



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:20 am BST

PDB ID : 4J5P
Title : Crystal Structure of a Covalently Bound alpha-Ketoheterocycle Inhibitor (Ph
enhexyl/Oxadiazole/Pyridine) to a Humanized Variant of Fatty Acid Amide
Hydrolase
Authors : Otrubova, K.; Brown, M.; McCormick, M.S.; Han, G.W.; O'Neal, S.T.; Cra-
vatt, B.F.; Stevens, R.C.; Lichtman, A.H.; Boger, D.L.
Deposited on : 2013-02-08
Resolution : 2.30 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

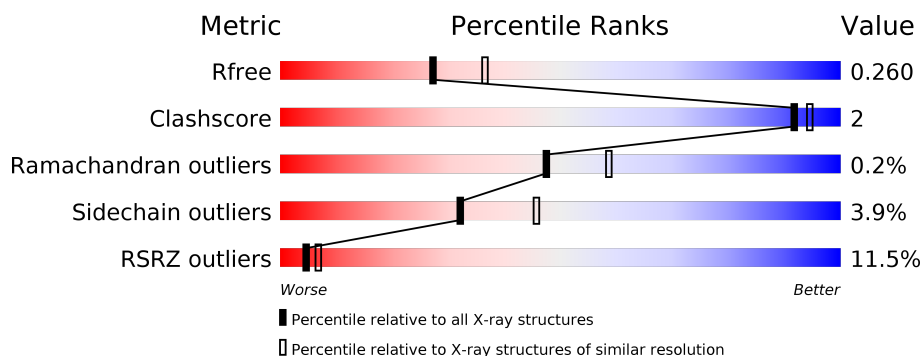
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	573	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>7% • 5%</div> </div> </div>
1	B	573	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>6% • 5%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8787 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	544	Total	C	N	O	S	0	0	0
			4198	2679	717	772	30			
1	B	545	Total	C	N	O	S	0	0	0
			4207	2684	719	774	30			

There are 58 discrepancies between the modelled and reference sequences:

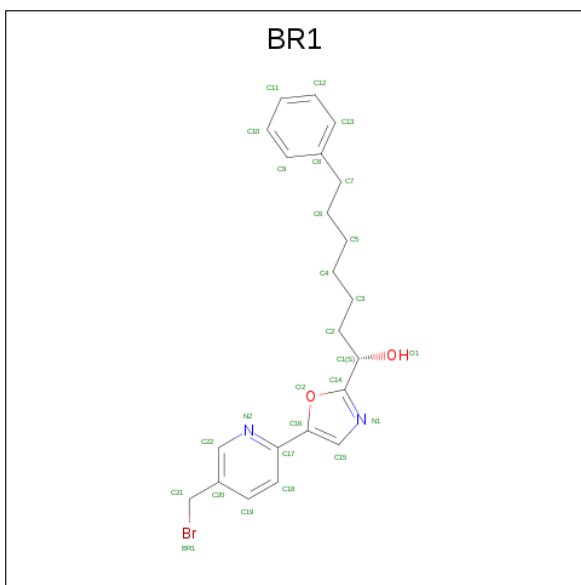
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P97612
A	8	GLY	-	EXPRESSION TAG	UNP P97612
A	9	SER	-	EXPRESSION TAG	UNP P97612
A	10	SER	-	EXPRESSION TAG	UNP P97612
A	11	HIS	-	EXPRESSION TAG	UNP P97612
A	12	HIS	-	EXPRESSION TAG	UNP P97612
A	13	HIS	-	EXPRESSION TAG	UNP P97612
A	14	HIS	-	EXPRESSION TAG	UNP P97612
A	15	HIS	-	EXPRESSION TAG	UNP P97612
A	16	HIS	-	EXPRESSION TAG	UNP P97612
A	17	SER	-	EXPRESSION TAG	UNP P97612
A	18	SER	-	EXPRESSION TAG	UNP P97612
A	19	GLY	-	EXPRESSION TAG	UNP P97612
A	20	LEU	-	EXPRESSION TAG	UNP P97612
A	21	VAL	-	EXPRESSION TAG	UNP P97612
A	22	PRO	-	EXPRESSION TAG	UNP P97612
A	23	ARG	-	EXPRESSION TAG	UNP P97612
A	24	GLY	-	EXPRESSION TAG	UNP P97612
A	25	SER	-	EXPRESSION TAG	UNP P97612
A	26	HIS	-	EXPRESSION TAG	UNP P97612
A	27	MET	-	EXPRESSION TAG	UNP P97612
A	28	ALA	-	EXPRESSION TAG	UNP P97612
A	29	SER	-	EXPRESSION TAG	UNP P97612
A	192	PHE	LEU	ENGINEERED MUTATION	UNP P97612
A	194	TYR	PHE	ENGINEERED MUTATION	UNP P97612

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Chain	Residue	Modelled	Actual	Comment	Reference
A	377	THR	ALA	ENGINEERED MUTATION	UNP P97612
A	435	ASN	SER	ENGINEERED MUTATION	UNP P97612
A	491	VAL	ILE	ENGINEERED MUTATION	UNP P97612
A	495	MET	VAL	ENGINEERED MUTATION	UNP P97612
B	7	MET	-	EXPRESSION TAG	UNP P97612
B	8	GLY	-	EXPRESSION TAG	UNP P97612
B	9	SER	-	EXPRESSION TAG	UNP P97612
B	10	SER	-	EXPRESSION TAG	UNP P97612
B	11	HIS	-	EXPRESSION TAG	UNP P97612
B	12	HIS	-	EXPRESSION TAG	UNP P97612
B	13	HIS	-	EXPRESSION TAG	UNP P97612
B	14	HIS	-	EXPRESSION TAG	UNP P97612
B	15	HIS	-	EXPRESSION TAG	UNP P97612
B	16	HIS	-	EXPRESSION TAG	UNP P97612
B	17	SER	-	EXPRESSION TAG	UNP P97612
B	18	SER	-	EXPRESSION TAG	UNP P97612
B	19	GLY	-	EXPRESSION TAG	UNP P97612
B	20	LEU	-	EXPRESSION TAG	UNP P97612
B	21	VAL	-	EXPRESSION TAG	UNP P97612
B	22	PRO	-	EXPRESSION TAG	UNP P97612
B	23	ARG	-	EXPRESSION TAG	UNP P97612
B	24	GLY	-	EXPRESSION TAG	UNP P97612
B	25	SER	-	EXPRESSION TAG	UNP P97612
B	26	HIS	-	EXPRESSION TAG	UNP P97612
B	27	MET	-	EXPRESSION TAG	UNP P97612
B	28	ALA	-	EXPRESSION TAG	UNP P97612
B	29	SER	-	EXPRESSION TAG	UNP P97612
B	192	PHE	LEU	ENGINEERED MUTATION	UNP P97612
B	194	TYR	PHE	ENGINEERED MUTATION	UNP P97612
B	377	THR	ALA	ENGINEERED MUTATION	UNP P97612
B	435	ASN	SER	ENGINEERED MUTATION	UNP P97612
B	491	VAL	ILE	ENGINEERED MUTATION	UNP P97612
B	495	MET	VAL	ENGINEERED MUTATION	UNP P97612

- Molecule 2 is (1S)-1-{5-[5-(bromomethyl)pyridin-2-yl]-1,3-oxazol-2-yl}-7-phenylheptan-1-ol (three-letter code: BR1) (formula: C₂₂H₂₅BrN₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	22	2	2		
2	B	1	Total	C	N	O	0	0
			26	22	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

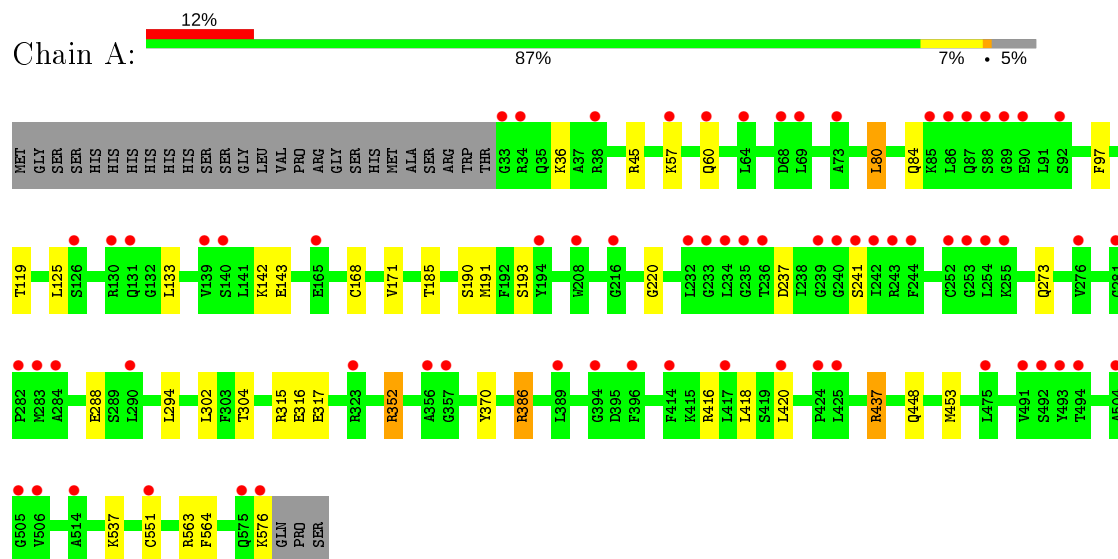
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	170	Total	O	0	0
			170	170		

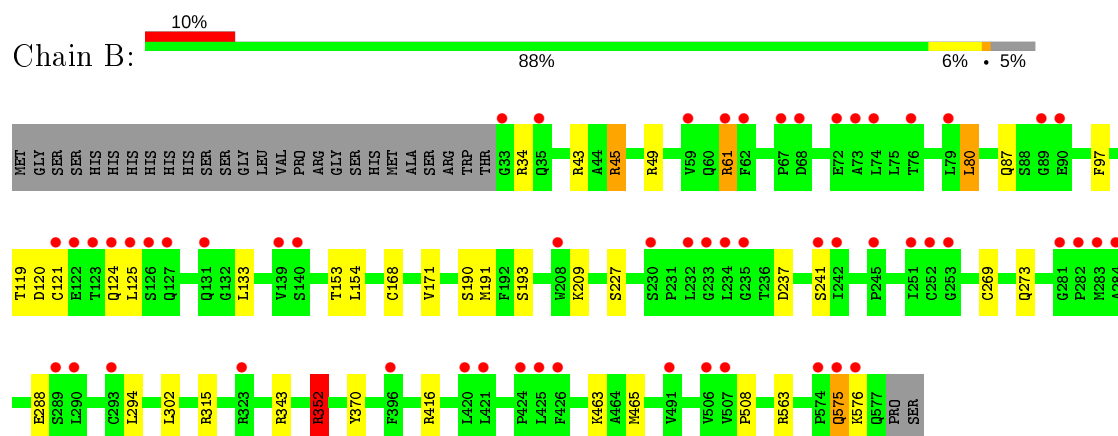
3 Residue-property plots [i](#)

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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.07Å 104.07Å 261.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.38 – 2.30 33.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (33.38-2.30) 97.3 (33.38-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	48.72 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.220 , 0.265 0.222 , 0.260	Depositor DCC
R_{free} test set	3602 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8787	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, BR1, 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	0.79	0/4292	0.87	7/5822 (0.1%)
1	B	0.84	1/4301 (0.0%)	0.89	6/5834 (0.1%)
All	All	0.82	1/8593 (0.0%)	0.88	13/11656 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	SER	CB-OG	-5.83	1.34	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	315	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	A	45	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	B	45	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	A	386	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	352	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	49	ARG	CG-CD-NE	-5.47	100.31	111.80
1	A	437	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	315	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	453	MET	CG-SD-CE	5.19	108.50	100.20
1	B	43	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	352	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	352	ARG	NE-CZ-NH1	-5.01	117.80	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	4198	0	4252	11	0
1	B	4207	0	4260	17	0
2	A	26	0	22	0	0
2	B	26	0	22	1	0
3	A	14	0	20	0	0
3	B	21	0	30	0	0
4	B	1	0	0	0	0
5	A	124	0	0	1	0
5	B	170	0	0	7	0
All	All	8787	0	8606	27	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 2.

All (27) 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:304:THR:O	1:B:463:LYS:HE3	1.77	0.84
1:B:34:ARG:HA	5:B:704:HOH:O	1.92	0.70
1:A:80:LEU:HD13	1:A:288:GLU:HG3	1.84	0.59
1:A:237:ASP:HA	1:A:241:SER:HB2	1.85	0.58
1:B:80:LEU:HD13	1:B:288:GLU:HG3	1.86	0.56
1:B:352:ARG:HD2	5:B:710:HOH:O	2.05	0.56
1:B:237:ASP:HA	1:B:241:SER:HB2	1.89	0.55
1:B:121:CYS:HA	1:B:124:GLN:HB2	1.89	0.54
1:B:168:CYS:SG	1:B:171:VAL:HG23	2.48	0.54
1:B:45:ARG:NH2	5:B:763:HOH:O	2.41	0.52
1:B:61:ARG:N	5:B:719:HOH:O	2.42	0.51
1:A:168:CYS:SG	1:A:171:VAL:HG23	2.53	0.48
1:B:575:GLN:H	1:B:575:GLN:CD	2.16	0.47
1:B:209:LYS:NZ	5:B:822:HOH:O	2.45	0.47
1:B:508:PRO:HB3	5:B:742:HOH:O	2.16	0.46
1:B:87:GLN:NE2	5:B:714:HOH:O	2.50	0.44
1:B:269:CYS:N	2:B:601:BR1:C21	2.81	0.44
1:A:448:GLN:HG2	5:A:701:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PHE:HB2	1:B:125:LEU:HD21	2.00	0.43
1:A:185:THR:HB	1:A:220:GLY:HA3	2.01	0.43
1:B:190:SER:O	1:B:191:MET:HB2	2.20	0.42
1:A:97:PHE:HB2	1:A:125:LEU:HD21	2.01	0.41
1:A:416:ARG:HG3	1:A:437:ARG:CZ	2.50	0.41
1:A:190:SER:O	1:A:191:MET:HB2	2.21	0.41
1:A:142:LYS:HE2	1:A:191:MET:SD	2.61	0.41
1:A:551:CYS:HB3	1:A:564:PHE:CD1	2.56	0.41
1:B:153:THR:O	1:B:154:LEU:HB2	2.22	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	542/573 (95%)	523 (96%)	18 (3%)	1 (0%)	47	58
1	B	543/573 (95%)	524 (96%)	18 (3%)	1 (0%)	47	58
All	All	1085/1146 (95%)	1047 (96%)	36 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	SER
1	A	193	SER

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	462/487 (95%)	441 (96%)	21 (4%)	27	39
1	B	463/487 (95%)	448 (97%)	15 (3%)	39	54
All	All	925/974 (95%)	889 (96%)	36 (4%)	32	46

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	57	LYS
1	A	60	GLN
1	A	80	LEU
1	A	84	GLN
1	A	119	THR
1	A	133	LEU
1	A	143	GLU
1	A	273	GLN
1	A	294	LEU
1	A	302	LEU
1	A	316	GLU
1	A	317	GLU
1	A	352	ARG
1	A	370	TYR
1	A	386	ARG
1	A	418	LEU
1	A	420	LEU
1	A	537	LYS
1	A	563	ARG
1	A	576	LYS
1	B	61	ARG
1	B	80	LEU
1	B	119	THR
1	B	120	ASP
1	B	133	LEU
1	B	273	GLN
1	B	294	LEU
1	B	302	LEU
1	B	352	ARG
1	B	370	TYR
1	B	416	ARG
1	B	465	MET

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Mol	Chain	Res	Type
1	B	563	ARG
1	B	575	GLN
1	B	576	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	351	GLN
1	A	557	GLN
1	B	87	GLN
1	B	124	GLN
1	B	351	GLN

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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
2	BR1	B	601	1	25,28,29	1.08	1 (4%)	28,36,37	1.57	3 (10%)
3	PEG	B	602	-	6,6,6	0.56	0	5,5,5	0.40	0
2	BR1	A	601	1	25,28,29	1.14	2 (8%)	28,36,37	1.56	6 (21%)
3	PEG	B	603	-	6,6,6	0.63	0	5,5,5	0.29	0
3	PEG	B	604	-	6,6,6	0.78	0	5,5,5	0.50	0
3	PEG	A	603	-	6,6,6	0.72	0	5,5,5	0.38	0
3	PEG	A	602	-	6,6,6	0.44	0	5,5,5	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BR1	B	601	1	-	3/9/17/19	0/3/3/3
3	PEG	B	602	-	-	2/4/4/4	-
2	BR1	A	601	1	-	3/9/17/19	0/3/3/3
3	PEG	B	603	-	-	2/4/4/4	-
3	PEG	B	604	-	-	2/4/4/4	-
3	PEG	A	603	-	-	3/4/4/4	-
3	PEG	A	602	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BR1	C7-C8	-3.09	1.42	1.51
2	A	601	BR1	C7-C8	-2.69	1.43	1.51
2	A	601	BR1	C16-C17	-2.61	1.43	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BR1	C18-C19-C20	-4.12	115.86	121.38
2	A	601	BR1	C18-C19-C20	-3.58	116.59	121.38
2	B	601	BR1	C5-C6-C7	-3.43	100.40	113.76
2	A	601	BR1	C21-C20-C22	-2.98	115.33	121.11
2	A	601	BR1	C20-C22-N2	-2.50	121.87	124.81
2	A	601	BR1	C5-C6-C7	-2.46	104.19	113.76
2	A	601	BR1	C2-C1-C14	-2.05	106.42	112.34
2	A	601	BR1	C19-C20-C22	2.02	121.24	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BR1	C3-C2-C1	-2.00	107.74	113.82

There are no chirality outliers.

All (17) torsion outliers are listed below:

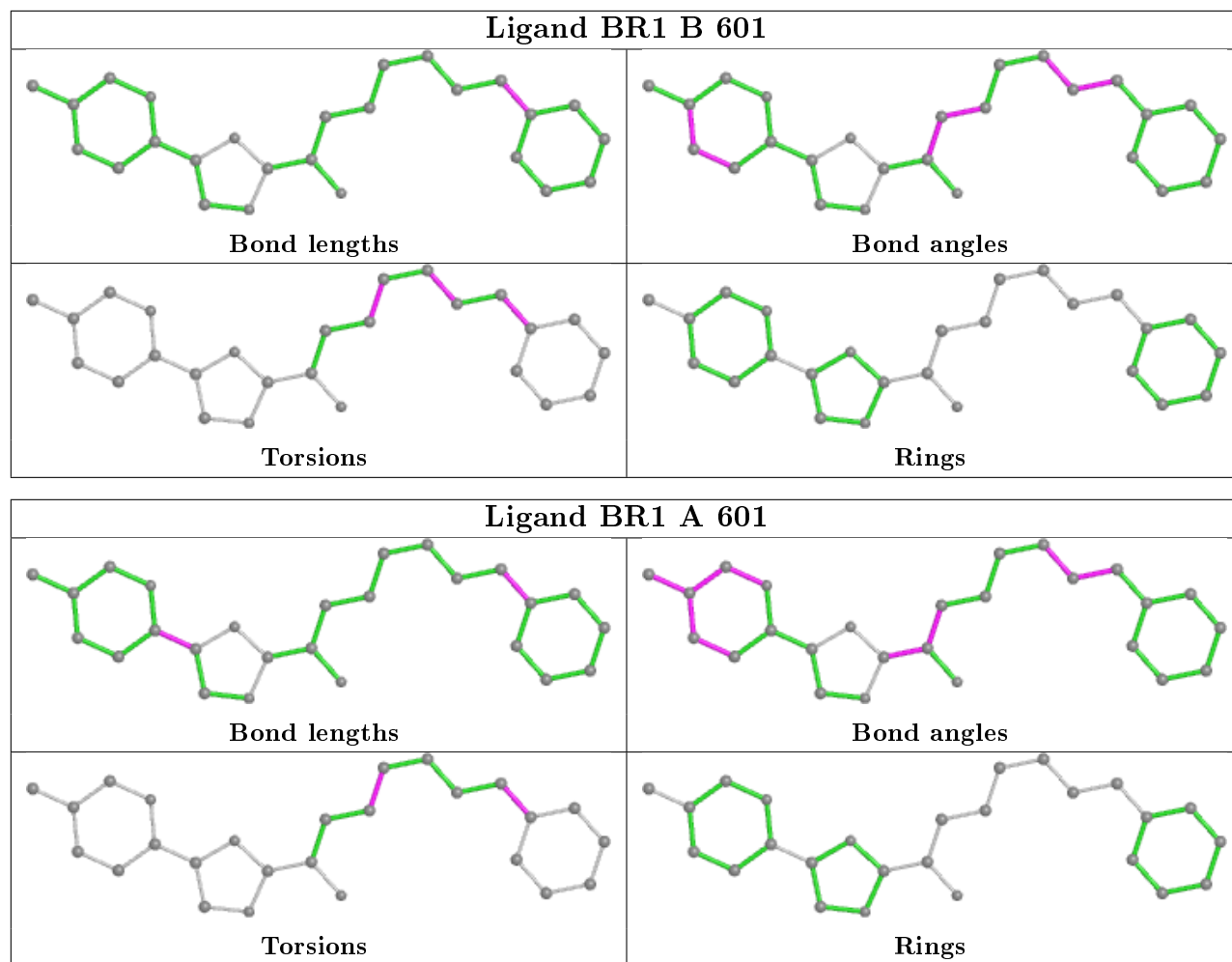
Mol	Chain	Res	Type	Atoms
3	B	604	PEG	O2-C3-C4-O4
3	B	602	PEG	O2-C3-C4-O4
3	A	603	PEG	O2-C3-C4-O4
3	A	602	PEG	O2-C3-C4-O4
3	A	603	PEG	C4-C3-O2-C2
3	B	603	PEG	C1-C2-O2-C3
3	B	602	PEG	O1-C1-C2-O2
3	A	602	PEG	O1-C1-C2-O2
2	A	601	BR1	C2-C3-C4-C5
3	B	604	PEG	C4-C3-O2-C2
2	B	601	BR1	C4-C5-C6-C7
3	A	603	PEG	O1-C1-C2-O2
2	B	601	BR1	C6-C7-C8-C9
2	B	601	BR1	C2-C3-C4-C5
2	A	601	BR1	C6-C7-C8-C13
2	A	601	BR1	C6-C7-C8-C9
3	B	603	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	BR1	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 [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(Å ²)	Q<0.9
1	A	544/573 (94%)	0.51	69 (12%) 3 5	37, 57, 88, 136	0
1	B	545/573 (95%)	0.38	56 (10%) 6 9	39, 57, 98, 117	0
All	All	1089/1146 (95%)	0.44	125 (11%) 4 7	37, 57, 95, 136	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	THR	6.7
1	B	575	GLN	5.5
1	A	69	LEU	5.5
1	A	242	ILE	5.1
1	A	64	LEU	4.8
1	B	126	SER	4.7
1	B	290	LEU	4.6
1	A	253	GLY	4.5
1	B	122	GLU	4.4
1	A	234	LEU	4.4
1	A	506	VAL	4.4
1	B	284	ALA	4.4
1	A	282	PRO	4.3
1	A	576	LYS	4.3
1	A	254	LEU	4.3
1	B	73	ALA	4.2
1	B	124	GLN	4.2
1	A	283	MET	4.1
1	B	234	LEU	4.1
1	B	125	LEU	4.0
1	A	491	VAL	4.0
1	B	283	MET	4.0
1	A	131	GLN	3.9
1	A	235	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	76	THR	3.9
1	A	323	ARG	3.8
1	B	232	LEU	3.8
1	B	59	VAL	3.8
1	A	414	PHE	3.6
1	B	251	ILE	3.6
1	B	139	VAL	3.6
1	A	68	ASP	3.5
1	B	424	PRO	3.5
1	B	282	PRO	3.4
1	B	242	ILE	3.4
1	A	425	LEU	3.4
1	A	417	LEU	3.3
1	B	72	GLU	3.3
1	A	290	LEU	3.3
1	A	89	GLY	3.3
1	B	127	GLN	3.2
1	A	239	GLY	3.1
1	B	33	GLY	3.1
1	A	244	PHE	3.1
1	A	575	GLN	3.1
1	A	73	ALA	3.1
1	A	504	ALA	3.1
1	A	240	GLY	3.0
1	A	252	CYS	3.0
1	A	394	GLY	3.0
1	B	233	GLY	2.9
1	B	121	CYS	2.9
1	B	74	LEU	2.9
1	A	87	GLN	2.9
1	A	88	SER	2.8
1	A	194	TYR	2.8
1	B	35	GLN	2.8
1	A	165	GLU	2.8
1	B	425	LEU	2.8
1	B	420	LEU	2.7
1	A	357	GLY	2.7
1	A	85	LYS	2.7
1	A	424	PRO	2.7
1	A	38	ARG	2.7
1	A	90	GLU	2.6
1	A	505	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	252	CYS	2.6
1	B	131	GLN	2.6
1	B	235	GLY	2.6
1	A	233	GLY	2.6
1	A	494	THR	2.5
1	B	61	ARG	2.5
1	B	245	PRO	2.5
1	A	276	VAL	2.5
1	B	281	GLY	2.5
1	B	90	GLU	2.5
1	A	130	ARG	2.5
1	A	420	LEU	2.5
1	A	492	SER	2.5
1	B	289	SER	2.4
1	A	57	LYS	2.4
1	A	493	TYR	2.4
1	A	139	VAL	2.4
1	B	421	LEU	2.4
1	A	140	SER	2.4
1	B	506	VAL	2.4
1	A	34	ARG	2.4
1	A	241	SER	2.4
1	A	232	LEU	2.3
1	A	284	ALA	2.3
1	A	396	PHE	2.3
1	A	216	GLY	2.3
1	A	475	LEU	2.3
1	B	208	TRP	2.3
1	B	396	PHE	2.3
1	B	253	GLY	2.2
1	A	551	CYS	2.2
1	B	62	PHE	2.2
1	A	92	SER	2.2
1	A	243	ARG	2.2
1	A	60	GLN	2.2
1	B	507	VAL	2.2
1	B	241	SER	2.2
1	A	514	ALA	2.2
1	B	230	SER	2.2
1	B	89	GLY	2.2
1	B	323	ARG	2.1
1	A	126	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	236	THR	2.1
1	B	491	VAL	2.1
1	B	426	PHE	2.1
1	A	86	LEU	2.1
1	B	576	LYS	2.1
1	A	255	LYS	2.1
1	A	389	LEU	2.1
1	B	79	LEU	2.1
1	B	67	PRO	2.1
1	B	140	SER	2.0
1	B	574	PRO	2.0
1	A	208	TRP	2.0
1	B	293	CYS	2.0
1	A	33	GLY	2.0
1	A	281	GLY	2.0
1	B	68	ASP	2.0
1	A	356	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	B	603	7/7	0.60	0.16	82,93,106,107	0
3	PEG	B	602	7/7	0.83	0.24	68,76,81,82	0
2	BR1	A	601	26/27	0.85	0.27	48,68,77,81	0
3	PEG	B	604	7/7	0.85	0.12	62,69,78,84	0
2	BR1	B	601	26/27	0.88	0.22	49,62,68,71	0
3	PEG	A	602	7/7	0.91	0.17	69,69,74,74	0

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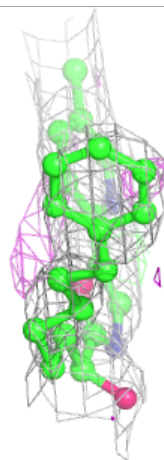
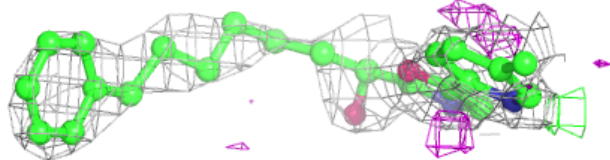
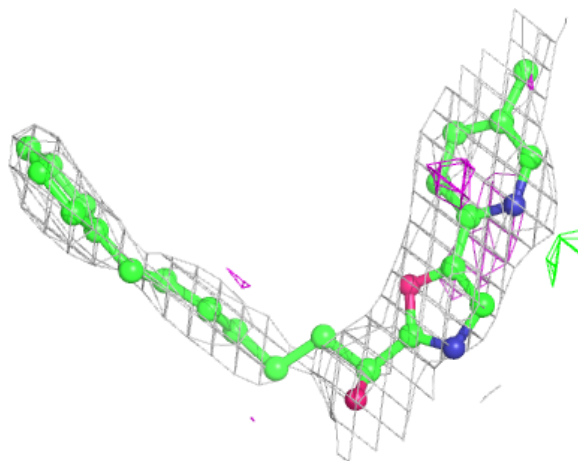
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	A	603	7/7	0.93	0.20	54,59,75,76	0
4	CL	B	605	1/1	0.94	0.15	48,48,48,48	0

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.

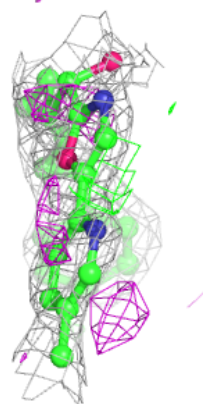
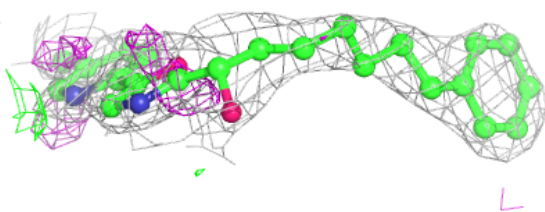
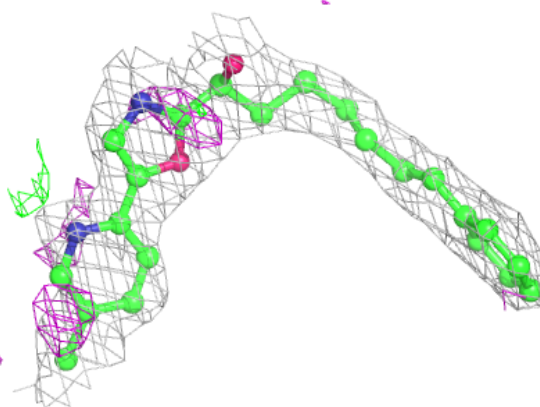
Electron density around BR1 A 601:

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 BR1 B 601:

$2mF_o-DF_c$ (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.