Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:31 am BST

PDB ID	:	7ZOG
Title	:	Crystal structure of Cryptosporidium parvum -Plasmodium falciparum mutant lysyl tRNA synthetase in complex with inhibitor
Authors	:	Dawson, A.; Wyllie, S.
Deposited on	:	2022-04-25
Resolution	:	1.80 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:

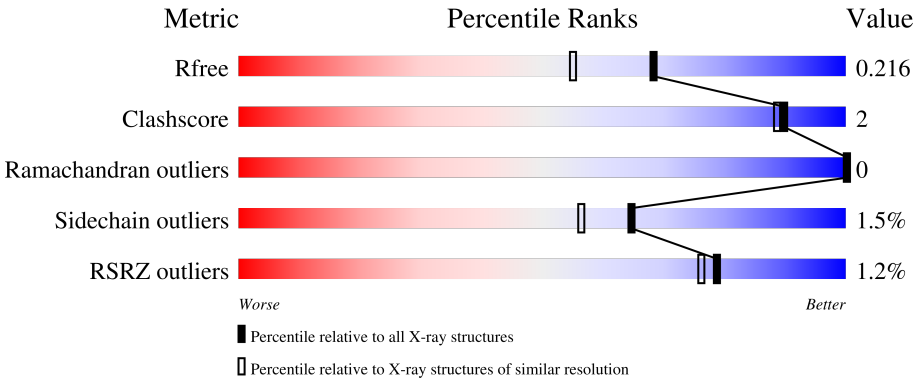
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	535	88% · 7%
1	B	535	88% · 7%
1	C	535	86% · 9%
1	D	535	87% 5% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17759 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	496	Total	C	N	O	S	0	3	0
			4024	2579	668	749	28			
1	B	497	Total	C	N	O	S	0	3	0
			4032	2583	670	751	28			
1	C	485	Total	C	N	O	S	0	3	0
			3950	2536	656	731	27			
1	D	495	Total	C	N	O	S	0	3	0
			4016	2575	667	746	28			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q5CR27
A	26	ALA	-	expression tag	UNP Q5CR27
A	27	HIS	-	expression tag	UNP Q5CR27
A	28	HIS	-	expression tag	UNP Q5CR27
A	29	HIS	-	expression tag	UNP Q5CR27
A	30	HIS	-	expression tag	UNP Q5CR27
A	31	HIS	-	expression tag	UNP Q5CR27
A	32	HIS	-	expression tag	UNP Q5CR27
A	33	MET	-	expression tag	UNP Q5CR27
A	34	GLY	-	expression tag	UNP Q5CR27
A	35	THR	-	expression tag	UNP Q5CR27
A	36	LEU	-	expression tag	UNP Q5CR27
A	37	GLU	-	expression tag	UNP Q5CR27
A	38	ALA	-	expression tag	UNP Q5CR27
A	39	GLN	-	expression tag	UNP Q5CR27
A	40	THR	-	expression tag	UNP Q5CR27
A	41	GLN	-	expression tag	UNP Q5CR27
A	42	GLY	-	expression tag	UNP Q5CR27
A	43	PRO	-	expression tag	UNP Q5CR27
A	44	GLY	-	expression tag	UNP Q5CR27
A	45	SER	-	expression tag	UNP Q5CR27

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Chain	Residue	Modelled	Actual	Comment	Reference
A	272	THR	PRO	engineered mutation	UNP Q5CR27
A	293	VAL	ASN	engineered mutation	UNP Q5CR27
A	309	SER	ALA	engineered mutation	UNP Q5CR27
B	25	MET	-	initiating methionine	UNP Q5CR27
B	26	ALA	-	expression tag	UNP Q5CR27
B	27	HIS	-	expression tag	UNP Q5CR27
B	28	HIS	-	expression tag	UNP Q5CR27
B	29	HIS	-	expression tag	UNP Q5CR27
B	30	HIS	-	expression tag	UNP Q5CR27
B	31	HIS	-	expression tag	UNP Q5CR27
B	32	HIS	-	expression tag	UNP Q5CR27
B	33	MET	-	expression tag	UNP Q5CR27
B	34	GLY	-	expression tag	UNP Q5CR27
B	35	THR	-	expression tag	UNP Q5CR27
B	36	LEU	-	expression tag	UNP Q5CR27
B	37	GLU	-	expression tag	UNP Q5CR27
B	38	ALA	-	expression tag	UNP Q5CR27
B	39	GLN	-	expression tag	UNP Q5CR27
B	40	THR	-	expression tag	UNP Q5CR27
B	41	GLN	-	expression tag	UNP Q5CR27
B	42	GLY	-	expression tag	UNP Q5CR27
B	43	PRO	-	expression tag	UNP Q5CR27
B	44	GLY	-	expression tag	UNP Q5CR27
B	45	SER	-	expression tag	UNP Q5CR27
B	272	THR	PRO	engineered mutation	UNP Q5CR27
B	293	VAL	ASN	engineered mutation	UNP Q5CR27
B	309	SER	ALA	engineered mutation	UNP Q5CR27
C	25	MET	-	initiating methionine	UNP Q5CR27
C	26	ALA	-	expression tag	UNP Q5CR27
C	27	HIS	-	expression tag	UNP Q5CR27
C	28	HIS	-	expression tag	UNP Q5CR27
C	29	HIS	-	expression tag	UNP Q5CR27
C	30	HIS	-	expression tag	UNP Q5CR27
C	31	HIS	-	expression tag	UNP Q5CR27
C	32	HIS	-	expression tag	UNP Q5CR27
C	33	MET	-	expression tag	UNP Q5CR27
C	34	GLY	-	expression tag	UNP Q5CR27
C	35	THR	-	expression tag	UNP Q5CR27
C	36	LEU	-	expression tag	UNP Q5CR27
C	37	GLU	-	expression tag	UNP Q5CR27
C	38	ALA	-	expression tag	UNP Q5CR27
C	39	GLN	-	expression tag	UNP Q5CR27

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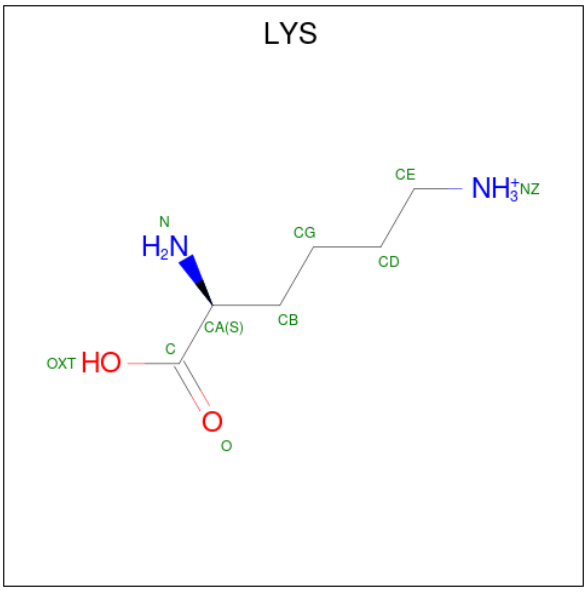
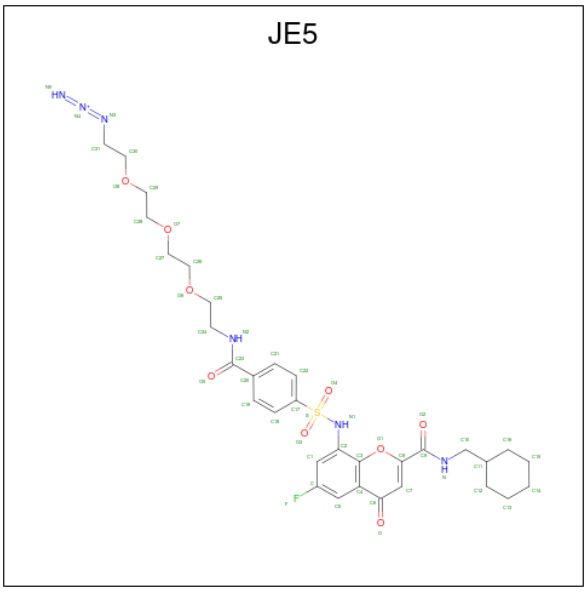
Chain	Residue	Modelled	Actual	Comment	Reference
C	40	THR	-	expression tag	UNP Q5CR27
C	41	GLN	-	expression tag	UNP Q5CR27
C	42	GLY	-	expression tag	UNP Q5CR27
C	43	PRO	-	expression tag	UNP Q5CR27
C	44	GLY	-	expression tag	UNP Q5CR27
C	45	SER	-	expression tag	UNP Q5CR27
C	272	THR	PRO	engineered mutation	UNP Q5CR27
C	293	VAL	ASN	engineered mutation	UNP Q5CR27
C	309	SER	ALA	engineered mutation	UNP Q5CR27
D	25	MET	-	initiating methionine	UNP Q5CR27
D	26	ALA	-	expression tag	UNP Q5CR27
D	27	HIS	-	expression tag	UNP Q5CR27
D	28	HIS	-	expression tag	UNP Q5CR27
D	29	HIS	-	expression tag	UNP Q5CR27
D	30	HIS	-	expression tag	UNP Q5CR27
D	31	HIS	-	expression tag	UNP Q5CR27
D	32	HIS	-	expression tag	UNP Q5CR27
D	33	MET	-	expression tag	UNP Q5CR27
D	34	GLY	-	expression tag	UNP Q5CR27
D	35	THR	-	expression tag	UNP Q5CR27
D	36	LEU	-	expression tag	UNP Q5CR27
D	37	GLU	-	expression tag	UNP Q5CR27
D	38	ALA	-	expression tag	UNP Q5CR27
D	39	GLN	-	expression tag	UNP Q5CR27
D	40	THR	-	expression tag	UNP Q5CR27
D	41	GLN	-	expression tag	UNP Q5CR27
D	42	GLY	-	expression tag	UNP Q5CR27
D	43	PRO	-	expression tag	UNP Q5CR27
D	44	GLY	-	expression tag	UNP Q5CR27
D	45	SER	-	expression tag	UNP Q5CR27
D	272	THR	PRO	engineered mutation	UNP Q5CR27
D	293	VAL	ASN	engineered mutation	UNP Q5CR27
D	309	SER	ALA	engineered mutation	UNP Q5CR27

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



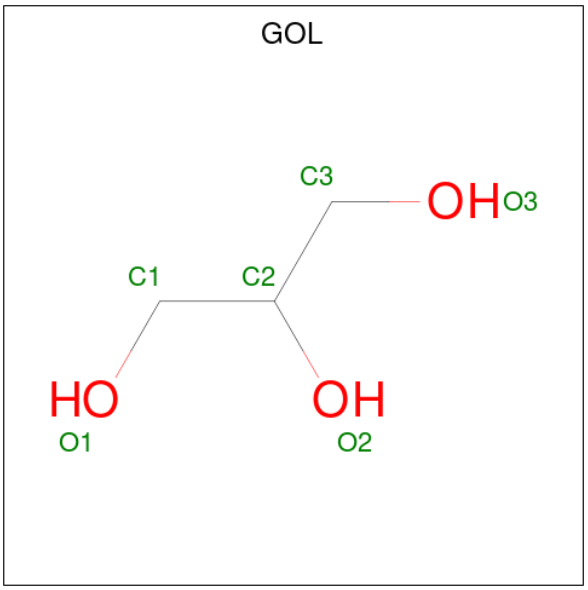
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 10 6 2 2	0	0
2	B	1	Total C N O 10 6 2 2	0	0
2	C	1	Total C N O 10 6 2 2	0	0
2	D	1	Total C N O 10 6 2 2	0	0

- Molecule 3 is 8-[[4-[2-[2-[2-[2-[(azanylidene-$l^{4}-azanylidene)amino]ethoxy]ethoxy]ethoxy]ethylcarbamoyl]phenyl]sulfonylamino]- {N}-(cyclohexylmethyl)-6-fluoranyl-4-oxidanylidene-chromene-2-carboxamide (three-letter code: JE5) (formula: $C_{32}H_{40}FN_6O_9S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			49	32	1	6	9	1		
3	B	1	Total	C	F	N	O	S	0	0
			49	32	1	6	9	1		
3	C	1	Total	C	F	N	O	S	0	0
			49	32	1	6	9	1		
3	D	1	Total	C	F	N	O	S	0	0
			49	32	1	6	9	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

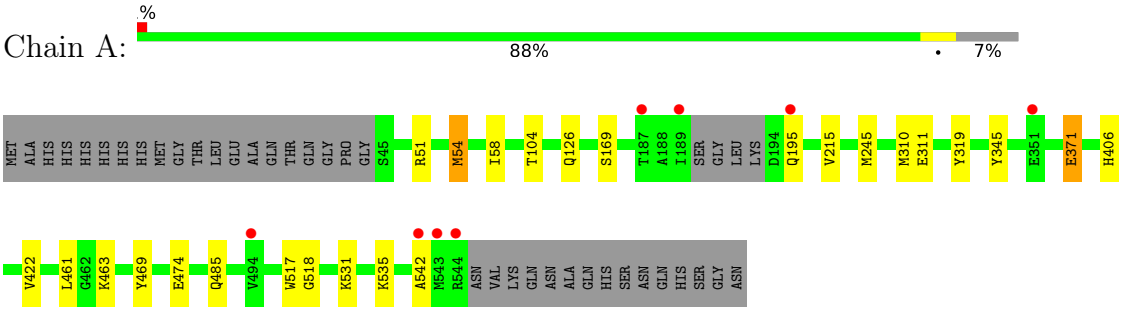
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	361	Total O 361 361	0	0
5	B	400	Total O 400 400	0	0
5	C	365	Total O 365 365	0	0
5	D	339	Total O 339 339	0	0

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.

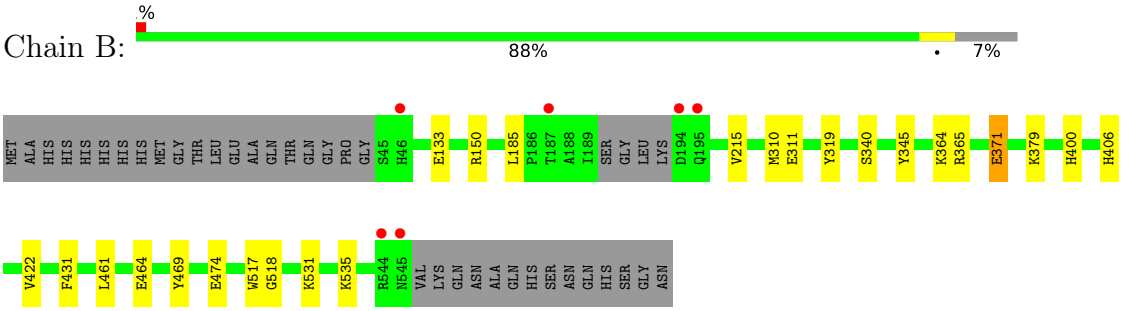
• Molecule 1: Lysine-tRNA ligase

Chain A:



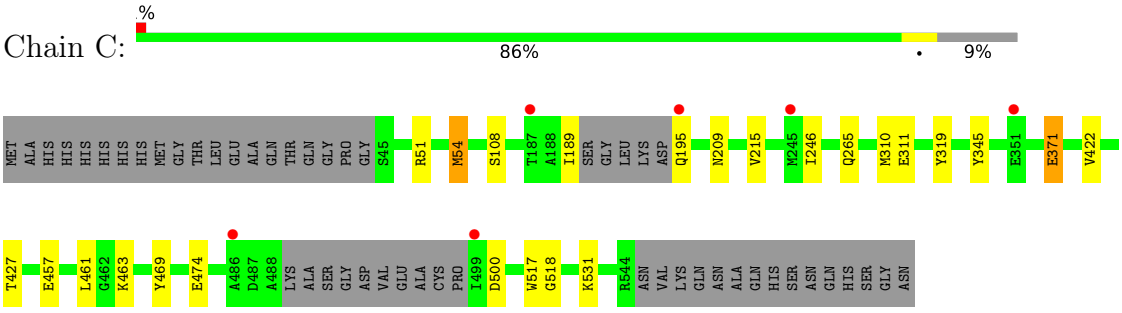
• Molecule 1: Lysine-tRNA ligase

Chain B:



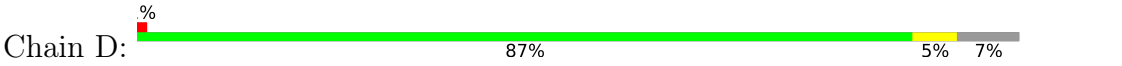
• Molecule 1: Lysine-tRNA ligase

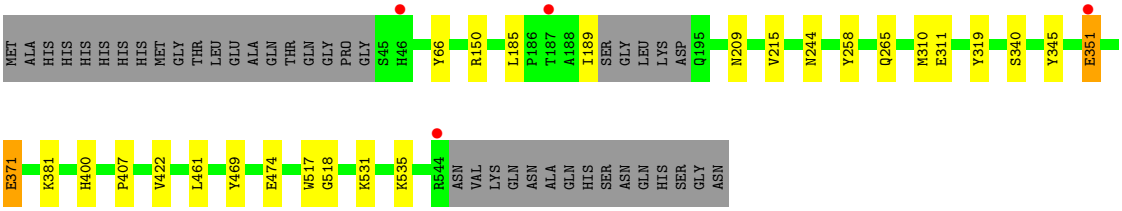
Chain C:



• Molecule 1: Lysine-tRNA ligase

Chain D:




MET ALA HIS HIS HIS HIS HIS MET GLY THR LEU GLU ALA GLN THR GLN GLY PRO GLY S45 H46 Y66 R150 L185 P186 T187 A188 I189 SER GLY LEU LYS ASP Q195 N209 V215 N244 Y258 Q265 M310 E311 Y319 S340 Y345 E351
E371 K381 H400 P407 V422 L461 Y469 E474 W517 G518 K531 K535 R544 ASN VAL LYS GLN ASN ALA GLN HIS SER ASN GLN HIS SER GLY ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.10Å 118.73Å 143.45Å 90.00° 90.69° 90.00°	Depositor
Resolution (Å)	64.90 – 1.80 64.81 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.90-1.80) 100.0 (64.81-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.210 0.190 , 0.216	Depositor DCC
R_{free} test set	11382 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.903	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17759	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: JE5, GOL

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	0.73	0/4131	0.77	0/5571
1	B	0.72	0/4139	0.77	0/5582
1	C	0.73	1/4055 (0.0%)	0.77	0/5466
1	D	0.72	0/4123	0.77	0/5560
All	All	0.73	1/16448 (0.0%)	0.77	0/22179

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	457	GLU	CD-OE2	-5.60	1.19	1.25

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	4024	0	3977	15	0
1	B	4032	0	3983	17	0
1	C	3950	0	3910	11	0
1	D	4016	0	3973	16	0
2	A	10	0	12	0	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	0	0
2	D	10	0	12	0	0
3	A	49	0	0	0	0
3	B	49	0	0	0	0
3	C	49	0	0	0	0
3	D	49	0	0	0	0
4	A	12	0	16	1	0
4	B	6	0	8	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
5	A	361	0	0	5	0
5	B	400	0	0	9	1
5	C	365	0	0	1	0
5	D	339	0	0	6	1
All	All	17759	0	15939	57	1

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 2.

All (57) 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:C:463:LYS:HD2	5:C:1159:HOH:O	1.56	1.03
1:B:464:GLU:OE1	5:B:901:HOH:O	1.99	0.81
1:B:406:HIS:HD2	5:B:1241:HOH:O	1.69	0.76
1:D:351:GLU:N	1:D:351:GLU:OE1	2.24	0.71
1:A:463:LYS:HD2	5:A:1017:HOH:O	1.95	0.65
1:D:150:ARG:NH1	1:D:185:LEU:O	2.32	0.62
1:A:535:LYS:HE2	5:A:811:HOH:O	1.98	0.62
1:B:150:ARG:NH1	1:B:185:LEU:O	2.33	0.62
1:D:381:LYS:NZ	5:D:904:HOH:O	2.32	0.59
1:C:371:GLU:HB3	1:C:422:VAL:HG22	1.86	0.57
1:B:371:GLU:HB3	1:B:422:VAL:HG22	1.87	0.57
1:D:150:ARG:NH2	5:D:905:HOH:O	2.38	0.55
1:D:371:GLU:HB3	1:D:422:VAL:HG22	1.89	0.54
1:A:371:GLU:HB3	1:A:422:VAL:HG22	1.89	0.53
1:A:542:ALA:HB3	5:A:846:HOH:O	2.09	0.53
1:B:535:LYS:HE3	5:B:1084:HOH:O	2.07	0.53
1:B:150:ARG:NH2	5:B:910:HOH:O	2.42	0.52
1:C:51:ARG:HH21	1:C:54:MET:HE2	1.76	0.51
1:B:400:HIS:HE1	5:B:965:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:LYS:HE3	5:D:1108:HOH:O	2.11	0.49
1:A:406:HIS:CE1	1:D:258:TYR:HB2	2.48	0.48
1:A:51:ARG:HH21	1:A:54:MET:HE2	1.77	0.48
1:A:535:LYS:CE	5:A:811:HOH:O	2.60	0.48
1:B:215:VAL:CG2	1:B:531:LYS:HE3	2.43	0.48
1:D:215:VAL:CG2	1:D:531:LYS:HE3	2.46	0.46
1:D:345:TYR:CD2	1:D:461:LEU:CD1	2.99	0.45
1:A:215:VAL:CG2	1:A:531:LYS:HE3	2.47	0.45
1:D:244:ASN:HB3	5:D:1095:HOH:O	2.17	0.45
1:C:189:ILE:CG2	1:C:209:ASN:HB2	2.48	0.44
1:D:310:MET:O	1:D:518:GLY:HA2	2.18	0.44
1:A:345:TYR:CD2	1:A:461:LEU:CD1	3.00	0.44
1:B:133:GLU:HG3	5:B:1272:HOH:O	2.17	0.44
1:B:311:GLU:HA	1:B:517:TRP:O	2.18	0.43
1:C:215:VAL:CG2	1:C:531:LYS:HE3	2.49	0.43
1:C:311:GLU:HA	1:C:517:TRP:O	2.18	0.43
1:C:246:ILE:HD12	1:C:500:ASP:HA	2.00	0.43
1:B:379:LYS:HE3	5:B:1062:HOH:O	2.19	0.43
1:D:400:HIS:HE1	5:D:909:HOH:O	2.00	0.43
1:A:104:THR:HG21	4:A:603:GOL:O3	2.19	0.43
1:D:244:ASN:HB2	5:D:968:HOH:O	2.20	0.42
1:A:54:MET:HE3	1:A:58:ILE:CD1	2.50	0.42
1:A:310:MET:O	1:A:518:GLY:HA2	2.20	0.42
1:A:311:GLU:HA	1:A:517:TRP:O	2.20	0.42
1:C:427:THR:HG23	1:C:461:LEU:HD23	2.01	0.42
1:B:310:MET:O	1:B:518:GLY:HA2	2.20	0.42
1:C:345:TYR:CD2	1:C:461:LEU:CD1	3.02	0.42
1:D:311:GLU:HA	1:D:517:TRP:O	2.19	0.42
1:B:215:VAL:HG21	1:B:531:LYS:HE3	2.01	0.42
1:B:345:TYR:CD2	1:B:461:LEU:CD1	3.02	0.41
1:A:485:GLN:NE2	5:A:803:HOH:O	2.36	0.41
1:B:406:HIS:HE1	5:B:1240:HOH:O	2.03	0.41
1:D:189:ILE:CG2	1:D:209:ASN:HB2	2.50	0.41
1:B:365:ARG:HG3	1:B:431:PHE:HB2	2.03	0.41
1:C:474:GLU:HG2	1:D:66:TYR:CE2	2.55	0.41
1:B:364:LYS:NZ	5:B:926:HOH:O	2.53	0.41
1:C:310:MET:O	1:C:518:GLY:HA2	2.20	0.40
1:A:126:GLN:O	1:A:169:SER:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1247:HOH:O	5:D:1198:HOH:O[1_565]	2.13	0.07

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	495/535 (92%)	486 (98%)	9 (2%)	0	100	100
1	B	496/535 (93%)	486 (98%)	10 (2%)	0	100	100
1	C	482/535 (90%)	474 (98%)	8 (2%)	0	100	100
1	D	494/535 (92%)	486 (98%)	8 (2%)	0	100	100
All	All	1967/2140 (92%)	1932 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	444/472 (94%)	437 (98%)	7 (2%)	62	54
1	B	445/472 (94%)	440 (99%)	5 (1%)	73	68
1	C	436/472 (92%)	429 (98%)	7 (2%)	62	54
1	D	443/472 (94%)	435 (98%)	8 (2%)	59	48
All	All	1768/1888 (94%)	1741 (98%)	27 (2%)	65	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	MET
1	A	195	GLN
1	A	245	MET
1	A	319	TYR
1	A	371	GLU
1	A	469	TYR
1	A	474	GLU
1	B	319	TYR
1	B	340	SER
1	B	371	GLU
1	B	469	TYR
1	B	474	GLU
1	C	54	MET
1	C	108	SER
1	C	195	GLN
1	C	265	GLN
1	C	319	TYR
1	C	371	GLU
1	C	469	TYR
1	D	265	GLN
1	D	319	TYR
1	D	340	SER
1	D	351	GLU
1	D	371	GLU
1	D	407	PRO
1	D	469	TYR
1	D	474	GLU

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	195	GLN
1	A	406	HIS
1	B	400	HIS
1	B	406	HIS
1	C	406	HIS
1	D	400	HIS

5.3.3 RNA

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)

14 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	A	601	-	8,9,9	0.53	0	9,10,10	0.91	0
3	JE5	C	604	-	51,52,52	0.52	1 (1%)	67,69,69	0.45	0
3	JE5	B	603	-	51,52,52	0.55	1 (1%)	67,69,69	0.56	1 (1%)
4	GOL	C	602	-	5,5,5	0.17	0	5,5,5	0.33	0
3	JE5	D	603	-	51,52,52	0.59	1 (1%)	67,69,69	0.61	1 (1%)
2	LYS	D	601	-	8,9,9	0.75	0	9,10,10	0.89	0
2	LYS	C	601	-	8,9,9	0.69	0	9,10,10	0.64	0
3	JE5	A	602	-	51,52,52	0.59	1 (1%)	67,69,69	0.58	1 (1%)
4	GOL	C	603	-	5,5,5	0.16	0	5,5,5	0.46	0
4	GOL	B	602	-	5,5,5	0.11	0	5,5,5	0.22	0
2	LYS	B	601	-	8,9,9	0.77	0	9,10,10	0.74	0
4	GOL	D	602	-	5,5,5	0.12	0	5,5,5	0.27	0
4	GOL	A	604	-	5,5,5	0.11	0	5,5,5	0.36	0
4	GOL	A	603	-	5,5,5	0.22	0	5,5,5	0.29	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
2	LYS	A	601	-	-	0/9/9/9	-
3	JE5	C	604	-	-	7/39/47/47	0/4/4/4
3	JE5	B	603	-	-	8/39/47/47	0/4/4/4
4	GOL	C	602	-	-	2/4/4/4	-
3	JE5	D	603	-	-	8/39/47/47	0/4/4/4
2	LYS	D	601	-	-	0/9/9/9	-
2	LYS	C	601	-	-	0/9/9/9	-
3	JE5	A	602	-	-	7/39/47/47	0/4/4/4
4	GOL	C	603	-	-	0/4/4/4	-
4	GOL	B	602	-	-	2/4/4/4	-
2	LYS	B	601	-	-	0/9/9/9	-
4	GOL	D	602	-	-	2/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	A	603	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	JE5	N4-N3	2.54	1.30	1.23
3	A	602	JE5	N4-N3	2.35	1.29	1.23
3	B	603	JE5	N4-N3	2.28	1.29	1.23
3	C	604	JE5	N4-N3	2.17	1.29	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	603	JE5	C31-N3-N4	2.35	127.10	115.95
3	A	602	JE5	C31-N3-N4	2.12	126.02	115.95
3	B	603	JE5	O3-S-N1	2.04	111.85	106.73

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	JE5	O8-C30-C31-N3
3	D	603	JE5	O8-C30-C31-N3
4	A	604	GOL	C1-C2-C3-O3
4	B	602	GOL	O1-C1-C2-O2
4	B	602	GOL	O1-C1-C2-C3
4	C	602	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	D	602	GOL	O1-C1-C2-C3
3	C	604	JE5	O8-C30-C31-N3
4	A	603	GOL	C1-C2-C3-O3
3	A	602	JE5	C18-C17-S-O4
3	A	602	JE5	C22-C17-S-O4
4	A	603	GOL	O2-C2-C3-O3
4	A	604	GOL	O2-C2-C3-O3
4	C	602	GOL	O1-C1-C2-O2
4	D	602	GOL	O1-C1-C2-O2
3	C	604	JE5	C18-C17-S-O4
3	C	604	JE5	C22-C17-S-O4
3	B	603	JE5	C18-C17-S-O4
3	A	602	JE5	C18-C17-S-N1
3	B	603	JE5	C30-C31-N3-N4
3	D	603	JE5	C30-C31-N3-N4
3	A	602	JE5	C22-C17-S-N1
3	B	603	JE5	C22-C17-S-O4
3	B	603	JE5	C18-C17-S-N1
3	C	604	JE5	C22-C17-S-N1
3	D	603	JE5	C18-C17-S-O4
3	C	604	JE5	C18-C17-S-N1
4	A	603	GOL	O1-C1-C2-O2
3	D	603	JE5	C22-C17-S-O4
3	D	603	JE5	C18-C17-S-N1
3	C	604	JE5	C29-C28-O7-C27
3	B	603	JE5	C29-C28-O7-C27
3	B	603	JE5	C22-C17-S-N1
3	A	602	JE5	C30-C31-N3-N4
3	C	604	JE5	C30-C31-N3-N4
3	D	603	JE5	C22-C17-S-N1
3	A	602	JE5	C28-C29-O8-C30
3	B	603	JE5	C31-C30-O8-C29
3	D	603	JE5	C28-C29-O8-C30
3	D	603	JE5	C29-C28-O7-C27
3	B	603	JE5	O6-C26-C27-O7

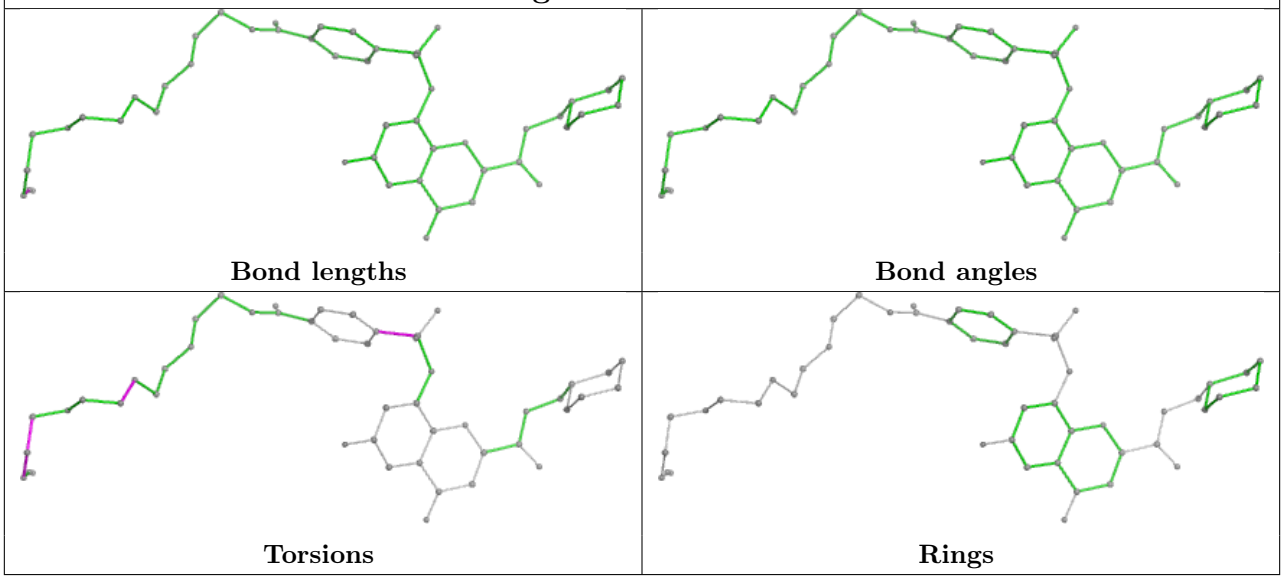
There are no ring outliers.

1 monomer is involved in 1 short contact:

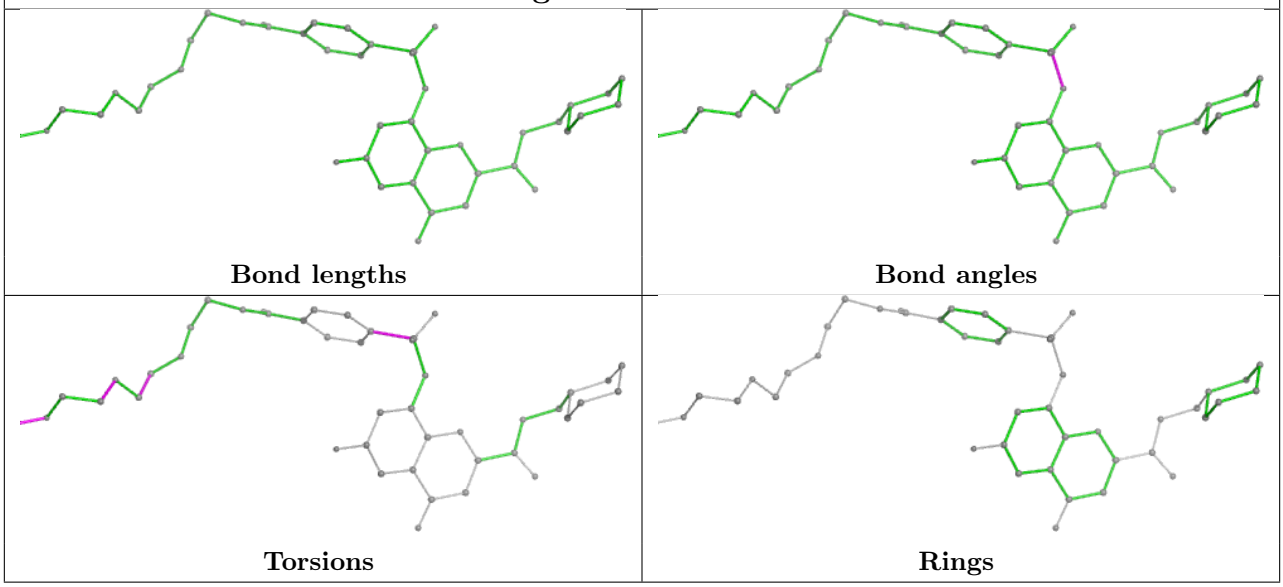
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	1	0

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 then 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.

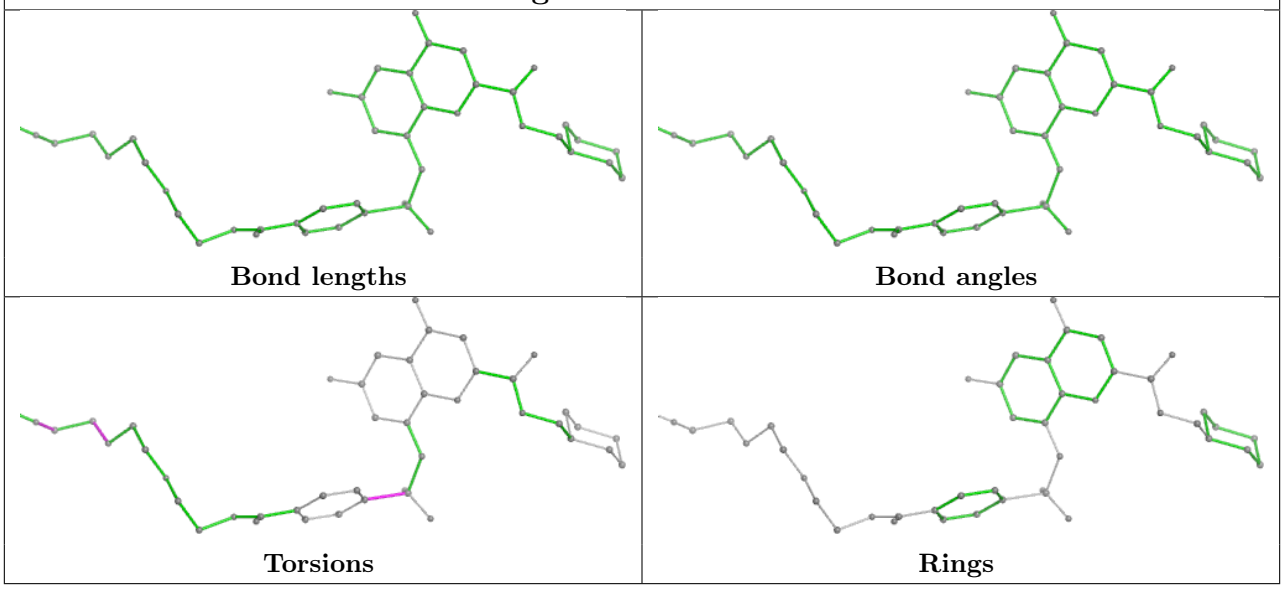
Ligand JE5 C 604



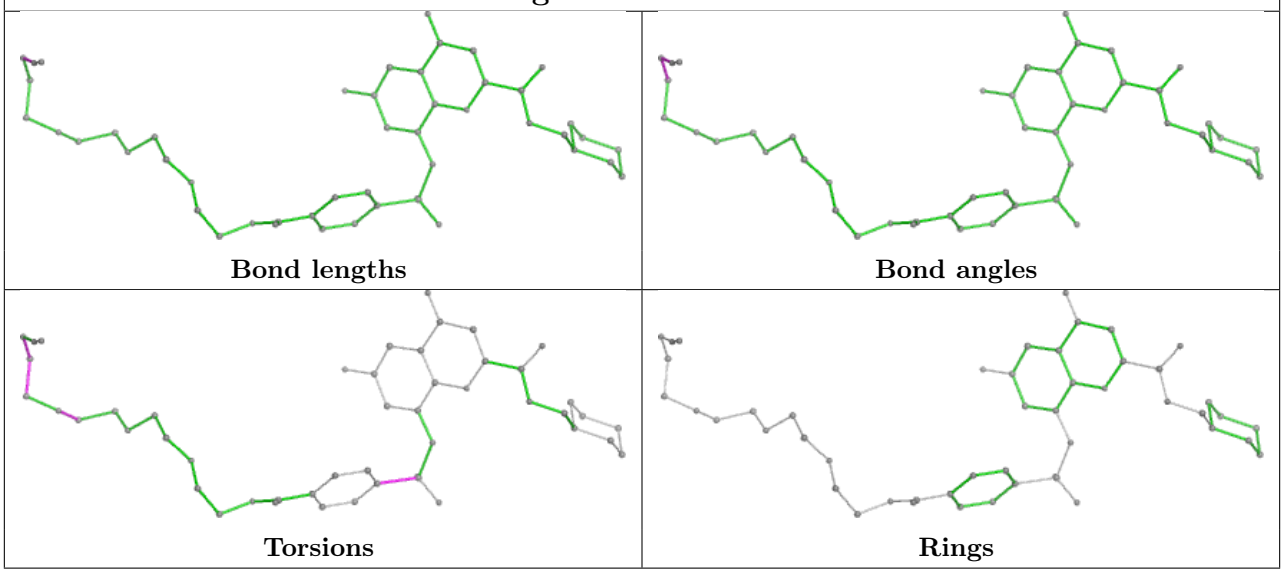
Ligand JE5 B 603



Ligand JE5 D 603



Ligand JE5 A 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, 95^{th} 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	496/535 (92%)	-0.37	8 (1%)	72	68	21, 30, 56, 81	0
1	B	497/535 (92%)	-0.25	6 (1%)	79	76	20, 30, 55, 86	0
1	C	485/535 (90%)	-0.19	6 (1%)	79	76	22, 30, 55, 78	0
1	D	495/535 (92%)	-0.20	4 (0%)	86	84	23, 34, 54, 80	0
All	All	1973/2140 (92%)	-0.25	24 (1%)	79	76	20, 31, 55, 86	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLN	4.2
1	C	351	GLU	4.2
1	C	195	GLN	3.6
1	C	486	ALA	3.2
1	D	46	HIS	3.1
1	A	351	GLU	3.0
1	B	544	ARG	2.9
1	D	187	THR	2.8
1	B	194	ASP	2.8
1	C	187	THR	2.8
1	C	499	ILE	2.7
1	C	245	MET	2.7
1	A	544	ARG	2.5
1	D	544	ARG	2.4
1	A	187	THR	2.3
1	A	189	ILE	2.3
1	B	46	HIS	2.2
1	B	195	GLN	2.2
1	B	545	ASN	2.2
1	B	187	THR	2.2
1	D	351	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	2.0
1	A	494	VAL	2.0
1	A	543	MET	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)

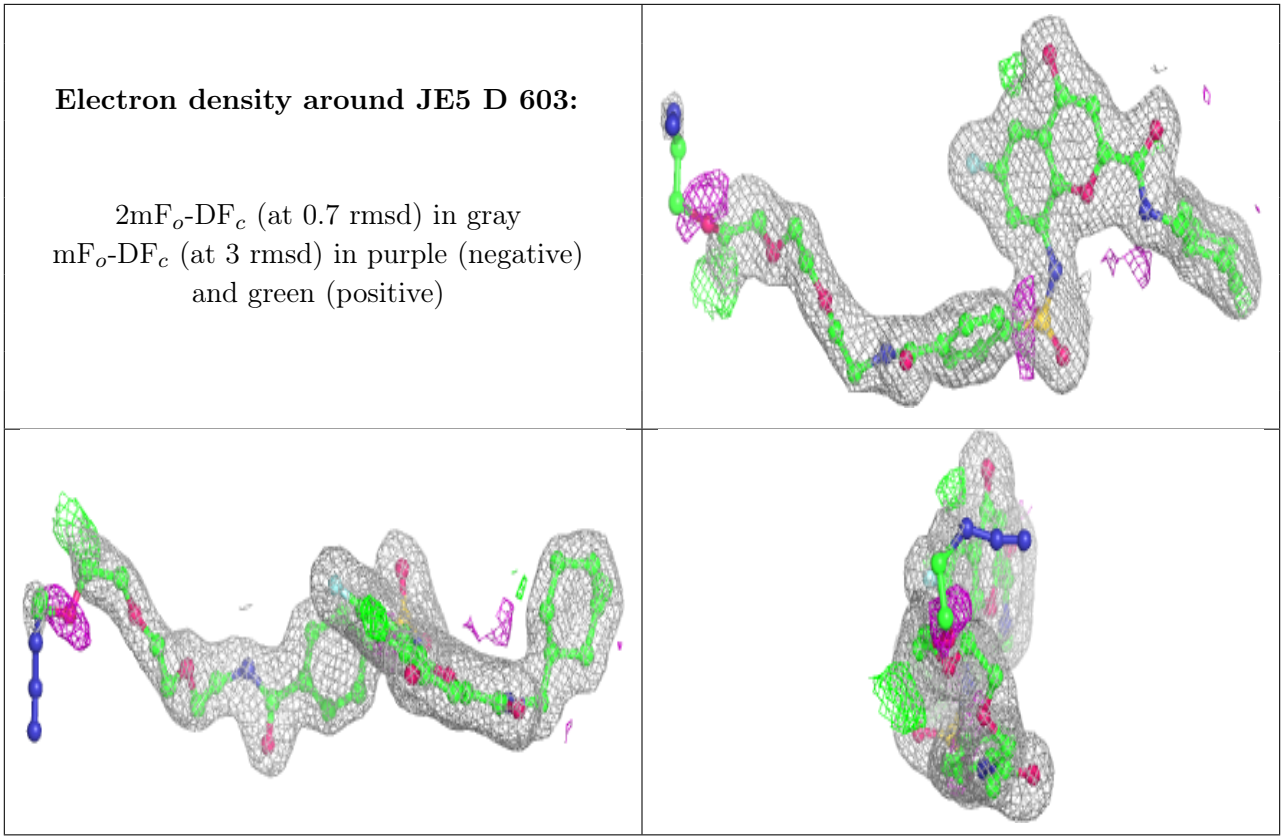
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GOL	D	602	6/6	0.84	0.22	47,55,59,66	0
4	GOL	B	602	6/6	0.88	0.18	44,45,52,59	0
4	GOL	C	602	6/6	0.88	0.17	40,47,50,52	0
4	GOL	C	603	6/6	0.88	0.12	34,46,46,51	0
4	GOL	A	603	6/6	0.88	0.15	35,44,47,56	0
2	LYS	D	601	10/10	0.92	0.11	26,27,29,29	0
4	GOL	A	604	6/6	0.93	0.14	34,44,51,51	0
3	JE5	D	603	49/49	0.94	0.12	26,34,104,109	0
2	LYS	C	601	10/10	0.95	0.10	21,23,26,27	0
3	JE5	A	602	49/49	0.97	0.10	23,28,100,107	0
3	JE5	B	603	49/49	0.97	0.11	23,27,113,117	0
3	JE5	C	604	49/49	0.97	0.12	24,31,118,123	0
2	LYS	A	601	10/10	0.97	0.07	20,22,23,24	0
2	LYS	B	601	10/10	0.97	0.10	22,23,25,25	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.

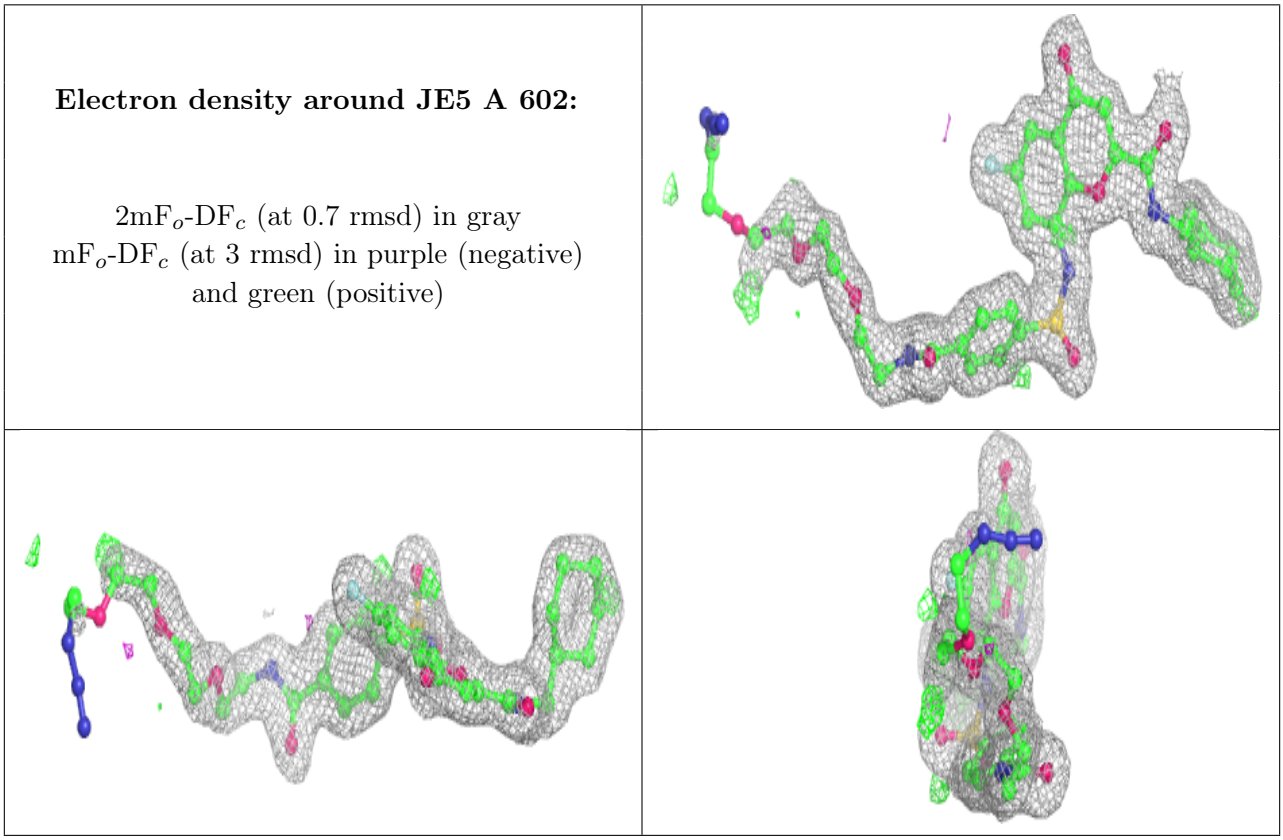
Electron density around JE5 D 603:

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



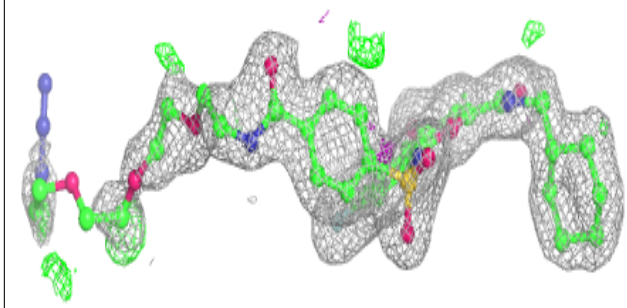
Electron density around JE5 A 602:

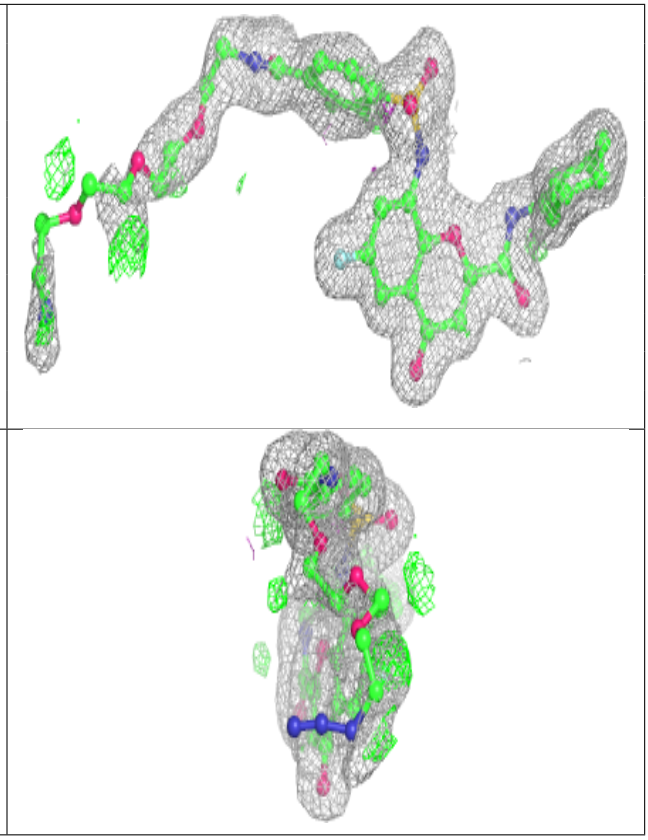
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around JE5 B 603:

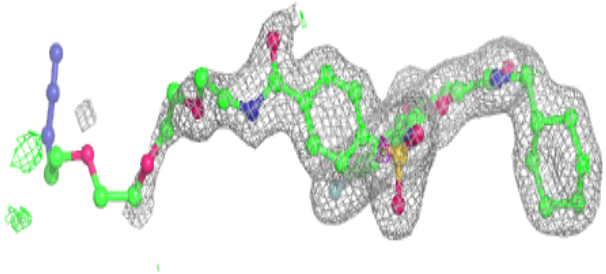
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

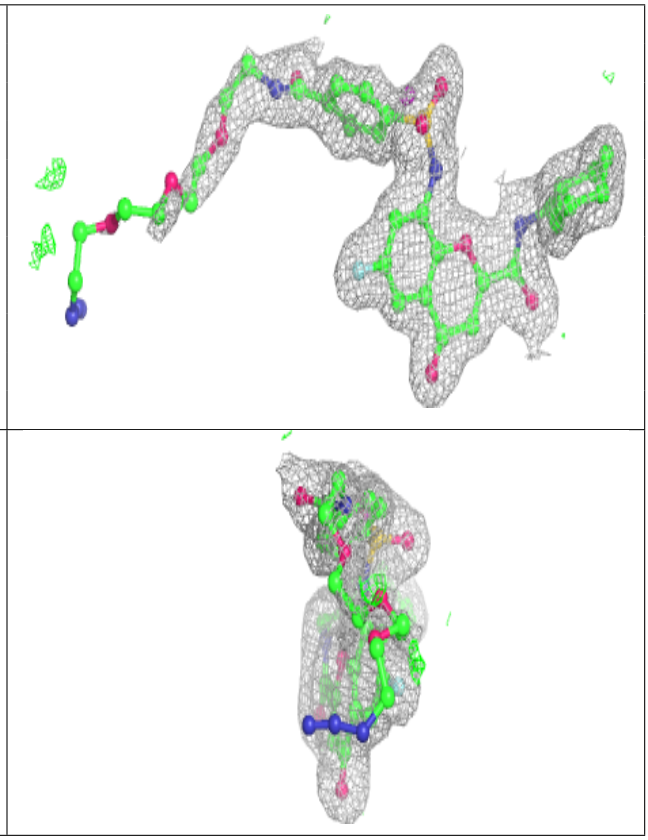




Electron density around JE5 C 604:

$2mF_o$-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.