



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:03 am BST

PDB ID : 3W1V  
Title : Crystal Structure of Capsular Polysaccharide Synthesizing Enzyme CapE from Staphylococcus aureus in complex with inhibitor  
Authors : Miyafusa, T.; Caaveiro, J.M.; Tanaka, Y.; Tsumoto, K.  
Deposited on : 2012-11-21  
Resolution : 2.10 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.

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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

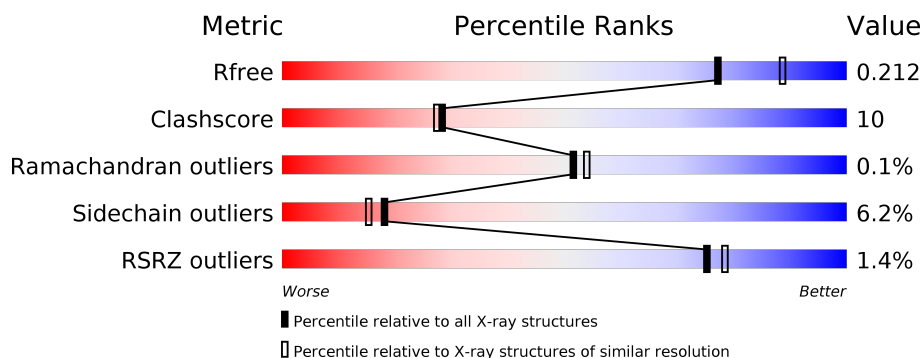
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>76%</span> <span>16%</span> <span>• • •</span> </div> </div>
1	B	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>77%</span> <span>15%</span> <span>• 5%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	406	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6115 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 Capsular polysaccharide synthesis enzyme Cap8E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	4	0
			2770	1738	475	542	15			
1	B	346	Total	C	N	O	S	0	8	0
			2792	1751	479	547	15			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q7A2Y4
A	-19	ASN	-	EXPRESSION TAG	UNP Q7A2Y4
A	-18	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-17	LYS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-16	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-15	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-14	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-13	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-12	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-11	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
A	-10	SER	-	EXPRESSION TAG	UNP Q7A2Y4
A	-9	SER	-	EXPRESSION TAG	UNP Q7A2Y4
A	-8	GLY	-	EXPRESSION TAG	UNP Q7A2Y4
A	-7	LEU	-	EXPRESSION TAG	UNP Q7A2Y4
A	-6	VAL	-	EXPRESSION TAG	UNP Q7A2Y4
A	-5	PRO	-	EXPRESSION TAG	UNP Q7A2Y4
A	-4	ARG	-	EXPRESSION TAG	UNP Q7A2Y4
A	-3	GLY	-	EXPRESSION TAG	UNP Q7A2Y4
A	-2	SER	-	EXPRESSION TAG	UNP Q7A2Y4
A	-1	ALA	-	EXPRESSION TAG	UNP Q7A2Y4
A	0	MET	-	EXPRESSION TAG	UNP Q7A2Y4
A	1	GLY	-	EXPRESSION TAG	UNP Q7A2Y4
B	-20	MET	-	EXPRESSION TAG	UNP Q7A2Y4
B	-19	ASN	-	EXPRESSION TAG	UNP Q7A2Y4
B	-18	HIS	-	EXPRESSION TAG	UNP Q7A2Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	LYS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-16	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-15	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-14	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-13	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-12	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-11	HIS	-	EXPRESSION TAG	UNP Q7A2Y4
B	-10	SER	-	EXPRESSION TAG	UNP Q7A2Y4
B	-9	SER	-	EXPRESSION TAG	UNP Q7A2Y4
B	-8	GLY	-	EXPRESSION TAG	UNP Q7A2Y4
B	-7	LEU	-	EXPRESSION TAG	UNP Q7A2Y4
B	-6	VAL	-	EXPRESSION TAG	UNP Q7A2Y4
B	-5	PRO	-	EXPRESSION TAG	UNP Q7A2Y4
B	-4	ARG	-	EXPRESSION TAG	UNP Q7A2Y4
B	-3	GLY	-	EXPRESSION TAG	UNP Q7A2Y4
B	-2	SER	-	EXPRESSION TAG	UNP Q7A2Y4
B	-1	ALA	-	EXPRESSION TAG	UNP Q7A2Y4
B	0	MET	-	EXPRESSION TAG	UNP Q7A2Y4
B	1	GLY	-	EXPRESSION TAG	UNP Q7A2Y4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



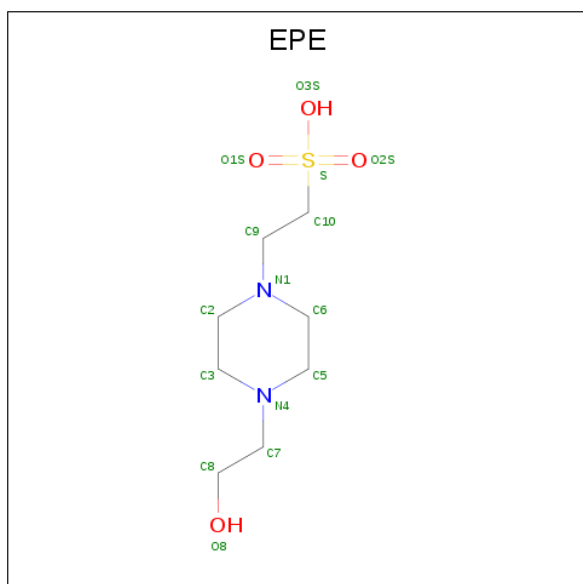
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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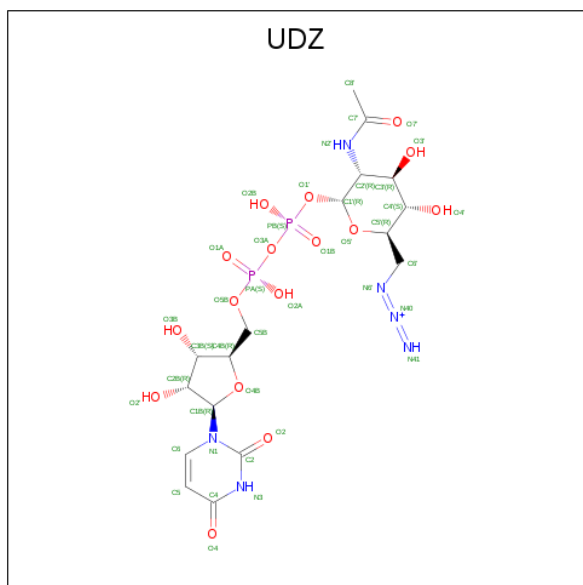
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is [(2R,3S,4R,5R,6R)-5-acetamido-6-[[[(2R,3S,4R,5R)-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,4-bis(oxidanyl)oxan-2-yl]methylimino-azanylidene-azanium (three-letter code: UDZ) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>6</sub>O<sub>16</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			41	17	6	16	2		
4	B	1	Total	C	N	O	P	0	0
			41	17	6	16	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

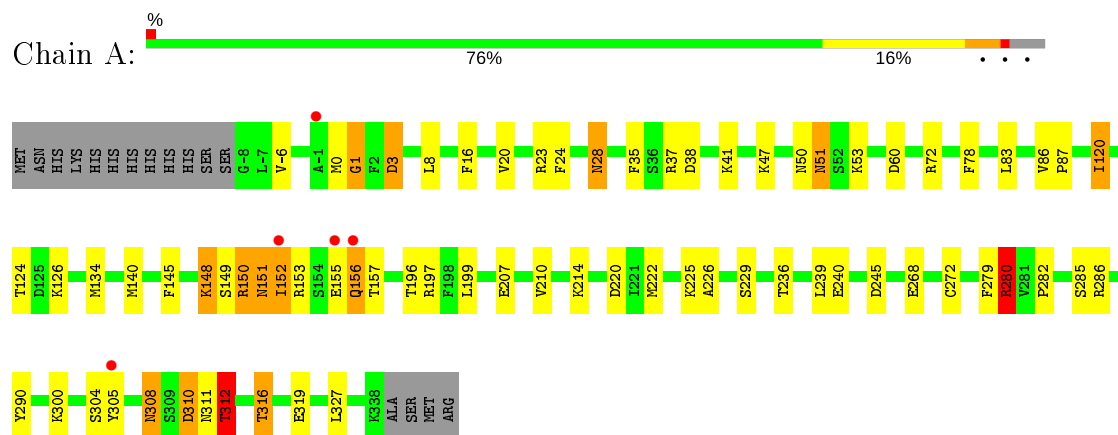
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		
6	B	195	Total	O	0	0
			195	195		

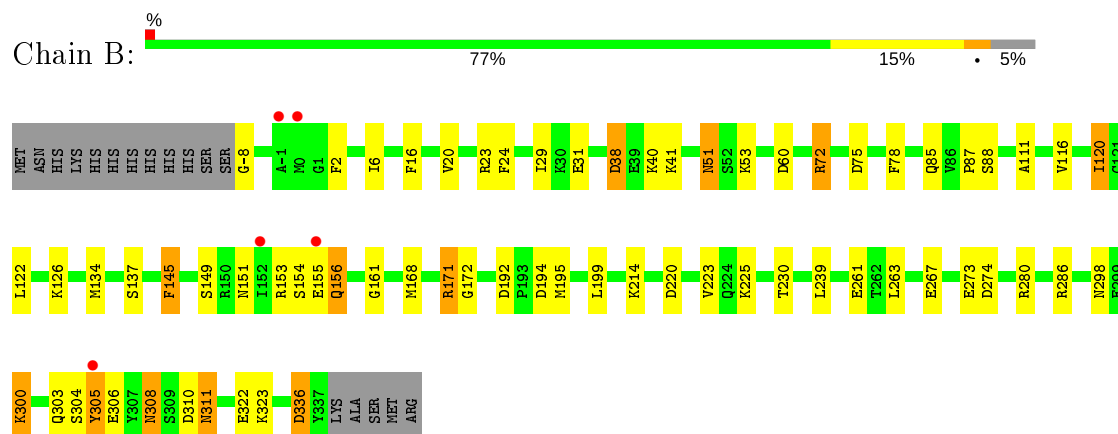
### 3 Residue-property plots [i](#)

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: Capsular polysaccharide synthesis enzyme Cap8E



- Molecule 1: Capsular polysaccharide synthesis enzyme Cap8E





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.78Å 123.78Å 104.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.80 – 2.10 34.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.80-2.10) 99.9 (34.82-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.164 , 0.207 0.168 , 0.212	Depositor DCC
$R_{free}$ test set	2755 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.168 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDZ, NA, EPE, 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	1.12	1/2811 (0.0%)	1.13	13/3787 (0.3%)
1	B	1.13	4/2833 (0.1%)	1.13	12/3815 (0.3%)
All	All	1.13	5/5644 (0.1%)	1.13	25/7602 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	GLU	CD-OE1	6.75	1.33	1.25
1	A	151	ASN	N-CA	6.62	1.59	1.46
1	B	151	ASN	N-CA	5.27	1.56	1.46
1	B	261	GLU	CD-OE2	5.09	1.31	1.25
1	B	267	GLU	CG-CD	5.07	1.59	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	NE-CZ-NH1	-10.56	115.02	120.30
1	B	72	ARG	NE-CZ-NH2	9.95	125.27	120.30
1	A	280[A]	ARG	NE-CZ-NH1	-9.41	115.60	120.30
1	A	280[B]	ARG	NE-CZ-NH1	-9.41	115.60	120.30
1	A	72	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	B	286	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	38	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	222	MET	CG-SD-CE	6.67	110.86	100.20
1	A	197	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	150	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	286	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	310	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	72	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	B	72	ARG	CD-NE-CZ	-5.92	115.31	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	280[A]	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	A	280[B]	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	B	38	ASP	CB-CG-OD1	-5.72	113.16	118.30
1	A	312	THR	CB-CA-C	-5.57	96.57	111.60
1	B	194	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	B	122	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	83	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	75	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	A	1	GLY	N-CA-C	-5.20	100.11	113.10
1	B	151	ASN	N-CA-C	5.18	124.99	111.00

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	2770	0	2770	53	0
1	B	2792	0	2792	61	0
2	A	35	0	0	1	0
2	B	35	0	0	5	0
3	A	15	0	17	0	0
4	A	41	0	25	0	0
4	B	41	0	26	0	0
5	B	1	0	0	0	0
6	A	190	0	0	4	0
6	B	195	0	0	4	0
All	All	6115	0	5630	111	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 10.

All (111) 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:280[A]:ARG:CG	1:A:280[A]:ARG:HH11	1.64	1.10
1:A:280[A]:ARG:HG2	1:A:280[A]:ARG:NH1	1.57	1.09
1:A:226:ALA:O	1:A:312:THR:HG21	1.62	1.00
1:A:280[A]:ARG:HG2	1:A:280[A]:ARG:HH11	0.79	0.93
1:B:38:ASP:OD1	1:B:41[A]:LYS:HG3	1.71	0.90
1:A:38:ASP:OD1	1:A:41:LYS:HE2	1.74	0.85
1:B:72:ARG:HD2	6:B:695:HOH:O	1.73	0.85
1:B:168:MET:HE1	1:B:199:LEU:HB3	1.60	0.84
1:A:20:VAL:HG11	1:A:78:PHE:HD2	1.43	0.81
1:B:149:SER:HB3	6:B:631:HOH:O	1.79	0.81
1:B:153[B]:ARG:HG2	2:B:406:SO4:O4	1.83	0.79
1:A:153:ARG:HG2	6:A:562:HOH:O	1.81	0.78
1:A:316:THR:HG22	1:A:319:GLU:H	1.49	0.78
1:B:171:ARG:HD2	1:B:172:GLY:H	1.48	0.77
1:B:38:ASP:CG	1:B:41[A]:LYS:HG3	2.04	0.77
1:A:20:VAL:HG11	1:A:78:PHE:CD2	2.21	0.74
1:A:308:ASN:C	1:A:308:ASN:HD22	1.91	0.74
1:B:38:ASP:OD1	1:B:41[A]:LYS:CE	2.35	0.73
1:A:280[A]:ARG:CG	1:A:280[A]:ARG:NH1	2.34	0.73
1:B:85[A]:GLN:HB2	1:B:88[A]:SER:OG	1.86	0.73
1:B:51:ASN:HD22	1:B:53:LYS:H	1.36	0.73
1:B:38:ASP:OD1	1:B:41[A]:LYS:NZ	2.23	0.72
1:A:152:ILE:HD12	1:A:153:ARG:N	2.06	0.71
1:B:171:ARG:HD2	1:B:172:GLY:N	2.06	0.70
1:A:149:SER:HB3	6:A:604:HOH:O	1.91	0.69
1:B:153[A]:ARG:HB2	1:B:156:GLN:HG3	1.74	0.69
1:A:51:ASN:HD22	1:A:53:LYS:H	1.42	0.68
1:A:316:THR:CG2	1:A:319:GLU:H	2.09	0.65
1:B:308:ASN:HD22	1:B:308:ASN:C	2.00	0.64
1:B:154:SER:N	2:B:406:SO4:O2	2.26	0.64
1:B:126:LYS:HD2	1:B:134:MET:CE	2.29	0.62
1:A:152:ILE:HD11	1:A:157:THR:H	1.65	0.61
1:A:148:LYS:HD3	1:A:148:LYS:N	2.17	0.60
1:A:126:LYS:HD2	1:A:134:MET:CE	2.33	0.58
1:B:153[B]:ARG:HA	2:B:406:SO4:O2	2.05	0.57
1:A:3[B]:ASP:OD1	1:A:28:ASN:OD1	2.24	0.56
1:A:225:LYS:HE2	1:A:279:PHE:CZ	2.41	0.55
1:A:280[A]:ARG:NH1	1:A:282:PRO:HG3	2.21	0.55
1:B:273:GLU:OE2	1:B:280[B]:ARG:NH1	2.40	0.55
1:B:300:LYS:NZ	1:B:304:SER:HB2	2.22	0.55
1:B:38:ASP:OD1	1:B:41[A]:LYS:HE2	2.07	0.54
1:B:38:ASP:OD1	1:B:41[A]:LYS:CG	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LYS:HD2	1:B:134:MET:HE1	1.90	0.53
1:B:168:MET:HE1	1:B:323:LYS:HD3	1.91	0.52
1:B:145:PHE:CZ	1:B:161:GLY:HA3	2.44	0.52
1:B:195:MET:O	1:B:230:THR:HA	2.09	0.52
1:A:0:MET:HG3	1:A:1:GLY:O	2.09	0.52
1:B:308:ASN:ND2	1:B:310:ASP:H	2.08	0.52
1:A:308:ASN:ND2	1:A:308:ASN:C	2.62	0.51
1:B:153[A]:ARG:HG3	2:B:407:SO4:O2	2.09	0.51
1:B:192:ASP:HB3	1:B:195:MET:HG3	1.91	0.51
1:B:168:MET:CE	1:B:199:LEU:HB3	2.35	0.51
1:A:236:THR:O	1:A:240:GLU:HG3	2.10	0.50
1:A:140:MET:CE	1:B:137:SER:HB3	2.42	0.50
1:A:140:MET:HE1	1:B:137:SER:HB3	1.94	0.49
1:B:20:VAL:HG11	1:B:78:PHE:CD2	2.46	0.49
1:A:308:ASN:ND2	1:A:311:ASN:H	2.11	0.48
1:A:308:ASN:ND2	1:A:310:ASP:H	2.12	0.48
1:B:120:ILE:CD1	1:B:120:ILE:N	2.77	0.48
1:B:-8:GLY:O	1:B:214:LYS:HE3	2.14	0.48
1:A:148:LYS:N	1:A:148:LYS:CD	2.78	0.47
1:B:153[A]:ARG:HA	2:B:406:SO4:O2	2.13	0.47
1:B:220:ASP:OD2	1:B:280[A]:ARG:HD3	2.13	0.47
1:A:86:VAL:HB	1:A:87:PRO:HD3	1.97	0.47
1:A:24:PHE:CE2	1:A:78:PHE:HE2	2.33	0.47
1:B:51:ASN:ND2	6:B:623:HOH:O	2.44	0.47
1:A:23[B]:ARG:NH1	1:A:207:GLU:OE2	2.44	0.47
1:B:126:LYS:HD2	1:B:134:MET:HE3	1.96	0.46
1:B:308:ASN:HD22	1:B:310:ASP:H	1.61	0.46
1:B:153[A]:ARG:HB2	1:B:156:GLN:CG	2.44	0.46
1:B:308:ASN:ND2	1:B:311:ASN:H	2.14	0.46
1:A:47:LYS:HE2	1:A:47:LYS:HB2	1.80	0.45
1:B:153[B]:ARG:O	1:B:156:GLN:N	2.40	0.45
1:B:153[A]:ARG:O	1:B:156:GLN:N	2.46	0.45
1:A:150:ARG:HD3	1:A:285:SER:O	2.17	0.45
1:A:148:LYS:HD3	1:A:148:LYS:H	1.81	0.44
1:A:51:ASN:ND2	1:A:53:LYS:H	2.12	0.44
1:A:38:ASP:OD1	1:A:41:LYS:HG3	2.17	0.44
1:B:153[B]:ARG:NH1	1:B:155:GLU:HB2	2.32	0.44
1:A:290:TYR:CD2	1:B:87:PRO:HB2	2.53	0.44
1:B:40[A]:LYS:HB3	6:B:660:HOH:O	2.18	0.44
1:A:16:PHE:HD1	6:A:615:HOH:O	1.99	0.43
1:A:196:THR:HA	1:A:229:SER:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ASP:N	1:B:336:ASP:OD1	2.51	0.43
1:B:120:ILE:HD13	1:B:120:ILE:N	2.33	0.43
1:A:280[A]:ARG:HH12	1:A:282:PRO:CA	2.30	0.43
1:B:223:VAL:CG1	1:B:263:LEU:HD13	2.48	0.43
1:B:16:PHE:CE2	1:B:20:VAL:HG21	2.54	0.43
1:B:16:PHE:CE2	1:B:20:VAL:CG2	3.02	0.43
1:B:2:PHE:HB3	1:B:29:ILE:HA	2.01	0.43
1:B:24:PHE:CE2	1:B:78:PHE:HE2	2.36	0.43
1:A:37:ARG:NH1	1:A:60:ASP:OD2	2.52	0.42
1:B:6:ILE:HG12	1:B:31:GLU:HB3	2.01	0.42
1:A:20:VAL:CG1	1:A:78:PHE:CD2	2.98	0.42
1:A:153:ARG:O	1:A:156:GLN:HB2	2.19	0.42
1:A:120:ILE:N	1:A:120:ILE:HD12	2.35	0.42
1:B:225:LYS:NZ	1:B:274:ASP:OD2	2.52	0.42
1:A:23[B]:ARG:NH2	1:A:207:GLU:OE2	2.52	0.42
1:A:268:GLU:O	1:A:272:CYS:HB3	2.20	0.42
1:A:220:ASP:OD1	1:A:280[A]:ARG:CZ	2.69	0.41
1:A:312:THR:HG22	6:A:520:HOH:O	2.20	0.41
1:A:8:LEU:HD11	1:A:35:PHE:HB2	2.01	0.41
1:B:311:ASN:C	1:B:311:ASN:HD22	2.23	0.41
1:B:298:ASN:HD21	1:B:300:LYS:HB3	1.85	0.41
1:B:153[A]:ARG:HB2	1:B:156:GLN:OE1	2.21	0.41
1:A:327:LEU:HB3	2:A:402:SO4:O3	2.21	0.41
1:A:280[B]:ARG:HG3	1:A:280[B]:ARG:O	2.19	0.40
1:A:210:VAL:HG12	1:A:214:LYS:HD2	2.02	0.40
1:B:111:ALA:HB1	1:B:116:VAL:HB	2.02	0.40
1:B:305:TYR:HD2	1:B:306:GLU:H	1.69	0.40
1:B:308:ASN:HD22	1:B:310:ASP:N	2.18	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	349/363 (96%)	342 (98%)	7 (2%)	0	100	100
1	B	352/363 (97%)	342 (97%)	9 (3%)	1 (0%)	41	41
All	All	701/726 (97%)	684 (98%)	16 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	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	305/316 (96%)	279 (92%)	26 (8%)	10	7
1	B	308/316 (98%)	295 (96%)	13 (4%)	30	30
All	All	613/632 (97%)	574 (94%)	39 (6%)	18	14

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	VAL
1	A	3[A]	ASP
1	A	3[B]	ASP
1	A	28	ASN
1	A	50	ASN
1	A	51	ASN
1	A	120	ILE
1	A	124	THR
1	A	145	PHE
1	A	148	LYS
1	A	151	ASN
1	A	152	ILE
1	A	155	GLU
1	A	156	GLN
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	239	LEU
1	A	245	ASP
1	A	280[A]	ARG
1	A	280[B]	ARG
1	A	286	ARG
1	A	300	LYS
1	A	304	SER
1	A	305	TYR
1	A	308	ASN
1	A	312	THR
1	A	316	THR
1	B	23	ARG
1	B	51	ASN
1	B	120	ILE
1	B	145	PHE
1	B	156	GLN
1	B	171	ARG
1	B	239	LEU
1	B	300	LYS
1	B	303	GLN
1	B	305	TYR
1	B	308	ASN
1	B	311	ASN
1	B	322	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	113	HIS
1	A	289	ASN
1	A	308	ASN
1	B	51	ASN
1	B	271	GLN
1	B	308	ASN
1	B	311	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
2	SO4	B	404	-	4,4,4	0.34	0	6,6,6	0.29	0
2	SO4	A	405	-	4,4,4	0.45	0	6,6,6	0.44	0
2	SO4	B	401	-	4,4,4	0.55	0	6,6,6	0.91	1 (16%)
2	SO4	A	401	-	4,4,4	0.53	0	6,6,6	0.96	0
2	SO4	A	406	-	4,4,4	0.43	0	6,6,6	0.31	0
4	UDZ	A	409	-	35,43,43	1.39	5 (14%)	44,64,64	1.52	9 (20%)
2	SO4	B	402	-	4,4,4	0.36	0	6,6,6	0.90	0
2	SO4	B	406	-	4,4,4	0.22	0	6,6,6	0.72	0
2	SO4	A	404	-	4,4,4	0.42	0	6,6,6	0.28	0
4	UDZ	B	409	-	35,43,43	1.24	3 (8%)	44,64,64	1.24	7 (15%)
2	SO4	B	405	-	4,4,4	0.27	0	6,6,6	0.44	0
2	SO4	A	407	-	4,4,4	0.43	0	6,6,6	0.45	0
2	SO4	B	407	-	4,4,4	0.44	0	6,6,6	0.32	0
3	EPE	A	408	-	15,15,15	2.27	2 (13%)	18,20,20	2.39	8 (44%)
2	SO4	A	403	-	4,4,4	0.50	0	6,6,6	0.38	0
2	SO4	B	403	-	4,4,4	0.38	0	6,6,6	0.45	0
2	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.16	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
4	UDZ	B	409	-	-	10/26/65/65	0/3/3/3
4	UDZ	A	409	-	-	9/26/65/65	0/3/3/3
3	EPE	A	408	-	-	3/9/19/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	408	EPE	O1S-S	7.07	1.65	1.45
3	A	408	EPE	C10-S	-4.94	1.70	1.77
4	B	409	UDZ	N40-N6'	3.64	1.32	1.23
4	A	409	UDZ	O4B-C1B	3.32	1.45	1.41
4	A	409	UDZ	N40-N6'	3.15	1.31	1.23
4	A	409	UDZ	C4-N3	2.61	1.37	1.33
4	A	409	UDZ	C3'-C2'	2.54	1.58	1.53
4	A	409	UDZ	C6'-C5'	2.50	1.55	1.51
4	B	409	UDZ	C6-N1	2.02	1.38	1.35
4	B	409	UDZ	C2-N3	-2.02	1.34	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	EPE	O3S-S-C10	4.93	113.74	105.77
3	A	408	EPE	O1S-S-C10	-4.42	101.59	106.92
4	A	409	UDZ	C4'-C3'-C2'	3.56	115.56	110.34
4	B	409	UDZ	O3A-PB-O1'	-3.41	95.61	102.48
3	A	408	EPE	O2S-S-C10	3.29	110.87	106.92
4	A	409	UDZ	PB-O3A-PA	-3.22	121.78	132.83
3	A	408	EPE	O3S-S-O2S	-3.14	103.59	111.27
4	A	409	UDZ	C6'-N6'-N40	3.07	122.28	115.60
4	B	409	UDZ	PB-O3A-PA	-2.98	122.61	132.83
4	B	409	UDZ	O5'-C1'-C2'	-2.92	104.88	110.58
3	A	408	EPE	C9-N1-C6	-2.82	104.01	111.23
4	B	409	UDZ	C4'-C3'-C2'	2.77	114.40	110.34
4	A	409	UDZ	O4'-C4'-C5'	-2.67	102.68	109.30
3	A	408	EPE	C3-C2-N1	-2.42	105.67	110.64
4	A	409	UDZ	O3B-C3B-C4B	2.39	117.96	111.05
4	A	409	UDZ	O5'-C5'-C4'	2.37	114.01	109.69
3	A	408	EPE	O3S-S-O1S	2.36	117.03	111.27
3	A	408	EPE	C7-N4-C5	-2.31	105.32	111.23
4	A	409	UDZ	O2A-PA-O1A	2.28	123.53	112.24
4	B	409	UDZ	O2A-PA-O5B	-2.20	97.53	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	409	UDZ	C5-C4-N3	-2.18	118.51	123.31
4	A	409	UDZ	O3'-C3'-C4'	2.15	115.31	110.35
4	B	409	UDZ	O2B-PB-O1B	2.13	122.80	112.24
4	B	409	UDZ	O5'-C5'-C4'	2.08	113.47	109.69
2	B	401	SO4	O4-S-O1	2.03	119.90	109.31

There are no chirality outliers.

All (22) torsion outliers are listed below:

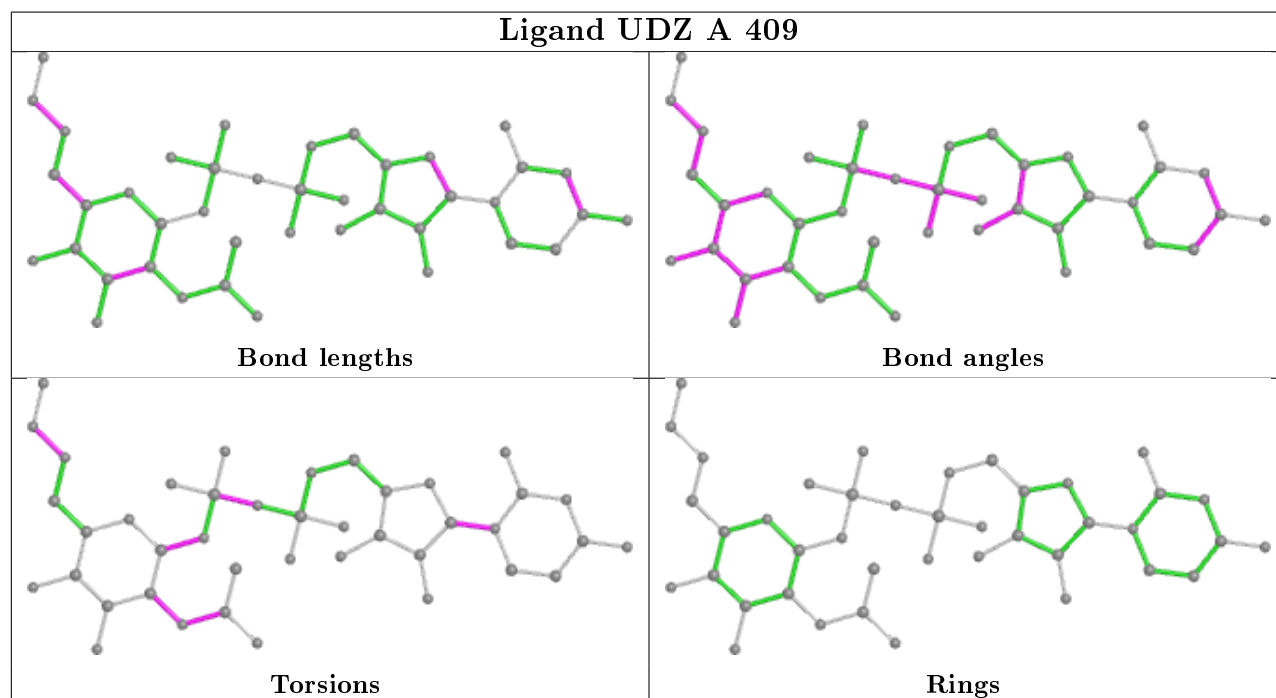
Mol	Chain	Res	Type	Atoms
4	A	409	UDZ	C2B-C1B-N1-C6
4	A	409	UDZ	O4B-C1B-N1-C6
4	A	409	UDZ	C1'-C2'-N2'-C7'
4	A	409	UDZ	O7'-C7'-N2'-C2'
4	A	409	UDZ	C8'-C7'-N2'-C2'
4	B	409	UDZ	C2B-C1B-N1-C6
4	B	409	UDZ	O4B-C1B-N1-C6
4	B	409	UDZ	C4'-C5'-C6'-N6'
4	B	409	UDZ	O5'-C5'-C6'-N6'
3	A	408	EPE	N4-C7-C8-O8
4	B	409	UDZ	O7'-C7'-N2'-C2'
4	B	409	UDZ	C8'-C7'-N2'-C2'
3	A	408	EPE	C8-C7-N4-C3
3	A	408	EPE	C8-C7-N4-C5
4	A	409	UDZ	N41-N40-N6'-C6'
4	B	409	UDZ	N41-N40-N6'-C6'
4	A	409	UDZ	O5'-C1'-O1'-PB
4	B	409	UDZ	O5'-C1'-O1'-PB
4	B	409	UDZ	PA-O3A-PB-O2B
4	A	409	UDZ	PA-O3A-PB-O2B
4	B	409	UDZ	PA-O3A-PB-O1B
4	A	409	UDZ	C3'-C2'-N2'-C7'

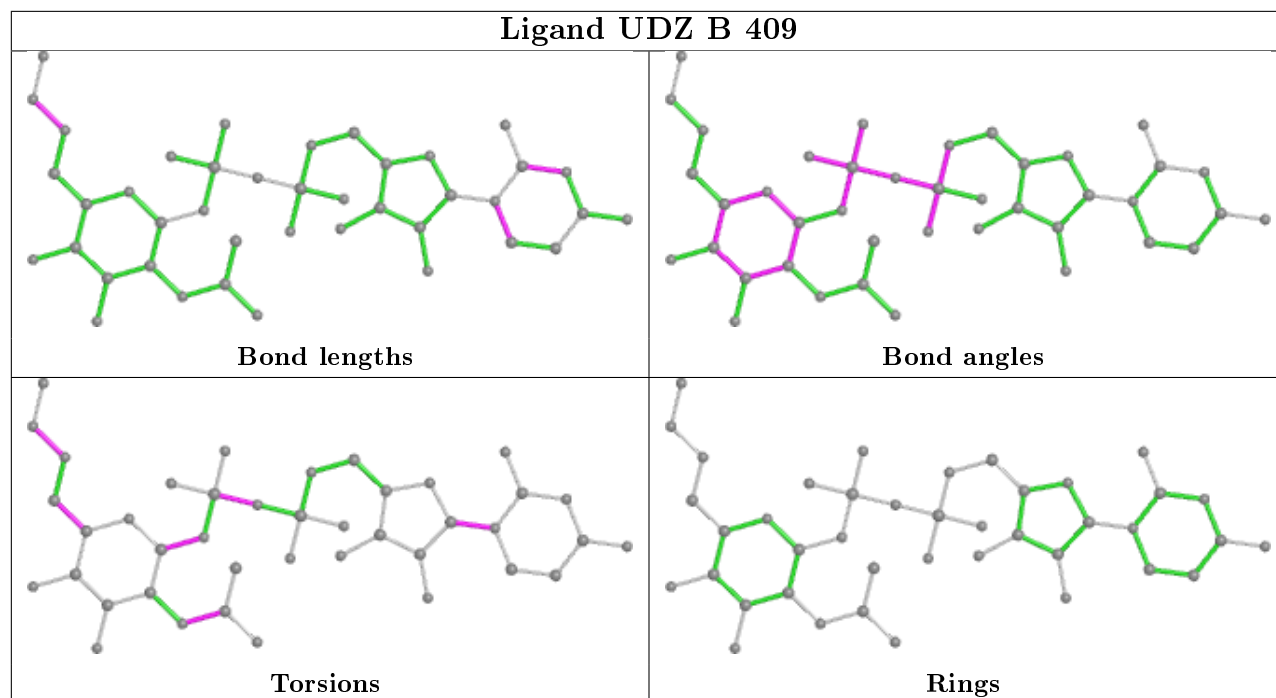
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	406	SO4	4	0
2	B	407	SO4	1	0
2	A	402	SO4	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, 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	347/363 (95%)	-0.43	5 (1%) 75 78	10, 26, 50, 72	0
1	B	346/363 (95%)	-0.43	5 (1%) 75 78	10, 27, 54, 76	1 (0%)
All	All	693/726 (95%)	-0.43	10 (1%) 75 78	10, 26, 53, 76	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	GLU	3.4
1	A	155	GLU	3.2
1	B	152	ILE	2.8
1	A	305	TYR	2.3
1	A	-1	ALA	2.3
1	A	152	ILE	2.2
1	B	-1	ALA	2.2
1	A	156	GLN	2.2
1	B	0	MET	2.1
1	B	305	TYR	2.1

### 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 ⓘ

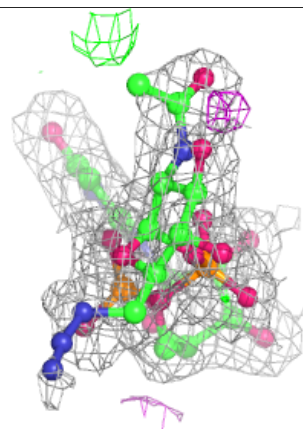
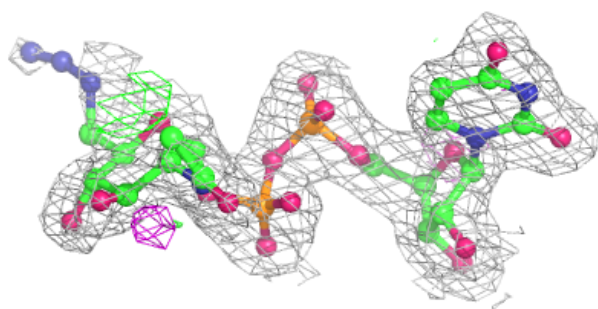
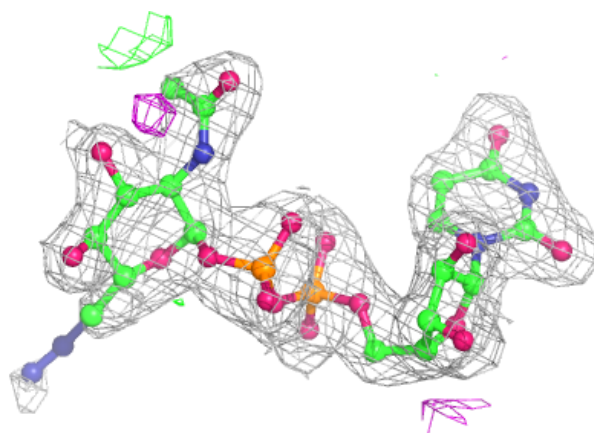
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	SO4	A	407	5/5	0.79	0.32	95,102,111,112	0
2	SO4	B	407	5/5	0.88	0.28	88,90,101,106	0
3	EPE	A	408	15/15	0.88	0.18	40,55,65,67	0
2	SO4	A	405	5/5	0.92	0.12	59,70,77,77	0
2	SO4	B	402	5/5	0.94	0.12	61,65,70,72	0
2	SO4	B	406	5/5	0.94	0.14	70,78,82,82	0
2	SO4	A	403	5/5	0.94	0.21	65,78,93,95	0
2	SO4	A	404	5/5	0.95	0.12	58,71,73,76	0
2	SO4	A	406	5/5	0.95	0.14	48,59,67,72	0
2	SO4	B	404	5/5	0.95	0.16	76,77,81,89	0
2	SO4	B	403	5/5	0.95	0.17	43,62,71,75	0
2	SO4	B	405	5/5	0.96	0.14	38,39,43,45	5
4	UDZ	B	409	41/41	0.97	0.11	24,32,61,80	0
4	UDZ	A	409	41/41	0.97	0.10	24,33,58,66	0
2	SO4	A	402	5/5	0.97	0.14	62,70,76,78	0
2	SO4	A	401	5/5	0.99	0.10	31,35,36,38	0
2	SO4	B	401	5/5	0.99	0.08	37,37,41,45	0
5	NA	B	408	1/1	1.00	0.12	22,22,22,22	0

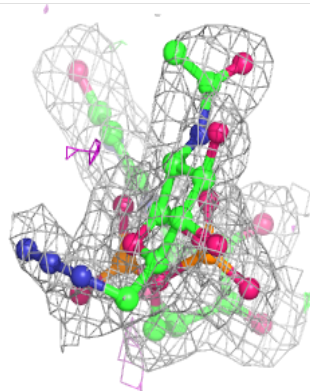
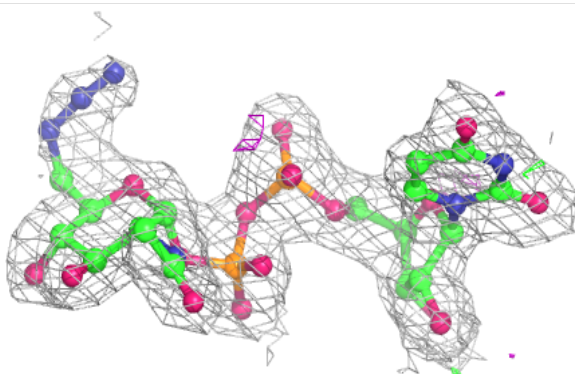
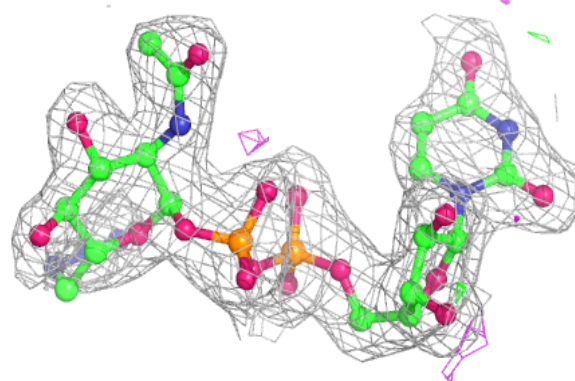
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UDZ B 409:**

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

**Electron density around UDZ A 409:**

$2mF_o-DF_c$  (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.