Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 03:16 pm GMT

PDB ID	:	6SLF
Title	:	Nalpha-acylglutamine aminoacylase from Corynebacterium sp.releasing human axilla odorants co-crystallised with high affinity inhibitor
Authors	:	Natsch, A.; Emter, R.
Deposited on	:	2019-08-19
Resolution	:	1.75 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:

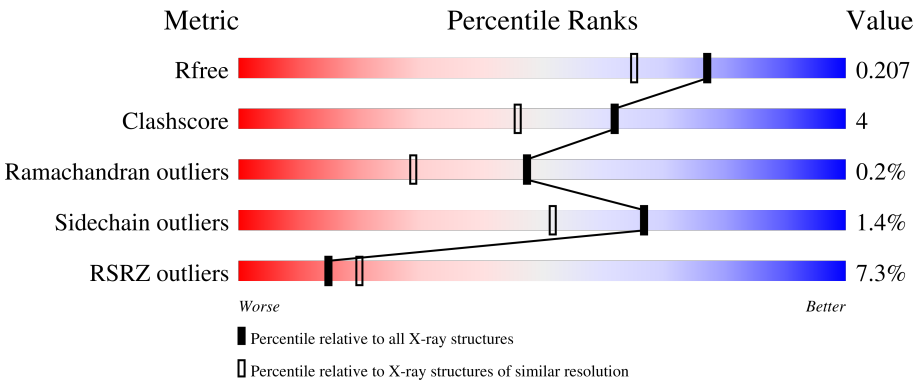
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	400	4% 90% 10%
1	B	400	5% 93% 6% •
1	C	400	4% 94% 6% •
1	D	400	16% 85% 14% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BTB	D	405	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13313 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.

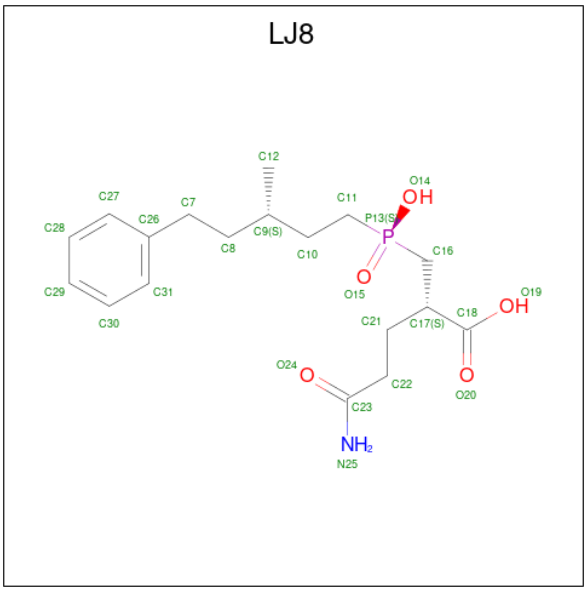
- Molecule 1 is a protein called N-alpha-acyl-glutamine aminoacylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3047	1917	518	601	11	0	0	0
1	B	396	3033	1909	515	598	11	0	0	0
1	C	396	3033	1910	516	596	11	0	0	0
1	D	395	3024	1904	514	595	11	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

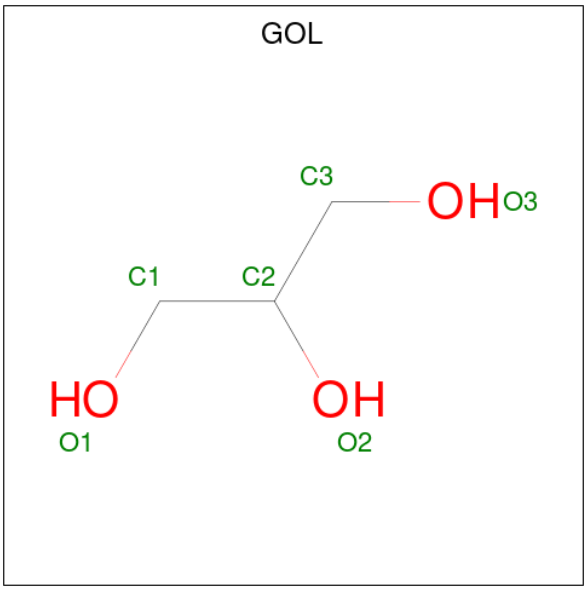
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is (2 {S})-5-azanyl-2-[[[(3 {S})-3-methyl-5-phenyl-pentyl]-oxidanyl-phosphoryl]methyl]-5-oxidanylidene-pentanoic acid (three-letter code: LJ8) (formula: $C_{18}H_{28}NO_5P$) (labeled as "Ligand of Interest" by depositor).



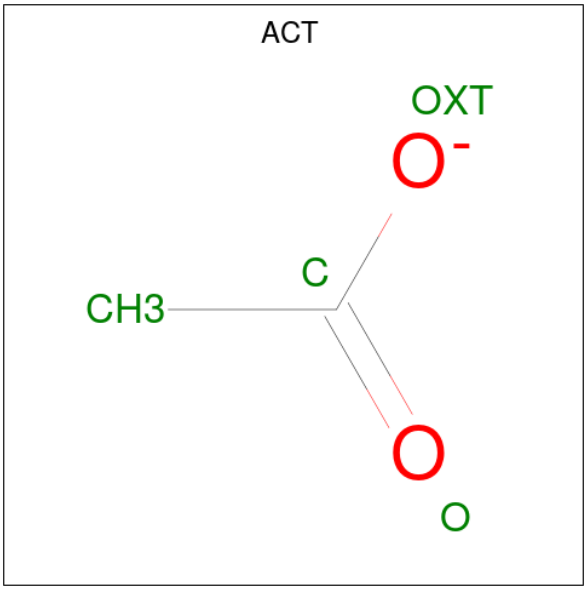
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	25	18	1	5	1	0	0
			Total	C	N	O	P		
3	B	1	25	18	1	5	1	0	0
			Total	C	N	O	P		
3	C	1	25	18	1	5	1	0	0
			Total	C	N	O	P		
3	D	1	25	18	1	5	1	0	0

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



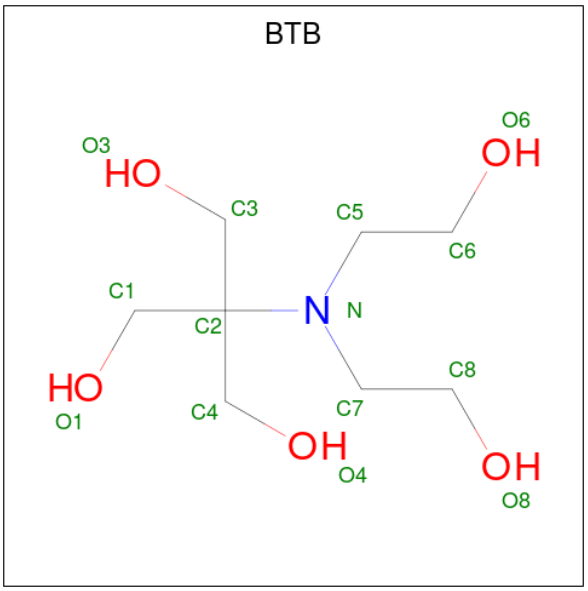
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	1	14	8	1	5	0	0

- Molecule 7 is water.

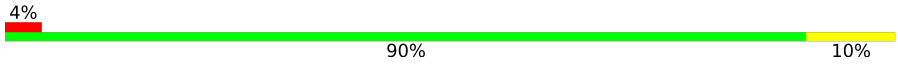
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	309	309	309	0	0
			Total	O		
7	B	255	255	255	0	0
			Total	O		
7	C	284	284	284	0	0
			Total	O		
7	D	172	172	172	0	0

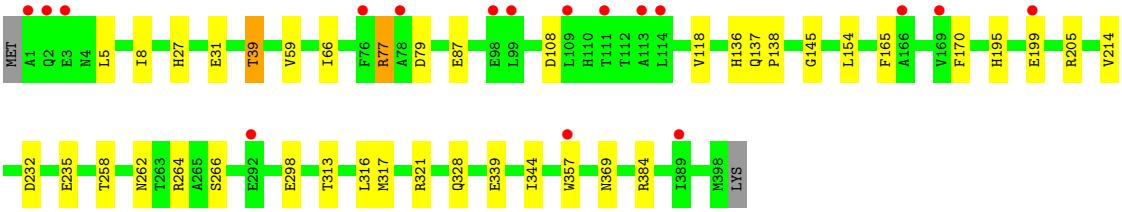
3 Residue-property plots (i)

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: N-alpha-acyl-glutamine aminoacylase

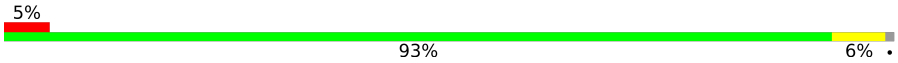
Chain A:

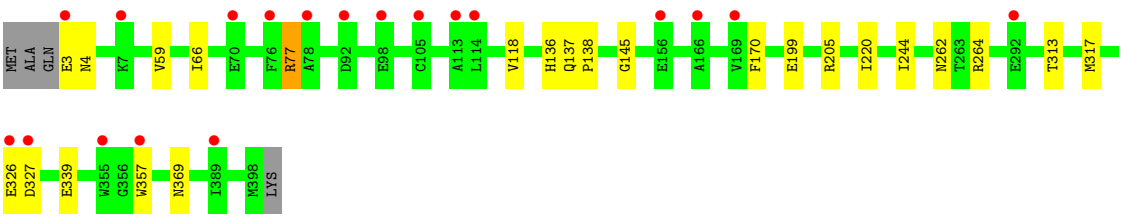




• Molecule 1: N-alpha-acyl-glutamine aminoacylase

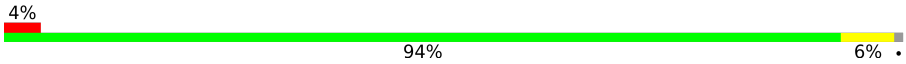
Chain B:

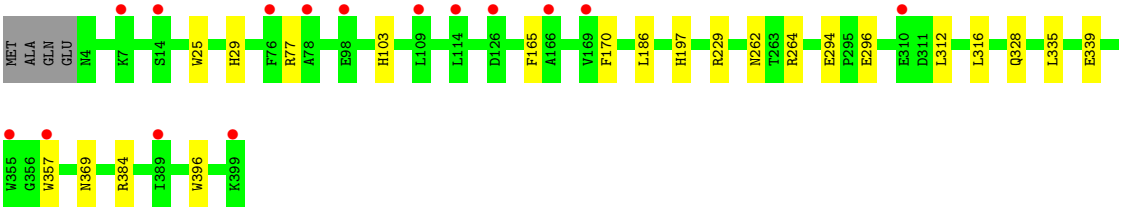




• Molecule 1: N-alpha-acyl-glutamine aminoacylase

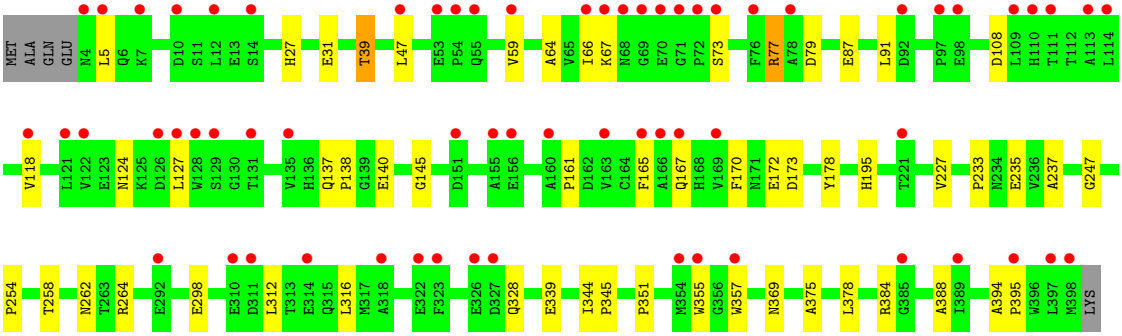
Chain C:





• Molecule 1: N-alpha-acyl-glutamine aminoacylase

Chain D:


MET
ALA
GLN
GLU
N4
L5
Q6
K7
D10
S11
L12
E13
S14
H27
E31
T39
L47
E53
P54
Q55
V59
A64
V65
I66
K67
N68
G69
E70
G71
P72
S73
F76
R77
A78
D79
E87
L91
D92
P97
E98
D108
L109
H110
T111
T112
A113
L114
V118
L121
V122
E123
N124
K125
D126
L127
W128
S129
G130
T131
V135
H136
Q137
P138
G139
E140
G145
D151
A155
E156
A160
P161
D162
V163
C164
F165
A166
Q167
H168
V169
F170
N171
E172
D173
Y178
H196
T221
V227
P233
N234
E235
V236
A237
G247
P254
T258
N262
T263
R264
E292
E298
E310
D311
L312
T313
E314
Q315
L316
M317
A318
E322
F323
E326
D327
Q328
E339
I344
P345
P351
M354
W355
G356
W357
N369
A375
L378
R384
G385
A388
I389
A394
P395
W396
L397
M398
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.69Å 181.92Å 93.12Å 90.00° 104.14° 90.00°	Depositor
Resolution (Å)	29.58 – 1.75 29.58 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.58-1.75) 100.0 (29.58-1.75)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.210 0.181 , 0.207	Depositor DCC
R_{free} test set	8738 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13313	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, ACT, LJ8, ZN, BTB

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	0/3121	0.70	2/4251 (0.0%)
1	B	0.68	0/3107	0.66	0/4232
1	C	0.71	0/3107	0.70	0/4231
1	D	0.59	0/3098	0.63	0/4220
All	All	0.68	0/12433	0.67	2/16934 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	232	ASP	CB-CG-OD1	5.47	123.22	118.30

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	3047	0	2910	33	0
1	B	3033	0	2894	17	0
1	C	3033	0	2901	14	0
1	D	3024	0	2888	41	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	25	0	0	1	0
3	B	25	0	0	1	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	D	14	0	19	15	0
7	A	309	0	0	3	0
7	B	255	0	0	2	0
7	C	284	0	0	2	0
7	D	172	0	0	0	0
All	All	13313	0	11648	105	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 (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:O	6:D:405:BTB:H42	1.43	1.18
1:D:227:VAL:HG13	6:D:405:BTB:H72	1.52	0.90
1:C:294:GLU:HG2	7:C:757:HOH:O	1.70	0.90
1:A:199:GLU:HG3	7:A:699:HOH:O	1.76	0.84
1:A:328:GLN:HE21	1:A:384:ARG:HH22	1.24	0.84
1:D:237:ALA:H	6:D:405:BTB:C8	1.93	0.82
1:B:199:GLU:HG3	7:B:555:HOH:O	1.82	0.80
1:D:237:ALA:H	6:D:405:BTB:H81	1.47	0.80
1:D:31:GLU:OE1	1:D:39:THR:HG23	1.82	0.78
1:A:31:GLU:OE1	1:A:39:THR:HG23	1.86	0.75
1:C:262:ASN:HD21	1:C:264:ARG:HE	1.35	0.73
1:A:328:GLN:HE21	1:A:384:ARG:NH2	1.88	0.72
1:A:262:ASN:HD21	1:A:264:ARG:HE	1.37	0.72
1:B:262:ASN:HD21	1:B:264:ARG:HE	1.38	0.71
1:A:66:ILE:HD11	1:A:118:VAL:HG13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:VAL:CG1	6:D:405:BTB:H72	2.20	0.68
1:A:369:ASN:HD22	1:A:369:ASN:H	1.40	0.68
1:D:233:PRO:O	6:D:405:BTB:H41	1.95	0.66
1:B:313:THR:O	1:B:317:MET:HG3	1.98	0.64
1:B:66:ILE:HD11	1:B:118:VAL:HG13	1.79	0.64
1:A:31:GLU:OE1	1:A:39:THR:CG2	2.46	0.62
1:D:27:HIS:HE1	1:D:87:GLU:OE1	1.83	0.62
1:D:369:ASN:HD22	1:D:369:ASN:H	1.48	0.61
1:D:27:HIS:HD2	1:D:108:ASP:OD2	1.84	0.61
1:B:369:ASN:H	1:B:369:ASN:HD22	1.50	0.60
1:C:328:GLN:HE21	1:C:384:ARG:NH2	1.99	0.60
1:D:237:ALA:N	6:D:405:BTB:H81	2.15	0.60
1:A:27:HIS:HE1	1:A:87:GLU:OE1	1.86	0.59
1:C:25:TRP:O	1:C:29:HIS:HD2	1.86	0.58
1:C:369:ASN:H	1:C:369:ASN:HD22	1.51	0.57
1:D:262:ASN:HD21	1:D:264:ARG:HE	1.51	0.57
1:A:235:GLU:O	6:D:405:BTB:C4	2.34	0.56
1:D:5:LEU:HD13	1:D:394:ALA:HB2	1.88	0.56
1:D:233:PRO:HA	6:D:405:BTB:H51	1.87	0.56
1:C:328:GLN:HE21	1:C:384:ARG:HH22	1.55	0.54
1:B:77:ARG:HH21	1:B:137:GLN:HE22	1.55	0.53
1:D:27:HIS:CD2	1:D:108:ASP:OD2	2.62	0.53
1:D:77:ARG:HE	1:D:137:GLN:NE2	2.05	0.53
1:D:227:VAL:O	6:D:405:BTB:C6	2.56	0.53
1:D:66:ILE:HD11	1:D:118:VAL:HG13	1.90	0.53
1:A:77:ARG:HH21	1:A:137:GLN:HE22	1.55	0.52
1:A:27:HIS:HD2	1:A:108:ASP:OD2	1.93	0.51
1:A:77:ARG:HE	1:A:137:GLN:NE2	2.08	0.51
1:B:136:HIS:HD2	7:B:600:HOH:O	1.93	0.51
1:D:165:PHE:CE1	1:D:316:LEU:HD11	2.46	0.51
1:D:170:PHE:HB2	1:D:369:ASN:HD21	1.75	0.51
1:B:77:ARG:HE	1:B:137:GLN:NE2	2.08	0.50
1:D:344:ILE:HB	1:D:345:PRO:CD	2.42	0.50
1:D:235:GLU:O	6:D:405:BTB:O4	2.22	0.49
1:A:27:HIS:CD2	1:A:108:ASP:OD2	2.66	0.49
1:B:170:PHE:HB2	1:B:369:ASN:HD21	1.78	0.49
1:D:91:LEU:HD11	1:D:375:ALA:HB1	1.95	0.49
1:A:170:PHE:HB2	1:A:369:ASN:HD21	1.78	0.49
1:C:170:PHE:HB2	1:C:369:ASN:HD21	1.78	0.48
1:D:237:ALA:N	6:D:405:BTB:C8	2.69	0.48
1:D:394:ALA:HB3	1:D:395:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ASN:HB3	1:D:127:LEU:HD12	1.95	0.48
1:A:154:LEU:HD22	1:A:344:ILE:HD12	1.95	0.48
1:C:197:HIS:NE2	1:C:296:GLU:OE2	2.43	0.48
1:D:227:VAL:O	6:D:405:BTB:H62	2.15	0.47
1:A:317:MET:HE1	1:A:321:ARG:NH2	2.31	0.46
1:C:262:ASN:HD21	1:C:264:ARG:NE	2.08	0.46
1:D:237:ALA:O	6:D:405:BTB:H81	2.14	0.46
1:A:235:GLU:OE1	1:A:266:SER:OG	2.23	0.46
1:D:47:LEU:HD13	1:D:64:ALA:HB2	1.98	0.46
1:C:103:HIS:HE1	7:C:611:HOH:O	1.99	0.46
3:A:403:LJ8:C29	1:B:205:ARG:HD3	2.46	0.46
1:C:312:LEU:HD11	1:C:396:TRP:CZ2	2.51	0.46
1:D:138:PRO:O	1:D:145:GLY:HA3	2.15	0.46
1:D:170:PHE:CB	1:D:369:ASN:HD21	2.29	0.46
1:C:165:PHE:CE1	1:C:316:LEU:HD11	2.51	0.46
1:D:328:GLN:HE21	1:D:384:ARG:NH2	2.13	0.46
1:B:170:PHE:CB	1:B:369:ASN:HD21	2.28	0.45
1:A:39:THR:HG21	7:A:650:HOH:O	2.16	0.45
1:C:186:LEU:HD23	1:C:335:LEU:HB2	1.99	0.45
1:D:77:ARG:HH21	1:D:137:GLN:HE22	1.63	0.45
1:A:369:ASN:H	1:A:369:ASN:ND2	2.10	0.45
1:A:170:PHE:CB	1:A:369:ASN:HD21	2.30	0.45
1:D:167:GLN:HA	1:D:355:TRP:O	2.16	0.45
1:B:138:PRO:O	1:B:145:GLY:HA3	2.17	0.44
1:B:3:GLU:HG3	1:B:4:ASN:H	1.82	0.44
1:B:77:ARG:HH21	1:B:137:GLN:NE2	2.15	0.44
1:A:195:HIS:HE1	1:A:298:GLU:OE1	2.00	0.44
1:D:312:LEU:HD22	1:D:351:PRO:HB2	1.98	0.44
1:D:178:TYR:CE1	1:D:388:ALA:HB2	2.52	0.44
1:B:262:ASN:HD21	1:B:264:ARG:NE	2.13	0.43
6:D:405:BTB:H52	6:D:405:BTB:H82	1.74	0.43
1:A:195:HIS:HD2	1:A:258:THR:OG1	2.01	0.43
1:A:136:HIS:HD2	7:A:579:HOH:O	2.00	0.43
1:B:220:ILE:HD11	1:B:244:ILE:HD12	2.00	0.43
1:A:165:PHE:CE1	1:A:316:LEU:HD11	2.54	0.42
1:D:73:SER:HB3	1:D:161:PRO:HA	2.01	0.42
1:A:77:ARG:HH21	1:A:137:GLN:NE2	2.17	0.42
1:A:205:ARG:HD3	3:B:403:LJ8:C29	2.50	0.41
1:A:313:THR:O	1:A:317:MET:HG3	2.20	0.41
1:A:5:LEU:O	1:A:8:ILE:HG22	2.20	0.41
1:A:317:MET:CE	1:A:321:ARG:NH2	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:HIS:HD2	1:D:258:THR:OG1	2.04	0.41
1:D:195:HIS:HE1	1:D:298:GLU:OE1	2.04	0.41
1:B:3:GLU:HG3	1:B:4:ASN:N	2.36	0.41
1:A:138:PRO:O	1:A:145:GLY:HA3	2.21	0.41
1:D:172:GLU:HG3	1:D:173:ASP:N	2.36	0.41
1:D:79:ASP:OD2	1:D:140:GLU:HG3	2.21	0.40
1:A:214:VAL:HG21	1:C:229:ARG:HD2	2.03	0.40
1:D:247:GLY:HA2	1:D:254:PRO:HB3	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	396/400 (99%)	389 (98%)	6 (2%)	1 (0%)	41	22
1	B	394/400 (98%)	389 (99%)	4 (1%)	1 (0%)	41	22
1	C	394/400 (98%)	385 (98%)	9 (2%)	0	100	100
1	D	393/400 (98%)	383 (98%)	9 (2%)	1 (0%)	41	22
All	All	1577/1600 (99%)	1546 (98%)	28 (2%)	3 (0%)	47	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	B	59	VAL
1	D	59	VAL

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	321/323 (99%)	317 (99%)	4 (1%)	71	56
1	B	320/323 (99%)	315 (98%)	5 (2%)	62	45
1	C	320/323 (99%)	317 (99%)	3 (1%)	78	67
1	D	319/323 (99%)	313 (98%)	6 (2%)	57	37
All	All	1280/1292 (99%)	1262 (99%)	18 (1%)	67	52

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	77	ARG
1	A	339	GLU
1	A	357	TRP
1	B	77	ARG
1	B	326	GLU
1	B	327	ASP
1	B	339	GLU
1	B	357	TRP
1	C	77	ARG
1	C	339	GLU
1	C	357	TRP
1	D	39	THR
1	D	67	LYS
1	D	77	ARG
1	D	339	GLU
1	D	357	TRP
1	D	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS

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Mol	Chain	Res	Type
1	A	136	HIS
1	A	137	GLN
1	A	195	HIS
1	A	224	GLN
1	A	234	ASN
1	A	262	ASN
1	A	328	GLN
1	A	346	ASN
1	A	369	ASN
1	B	56	ASN
1	B	136	HIS
1	B	137	GLN
1	B	234	ASN
1	B	262	ASN
1	B	369	ASN
1	C	29	HIS
1	C	56	ASN
1	C	103	HIS
1	C	136	HIS
1	C	195	HIS
1	C	234	ASN
1	C	262	ASN
1	C	276	ASN
1	C	293	GLN
1	C	328	GLN
1	C	346	ASN
1	C	369	ASN
1	D	27	HIS
1	D	136	HIS
1	D	137	GLN
1	D	195	HIS
1	D	224	GLN
1	D	234	ASN
1	D	262	ASN
1	D	293	GLN
1	D	328	GLN
1	D	346	ASN
1	D	369	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)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	B	406	-	3,3,3	0.99	0	3,3,3	0.90	0
3	LJ8	A	403	2	21,25,25	0.77	1 (4%)	26,33,33	0.95	1 (3%)
5	ACT	C	404	-	3,3,3	0.60	0	3,3,3	1.35	0
4	GOL	B	405	-	5,5,5	0.46	0	5,5,5	0.62	0
3	LJ8	D	403	2	21,25,25	0.77	1 (4%)	26,33,33	0.94	1 (3%)
4	GOL	B	404	-	5,5,5	0.37	0	5,5,5	0.62	0
3	LJ8	B	403	2	21,25,25	0.77	1 (4%)	26,33,33	0.94	1 (3%)
4	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.39	0
5	ACT	A	405	-	3,3,3	0.57	0	3,3,3	1.27	0
5	ACT	D	404	-	3,3,3	0.71	0	3,3,3	1.42	0
3	LJ8	C	403	2	21,25,25	1.10	1 (4%)	26,33,33	0.55	0
6	BTB	D	405	-	13,13,13	1.25	2 (15%)	7,16,16	1.79	2 (28%)

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	LJ8	A	403	2	-	5/25/25/25	0/1/1/1
4	GOL	B	405	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LJ8	D	403	2	-	7/25/25/25	0/1/1/1
4	GOL	B	404	-	-	2/4/4/4	-
3	LJ8	B	403	2	-	8/25/25/25	0/1/1/1
4	GOL	A	404	-	-	1/4/4/4	-
3	LJ8	C	403	2	-	5/25/25/25	0/1/1/1
6	BTB	D	405	-	-	11/21/21/21	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	LJ8	P13-C16	3.09	1.82	1.79
6	D	405	BTB	C3-C2	-2.89	1.49	1.53
6	D	405	BTB	C7-N	-2.13	1.44	1.48
3	B	403	LJ8	P13-C16	2.11	1.81	1.79
3	A	403	LJ8	P13-C16	2.11	1.81	1.79
3	D	403	LJ8	P13-C16	2.06	1.81	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	405	BTB	C8-C7-N	-3.14	99.31	111.59
6	D	405	BTB	O3-C3-C2	-2.81	103.75	111.44
3	A	403	LJ8	P13-C11-C10	-2.72	109.49	114.56
3	D	403	LJ8	P13-C11-C10	-2.69	109.53	114.56
3	B	403	LJ8	P13-C11-C10	-2.68	109.56	114.56

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	LJ8	C17-C16-P13-O15
3	B	403	LJ8	C17-C16-P13-O15
3	B	403	LJ8	C11-C10-C9-C12
3	C	403	LJ8	C17-C16-P13-O15
3	D	403	LJ8	C17-C16-P13-O15
4	B	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-C3
6	D	405	BTB	C1-C2-C3-O3
6	D	405	BTB	C4-C2-C3-O3
6	D	405	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	D	405	BTB	C1-C2-C4-O4
6	D	405	BTB	C1-C2-N-C7
6	D	405	BTB	C3-C2-N-C7
6	D	405	BTB	C4-C2-N-C7
6	D	405	BTB	N-C5-C6-O6
3	C	403	LJ8	C17-C16-P13-C11
3	B	403	LJ8	C10-C11-P13-O14
3	D	403	LJ8	C17-C16-P13-C11
6	D	405	BTB	N-C7-C8-O8
6	D	405	BTB	O1-C1-C2-C4
3	A	403	LJ8	C11-C10-C9-C12
3	C	403	LJ8	C17-C16-P13-O14
3	D	403	LJ8	C11-C10-C9-C12
3	B	403	LJ8	C11-C10-C9-C8
3	A	403	LJ8	C17-C16-P13-C11
3	A	403	LJ8	C16-C17-C18-O20
3	B	403	LJ8	C16-C17-C18-O20
3	B	403	LJ8	C16-C17-C18-O19
3	C	403	LJ8	C16-C17-C18-O20
3	C	403	LJ8	C16-C17-C18-O19
3	D	403	LJ8	C16-C17-C18-O20
3	D	403	LJ8	C16-C17-C18-O19
3	B	403	LJ8	C17-C16-P13-C11
4	A	404	GOL	C1-C2-C3-O3
3	D	403	LJ8	C10-C11-P13-O14
3	B	403	LJ8	C16-C17-C21-C22
6	D	405	BTB	O1-C1-C2-C3
3	A	403	LJ8	C10-C11-P13-O15
3	D	403	LJ8	C10-C11-P13-O15

There are no ring outliers.

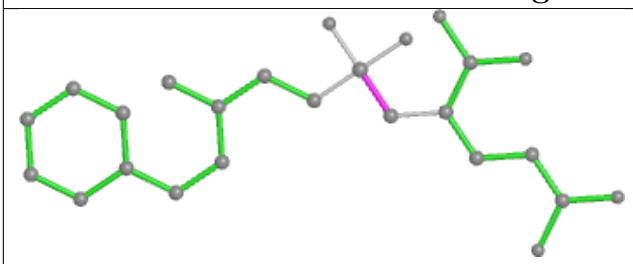
3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	LJ8	1	0
3	B	403	LJ8	1	0
6	D	405	BTB	15	0

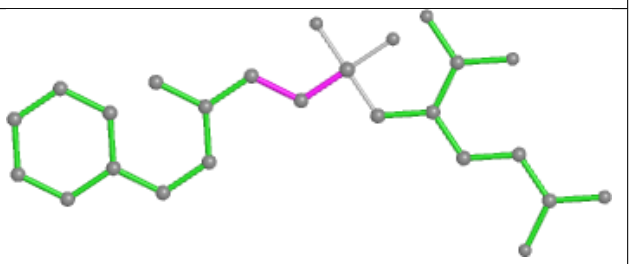
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

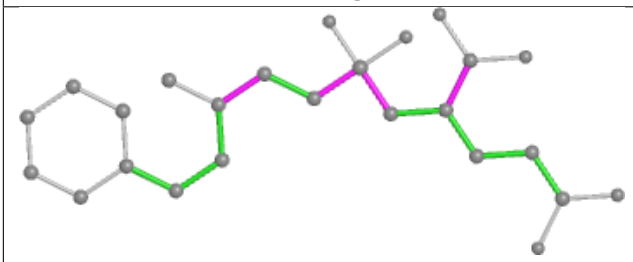
Ligand LJ8 A 403



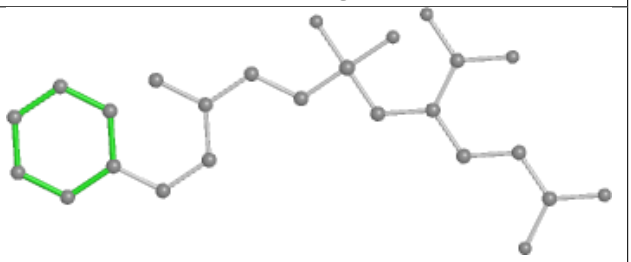
Bond lengths



Bond angles

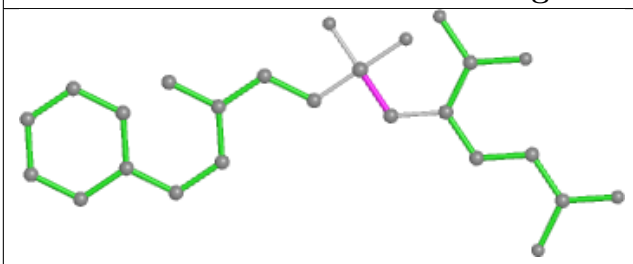


Torsions

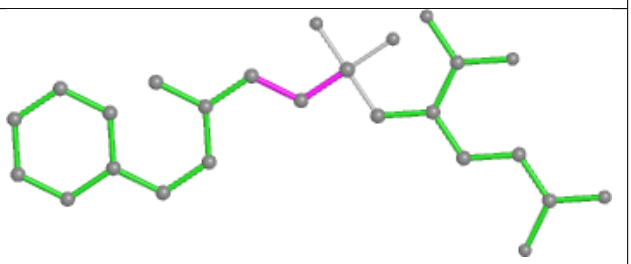


Rings

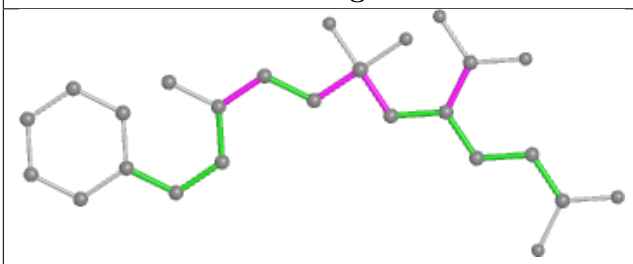
Ligand LJ8 D 403



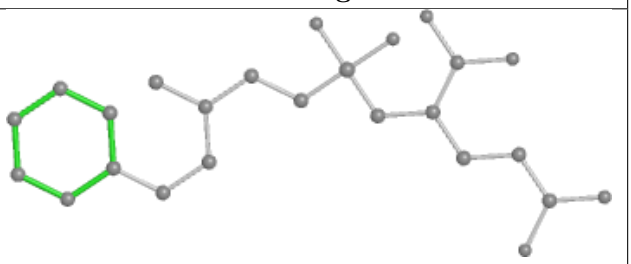
Bond lengths



Bond angles

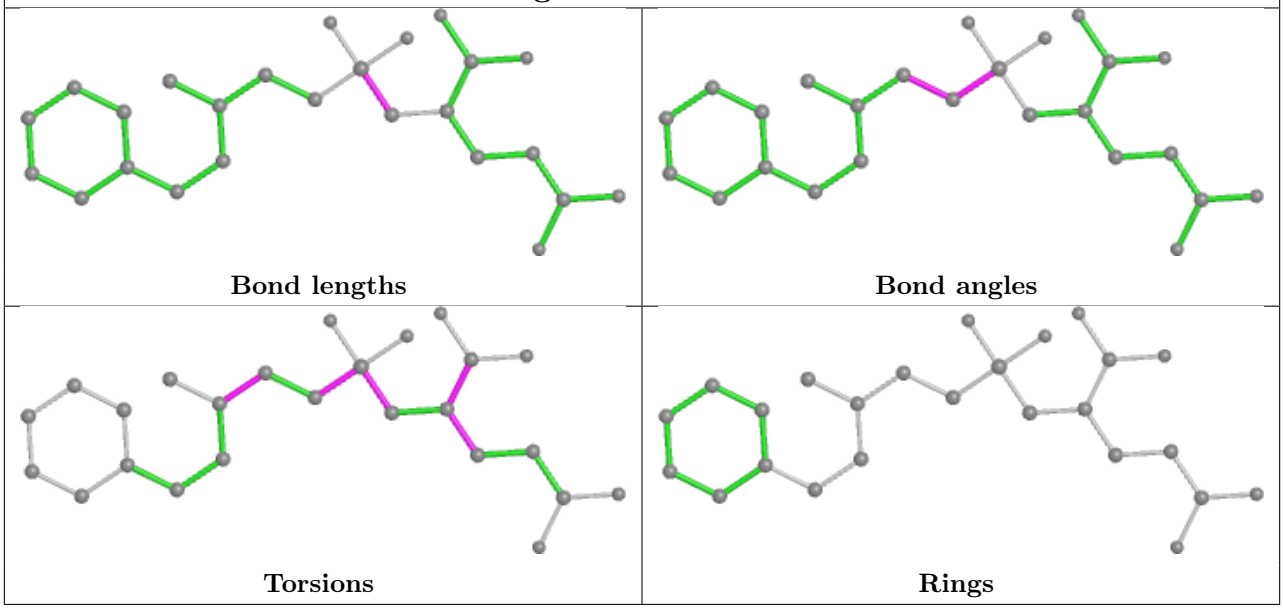


Torsions

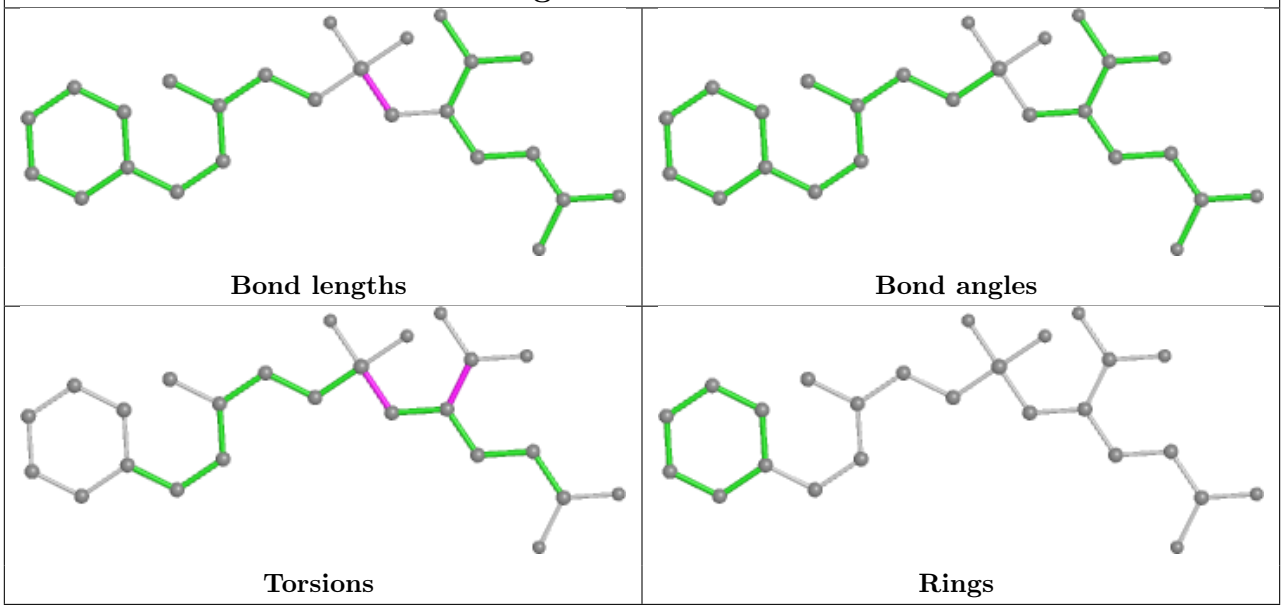


Rings

Ligand LJ8 B 403



Ligand LJ8 C 403



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	398/400 (99%)	-0.06	17 (4%)	35	41	13, 20, 30, 45	0
1	B	396/400 (99%)	0.14	19 (4%)	30	36	13, 24, 37, 46	0
1	C	396/400 (99%)	0.02	15 (3%)	40	47	12, 21, 34, 45	0
1	D	395/400 (98%)	0.70	65 (16%)	1	2	15, 32, 57, 63	0
All	All	1585/1600 (99%)	0.20	116 (7%)	15	20	12, 23, 47, 63	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	LEU	6.0
1	A	1	ALA	5.0
1	D	126	ASP	4.6
1	D	389	ILE	4.6
1	D	127	LEU	4.5
1	D	7	LYS	4.4
1	D	10	ASP	4.3
1	D	156	GLU	4.2
1	D	326	GLU	4.1
1	D	70	GLU	4.0
1	A	114	LEU	3.9
1	B	327	ASP	3.9
1	D	323	PHE	3.9
1	D	92	ASP	3.8
1	A	2	GLN	3.7
1	D	76	PHE	3.7
1	D	78	ALA	3.6
1	B	3	GLU	3.6
1	D	155	ALA	3.6
1	D	169	VAL	3.6
1	B	169	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	3.4
1	D	69	GLY	3.3
1	B	70	GLU	3.3
1	D	166	ALA	3.3
1	A	292	GLU	3.2
1	D	73	SER	3.1
1	C	78	ALA	3.1
1	B	292	GLU	3.1
1	B	326	GLU	3.1
1	D	165	PHE	3.1
1	B	114	LEU	3.1
1	D	67	LYS	3.1
1	D	4	ASN	3.0
1	A	389	ILE	3.0
1	D	98	GLU	3.0
1	D	129	SER	3.0
1	D	318	ALA	3.0
1	D	311	ASP	3.0
1	D	66	ILE	2.9
1	D	131	THR	2.9
1	A	76	PHE	2.8
1	C	169	VAL	2.8
1	C	7	LYS	2.8
1	A	113	ALA	2.8
1	C	166	ALA	2.8
1	D	14	SER	2.7
1	C	357	TRP	2.7
1	C	399	LYS	2.7
1	D	109	LEU	2.7
1	C	114	LEU	2.6
1	D	327	ASP	2.6
1	B	78	ALA	2.6
1	A	169	VAL	2.6
1	C	76	PHE	2.6
1	D	53	GLU	2.6
1	D	357	TRP	2.5
1	B	76	PHE	2.5
1	A	109	LEU	2.5
1	D	47	LEU	2.5
1	D	292	GLU	2.5
1	B	92	ASP	2.5
1	A	166	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	14	SER	2.5
1	D	314	GLU	2.5
1	D	113	ALA	2.4
1	D	111	THR	2.4
1	C	109	LEU	2.4
1	D	397	LEU	2.4
1	D	322	GLU	2.4
1	B	166	ALA	2.4
1	A	78	ALA	2.4
1	D	160	ALA	2.4
1	A	98	GLU	2.4
1	C	126	ASP	2.4
1	D	110	HIS	2.4
1	D	354	MET	2.4
1	D	398	MET	2.4
1	D	121	LEU	2.4
1	C	355	TRP	2.4
1	D	355	TRP	2.4
1	D	59	VAL	2.3
1	D	395	PRO	2.3
1	B	355	TRP	2.3
1	D	167	GLN	2.3
1	D	163	VAL	2.3
1	B	156	GLU	2.3
1	D	151	ASP	2.3
1	B	357	TRP	2.3
1	D	71	GLY	2.2
1	D	55	GLN	2.2
1	C	98	GLU	2.2
1	D	135	VAL	2.2
1	D	68	ASN	2.2
1	C	389	ILE	2.2
1	C	310	GLU	2.2
1	D	97	PRO	2.2
1	D	310	GLU	2.2
1	B	7	LYS	2.2
1	D	128	TRP	2.2
1	B	105	CYS	2.2
1	A	199	GLU	2.1
1	D	122	VAL	2.1
1	B	98	GLU	2.1
1	D	54	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	385	GLY	2.1
1	D	118	VAL	2.1
1	A	111	THR	2.1
1	B	113	ALA	2.1
1	D	5	LEU	2.1
1	B	389	ILE	2.1
1	A	357	TRP	2.0
1	D	221	THR	2.0
1	A	99	LEU	2.0
1	D	12	LEU	2.0
1	D	72	PRO	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
4	GOL	B	404	6/6	0.69	0.17	32,34,36,36	0
4	GOL	B	405	6/6	0.79	0.14	46,48,50,51	0
6	BTB	D	405	14/14	0.80	0.25	37,41,43,43	0
4	GOL	A	404	6/6	0.86	0.18	46,49,49,50	0
5	ACT	B	406	4/4	0.89	0.12	27,29,29,29	0
3	LJ8	D	403	25/25	0.94	0.12	23,27,29,30	0
3	LJ8	A	403	25/25	0.94	0.13	14,19,23,24	0
5	ACT	A	405	4/4	0.95	0.07	28,28,29,30	0
3	LJ8	C	403	25/25	0.96	0.11	15,19,21,23	0
5	ACT	C	404	4/4	0.96	0.11	26,28,28,28	0
5	ACT	D	404	4/4	0.96	0.14	42,43,43,43	0
3	LJ8	B	403	25/25	0.96	0.11	16,20,23,24	0

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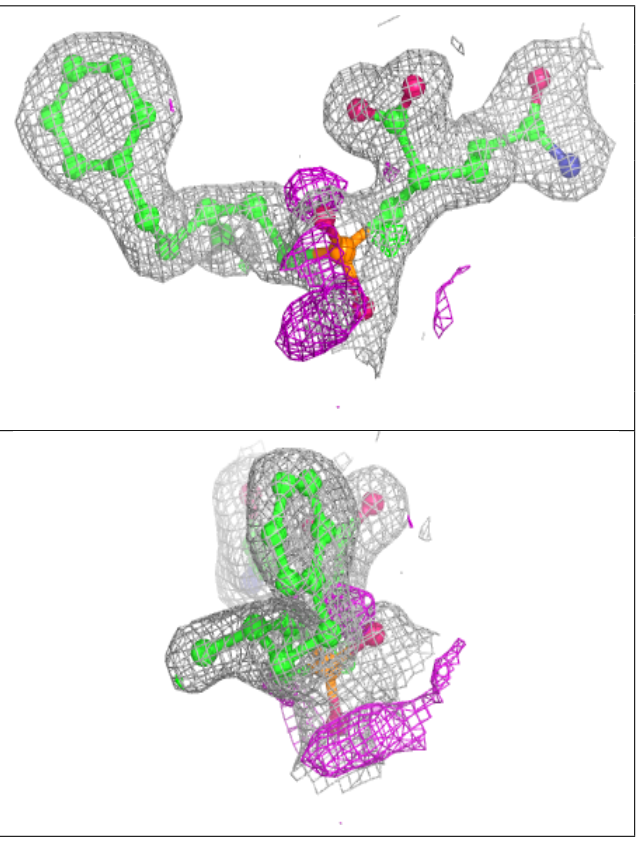
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	402	1/1	0.98	0.03	29,29,29,29	0
2	ZN	A	402	1/1	0.99	0.02	24,24,24,24	0
2	ZN	C	402	1/1	0.99	0.03	28,28,28,28	0
2	ZN	D	401	1/1	0.99	0.02	30,30,30,30	0
2	ZN	D	402	1/1	0.99	0.03	39,39,39,39	0
2	ZN	B	401	1/1	1.00	0.03	25,25,25,25	0
2	ZN	A	401	1/1	1.00	0.03	27,27,27,27	0
2	ZN	C	401	1/1	1.00	0.03	22,22,22,22	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.

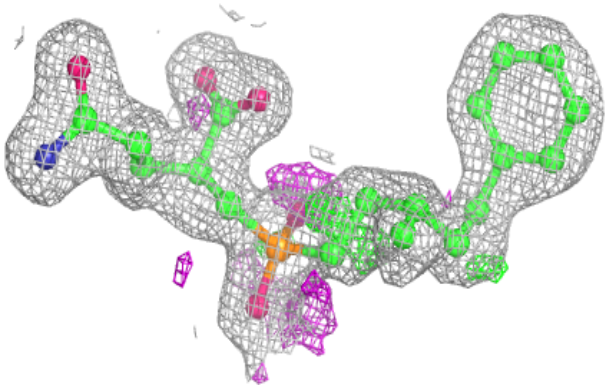
Electron density around LJ8 D 403:

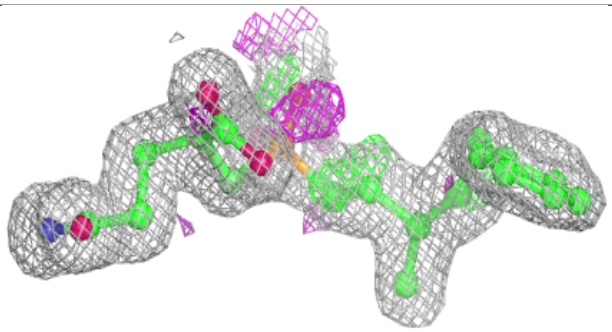
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

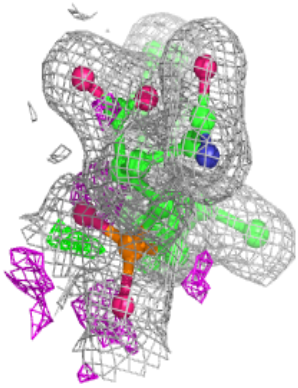


Electron density around LJ8 A 403:

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

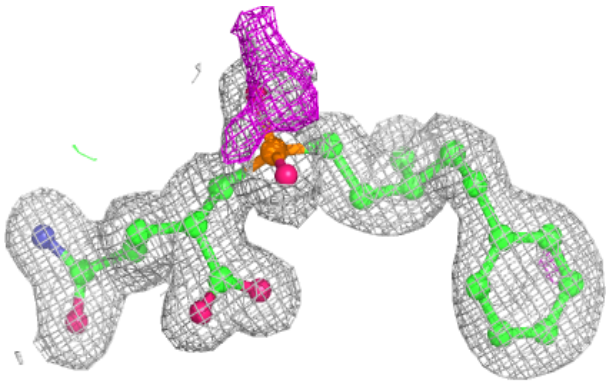


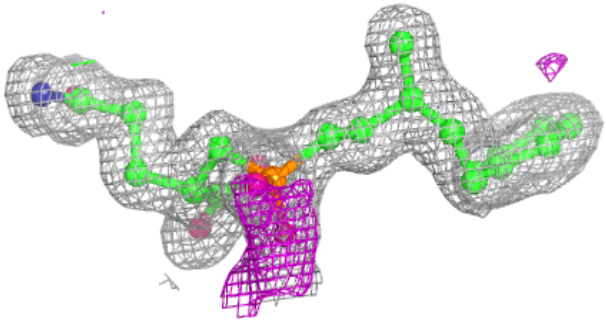


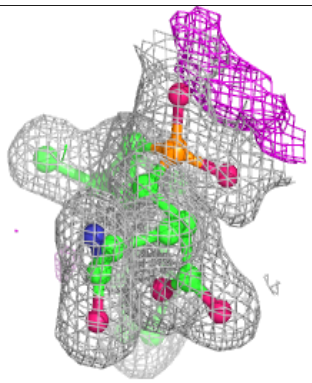


Electron density around LJ8 C 403:

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

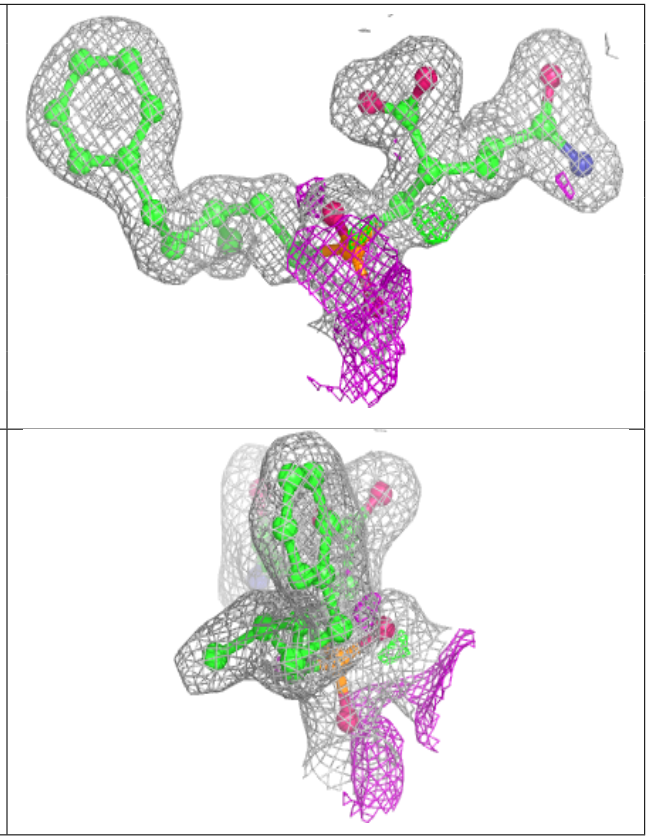






Electron density around LJ8 B 403:

$2mF_o$-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.