



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:52 am BST

PDB ID : 4DO3
Title : Structure of FAAH with a non-steroidal anti-inflammatory drug
Authors : Garau, G.
Deposited on : 2012-02-09
Resolution : 2.25 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 : 2.11
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) : 2.11

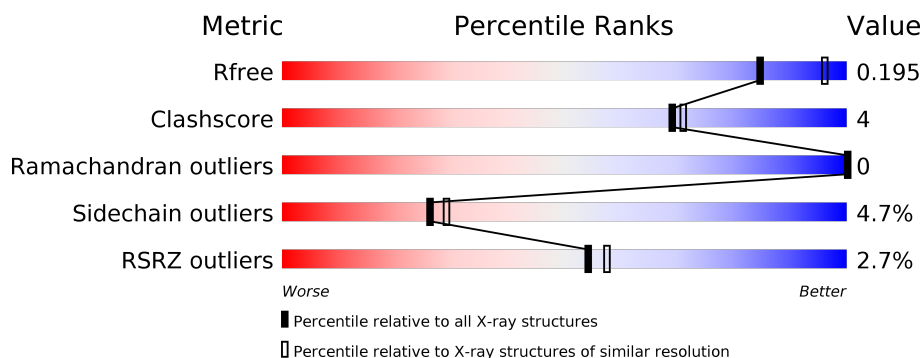
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	B	571	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8986 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 Fatty-acid amide hydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	3	0
			4196	2680	715	770	31			
1	B	544	Total	C	N	O	S	0	2	0
			4199	2681	716	772	30			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP P97612
A	12	GLY	-	EXPRESSION TAG	UNP P97612
A	13	SER	-	EXPRESSION TAG	UNP P97612
A	14	SER	-	EXPRESSION TAG	UNP P97612
A	15	HIS	-	EXPRESSION TAG	UNP P97612
A	16	HIS	-	EXPRESSION TAG	UNP P97612
A	17	HIS	-	EXPRESSION TAG	UNP P97612
A	18	HIS	-	EXPRESSION TAG	UNP P97612
A	19	HIS	-	EXPRESSION TAG	UNP P97612
A	20	HIS	-	EXPRESSION TAG	UNP P97612
A	21	SER	-	EXPRESSION TAG	UNP P97612
A	22	SER	-	EXPRESSION TAG	UNP P97612
A	23	GLY	-	EXPRESSION TAG	UNP P97612
A	24	LEU	-	EXPRESSION TAG	UNP P97612
A	25	VAL	-	EXPRESSION TAG	UNP P97612
A	26	PRO	-	EXPRESSION TAG	UNP P97612
A	27	ARG	-	EXPRESSION TAG	UNP P97612
A	28	GLY	-	EXPRESSION TAG	UNP P97612
A	29	SER	-	EXPRESSION TAG	UNP P97612
A	30	HIS	-	EXPRESSION TAG	UNP P97612
A	31	MET	-	EXPRESSION TAG	UNP P97612
A	576	HIS	-	EXPRESSION TAG	UNP P97612
A	577	HIS	-	EXPRESSION TAG	UNP P97612
A	578	HIS	-	EXPRESSION TAG	UNP P97612
A	579	HIS	-	EXPRESSION TAG	UNP P97612

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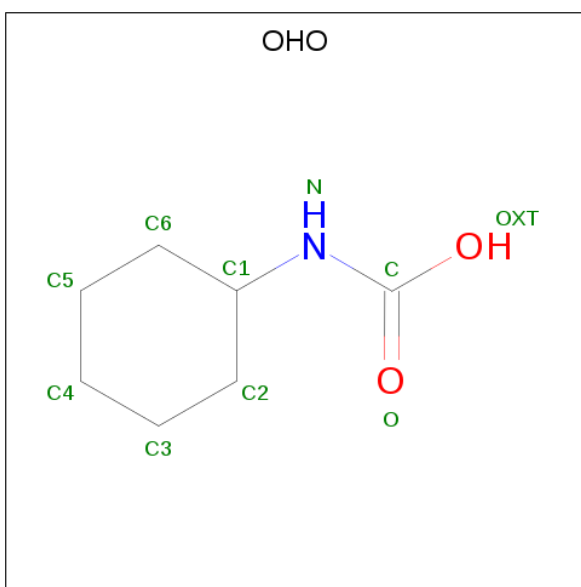
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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	HIS	-	EXPRESSION TAG	UNP P97612
A	581	HIS	-	EXPRESSION TAG	UNP P97612
B	11	MET	-	EXPRESSION TAG	UNP P97612
B	12	GLY	-	EXPRESSION TAG	UNP P97612
B	13	SER	-	EXPRESSION TAG	UNP P97612
B	14	SER	-	EXPRESSION TAG	UNP P97612
B	15	HIS	-	EXPRESSION TAG	UNP P97612
B	16	HIS	-	EXPRESSION TAG	UNP P97612
B	17	HIS	-	EXPRESSION TAG	UNP P97612
B	18	HIS	-	EXPRESSION TAG	UNP P97612
B	19	HIS	-	EXPRESSION TAG	UNP P97612
B	20	HIS	-	EXPRESSION TAG	UNP P97612
B	21	SER	-	EXPRESSION TAG	UNP P97612
B	22	SER	-	EXPRESSION TAG	UNP P97612
B	23	GLY	-	EXPRESSION TAG	UNP P97612
B	24	LEU	-	EXPRESSION TAG	UNP P97612
B	25	VAL	-	EXPRESSION TAG	UNP P97612
B	26	PRO	-	EXPRESSION TAG	UNP P97612
B	27	ARG	-	EXPRESSION TAG	UNP P97612
B	28	GLY	-	EXPRESSION TAG	UNP P97612
B	29	SER	-	EXPRESSION TAG	UNP P97612
B	30	HIS	-	EXPRESSION TAG	UNP P97612
B	31	MET	-	EXPRESSION TAG	UNP P97612
B	576	HIS	-	EXPRESSION TAG	UNP P97612
B	577	HIS	-	EXPRESSION TAG	UNP P97612
B	578	HIS	-	EXPRESSION TAG	UNP P97612
B	579	HIS	-	EXPRESSION TAG	UNP P97612
B	580	HIS	-	EXPRESSION TAG	UNP P97612
B	581	HIS	-	EXPRESSION TAG	UNP P97612

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

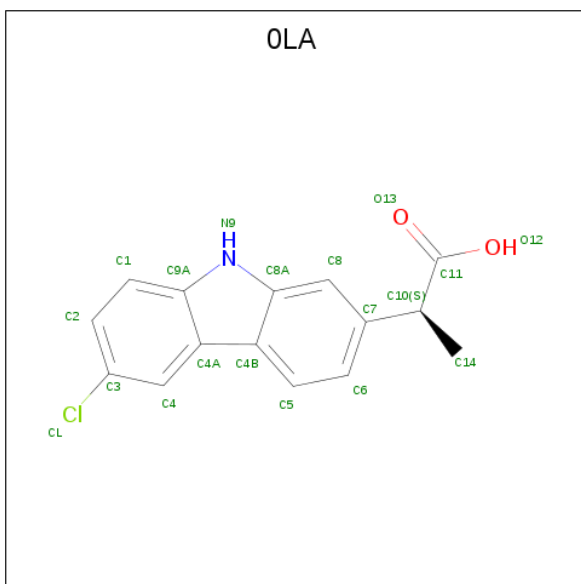
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is CYCLOHEXANE AMINOCARBOXYLIC ACID (three-letter code: OHO) (formula: C₇H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	7	1	1		
3	B	1	Total	C	N	O	0	0
			9	7	1	1		

- Molecule 4 is (2S)-2-(6-chloro-9H-carbazol-2-yl)propanoic acid (three-letter code: OLA) (formula: $C_{15}H_{12}ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			19	15	1	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			19	15	1	1	2		

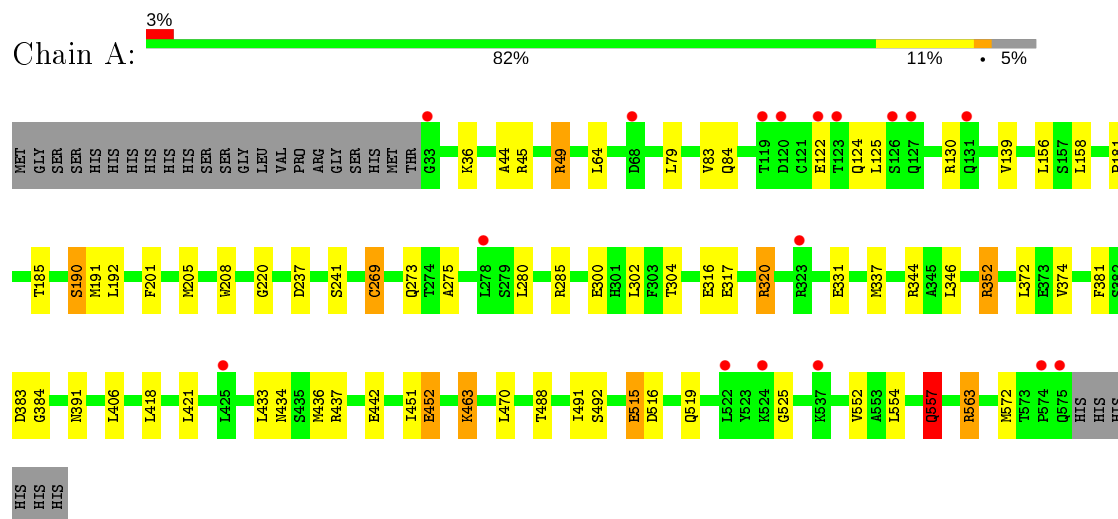
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		
5	B	281	Total	O	0	1
			282	282		

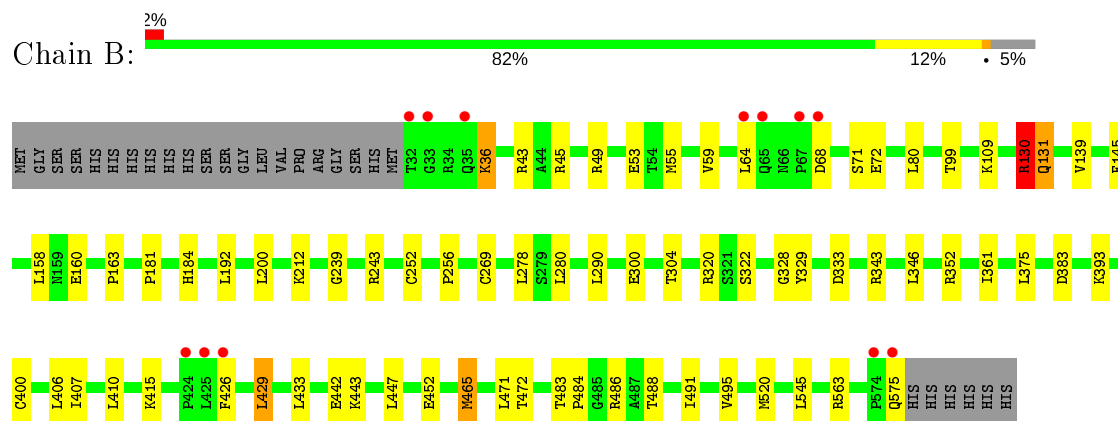
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Fatty-acid amide hydrolase 1



• Molecule 1: Fatty-acid amide hydrolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.47Å 104.37Å 147.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.50 – 2.25 44.44 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.50-2.25) 99.8 (44.44-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.164 , 0.199 0.162 , 0.195	Depositor DCC
R_{free} test set	3838 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8986	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: OHO, 0LA, CL

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	1.20	10/4299 (0.2%)	0.97	4/5832 (0.1%)
1	B	1.21	7/4298 (0.2%)	1.02	11/5831 (0.2%)
All	All	1.21	17/8597 (0.2%)	0.99	15/11663 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	CYS	CB-SG	-10.23	1.64	1.82
1	A	452	GLU	CG-CD	9.98	1.67	1.51
1	B	269	CYS	CB-SG	-7.97	1.68	1.82
1	A	563	ARG	CG-CD	-6.60	1.35	1.51
1	A	374	VAL	CB-CG2	6.05	1.65	1.52
1	B	452	GLU	CG-CD	5.92	1.60	1.51
1	A	557	GLN	CB-CG	-5.57	1.37	1.52
1	B	452	GLU	CD-OE1	5.57	1.31	1.25
1	A	317	GLU	CG-CD	5.56	1.60	1.51
1	A	208	TRP	CE3-CZ3	5.55	1.47	1.38
1	A	515	GLU	CG-CD	5.41	1.60	1.51
1	A	331	GLU	CD-OE2	5.39	1.31	1.25
1	B	53	GLU	CG-CD	5.35	1.59	1.51
1	B	145	PHE	CD2-CE2	5.25	1.49	1.39
1	B	36	LYS	CD-CE	5.17	1.64	1.51
1	B	72	GLU	CG-CD	5.16	1.59	1.51
1	A	190	SER	CB-OG	5.01	1.48	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	A	269	CYS	CA-CB-SG	-8.82	98.12	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	130	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	B	130	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	A	49	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	333	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	465	MET	CG-SD-CE	-6.16	90.35	100.20
1	A	452	GLU	CA-CB-CG	6.12	126.86	113.40
1	B	243	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	516	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	269	CYS	CA-CB-SG	-5.29	104.47	114.00
1	B	49	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	520	MET	CG-SD-CE	5.11	108.38	100.20
1	B	486	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	4196	0	4263	35	0
1	B	4199	0	4265	31	0
2	A	1	0	0	0	0
3	A	9	0	12	1	0
3	B	9	0	12	0	0
4	A	19	0	11	1	0
4	B	19	0	11	2	0
5	A	252	0	0	4	0
5	B	282	0	0	0	0
All	All	8986	0	8574	63	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 (63) 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:337[B]:MET:CE	1:A:525:GLY:H	1.90	0.85
1:B:45:ARG:NH2	1:B:200:LEU:O	2.14	0.79
1:B:407:ILE:CD1	4:B:602:OLA:H8	2.14	0.78
1:B:45:ARG:CG	1:B:45:ARG:HH21	2.07	0.67
1:B:45:ARG:HH21	1:B:45:ARG:HG2	1.60	0.67
1:A:434:ASN:HD21	1:A:437:ARG:HH21	1.47	0.60
1:A:205:MET:HE2	5:A:727:HOH:O	2.05	0.56
1:A:237:ASP:HA	1:A:241:SER:HB2	1.91	0.53
1:A:316:GLU:OE1	1:A:320:ARG:HD2	2.09	0.52
1:B:55:MET:O	1:B:59:VAL:HG23	2.10	0.52
1:A:122:GLU:O	1:A:125:LEU:HB3	2.11	0.51
1:A:124:GLN:NE2	5:A:734:HOH:O	2.10	0.50
1:A:300:GLU:O	1:A:304:THR:HG23	2.12	0.50
1:B:256:PRO:HD2	1:B:280:LEU:O	2.14	0.48
1:A:45:ARG:NH1	5:A:945:HOH:O	2.47	0.48
1:B:328:GLY:HA2	1:B:361:ILE:O	2.14	0.48
1:A:554:LEU:O	1:A:557:GLN:HB2	2.14	0.48
1:A:285:ARG:HD3	5:A:842:HOH:O	2.14	0.47
1:B:71:SER:HB2	1:B:99:THR:HG23	1.95	0.47
1:B:443:LYS:HA	1:B:443:LYS:HD3	1.76	0.47
1:A:434:ASN:ND2	1:A:437:ARG:HH21	2.12	0.47
1:A:383:ASP:HB2	1:B:442:GLU:HB2	1.97	0.47
1:A:139:VAL:O	1:A:181:PRO:HA	2.15	0.47
1:B:45:ARG:CG	1:B:45:ARG:NH2	2.75	0.47
1:A:442:GLU:HB2	1:B:383:ASP:HB2	1.97	0.46
1:A:384:GLY:HA2	1:A:436:MET:O	2.16	0.46
1:B:212:LYS:HG3	1:B:545:LEU:HD11	1.96	0.46
1:B:346:LEU:HD13	1:B:346:LEU:C	2.36	0.46
1:A:346:LEU:C	1:A:346:LEU:HD13	2.36	0.46
1:B:43:ARG:NH2	1:B:160:GLU:OE1	2.49	0.46
1:B:300:GLU:O	1:B:304:THR:HG23	2.16	0.46
1:A:337[B]:MET:HE1	1:A:525:GLY:H	1.77	0.45
1:B:483:THR:N	1:B:484:PRO:CD	2.80	0.45
1:A:488:THR:O	1:A:491:ILE:HG12	2.17	0.45
1:B:239:GLY:HA2	1:B:495:VAL:HG23	1.99	0.45
1:B:375:LEU:HA	1:B:447:LEU:HD11	1.99	0.45
1:B:488:THR:O	1:B:491:ILE:HG12	2.17	0.45
1:B:131:GLN:H	1:B:131:GLN:CD	2.20	0.44
1:A:337[B]:MET:CE	1:A:525:GLY:N	2.70	0.44
1:B:410:LEU:O	1:B:415:LYS:HE3	2.17	0.44
1:A:185:THR:HB	1:A:220:GLY:HA3	1.99	0.44
1:A:515:GLU:O	1:A:519:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HB3	1:B:130:ARG:HE	1.54	0.44
1:A:156:LEU:HD13	1:A:391:ASN:HB3	2.01	0.43
1:A:463:LYS:HE3	1:B:304:THR:O	2.17	0.43
1:B:109:LYS:HE3	1:B:109:LYS:HB3	1.88	0.43
1:A:275:ALA:HB1	1:A:451:ILE:CD1	2.48	0.43
1:A:491:ILE:HG21	3:A:601:OHO:H32	2.01	0.43
1:A:381:PHE:HE2	4:A:602:OLA:CL	2.37	0.43
1:B:407:ILE:HD12	4:B:602:OLA:H8	1.96	0.43
1:B:426:PHE:HB3	1:B:429:LEU:HG	2.00	0.42
1:B:252:CYS:HB3	1:B:290:LEU:HD11	2.00	0.42
1:B:131:GLN:NE2	1:B:131:GLN:H	2.17	0.42
1:A:190:SER:O	1:A:191:MET:HB2	2.20	0.42
1:A:45:ARG:HB3	1:A:49:ARG:NH2	2.34	0.42
1:B:329:TYR:HA	1:B:471:LEU:O	2.20	0.42
1:A:44:ALA:HB1	1:A:201:PHE:CE2	2.55	0.41
1:B:139:VAL:O	1:B:181:PRO:HA	2.19	0.41
1:A:372:LEU:HD11	1:A:492:SER:HB2	2.02	0.41
1:A:344:ARG:HG2	1:A:344:ARG:NH2	2.36	0.41
1:A:352:ARG:HG3	1:A:572:MET:SD	2.61	0.40
1:A:79:LEU:O	1:A:83:VAL:HG23	2.21	0.40
1:A:470:LEU:HB3	1:A:552:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	544/571 (95%)	529 (97%)	15 (3%)	0	100	100
1	B	544/571 (95%)	532 (98%)	12 (2%)	0	100	100
All	All	1088/1142 (95%)	1061 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/485 (96%)	443 (96%)	20 (4%)	29	33
1	B	463/485 (96%)	440 (95%)	23 (5%)	24	26
All	All	926/970 (96%)	883 (95%)	43 (5%)	26	30

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	64	LEU
1	A	84	GLN
1	A	130	ARG
1	A	158	LEU
1	A	192	LEU
1	A	269	CYS
1	A	273	GLN
1	A	280	LEU
1	A	302	LEU
1	A	320	ARG
1	A	352	ARG
1	A	406	LEU
1	A	418	LEU
1	A	421	LEU
1	A	433	LEU
1	A	452	GLU
1	A	463	LYS
1	A	557	GLN
1	A	563	ARG
1	B	36	LYS
1	B	64	LEU
1	B	68	ASP
1	B	80	LEU
1	B	130	ARG

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	158	LEU
1	B	163	PRO
1	B	184	HIS
1	B	192	LEU
1	B	278	LEU
1	B	320	ARG
1	B	322	SER
1	B	352	ARG
1	B	393	LYS
1	B	400	CYS
1	B	406	LEU
1	B	429	LEU
1	B	433	LEU
1	B	465	MET
1	B	472	THR
1	B	563	ARG
1	B	575	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	334	ASN
1	A	351	GLN
1	A	434	ASN
1	A	449	HIS
1	A	466	ASN
1	B	124	GLN
1	B	127	GLN
1	B	131	GLN
1	B	351	GLN
1	B	466	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	OHO	A	601	1	9,9,10	1.20	1 (11%)	9,10,12	1.32	1 (11%)
3	OHO	B	601	1	9,9,10	0.84	0	9,10,12	1.32	1 (11%)
4	0LA	B	602	-	18,21,21	1.47	5 (27%)	27,31,31	1.81	6 (22%)
4	0LA	A	602	-	18,21,21	1.40	2 (11%)	27,31,31	2.11	9 (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	OHO	A	601	1	-	0/3/11/12	0/1/1/1
3	OHO	B	601	1	-	0/3/11/12	0/1/1/1
4	0LA	B	602	-	-	0/4/8/8	0/3/3/3
4	0LA	A	602	-	-	0/4/8/8	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	OHO	C1-N	-3.34	1.44	1.47
4	B	602	0LA	C4-C3	3.28	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	0LA	C6-C7	2.83	1.43	1.39
4	B	602	0LA	C6-C7	2.51	1.43	1.39
4	A	602	0LA	C5-C6	2.35	1.41	1.36
4	B	602	0LA	C3-CL	2.19	1.79	1.74
4	B	602	0LA	C8-C7	2.10	1.41	1.37
4	B	602	0LA	C4B-C4A	-2.04	1.39	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	0LA	C3-C4-C4A	-4.67	114.74	120.26
4	A	602	0LA	C6-C5-C4B	-4.61	114.99	121.63
4	B	602	0LA	C14-C10-C11	-4.04	101.69	112.14
4	B	602	0LA	C6-C5-C4B	-3.60	116.45	121.63
3	B	601	OHO	C4-C3-C2	3.44	118.42	111.42
4	A	602	0LA	C5-C4B-C8A	3.33	122.58	118.17
4	A	602	0LA	C2-C1-C9A	-3.25	116.75	120.84
4	B	602	0LA	C5-C4B-C8A	3.25	122.47	118.17
4	B	602	0LA	C3-C4-C4A	-3.06	116.64	120.26
4	A	602	0LA	C4B-C4A-C9A	2.98	109.35	106.09
4	A	602	0LA	C8-C7-C10	-2.74	115.96	122.20
4	A	602	0LA	C4-C4A-C9A	2.63	121.85	118.26
4	A	602	0LA	C4-C4A-C4B	-2.52	128.80	132.28
4	B	602	0LA	C4B-C4A-C9A	2.46	108.78	106.09
3	A	601	OHO	C4-C3-C2	2.41	116.33	111.42
4	A	602	0LA	C8A-N9-C9A	2.06	111.32	107.09
4	B	602	0LA	C8-C7-C10	-2.03	117.59	122.20

There are no chirality outliers.

There are no torsion outliers.

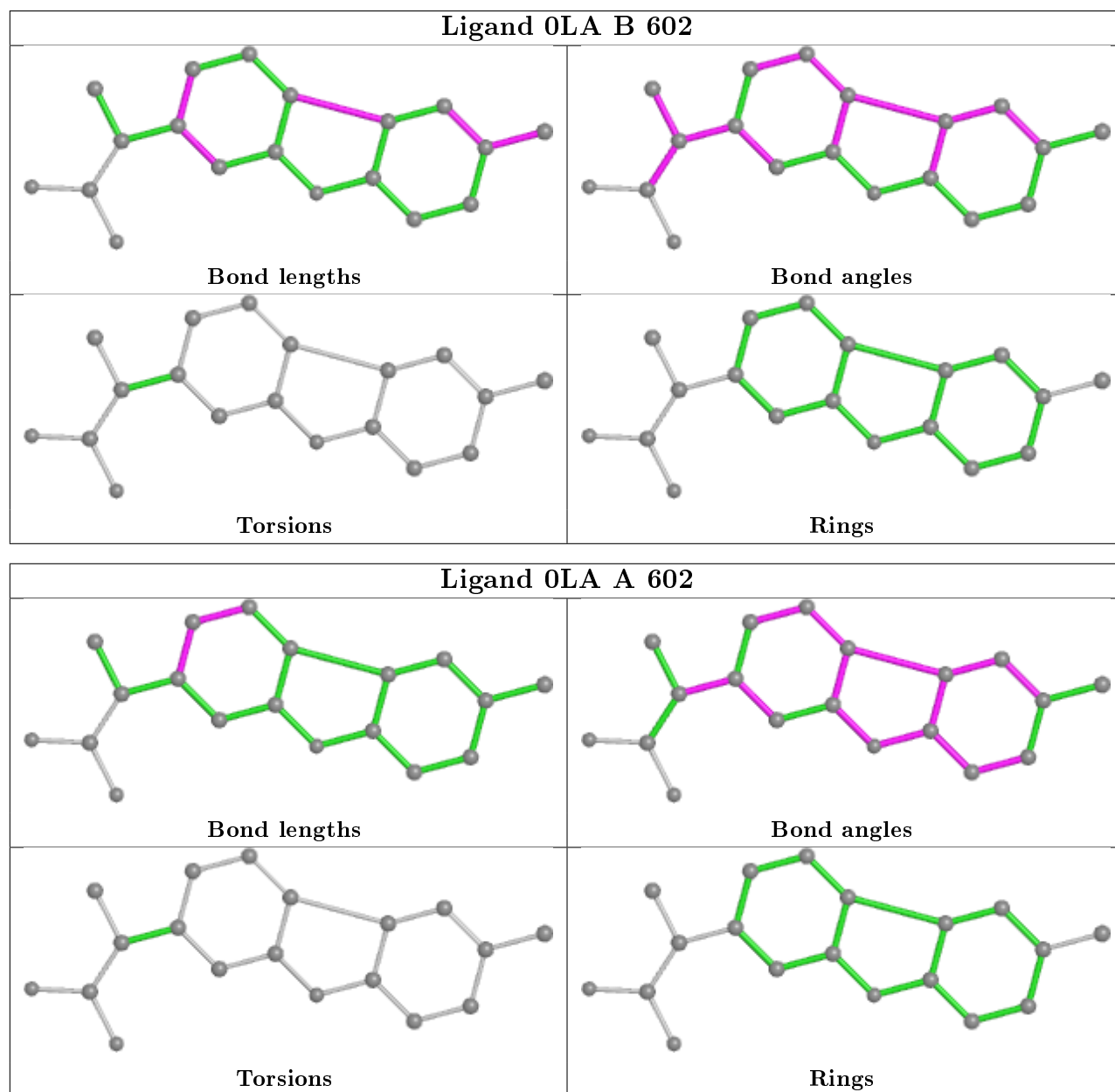
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	OHO	1	0
4	B	602	0LA	2	0
4	A	602	0LA	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/571 (95%)	-0.29	17 (3%) 49 52	17, 27, 48, 69	0
1	B	544/571 (95%)	-0.43	12 (2%) 62 65	15, 24, 48, 71	0
All	All	1087/1142 (95%)	-0.36	29 (2%) 54 57	15, 25, 48, 71	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	THR	6.7
1	B	575	GLN	5.9
1	A	425	LEU	5.4
1	A	575	GLN	5.2
1	B	64	LEU	3.9
1	A	574	PRO	3.8
1	B	65	GLN	3.8
1	B	68	ASP	3.7
1	A	119	THR	3.7
1	B	33	GLY	3.6
1	A	323	ARG	3.3
1	A	524	LYS	3.2
1	A	33	GLY	3.2
1	B	425	LEU	2.9
1	A	126	SER	2.8
1	B	67	PRO	2.8
1	A	123	THR	2.6
1	A	68	ASP	2.5
1	B	426	PHE	2.4
1	B	574	PRO	2.4
1	B	35	GLN	2.4
1	A	522	LEU	2.4
1	B	424	PRO	2.3
1	A	122	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	ASP	2.2
1	A	278	LEU	2.2
1	A	131	GLN	2.1
1	A	127	GLN	2.0
1	A	537	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

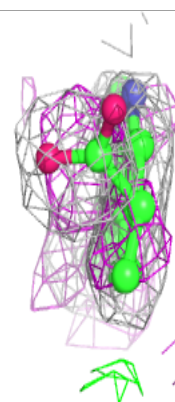
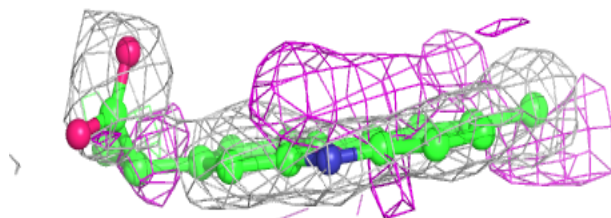
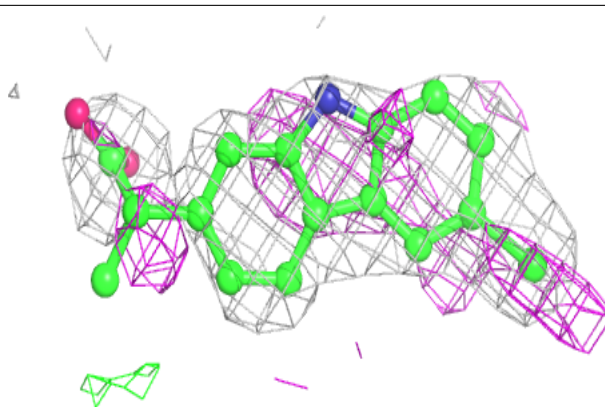
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OLA	B	602	19/19	0.80	0.32	54,57,66,67	0
4	OLA	A	602	19/19	0.82	0.26	54,58,65,67	0
3	OHO	A	601	9/10	0.97	0.15	31,32,34,34	0
3	OHO	B	601	9/10	0.97	0.10	28,30,33,33	0
2	CL	A	600	1/1	0.99	0.20	18,18,18,18	0

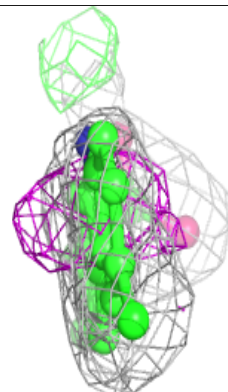
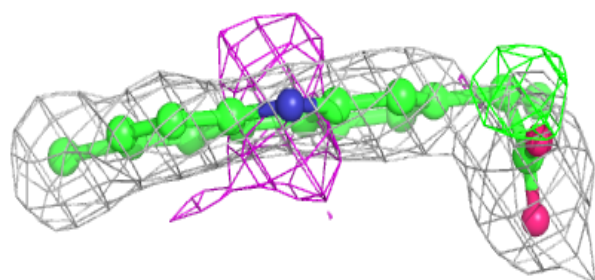
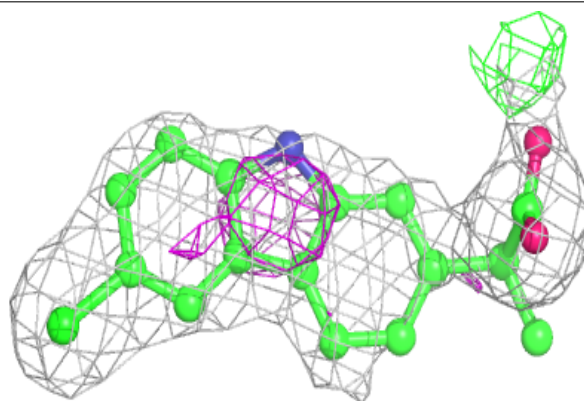
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0LA B 602:

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

**Electron density around 0LA A 602:**

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



6.5 Other polymers

There are no such residues in this entry.