



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2021 – 04:21 PM JST

PDB ID : 7F3O
Title : Crystal structure of the GluA2o LBD in complex with glutamate and TAK-653
Authors : Sogabe, S.; Igaki, S.; Hirokawa, A.; Zama, Y.; Lane, W.; Snell, G.
Deposited on : 2021-06-16
Resolution : 1.44 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

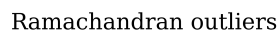
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
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) : 2.22

i

X-RAY DIFFRACTION

A.



R_{free}
Clashscore
Ramachandran outliers
Sidechain outliers
BSRZ outliers

The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Order	Channel	Duration	Quality of Channel
1	A	263	<div> <div></div> <div>3%</div> <div>90%</div> <div>8%</div> <div></div> </div>
1	B	263	<div> <div></div> <div>%</div> <div>92%</div> <div>8%</div> <div></div> </div>
1	C	263	<div> <div></div> <div></div> <div>93%</div> <div>6%</div> <div></div> </div>
1	D	263	<div> <div></div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div>
1	E	263	<div> <div></div> <div>%</div> <div>93%</div> <div>7%</div> <div></div> </div>
1	F	263	<div> <div></div> <div>2%</div> <div>94%</div> <div>5%</div> <div></div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13970 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	5	0
			2075	1326	344	389	16			
1	B	261	Total	C	N	O	S	0	1	0
			2048	1303	343	387	15			
1	C	262	Total	C	N	O	S	0	8	0
			2089	1333	346	394	16			
1	D	262	Total	C	N	O	S	0	9	0
			2097	1338	349	394	16			
1	E	262	Total	C	N	O	S	0	4	0
			2070	1322	344	389	15			
1	F	261	Total	C	N	O	S	0	2	0
			2054	1307	343	389	15			

There are 24 discrepancies between the modelled and reference sequences:

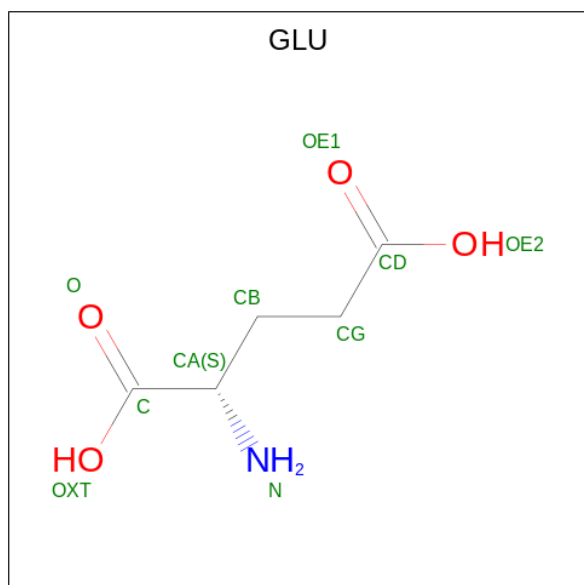
Chain	Residue	Modelled	Actual	Comment	Reference
A	411	GLY	-	expression tag	UNP P42262
A	412	SER	-	expression tag	UNP P42262
A	641	GLY	-	linker	UNP P42262
A	642	THR	-	linker	UNP P42262
B	411	GLY	-	expression tag	UNP P42262
B	412	SER	-	expression tag	UNP P42262
B	641	GLY	-	linker	UNP P42262
B	642	THR	-	linker	UNP P42262
C	411	GLY	-	expression tag	UNP P42262
C	412	SER	-	expression tag	UNP P42262
C	641	GLY	-	linker	UNP P42262
C	642	THR	-	linker	UNP P42262
D	411	GLY	-	expression tag	UNP P42262
D	412	SER	-	expression tag	UNP P42262
D	641	GLY	-	linker	UNP P42262
D	642	THR	-	linker	UNP P42262
E	411	GLY	-	expression tag	UNP P42262

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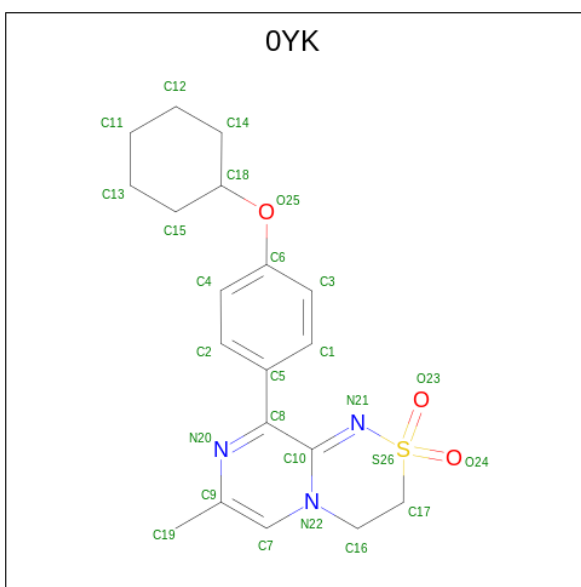
Chain	Residue	Modelled	Actual	Comment	Reference
E	412	SER	-	expression tag	UNP P42262
E	641	GLY	-	linker	UNP P42262
E	642	THR	-	linker	UNP P42262
F	411	GLY	-	expression tag	UNP P42262
F	412	SER	-	expression tag	UNP P42262
F	641	GLY	-	linker	UNP P42262
F	642	THR	-	linker	UNP P42262

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is 7-(4-cyclohexyloxyphenyl)-9-methyl-4 λ^6 -thia-1 λ^4 ,5,8-triazabicyclo[4.4.0]deca-1(10),6,8-triene 4,4-dioxide (three-letter code: 0YK) (formula: C₁₉H₂₃N₃O₃S) (labeled as "Ligand of Interest" by depositor).

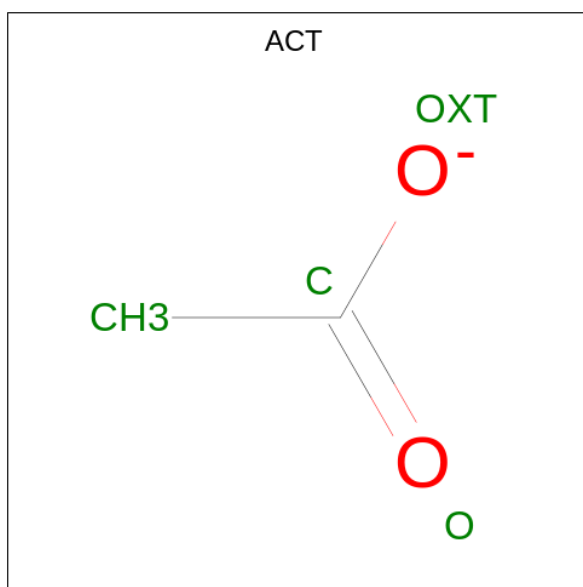


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
3	C	1	Total	C	N	O	S	0	1
			52	38	6	6	2		
3	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

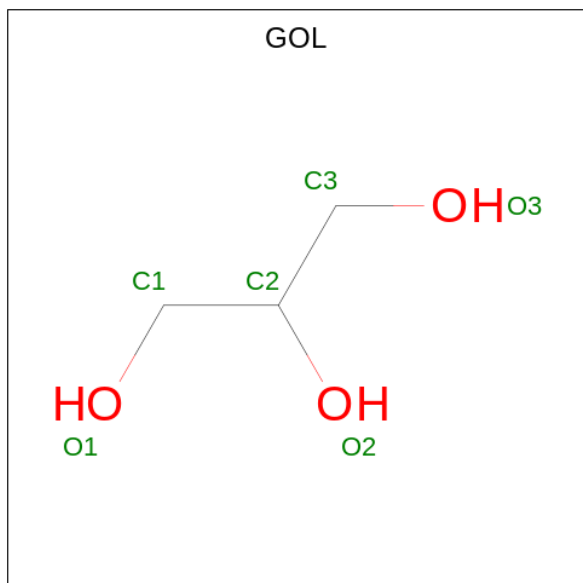
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	2	Total	Zn	0	0
			2	2		
4	D	3	Total	Zn	0	0
			3	3		
4	E	1	Total	Zn	0	0
			1	1		
4	F	3	Total	Zn	0	0
			3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

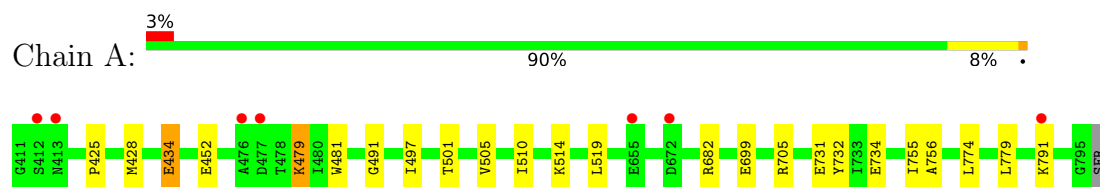
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	191	Total	O	0	0
			191	191		
7	B	178	Total	O	0	0
			178	178		
7	C	303	Total	O	0	0
			303	303		
7	D	291	Total	O	0	0
			291	291		
7	E	193	Total	O	0	0
			193	193		
7	F	179	Total	O	0	0
			179	179		

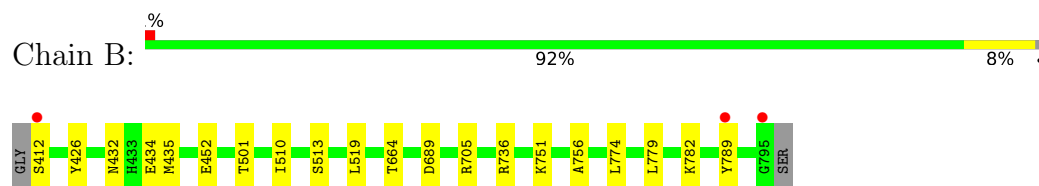
3 Residue-property plots [i](#)

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.

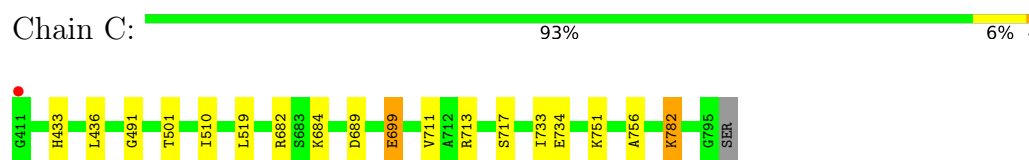
- Molecule 1: Glutamate receptor 2



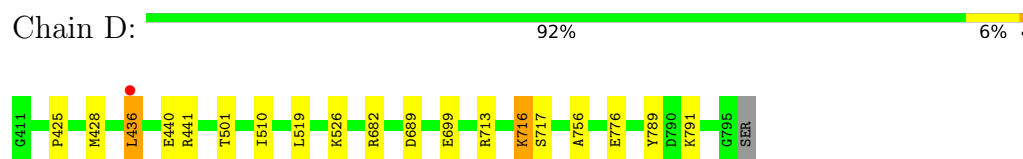
- Molecule 1: Glutamate receptor 2



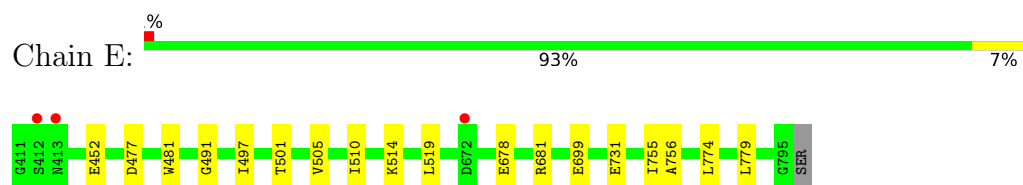
- Molecule 1: Glutamate receptor 2



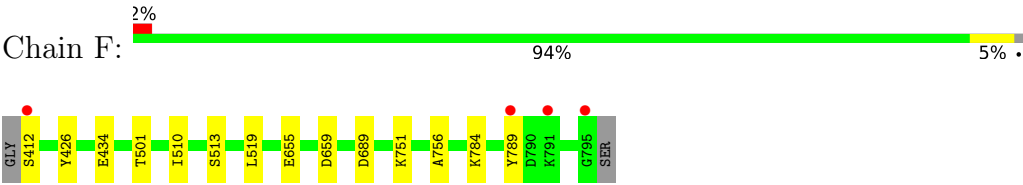
- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.31Å 163.51Å 47.56Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	40.00 – 1.44 42.41 – 1.44	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-1.44) 97.0 (42.41-1.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.214 0.194 , 0.213	Depositor DCC
R_{free} test set	15337 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13970	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 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0YK, ACT, GOL, ZN

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	0.61	3/2127 (0.1%)	0.86	3/2859 (0.1%)
1	B	0.48	0/2087	0.81	3/2805 (0.1%)
1	C	0.67	2/2150 (0.1%)	0.95	0/2888
1	D	0.69	2/2161 (0.1%)	0.95	3/2902 (0.1%)
1	E	0.58	2/2119 (0.1%)	0.86	1/2849 (0.0%)
1	F	0.49	0/2096	0.81	2/2817 (0.1%)
All	All	0.59	9/12740 (0.1%)	0.88	12/17120 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	699	GLU	CD-OE2	12.48	1.39	1.25
1	C	699	GLU	CD-OE2	9.89	1.36	1.25
1	E	731	GLU	CD-OE1	8.46	1.34	1.25
1	A	699	GLU	CD-OE2	7.64	1.34	1.25
1	A	699	GLU	CB-CG	7.58	1.66	1.52
1	A	731	GLU	CD-OE2	7.20	1.33	1.25
1	D	776	GLU	CD-OE2	-5.91	1.19	1.25
1	C	734	GLU	CD-OE2	-5.48	1.19	1.25
1	E	699	GLU	CD-OE1	-5.17	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	GLU	OE1-CD-OE2	-11.80	109.13	123.30
1	E	699	GLU	OE1-CD-OE2	-11.56	109.43	123.30
1	D	789	TYR	CB-CA-C	11.31	133.03	110.40
1	B	705	ARG	CG-CD-NE	-6.95	97.20	111.80
1	F	789	TYR	CB-CA-C	6.26	122.92	110.40
1	F	426	TYR	CB-CG-CD1	-5.85	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	789	TYR	CB-CA-C	5.69	121.78	110.40
1	D	699	GLU	CG-CD-OE2	5.66	129.61	118.30
1	A	734	GLU	CB-CG-CD	-5.52	99.30	114.20
1	B	426	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	D	441	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	732	TYR	CB-CG-CD2	-5.03	117.98	121.00

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	2075	0	2124	12	0
1	B	2048	0	2083	13	0
1	C	2089	0	2139	10	0
1	D	2097	0	2152	11	0
1	E	2070	0	2115	9	0
1	F	2054	0	2089	8	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	10	0	5	1	0
2	D	10	0	5	1	0
2	E	10	0	5	1	0
2	F	10	0	5	1	0
3	A	26	0	0	1	0
3	C	52	0	0	4	0
3	E	26	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	1	0
4	D	3	0	0	0	0
4	E	1	0	0	0	0
4	F	3	0	0	0	0
5	C	4	0	3	0	0
5	D	8	0	6	0	0
5	F	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	191	0	0	3	0
7	B	178	0	0	3	0
7	C	303	0	0	6	0
7	D	291	0	0	6	0
7	E	193	0	0	1	0
7	F	179	0	0	3	0
All	All	13970	0	12760	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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)
3:C:806[A]:0YK:O24	7:C:902:HOH:O	1.54	1.26
1:E:678:GLU:OE1	1:E:681:ARG:NH2	1.76	1.18
1:B:774:LEU:HD22	1:B:779:LEU:HD23	1.41	1.01
1:B:434:GLU:HG2	7:B:1007:HOH:O	1.69	0.92
1:B:432:ASN:HB2	1:B:435:MET:HE2	1.52	0.90
3:C:806[A]:0YK:C16	7:D:1042:HOH:O	2.26	0.84
1:B:689:ASP:OD1	7:B:901:HOH:O	1.95	0.83
1:F:655:GLU:HG2	1:F:659:ASP:OD1	1.77	0.83
1:A:434:GLU:HG3	7:A:925:HOH:O	1.83	0.79
3:C:806[B]:0YK:C16	7:C:1062:HOH:O	2.30	0.78
1:D:716:LYS:HG2	7:D:1015:HOH:O	1.85	0.75
1:D:682[B]:ARG:HD3	7:D:905:HOH:O	1.93	0.68
1:C:699:GLU:OE2	4:C:801:ZN:ZN	1.41	0.68
1:A:774:LEU:HD22	1:A:779:LEU:HD23	1.75	0.67
1:D:436:LEU:HD22	1:D:440:GLU:OE1	1.97	0.64
1:F:689:ASP:OD2	7:F:901:HOH:O	2.13	0.64
1:A:497:ILE:HG12	1:A:755[B]:ILE:HD12	1.82	0.61
1:C:689:ASP:OD2	7:C:903:HOH:O	2.16	0.60
1:E:774:LEU:HD22	1:E:779:LEU:HD23	1.83	0.60
1:E:497:ILE:HG12	1:E:755[B]:ILE:HD12	1.83	0.59
1:A:425:PRO:HA	1:A:428[B]:MET:SD	2.43	0.58
1:B:452:GLU:HG3	1:B:779:LEU:HD21	1.85	0.58
1:F:784:LYS:NZ	7:F:902:HOH:O	2.38	0.57
1:D:689:ASP:OD1	7:D:901:HOH:O	2.19	0.53
3:C:806[B]:0YK:C17	7:C:1044:HOH:O	0.83	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:THR:HG1	2:A:801:GLU:N	2.08	0.52
1:C:510:ILE:HD12	1:C:756:ALA:HB1	1.92	0.52
1:E:452:GLU:HG3	1:E:779:LEU:HD21	1.92	0.52
1:D:716:LYS:CG	7:D:1015:HOH:O	2.53	0.50
1:C:433:HIS:CD2	1:C:436:LEU:HD22	2.47	0.49
1:C:711:VAL:HG21	1:C:733:ILE:HD13	1.93	0.49
1:D:510:ILE:HD12	1:D:756:ALA:HB1	1.94	0.49
1:E:501:THR:HG1	2:E:801:GLU:N	2.11	0.49
1:A:452:GLU:HG3	1:A:779:LEU:HD21	1.95	0.49
1:D:436:LEU:CD2	1:D:440:GLU:OE1	2.60	0.49
1:A:510:ILE:HD12	1:A:756:ALA:HB1	1.96	0.48
1:B:501:THR:HG1	2:B:801:GLU:N	2.11	0.48
1:F:434:GLU:HG2	5:F:805:ACT:O	2.14	0.48
1:C:713:ARG:O	1:C:717:SER:HB3	2.14	0.48
1:E:481:TRP:HH2	1:E:505[B]:VAL:HG12	1.79	0.47
1:D:501:THR:HG1	2:D:801:GLU:N	2.13	0.47
1:B:432:ASN:CB	1:B:435:MET:HE2	2.33	0.46
1:D:713:ARG:O	1:D:717:SER:HB3	2.15	0.46
1:E:510:ILE:HD12	1:E:756:ALA:HB1	1.97	0.46
1:F:501:THR:HG1	2:F:801:GLU:N	2.13	0.46
1:A:491:GLY:HA2	7:A:940:HOH:O	2.15	0.45
1:A:481:TRP:HH2	1:A:505[B]:VAL:HG12	1.82	0.45
1:E:514:LYS:HE3	1:F:513:SER:O	2.17	0.45
1:C:501:THR:HG1	2:C:802:GLU:N	2.16	0.44
1:F:751:LYS:HB2	7:F:1038:HOH:O	2.17	0.44
1:F:510:ILE:HD12	1:F:756:ALA:HB1	1.99	0.44
1:E:491:GLY:HA2	7:E:935:HOH:O	2.18	0.44
1:C:782:LYS:HB2	1:C:782:LYS:HE2	1.34	0.43
1:B:432:ASN:HD22	1:B:435:MET:CE	2.31	0.43
1:B:751:LYS:HB2	7:B:1039:HOH:O	2.18	0.43
1:A:514:LYS:HE3	1:B:513:SER:O	2.19	0.42
1:B:782:LYS:HE3	1:B:782:LYS:HB2	1.78	0.42
1:D:425:PRO:HA	1:D:428[B]:MET:SD	2.60	0.42
1:B:774:LEU:HD22	1:B:779:LEU:CD2	2.30	0.42
1:A:479:LYS:HD2	1:A:479:LYS:N	2.35	0.41
1:B:510:ILE:HD12	1:B:756:ALA:HB1	2.01	0.41
1:A:682:ARG:NH2	7:A:907:HOH:O	2.53	0.41
1:C:751:LYS:HB2	7:C:902:HOH:O	2.20	0.41
1:D:717:SER:HB3	7:D:982:HOH:O	2.21	0.41
1:C:491:GLY:HA2	7:C:966:HOH:O	2.21	0.41
3:A:802:OYK:C1	3:A:802:OYK:N21	2.83	0.41

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	265/263 (101%)	262 (99%)	3 (1%)	0	100	100
1	B	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
1	C	268/263 (102%)	266 (99%)	2 (1%)	0	100	100
1	D	269/263 (102%)	266 (99%)	3 (1%)	0	100	100
1	E	264/263 (100%)	262 (99%)	2 (1%)	0	100	100
1	F	261/263 (99%)	259 (99%)	2 (1%)	0	100	100
All	All	1587/1578 (101%)	1573 (99%)	14 (1%)	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	225/221 (102%)	220 (98%)	5 (2%)	52	17
1	B	221/221 (100%)	217 (98%)	4 (2%)	59	25
1	C	228/221 (103%)	224 (98%)	4 (2%)	59	25
1	D	229/221 (104%)	223 (97%)	6 (3%)	46	12
1	E	224/221 (101%)	222 (99%)	2 (1%)	78	54
1	F	222/221 (100%)	220 (99%)	2 (1%)	78	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1349/1326 (102%)	1326 (98%)	23 (2%)	60 28

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	A	479	LYS
1	A	519	LEU
1	A	705	ARG
1	A	791	LYS
1	B	412	SER
1	B	519	LEU
1	B	664	THR
1	B	736	ARG
1	C	519	LEU
1	C	682	ARG
1	C	684	LYS
1	C	782	LYS
1	D	436	LEU
1	D	519	LEU
1	D	526[A]	LYS
1	D	526[B]	LYS
1	D	716	LYS
1	D	791	LYS
1	E	477	ASP
1	E	519	LEU
1	F	412	SER
1	F	519	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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$
3	0YK	C	806[A]	-	27,29,29	1.70	5 (18%)	36,42,42	2.62	11 (30%)
2	GLU	C	802	-	2,9,9	1.67	1 (50%)	2,11,11	1.00	0
5	ACT	C	804	-	1,3,3	4.72	1 (100%)	0,3,3	0.00	-
5	ACT	F	805	4	1,3,3	4.93	1 (100%)	0,3,3	0.00	-
2	GLU	E	801	-	2,9,9	0.18	0	2,11,11	0.69	0
5	ACT	D	804	-	1,3,3	4.32	1 (100%)	0,3,3	0.00	-
6	GOL	D	806	-	5,5,5	0.10	0	5,5,5	0.23	0
3	0YK	C	806[B]	-	27,29,29	1.64	4 (14%)	36,42,42	2.45	10 (27%)
2	GLU	F	801	-	2,9,9	1.72	1 (50%)	2,11,11	1.25	0
2	GLU	A	801	-	2,9,9	0.46	0	2,11,11	0.77	0
5	ACT	D	805	4	1,3,3	4.57	1 (100%)	0,3,3	0.00	-
6	GOL	C	805	-	5,5,5	0.12	0	5,5,5	0.29	0
2	GLU	B	801	-	2,9,9	1.44	1 (50%)	2,11,11	1.12	0
3	0YK	E	803	-	27,29,29	1.72	6 (22%)	36,42,42	2.50	9 (25%)
2	GLU	D	801	-	2,9,9	1.40	0	2,11,11	1.41	0
3	0YK	A	802	-	27,29,29	1.82	8 (29%)	36,42,42	2.64	12 (33%)

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	0YK	C	806[A]	-	-	0/8/27/27	0/3/4/4
2	GLU	C	802	-	-	0/3/9/9	-
2	GLU	E	801	-	-	0/3/9/9	-
6	GOL	D	806	-	-	1/4/4/4	-
3	0YK	C	806[B]	-	-	0/8/27/27	0/3/4/4
2	GLU	F	801	-	-	0/3/9/9	-
2	GLU	A	801	-	-	0/3/9/9	-
6	GOL	C	805	-	-	1/4/4/4	-
2	GLU	B	801	-	-	0/3/9/9	-
3	0YK	E	803	-	-	0/8/27/27	0/3/4/4
2	GLU	D	801	-	-	0/3/9/9	-
3	0YK	A	802	-	-	0/8/27/27	0/3/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	805	ACT	CH3-C	4.93	1.55	1.48
3	C	806[A]	0YK	C7-C9	-4.92	1.33	1.39
3	C	806[A]	0YK	C10-C8	4.89	1.50	1.40
3	C	806[B]	0YK	C7-C9	-4.83	1.33	1.39
3	C	806[B]	0YK	C10-C8	4.78	1.50	1.40
5	C	804	ACT	CH3-C	4.72	1.54	1.48
5	D	805	ACT	CH3-C	4.57	1.54	1.48
3	A	802	0YK	C7-C9	-4.50	1.33	1.39
3	E	803	0YK	C7-C9	-4.34	1.33	1.39
5	D	804	ACT	CH3-C	4.32	1.54	1.48
3	E	803	0YK	C10-C8	4.09	1.49	1.40
3	E	803	0YK	C17-S26	4.06	1.81	1.76
3	A	802	0YK	C17-S26	3.77	1.81	1.76
3	A	802	0YK	C10-C8	3.76	1.48	1.40
3	C	806[A]	0YK	C16-N22	-3.05	1.44	1.48
3	A	802	0YK	C5-C8	-2.86	1.45	1.49
3	C	806[B]	0YK	C16-N22	-2.78	1.44	1.48
3	A	802	0YK	O24-S26	2.70	1.47	1.43
3	A	802	0YK	O25-C6	2.64	1.43	1.38
3	A	802	0YK	C16-N22	-2.54	1.45	1.48
2	F	801	GLU	CA-N	2.42	1.52	1.47
2	C	802	GLU	CA-N	2.36	1.52	1.47
3	C	806[A]	0YK	C8-N20	-2.36	1.30	1.34
3	A	802	0YK	C8-N20	-2.33	1.30	1.34
3	C	806[A]	0YK	O24-S26	2.31	1.46	1.43
3	C	806[B]	0YK	C8-N20	-2.27	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	803	OYK	O25-C6	2.23	1.42	1.38
3	E	803	OYK	C16-N22	-2.07	1.45	1.48
3	E	803	OYK	O24-S26	2.06	1.46	1.43
2	B	801	GLU	CA-N	2.03	1.51	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	OYK	C8-C10-N22	-6.77	115.32	120.44
3	A	802	OYK	C10-C8-C5	-6.70	114.93	123.18
3	C	806[A]	OYK	C10-C8-C5	-6.59	115.07	123.18
3	E	803	OYK	C10-C8-C5	-6.47	115.21	123.18
3	C	806[B]	OYK	C10-C8-C5	-6.45	115.24	123.18
3	C	806[B]	OYK	C8-C10-N22	-6.14	115.80	120.44
3	E	803	OYK	C8-C10-N22	-6.09	115.84	120.44
3	C	806[A]	OYK	C8-C10-N22	-6.00	115.90	120.44
3	C	806[A]	OYK	C5-C8-N20	5.80	122.78	115.09
3	E	803	OYK	C5-C8-N20	5.57	122.49	115.09
3	C	806[B]	OYK	C5-C8-N20	5.57	122.48	115.09
3	E	803	OYK	C2-C5-C8	-5.36	112.11	120.61
3	C	806[A]	OYK	O23-S26-C17	-5.34	102.51	109.50
3	A	802	OYK	C5-C8-N20	5.24	122.05	115.09
3	A	802	OYK	C2-C5-C8	-5.20	112.37	120.61
3	C	806[B]	OYK	C2-C5-C8	-4.79	113.01	120.61
3	C	806[A]	OYK	C2-C5-C8	-4.70	113.16	120.61
3	A	802	OYK	O24-S26-C17	4.68	115.63	109.50
3	E	803	OYK	O24-S26-C17	4.65	115.58	109.50
3	C	806[A]	OYK	C1-C5-C8	4.30	127.43	120.61
3	C	806[B]	OYK	O23-S26-C17	-4.27	103.91	109.50
3	C	806[B]	OYK	C1-C5-C8	4.22	127.30	120.61
3	C	806[A]	OYK	O24-S26-N21	4.21	115.06	108.93
3	E	803	OYK	C1-C5-C8	4.05	127.02	120.61
3	A	802	OYK	C1-C5-C8	3.74	126.54	120.61
3	A	802	OYK	O23-S26-C17	-3.63	104.74	109.50
3	A	802	OYK	O24-S26-O23	-3.41	113.53	118.28
3	E	803	OYK	C16-C17-S26	-3.15	107.78	113.13
3	C	806[A]	OYK	C7-C9-N20	3.03	123.05	120.94
3	C	806[B]	OYK	O24-S26-N21	2.98	113.26	108.93
3	C	806[A]	OYK	C16-N22-C10	2.92	122.31	118.06
3	C	806[B]	OYK	C7-C9-N20	2.85	122.92	120.94
3	A	802	OYK	C16-C17-S26	-2.66	108.62	113.13
3	A	802	OYK	O25-C18-C14	-2.61	102.53	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	803	0YK	O24-S26-O23	-2.53	114.75	118.28
3	C	806[B]	0YK	O23-S26-N21	2.37	112.37	108.93
3	C	806[A]	0YK	O23-S26-N21	2.35	112.35	108.93
3	C	806[B]	0YK	C16-N22-C10	2.26	121.36	118.06
3	A	802	0YK	C17-C16-N22	2.24	112.40	109.52
3	E	803	0YK	O23-S26-C17	-2.20	106.62	109.50
3	C	806[A]	0YK	O24-S26-O23	-2.12	115.32	118.28
3	A	802	0YK	C7-C9-N20	2.12	122.42	120.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	805	GOL	O1-C1-C2-C3
6	D	806	GOL	O1-C1-C2-C3

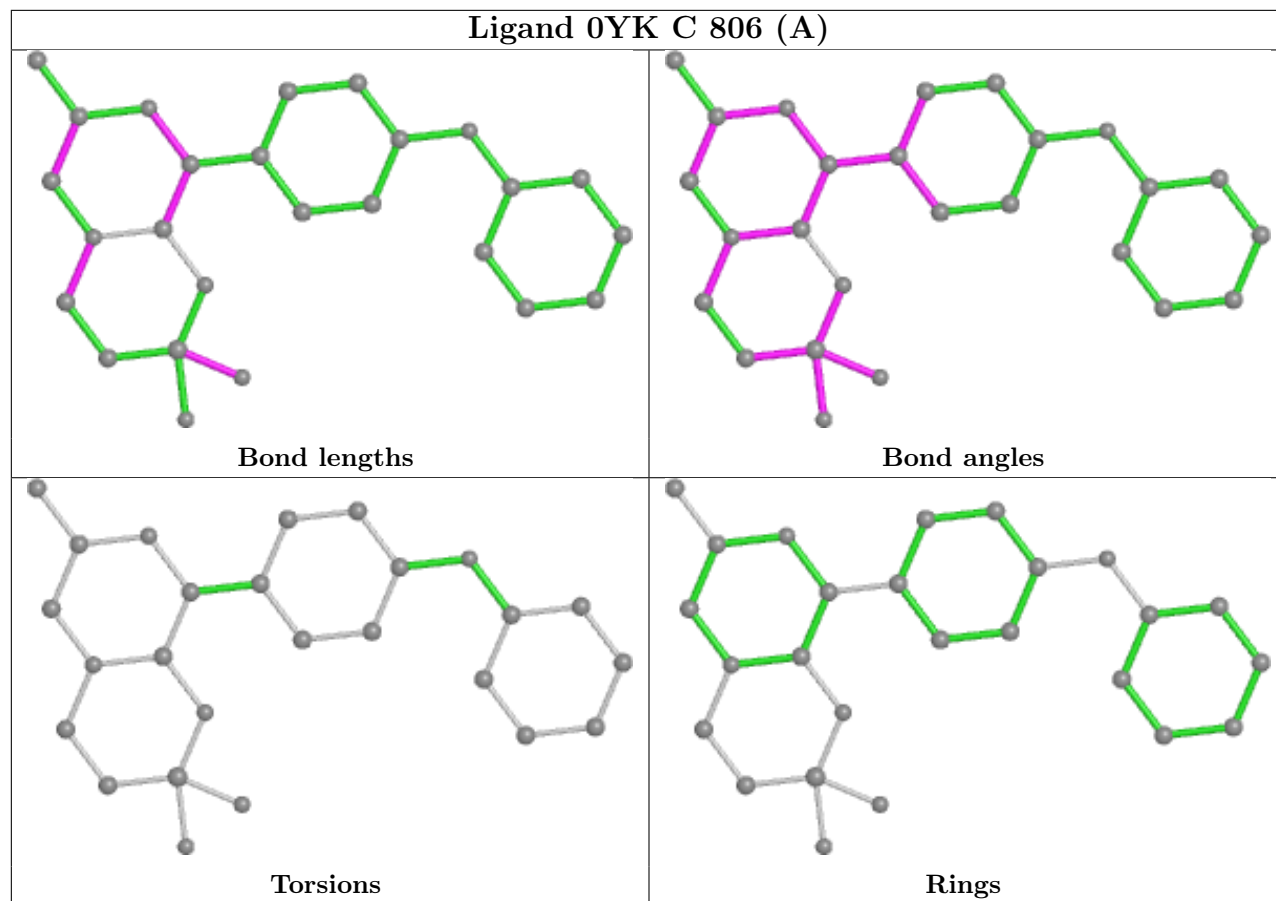
There are no ring outliers.

10 monomers are involved in 12 short contacts:

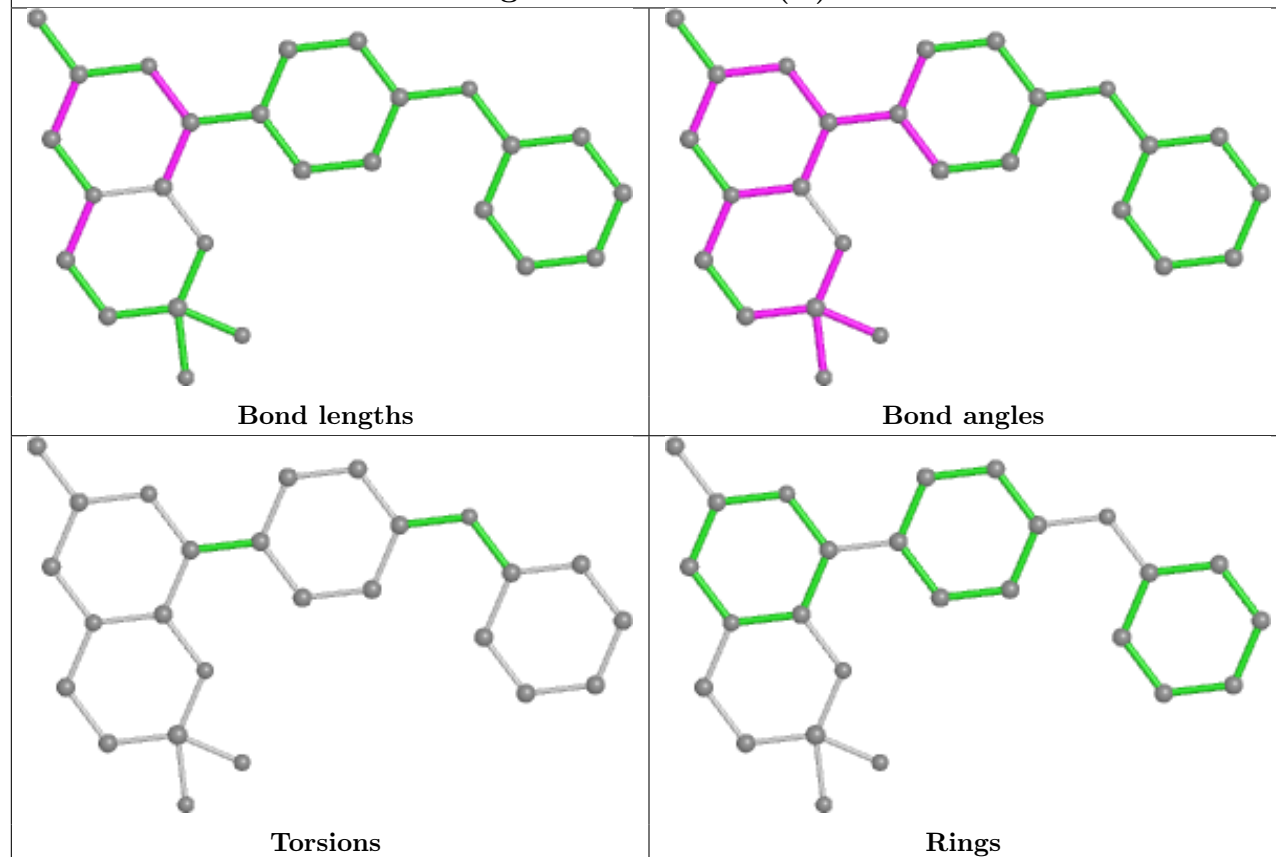
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	806[A]	0YK	2	0
2	C	802	GLU	1	0
5	F	805	ACT	1	0
2	E	801	GLU	1	0
3	C	806[B]	0YK	2	0
2	F	801	GLU	1	0
2	A	801	GLU	1	0
2	B	801	GLU	1	0
2	D	801	GLU	1	0
3	A	802	0YK	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

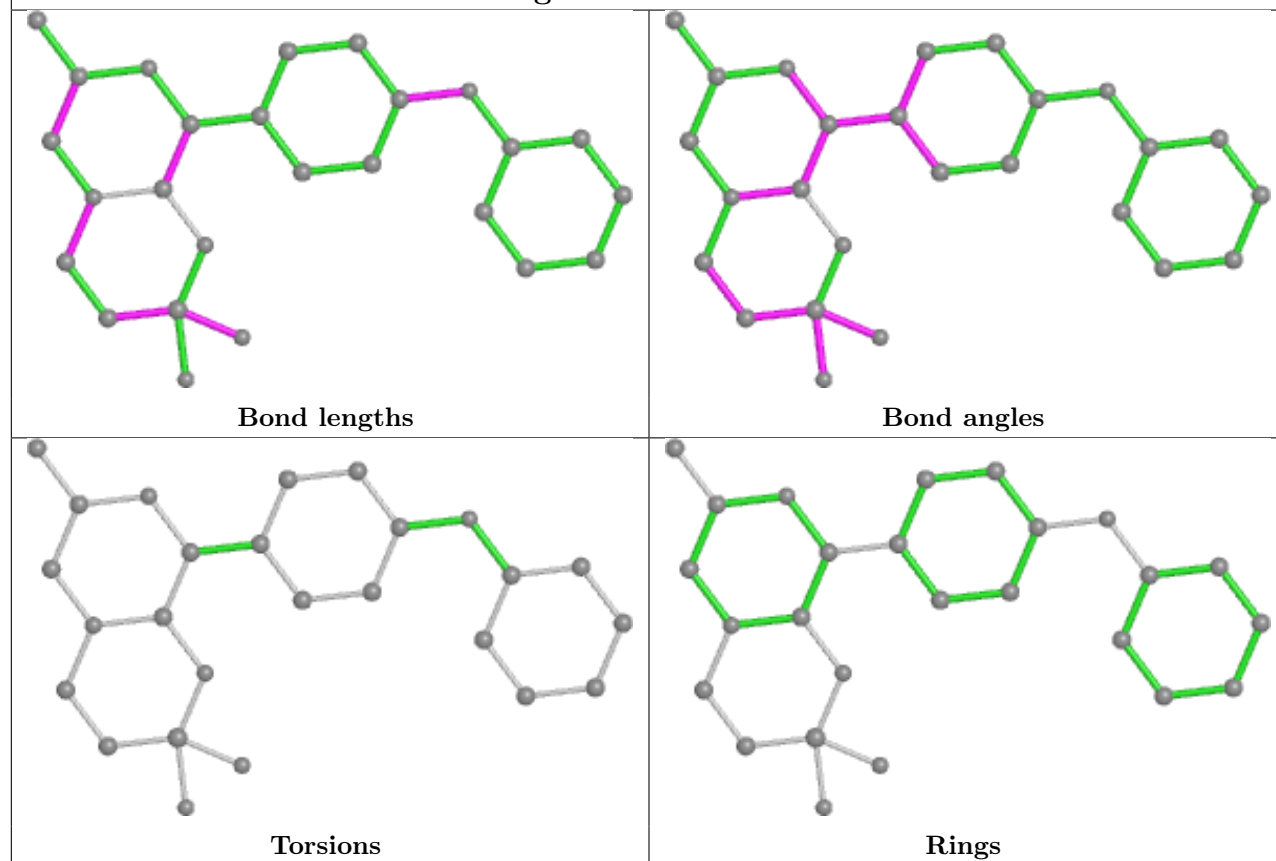
equivalents in the CSD to analyse the geometry.

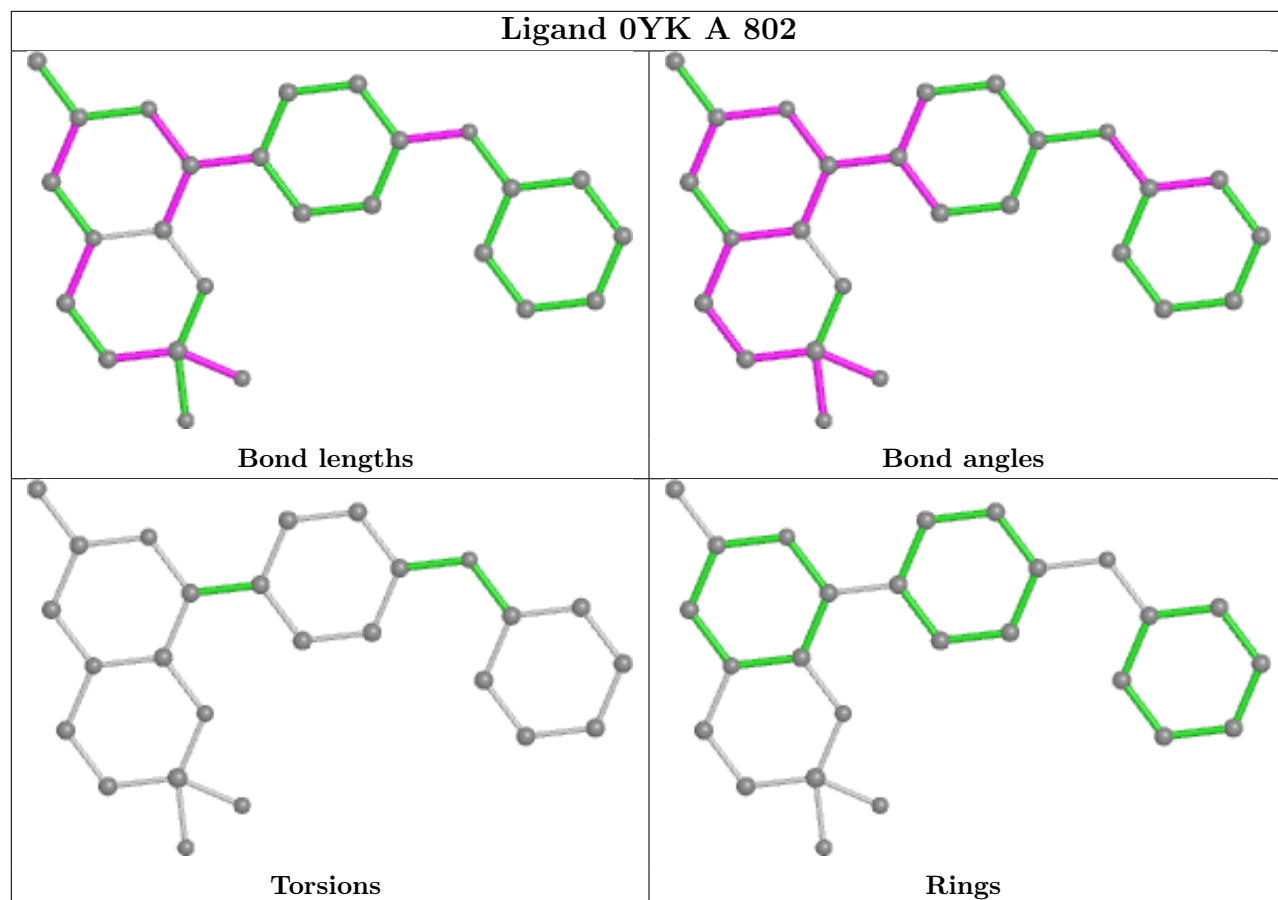


Ligand 0YK C 806 (B)



Ligand 0YK E 803





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	262/263 (99%)	-0.14	7 (2%)	54	55	15, 24, 43, 60	0
1	B	261/263 (99%)	-0.17	3 (1%)	80	81	16, 25, 46, 70	0
1	C	262/263 (99%)	-0.22	1 (0%)	92	93	11, 19, 36, 57	0
1	D	262/263 (99%)	-0.24	1 (0%)	92	93	11, 19, 35, 59	0
1	E	262/263 (99%)	-0.13	3 (1%)	80	81	15, 24, 43, 61	0
1	F	261/263 (99%)	-0.19	4 (1%)	73	73	16, 26, 47, 80	0
All	All	1570/1578 (99%)	-0.18	19 (1%)	79	79	11, 23, 43, 80	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	789	TYR	4.1
1	E	412	SER	4.1
1	B	789	TYR	3.6
1	A	413	ASN	3.4
1	D	436	LEU	3.3
1	B	412	SER	3.2
1	C	411	GLY	3.1
1	E	413	ASN	3.0
1	A	672	ASP	2.8
1	A	412	SER	2.8
1	F	412	SER	2.6
1	B	795	GLY	2.5
1	F	791	LYS	2.5
1	A	791	LYS	2.4
1	E	672	ASP	2.4
1	F	795	GLY	2.3
1	A	477	ASP	2.2
1	A	476	ALA	2.1
1	A	655	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](#)

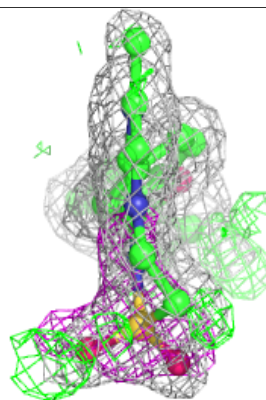
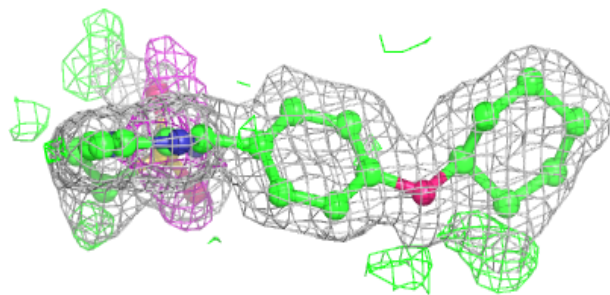
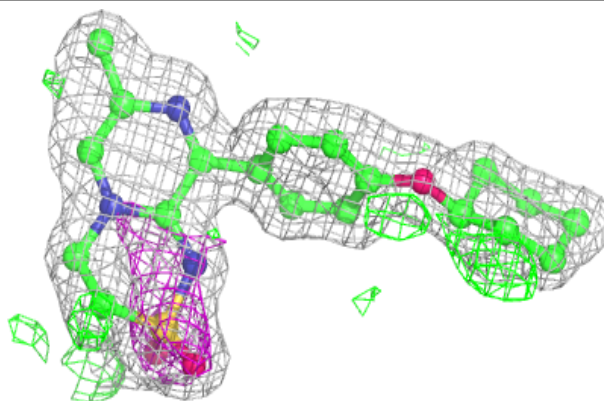
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	D	806	6/6	0.78	0.24	27,39,45,45	0
6	GOL	C	805	6/6	0.86	0.20	27,41,42,45	0
5	ACT	C	804	4/4	0.86	0.19	25,28,28,39	0
5	ACT	F	805	4/4	0.87	0.21	32,36,44,46	0
5	ACT	D	804	4/4	0.89	0.17	26,26,27,39	0
4	ZN	E	802	1/1	0.91	0.08	25,25,25,25	0
4	ZN	F	803	1/1	0.93	0.07	26,26,26,26	0
3	0YK	E	803	26/26	0.93	0.10	21,24,27,31	0
4	ZN	F	802	1/1	0.93	0.08	42,42,42,42	0
3	0YK	A	802	26/26	0.94	0.09	20,24,27,32	0
5	ACT	D	805	4/4	0.95	0.15	28,36,45,51	0
4	ZN	B	802	1/1	0.95	0.06	41,41,41,41	0
3	0YK	C	806[B]	26/26	0.95	0.11	14,18,20,22	26
3	0YK	C	806[A]	26/26	0.95	0.11	14,18,20,22	26
2	GLU	F	801	10/10	0.96	0.07	15,16,19,20	0
2	GLU	C	802	10/10	0.97	0.07	12,13,14,14	0
2	GLU	B	801	10/10	0.97	0.06	15,16,19,20	0
4	ZN	F	804	1/1	0.97	0.04	21,21,21,21	0
4	ZN	D	802	1/1	0.98	0.04	21,21,21,21	0
4	ZN	D	803	1/1	0.98	0.06	20,20,20,20	0
2	GLU	A	801	10/10	0.98	0.06	16,18,20,20	0
2	GLU	D	801	10/10	0.98	0.07	12,13,14,14	0
2	GLU	E	801	10/10	0.98	0.05	16,18,21,21	0
4	ZN	C	803	1/1	0.98	0.06	20,20,20,20	0
4	ZN	C	801	1/1	0.99	0.04	19,19,19,19	0
4	ZN	D	807	1/1	0.99	0.05	19,19,19,19	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.

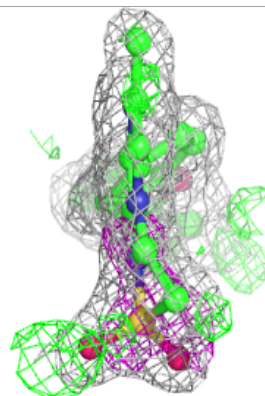
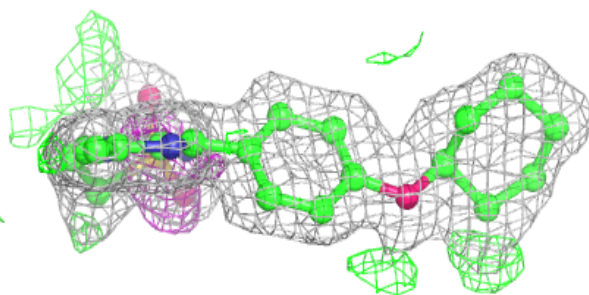
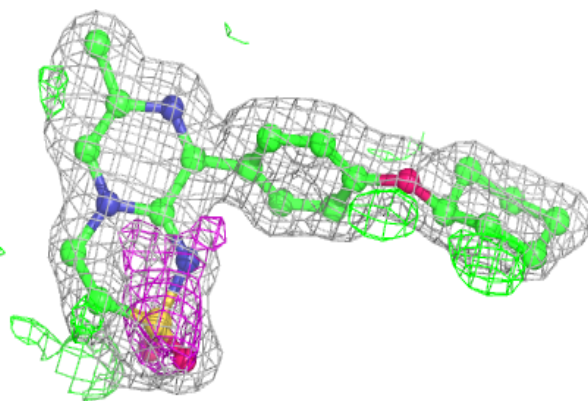
Electron density around 0YK E 803:

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

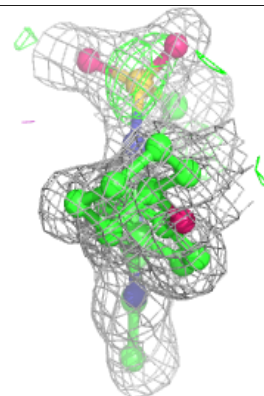
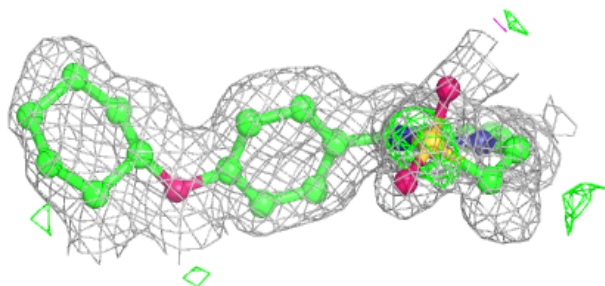
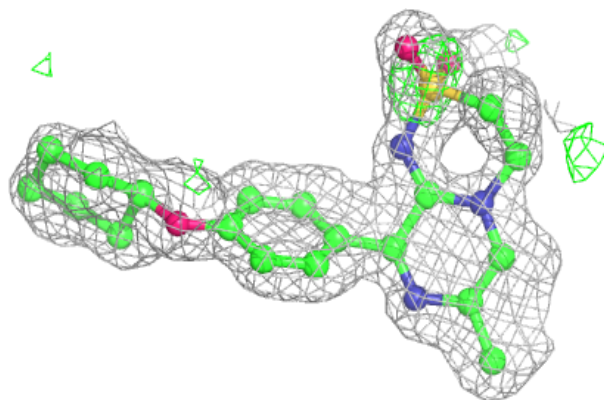


Electron density around 0YK A 802:

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

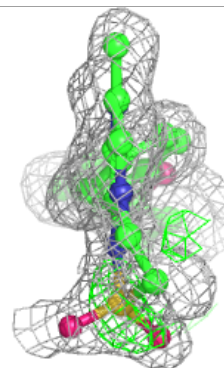
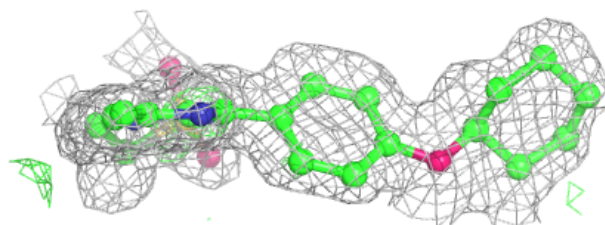
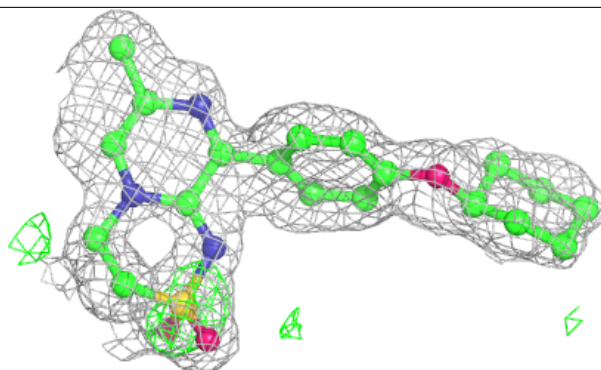
**Electron density around 0YK C 806 (B):**

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



Electron density around 0YK C 806 (A):

$2mF_o-DF_c$ (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.