



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:46 AM UTC

PDB ID : 5UXZ / pdb_00005uxz
Title : X-ray crystal structure of Halotag bound to the P9 benzothiadiazole fluorogenic ligand
Authors : Dunham, N.P.; Boal, A.K.
Deposited on : 2017-02-23
Resolution : 1.92 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

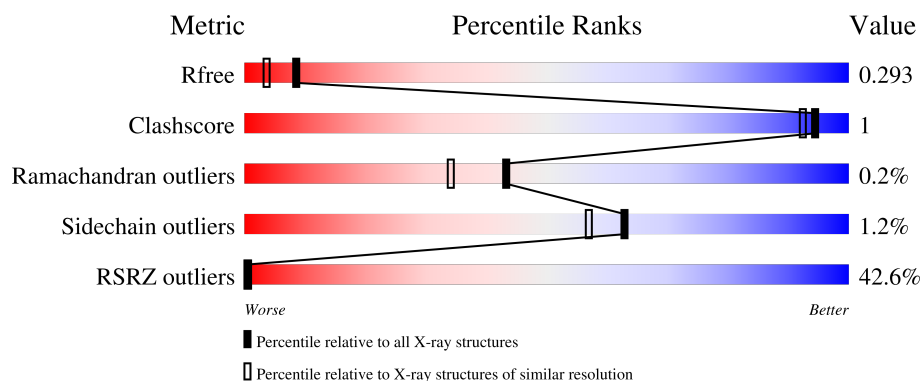
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	307	25% 92% 6%
1	B	307	56% 90% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4827 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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2328	1515	392	412	9			
1	B	295	Total	C	N	O	S	0	0	0
			2363	1537	397	420	9			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	VAL	LEU	conflict	UNP P0A3G2
A	58	THR	SER	conflict	UNP P0A3G2
A	78	GLY	ASP	conflict	UNP P0A3G2
A	87	PHE	TYR	conflict	UNP P0A3G2
A	88	MET	LEU	conflict	UNP P0A3G2
A	128	PHE	CYS	conflict	UNP P0A3G2
A	155	THR	ALA	conflict	UNP P0A3G2
A	160	LYS	GLU	conflict	UNP P0A3G2
A	167	VAL	ALA	conflict	UNP P0A3G2
A	172	THR	ALA	conflict	UNP P0A3G2
A	175	MET	LYS	conflict	UNP P0A3G2
A	176	GLY	CYS	conflict	UNP P0A3G2
A	195	ASN	LYS	conflict	UNP P0A3G2
A	224	GLU	ALA	conflict	UNP P0A3G2
A	227	ASP	ASN	conflict	UNP P0A3G2
A	257	LYS	GLU	conflict	UNP P0A3G2
A	264	ALA	THR	conflict	UNP P0A3G2
A	272	ASN	HIS	conflict	UNP P0A3G2
A	273	LEU	TYR	conflict	UNP P0A3G2
A	291	SER	-	expression tag	UNP P0A3G2
A	293	THR	-	expression tag	UNP P0A3G2
A	294	LEU	-	expression tag	UNP P0A3G2
A	295	GLU	-	expression tag	UNP P0A3G2
A	296	ILE	-	expression tag	UNP P0A3G2
A	297	SER	-	expression tag	UNP P0A3G2

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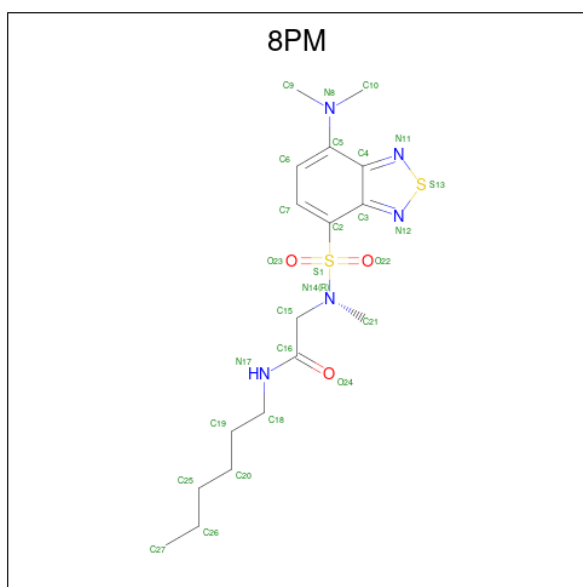
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLY	-	expression tag	UNP P0A3G2
A	299	LEU	-	expression tag	UNP P0A3G2
A	300	GLU	-	expression tag	UNP P0A3G2
A	301	ILE	-	expression tag	UNP P0A3G2
A	302	SER	-	expression tag	UNP P0A3G2
A	303	GLY	-	expression tag	UNP P0A3G2
A	304	LEU	-	expression tag	UNP P0A3G2
A	305	GLU	-	expression tag	UNP P0A3G2
A	306	HIS	-	expression tag	UNP P0A3G2
A	307	HIS	-	expression tag	UNP P0A3G2
A	308	HIS	-	expression tag	UNP P0A3G2
A	309	HIS	-	expression tag	UNP P0A3G2
A	310	HIS	-	expression tag	UNP P0A3G2
A	311	HIS	-	expression tag	UNP P0A3G2
B	47	VAL	LEU	conflict	UNP P0A3G2
B	58	THR	SER	conflict	UNP P0A3G2
B	78	GLY	ASP	conflict	UNP P0A3G2
B	87	PHE	TYR	conflict	UNP P0A3G2
B	88	MET	LEU	conflict	UNP P0A3G2
B	128	PHE	CYS	conflict	UNP P0A3G2
B	155	THR	ALA	conflict	UNP P0A3G2
B	160	LYS	GLU	conflict	UNP P0A3G2
B	167	VAL	ALA	conflict	UNP P0A3G2
B	172	THR	ALA	conflict	UNP P0A3G2
B	175	MET	LYS	conflict	UNP P0A3G2
B	176	GLY	CYS	conflict	UNP P0A3G2
B	195	ASN	LYS	conflict	UNP P0A3G2
B	224	GLU	ALA	conflict	UNP P0A3G2
B	227	ASP	ASN	conflict	UNP P0A3G2
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B	264	ALA	THR	conflict	UNP P0A3G2
B	272	ASN	HIS	conflict	UNP P0A3G2
B	273	LEU	TYR	conflict	UNP P0A3G2
B	291	SER	-	expression tag	UNP P0A3G2
B	292	THR	-	expression tag	UNP P0A3G2
B	293	LEU	-	expression tag	UNP P0A3G2
B	294	GLU	-	expression tag	UNP P0A3G2
B	295	ILE	-	expression tag	UNP P0A3G2
B	296	SER	-	expression tag	UNP P0A3G2
B	297	GLY	-	expression tag	UNP P0A3G2
B	298	LEU	-	expression tag	UNP P0A3G2
B	299	GLU	-	expression tag	UNP P0A3G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	ILE	-	expression tag	UNP P0A3G2
B	301	SER	-	expression tag	UNP P0A3G2
B	302	GLY	-	expression tag	UNP P0A3G2
B	303	LEU	-	expression tag	UNP P0A3G2
B	304	GLU	-	expression tag	UNP P0A3G2
B	305	HIS	-	expression tag	UNP P0A3G2
B	306	HIS	-	expression tag	UNP P0A3G2
B	307	HIS	-	expression tag	UNP P0A3G2
B	308	HIS	-	expression tag	UNP P0A3G2
B	309	HIS	-	expression tag	UNP P0A3G2
B	310	HIS	-	expression tag	UNP P0A3G2

- Molecule 2 is N 2 -{[7-(dimethylamino)-2,1,3-benzothiadiazol-4-yl]sulfonyl}-N-hexyl-N 2 -methylglycinamide (CCD ID: 8PM) (formula: C₁₇H₂₇N₅O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	17	5	3	2		
2	B	1	Total	C	N	O	S	0	0
			27	17	5	3	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	19	Total	O	0	0
			19	19		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.94Å 69.12Å 83.90Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 50.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	81.9 (50.00-1.92) 81.9 (50.00-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.269 , 0.287 0.274 , 0.293	Depositor DCC
R_{free} test set	1806 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4827	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: EDO, CL, 8PM

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	0.48	1/2407 (0.0%)	0.68	0/3292
1	B	0.47	1/2442 (0.0%)	0.67	0/3339
All	All	0.48	2/4849 (0.0%)	0.68	0/6631

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	ASP	CG-OD1	10.85	1.46	1.25
1	A	106	ASP	CG-OD1	10.53	1.45	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2328	0	2271	2	0
1	B	2363	0	2307	10	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	0	0	0
5	B	19	0	0	0	0
All	All	4827	0	4590	12	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 1.

All (12) 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:275:GLN:HE21	1:A:275:GLN:H	1.53	0.56
1:B:275:GLN:HE21	1:B:275:GLN:H	1.59	0.51
1:B:200:GLU:N	1:B:201:PRO:HD2	2.29	0.46
1:B:245:VAL:HG11	2:B:401:8PM:O24	2.17	0.44
1:B:193:PHE:CZ	1:B:202:LEU:HD21	2.53	0.44
1:B:56:ALA:N	1:B:57:PRO:CD	2.82	0.43
1:B:129:MET:O	1:B:130:GLU:C	2.62	0.43
1:B:64:PRO:HB3	1:B:91:PHE:CZ	2.54	0.42
1:B:42:PRO:HB3	1:B:202:LEU:HD22	2.02	0.42
1:B:172:THR:HA	1:B:175:MET:HE3	2.02	0.42
1:B:107:TRP:CD2	1:B:132:ILE:CD1	3.05	0.40
1:A:200:GLU:N	1:A:201:PRO:CD	2.85	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	288/307 (94%)	275 (96%)	13 (4%)	0	100	100
1	B	293/307 (95%)	278 (95%)	14 (5%)	1 (0%)	36	26
All	All	581/614 (95%)	553 (95%)	27 (5%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	ASN

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	250/265 (94%)	246 (98%)	4 (2%)	55	44
1	B	254/265 (96%)	252 (99%)	2 (1%)	73	71
All	All	504/530 (95%)	498 (99%)	6 (1%)	63	57

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	156	ASP
1	A	267	ILE
1	A	275	GLN
1	B	275	GLN
1	B	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	59	HIS
1	A	114	HIS
1	A	119	ASN
1	A	272	ASN
1	A	275	GLN
1	A	278	ASN
1	B	217	ASN
1	B	275	GLN
1	B	278	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 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$
4	EDO	A	404	-	3,3,3	0.41	0	2,2,2	0.30	0
4	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.18	0
2	8PM	A	401	1	28,28,28	3.29	6 (21%)	33,39,39	2.74	10 (30%)
2	8PM	B	401	1	28,28,28	3.24	6 (21%)	33,39,39	2.66	11 (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
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
2	8PM	A	401	1	-	10/27/27/27	0/2/2/2
2	8PM	B	401	1	-	8/27/27/27	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	8PM	C2-S1	-12.19	1.60	1.77
2	B	401	8PM	C2-S1	-11.61	1.61	1.77
2	B	401	8PM	C2-C3	9.83	1.49	1.42
2	A	401	8PM	C2-C3	9.75	1.49	1.42
2	A	401	8PM	S13-N12	4.21	1.69	1.62
2	B	401	8PM	S13-N12	4.10	1.69	1.62
2	B	401	8PM	S13-N11	4.05	1.68	1.62
2	A	401	8PM	S13-N11	4.03	1.68	1.62
2	B	401	8PM	C5-C4	3.98	1.50	1.41
2	A	401	8PM	C5-C4	3.96	1.50	1.41
2	B	401	8PM	C3-C4	2.14	1.51	1.45
2	A	401	8PM	C3-C4	2.05	1.51	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	8PM	O23-S1-O22	-7.75	107.50	119.59
2	A	401	8PM	O23-S1-O22	-7.56	107.79	119.59
2	A	401	8PM	C7-C6-C5	6.77	122.76	116.82
2	B	401	8PM	C7-C6-C5	6.64	122.65	116.82
2	A	401	8PM	C2-C3-C4	-5.24	117.68	121.86
2	B	401	8PM	C2-C3-C4	-5.11	117.79	121.86
2	A	401	8PM	O22-S1-N14	4.86	112.83	107.02
2	A	401	8PM	C4-N11-S13	4.56	107.17	104.58
2	B	401	8PM	C3-N12-S13	4.56	107.17	104.58
2	B	401	8PM	C4-N11-S13	4.51	107.14	104.58
2	B	401	8PM	C2-S1-N14	4.36	117.12	106.39
2	A	401	8PM	C3-N12-S13	4.22	106.97	104.58
2	A	401	8PM	O23-S1-N14	3.63	111.35	107.02
2	A	401	8PM	C7-C2-S1	2.46	120.83	117.48
2	A	401	8PM	C16-C15-N14	-2.40	109.49	116.15
2	B	401	8PM	C15-C16-N17	2.22	120.48	115.64
2	B	401	8PM	C10-N8-C5	2.19	121.94	115.16
2	B	401	8PM	O24-C16-N17	-2.15	118.81	123.03
2	A	401	8PM	C21-N14-C15	-2.12	109.75	115.09
2	B	401	8PM	C18-N17-C16	2.09	126.71	122.82
2	B	401	8PM	C7-C2-C3	-2.02	119.50	121.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

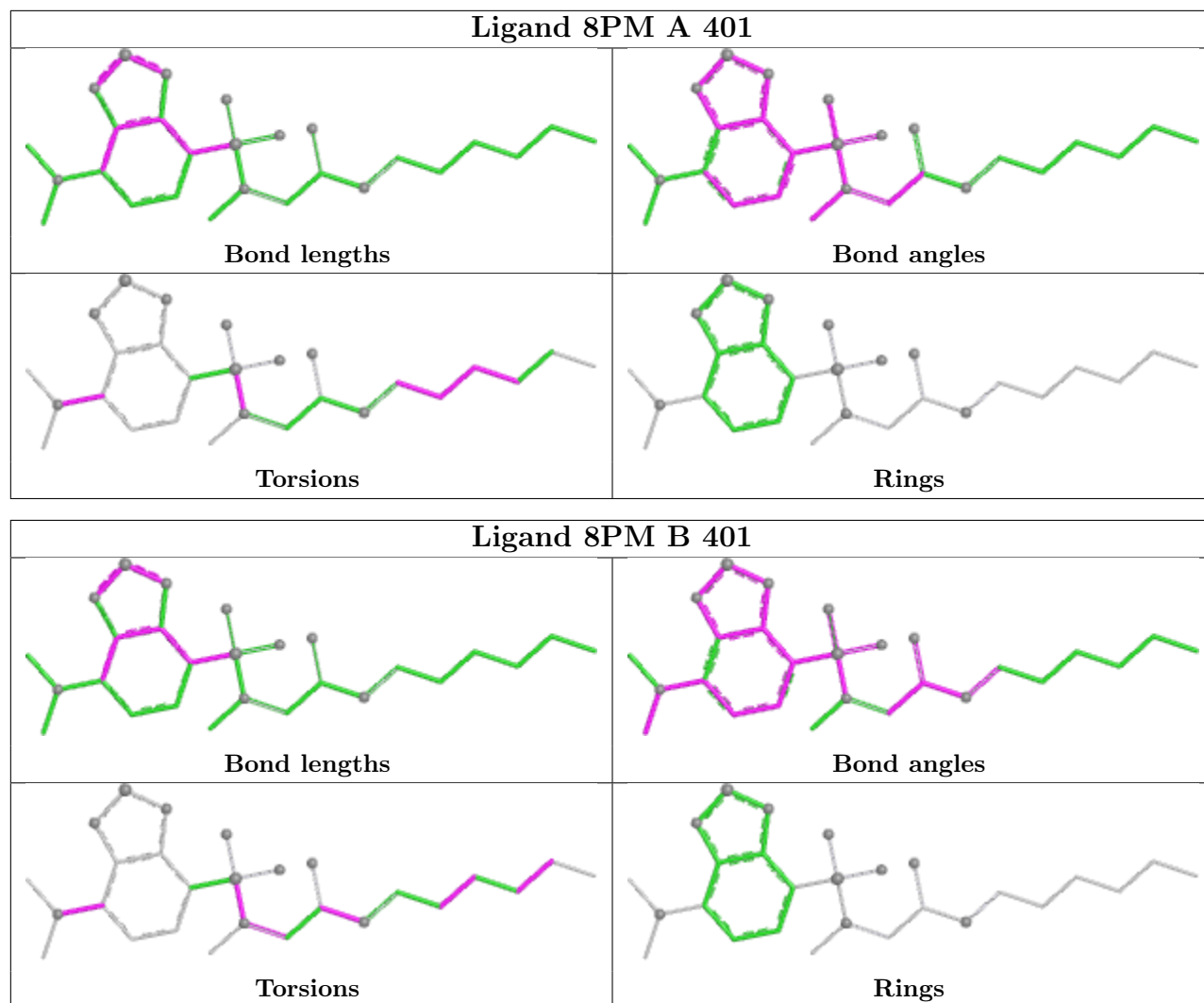
Mol	Chain	Res	Type	Atoms
2	A	401	8PM	C21-N14-S1-O22
2	B	401	8PM	C16-C15-N14-C21
2	B	401	8PM	O24-C16-N17-C18
2	A	401	8PM	N17-C18-C19-C20
2	B	401	8PM	C15-C16-N17-C18
2	B	401	8PM	C18-C19-C20-C25
4	A	404	EDO	O1-C1-C2-O2
2	A	401	8PM	C19-C20-C25-C26
2	B	401	8PM	C20-C25-C26-C27
2	A	401	8PM	C15-N14-S1-O23
2	A	401	8PM	C21-N14-S1-C2
2	A	401	8PM	C6-C5-N8-C9
2	B	401	8PM	C6-C5-N8-C10
2	A	401	8PM	C18-C19-C20-C25
2	A	401	8PM	C15-N14-S1-C2
2	A	401	8PM	C15-N14-S1-O22
2	A	401	8PM	C21-N14-S1-O23
2	B	401	8PM	C21-N14-S1-O23
2	B	401	8PM	C4-C5-N8-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	8PM	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	290/307 (94%)	1.32	78 (26%) 1 1	5, 16, 36, 41	33 (11%)
1	B	295/307 (96%)	2.45	171 (57%) 0 0	11, 30, 50, 57	33 (11%)
All	All	585/614 (95%)	1.89	249 (42%) 0 0	5, 23, 46, 57	66 (11%)

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	LEU	8.3
1	B	17	VAL	7.8
1	B	193	PHE	7.0
1	A	157	VAL	6.7
1	B	157	VAL	6.6
1	B	203	TRP	6.5
1	B	137	THR	6.4
1	B	212	ALA	6.2
1	B	162	ILE	5.9
1	B	298	LEU	5.7
1	B	144	PHE	5.5
1	B	138	TRP	5.5
1	B	56	ALA	5.5
1	B	165	GLN	5.5
1	B	136	PRO	5.4
1	A	288	ARG	5.3
1	B	28	GLY	5.2
1	B	192	PRO	5.2
1	B	211	ILE	5.2
1	B	288	ARG	5.1
1	B	142	PRO	5.1
1	B	31	ASP	4.9
1	B	25	VAL	4.9
1	A	135	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	29	PRO	4.9
1	B	156	ASP	4.8
1	B	71	LYS	4.8
1	B	167	VAL	4.7
1	A	229	LEU	4.7
1	B	79	TYR	4.7
1	A	144	PHE	4.6
1	B	140	GLU	4.6
1	B	76	ASP	4.6
1	B	155	THR	4.6
1	B	77	LEU	4.6
1	B	188	HIS	4.5
1	B	90	ALA	4.5
1	B	161	LEU	4.5
1	A	261	ASN	4.5
1	B	160	LYS	4.4
1	B	197	VAL	4.4
1	A	256	ALA	4.4
1	B	21	ARG	4.4
1	B	147	GLU	4.4
1	B	152	PHE	4.3
1	B	14	TYR	4.3
1	B	135	ILE	4.3
1	B	16	GLU	4.3
1	A	137	THR	4.2
1	B	154	THR	4.2
1	B	143	GLU	4.2
1	B	141	TRP	4.2
1	A	293	THR	4.2
1	B	19	GLY	4.2
1	A	215	PRO	4.1
1	A	220	ALA	4.1
1	A	227	ASP	4.1
1	B	213	GLY	4.1
1	A	219	VAL	4.0
1	B	27	VAL	4.0
1	B	196	PRO	4.0
1	B	74	LYS	4.0
1	B	98	GLU	4.0
1	B	151	ALA	4.0
1	B	254	ARG	3.9
1	A	263	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	254	ARG	3.8
1	B	184	VAL	3.8
1	B	148	THR	3.8
1	B	149	PHE	3.8
1	B	207	ASN	3.8
1	A	203	TRP	3.8
1	B	163	ILE	3.7
1	B	158	GLY	3.7
1	A	136	PRO	3.7
1	B	218	ILE	3.7
1	B	209	LEU	3.7
1	A	188	HIS	3.7
1	B	145	ALA	3.6
1	B	24	TYR	3.6
1	B	15	VAL	3.6
1	B	58	THR	3.6
1	B	169	ILE	3.6
1	A	228	TRP	3.6
1	B	164	ASP	3.6
1	A	156	ASP	3.5
1	A	221	LEU	3.5
1	B	75	PRO	3.5
1	B	245	VAL	3.5
1	B	20	GLU	3.5
1	A	145	ALA	3.5
1	B	10	PHE	3.5
1	B	297	GLY	3.5
1	B	198	ASP	3.5
1	A	138	TRP	3.4
1	A	148	THR	3.4
1	B	94	ALA	3.4
1	B	215	PRO	3.4
1	A	226	MET	3.4
1	B	191	GLU	3.4
1	A	231	GLN	3.4
1	B	195	ASN	3.4
1	A	230	HIS	3.3
1	A	99	GLU	3.3
1	A	147	GLU	3.3
1	B	99	GLU	3.3
1	B	8	PHE	3.3
1	A	151	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	229	LEU	3.3
1	B	57	PRO	3.2
1	B	171	GLY	3.2
1	A	216	ALA	3.2
1	A	224	GLU	3.2
1	A	119	ASN	3.2
1	B	70	GLY	3.2
1	B	82	ASP	3.2
1	B	80	PHE	3.2
1	B	124	LYS	3.1
1	B	153	ARG	3.1
1	B	139	ASP	3.1
1	B	182	THR	3.1
1	B	12	PRO	3.1
1	B	202	LEU	3.1
1	A	141	TRP	3.1
1	B	246	LEU	3.1
1	A	197	VAL	3.1
1	A	152	PHE	3.0
1	B	13	HIS	3.0
1	A	213	GLY	3.0
1	B	7	GLY	3.0
1	A	98	GLU	3.0
1	B	201	PRO	3.0
1	B	260	PRO	3.0
1	A	250	ALA	3.0
1	B	30	ARG	3.0
1	B	18	LEU	3.0
1	A	225	TYR	3.0
1	B	258	SER	3.0
1	A	133	ARG	3.0
1	B	287	ALA	3.0
1	A	217	ASN	3.0
1	B	200	GLU	3.0
1	B	59	HIS	2.9
1	A	255	LEU	2.9
1	B	231	GLN	2.9
1	B	227	ASP	2.9
1	B	146	ARG	2.9
1	B	78	GLY	2.9
1	B	221	LEU	2.8
1	B	230	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	139	ASP	2.8
1	B	168	PHE	2.8
1	B	204	ARG	2.8
1	A	155	THR	2.8
1	B	23	HIS	2.8
1	B	292	THR	2.8
1	A	260	PRO	2.8
1	A	31	ASP	2.8
1	A	253	ALA	2.8
1	A	160	LYS	2.8
1	B	255	LEU	2.8
1	B	134	PRO	2.8
1	B	97	LEU	2.7
1	B	26	ASP	2.7
1	B	11	ASP	2.7
1	B	159	ARG	2.7
1	B	199	ARG	2.7
1	B	259	LEU	2.7
1	B	252	ALA	2.6
1	B	294	GLU	2.6
1	B	180	PRO	2.6
1	B	217	ASN	2.6
1	A	252	ALA	2.6
1	A	259	LEU	2.6
1	B	4	ILE	2.6
1	B	96	GLY	2.6
1	A	163	ILE	2.6
1	A	212	ALA	2.6
1	B	234	VAL	2.6
1	B	87	PHE	2.5
1	B	290	LEU	2.5
1	B	33	THR	2.5
1	A	214	GLU	2.5
1	B	247	ILE	2.5
1	B	6	THR	2.5
1	B	121	GLU	2.5
1	A	258	SER	2.5
1	B	295	ILE	2.5
1	A	123	VAL	2.5
1	A	142	PRO	2.4
1	B	222	VAL	2.4
1	A	158	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	95	LEU	2.4
1	B	9	PRO	2.4
1	A	265	VAL	2.4
1	B	85	VAL	2.4
1	A	195	ASN	2.4
1	B	173	LEU	2.4
1	B	181	LEU	2.4
1	B	91	PHE	2.4
1	A	211	ILE	2.4
1	B	67	ILE	2.4
1	B	250	ALA	2.4
1	B	214	GLU	2.4
1	B	190	ARG	2.3
1	A	264	ALA	2.3
1	B	120	PRO	2.3
1	B	22	MET	2.3
1	B	187	ASP	2.3
1	B	166	ASN	2.3
1	A	232	SER	2.3
1	B	81	PHE	2.3
1	B	64	PRO	2.3
1	B	216	ALA	2.3
1	A	218	ILE	2.3
1	B	92	ILE	2.3
1	A	154	THR	2.3
1	A	294	LEU	2.3
1	B	175	MET	2.3
1	B	189	TYR	2.2
1	B	220	ALA	2.2
1	A	235	PRO	2.2
1	A	234	VAL	2.2
1	A	140	GLU	2.2
1	A	223	GLU	2.2
1	A	249	PRO	2.2
1	A	116	ALA	2.2
1	B	208	GLU	2.2
1	B	100	VAL	2.2
1	A	82	ASP	2.2
1	B	66	LEU	2.2
1	B	51	ILE	2.1
1	B	150	GLN	2.1
1	B	219	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	72	SER	2.1
1	A	233	PRO	2.1
1	B	261	ASN	2.1
1	A	291	SER	2.1
1	A	71	LYS	2.1
1	B	205	PHE	2.1
1	B	257	LYS	2.1
1	A	245	VAL	2.1
1	B	73	ASP	2.1
1	A	284	SER	2.0
1	B	263	LYS	2.0
1	B	5	GLY	2.0
1	B	32	GLY	2.0
1	B	101	VAL	2.0
1	B	123	VAL	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 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.

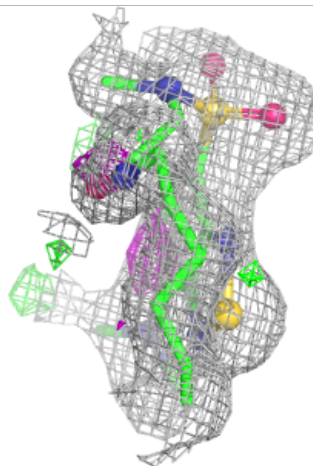
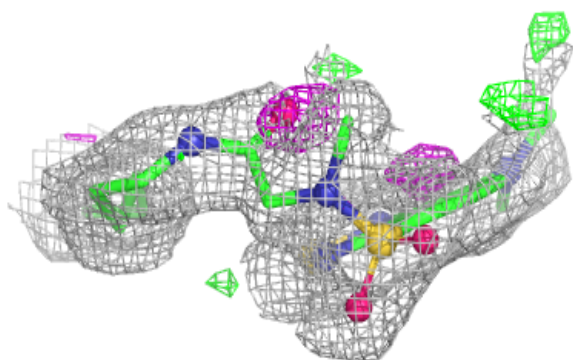
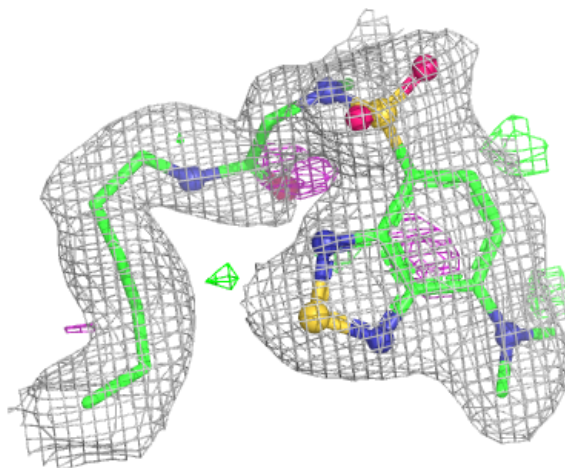
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8PM	B	401	27/27	0.84	0.14	20,31,33,33	0
2	8PM	A	401	27/27	0.85	0.12	14,23,25,25	0
4	EDO	A	403	4/4	0.87	0.11	17,18,18,18	0
4	EDO	A	404	4/4	0.89	0.19	16,16,16,16	0
3	CL	B	402	1/1	0.91	0.09	26,26,26,26	0
3	CL	A	402	1/1	0.97	0.04	16,16,16,16	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.

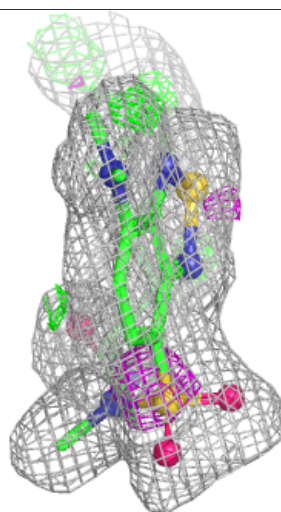
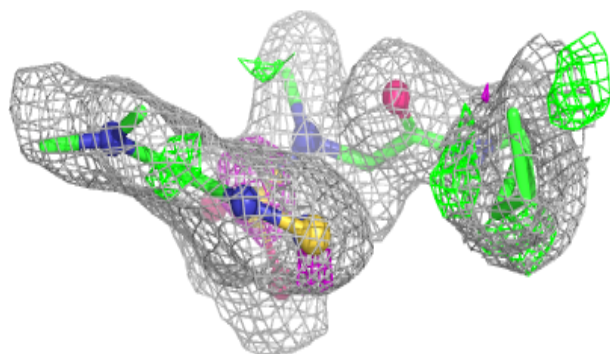
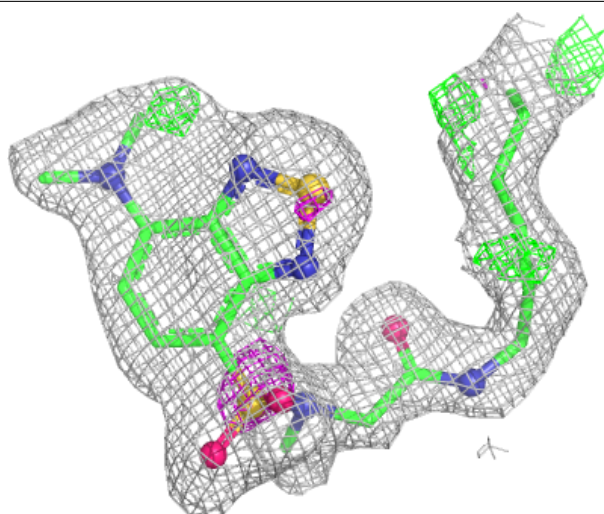
Electron density around 8PM B 401:

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



Electron density around 8PM A 401:

$2mF_o-DF_c$ (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.