molecule 1: Lysine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.12Å 97.20Å 105.83Å 90.05° 104.28° 117.86°	Depositor
Resolution (Å)	41.32 – 2.25 41.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.32-2.25) 98.3 (41.32-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.153 , 0.195 0.155 , 0.198	Depositor DCC
R_{free} test set	1954 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16277	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: KRS, MPD

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	0.36	0/3843	0.53	0/5221
1	B	0.36	0/3838	0.53	0/5213
1	C	0.31	0/3865	0.49	0/5253
1	D	0.31	0/3844	0.50	0/5221
All	All	0.34	0/15390	0.52	0/20908

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	TYR	Peptide
1	B	420	TYR	Peptide
1	C	420	TYR	Peptide
1	D	420	TYR	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	3768	0	3693	15	0
1	B	3766	0	3683	18	0
1	C	3787	0	3681	24	0
1	D	3774	0	3676	20	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
2	C	10	0	12	0	0
2	D	10	0	12	0	0
3	A	21	0	20	0	0
3	B	21	0	19	0	0
3	C	21	0	19	4	0
3	D	21	0	18	4	0
4	A	24	0	42	2	0
4	B	32	0	56	4	0
4	C	8	0	14	0	0
4	D	8	0	14	0	0
5	A	280	0	0	1	0
5	B	274	0	0	1	0
5	C	210	0	0	1	0
5	D	222	0	0	0	0
All	All	16277	0	14983	76	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 3.

All (76) 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:476:LEU:HD23	1:A:487:THR:HB	1.62	0.81
1:C:237:LYS:HG2	1:C:462:MET:HE1	1.67	0.76
1:B:476:LEU:HD23	1:B:487:THR:HB	1.69	0.73
1:B:228:LEU:HD21	1:C:228:LEU:HD21	1.75	0.67
1:C:240:ILE:HB	1:C:462:MET:HE3	1.77	0.67
1:C:11:GLN:NE2	5:C:701:HOH:O	2.21	0.66
4:B:605:MPD:O4	4:B:605:MPD:O2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG13	1:A:491:PRO:HG2	1.79	0.65
1:C:462:MET:HE2	1:C:465:CYS:SG	2.39	0.63
1:C:418:THR:HG22	3:C:602:KRS:H15	1.83	0.60
1:B:262:THR:HG22	1:B:477:MET:HE1	1.83	0.60
1:D:473:ASP:O	1:D:477:MET:HG3	2.01	0.60
1:D:476:LEU:HD13	1:D:487:THR:HB	1.84	0.59
1:A:262:THR:HG22	1:A:477:MET:HE1	1.84	0.59
1:D:160:ARG:NH2	1:D:494:ARG:O	2.35	0.59
1:B:159:VAL:HG13	1:B:491:PRO:HG2	1.85	0.59
1:A:228:LEU:HD21	1:D:228:LEU:HD21	1.89	0.54
1:A:222:LEU:O	1:D:494:ARG:NH1	2.41	0.53
1:D:303:LEU:HD13	1:D:479:LEU:HA	1.89	0.53
1:C:311:TYR:CE2	1:C:412:ARG:HG3	2.42	0.53
1:A:99:ARG:NH1	1:A:103:ASP:OD1	2.41	0.53
1:D:397:HIS:HA	1:D:405:GLU:HG3	1.89	0.53
1:D:50:LEU:HD12	1:D:51:PRO:HD2	1.91	0.53
1:D:311:TYR:CE2	1:D:412:ARG:HG3	2.43	0.52
1:B:222:LEU:O	1:C:494[B]:ARG:NH1	2.43	0.51
1:C:473:ASP:O	1:C:477[B]:MET:HG3	2.11	0.50
1:A:282:SER:HB2	1:A:468:THR:CG2	2.41	0.50
1:C:477[B]:MET:HE2	1:C:484:ILE:HB	1.94	0.49
1:C:197:GLU:HB2	1:C:248:PHE:CZ	2.47	0.49
1:B:412:ARG:NH2	5:B:707:HOH:O	2.42	0.49
1:D:317:TRP:CG	1:D:380:PRO:HB2	2.48	0.48
1:B:179:ARG:HD2	1:B:487:THR:O	2.13	0.48
1:C:147:PRO:HD2	1:C:168:VAL:HG11	1.95	0.48
1:C:476:LEU:HD13	1:C:487:THR:HB	1.94	0.48
1:A:179:ARG:HD2	1:A:487:THR:O	2.14	0.47
1:C:257:GLU:OE2	3:C:602:KRS:O2	2.23	0.47
1:B:450:LEU:HD21	1:B:455:LEU:HD11	1.97	0.46
1:D:272:THR:O	1:D:467:GLY:HA2	2.16	0.46
1:B:100:GLU:O	1:B:104:ARG:HG3	2.16	0.46
1:B:336:PRO:HD3	4:B:606:MPD:HM2	1.98	0.46
1:D:474:ARG:NH1	3:D:503:KRS:H8	2.32	0.45
1:B:485:ARG:HH22	1:B:493:VAL:HG12	1.81	0.44
1:C:200:THR:HB	1:C:201:PRO:HD2	1.99	0.44
1:C:405:GLU:HB2	1:C:421:SER:HB2	1.98	0.44
1:D:415:GLU:OE2	3:D:503:KRS:H14	2.17	0.44
1:B:222:LEU:HD22	1:C:494[B]:ARG:HG3	2.00	0.44
1:C:311:TYR:CD2	1:C:412:ARG:HG3	2.52	0.44
1:B:282:SER:HB2	1:B:468:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:HD11	1:C:313:ILE:HD13	1.99	0.43
1:C:474:ARG:HG2	1:C:477[B]:MET:HE3	1.99	0.43
1:D:418:THR:HG22	3:D:503:KRS:H15	2.00	0.43
1:D:303:LEU:HD11	1:D:313:ILE:HD13	2.00	0.43
1:A:485[B]:ARG:HB2	5:A:880:HOH:O	2.18	0.43
4:A:604:MPD:H11	4:A:604:MPD:H4	1.77	0.42
4:B:605:MPD:HO2	4:B:605:MPD:HO4	1.62	0.42
1:D:271:GLU:HA	1:D:468:THR:O	2.19	0.42
1:C:474:ARG:NH1	3:C:602:KRS:H8	2.34	0.42
1:A:311:TYR:CE2	1:A:412:ARG:HG3	2.54	0.42
1:A:473:ASP:O	1:A:477:MET:HG3	2.19	0.42
1:D:8:ILE:H	1:D:9:PRO:HD2	1.85	0.42
4:B:604:MPD:H11	4:B:604:MPD:H4	1.82	0.42
1:B:433:PHE:HE1	1:B:448:MET:HE3	1.84	0.42
1:B:91:MET:HE3	1:B:130:SER:OG	2.20	0.41
1:A:67:VAL:HB	4:A:605:MPD:H32	2.01	0.41
1:A:358:VAL:HG13	1:A:363:LYS:HB3	2.02	0.41
1:B:99:ARG:HA	1:B:99:ARG:HD3	1.89	0.41
1:D:358:VAL:HG13	1:D:444:ASP:HB2	2.02	0.41
1:C:264:SER:H	3:C:602:KRS:H3	1.85	0.41
1:B:272:THR:O	1:B:467:GLY:HA2	2.21	0.41
1:D:385:ASP:HB3	1:D:403:VAL:HG11	2.02	0.41
1:A:252:ARG:NH1	1:A:266:GLU:OE2	2.53	0.41
1:D:257:GLU:OE1	3:D:503:KRS:O2	2.38	0.41
1:A:197:GLU:HB2	1:A:248:PHE:CZ	2.55	0.40
1:C:272:THR:O	1:C:467:GLY:HA2	2.21	0.40
1:B:473:ASP:O	1:B:477:MET:HG3	2.21	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	487/506 (96%)	474 (97%)	13 (3%)	0	100	100
1	B	486/506 (96%)	470 (97%)	16 (3%)	0	100	100
1	C	491/506 (97%)	480 (98%)	11 (2%)	0	100	100
1	D	484/506 (96%)	473 (98%)	11 (2%)	0	100	100
All	All	1948/2024 (96%)	1897 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	393/424 (93%)	386 (98%)	7 (2%)	51	63
1	B	393/424 (93%)	387 (98%)	6 (2%)	57	68
1	C	391/424 (92%)	388 (99%)	3 (1%)	73	80
1	D	393/424 (93%)	390 (99%)	3 (1%)	73	80
All	All	1570/1696 (93%)	1551 (99%)	19 (1%)	63	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	52	THR
1	A	72	THR
1	A	120	THR
1	A	279	TYR
1	A	378	THR
1	A	473	ASP
1	B	11	GLN
1	B	54	SER
1	B	151	LYS
1	B	279	TYR
1	B	348	SER
1	B	473	ASP

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Mol	Chain	Res	Type
1	C	260	ASP
1	C	279	TYR
1	C	473	ASP
1	D	156	GLU
1	D	279	TYR
1	D	345	ASP

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

Mol	Chain	Res	Type
1	A	178	GLN
1	B	11	GLN
1	B	178	GLN
1	C	178	GLN
1	C	302	GLN
1	D	178	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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
4	MPD	C	603	-	7,7,7	0.27	0	9,10,10	0.22	0
2	LYS	D	502	-	8,9,9	0.76	0	7,10,10	0.87	0
4	MPD	A	603	-	7,7,7	0.34	0	9,10,10	0.35	0
3	KRS	C	602	-	23,23,23	0.69	0	33,33,33	1.53	5 (15%)
4	MPD	B	605	-	7,7,7	0.35	0	9,10,10	0.25	0
4	MPD	B	606	-	7,7,7	0.35	0	9,10,10	0.41	0
4	MPD	D	501	-	7,7,7	0.27	0	9,10,10	0.36	0
3	KRS	A	602	-	23,23,23	1.06	1 (4%)	33,33,33	1.87	8 (24%)
3	KRS	B	602	-	23,23,23	0.86	1 (4%)	33,33,33	1.89	9 (27%)
2	LYS	A	601	-	8,9,9	0.74	0	7,10,10	1.07	1 (14%)
4	MPD	A	605	-	7,7,7	0.31	0	9,10,10	0.23	0
4	MPD	B	604	-	7,7,7	0.31	0	9,10,10	0.25	0
2	LYS	B	601	-	8,9,9	0.80	0	7,10,10	0.67	0
4	MPD	B	603	-	7,7,7	0.39	0	9,10,10	0.60	0
4	MPD	A	604	-	7,7,7	0.35	0	9,10,10	0.37	0
3	KRS	D	503	-	23,23,23	0.68	0	33,33,33	1.45	5 (15%)
2	LYS	C	601	-	8,9,9	0.83	0	7,10,10	0.91	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
4	MPD	C	603	-	-	2/5/5/5	-
2	LYS	D	502	-	-	1/9/9/9	-
4	MPD	A	603	-	-	3/5/5/5	-
3	KRS	C	602	-	-	0/4/26/26	0/3/3/3
4	MPD	B	605	-	-	4/5/5/5	-
4	MPD	B	606	-	-	0/5/5/5	-
4	MPD	D	501	-	-	3/5/5/5	-
3	KRS	A	602	-	-	0/4/26/26	0/3/3/3
3	KRS	B	602	-	-	0/4/26/26	0/3/3/3
2	LYS	A	601	-	-	1/9/9/9	-
4	MPD	A	605	-	-	0/5/5/5	-
4	MPD	B	604	-	-	2/5/5/5	-
2	LYS	B	601	-	-	1/9/9/9	-
4	MPD	B	603	-	-	0/5/5/5	-
4	MPD	A	604	-	-	3/5/5/5	-
3	KRS	D	503	-	-	0/4/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	C	601	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	KRS	O3-C8	3.03	1.39	1.34
3	B	602	KRS	O3-C8	2.28	1.38	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	KRS	C7-O3-C8	5.15	126.36	118.78
3	A	602	KRS	C7-O3-C8	4.65	125.62	118.78
3	A	602	KRS	O3-C7-C10	4.16	112.66	106.10
3	C	602	KRS	C7-O3-C8	3.75	124.30	118.78
3	B	602	KRS	C12-O5-C11	3.66	121.52	114.00
3	B	602	KRS	O3-C7-C10	3.66	111.86	106.10
3	A	602	KRS	C12-O5-C11	3.63	121.47	114.00
3	B	602	KRS	C14-C13-C12	3.44	113.34	111.00
3	A	602	KRS	C14-C13-C12	3.41	113.33	111.00
3	D	503	KRS	C7-O3-C8	3.08	123.32	118.78
3	C	602	KRS	C14-C13-C12	2.98	113.03	111.00
3	D	503	KRS	O3-C8-C9	-2.97	115.22	119.08
3	D	503	KRS	O5-C11-C10	-2.96	100.65	107.84
3	A	602	KRS	O5-C11-C15	2.96	113.02	109.91
3	C	602	KRS	O3-C8-C9	-2.94	115.26	119.08
3	B	602	KRS	O5-C12-C13	2.71	111.96	109.91
3	B	602	KRS	O3-C8-C9	-2.59	115.72	119.08
3	C	602	KRS	O5-C11-C10	-2.56	101.64	107.84
3	B	602	KRS	O5-C12-C16	2.48	111.53	106.88
3	A	602	KRS	O5-C12-C13	2.47	111.78	109.91
2	A	601	LYS	OXT-C-O	-2.33	118.80	124.08
3	D	503	KRS	O5-C12-C13	-2.30	108.17	109.91
3	A	602	KRS	O5-C11-C10	-2.30	102.27	107.84
3	B	602	KRS	O5-C11-C10	-2.29	102.29	107.84
3	C	602	KRS	C1-C9-C8	-2.18	117.36	119.77
3	A	602	KRS	O5-C12-C16	2.07	110.75	106.88
3	D	503	KRS	C1-C9-C8	-2.07	117.49	119.77
3	B	602	KRS	O5-C11-C15	2.01	112.02	109.91

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	MPD	C1-C2-C3-C4
4	B	605	MPD	C2-C3-C4-O4
4	A	604	MPD	O2-C2-C3-C4
4	A	604	MPD	CM-C2-C3-C4
4	B	605	MPD	CM-C2-C3-C4
4	D	501	MPD	CM-C2-C3-C4
4	B	605	MPD	C2-C3-C4-C5
2	A	601	LYS	CG-CD-CE-NZ
4	A	603	MPD	O2-C2-C3-C4
4	B	604	MPD	O2-C2-C3-C4
4	C	603	MPD	O2-C2-C3-C4
4	C	603	MPD	C2-C3-C4-O4
4	D	501	MPD	C2-C3-C4-O4
4	A	603	MPD	C1-C2-C3-C4
4	A	603	MPD	CM-C2-C3-C4
4	B	604	MPD	CM-C2-C3-C4
4	B	605	MPD	C1-C2-C3-C4
4	D	501	MPD	C1-C2-C3-C4
2	D	502	LYS	CG-CD-CE-NZ
2	B	601	LYS	OXT-C-CA-N

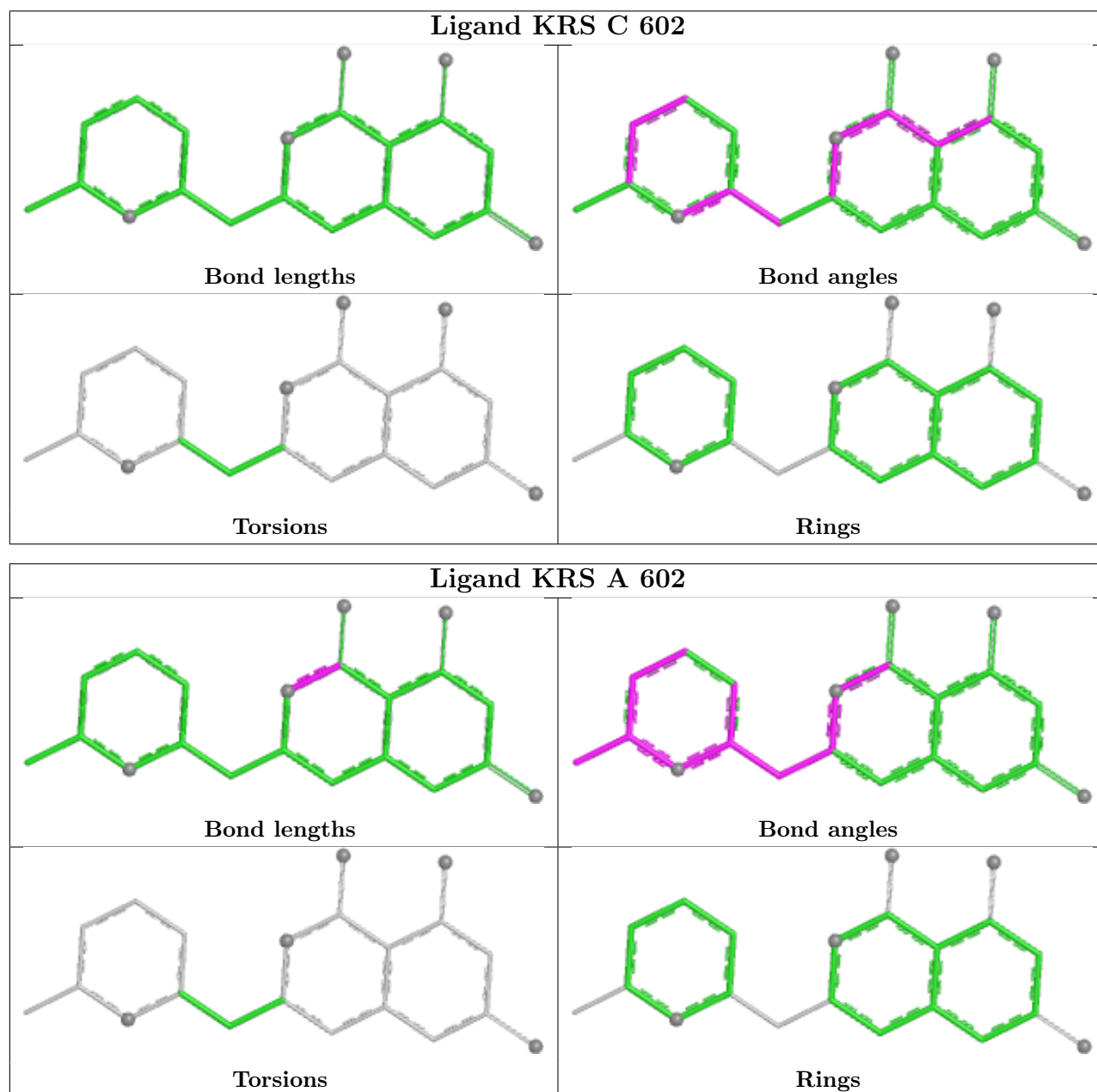
There are no ring outliers.

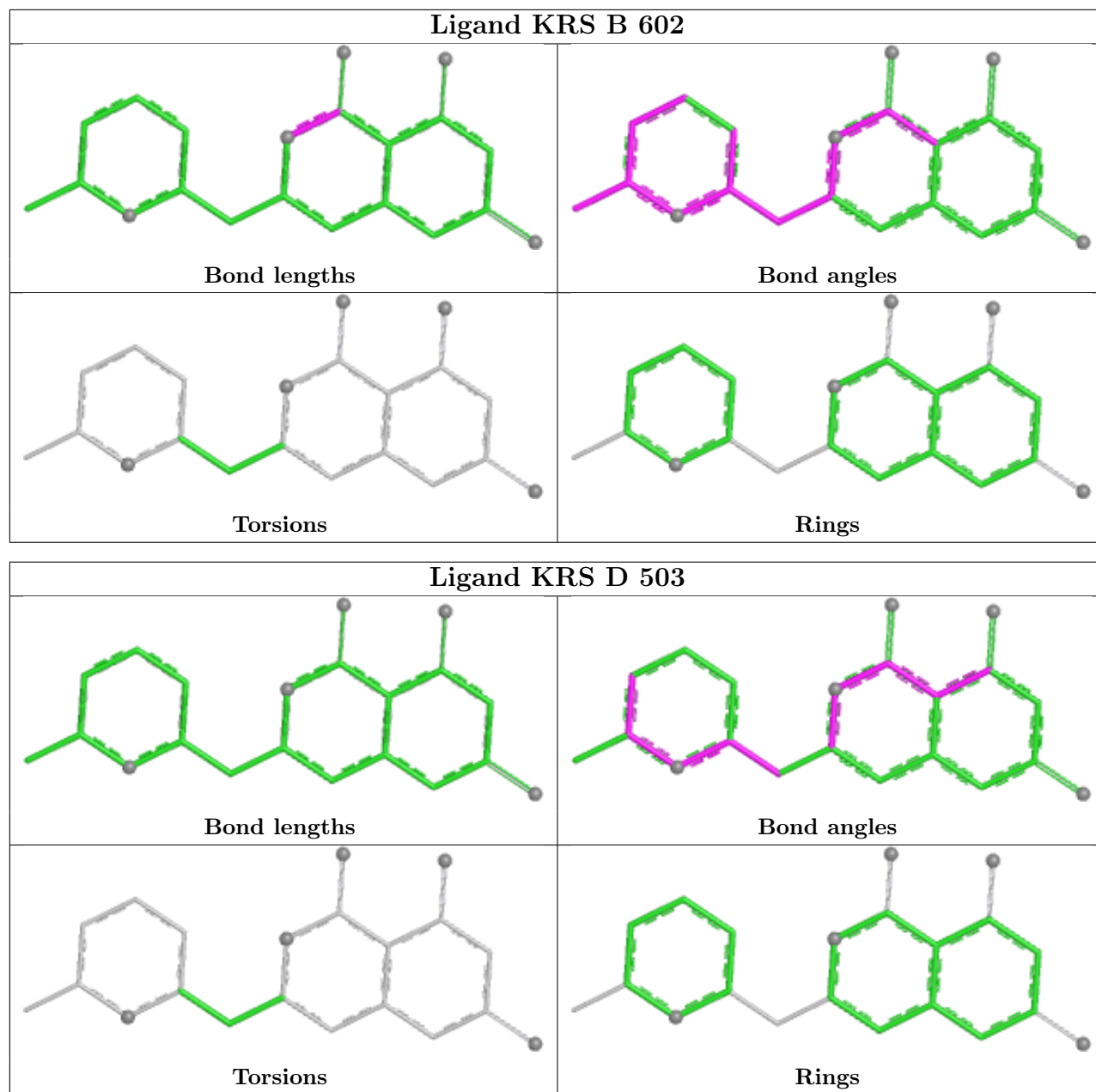
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	KRS	4	0
4	B	605	MPD	2	0
4	B	606	MPD	1	0
4	A	605	MPD	1	0
4	B	604	MPD	1	0
4	A	604	MPD	1	0
3	D	503	KRS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/506 (96%)	-0.31	6 (1%) 76 77	25, 45, 87, 111	2 (0%)
1	B	487/506 (96%)	-0.30	5 (1%) 79 81	24, 45, 90, 106	1 (0%)
1	C	490/506 (96%)	-0.17	13 (2%) 56 57	28, 52, 102, 134	3 (0%)
1	D	487/506 (96%)	-0.09	15 (3%) 51 51	27, 53, 101, 129	1 (0%)
All	All	1951/2024 (96%)	-0.22	39 (1%) 65 65	24, 50, 94, 134	7 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	4.9
1	C	358	VAL	4.7
1	B	9	PRO	4.7
1	C	261	SER	4.5
1	D	358	VAL	4.3
1	D	357	SER	4.2
1	D	258	GLY	3.9
1	C	258	GLY	3.5
1	D	7	ASN	3.5
1	C	7	ASN	3.3
1	D	496	HIS	3.3
1	B	72	THR	3.2
1	D	356	ASN	3.2
1	D	352	VAL	3.0
1	A	72	THR	3.0
1	D	261	SER	2.9
1	A	10	GLU	2.9
1	C	150	HIS	2.9
1	D	148	VAL	2.9
1	C	357	SER	2.8
1	D	359	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	351	ASP	2.7
1	C	359	PHE	2.7
1	A	71	ASN	2.6
1	B	495	PRO	2.6
1	A	95	ASP	2.5
1	D	8	ILE	2.5
1	D	259	SER	2.4
1	C	496	HIS	2.4
1	C	356	ASN	2.3
1	C	351	ASP	2.3
1	B	70	ARG	2.1
1	C	352	VAL	2.1
1	D	413	GLY	2.1
1	C	494[A]	ARG	2.1
1	C	151	LYS	2.0
1	D	262	THR	2.0
1	B	10	GLU	2.0
1	A	356	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	B	606	8/8	0.84	0.25	47,83,93,94	0
4	MPD	B	604	8/8	0.87	0.21	92,98,100,102	0
4	MPD	A	604	8/8	0.87	0.24	94,98,101,103	0
3	KRS	C	602	21/21	0.88	0.17	72,81,91,99	0
3	KRS	D	503	21/21	0.90	0.16	61,78,93,95	0

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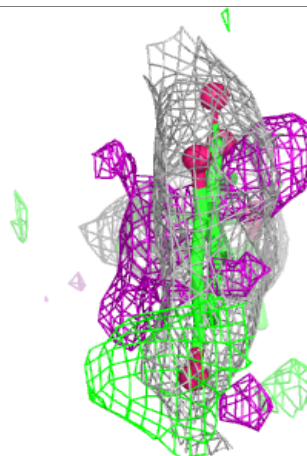
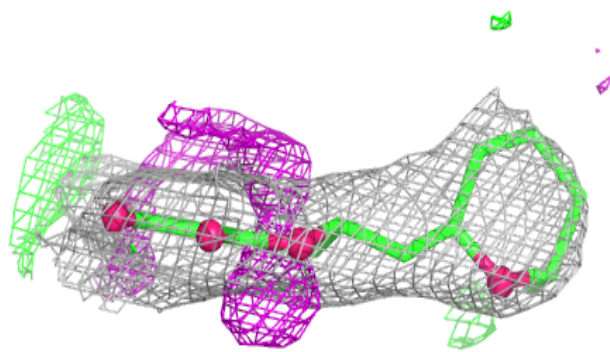
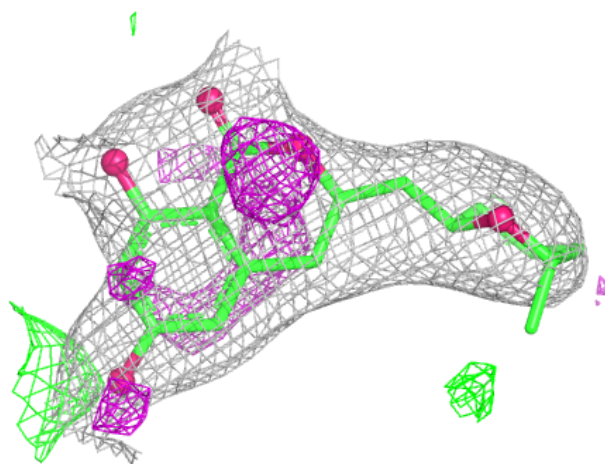
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MPD	B	605	8/8	0.93	0.14	60,70,74,75	0
4	MPD	A	605	8/8	0.94	0.14	78,83,90,93	0
4	MPD	A	603	8/8	0.94	0.12	41,51,55,62	0
4	MPD	D	501	8/8	0.94	0.12	46,55,58,60	0
2	LYS	C	601	10/10	0.95	0.08	43,47,55,55	0
3	KRS	A	602	21/21	0.95	0.07	34,38,40,47	0
3	KRS	B	602	21/21	0.95	0.07	32,38,42,47	0
2	LYS	B	601	10/10	0.96	0.07	27,31,37,42	0
4	MPD	C	603	8/8	0.96	0.09	38,50,58,59	0
4	MPD	B	603	8/8	0.96	0.09	41,53,59,61	0
2	LYS	D	502	10/10	0.97	0.07	44,51,55,57	0
2	LYS	A	601	10/10	0.98	0.05	26,30,40,42	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.

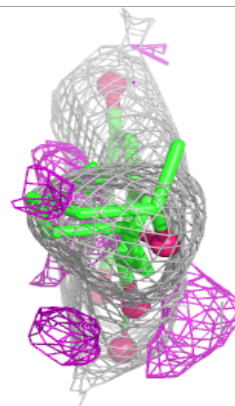
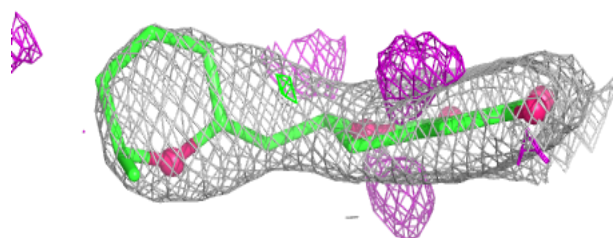
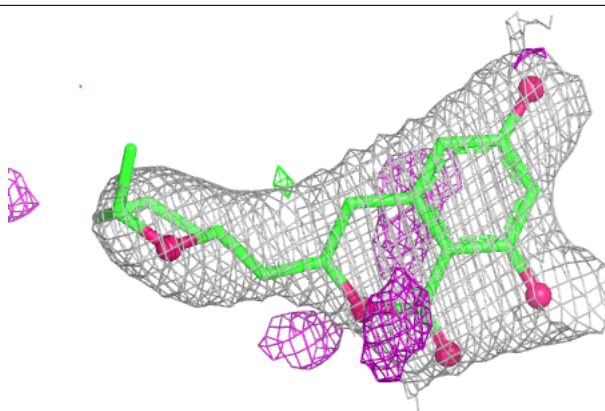
Electron density around KRS C 602:

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

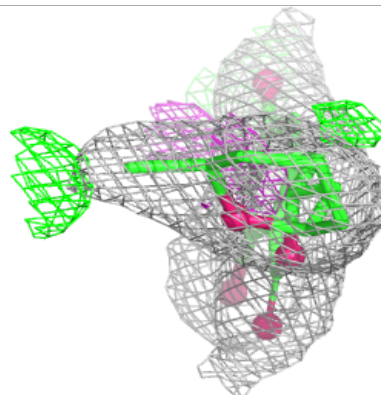
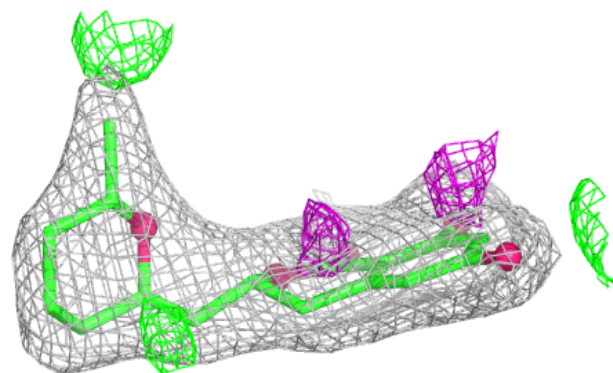
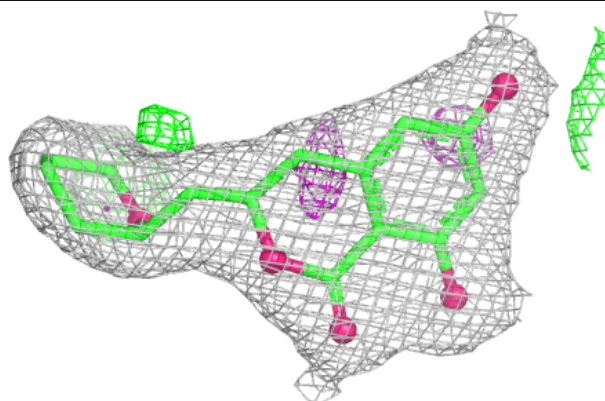


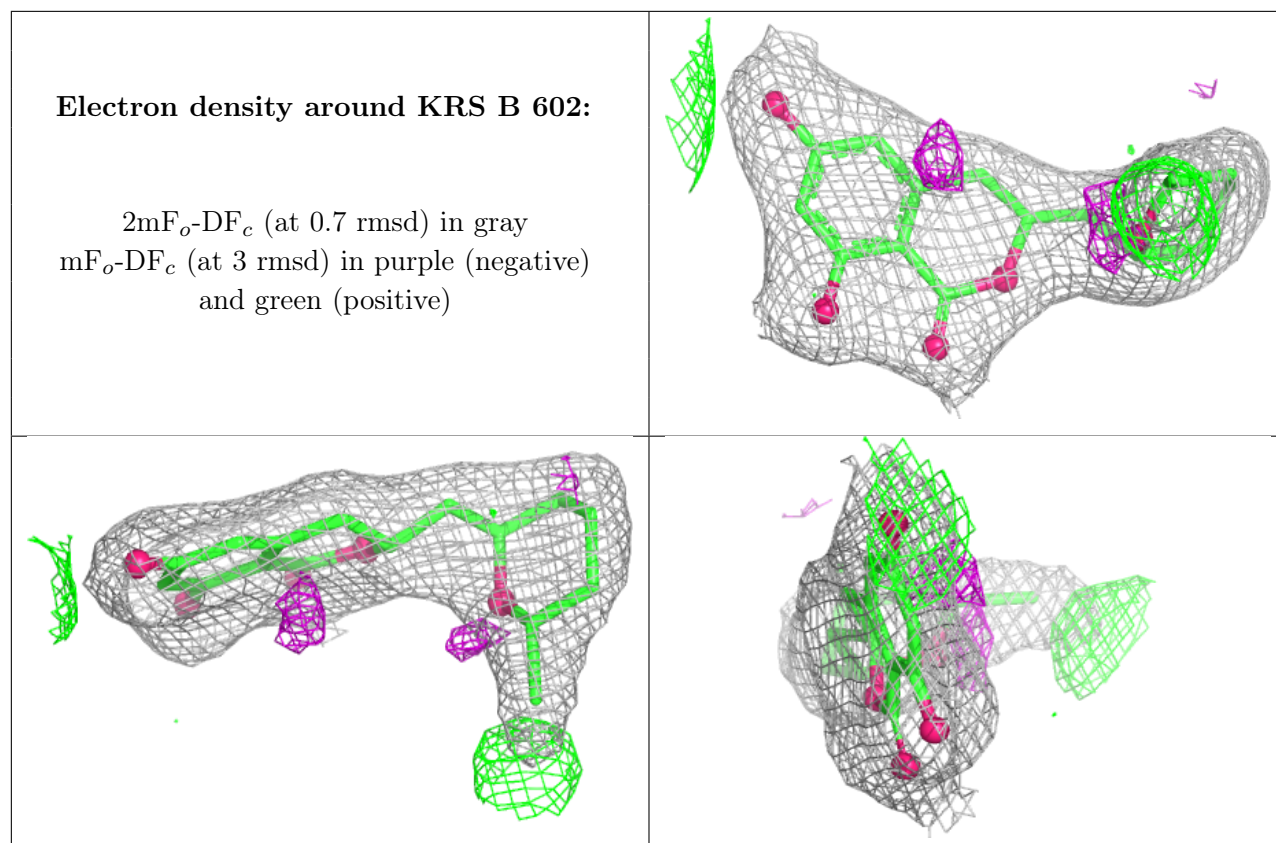
Electron density around KRS D 503:

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

**Electron density around KRS A 602:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.