



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2025 – 10:12 AM JST

PDB ID : 9M7D / pdb\_00009m7d  
Title : Crystal structure of AsDMS D333N mutant  
Authors : Fujiyama, K.; Vo, N.N.Q.; Takahashi, S.  
Deposited on : 2025-03-10  
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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

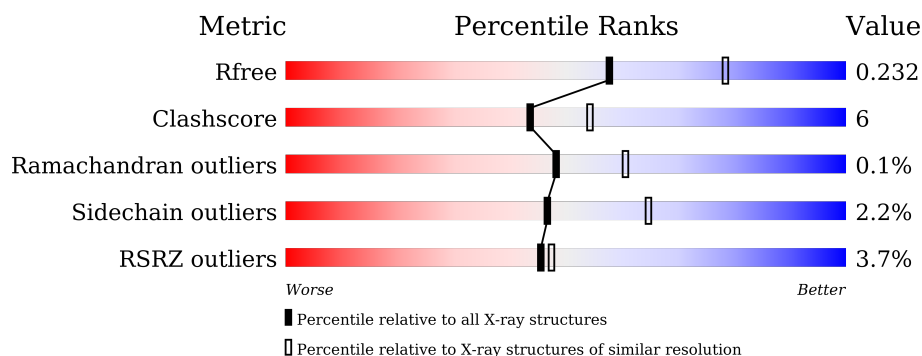
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	521	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
1	B	521	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8967 atoms, of which 50 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 Haloacid dehalogenase superfamily, subfamily IA, variant 3 with third motif having DD or ED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4230	2739	691	784	16			
1	B	511	Total	C	N	O	S	0	2	0
			4182	2708	682	776	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A1M6CXF0
A	-1	SER	-	expression tag	UNP A0A1M6CXF0
A	0	HIS	-	expression tag	UNP A0A1M6CXF0
A	333	ASN	ASP	engineered mutation	UNP A0A1M6CXF0
B	-2	GLY	-	expression tag	UNP A0A1M6CXF0
B	-1	SER	-	expression tag	UNP A0A1M6CXF0
B	0	HIS	-	expression tag	UNP A0A1M6CXF0
B	333	ASN	ASP	engineered mutation	UNP A0A1M6CXF0

- Molecule 2 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			49	15	25	7	2		
2	B	1	Total	C	H	O	P	0	0
			49	15	25	7	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	Cl	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	7	Total	Cl	0	0
			7	7		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

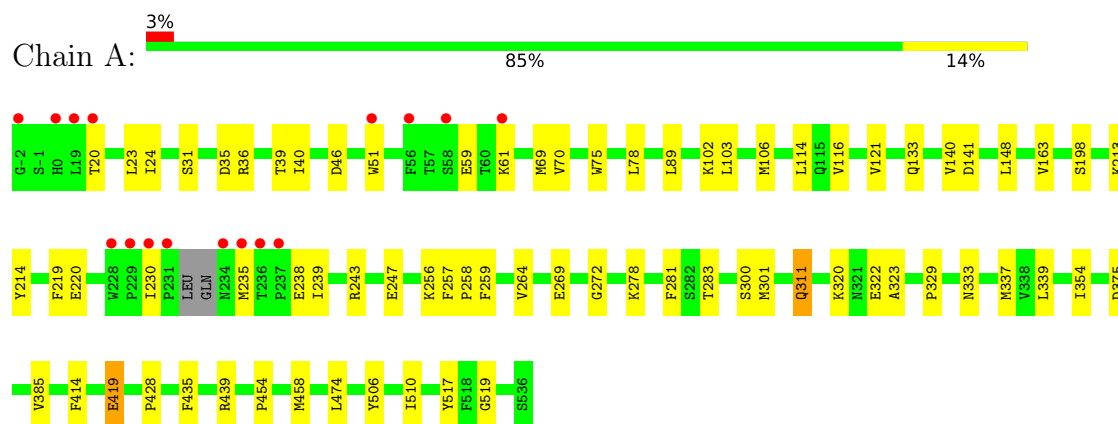
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		
5	B	163	Total	O	0	0
			163	163		

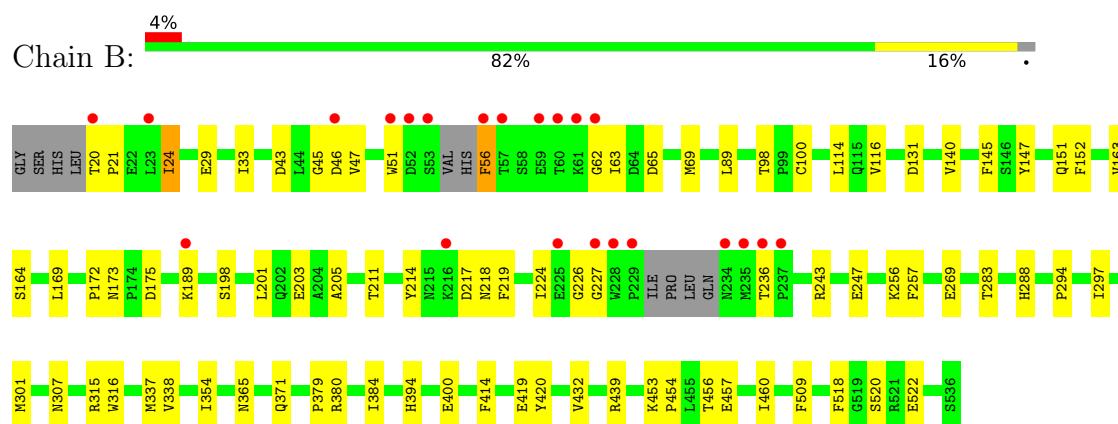
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Haloacid dehalogenase superfamily, subfamily IA, variant 3 with third motif having DD or ED



- Molecule 1: Haloacid dehalogenase superfamily, subfamily IA, variant 3 with third motif having DD or ED



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.03Å 97.03Å 405.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 2.30 47.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.18-2.30) 100.0 (47.18-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0403, PHENIX 1.11.1	Depositor
R, $R_{free}$	0.184 , 0.226 0.190 , 0.232	Depositor DCC
$R_{free}$ test set	4390 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: UNL, CL, SO4

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	0.59	0/4329	0.70	0/5863
1	B	0.60	0/4284	0.72	0/5800
All	All	0.60	0/8613	0.71	0/11663

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	4230	0	4223	45	0
1	B	4182	0	4172	56	0
2	A	24	25	0	0	0
2	B	24	25	0	1	0
3	A	8	0	0	1	0
3	B	7	0	0	1	0
4	A	50	0	0	1	0
4	B	35	0	0	1	0
5	A	194	0	0	4	0
5	B	163	0	0	6	0
All	All	8917	50	8395	102	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 6.

All (102) 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:51:TRP:HB3	1:A:114:LEU:HD23	1.35	1.05
1:B:173[B]:ASN:HD21	1:B:175:ASP:HB2	1.32	0.93
1:B:189:LYS:HE3	1:B:227:GLY:HA3	1.61	0.83
1:B:173[B]:ASN:ND2	1:B:175:ASP:HB2	1.96	0.78
1:B:63:ILE:HD12	1:B:65:ASP:O	1.84	0.78
1:A:243:ARG:O	1:A:247:GLU:HG3	1.85	0.76
1:A:36:ARG:NH1	5:A:702:HOH:O	2.21	0.73
1:B:51:TRP:HB3	1:B:114:LEU:HD23	1.71	0.71
1:A:51:TRP:HB3	1:A:114:LEU:CD2	2.20	0.67
1:B:189:LYS:HE2	5:B:791:HOH:O	1.98	0.63
1:A:214:TYR:HD1	1:A:219:PHE:CE1	2.16	0.62
1:B:62:GLY:HA3	1:B:98:THR:HG23	1.82	0.62
1:A:414:PHE:CE1	1:A:419:GLU:HG2	2.35	0.61
1:A:272:GLY:HA2	1:B:100:CYS:SG	2.41	0.60
1:B:24:ILE:HD12	1:B:33:ILE:HD11	1.84	0.59
1:B:243:ARG:O	1:B:247:GLU:HG3	2.03	0.58
1:B:283:THR:HG23	1:B:301:MET:HE2	1.85	0.58
1:A:235:MET:HA	1:A:238:GLU:OE1	2.05	0.57
1:B:173[A]:ASN:ND2	3:B:607:CL:CL	2.76	0.56
1:A:23:LEU:C	1:A:24:ILE:HD13	2.30	0.55
1:A:283:THR:HG23	1:A:301:MET:HE2	1.88	0.55
1:A:23:LEU:O	1:A:24:ILE:HD13	2.07	0.55
1:B:69:MET:HE1	1:B:89:LEU:CD2	2.37	0.54
1:A:439:ARG:HD2	5:A:823:HOH:O	2.09	0.53
1:B:24:ILE:HD12	1:B:33:ILE:CD1	2.38	0.53
1:A:59:GLU:OE1	1:A:61:LYS:HD3	2.09	0.53
1:A:322:GLU:HG2	5:A:703:HOH:O	2.10	0.52
1:B:457:GLU:HB3	5:B:833:HOH:O	2.11	0.51
1:A:333:ASN:HB2	1:A:385:VAL:HG22	1.92	0.50
1:A:24:ILE:HB	1:A:219:PHE:HB2	1.94	0.50
1:B:189:LYS:HG3	1:B:227:GLY:CA	2.41	0.50
1:B:140:VAL:HG13	1:B:163:VAL:HG13	1.94	0.50
1:B:414:PHE:CE1	1:B:419:GLU:HG2	2.47	0.50
1:B:147:TYR:CZ	1:B:151:GLN:HG3	2.47	0.50
1:A:258:PRO:HD2	3:A:606:CL:CL	2.48	0.49
4:A:614:SO4:O3	5:A:701:HOH:O	2.14	0.49
1:A:419:GLU:O	1:A:419:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TYR:O	1:A:519:GLY:HA3	2.12	0.49
1:B:45:GLY:C	1:B:47:VAL:H	2.22	0.48
1:A:281:PHE:CE1	1:A:337:MET:HE3	2.48	0.48
1:A:78:LEU:HG	1:A:141:ASP:HB3	1.96	0.48
1:B:24:ILE:CD1	1:B:33:ILE:HD11	2.43	0.48
1:A:256:LYS:HD3	1:A:257:PHE:CE2	2.48	0.47
1:B:214:TYR:HD1	1:B:219:PHE:CE1	2.33	0.47
1:B:456:THR:O	1:B:460:ILE:HG13	2.15	0.47
1:A:278:LYS:HE3	1:A:322:GLU:OE2	2.15	0.47
1:B:152:PHE:O	1:B:453:LYS:NZ	2.48	0.47
1:B:189:LYS:HG3	1:B:227:GLY:HA3	1.97	0.47
1:A:259:PHE:CE2	1:A:320:LYS:HE3	2.50	0.46
1:A:114:LEU:HD13	1:A:148:LEU:HD21	1.98	0.46
1:A:281:PHE:HE1	1:A:337:MET:HE3	1.79	0.46
1:A:311:GLN:O	1:A:311:GLN:HG3	2.15	0.46
2:B:601:UNL:C03	2:B:601:UNL:C07	2.93	0.46
1:B:145:PHE:CE2	1:B:460:ILE:HD13	2.51	0.46
1:B:394:HIS:HE1	5:B:702:HOH:O	1.99	0.46
1:A:89:LEU:HD22	1:A:103:LEU:HB3	1.98	0.46
1:B:201:LEU:HD22	1:B:211:THR:HB	1.98	0.46
1:A:69:MET:HE1	1:A:89:LEU:HD21	1.98	0.46
1:B:189:LYS:CE	1:B:227:GLY:HA3	2.41	0.46
1:B:294:PRO:HD2	1:B:297:ILE:HD12	1.97	0.46
1:B:147:TYR:CE1	1:B:151:GLN:HG3	2.51	0.45
1:B:217:ASP:HB2	1:B:218:ASN:HD22	1.81	0.45
1:B:520:SER:HB2	1:B:522:GLU:OE2	2.16	0.45
1:B:189:LYS:HG3	1:B:227:GLY:N	2.32	0.45
1:A:40:ILE:HD12	1:A:40:ILE:N	2.33	0.44
1:B:116:VAL:HG13	1:B:152:PHE:CD1	2.53	0.43
1:B:140:VAL:CG1	1:B:163:VAL:HG13	2.47	0.43
1:A:428:PRO:HG3	1:A:510:ILE:HD13	2.01	0.43
1:A:454:PRO:O	1:A:458:MET:HG2	2.18	0.43
1:B:164:SER:HB2	1:B:169:LEU:O	2.18	0.43
1:B:256:LYS:HD3	1:B:257:PHE:CE2	2.54	0.43
1:B:20:THR:HA	1:B:21:PRO:HD3	1.82	0.43
1:A:31:SER:O	1:A:35:ASP:HB2	2.19	0.43
1:A:278:LYS:HE2	1:A:323:ALA:HB2	1.99	0.43
1:B:371:GLN:HB3	5:B:798:HOH:O	2.19	0.43
1:B:384:ILE:HD13	1:B:432:VAL:HG12	2.01	0.43
1:A:116:VAL:HB	1:A:121:VAL:HG21	2.01	0.42
1:B:172:PRO:O	1:B:203:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LYS:N	1:B:454:PRO:HD2	2.34	0.42
1:B:56:PHE:CD2	1:B:56:PHE:N	2.87	0.42
1:B:315:ARG:HD3	5:B:812:HOH:O	2.18	0.42
1:A:102:LYS:O	1:A:106:MET:HG3	2.19	0.42
1:A:235:MET:O	1:A:239:ILE:HG13	2.19	0.42
1:B:189:LYS:HG3	1:B:226:GLY:C	2.45	0.42
1:A:213:LYS:HB3	1:A:220:GLU:HB2	2.01	0.42
1:B:316:TRP:CE2	1:B:338:VAL:HG11	2.55	0.42
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.83	0.42
1:A:70:VAL:HA	1:A:75:TRP:CG	2.55	0.41
1:B:365:ASN:HB3	1:B:371:GLN:CD	2.45	0.41
1:B:509:PHE:CE1	1:B:518:PHE:HB2	2.55	0.41
1:B:43:ASP:OD1	4:B:613:SO4:O3	2.39	0.41
1:B:205:ALA:HB1	1:B:224:ILE:CD1	2.51	0.41
1:A:264:VAL:HA	1:A:517:TYR:O	2.21	0.41
1:B:414:PHE:CE2	1:B:420:TYR:HA	2.55	0.41
1:A:20:THR:O	1:A:20:THR:HG23	2.19	0.41
1:B:379:PRO:O	1:B:380:ARG:HD3	2.21	0.41
1:A:39:THR:HA	1:A:133:GLN:O	2.21	0.40
1:A:329:PRO:HB3	1:A:375:ASP:HB2	2.01	0.40
1:A:435:PHE:CG	1:A:474:LEU:HD22	2.55	0.40
1:B:288:HIS:NE2	1:B:439:ARG:NH1	2.70	0.40
1:B:419:GLU:CD	5:B:725:HOH:O	2.65	0.40
1:B:205:ALA:HB1	1:B:224:ILE:HD13	2.03	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	515/521 (99%)	500 (97%)	15 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	507/521 (97%)	497 (98%)	9 (2%)	1 (0%)	44 55
All	All	1022/1042 (98%)	997 (98%)	24 (2%)	1 (0%)	48 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	ASP

### 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	474/476 (100%)	464 (98%)	10 (2%)	48 66
1	B	469/476 (98%)	458 (98%)	11 (2%)	45 63
All	All	943/952 (99%)	922 (98%)	21 (2%)	47 65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	140	VAL
1	A	163	VAL
1	A	198	SER
1	A	230	ILE
1	A	269	GLU
1	A	300	SER
1	A	311	GLN
1	A	354	ILE
1	A	419	GLU
1	B	24	ILE
1	B	29	GLU
1	B	56	PHE
1	B	131	ASP
1	B	198	SER

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Mol	Chain	Res	Type
1	B	236	THR
1	B	269	GLU
1	B	307	ASN
1	B	337	MET
1	B	354	ILE
1	B	400	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	B	202	GLN
1	B	234	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are unknown and 15 are monoatomic - leaving 17 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	SO4	B	614	-	4,4,4	0.23	0	6,6,6	0.22	0
4	SO4	B	609	-	4,4,4	0.24	0	6,6,6	0.48	0
4	SO4	B	611	-	4,4,4	0.17	0	6,6,6	0.23	0
4	SO4	A	612	-	4,4,4	0.21	0	6,6,6	0.47	0
4	SO4	A	610	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	A	613	-	4,4,4	0.23	0	6,6,6	0.24	0
4	SO4	A	615	-	4,4,4	0.57	0	6,6,6	0.64	0
4	SO4	A	617	-	4,4,4	0.09	0	6,6,6	0.27	0
4	SO4	A	614	-	4,4,4	0.26	0	6,6,6	0.34	0
4	SO4	A	618	-	4,4,4	0.31	0	6,6,6	0.36	0
4	SO4	B	610	-	4,4,4	0.12	0	6,6,6	0.28	0
4	SO4	B	613	-	4,4,4	0.51	0	6,6,6	0.30	0
4	SO4	A	616	-	4,4,4	0.20	0	6,6,6	0.25	0
4	SO4	B	615	-	4,4,4	0.15	0	6,6,6	0.19	0
4	SO4	A	611	-	4,4,4	0.18	0	6,6,6	0.31	0
4	SO4	A	619	-	4,4,4	0.19	0	6,6,6	0.28	0
4	SO4	B	612	-	4,4,4	0.15	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	614	SO4	1	0
4	B	613	SO4	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/521 (99%)	-0.13	16 (3%)	51 53	34, 45, 80, 107	0
1	B	511/521 (98%)	-0.07	22 (4%)	40 41	28, 46, 81, 126	2 (0%)
All	All	1030/1042 (98%)	-0.10	38 (3%)	45 47	28, 46, 80, 126	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	TRP	7.2
1	B	56	PHE	7.2
1	B	229	PRO	6.8
1	A	231	PRO	5.7
1	A	234	ASN	5.4
1	B	60	THR	5.0
1	A	51	TRP	4.8
1	A	230	ILE	4.1
1	A	229	PRO	4.1
1	B	234	ASN	4.0
1	B	61	LYS	3.9
1	A	236	THR	3.9
1	B	228	TRP	3.9
1	B	57	THR	3.8
1	B	237	PRO	3.7
1	A	235	MET	3.6
1	A	20	THR	3.6
1	B	236	THR	3.4
1	B	53	SER	3.3
1	B	20	THR	3.1
1	A	56	PHE	3.1
1	A	237	PRO	3.0
1	B	216	LYS	2.8
1	B	235	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	61	LYS	2.7
1	A	228	TRP	2.6
1	B	46	ASP	2.6
1	B	52	ASP	2.6
1	B	225	GLU	2.5
1	A	-2	GLY	2.2
1	B	62	GLY	2.2
1	A	58	SER	2.2
1	A	19	LEU	2.2
1	B	23	LEU	2.2
1	A	0	HIS	2.2
1	B	189	LYS	2.1
1	B	59	GLU	2.1
1	B	227	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	B	615	5/5	0.62	0.14	111,111,142,170	0
4	SO4	A	617	5/5	0.63	0.12	120,125,127,130	0
4	SO4	B	614	5/5	0.64	0.14	80,98,143,146	0
4	SO4	A	618	5/5	0.64	0.14	89,91,132,146	0
4	SO4	A	619	5/5	0.66	0.10	93,117,145,148	0
4	SO4	A	615	5/5	0.69	0.16	62,65,101,129	0
4	SO4	A	613	5/5	0.69	0.14	98,107,146,152	0
4	SO4	A	610	5/5	0.73	0.11	84,89,118,122	0
4	SO4	B	613	5/5	0.73	0.16	68,69,99,137	0

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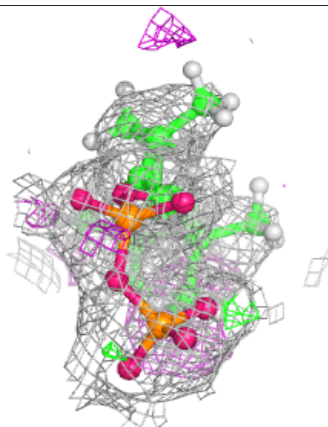
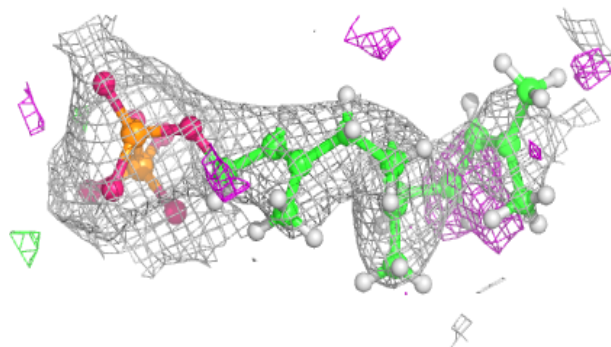
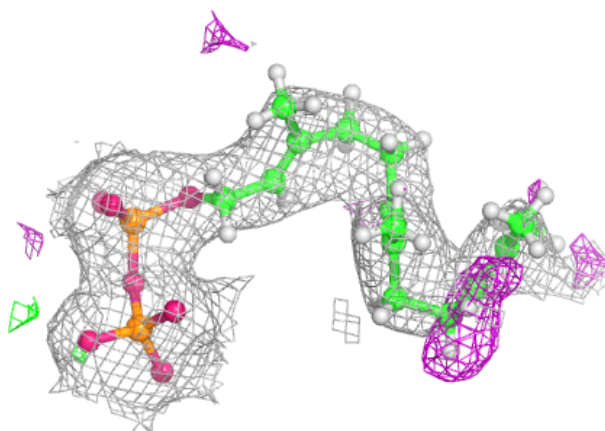
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	611	5/5	0.74	0.14	71,86,117,118	0
4	SO4	B	611	5/5	0.77	0.14	96,96,141,154	0
4	SO4	A	614	5/5	0.77	0.14	79,103,114,122	0
4	SO4	A	612	5/5	0.79	0.12	79,83,107,109	0
4	SO4	B	610	5/5	0.79	0.10	82,103,126,129	0
4	SO4	B	612	5/5	0.80	0.13	71,95,116,127	0
4	SO4	A	616	5/5	0.83	0.12	82,92,126,147	0
3	CL	A	604	1/1	0.86	0.20	75,75,75,75	0
4	SO4	B	609	5/5	0.86	0.08	66,78,95,109	0
3	CL	B	603	1/1	0.89	0.15	71,71,71,71	0
3	CL	B	607	1/1	0.92	0.12	85,85,85,85	0
3	CL	A	608	1/1	0.93	0.12	64,64,64,64	0
3	CL	B	608	1/1	0.96	0.10	63,63,63,63	0
2	UNL	A	601	49/-	0.96	0.10	37,53,77,77	0
3	CL	A	602	1/1	0.96	0.12	53,53,53,53	0
3	CL	A	606	1/1	0.97	0.16	61,61,61,61	0
3	CL	A	607	1/1	0.97	0.08	64,64,64,64	0
3	CL	A	603	1/1	0.97	0.07	50,50,50,50	0
3	CL	A	609	1/1	0.97	0.16	56,56,56,56	0
3	CL	B	602	1/1	0.97	0.07	54,54,54,54	0
3	CL	B	606	1/1	0.98	0.04	66,66,66,66	0
2	UNL	B	601	49/-	0.98	0.07	38,52,62,70	0
3	CL	A	605	1/1	0.98	0.13	51,51,51,51	0
3	CL	B	605	1/1	0.98	0.09	57,57,57,57	0
3	CL	B	604	1/1	0.99	0.12	54,54,54,54	0

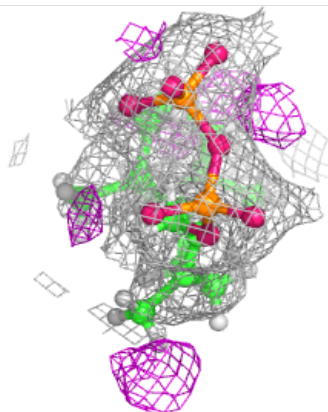
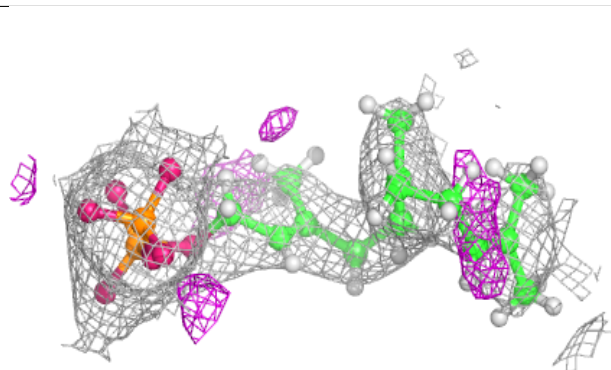
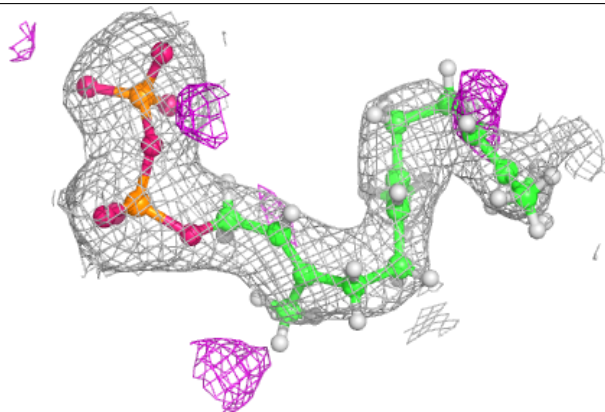
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UNL 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 UNL 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.