



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:01 AM UTC

PDB ID : 7ZBD / pdb_00007zbd
Title : HaloTag with TRaQ-G ligand
Authors : Emmert, S.; Rivera-Fuentes, P.; Pojer, F.; Lau, K.
Deposited on : 2022-03-23
Resolution : 1.68 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

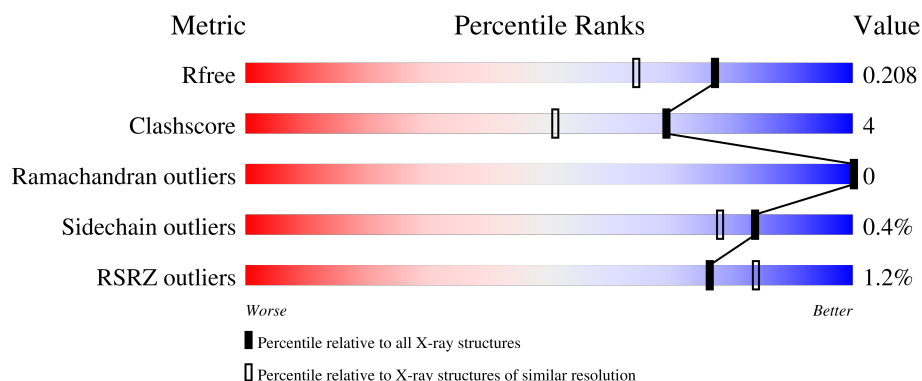
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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 $\leq 5\%$. 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	303	% 89% 7% .
1	B	303	% 87% 8% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5333 atoms, of which 101 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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	1	0
			2350	1529	395	417	9			
1	B	290	Total	C	N	O	S	0	2	0
			2344	1524	397	414	9			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P0A3G3
A	47	VAL	LEU	engineered mutation	UNP P0A3G3
A	58	THR	SER	engineered mutation	UNP P0A3G3
A	78	GLY	ASP	engineered mutation	UNP P0A3G3
A	87	PHE	TYR	engineered mutation	UNP P0A3G3
A	88	MET	LEU	engineered mutation	UNP P0A3G3
A	128	PHE	CYS	engineered mutation	UNP P0A3G3
A	155	THR	ALA	engineered mutation	UNP P0A3G3
A	160	LYS	GLU	engineered mutation	UNP P0A3G3
A	167	VAL	ALA	engineered mutation	UNP P0A3G3
A	172	THR	ALA	engineered mutation	UNP P0A3G3
A	175	MET	LYS	engineered mutation	UNP P0A3G3
A	176	GLY	CYS	engineered mutation	UNP P0A3G3
A	195	ASN	LYS	engineered mutation	UNP P0A3G3
A	224	GLU	ALA	engineered mutation	UNP P0A3G3
A	227	ASP	ASN	engineered mutation	UNP P0A3G3
A	257	LYS	GLU	engineered mutation	UNP P0A3G3
A	264	ALA	THR	engineered mutation	UNP P0A3G3
A	272	ASN	HIS	engineered mutation	UNP P0A3G3
A	273	LEU	TYR	engineered mutation	UNP P0A3G3
A	291	SER	-	expression tag	UNP P0A3G3
A	292	THR	-	expression tag	UNP P0A3G3
A	293	LEU	-	expression tag	UNP P0A3G3
A	294	GLU	-	expression tag	UNP P0A3G3
A	295	ILE	-	expression tag	UNP P0A3G3

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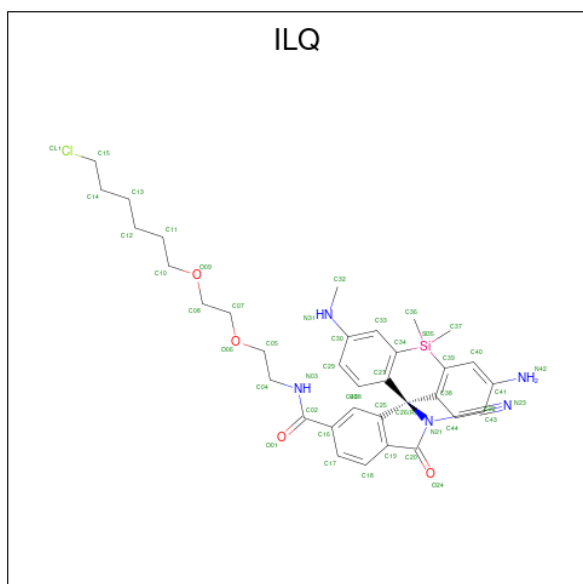
Chain	Residue	Modelled	Actual	Comment	Reference
A	296	SER	-	expression tag	UNP P0A3G3
A	297	GLY	-	expression tag	UNP P0A3G3
A	298	HIS	-	expression tag	UNP P0A3G3
A	299	HIS	-	expression tag	UNP P0A3G3
A	300	HIS	-	expression tag	UNP P0A3G3
A	301	HIS	-	expression tag	UNP P0A3G3
A	302	HIS	-	expression tag	UNP P0A3G3
A	303	HIS	-	expression tag	UNP P0A3G3
B	2	ALA	SER	engineered mutation	UNP P0A3G3
B	47	VAL	LEU	engineered mutation	UNP P0A3G3
B	58	THR	SER	engineered mutation	UNP P0A3G3
B	78	GLY	ASP	engineered mutation	UNP P0A3G3
B	87	PHE	TYR	engineered mutation	UNP P0A3G3
B	88	MET	LEU	engineered mutation	UNP P0A3G3
B	128	PHE	CYS	engineered mutation	UNP P0A3G3
B	155	THR	ALA	engineered mutation	UNP P0A3G3
B	160	LYS	GLU	engineered mutation	UNP P0A3G3
B	167	VAL	ALA	engineered mutation	UNP P0A3G3
B	172	THR	ALA	engineered mutation	UNP P0A3G3
B	175	MET	LYS	engineered mutation	UNP P0A3G3
B	176	GLY	CYS	engineered mutation	UNP P0A3G3
B	195	ASN	LYS	engineered mutation	UNP P0A3G3
B	224	GLU	ALA	engineered mutation	UNP P0A3G3
B	227	ASP	ASN	engineered mutation	UNP P0A3G3
B	257	LYS	GLU	engineered mutation	UNP P0A3G3
B	264	ALA	THR	engineered mutation	UNP P0A3G3
B	272	ASN	HIS	engineered mutation	UNP P0A3G3
B	273	LEU	TYR	engineered mutation	UNP P0A3G3
B	291	SER	-	expression tag	UNP P0A3G3
B	292	THR	-	expression tag	UNP P0A3G3
B	293	LEU	-	expression tag	UNP P0A3G3
B	294	GLU	-	expression tag	UNP P0A3G3
B	295	ILE	-	expression tag	UNP P0A3G3
B	296	SER	-	expression tag	UNP P0A3G3
B	297	GLY	-	expression tag	UNP P0A3G3
B	298	HIS	-	expression tag	UNP P0A3G3
B	299	HIS	-	expression tag	UNP P0A3G3
B	300	HIS	-	expression tag	UNP P0A3G3
B	301	HIS	-	expression tag	UNP P0A3G3
B	302	HIS	-	expression tag	UNP P0A3G3
B	303	HIS	-	expression tag	UNP P0A3G3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is (10R)-7-azanyl-N-[2-[2-(6-chloranylhexoxy)ethoxy]ethyl]-2'-cyano-5,5-dimethyl-3-(methylamino)-1'-oxidanylidene-spiro[benzo[b][1]benzosilole-10,3'-isoindole]-5'-carboxamide (CCD ID: ILQ) (formula: C₃₅H₄₂ClN₅O₄Si) (labeled as "Ligand of Interest" by depositor).

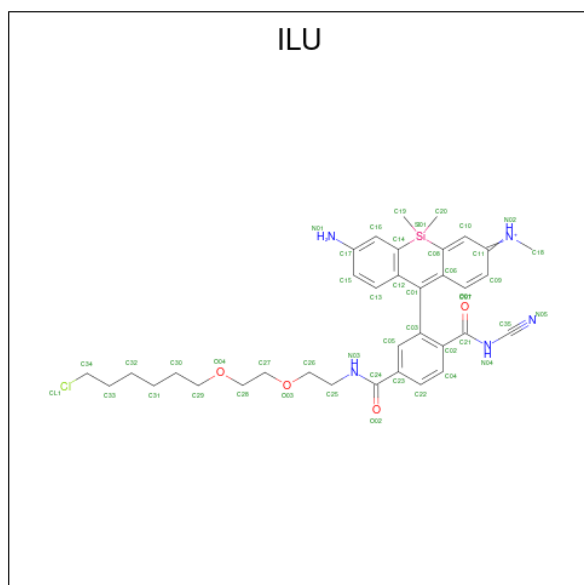


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	Si	0	0
			87	35	42	5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

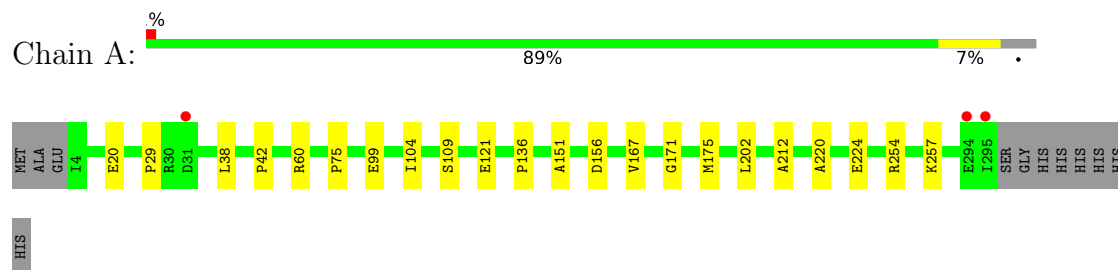
- Molecule 5 is [7-azanyl-10-[5-[2-[2-(6-chloranylhexoxy)ethoxy]ethylcarbamoyl]-2-(cyanocarbamoyl)phenyl]-5,5-dimethyl-benzo[b][1]benzosilin-3-ylidene]-methyl-azanium (CCD ID: ILU) (formula: C₃₅H₄₃ClN₅O₄Si) (labeled as "Ligand of Interest" by depositor).



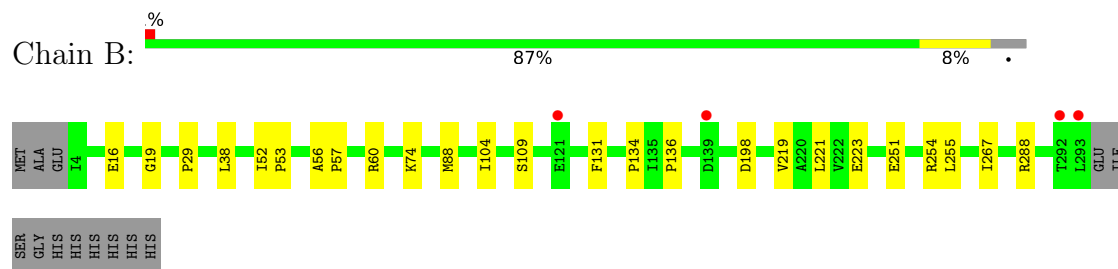
3 Residue-property plots

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: Haloalkane dehalogenase



- Molecule 1: Haloalkane dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.91Å 50.46Å 79.48Å 90.00° 117.74° 90.00°	Depositor
Resolution (Å)	47.75 – 1.68 47.75 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.75-1.68) 99.3 (47.75-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.222 (Not available) , 0.208	Depositor DCC
R_{free} test set	3303 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: CL, ILU, GOL, ILQ

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	0.52	0/2432	0.65	0/3326
1	B	0.49	0/2426	0.64	0/3317
All	All	0.51	0/4858	0.64	0/6643

There are no bond length outliers.

There are no bond angle outliers.

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	2350	0	2294	16	0
1	B	2344	0	2289	16	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
3	A	45	42	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	45	43	0	1	0
6	A	223	0	0	1	0
6	B	211	0	0	2	0
All	All	5232	101	4599	33	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 (33) 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:171:GLY:O	1:A:175:MET:HG3	1.56	1.05
1:A:20:GLU:HG3	1:A:75:PRO:HG3	1.64	0.79
1:A:29:PRO:O	1:A:60:ARG:HB2	1.99	0.63
1:B:16:GLU:HG3	6:B:678:HOH:O	1.99	0.62
1:A:121:GLU:H	1:A:121:GLU:CD	2.10	0.58
1:B:288[A]:ARG:HB3	1:B:288[A]:ARG:CZ	2.35	0.56
1:A:220:ALA:O	1:A:224:GLU:HG3	2.07	0.54
1:B:221:LEU:C	1:B:221:LEU:HD23	2.32	0.53
1:B:104:ILE:HB	1:B:109:SER:HA	1.90	0.52
1:A:42:PRO:HB3	1:A:202:LEU:HD22	1.91	0.52
1:A:99:GLU:OE1	1:A:99:GLU:N	2.39	0.51
1:A:254:ARG:NH1	1:A:254:ARG:HG2	2.27	0.49
1:A:104:ILE:HB	1:A:109:SER:HA	1.94	0.49
1:A:175:MET:HE1	3:A:402:ILQ:C43	2.44	0.48
1:B:134:PRO:O	1:B:136:PRO:HD3	2.15	0.46
1:B:29:PRO:O	1:B:60:ARG:HB2	2.16	0.46
1:B:38:LEU:HD22	1:B:88:MET:HE3	1.99	0.45
1:B:74:LYS:HE2	1:B:198:ASP:CG	2.41	0.45
1:B:219:VAL:O	1:B:223:GLU:HG3	2.16	0.45
1:B:74:LYS:HE3	6:B:503:HOH:O	2.15	0.45
1:A:156:ASP:OD1	1:A:156:ASP:N	2.50	0.44
1:B:131:PHE:HZ	1:B:255:LEU:HD13	1.82	0.44
1:A:151:ALA:HB3	3:A:402:ILQ:C32	2.48	0.43
1:B:56:ALA:N	1:B:57:PRO:CD	2.82	0.43
1:A:257:LYS:HB3	1:A:257:LYS:HE2	1.86	0.42
1:A:151:ALA:CB	3:A:402:ILQ:C32	2.98	0.42
1:B:16:GLU:OE2	1:B:19:GLY:HA2	2.20	0.42
1:B:251:GLU:OE1	1:B:254:ARG:NH1	2.53	0.41
1:B:74:LYS:CE	1:B:198:ASP:HB3	2.50	0.41
5:B:402:ILU:O01	5:B:402:ILU:C01	2.68	0.41
1:B:52:ILE:N	1:B:53:PRO:CD	2.84	0.41
1:A:136:PRO:O	1:A:212:ALA:HA	2.20	0.41
1:A:38:LEU:HA	6:A:592:HOH:O	2.21	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	291/303 (96%)	279 (96%)	12 (4%)	0	100	100
1	B	290/303 (96%)	280 (97%)	10 (3%)	0	100	100
All	All	581/606 (96%)	559 (96%)	22 (4%)	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	253/261 (97%)	252 (100%)	1 (0%)	84	78
1	B	252/261 (97%)	251 (100%)	1 (0%)	84	78
All	All	505/522 (97%)	503 (100%)	2 (0%)	84	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	VAL
1	B	267	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are 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	ILQ	A	402	1	47,49,50	2.73	10 (21%)	66,71,72	2.14	19 (28%)
5	ILU	B	402	1	46,48,49	2.71	13 (28%)	56,66,67	2.25	14 (25%)
2	GOL	B	401	-	5,5,5	0.76	0	5,5,5	1.08	1 (20%)
2	GOL	A	401	-	5,5,5	0.92	0	5,5,5	1.37	1 (20%)

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	ILQ	A	402	1	-	1/19/65/66	0/5/5/5
5	ILU	B	402	1	-	10/29/63/64	0/3/4/4
2	GOL	B	401	-	-	3/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	ILQ	C26-C27	10.85	1.67	1.51
5	B	402	ILU	C21-N04	9.49	1.45	1.35
5	B	402	ILU	C11-N02	9.09	1.44	1.30
3	A	402	ILQ	C26-C38	8.88	1.64	1.51
5	B	402	ILU	C35-N05	6.33	1.25	1.15
5	B	402	ILU	C24-N03	5.22	1.45	1.33
3	A	402	ILQ	C30-N31	5.01	1.47	1.37
3	A	402	ILQ	SI35-C34	-4.90	1.79	1.86
3	A	402	ILQ	C02-N03	4.52	1.43	1.33
3	A	402	ILQ	SI35-C39	-4.42	1.80	1.86
5	B	402	ILU	C06-C01	3.92	1.51	1.40
3	A	402	ILQ	C19-C20	3.59	1.54	1.48
3	A	402	ILQ	C34-C27	-3.51	1.37	1.41
5	B	402	ILU	SI01-C08	3.39	1.92	1.87
5	B	402	ILU	C10-C11	-3.16	1.39	1.45
5	B	402	ILU	C02-C21	3.02	1.56	1.50
3	A	402	ILQ	C19-C25	2.88	1.43	1.39
3	A	402	ILQ	C41-N42	2.33	1.46	1.38
5	B	402	ILU	C17-N01	2.31	1.46	1.38
5	B	402	ILU	SI01-C20	2.27	1.89	1.86
5	B	402	ILU	SI01-C19	2.12	1.89	1.86
5	B	402	ILU	C09-C11	-2.02	1.39	1.44
5	B	402	ILU	C03-C01	2.01	1.52	1.49

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	ILU	C02-C21-N04	9.57	126.96	115.32
3	A	402	ILQ	C28-C27-C26	-7.39	108.68	122.22
5	B	402	ILU	O01-C21-N04	-7.13	112.65	122.74
3	A	402	ILQ	C44-C38-C26	-6.02	111.20	122.22
5	B	402	ILU	C03-C01-C06	-5.68	113.40	120.33
3	A	402	ILQ	C26-C25-C19	-4.71	107.56	111.04
3	A	402	ILQ	C25-C26-N21	3.77	106.05	100.29
5	B	402	ILU	C03-C01-C12	-3.51	115.37	119.91
3	A	402	ILQ	C26-C38-C39	3.50	125.47	121.98
3	A	402	ILQ	C19-C20-N21	-3.48	103.20	106.13
3	A	402	ILQ	C28-C27-C34	3.42	126.14	119.36
3	A	402	ILQ	C41-C40-C39	-3.36	119.89	122.68
5	B	402	ILU	C07-C06-C01	-3.30	117.08	123.90
3	A	402	ILQ	C25-C26-C38	-3.12	107.90	112.17
3	A	402	ILQ	C26-C27-C34	3.08	125.05	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ILQ	C17-C16-C45	2.99	122.70	119.25
3	A	402	ILQ	C29-C28-C27	-2.95	116.58	122.02
3	A	402	ILQ	C38-C26-C27	2.91	113.18	110.38
5	B	402	ILU	C27-O03-C26	2.87	125.82	113.26
3	A	402	ILQ	C30-C33-C34	-2.81	120.35	122.68
2	A	401	GOL	C3-C2-C1	-2.66	102.02	111.80
3	A	402	ILQ	C32-N31-C30	-2.61	117.57	122.51
5	B	402	ILU	C26-C25-N03	-2.61	105.61	111.82
5	B	402	ILU	C16-C14-C12	2.57	121.52	118.32
5	B	402	ILU	C05-C03-C02	2.49	122.02	119.16
5	B	402	ILU	C13-C12-C01	-2.41	118.47	123.22
3	A	402	ILQ	C43-C44-C38	-2.32	117.74	122.02
3	A	402	ILQ	C38-C26-N21	-2.32	109.43	111.25
5	B	402	ILU	C04-C02-C03	-2.28	116.70	119.26
3	A	402	ILQ	SI35-C34-C27	2.27	123.69	121.42
5	B	402	ILU	C12-C01-C06	2.26	124.83	120.00
2	B	401	GOL	C3-C2-C1	-2.20	103.72	111.80
5	B	402	ILU	C07-C06-C08	2.09	117.74	115.64
3	A	402	ILQ	C16-C45-C25	-2.09	117.57	121.32
5	B	402	ILU	C05-C03-C01	-2.00	115.54	118.97

There are no chirality outliers.

All (16) torsion outliers are listed below:

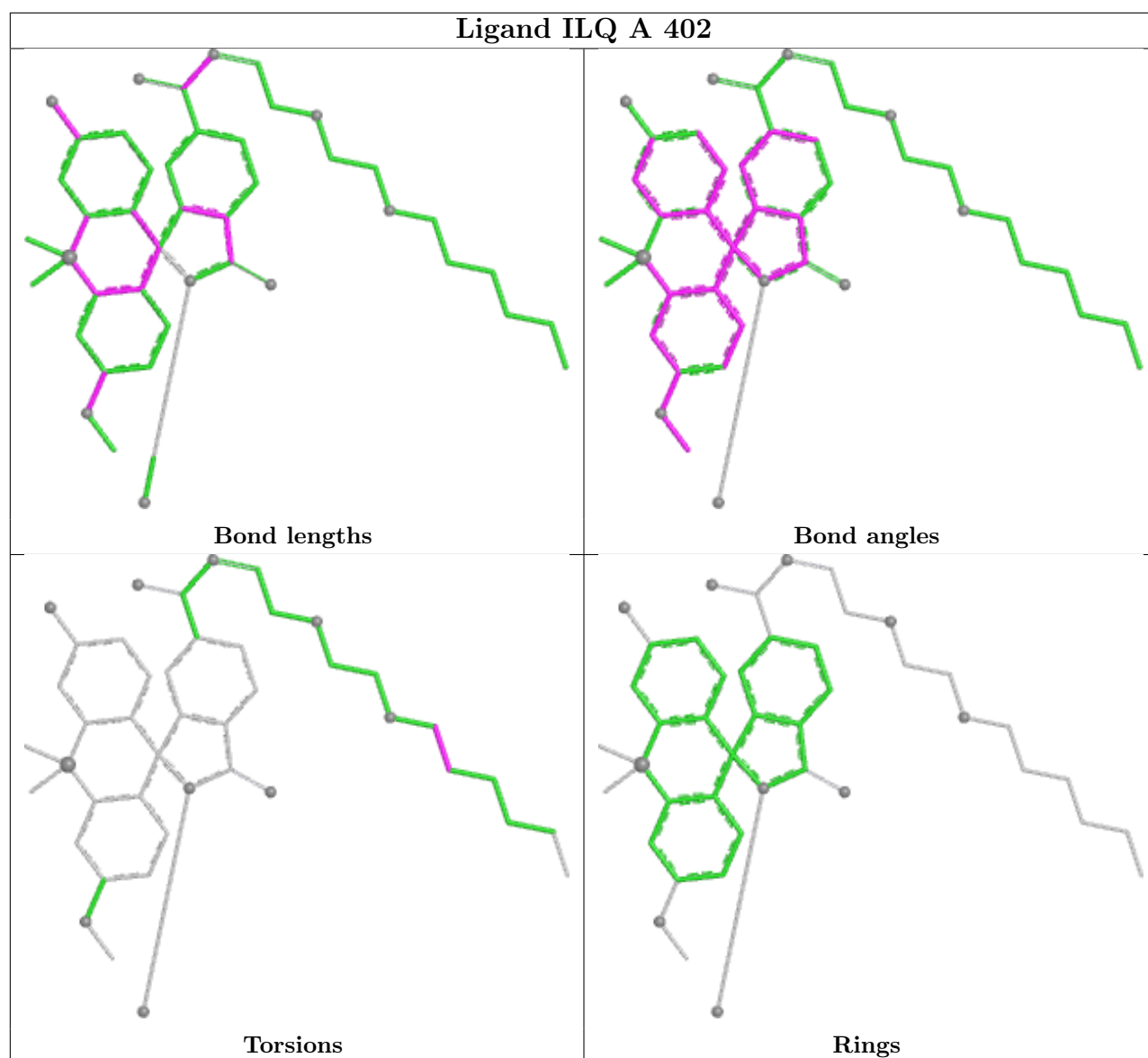
Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3
5	B	402	ILU	C03-C01-C12-C13
5	B	402	ILU	C06-C01-C12-C13
5	B	402	ILU	C02-C21-N04-C35
2	A	401	GOL	O2-C2-C3-O3
5	B	402	ILU	C03-C02-C21-O01
5	B	402	ILU	O01-C21-N04-C35
5	B	402	ILU	O03-C27-C28-O04
3	A	402	ILQ	O09-C10-C11-C12
5	B	402	ILU	C03-C02-C21-N04
5	B	402	ILU	N03-C25-C26-O03
2	B	401	GOL	O1-C1-C2-O2
5	B	402	ILU	C25-C26-O03-C27
5	B	402	ILU	C28-C27-O03-C26
2	B	401	GOL	C1-C2-C3-O3

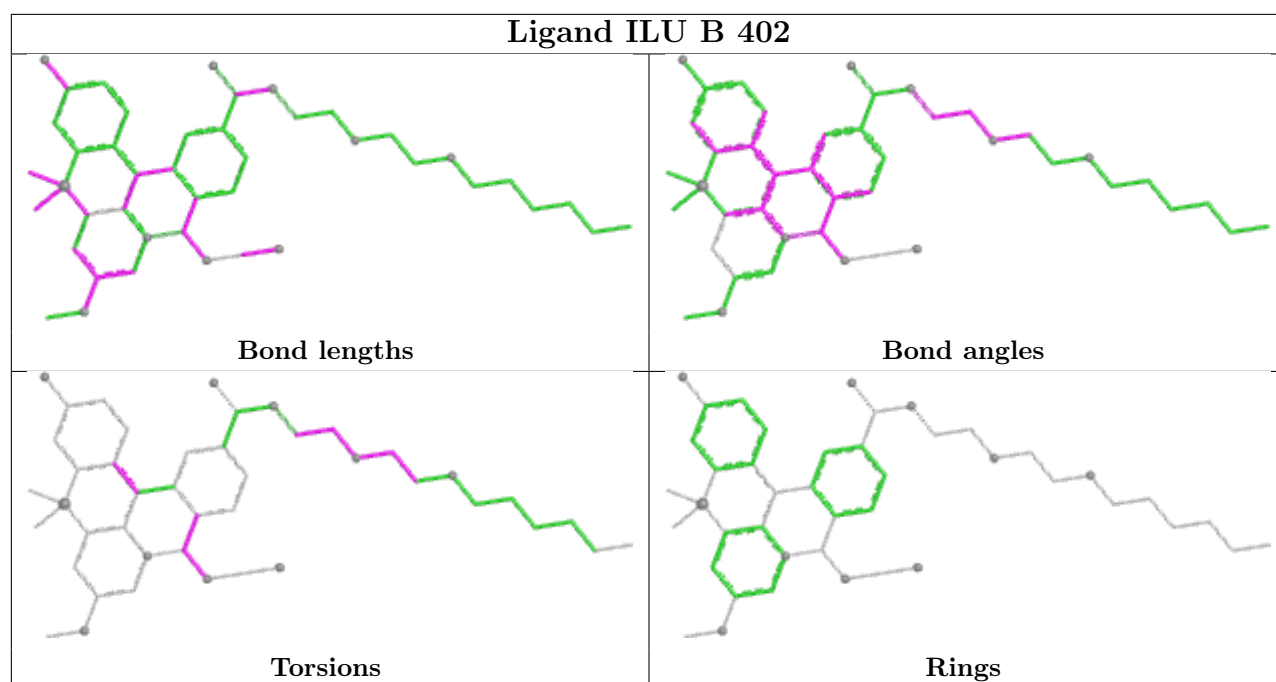
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	ILQ	3	0
5	B	402	ILU	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 [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	292/303 (96%)	0.18	3 (1%) 79 86	15, 25, 36, 55	1 (0%)
1	B	290/303 (95%)	0.32	4 (1%) 73 81	16, 26, 36, 51	2 (0%)
All	All	582/606 (96%)	0.25	7 (1%) 76 84	15, 25, 36, 55	3 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	3.2
1	B	293	LEU	3.0
1	A	31	ASP	2.7
1	A	294	GLU	2.6
1	B	139	ASP	2.5
1	B	121	GLU	2.1
1	B	292	THR	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

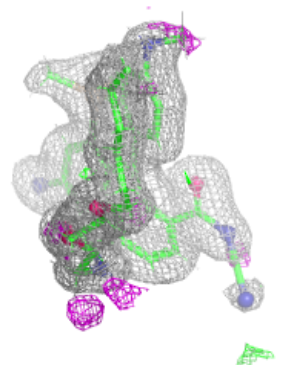
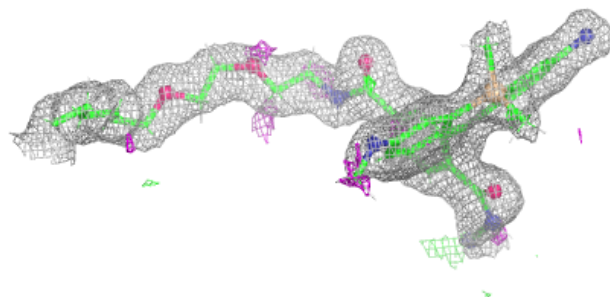
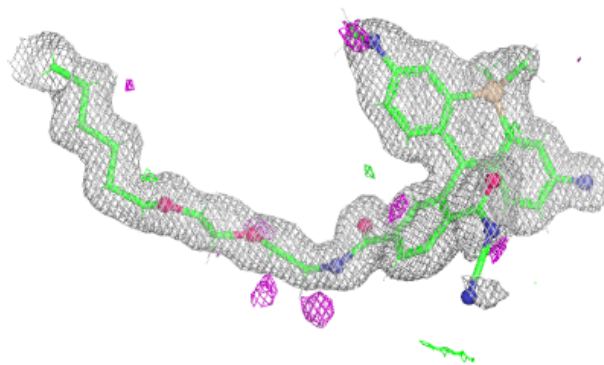
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	401	6/6	0.63	0.17	42,52,62,65	0
2	GOL	B	401	6/6	0.86	0.11	38,48,51,58	0
5	ILU	B	402	45/46	0.92	0.09	21,31,43,55	0
3	ILQ	A	402	45/46	0.94	0.09	18,27,44,77	0
4	CL	B	403	1/1	0.99	0.03	19,19,19,19	0
4	CL	A	403	1/1	1.00	0.03	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.

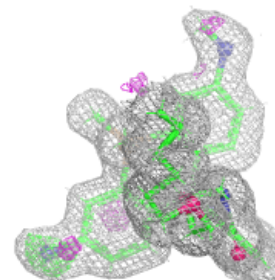
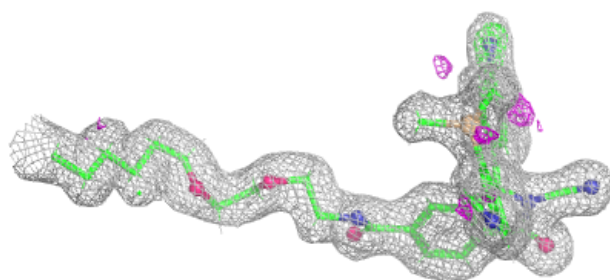
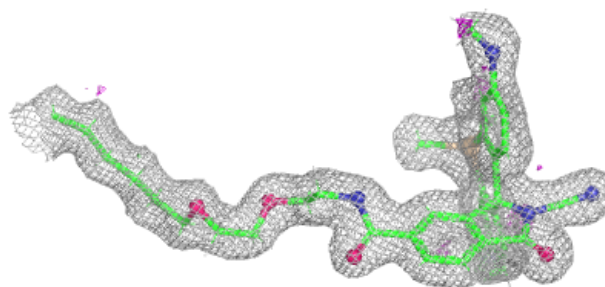
Electron density around ILU B 402:

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 ILQ A 402:

$2mF_o-DF_c$ (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.