Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:57 PM EDT

PDB ID	:	6J2V
Title	:	GABA aminotransferase from Corynebacterium glutamicum
Authors	:	Hong, J.; Kim, K.J.
Deposited on	:	2019-01-03
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

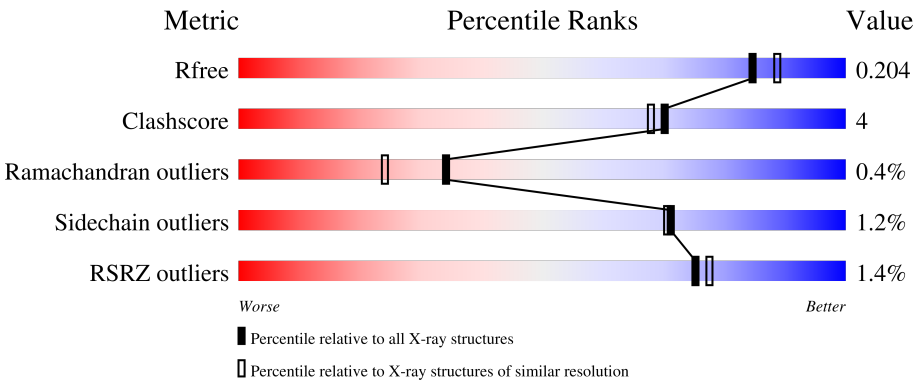
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	473	% 85% 8% • 7%
1	B	473	2% 89% • 7%
1	C	473	% 86% 7% 7%
1	D	473	2% 85% 8% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14304 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 PLP-dependent aminotransferases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	440	3200	2006	561	618	15	0	0	0
1	B	440	3200	2006	561	618	15	0	0	0
1	C	440	3200	2006	561	618	15	0	0	0
1	D	440	3200	2006	561	618	15	0	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q8NT35
A	-23	SER	-	expression tag	UNP Q8NT35
A	-22	TYR	-	expression tag	UNP Q8NT35
A	-21	TYR	-	expression tag	UNP Q8NT35
A	-20	HIS	-	expression tag	UNP Q8NT35
A	-19	HIS	-	expression tag	UNP Q8NT35
A	-18	HIS	-	expression tag	UNP Q8NT35
A	-17	HIS	-	expression tag	UNP Q8NT35
A	-16	HIS	-	expression tag	UNP Q8NT35
A	-15	HIS	-	expression tag	UNP Q8NT35
A	-14	ASP	-	expression tag	UNP Q8NT35
A	-13	TYR	-	expression tag	UNP Q8NT35
A	-12	ASP	-	expression tag	UNP Q8NT35
A	-11	ILE	-	expression tag	UNP Q8NT35
A	-10	PRO	-	expression tag	UNP Q8NT35
A	-9	THR	-	expression tag	UNP Q8NT35
A	-8	THR	-	expression tag	UNP Q8NT35
A	-7	GLU	-	expression tag	UNP Q8NT35
A	-6	ASN	-	expression tag	UNP Q8NT35
A	-5	LEU	-	expression tag	UNP Q8NT35
A	-4	TYR	-	expression tag	UNP Q8NT35

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	expression tag	UNP Q8NT35
A	-2	GLN	-	expression tag	UNP Q8NT35
A	-1	GLY	-	expression tag	UNP Q8NT35
A	0	HIS	-	expression tag	UNP Q8NT35
B	-24	MET	-	initiating methionine	UNP Q8NT35
B	-23	SER	-	expression tag	UNP Q8NT35
B	-22	TYR	-	expression tag	UNP Q8NT35
B	-21	TYR	-	expression tag	UNP Q8NT35
B	-20	HIS	-	expression tag	UNP Q8NT35
B	-19	HIS	-	expression tag	UNP Q8NT35
B	-18	HIS	-	expression tag	UNP Q8NT35
B	-17	HIS	-	expression tag	UNP Q8NT35
B	-16	HIS	-	expression tag	UNP Q8NT35
B	-15	HIS	-	expression tag	UNP Q8NT35
B	-14	ASP	-	expression tag	UNP Q8NT35
B	-13	TYR	-	expression tag	UNP Q8NT35
B	-12	ASP	-	expression tag	UNP Q8NT35
B	-11	ILE	-	expression tag	UNP Q8NT35
B	-10	PRO	-	expression tag	UNP Q8NT35
B	-9	THR	-	expression tag	UNP Q8NT35
B	-8	THR	-	expression tag	UNP Q8NT35
B	-7	GLU	-	expression tag	UNP Q8NT35
B	-6	ASN	-	expression tag	UNP Q8NT35
B	-5	LEU	-	expression tag	UNP Q8NT35
B	-4	TYR	-	expression tag	UNP Q8NT35
B	-3	PHE	-	expression tag	UNP Q8NT35
B	-2	GLN	-	expression tag	UNP Q8NT35
B	-1	GLY	-	expression tag	UNP Q8NT35
B	0	HIS	-	expression tag	UNP Q8NT35
C	-24	MET	-	initiating methionine	UNP Q8NT35
C	-23	SER	-	expression tag	UNP Q8NT35
C	-22	TYR	-	expression tag	UNP Q8NT35
C	-21	TYR	-	expression tag	UNP Q8NT35
C	-20	HIS	-	expression tag	UNP Q8NT35
C	-19	HIS	-	expression tag	UNP Q8NT35
C	-18	HIS	-	expression tag	UNP Q8NT35
C	-17	HIS	-	expression tag	UNP Q8NT35
C	-16	HIS	-	expression tag	UNP Q8NT35
C	-15	HIS	-	expression tag	UNP Q8NT35
C	-14	ASP	-	expression tag	UNP Q8NT35
C	-13	TYR	-	expression tag	UNP Q8NT35
C	-12	ASP	-	expression tag	UNP Q8NT35

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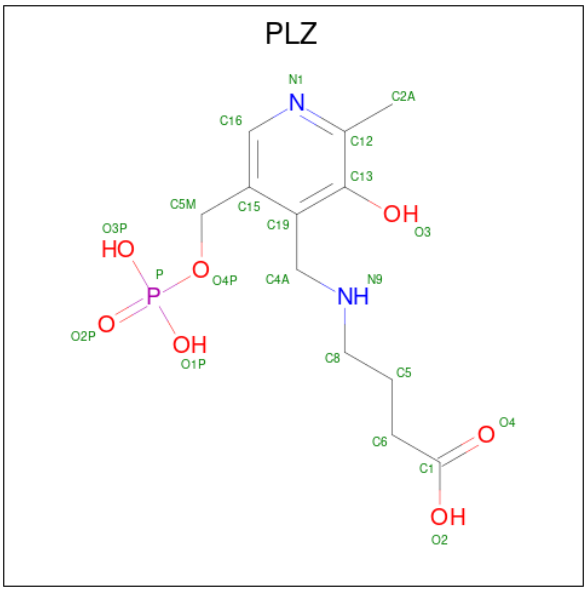
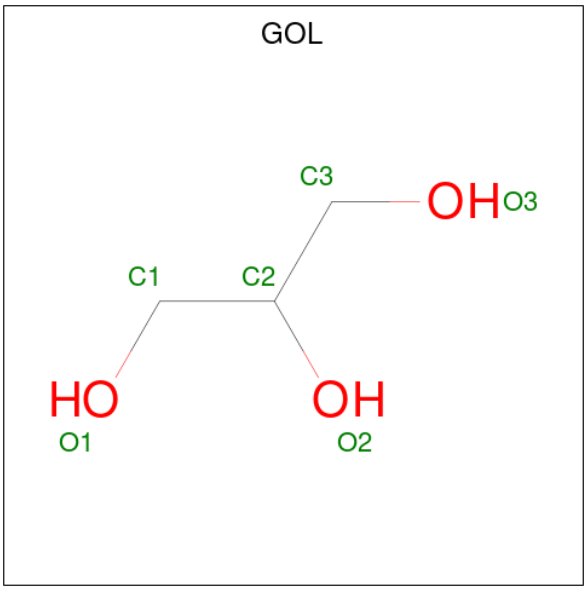
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	ILE	-	expression tag	UNP Q8NT35
C	-10	PRO	-	expression tag	UNP Q8NT35
C	-9	THR	-	expression tag	UNP Q8NT35
C	-8	THR	-	expression tag	UNP Q8NT35
C	-7	GLU	-	expression tag	UNP Q8NT35
C	-6	ASN	-	expression tag	UNP Q8NT35
C	-5	LEU	-	expression tag	UNP Q8NT35
C	-4	TYR	-	expression tag	UNP Q8NT35
C	-3	PHE	-	expression tag	UNP Q8NT35
C	-2	GLN	-	expression tag	UNP Q8NT35
C	-1	GLY	-	expression tag	UNP Q8NT35
C	0	HIS	-	expression tag	UNP Q8NT35
D	-24	MET	-	initiating methionine	UNP Q8NT35
D	-23	SER	-	expression tag	UNP Q8NT35
D	-22	TYR	-	expression tag	UNP Q8NT35
D	-21	TYR	-	expression tag	UNP Q8NT35
D	-20	HIS	-	expression tag	UNP Q8NT35
D	-19	HIS	-	expression tag	UNP Q8NT35
D	-18	HIS	-	expression tag	UNP Q8NT35
D	-17	HIS	-	expression tag	UNP Q8NT35
D	-16	HIS	-	expression tag	UNP Q8NT35
D	-15	HIS	-	expression tag	UNP Q8NT35
D	-14	ASP	-	expression tag	UNP Q8NT35
D	-13	TYR	-	expression tag	UNP Q8NT35
D	-12	ASP	-	expression tag	UNP Q8NT35
D	-11	ILE	-	expression tag	UNP Q8NT35
D	-10	PRO	-	expression tag	UNP Q8NT35
D	-9	THR	-	expression tag	UNP Q8NT35
D	-8	THR	-	expression tag	UNP Q8NT35
D	-7	GLU	-	expression tag	UNP Q8NT35
D	-6	ASN	-	expression tag	UNP Q8NT35
D	-5	LEU	-	expression tag	UNP Q8NT35
D	-4	TYR	-	expression tag	UNP Q8NT35
D	-3	PHE	-	expression tag	UNP Q8NT35
D	-2	GLN	-	expression tag	UNP Q8NT35
D	-1	GLY	-	expression tag	UNP Q8NT35
D	0	HIS	-	expression tag	UNP Q8NT35

- Molecule 2 is 4-[({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)AMINO]BUTANOIC ACID (three-letter code: PLZ) (formula: $C_{12}H_{19}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	22	12	2	7	1	0	0
			Total	C	N	O	P		
2	B	1	22	12	2	7	1	0	0
			Total	C	N	O	P		
2	C	1	22	12	2	7	1	0	0
			Total	C	N	O	P		
2	D	1	22	12	2	7	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

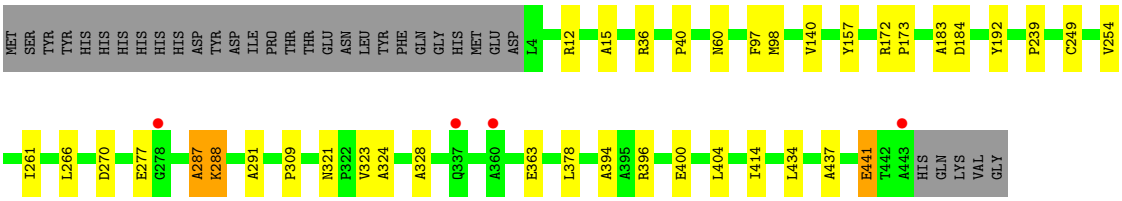
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	321	321	321	0	0
			Total	O		
4	B	355	355	355	0	0
			Total	O		
4	C	373	373	373	0	0
			Total	O		
4	D	319	319	319	0	0

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.

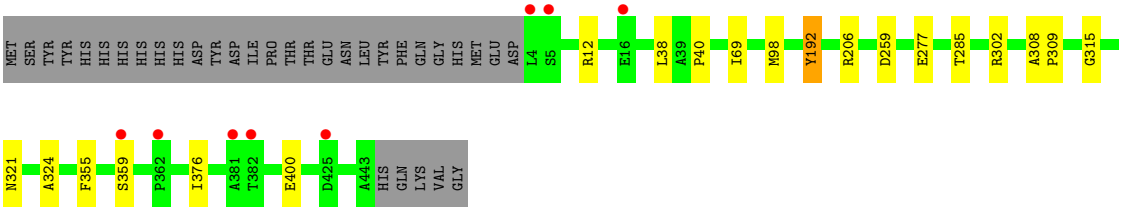
• Molecule 1: PLP-dependent aminotransferases

Chain A:



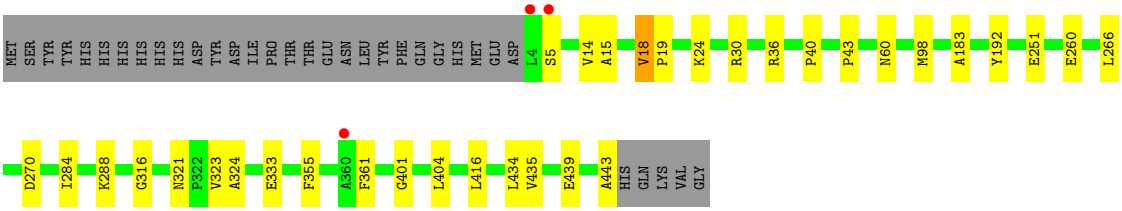
• Molecule 1: PLP-dependent aminotransferases

Chain B:



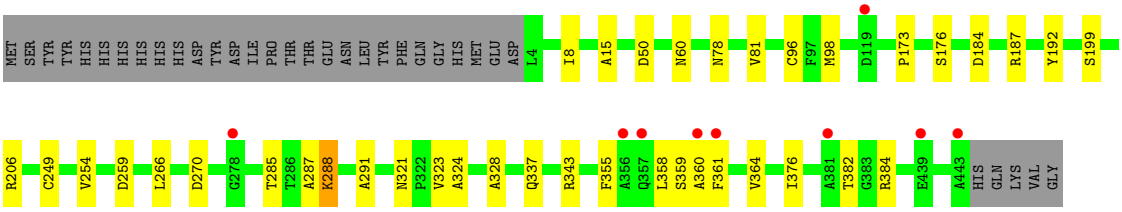
• Molecule 1: PLP-dependent aminotransferases

Chain C:



• Molecule 1: PLP-dependent aminotransferases

Chain D:


MET
SER
TYR
TYR
HIS
HIS
HIS
HIS
HIS
HIS
ASP
TYR
ASP
ILE
PRO
THR
THR
GLU
ASN
LEU
TYR
PHE
GLN
GLY
HIS
MET
GLU
ASP
L4
I8
A15
D50
N60
N78
V81
C96
F97
M98
D119
P173
S176
D184
R187
Y192
S199
R206
C249
V254
D259
L266
D270
G278
T285
T286
A287
K288
A291
N321
P322
V323
A324
A328
Q337
R343
F355
A356
Q357
L358
S359
A360
F361
V364
I376
A381
T382
G383
R384
E439
A443
HIS
GLN
LYS
VAL
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.72Å 70.50Å 97.02Å 106.57° 96.48° 110.66°	Depositor
Resolution (Å)	33.61 – 1.90 33.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (33.61-1.90) 96.9 (33.59-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.18 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.146 , 0.197 0.157 , 0.204	Depositor DCC
R_{free} test set	5902 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14304	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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 (i)

5.1 Standard geometry (i)

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

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	0/3253	0.88	0/4427
1	B	0.74	0/3253	0.88	2/4427 (0.0%)
1	C	0.75	1/3253 (0.0%)	0.89	2/4427 (0.0%)
1	D	0.74	0/3253	0.88	1/4427 (0.0%)
All	All	0.74	1/13012 (0.0%)	0.88	5/17708 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	GLU	CD-OE2	6.21	1.32	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	TYR	CB-CG-CD1	5.54	124.32	121.00
1	D	187	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	30	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	302	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	30	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3200	0	3205	30	0
1	B	3200	0	3205	12	0
1	C	3200	0	3205	27	0
1	D	3200	0	3205	24	0
2	A	22	0	16	6	0
2	B	22	0	16	1	0
2	C	22	0	16	4	0
2	D	22	0	15	2	0
3	A	12	0	16	2	0
3	B	12	0	16	1	0
3	C	12	0	16	3	0
3	D	12	0	16	1	0
4	A	321	0	0	1	0
4	B	355	0	0	2	0
4	C	373	0	0	2	0
4	D	319	0	0	5	0
All	All	14304	0	12947	92	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 4.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLU:OE1	4:B:601:HOH:O	1.83	0.96
1:A:288:LYS:NZ	2:A:501:PLZ:HN9	1.79	0.81
1:C:288:LYS:NZ	2:C:501:PLZ:N9	2.31	0.79
1:A:288:LYS:HZ1	2:A:501:PLZ:HN9	1.33	0.75
3:A:502:GOL:H31	1:B:38:LEU:HD21	1.68	0.75
3:D:503:GOL:H12	4:D:670:HOH:O	1.88	0.73
1:C:321:ASN:HD22	1:C:324:ALA:H	1.38	0.72
1:D:321:ASN:HD22	1:D:324:ALA:H	1.37	0.71
1:A:321:ASN:HD22	1:A:324:ALA:H	1.37	0.71
1:D:355:PHE:CE2	1:D:376:ILE:HD11	2.27	0.69
1:B:321:ASN:HD22	1:B:324:ALA:H	1.38	0.69
1:C:439:GLU:O	1:C:443:ALA:HB2	1.93	0.68
1:A:98:MET:HG3	3:A:502:GOL:O1	1.95	0.67
1:D:78:ASN:HD22	1:D:81:VAL:H	1.42	0.66
1:A:98:MET:O	1:B:40:PRO:HA	2.01	0.61
1:C:19:PRO:HG2	1:C:24:LYS:HG3	1.83	0.60
1:A:396:ARG:HD2	4:A:649:HOH:O	2.02	0.60
1:D:355:PHE:CZ	1:D:376:ILE:HD11	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:NZ	2:A:501:PLZ:N9	2.47	0.60
1:C:404:LEU:HD21	1:C:434:LEU:HD13	1.83	0.60
1:D:361:PHE:O	4:D:601:HOH:O	2.17	0.56
1:A:183:ALA:HB2	1:C:183:ALA:HB2	1.87	0.56
1:D:343:ARG:HD3	4:D:818:HOH:O	2.07	0.53
1:C:98:MET:HB2	4:D:839:HOH:O	2.09	0.53
1:D:288:LYS:NZ	2:D:502:PLZ:N9	2.57	0.52
1:B:308:ALA:HB3	1:B:309:PRO:HD3	1.93	0.51
1:D:358:LEU:O	1:D:361:PHE:N	2.43	0.51
1:C:404:LEU:CD2	1:C:434:LEU:HD13	2.41	0.50
3:C:503:GOL:H31	1:D:176:SER:O	2.11	0.50
4:C:870:HOH:O	1:D:98:MET:HB2	2.12	0.49
1:C:288:LYS:HZ1	2:C:501:PLZ:C8	2.25	0.48
1:C:288:LYS:HZ2	2:C:501:PLZ:C4A	2.26	0.48
1:A:266:LEU:HA	1:A:270:ASP:O	2.13	0.48
1:C:14:VAL:HG21	1:C:401:GLY:CA	2.44	0.48
1:D:321:ASN:HD21	1:D:323:VAL:HB	1.79	0.48
1:D:358:LEU:HD21	1:D:376:ILE:HD13	1.95	0.48
1:C:98:MET:SD	3:C:502:GOL:H32	2.54	0.47
1:A:404:LEU:HD13	1:A:414:ILE:HG23	1.95	0.47
1:A:15:ALA:H	1:A:60:ASN:ND2	2.13	0.47
1:D:249:CYS:HB3	1:D:254:VAL:O	2.14	0.47
1:A:404:LEU:CD2	1:A:434:LEU:HD13	2.45	0.47
1:D:337:GLN:NE2	1:D:337:GLN:HA	2.30	0.47
1:A:291:ALA:HA	1:A:328:ALA:HA	1.97	0.47
1:B:355:PHE:CE2	1:B:376:ILE:HD11	2.50	0.46
1:D:206:ARG:NH2	4:D:610:HOH:O	2.45	0.46
1:A:239:PRO:HA	1:A:277:GLU:OE2	2.15	0.46
1:B:12:ARG:HD2	1:B:400:GLU:O	2.16	0.46
1:A:404:LEU:C	1:A:404:LEU:HD12	2.37	0.46
1:A:404:LEU:HD12	1:A:404:LEU:O	2.16	0.45
1:A:261:ILE:HG23	1:A:287:ALA:HB3	1.98	0.45
1:A:394:ALA:HA	1:A:404:LEU:HD11	1.97	0.45
1:C:18:VAL:CG1	1:C:43:PRO:CG	2.94	0.45
1:C:321:ASN:HD21	1:C:323:VAL:HB	1.82	0.45
2:A:501:PLZ:N9	2:A:501:PLZ:O3	2.50	0.44
1:C:15:ALA:H	1:C:60:ASN:ND2	2.16	0.44
1:C:316:GLY:HA3	4:C:855:HOH:O	2.17	0.44
1:A:404:LEU:HD21	1:A:434:LEU:HD13	1.99	0.44
1:C:361:PHE:HZ	1:C:439:GLU:HG2	1.83	0.44
1:D:364:VAL:HG13	1:D:376:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:VAL:O	1:C:439:GLU:HG3	2.18	0.43
1:B:206:ARG:HD2	4:B:627:HOH:O	2.18	0.43
1:D:15:ALA:H	1:D:60:ASN:ND2	2.17	0.43
1:C:98:MET:HE1	2:D:502:PLZ:O2	2.18	0.43
1:B:315:GLY:HA2	3:B:503:GOL:H2	2.01	0.43
1:C:18:VAL:CG1	1:C:43:PRO:HG2	2.49	0.43
1:D:266:LEU:HA	1:D:270:ASP:O	2.19	0.43
1:D:291:ALA:HA	1:D:328:ALA:HA	2.01	0.43
1:A:288:LYS:HZ2	2:A:501:PLZ:HN9	1.61	0.43
1:B:259:ASP:HA	1:B:285:THR:OG1	2.18	0.43
1:C:40:PRO:HA	1:D:98:MET:O	2.19	0.43
1:A:157:TYR:CE1	2:A:501:PLZ:H81	2.53	0.42
1:A:437:ALA:O	1:A:441:GLU:HB2	2.19	0.42
1:A:249:CYS:HB3	1:A:254:VAL:O	2.20	0.42
1:A:321:ASN:HD21	1:A:323:VAL:HB	1.85	0.42
1:D:382:THR:HG21	1:D:384:ARG:NH2	2.35	0.42
1:A:172:ARG:HA	1:A:173:PRO:HA	1.85	0.42
2:B:502:PLZ:O3	2:B:502:PLZ:N9	2.53	0.42
1:D:358:LEU:O	1:D:360:ALA:N	2.52	0.42
1:C:316:GLY:O	3:C:502:GOL:H31	2.20	0.42
1:D:259:ASP:HA	1:D:285:THR:OG1	2.20	0.42
1:A:40:PRO:HA	1:B:98:MET:O	2.19	0.41
1:A:97:PHE:O	1:B:40:PRO:HB3	2.20	0.41
2:C:501:PLZ:N9	2:C:501:PLZ:O3	2.47	0.41
1:A:140:VAL:HG12	1:A:309:PRO:HG2	2.03	0.41
1:A:12:ARG:HD2	1:A:400:GLU:O	2.20	0.41
1:C:260:GLU:HG3	1:C:284:ILE:HD11	2.02	0.41
1:C:260:GLU:HG3	1:C:284:ILE:CD1	2.51	0.41
1:A:363:GLU:O	1:A:378:LEU:HA	2.21	0.41
1:C:14:VAL:HG21	1:C:401:GLY:HA3	2.02	0.41
1:C:266:LEU:HA	1:C:270:ASP:O	2.21	0.41
1:D:8:ILE:HG12	1:D:50:ASP:HB3	2.03	0.41
1:C:355:PHE:CZ	1:C:416:LEU:HD11	2.56	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	438/473 (93%)	420 (96%)	16 (4%)	2 (0%)	29 18
1	B	438/473 (93%)	421 (96%)	16 (4%)	1 (0%)	47 38
1	C	438/473 (93%)	418 (95%)	20 (5%)	0	100 100
1	D	438/473 (93%)	410 (94%)	24 (6%)	4 (1%)	17 7
All	All	1752/1892 (93%)	1669 (95%)	76 (4%)	7 (0%)	34 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	359	SER
1	A	288	LYS
1	A	287	ALA
1	D	96	CYS
1	D	287	ALA
1	D	288	LYS
1	B	69	ILE

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	317/348 (91%)	313 (99%)	4 (1%)	69 68
1	B	317/348 (91%)	315 (99%)	2 (1%)	86 87
1	C	317/348 (91%)	312 (98%)	5 (2%)	62 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	317/348 (91%)	313 (99%)	4 (1%)	69	68
All	All	1268/1392 (91%)	1253 (99%)	15 (1%)	71	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	184	ASP
1	A	192	TYR
1	A	441	GLU
1	B	192	TYR
1	B	359	SER
1	C	5	SER
1	C	18	VAL
1	C	36	ARG
1	C	192	TYR
1	C	333	GLU
1	D	173	PRO
1	D	184	ASP
1	D	192	TYR
1	D	199	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	60	ASN
1	A	128	ASN
1	A	155	ASN
1	A	321	ASN
1	B	31	GLN
1	B	128	ASN
1	B	321	ASN
1	C	60	ASN
1	C	128	ASN
1	C	321	ASN
1	D	60	ASN
1	D	78	ASN
1	D	128	ASN
1	D	321	ASN
1	D	337	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
3	GOL	B	503	-	5,5,5	0.23	0	5,5,5	0.62	0
3	GOL	A	502	-	5,5,5	0.11	0	5,5,5	0.34	0
2	PLZ	A	501	-	22,22,22	0.73	1 (4%)	29,30,30	0.86	1 (3%)
2	PLZ	C	501	-	22,22,22	0.76	0	29,30,30	0.63	0
3	GOL	D	503	-	5,5,5	0.17	0	5,5,5	0.12	0
2	PLZ	D	502	-	22,22,22	0.74	1 (4%)	29,30,30	0.82	0
3	GOL	C	503	-	5,5,5	0.22	0	5,5,5	0.54	0
3	GOL	A	503	-	5,5,5	0.07	0	5,5,5	0.22	0
3	GOL	C	502	-	5,5,5	0.09	0	5,5,5	0.27	0
3	GOL	D	501	-	5,5,5	0.14	0	5,5,5	0.24	0
3	GOL	B	501	-	5,5,5	0.24	0	5,5,5	0.21	0
2	PLZ	B	502	-	22,22,22	0.73	0	29,30,30	0.79	1 (3%)

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
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
2	PLZ	A	501	-	-	5/14/14/14	0/1/1/1
2	PLZ	C	501	-	-	3/14/14/14	0/1/1/1
3	GOL	D	503	-	-	2/4/4/4	-
2	PLZ	D	502	-	-	4/14/14/14	0/1/1/1
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	A	503	-	-	1/4/4/4	-
3	GOL	C	502	-	-	4/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	B	501	-	-	0/4/4/4	-
2	PLZ	B	502	-	-	6/14/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLZ	O2-C1	-2.11	1.23	1.30
2	D	502	PLZ	O2-C1	-2.03	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PLZ	O3P-P-O1P	2.10	115.69	107.80
2	B	502	PLZ	C19-C4A-N9	2.07	115.32	111.50

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLZ	C15-C19-C4A-N9
2	C	501	PLZ	C13-C19-C4A-N9
2	C	501	PLZ	C15-C19-C4A-N9
2	D	502	PLZ	C13-C19-C4A-N9
2	D	502	PLZ	C15-C19-C4A-N9
3	C	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
2	B	502	PLZ	C15-C19-C4A-N9
2	A	501	PLZ	C19-C4A-N9-C8
2	A	501	PLZ	C8-C5-C6-C1
3	A	502	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	503	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
2	A	501	PLZ	C13-C19-C4A-N9
2	B	502	PLZ	C13-C19-C4A-N9
3	A	502	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
2	B	502	PLZ	C8-C5-C6-C1
2	A	501	PLZ	C5M-O4P-P-O2P
3	D	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O2-C2-C3-O3
2	D	502	PLZ	O4-C1-C6-C5
2	D	502	PLZ	O2-C1-C6-C5
3	A	503	GOL	O2-C2-C3-O3
2	B	502	PLZ	O4-C1-C6-C5
2	B	502	PLZ	C5-C8-N9-C4A
2	B	502	PLZ	O2-C1-C6-C5
2	C	501	PLZ	O2-C1-C6-C5

There are no ring outliers.

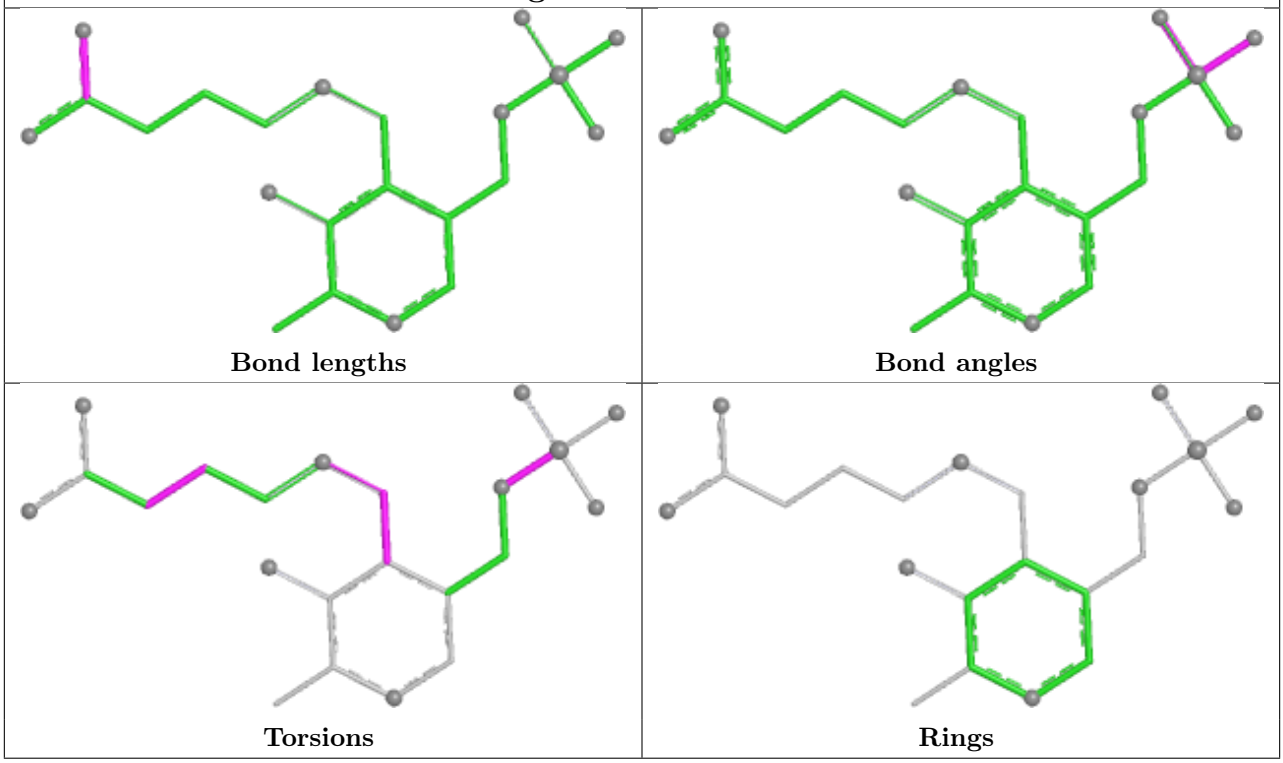
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	GOL	1	0
3	A	502	GOL	2	0
2	A	501	PLZ	6	0
2	C	501	PLZ	4	0
3	D	503	GOL	1	0
2	D	502	PLZ	2	0
3	C	503	GOL	1	0
3	C	502	GOL	2	0
2	B	502	PLZ	1	0

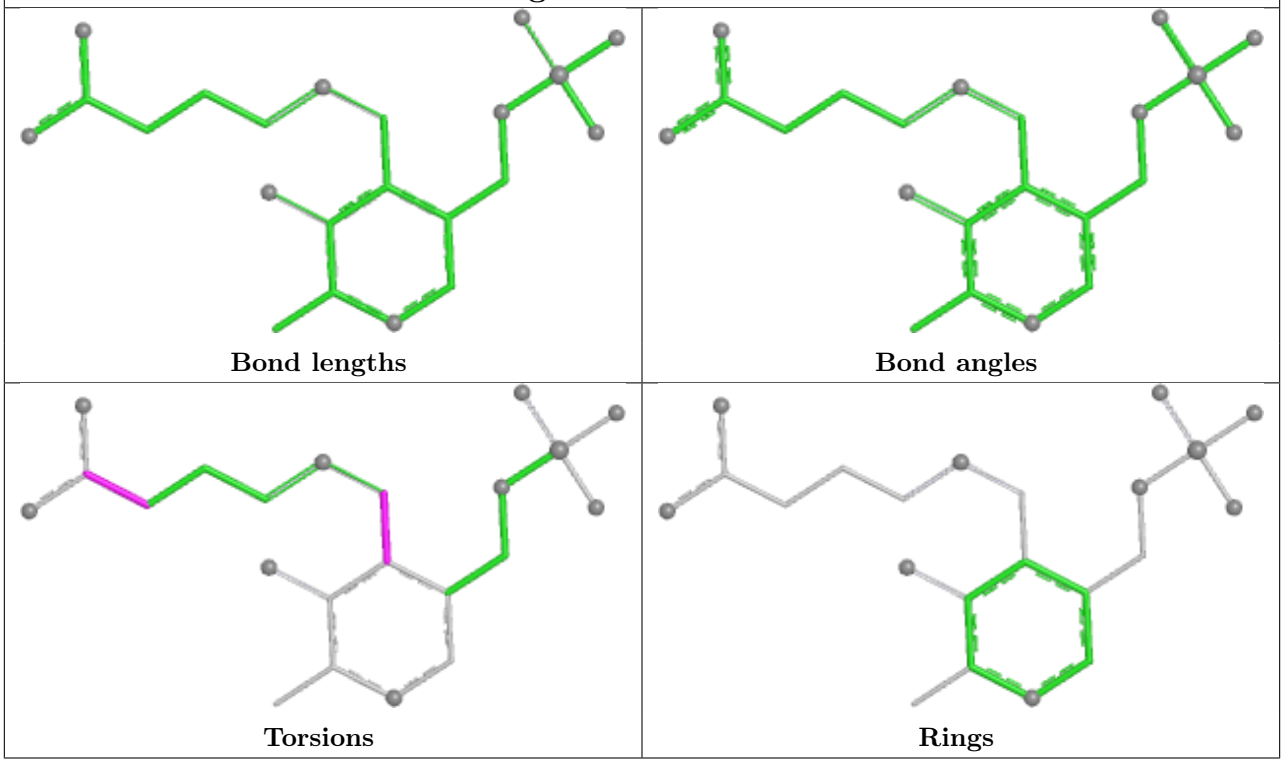
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

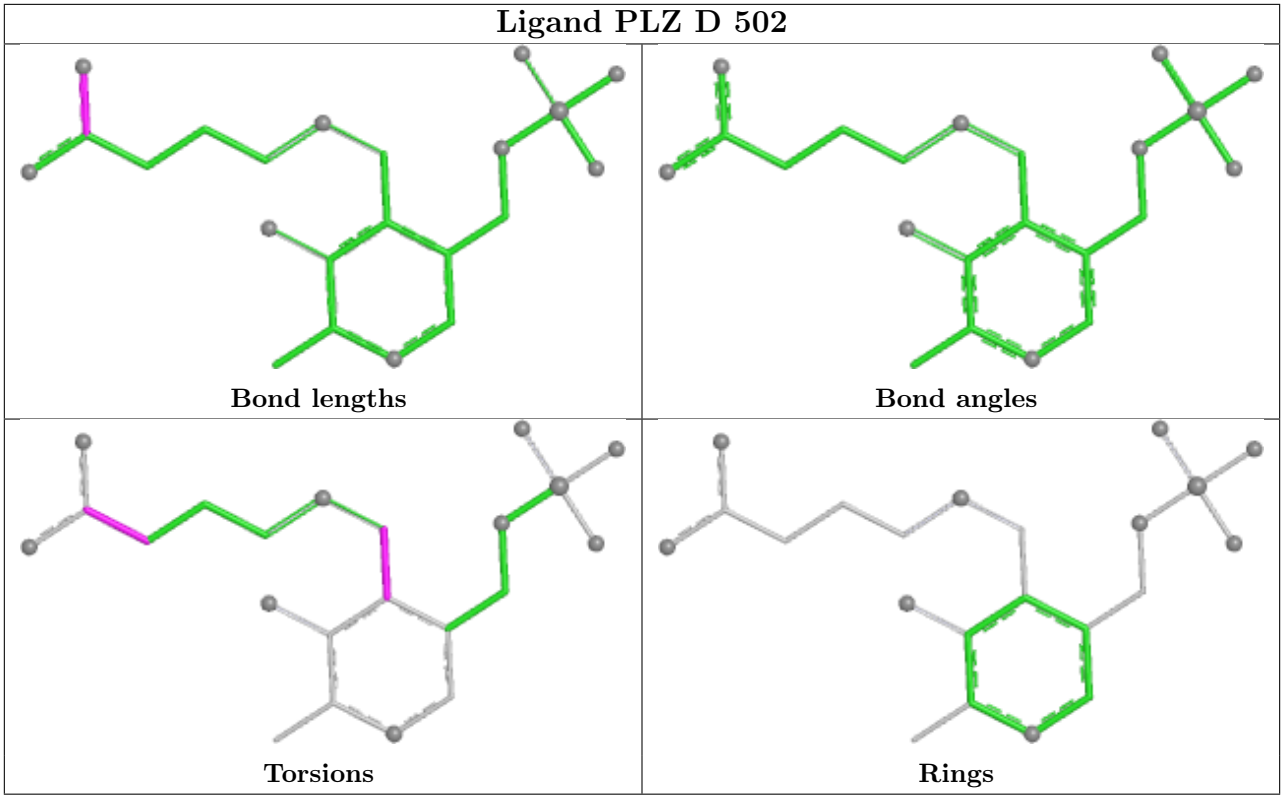
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

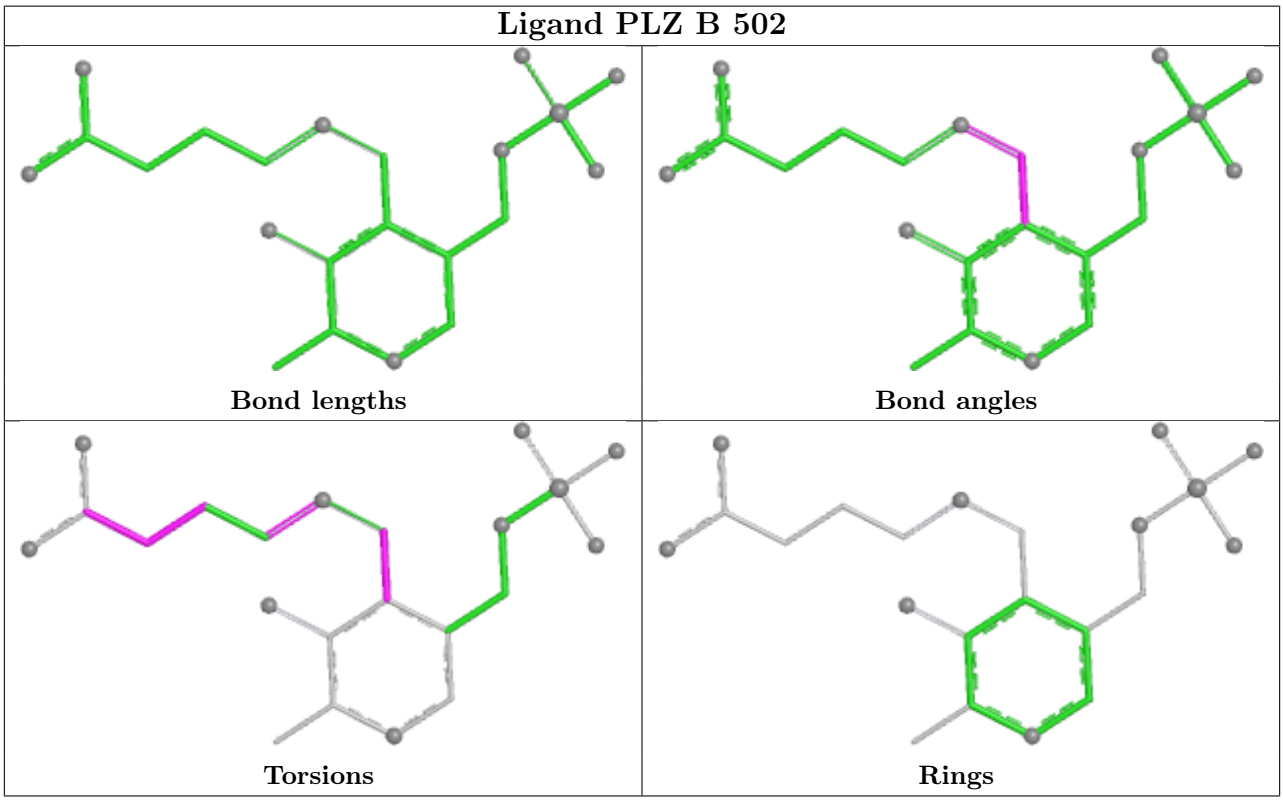
Ligand PLZ A 501



Ligand PLZ C 501







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	440/473 (93%)	-0.27	4 (0%)	84	85	14, 23, 40, 64	0
1	B	440/473 (93%)	-0.31	8 (1%)	68	71	14, 23, 38, 56	0
1	C	440/473 (93%)	-0.42	3 (0%)	87	88	13, 20, 33, 56	0
1	D	440/473 (93%)	-0.16	9 (2%)	65	68	15, 25, 43, 72	0
All	All	1760/1892 (93%)	-0.29	24 (1%)	75	77	13, 22, 39, 72	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	443	ALA	7.1
1	A	443	ALA	5.5
1	D	357	GLN	4.3
1	D	360	ALA	3.8
1	C	4	LEU	3.7
1	B	381	ALA	3.6
1	D	356	ALA	3.3
1	B	5	SER	3.3
1	B	4	LEU	3.2
1	A	360	ALA	3.1
1	A	278	GLY	3.1
1	D	278	GLY	2.9
1	D	361	PHE	2.7
1	D	381	ALA	2.6
1	B	362	PRO	2.6
1	B	359	SER	2.6
1	B	425	ASP	2.5
1	C	360	ALA	2.5
1	D	119	ASP	2.2
1	C	5	SER	2.1
1	A	337	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	16	GLU	2.1
1	B	382	THR	2.1
1	D	439	GLU	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)

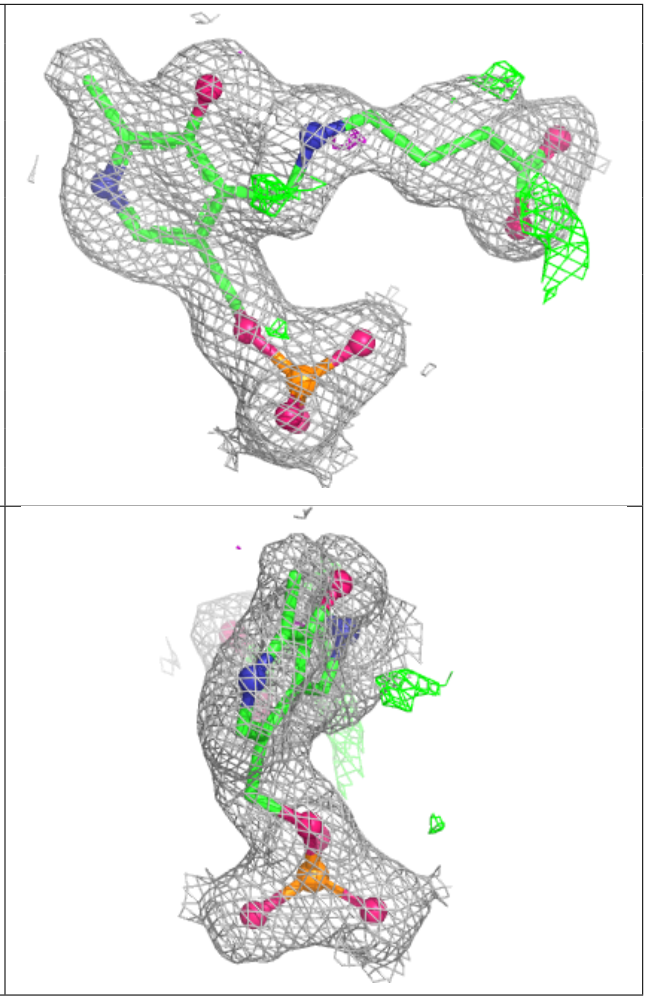
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	502	6/6	0.90	0.17	36,44,47,55	0
3	GOL	B	503	6/6	0.92	0.12	28,40,45,50	0
3	GOL	C	502	6/6	0.92	0.14	28,36,41,43	0
3	GOL	C	503	6/6	0.93	0.17	22,33,34,36	0
3	GOL	D	503	6/6	0.93	0.12	30,36,38,42	0
3	GOL	D	501	6/6	0.95	0.09	26,28,30,32	0
2	PLZ	A	501	22/22	0.97	0.11	17,22,38,41	0
3	GOL	A	503	6/6	0.97	0.12	26,31,34,37	0
3	GOL	B	501	6/6	0.97	0.08	20,24,26,29	0
2	PLZ	B	502	22/22	0.97	0.11	17,23,38,41	0
2	PLZ	C	501	22/22	0.98	0.10	15,19,33,39	0
2	PLZ	D	502	22/22	0.98	0.12	19,23,39,42	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.

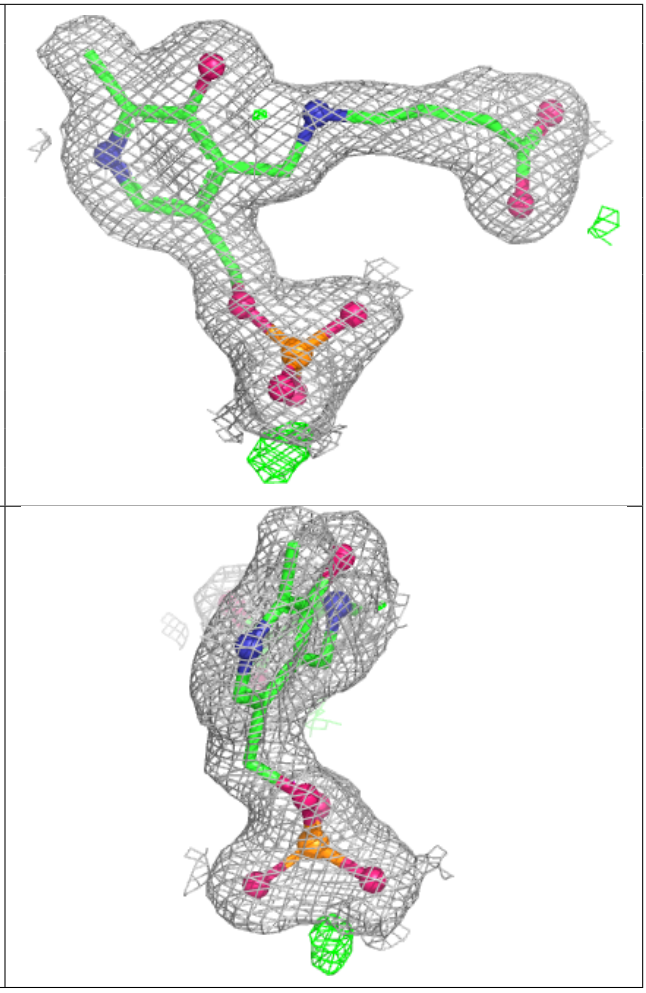
Electron density around PLZ A 501:

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



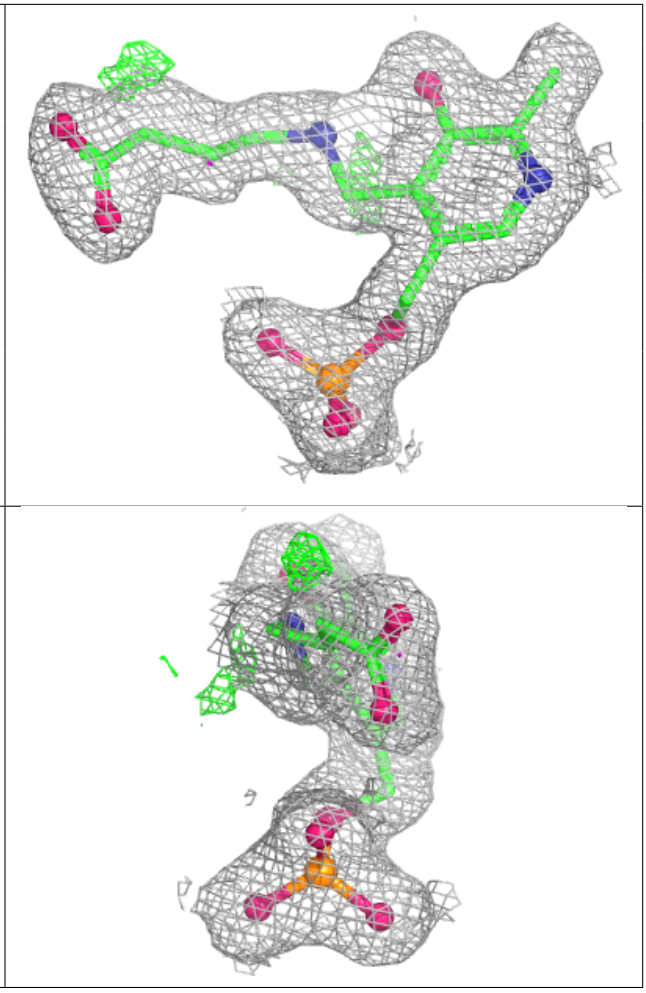
Electron density around PLZ B 502:

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



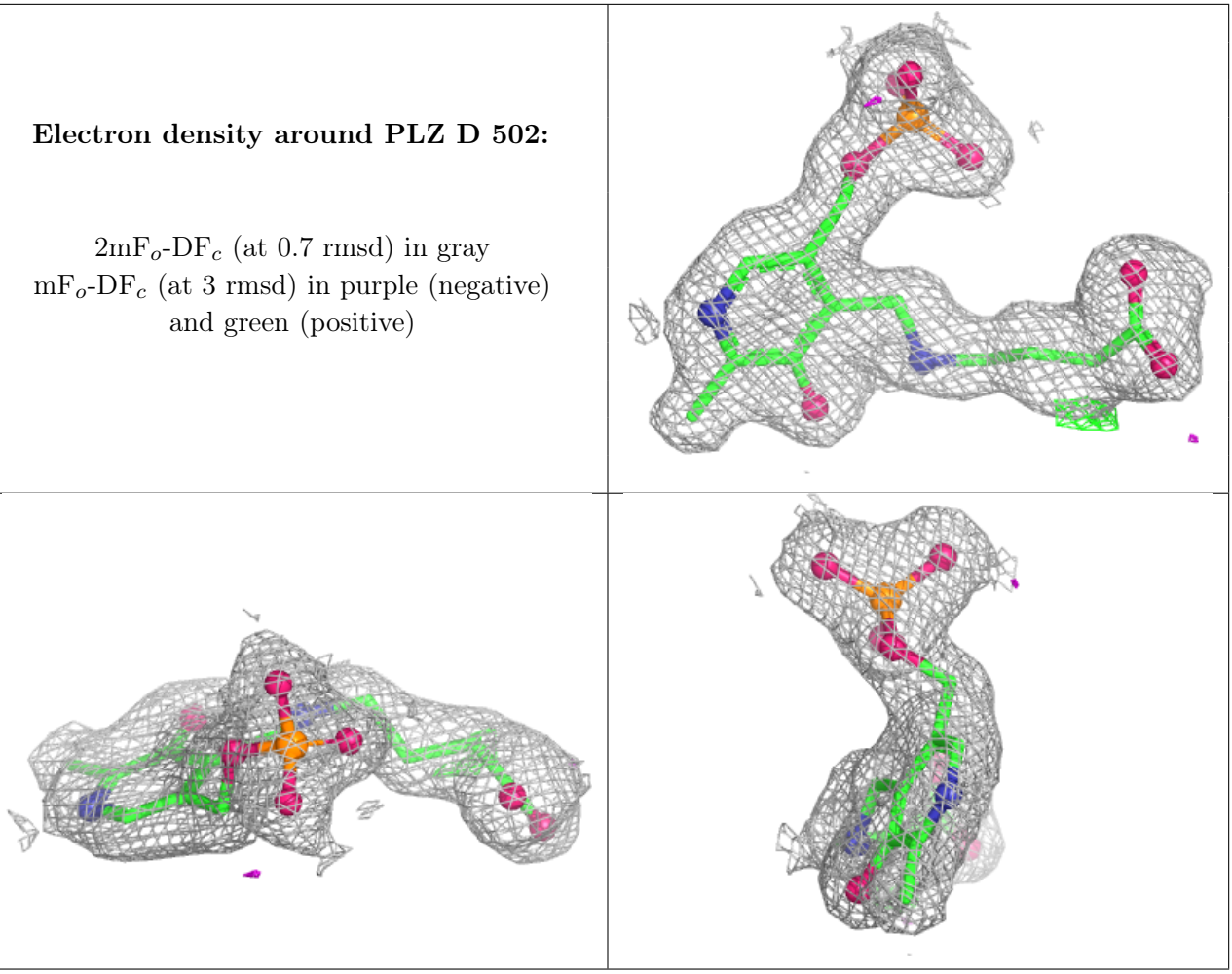
Electron density around PLZ C 501:

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



Electron density around PLZ D 502:

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.