



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 08:59 AM JST

PDB ID : 6M0T
Title : Crystal Structure of Lysyl-tRNA Synthetase from Plasmodium falciparum complexed with L-lysine and Cladosporin derivative (CL-2)
Authors : Babbar, P.; Sharma, A.; Manickam, Y.
Deposited on : 2020-02-22
Resolution : 2.68 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	:	2.18
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)	:	2.18

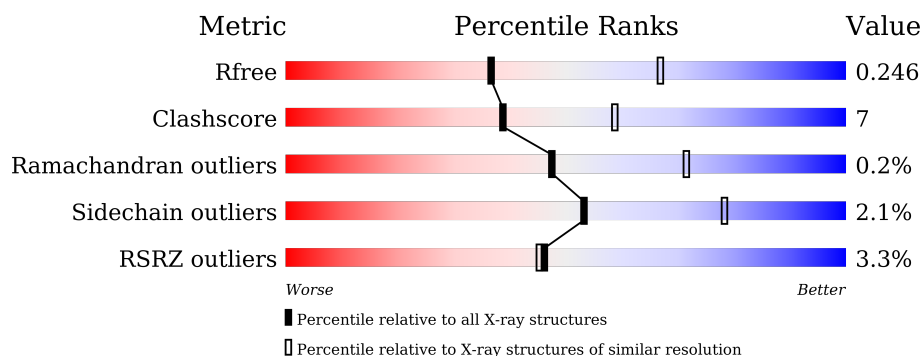
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	507	<div> <div>3%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	B	507	<div> <div>3%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
1	C	507	<div> <div>5%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	D	507	<div> <div>2%</div> <div>79%</div> <div>15%</div> <div>..</div> </div>

2 Entry composition [i](#)

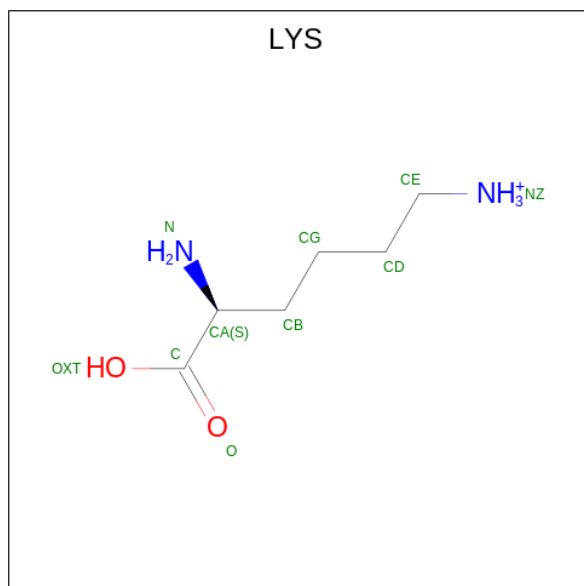
There are 4 unique types of molecules in this entry. The entry contains 16236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	493	Total	C	N	O	S	0	1	0
			4035	2599	674	745	17			
1	B	487	Total	C	N	O	S	0	0	0
			3980	2568	663	732	17			
1	C	485	Total	C	N	O	S	0	2	0
			3989	2578	662	732	17			
1	D	487	Total	C	N	O	S	0	1	0
			3990	2574	666	733	17			

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



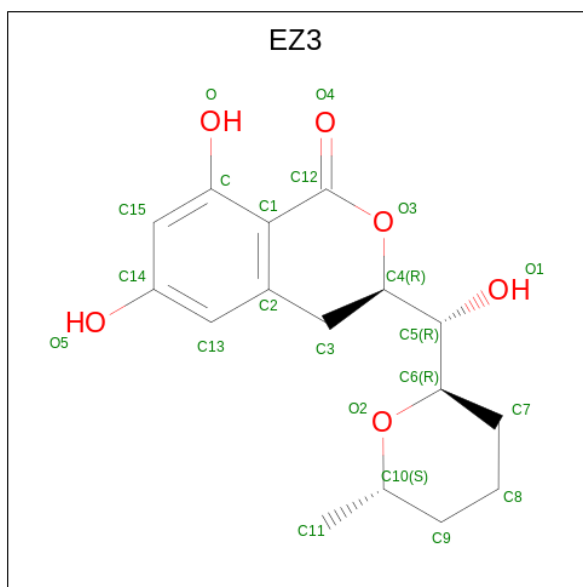
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (3R)-3-[(R)-[(2R,6S)-6-methyloxan-2-yl]-oxidanyl-methyl]-6,8-bis(oxidanyl)-3,4-dihydroisochromen-1-one (three-letter code: EZ3) (formula: C₁₆H₂₀O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	16	6		
3	B	1	Total	C	O	0	0
			22	16	6		
3	C	1	Total	C	O	0	0
			22	16	6		
3	D	1	Total	C	O	0	0
			22	16	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	33	Total	O	0	0
			33	33		

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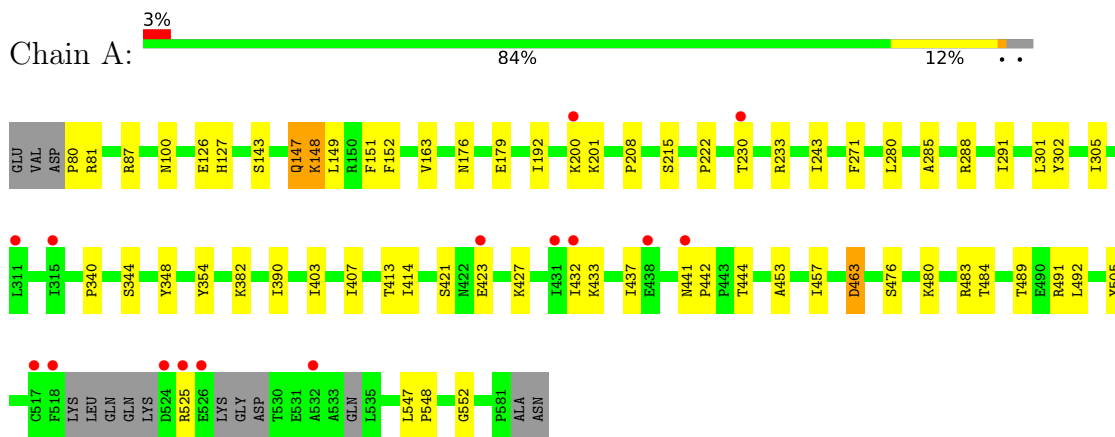
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	17	Total	O	0	0
			17	17		
4	D	23	Total	O	0	0
			23	23		

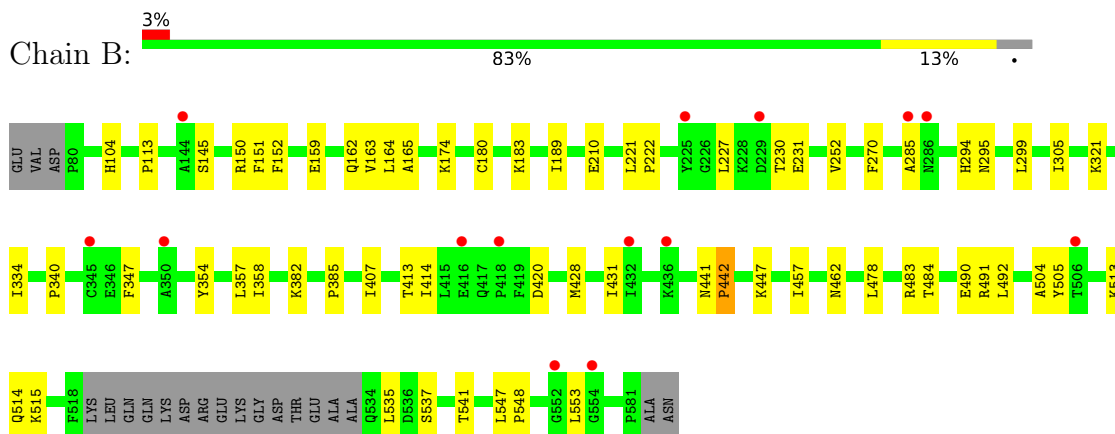
3 Residue-property plots [i](#)

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.

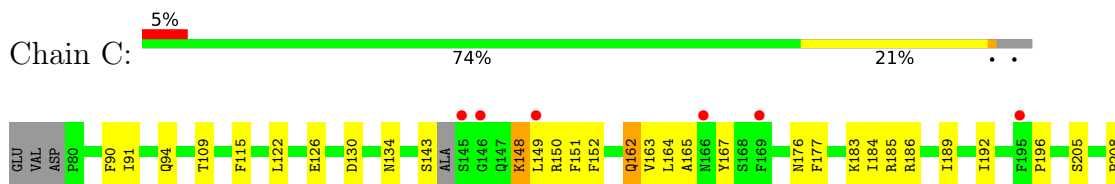
- Molecule 1: Lysine-tRNA ligase

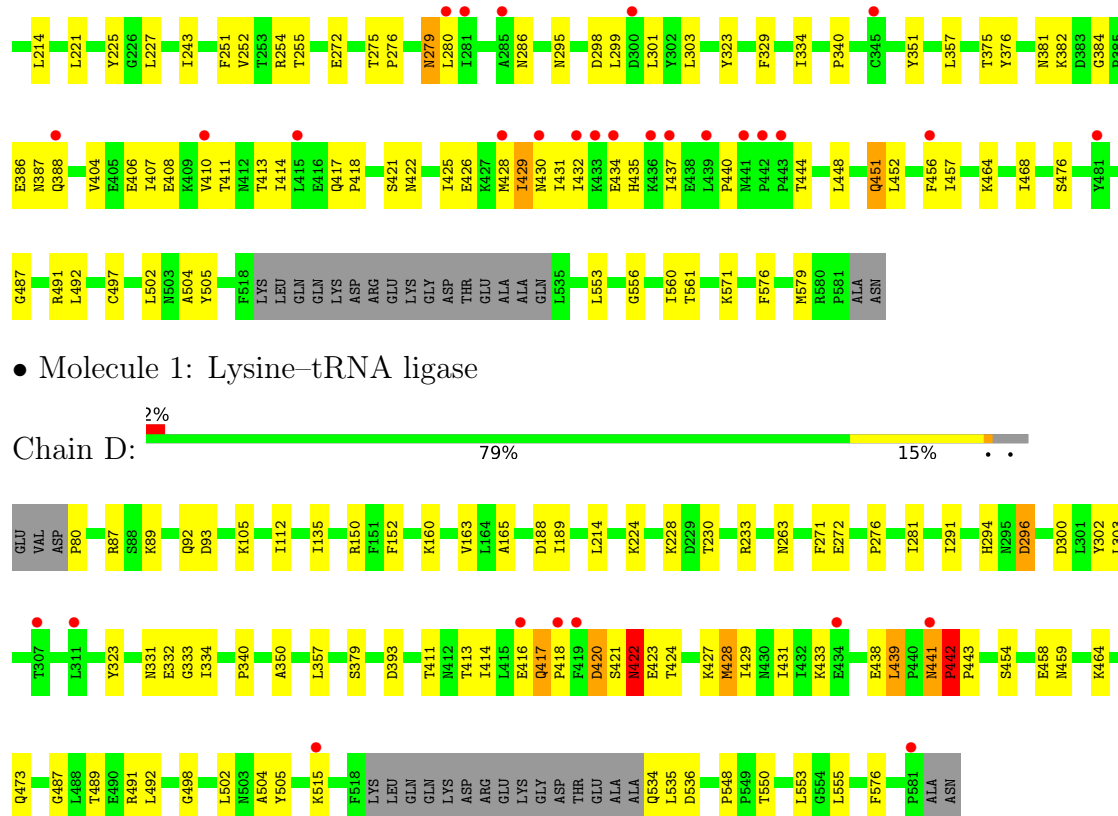


- Molecule 1: Lysine-tRNA ligase



- Molecule 1: Lysine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	299.56Å 59.14Å 141.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.84 – 2.68 36.84 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.84-2.68) 99.9 (36.84-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.15rc1_3423	Depositor
R, R_{free}	0.190 , 0.246 0.194 , 0.246	Depositor DCC
R_{free} test set	3505 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EZ3

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	0.30	0/4133	0.47	0/5579
1	B	0.30	0/4079	0.47	0/5509
1	C	0.30	0/4089	0.51	0/5521
1	D	0.32	0/4090	0.50	1/5524 (0.0%)
All	All	0.30	0/16391	0.49	1/22133 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	PRO	N-CA-C	-5.42	98.02	112.10

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	4035	0	3997	41	0
1	B	3980	0	3955	46	0
1	C	3989	0	3957	106	0
1	D	3990	0	3961	61	0
2	A	10	0	12	2	0
2	B	10	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	12	1	0
2	D	10	0	12	0	0
3	A	22	0	0	0	0
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	0	0
4	A	41	0	0	0	0
4	B	33	0	0	0	0
4	C	17	0	0	1	0
4	D	23	0	0	1	0
All	All	16236	0	15918	240	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 7.

All (240) 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:D:441:ASN:HB3	1:D:442:PRO:CD	1.36	1.47
1:D:441:ASN:CB	1:D:442:PRO:HD3	1.58	1.32
1:C:407:ILE:CD1	1:C:452:LEU:HG	1.68	1.23
1:C:407:ILE:HD13	1:C:452:LEU:CG	1.69	1.22
1:C:413:THR:HG22	1:C:414:ILE:N	1.54	1.15
1:C:426:GLU:CA	1:C:429:ILE:HG13	1.80	1.10
1:C:426:GLU:HA	1:C:429:ILE:CG1	1.83	1.07
1:C:425:ILE:HG22	1:C:429:ILE:HD11	1.34	1.05
1:C:407:ILE:HD13	1:C:452:LEU:HG	1.21	1.04
1:C:413:THR:CG2	1:C:414:ILE:N	2.20	1.04
1:B:441:ASN:HB3	1:B:442:PRO:HD3	1.39	1.04
1:C:407:ILE:HD13	1:C:452:LEU:CD2	1.89	1.03
1:C:407:ILE:HG21	1:C:452:LEU:HD21	1.46	0.97
1:D:417:GLN:HE21	1:D:417:GLN:HA	1.33	0.94
1:C:413:THR:CG2	1:C:414:ILE:H	1.79	0.94
1:C:407:ILE:CD1	1:C:452:LEU:CD2	2.44	0.94
1:C:431:ILE:HD11	1:C:435:HIS:CE1	2.08	0.89
1:C:431:ILE:HD11	1:C:435:HIS:HE1	1.37	0.88
1:C:407:ILE:CD1	1:C:452:LEU:CG	2.38	0.88
1:C:407:ILE:HD11	1:C:452:LEU:HG	1.56	0.88
1:C:556:GLY:O	1:C:560:ILE:HD12	1.73	0.86
1:A:463:ASP:OD1	1:A:463:ASP:N	2.09	0.84
1:D:413:THR:C	1:D:414:ILE:HD13	1.99	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ASP:N	1:D:420:ASP:OD1	2.09	0.82
1:C:152:PHE:HB2	1:C:163:VAL:HB	1.62	0.81
1:C:149:LEU:O	1:C:150:ARG:HD3	1.81	0.80
1:C:413:THR:HG22	1:C:414:ILE:H	1.35	0.80
1:C:428:MET:O	1:C:431:ILE:HG22	1.82	0.80
1:C:428:MET:O	1:C:432:ILE:HD12	1.80	0.80
1:D:417:GLN:OE1	1:D:487:GLY:HA3	1.84	0.78
1:D:441:ASN:CB	1:D:442:PRO:CD	2.28	0.77
1:C:407:ILE:HD13	1:C:452:LEU:HD21	1.66	0.76
1:D:414:ILE:HD13	1:D:414:ILE:N	2.01	0.76
1:A:348:TYR:OH	2:A:601:LYS:NZ	2.20	0.74
1:C:425:ILE:O	1:C:429:ILE:HG12	1.87	0.74
1:C:425:ILE:HG22	1:C:429:ILE:CD1	2.17	0.72
1:C:417:GLN:HG2	1:C:418:PRO:HA	1.72	0.71
1:C:428:MET:O	1:C:432:ILE:CD1	2.39	0.71
1:C:150:ARG:HB2	1:C:165:ALA:HB3	1.72	0.70
1:B:150:ARG:HB2	1:B:165:ALA:HB3	1.73	0.69
1:C:571:LYS:HD3	1:C:579:MET:CE	2.23	0.69
1:D:417:GLN:HE21	1:D:417:GLN:CA	1.99	0.69
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.75	0.69
1:C:426:GLU:HA	1:C:429:ILE:HG13	0.86	0.69
1:D:294:HIS:HE1	1:D:296:ASP:HB2	1.58	0.69
1:D:291:ILE:HD11	1:D:300:ASP:HB3	1.75	0.68
1:A:176:ASN:HD22	1:A:179:GLU:H	1.43	0.65
1:B:113:PRO:HG3	1:B:159:GLU:HG3	1.78	0.65
1:C:407:ILE:HD12	1:C:452:LEU:CD2	2.25	0.65
1:C:431:ILE:CD1	1:C:435:HIS:CE1	2.80	0.64
1:B:441:ASN:HB3	1:B:442:PRO:CD	2.24	0.62
1:C:413:THR:HG23	1:C:414:ILE:H	1.65	0.62
1:B:358:ILE:HG13	1:B:492:LEU:HD22	1.81	0.61
1:C:476:SER:HB3	1:C:491:ARG:HH11	1.66	0.61
1:D:441:ASN:HB3	1:D:442:PRO:HD3	0.63	0.60
1:B:441:ASN:CB	1:B:442:PRO:HD3	2.24	0.60
1:C:444:THR:O	1:C:448:LEU:HG	2.02	0.60
1:D:502:LEU:HD11	1:D:553:LEU:HD11	1.84	0.60
1:C:417:GLN:HG3	1:C:487:GLY:HA3	1.83	0.59
1:A:382:LYS:HD2	1:A:390:ILE:HD13	1.84	0.59
1:C:425:ILE:O	1:C:429:ILE:CG1	2.50	0.59
1:A:433:LYS:HA	1:A:433:LYS:HE3	1.84	0.58
1:B:442:PRO:HD2	1:B:447:LYS:NZ	2.18	0.58
1:D:421:SER:HB2	1:D:423:GLU:OE1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.84	0.58
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.85	0.58
1:D:491:ARG:HA	1:D:505:TYR:HB3	1.86	0.58
1:C:404:VAL:O	1:C:408:GLU:HG2	2.03	0.58
1:C:407:ILE:CD1	1:C:452:LEU:HD21	2.26	0.58
1:A:444:THR:HB	1:A:525:ARG:NH1	2.18	0.58
1:A:441:ASN:HB3	1:A:442:PRO:HD3	1.85	0.58
1:D:112:ILE:HG12	1:D:135:ILE:HD11	1.85	0.57
1:D:334:ILE:HD12	1:D:340:PRO:HD3	1.85	0.57
1:C:430:ASN:O	1:C:434:GLU:HG3	2.05	0.57
1:B:547:LEU:HD12	1:B:548:PRO:HD2	1.86	0.57
1:C:407:ILE:HD12	1:C:452:LEU:HD23	1.87	0.56
1:D:357:LEU:HD13	1:D:504:ALA:HB1	1.87	0.56
1:B:537:SER:O	1:B:541:THR:HG23	2.06	0.56
1:C:411:THR:HG22	1:C:411:THR:O	2.05	0.56
1:B:285:ALA:O	1:B:305:ILE:HD11	2.06	0.56
1:A:491:ARG:HA	1:A:505:TYR:HB3	1.88	0.56
1:B:513:LYS:HA	1:B:515:LYS:HE3	1.88	0.55
1:C:382:LYS:HD2	1:C:497:CYS:HB3	1.88	0.55
1:C:440:PRO:HG3	1:C:451:GLN:HG3	1.88	0.55
1:C:109:THR:HG23	1:C:134:ASN:HB2	1.89	0.54
1:C:432:ILE:HG22	1:C:437:ILE:O	2.08	0.54
1:A:403:ILE:HD11	1:A:453:ALA:HB2	1.89	0.54
1:C:571:LYS:HD3	1:C:579:MET:HE3	1.90	0.54
1:D:428:MET:HA	1:D:431:ILE:HD12	1.90	0.54
1:C:571:LYS:HD3	1:C:579:MET:HE1	1.90	0.53
1:A:148:LYS:O	1:A:149:LEU:HD23	2.08	0.53
1:B:442:PRO:HG2	1:B:447:LYS:HD3	1.89	0.53
1:D:439:LEU:HD11	1:D:443:PRO:HB3	1.90	0.53
1:D:502:LEU:HD12	1:D:555:LEU:HD21	1.90	0.53
1:A:201:LYS:HD3	1:A:201:LYS:N	2.23	0.53
1:B:151:PHE:HD1	1:B:162:GLN:NE2	2.06	0.53
1:B:354:TYR:CD2	1:B:490:GLU:HB3	2.43	0.53
1:C:386:GLU:HG3	1:C:386:GLU:O	2.09	0.53
1:D:429:ILE:O	1:D:433:LYS:HG3	2.08	0.52
1:C:254:ARG:HG3	1:C:561:THR:HG21	1.90	0.52
1:D:417:GLN:HG3	1:D:417:GLN:O	2.08	0.52
1:A:432:ILE:HG23	1:A:437:ILE:HB	1.91	0.52
1:C:90:PHE:HD2	1:C:91:ILE:HD13	1.74	0.51
1:A:407:ILE:HG13	1:A:457:ILE:HD11	1.93	0.51
1:C:252:VAL:HA	1:D:271:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ILE:CD1	1:C:452:LEU:HD23	2.38	0.51
1:C:276:PRO:HD3	1:D:576:PHE:HB2	1.93	0.51
1:B:180:CYS:HA	1:B:183:LYS:HE3	1.92	0.51
1:D:421:SER:O	1:D:423:GLU:N	2.43	0.50
1:D:263:ASN:ND2	4:D:701:HOH:O	2.40	0.50
1:D:272:GLU:HB2	1:D:323:TYR:CZ	2.46	0.50
1:D:417:GLN:CA	1:D:417:GLN:NE2	2.72	0.50
1:A:547:LEU:HD12	1:A:548:PRO:HD2	1.93	0.50
1:A:280:LEU:HD23	1:A:301:LEU:HD23	1.93	0.50
1:C:421:SER:O	1:C:425:ILE:HG13	2.12	0.49
1:A:143:SER:HB2	1:A:151:PHE:HB2	1.94	0.49
1:A:491:ARG:HG3	1:A:505:TYR:HD2	1.77	0.49
1:C:286:ASN:ND2	4:C:702:HOH:O	2.42	0.49
1:C:276:PRO:HG2	1:C:279:ASN:HD21	1.76	0.49
1:B:428:MET:HA	1:B:431:ILE:HD12	1.94	0.49
1:C:252:VAL:HA	1:D:271:PHE:HZ	1.77	0.49
1:C:406:GLU:HG2	1:C:457:ILE:HG22	1.95	0.49
1:D:189:ILE:HG22	1:D:214:LEU:HB2	1.94	0.49
1:C:425:ILE:CG2	1:C:429:ILE:HD11	2.25	0.49
1:A:230:THR:HB	1:A:233:ARG:HH21	1.78	0.49
1:C:189:ILE:HD13	1:D:548:PRO:HB3	1.95	0.49
1:C:334:ILE:HG12	1:C:340:PRO:HD3	1.94	0.48
1:D:454:SER:HA	1:D:458:GLU:HB2	1.96	0.48
1:D:291:ILE:HD12	1:D:302:TYR:CZ	2.48	0.48
1:D:414:ILE:O	1:D:427:LYS:NZ	2.43	0.48
1:B:230:THR:HG22	1:B:231:GLU:H	1.79	0.48
1:C:227:LEU:HD11	1:C:243:ILE:HD12	1.96	0.48
1:A:200:LYS:C	1:A:201:LYS:HD3	2.35	0.47
1:A:483:ARG:HG3	1:A:484:THR:HG23	1.95	0.47
1:D:152:PHE:HB2	1:D:163:VAL:HB	1.96	0.47
1:B:442:PRO:CD	1:B:447:LYS:NZ	2.77	0.47
1:C:299:LEU:HD22	1:C:301:LEU:HG	1.94	0.47
1:D:350:ALA:HA	1:D:550:THR:HG23	1.96	0.47
1:C:502:LEU:HD11	1:C:553:LEU:HD11	1.96	0.47
1:C:122:LEU:HD23	1:C:126:GLU:OE2	2.14	0.47
1:C:148:LYS:HG2	1:C:167:TYR:HB3	1.95	0.47
1:D:230:THR:HG22	1:D:233:ARG:HH12	1.80	0.47
1:D:294:HIS:CE1	1:D:296:ASP:HB2	2.46	0.47
1:B:382:LYS:HE3	1:B:462:ASN:ND2	2.31	0.46
1:D:424:THR:O	1:D:428:MET:HG3	2.15	0.46
1:C:162:GLN:HG3	1:C:163:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ILE:O	1:C:185:ARG:NH1	2.48	0.46
1:A:403:ILE:HG13	1:A:457:ILE:HD12	1.98	0.46
1:C:280:LEU:HG	1:C:299:LEU:HD21	1.97	0.46
1:C:413:THR:HG22	1:C:414:ILE:CA	2.40	0.46
2:C:601:LYS:HE2	2:C:601:LYS:HB3	1.67	0.46
1:C:90:PHE:O	1:C:94:GLN:HG3	2.16	0.46
1:D:87:ARG:NH2	1:D:188:ASP:OD1	2.48	0.46
1:D:473:GLN:HG2	1:D:489:THR:HG23	1.99	0.45
1:C:303:LEU:HD23	1:C:329:PHE:CG	2.52	0.45
1:D:459:ASN:ND2	1:D:498:GLY:HA3	2.31	0.45
1:D:416:GLU:O	1:D:424:THR:HG21	2.17	0.45
1:B:174:LYS:NZ	1:B:210:GLU:OE2	2.38	0.45
1:A:413:THR:O	1:A:414:ILE:HD13	2.16	0.45
1:B:222:PRO:HG2	1:B:227:LEU:HD11	1.99	0.45
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.52	0.45
1:A:291:ILE:HD12	1:A:302:TYR:CZ	2.52	0.45
1:D:393:ASP:O	1:D:464:LYS:HG3	2.17	0.45
1:C:295:ASN:OD1	1:D:331:ASN:ND2	2.44	0.45
1:C:457:ILE:HD12	1:C:468:ILE:HD13	1.99	0.45
1:B:413:THR:O	1:B:414:ILE:HD13	2.17	0.45
1:C:410:VAL:HG23	1:C:411:THR:N	2.32	0.45
1:C:351:TYR:O	1:D:105:LYS:NZ	2.48	0.44
1:C:407:ILE:HD13	1:C:452:LEU:CD1	2.42	0.44
1:D:417:GLN:N	1:D:418:PRO:CD	2.79	0.44
1:B:285:ALA:O	1:B:305:ILE:CD1	2.64	0.44
1:C:189:ILE:HG22	1:C:214:LEU:HB2	1.99	0.44
1:C:303:LEU:HD11	1:D:303:LEU:HD11	1.99	0.44
1:B:221:LEU:HD12	1:B:222:PRO:HD2	1.98	0.44
1:C:491:ARG:HA	1:C:505:TYR:HB3	1.98	0.44
1:D:417:GLN:N	1:D:418:PRO:HD3	2.32	0.44
1:C:115:PHE:CE2	1:C:196:PRO:HB3	2.53	0.44
1:C:186:ARG:NH1	1:C:221:LEU:HB3	2.32	0.44
1:D:150:ARG:HB2	1:D:165:ALA:HB3	1.98	0.44
1:D:89:LYS:NZ	1:D:93:ASP:OD2	2.50	0.44
1:A:480:LYS:HD3	1:B:104:HIS:CD2	2.52	0.44
1:B:478:LEU:HD21	1:B:535:LEU:HD21	2.00	0.43
1:A:552:GLY:C	2:A:601:LYS:HE2	2.39	0.43
1:C:432:ILE:HD12	1:C:432:ILE:H	1.82	0.43
1:C:476:SER:HB3	1:C:491:ARG:NH1	2.31	0.43
1:A:147:GLN:HE21	1:A:147:GLN:HB3	1.51	0.43
1:B:420:ASP:N	1:B:420:ASP:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:SER:HB2	1:C:151:PHE:HB2	2.00	0.43
1:C:162:GLN:HG2	1:C:164:LEU:HD12	2.01	0.43
1:D:416:GLU:N	1:D:424:THR:HG21	2.34	0.43
1:A:288:ARG:HD2	1:B:295:ASN:ND2	2.34	0.43
1:B:385:PRO:HG2	1:C:225:TYR:CE2	2.54	0.43
1:D:281:ILE:HG21	1:D:536:ASP:HB3	2.01	0.43
1:D:332:GLU:CG	1:D:333:GLY:H	2.32	0.43
1:B:152:PHE:HB2	1:B:163:VAL:CG1	2.49	0.43
1:B:442:PRO:HD2	1:B:447:LYS:CE	2.49	0.42
1:C:375:THR:OG1	1:C:376:TYR:N	2.52	0.42
1:C:410:VAL:HG21	1:C:456:PHE:HB3	2.00	0.42
1:D:411:THR:HG22	1:D:413:THR:OG1	2.19	0.42
1:C:272:GLU:HB2	1:C:323:TYR:CZ	2.53	0.42
1:B:334:ILE:HG12	1:B:340:PRO:HD3	2.00	0.42
1:C:192:ILE:HG23	1:C:208:PRO:HB3	2.01	0.42
1:C:251:PHE:O	1:C:255:THR:HG23	2.19	0.42
1:A:271:PHE:HZ	1:B:252:VAL:HA	1.84	0.42
1:B:357:LEU:HD13	1:B:504:ALA:HB1	2.01	0.42
1:C:417:GLN:HG3	1:C:487:GLY:CA	2.50	0.42
1:A:548:PRO:HB3	1:B:189:ILE:HG21	2.02	0.42
1:A:340:PRO:HG3	1:B:294:HIS:HE2	1.84	0.42
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.79	0.42
1:C:90:PHE:HZ	1:C:183:LYS:HB3	1.85	0.42
1:D:491:ARG:HD2	1:D:505:TYR:CD2	2.55	0.42
1:A:80:PRO:HB2	1:A:81:ARG:H	1.65	0.42
1:A:192:ILE:HG23	1:A:208:PRO:HB3	2.01	0.42
1:A:285:ALA:HB3	1:A:305:ILE:HD12	2.01	0.41
1:A:423:GLU:O	1:A:427:LYS:HG2	2.20	0.41
1:B:299:LEU:HD12	1:B:299:LEU:HA	1.85	0.41
1:C:162:GLN:HB3	1:C:205:SER:HB3	2.02	0.41
1:C:576:PHE:HB2	1:D:276:PRO:CG	2.50	0.41
1:D:291:ILE:HD12	1:D:302:TYR:CE2	2.54	0.41
1:D:421:SER:O	1:D:422:ASN:C	2.59	0.41
1:D:534:GLN:HG3	1:D:535:LEU:HD22	2.01	0.41
1:C:388:GLN:O	1:C:388:GLN:HG3	2.19	0.41
1:A:222:PRO:HG2	1:A:243:ILE:HG13	2.03	0.41
1:C:381:ASN:HB3	1:C:384:GLY:O	2.21	0.41
1:A:476:SER:HB2	1:A:489:THR:HG21	2.03	0.41
1:C:406:GLU:O	1:C:406:GLU:HG3	2.20	0.41
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.89	0.41
1:B:504:ALA:HB2	1:B:553:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:THR:HB	1:C:276:PRO:HD2	2.02	0.41
1:A:442:PRO:O	1:A:444:THR:N	2.49	0.41
1:C:176:ASN:OD1	1:C:177:PHE:N	2.54	0.41
1:C:122:LEU:HD12	1:C:122:LEU:H	1.85	0.40
1:C:410:VAL:CG2	1:C:411:THR:N	2.84	0.40
1:C:357:LEU:HD13	1:C:504:ALA:HB1	2.04	0.40
1:A:87:ARG:HD2	1:A:87:ARG:HA	1.89	0.40
1:A:126:GLU:O	1:A:127:HIS:ND1	2.54	0.40
1:B:347:PHE:CE2	1:B:553:LEU:HB3	2.57	0.40
1:C:186:ARG:HH11	1:C:221:LEU:HB3	1.85	0.40
1:B:270:PHE:CE1	1:B:321:LYS:HD2	2.56	0.40
1:B:483:ARG:HG3	1:B:484:THR:HG23	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	486/507 (96%)	464 (96%)	22 (4%)	0	100	100
1	B	483/507 (95%)	475 (98%)	7 (1%)	1 (0%)	47	71
1	C	481/507 (95%)	451 (94%)	30 (6%)	0	100	100
1	D	484/507 (96%)	467 (96%)	14 (3%)	3 (1%)	25	47
All	All	1934/2028 (95%)	1857 (96%)	73 (4%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	422	ASN
1	D	442	PRO
1	D	441	ASN

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Mol	Chain	Res	Type
1	B	442	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	446/457 (98%)	437 (98%)	9 (2%)	55	79
1	B	441/457 (96%)	439 (100%)	2 (0%)	88	95
1	C	442/457 (97%)	431 (98%)	11 (2%)	47	74
1	D	442/457 (97%)	427 (97%)	15 (3%)	37	63
All	All	1771/1828 (97%)	1734 (98%)	37 (2%)	53	78

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	147	GLN
1	A	148	LYS
1	A	215	SER
1	A	344	SER
1	A	354	TYR
1	A	421	SER
1	A	463	ASP
1	A	492	LEU
1	B	145	SER
1	B	514	GLN
1	C	130	ASP
1	C	148	LYS
1	C	162	GLN
1	C	279	ASN
1	C	298	ASP
1	C	387	ASN
1	C	422	ASN
1	C	429	ILE
1	C	451	GLN

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Mol	Chain	Res	Type
1	C	464	LYS
1	C	492	LEU
1	D	80	PRO
1	D	92	GLN
1	D	160	LYS
1	D	224	LYS
1	D	228	LYS
1	D	296	ASP
1	D	379	SER
1	D	417	GLN
1	D	420	ASP
1	D	422	ASN
1	D	428	MET
1	D	438	GLU
1	D	439	LEU
1	D	492	LEU
1	D	515	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	147	GLN
1	A	176	ASN
1	A	336	ASN
1	A	441	ASN
1	B	387	ASN
1	B	568	ASN
1	C	94	GLN
1	C	279	ASN
1	C	286	ASN
1	C	435	HIS
1	C	451	GLN
1	D	295	ASN
1	D	417	GLN
1	D	459	ASN
1	D	514	GLN
1	D	568	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	LYS	D	601	-	5,9,9	0.37	0	4,10,10	0.42	0
2	LYS	C	601	-	5,9,9	0.24	0	4,10,10	0.48	0
3	EZ3	B	602	-	24,24,24	0.18	0	33,35,35	0.33	0
2	LYS	A	601	-	5,9,9	0.22	0	4,10,10	0.45	0
3	EZ3	A	602	-	24,24,24	0.19	0	33,35,35	0.32	0
3	EZ3	D	602	-	24,24,24	0.17	0	33,35,35	0.25	0
3	EZ3	C	602	-	24,24,24	0.16	0	33,35,35	0.25	0
2	LYS	B	601	-	5,9,9	0.35	0	4,10,10	0.39	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	D	601	-	-	1/5/9/9	-
2	LYS	C	601	-	-	3/5/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EZ3	B	602	-	-	0/8/30/30	0/3/3/3
2	LYS	A	601	-	-	2/5/9/9	-
3	EZ3	A	602	-	-	0/8/30/30	0/3/3/3
3	EZ3	D	602	-	-	0/8/30/30	0/3/3/3
3	EZ3	C	602	-	-	0/8/30/30	0/3/3/3
2	LYS	B	601	-	-	0/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	LYS	C-CA-CB-CG
2	D	601	LYS	CA-CB-CG-CD
2	C	601	LYS	N-CA-CB-CG
2	C	601	LYS	CE-CD-CG-CB
2	A	601	LYS	CE-CD-CG-CB
2	A	601	LYS	CG-CD-CE-NZ

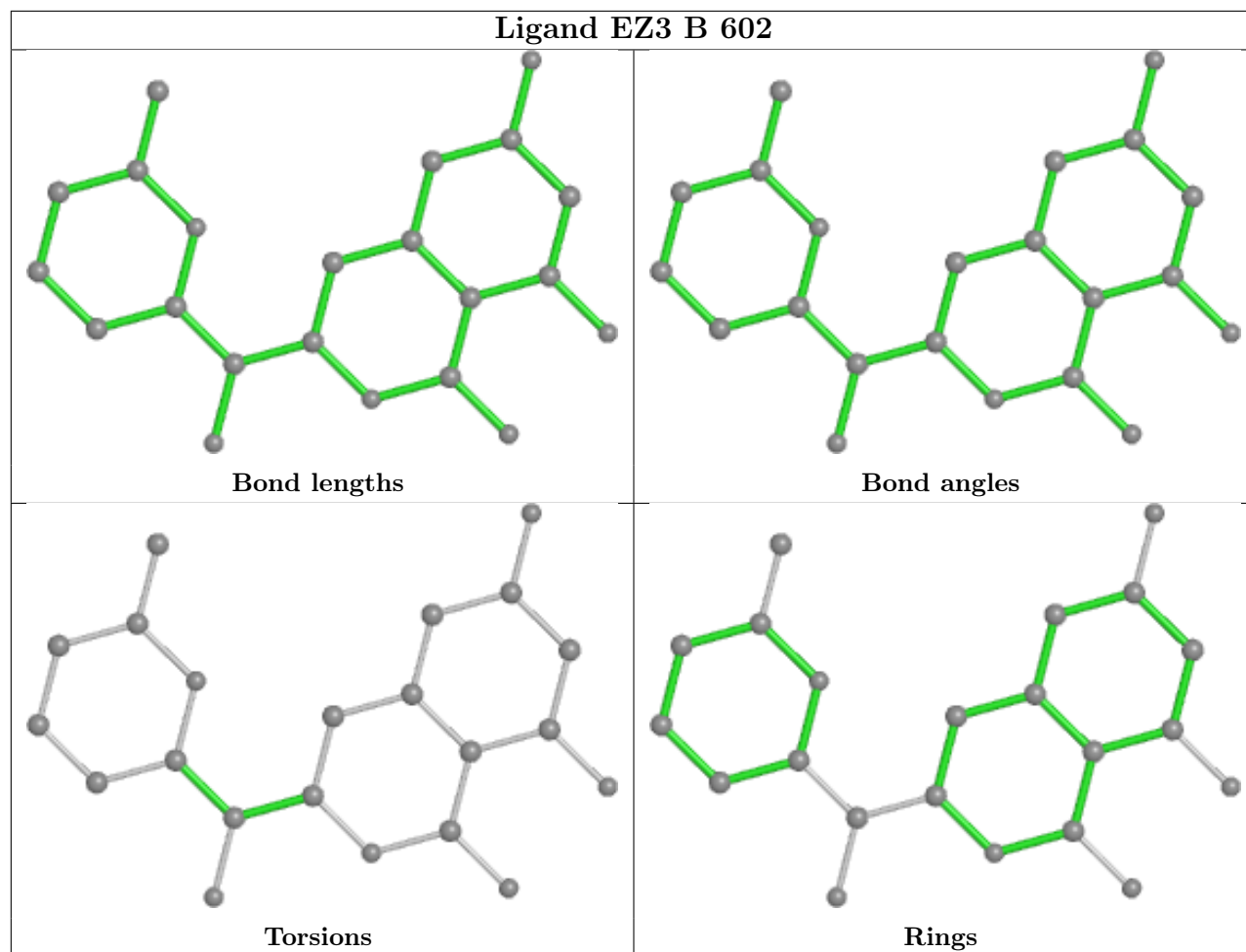
There are no ring outliers.

2 monomers are involved in 3 short contacts:

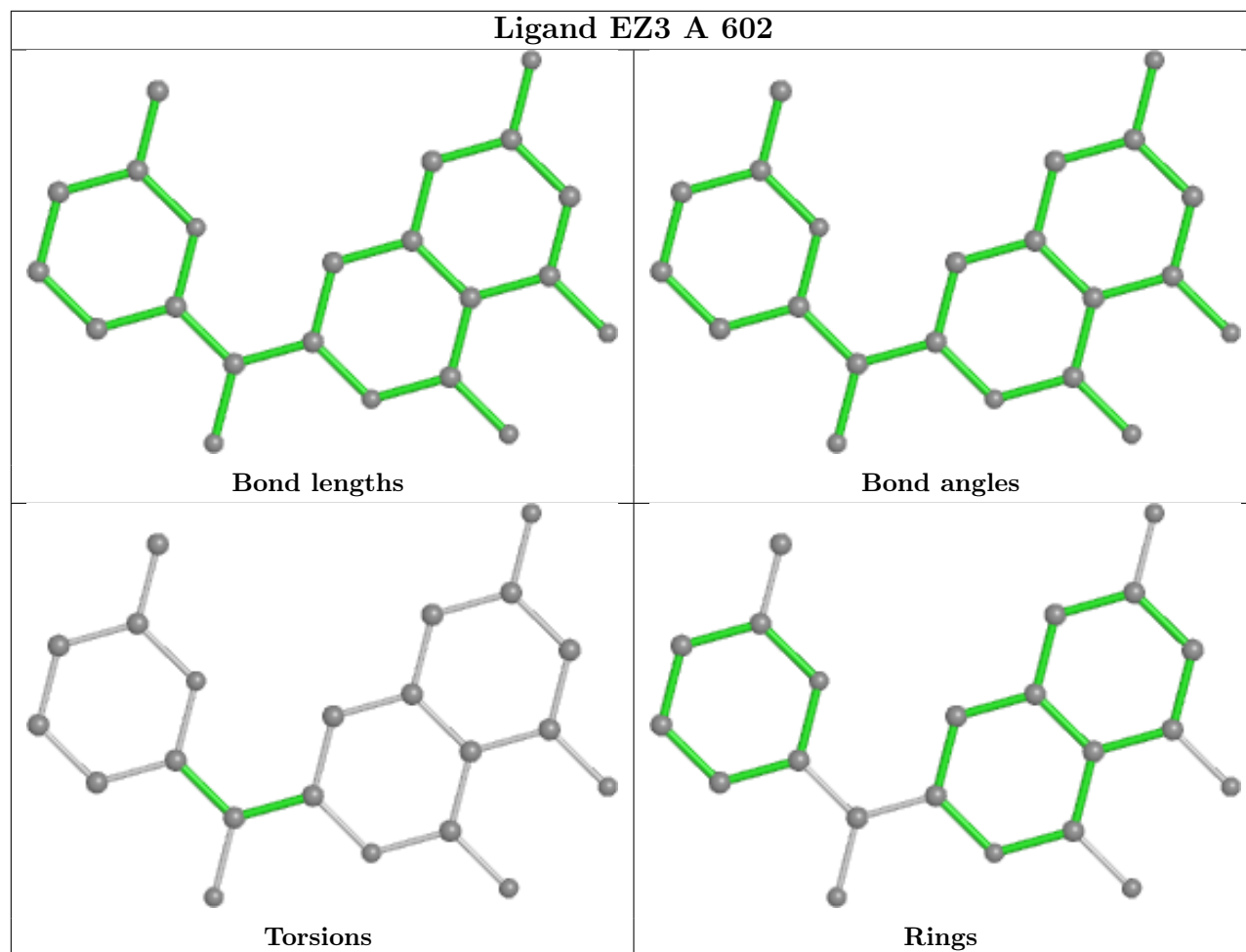
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	LYS	1	0
2	A	601	LYS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

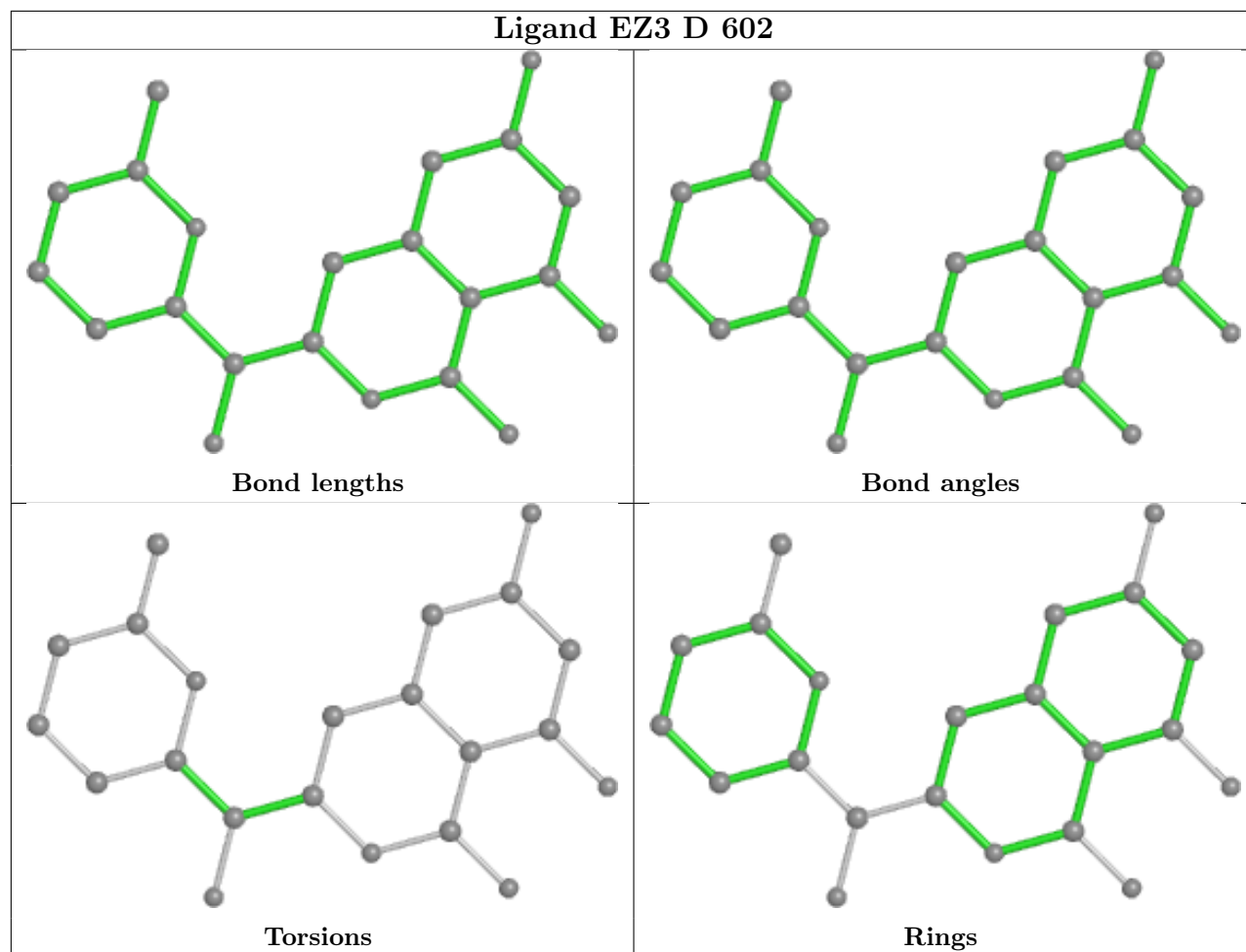
Ligand EZ3 B 602

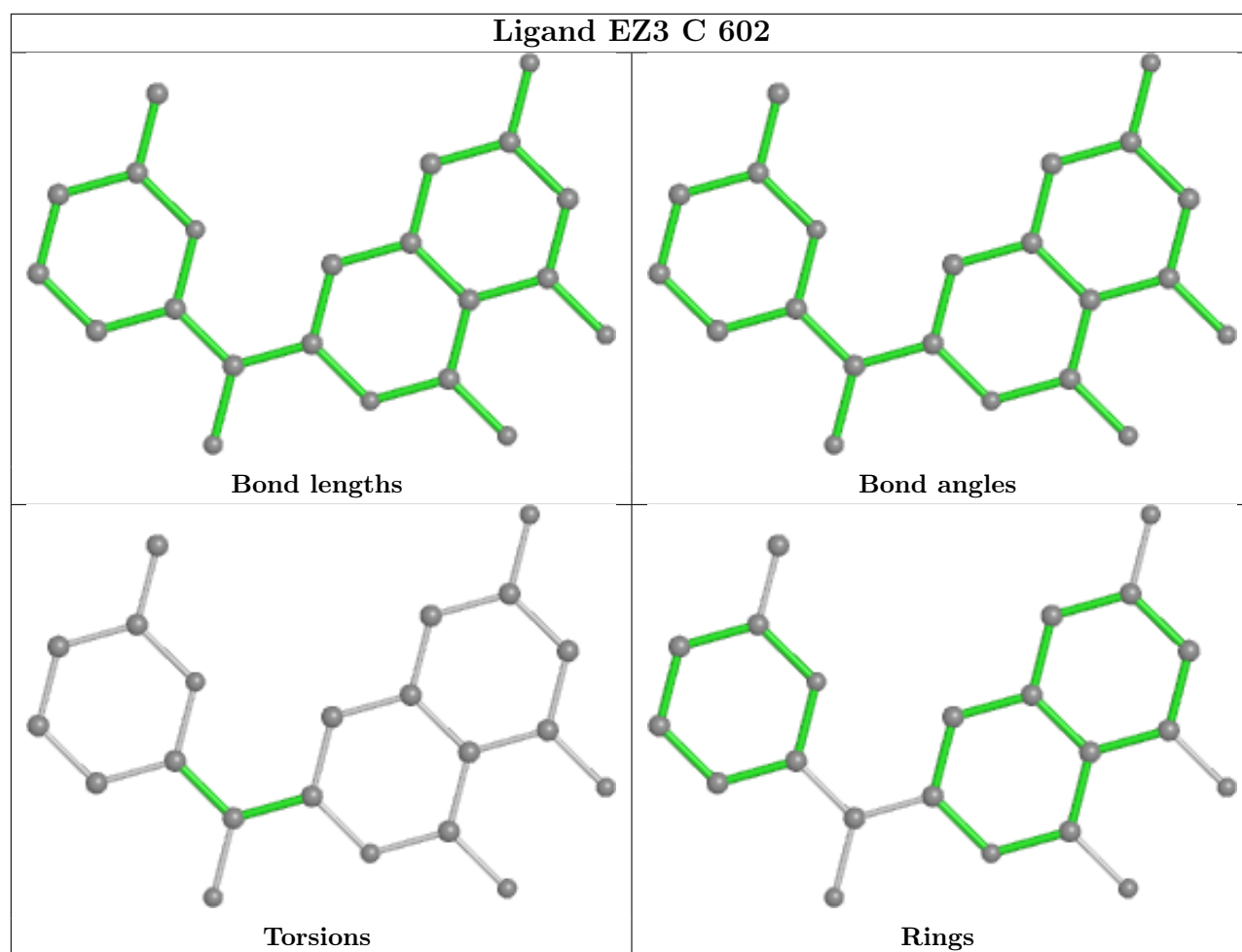


Ligand EZ3 A 602



Ligand EZ3 D 602





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	493/507 (97%)	0.17	15 (3%) 50 49	42, 66, 121, 161	0
1	B	487/507 (96%)	0.15	14 (2%) 51 51	40, 70, 116, 177	0
1	C	485/507 (95%)	0.31	27 (5%) 24 22	46, 84, 143, 183	0
1	D	487/507 (96%)	0.09	9 (1%) 68 69	30, 68, 113, 139	0
All	All	1952/2028 (96%)	0.18	65 (3%) 46 45	30, 72, 127, 183	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	532	ALA	8.0
1	B	225	TYR	6.1
1	C	443	PRO	5.7
1	C	456	PHE	4.5
1	C	437	ILE	4.4
1	A	526	GLU	4.3
1	A	230	THR	4.3
1	A	525	ARG	3.8
1	C	433	LYS	3.8
1	C	146	GLY	3.7
1	D	515	LYS	3.6
1	D	418	PRO	3.6
1	A	432	ILE	3.5
1	D	419	PHE	3.4
1	C	441	ASN	3.3
1	C	430	ASN	3.2
1	C	432	ILE	3.2
1	C	428	MET	3.2
1	B	229	ASP	3.1
1	C	481[A]	TYR	3.0
1	C	434	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	436	LYS	3.0
1	A	441	ASN	2.9
1	C	415	LEU	2.9
1	A	423	GLU	2.8
1	C	439	LEU	2.8
1	B	432	ILE	2.7
1	B	286	ASN	2.7
1	A	524	ASP	2.6
1	C	169	PHE	2.5
1	D	581	PRO	2.5
1	B	144	ALA	2.5
1	B	552	GLY	2.5
1	C	300	ASP	2.5
1	B	416	GLU	2.4
1	C	149	LEU	2.4
1	A	200	LYS	2.4
1	C	410	VAL	2.4
1	C	280	LEU	2.4
1	C	166	ASN	2.4
1	C	442	PRO	2.3
1	B	285	ALA	2.3
1	D	416	GLU	2.3
1	D	441	ASN	2.3
1	A	438	GLU	2.3
1	C	195	PHE	2.3
1	D	434	GLU	2.2
1	B	554	GLY	2.2
1	A	517	CYS	2.2
1	B	418	PRO	2.2
1	B	506	THR	2.2
1	C	281	ILE	2.1
1	C	285	ALA	2.1
1	A	311	LEU	2.1
1	A	431	ILE	2.1
1	B	436	LYS	2.1
1	C	145	SER	2.1
1	A	518	PHE	2.1
1	D	311	LEU	2.1
1	B	345	CYS	2.1
1	A	315	ILE	2.1
1	D	307	THR	2.1
1	B	350	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	388	GLN	2.0
1	C	345	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

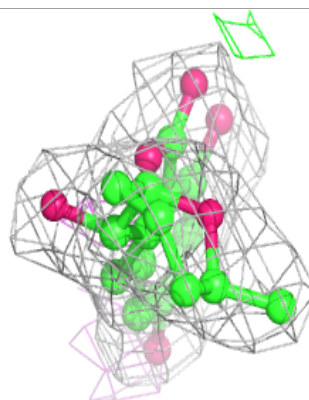
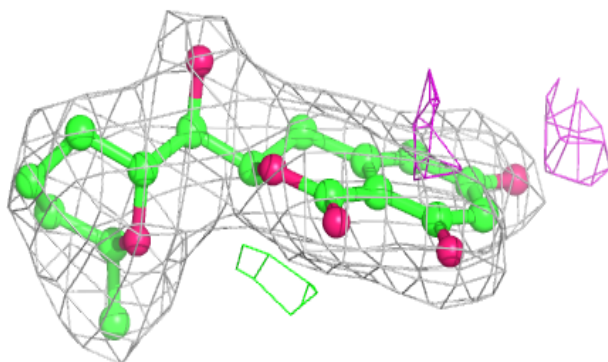
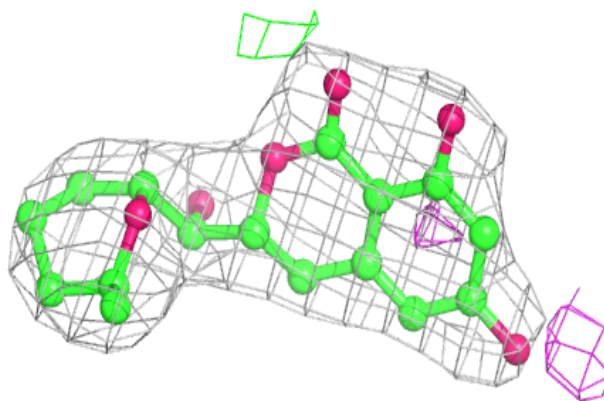
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LYS	A	601	10/10	0.88	0.42	55,60,97,101	0
2	LYS	C	601	10/10	0.90	0.33	78,84,88,93	0
3	EZ3	D	602	22/22	0.94	0.23	39,61,69,73	0
3	EZ3	B	602	22/22	0.95	0.21	36,51,59,62	0
2	LYS	B	601	10/10	0.96	0.30	50,52,57,58	0
3	EZ3	C	602	22/22	0.96	0.18	54,62,69,74	0
3	EZ3	A	602	22/22	0.96	0.20	41,53,59,63	0
2	LYS	D	601	10/10	0.97	0.37	53,58,68,69	0

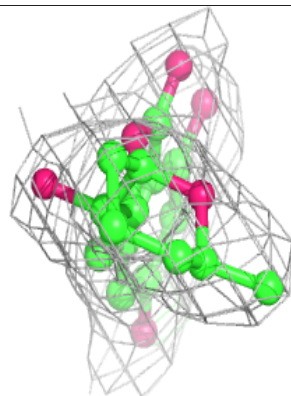
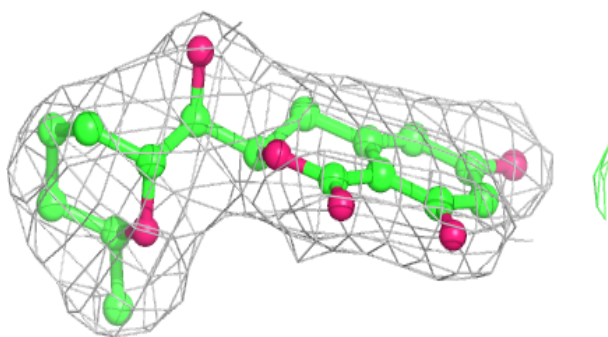
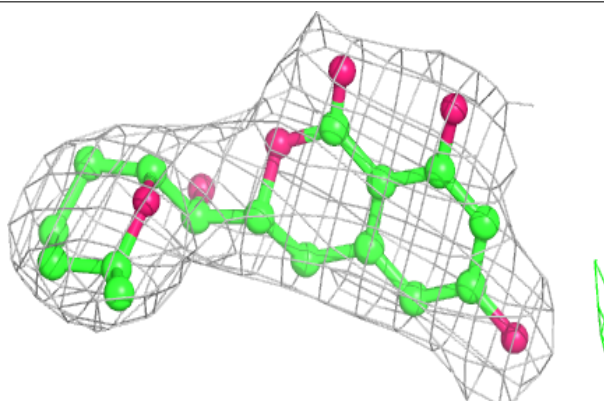
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EZ3 D 602:

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

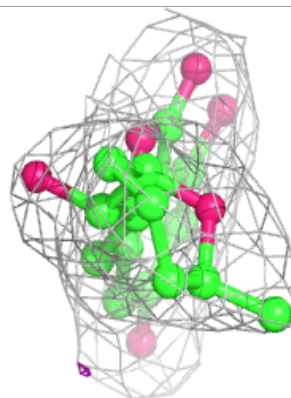
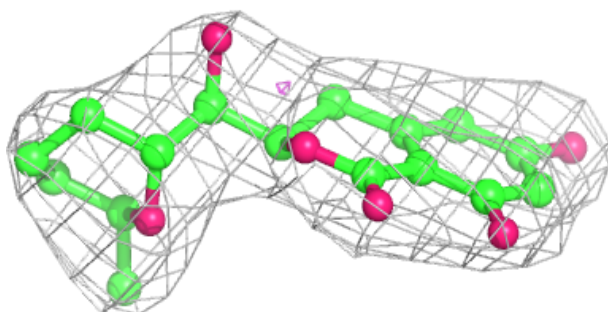
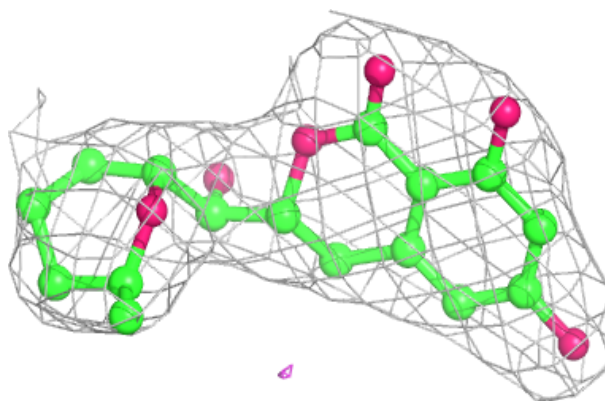
**Electron density around EZ3 B 602:**

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

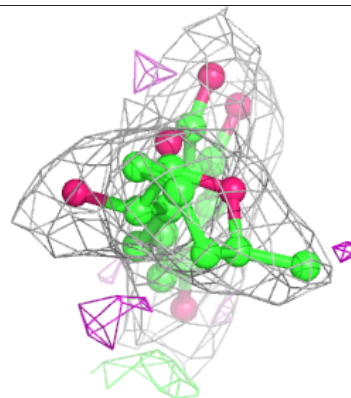
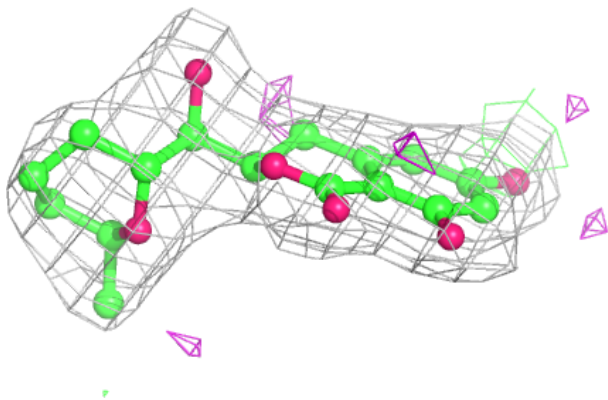
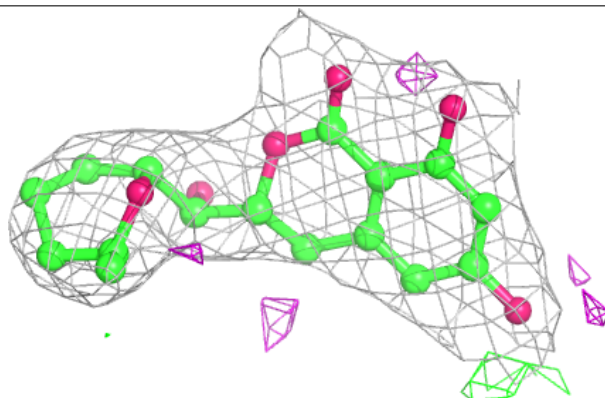


Electron density around EZ3 C 602:

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

**Electron density around EZ3 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 [i](#)

There are no such residues in this entry.