



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 07:40 PM JST

PDB ID : 7VZQ  
Title : The structure of GdmN V24Y/G157A/R158A/G188R mutant in complex with carbamoyl adenylate intermediate  
Authors : Wei, J.; Zheng, J.; Zhou, J.; Kang, Q.; Bai, L.  
Deposited on : 2021-11-16  
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.

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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

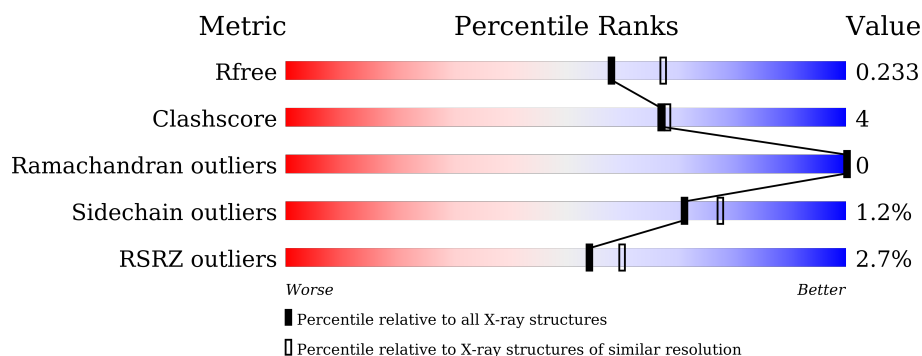
# 1 Overall quality at a glance

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 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	702	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 90%, yellow 90%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>90%</span> <span>6%</span> <span>.</span> </div> </div>
1	B	702	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 84%, yellow 84%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>84%</span> <span>12%</span> <span>..</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
4	EDO	A	703	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10814 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 GdmN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	1	0
			5208	3303	914	982	9			
1	B	679	Total	C	N	O	S	0	1	0
			5218	3309	913	988	8			

There are 48 discrepancies between the modelled and reference sequences:

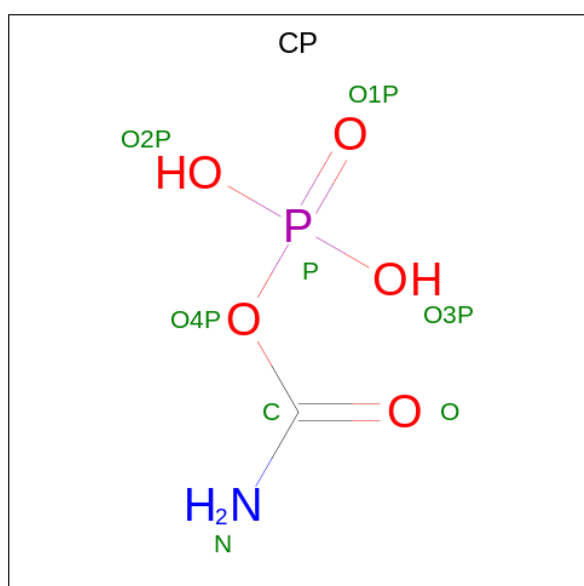
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q84G19
A	-18	GLY	-	expression tag	UNP Q84G19
A	-17	SER	-	expression tag	UNP Q84G19
A	-16	SER	-	expression tag	UNP Q84G19
A	-15	HIS	-	expression tag	UNP Q84G19
A	-14	HIS	-	expression tag	UNP Q84G19
A	-13	HIS	-	expression tag	UNP Q84G19
A	-12	HIS	-	expression tag	UNP Q84G19
A	-11	HIS	-	expression tag	UNP Q84G19
A	-10	HIS	-	expression tag	UNP Q84G19
A	-9	SER	-	expression tag	UNP Q84G19
A	-8	SER	-	expression tag	UNP Q84G19
A	-7	GLY	-	expression tag	UNP Q84G19
A	-6	LEU	-	expression tag	UNP Q84G19
A	-5	VAL	-	expression tag	UNP Q84G19
A	-4	PRO	-	expression tag	UNP Q84G19
A	-3	ARG	-	expression tag	UNP Q84G19
A	-2	GLY	-	expression tag	UNP Q84G19
A	-1	SER	-	expression tag	UNP Q84G19
A	0	HIS	-	expression tag	UNP Q84G19
A	24	TYR	VAL	engineered mutation	UNP Q84G19
A	157	ALA	GLY	engineered mutation	UNP Q84G19
A	158	ALA	ARG	engineered mutation	UNP Q84G19
A	188	ARG	GLY	engineered mutation	UNP Q84G19
B	-19	MET	-	initiating methionine	UNP Q84G19

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q84G19
B	-17	SER	-	expression tag	UNP Q84G19
B	-16	SER	-	expression tag	UNP Q84G19
B	-15	HIS	-	expression tag	UNP Q84G19
B	-14	HIS	-	expression tag	UNP Q84G19
B	-13	HIS	-	expression tag	UNP Q84G19
B	-12	HIS	-	expression tag	UNP Q84G19
B	-11	HIS	-	expression tag	UNP Q84G19
B	-10	HIS	-	expression tag	UNP Q84G19
B	-9	SER	-	expression tag	UNP Q84G19
B	-8	SER	-	expression tag	UNP Q84G19
B	-7	GLY	-	expression tag	UNP Q84G19
B	-6	LEU	-	expression tag	UNP Q84G19
B	-5	VAL	-	expression tag	UNP Q84G19
B	-4	PRO	-	expression tag	UNP Q84G19
B	-3	ARG	-	expression tag	UNP Q84G19
B	-2	GLY	-	expression tag	UNP Q84G19
B	-1	SER	-	expression tag	UNP Q84G19
B	0	HIS	-	expression tag	UNP Q84G19
B	24	TYR	VAL	engineered mutation	UNP Q84G19
B	157	ALA	GLY	engineered mutation	UNP Q84G19
B	158	ALA	ARG	engineered mutation	UNP Q84G19
B	188	ARG	GLY	engineered mutation	UNP Q84G19

- Molecule 2 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula:  $\text{CH}_4\text{NO}_5\text{P}$ ).

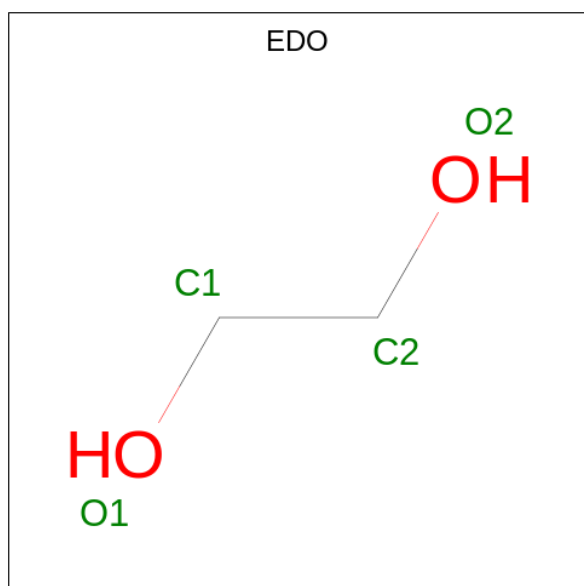


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			8	1	1	5	1		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

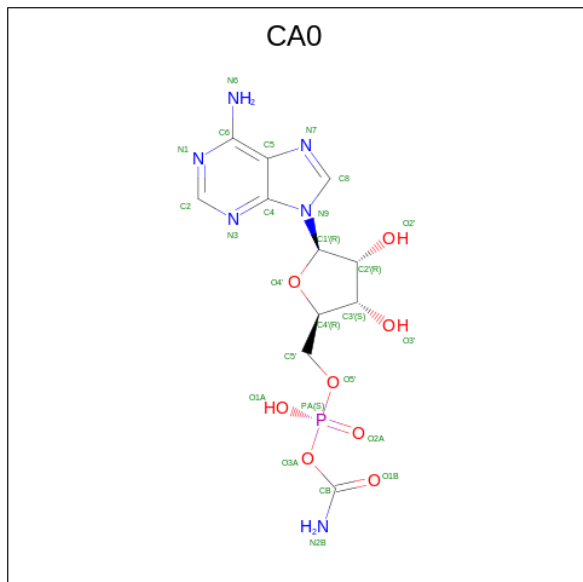
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



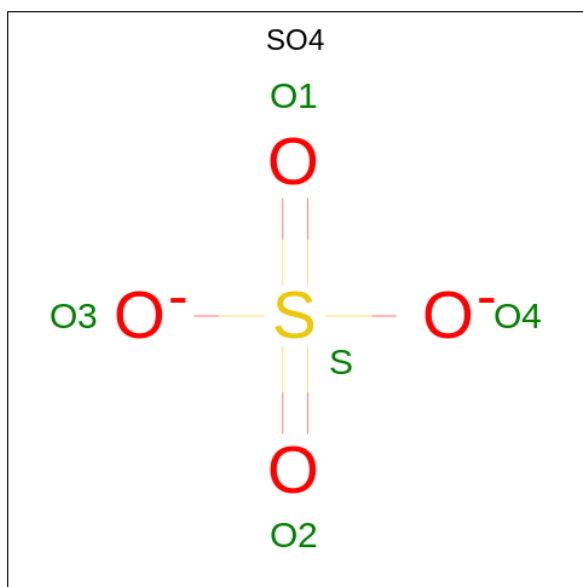
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 5'-O-[(S)-(carbamoyloxy)(hydroxy)phosphoryl]adenosine (three-letter code: CA0) (formula:  $C_{11}H_{15}N_6O_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			26	11	6	8	1		
5	B	1	Total	C	N	O	P	0	0
			26	11	6	8	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

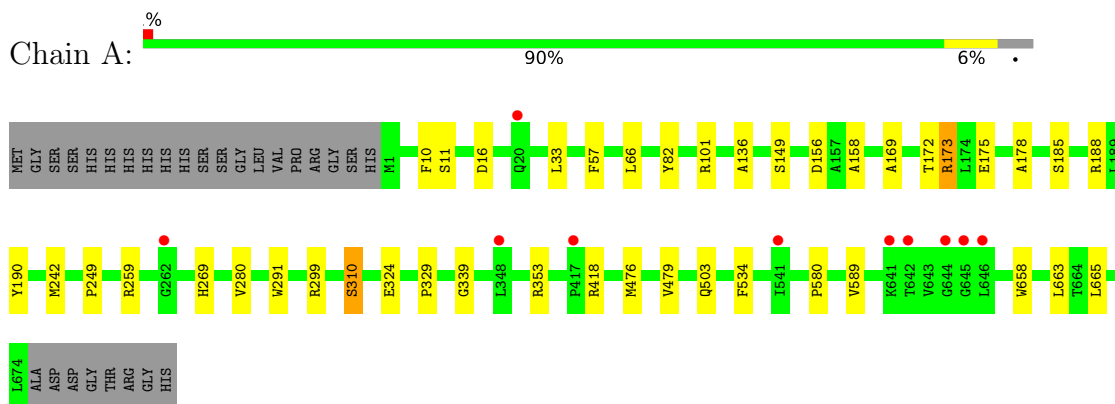
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	170	Total O 170 170	0	0
8	B	91	Total O 91 91	0	0

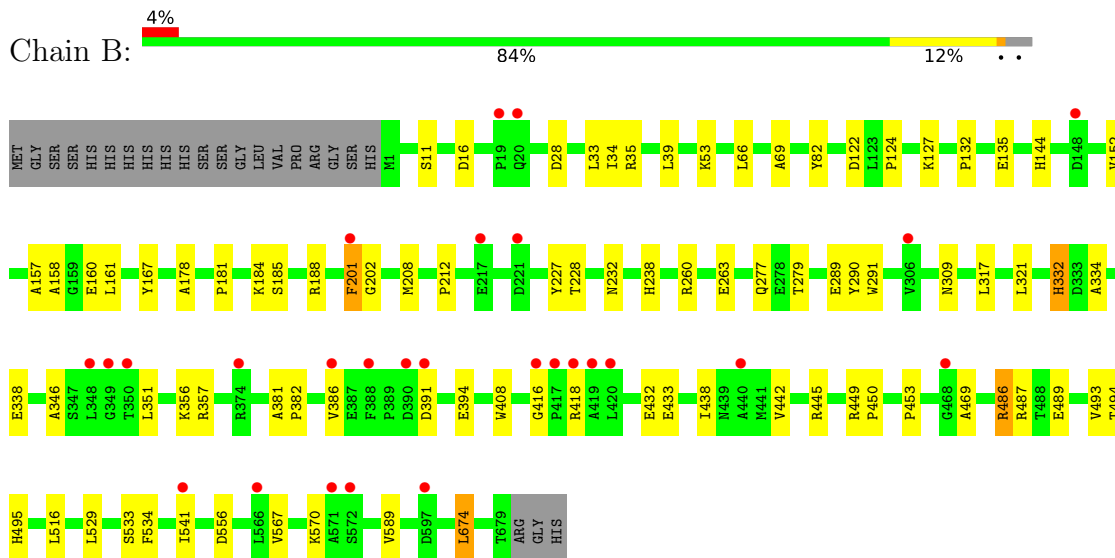
### 3 Residue-property plots [i](#)

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: GdmN



#### • Molecule 1: GdmN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.09Å 111.09Å 231.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.43 – 2.10 44.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.43-2.10) 99.5 (44.43-2.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.196 , 0.233 0.196 , 0.233	Depositor DCC
$R_{free}$ test set	4796 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: FE, EDO, CA0, CL, SO4, CP

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	0.42	0/5330	0.64	0/7250
1	B	0.39	0/5340	0.62	0/7268
All	All	0.40	0/10670	0.63	0/14518

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	5208	0	5115	28	0
1	B	5218	0	5097	55	0
2	A	8	0	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	16	0	24	5	0
4	B	8	0	12	4	0
5	A	26	0	14	2	0
5	B	26	0	14	3	0
6	A	25	0	0	0	0
6	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	170	0	0	1	0
8	B	91	0	0	0	0
All	All	10814	0	10278	82	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 (82) 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:B:346:ALA:HB2	1:B:351:LEU:HD12	1.51	0.90
1:B:418:ARG:HB2	4:B:702:EDO:H11	1.68	0.76
1:B:158:ALA:HB2	1:B:188:ARG:HH21	1.53	0.73
1:B:438:ILE:HA	1:B:442:VAL:HG22	1.76	0.66
1:B:277:GLN:HG2	4:B:703:EDO:H21	1.76	0.65
1:B:228:THR:HG23	1:B:238:HIS:NE2	2.11	0.65
1:B:442:VAL:HG12	1:B:556:ASP:HB2	1.78	0.64
1:B:208:MET:HE1	1:B:309:ASN:HA	1.81	0.62
1:A:476:MET:HG3	1:A:503:GLN:HB2	1.83	0.61
1:A:310:SER:HB2	1:A:479:VAL:HG23	1.84	0.58
1:B:445:ARG:HD2	1:B:449:ARG:HG3	1.87	0.57
1:B:450:PRO:HG3	1:B:495:HIS:CD2	2.40	0.57
1:A:418:ARG:HB2	4:A:703:EDO:H12	1.87	0.57
1:A:158:ALA:H	5:A:707:CA0:HN2B	1.54	0.56
1:A:418:ARG:N	4:A:703:EDO:H21	2.21	0.56
1:A:418:ARG:H	4:A:703:EDO:H21	1.71	0.55
1:A:156:ASP:HB2	5:A:707:CA0:HN2A	1.71	0.55
1:B:160:GLU:HG2	1:B:161:LEU:HG	1.89	0.55
1:B:212:PRO:HG3	4:B:703:EDO:H11	1.90	0.54
1:A:172:THR:HG22	1:A:353:ARG:HD2	1.89	0.53
1:B:486:ARG:NH1	1:B:489:GLU:OE1	2.43	0.51
1:B:438:ILE:HA	1:B:442:VAL:CG2	2.39	0.51
1:A:178:ALA:HB2	1:A:291:TRP:CZ2	2.46	0.51
1:B:208:MET:CE	5:B:704:CA0:HN6	2.23	0.50
1:B:232:ASN:HA	1:B:290:TYR:CE1	2.47	0.49
1:A:173:ARG:NH2	1:A:175:GLU:OE2	2.45	0.49
1:B:208:MET:CE	1:B:309:ASN:HA	2.43	0.49
1:B:35:ARG:NH2	1:B:69:ALA:O	2.45	0.49
1:A:580:PRO:HA	1:A:665:LEU:HD23	1.94	0.48
1:B:391:ASP:OD2	1:B:394:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:SER:HB3	1:B:16:ASP:HA	1.95	0.48
1:A:185:SER:HB3	1:A:188:ARG:HB2	1.96	0.48
1:B:386:VAL:HG12	1:B:567:VAL:HG22	1.96	0.48
1:B:453:PRO:HB3	1:B:493:VAL:HG21	1.95	0.48
1:A:101:ARG:HG2	1:A:101:ARG:HH11	1.79	0.48
1:B:201:PHE:HD1	1:B:202:GLY:H	1.63	0.47
1:A:11:SER:HB3	1:A:16:ASP:HA	1.95	0.47
1:B:124:PRO:HG2	1:B:127:LYS:HG3	1.97	0.47
1:A:589:VAL:HG13	1:B:589:VAL:HG13	1.95	0.47
1:B:28:ASP:OD1	1:B:53:LYS:HG2	2.16	0.46
1:B:132:PRO:HB2	1:B:135:GLU:HB2	1.98	0.45
1:B:289:GLU:HG3	1:B:321:LEU:HD11	1.96	0.45
1:A:190:TYR:HD2	1:A:280:VAL:HG21	1.81	0.45
1:A:101:ARG:NH2	8:A:807:HOH:O	2.49	0.45
1:B:34[A]:ILE:HD13	1:B:39:LEU:HA	1.98	0.45
1:A:299:ARG:HG2	1:A:324:GLU:HB2	1.98	0.44
1:B:260:ARG:O	1:B:263:GLU:HB2	2.17	0.44
1:A:33:LEU:HD11	1:A:66:LEU:HD23	1.99	0.44
1:A:418:ARG:O	4:A:703:EDO:H21	2.18	0.44
1:B:157:ALA:HB2	5:B:704:CA0:O3'	2.17	0.44
1:B:185:SER:HB3	1:B:188:ARG:HD2	1.98	0.44
1:A:242:MET:HE2	1:A:249:PRO:HB3	2.00	0.44
1:A:259:ARG:HB2	1:A:269:HIS:CE1	2.53	0.44
1:B:201:PHE:HD1	1:B:202:GLY:N	2.15	0.44
1:B:33:LEU:HD11	1:B:66:LEU:HD23	2.00	0.43
1:B:157:ALA:HB3	5:B:704:CA0:O1B	2.18	0.43
1:A:10:PHE:HA	1:A:57:PHE:HB2	2.01	0.43
1:B:381:ALA:O	1:B:570:LYS:HE2	2.18	0.43
1:A:329:PRO:CB	4:A:703:EDO:H11	2.48	0.43
1:A:658:TRP:CD1	1:A:665:LEU:HB2	2.53	0.43
1:B:332:HIS:HE1	1:B:334:ALA:HB3	1.83	0.43
1:B:442:VAL:HG12	1:B:556:ASP:CB	2.49	0.43
1:B:487:ARG:HG2	1:B:494:THR:HG21	2.00	0.43
1:B:317:LEU:HD12	1:B:469:ALA:HB3	2.00	0.42
1:B:332:HIS:CE1	1:B:334:ALA:HB3	2.54	0.42
1:B:433:GLU:H	1:B:433:GLU:CD	2.23	0.42
1:B:356:LYS:HE3	1:B:357:ARG:H	1.84	0.42
1:B:408:TRP:CH2	1:B:516:LEU:HD12	2.55	0.42
1:B:185:SER:HB3	1:B:188:ARG:HB2	2.02	0.42
1:B:674:LEU:HD12	1:B:674:LEU:HA	1.93	0.41
1:A:101:ARG:HG2	1:A:101:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HB	1:B:167:TYR:HB2	2.03	0.41
1:B:516:LEU:HD22	1:B:529:LEU:HD11	2.03	0.41
1:B:178:ALA:HB2	1:B:291:TRP:CZ2	2.56	0.41
1:B:416:GLY:C	4:B:702:EDO:H22	2.40	0.41
1:A:136:ALA:O	1:A:339:GLY:HA3	2.21	0.41
1:B:381:ALA:HB3	1:B:382:PRO:HD3	2.04	0.40
1:B:533:SER:HB2	1:B:541:ILE:HG12	2.03	0.40
1:B:181:PRO:HD2	1:B:184:LYS:HD2	2.04	0.40
1:B:144:HIS:NE2	1:B:338:GLU:OE2	2.35	0.40
1:B:227:TYR:CE1	1:B:279:THR:HG23	2.56	0.40
1:A:149:SER:HA	1:A:169:ALA:O	2.21	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	673/702 (96%)	656 (98%)	17 (2%)	0	100	100
1	B	678/702 (97%)	653 (96%)	25 (4%)	0	100	100
All	All	1351/1404 (96%)	1309 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	538/559 (96%)	533 (99%)	5 (1%)	78	84
1	B	535/559 (96%)	527 (98%)	8 (2%)	65	71
All	All	1073/1118 (96%)	1060 (99%)	13 (1%)	71	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	173	ARG
1	A	310	SER
1	A	534	PHE
1	A	663	LEU
1	B	82	TYR
1	B	122	ASP
1	B	201	PHE
1	B	332	HIS
1	B	432	GLU
1	B	486	ARG
1	B	534	PHE
1	B	674	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 3 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
6	SO4	A	709	-	4,4,4	0.14	0	6,6,6	0.25	0
4	EDO	A	703	-	3,3,3	0.18	0	2,2,2	0.53	0
6	SO4	A	710	-	4,4,4	0.18	0	6,6,6	0.37	0
4	EDO	B	702	-	3,3,3	0.45	0	2,2,2	0.33	0
6	SO4	B	705	-	4,4,4	0.15	0	6,6,6	0.17	0
4	EDO	A	706	-	3,3,3	0.50	0	2,2,2	0.44	0
4	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.34	0
6	SO4	A	712	-	4,4,4	0.35	0	6,6,6	0.15	0
5	CA0	A	707	3	24,28,28	3.83	10 (41%)	26,42,42	1.81	7 (26%)
4	EDO	A	705	-	3,3,3	0.51	0	2,2,2	0.41	0
5	CA0	B	704	3	24,28,28	3.94	10 (41%)	26,42,42	1.71	6 (23%)
2	CP	A	701	-	6,7,7	3.67	2 (33%)	7,10,10	2.46	2 (28%)
4	EDO	B	703	-	3,3,3	0.47	0	2,2,2	0.34	0
6	SO4	A	711	-	4,4,4	0.16	0	6,6,6	0.33	0
6	SO4	B	707	-	4,4,4	0.19	0	6,6,6	0.30	0
6	SO4	A	708	-	4,4,4	0.15	0	6,6,6	0.19	0
6	SO4	B	706	-	4,4,4	0.13	0	6,6,6	0.23	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	EDO	A	703	-	-	0/1/1/1	-
4	EDO	B	702	-	-	0/1/1/1	-
4	EDO	A	706	-	-	0/1/1/1	-
4	EDO	A	704	-	-	1/1/1/1	-
5	CA0	A	707	3	-	2/9/31/31	0/3/3/3
4	EDO	A	705	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CA0	B	704	3	-	2/9/31/31	0/3/3/3
2	CP	A	701	-	-	1/3/5/5	-
4	EDO	B	703	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	CA0	C3'-C2'	-9.54	1.27	1.53
5	A	707	CA0	C3'-C2'	-9.27	1.28	1.53
5	A	707	CA0	O4'-C1'	-8.83	1.28	1.41
5	B	704	CA0	C2'-C1'	8.81	1.67	1.53
5	B	704	CA0	O4'-C1'	-8.68	1.29	1.41
5	A	707	CA0	C2'-C1'	8.60	1.66	1.53
2	A	701	CP	C-N	6.36	1.45	1.33
2	A	701	CP	P-O4P	6.00	1.68	1.59
5	B	704	CA0	CB-N2B	5.61	1.44	1.33
5	A	707	CA0	CB-N2B	5.01	1.42	1.33
5	B	704	CA0	O4'-C4'	4.91	1.56	1.45
5	A	707	CA0	O4'-C4'	4.65	1.55	1.45
5	A	707	CA0	C5'-C4'	-4.30	1.38	1.51
5	B	704	CA0	C5'-C4'	-4.10	1.38	1.51
5	B	704	CA0	C6-N6	3.36	1.46	1.34
5	A	707	CA0	C6-N6	3.28	1.46	1.34
5	B	704	CA0	O3'-C3'	3.24	1.50	1.43
5	A	707	CA0	O3'-C3'	3.13	1.50	1.43
5	B	704	CA0	O1B-CB	-3.09	1.17	1.21
5	A	707	CA0	PA-O3A	2.58	1.65	1.60
5	A	707	CA0	O1B-CB	-2.54	1.18	1.21
5	B	704	CA0	PA-O3A	2.43	1.65	1.60

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CP	O-C-N	-5.44	116.53	125.51
5	A	707	CA0	N3-C2-N1	-4.69	121.35	128.68
5	B	704	CA0	N3-C2-N1	-4.39	121.81	128.68
5	A	707	CA0	O1B-CB-N2B	-4.18	118.61	125.51
5	B	704	CA0	O1B-CB-N2B	-3.90	119.08	125.51
5	B	704	CA0	C3'-C2'-C1'	3.45	106.17	100.98
5	A	707	CA0	C3'-C2'-C1'	3.41	106.11	100.98
5	B	704	CA0	O3A-PA-O5'	2.83	111.19	102.92
2	A	701	CP	O3P-P-O4P	2.77	113.70	105.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	707	CA0	O3A-PA-O5'	2.58	110.45	102.92
5	A	707	CA0	C4-C5-N7	-2.45	106.85	109.40
5	A	707	CA0	O1A-PA-O3A	2.44	112.11	104.14
5	B	704	CA0	O1A-PA-O3A	2.24	111.46	104.14
5	A	707	CA0	O4'-C1'-C2'	-2.24	103.65	106.93
5	B	704	CA0	N6-C6-N1	2.02	122.76	118.57

There are no chirality outliers.

All (8) torsion outliers are listed below:

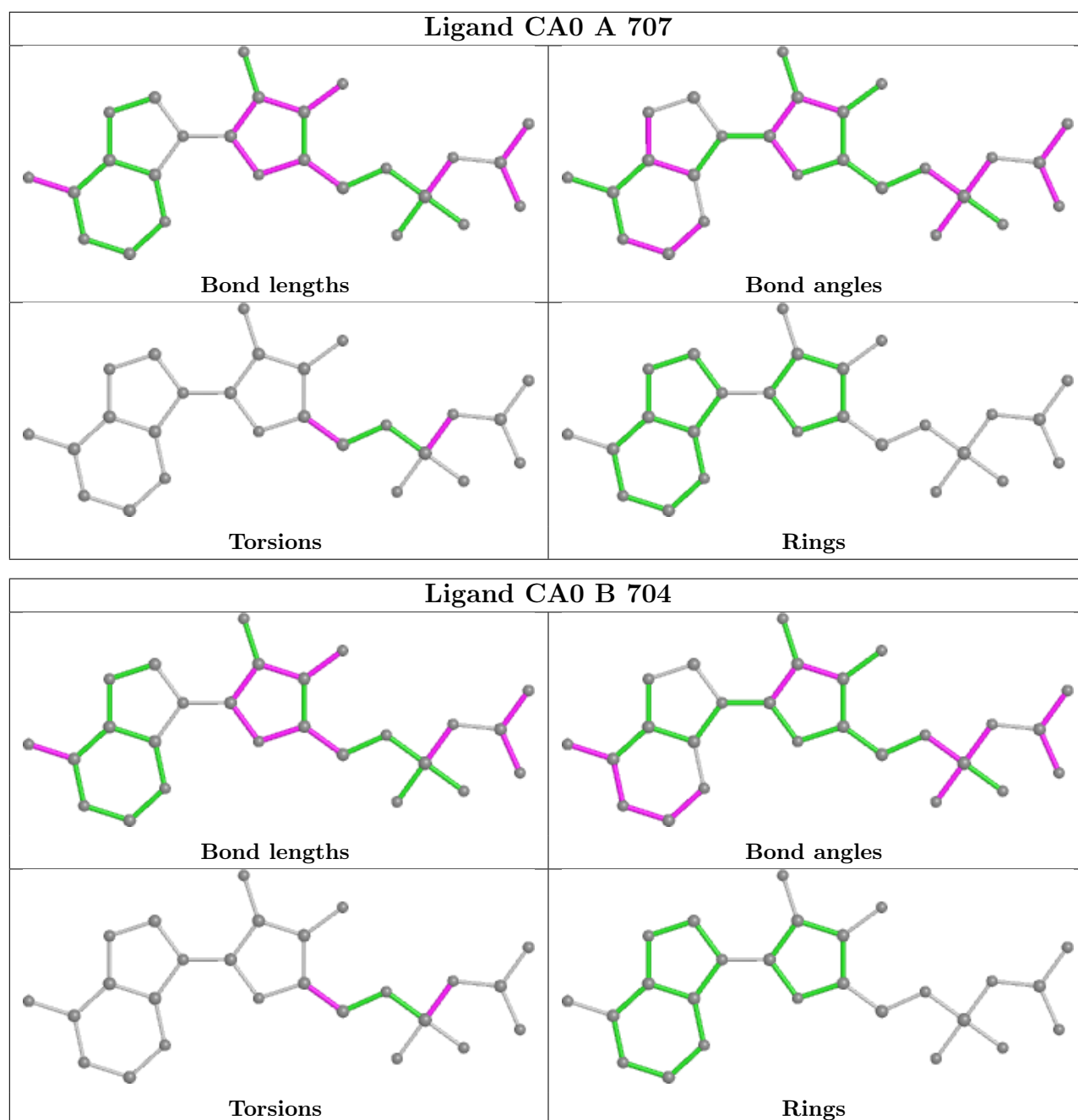
Mol	Chain	Res	Type	Atoms
2	A	701	CP	C-O4P-P-O1P
4	A	704	EDO	O1-C1-C2-O2
5	B	704	CA0	C3'-C4'-C5'-O5'
4	B	703	EDO	O1-C1-C2-O2
4	A	705	EDO	O1-C1-C2-O2
5	A	707	CA0	C3'-C4'-C5'-O5'
5	A	707	CA0	CB-O3A-PA-O5'
5	B	704	CA0	CB-O3A-PA-O5'

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	EDO	5	0
4	B	702	EDO	2	0
5	A	707	CA0	2	0
5	B	704	CA0	3	0
4	B	703	EDO	2	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	674/702 (96%)	0.01	10 (1%) 73 77	24, 35, 52, 66	0
1	B	679/702 (96%)	0.21	27 (3%) 38 44	27, 42, 62, 74	0
All	All	1353/1404 (96%)	0.11	37 (2%) 54 60	24, 38, 59, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	571	ALA	4.6
1	B	468	GLY	4.5
1	A	646	LEU	4.1
1	A	645	GLY	3.7
1	B	350	THR	3.5
1	B	541	ILE	3.5
1	B	417	PRO	3.2
1	B	386	VAL	3.1
1	B	440	ALA	2.9
1	A	642	THR	2.9
1	B	572	SER	2.9
1	A	348	LEU	2.9
1	B	348	LEU	2.8
1	B	390	ASP	2.7
1	B	388	PHE	2.6
1	A	644	GLY	2.5
1	B	201	PHE	2.5
1	B	20	GLN	2.4
1	B	597	ASP	2.4
1	B	148	ASP	2.4
1	A	20	GLN	2.3
1	B	349	GLY	2.3
1	B	221	ASP	2.2
1	B	418	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	641	LYS	2.2
1	B	217	GLU	2.2
1	B	566	LEU	2.2
1	A	262	GLY	2.1
1	A	541	ILE	2.1
1	A	417	PRO	2.1
1	B	306	VAL	2.1
1	B	419	ALA	2.1
1	B	19	PRO	2.0
1	B	374	ARG	2.0
1	B	391	ASP	2.0
1	B	416	GLY	2.0
1	B	420	LEU	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 monosaccharides 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	EDO	B	703	4/4	0.84	0.31	46,47,51,59	0
4	EDO	A	706	4/4	0.86	0.18	37,41,47,56	0
2	CP	A	701	8/8	0.87	0.18	41,45,56,61	0
7	CL	B	708	1/1	0.89	0.13	61,61,61,61	0
4	EDO	A	705	4/4	0.90	0.36	44,47,47,48	0
6	SO4	B	707	5/5	0.91	0.13	65,65,68,70	0
5	CA0	A	707	26/26	0.91	0.20	25,33,40,42	26
5	CA0	B	704	26/26	0.92	0.25	32,43,45,49	26
4	EDO	A	704	4/4	0.93	0.15	48,48,50,51	0
6	SO4	A	711	5/5	0.95	0.17	58,60,67,73	0

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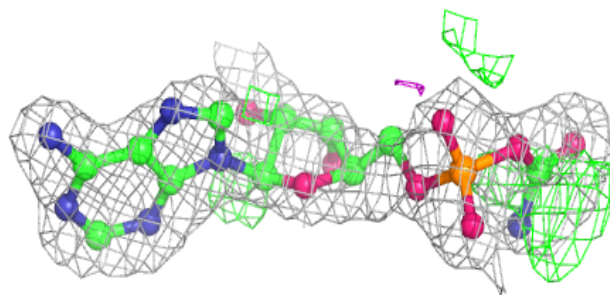
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	702	4/4	0.95	0.15	37,38,39,40	0
6	SO4	A	710	5/5	0.95	0.14	51,55,61,63	0
6	SO4	A	709	5/5	0.96	0.15	51,58,58,62	0
6	SO4	A	712	5/5	0.96	0.17	34,42,49,56	0
4	EDO	A	703	4/4	0.97	0.19	26,29,30,31	0
6	SO4	B	706	5/5	0.97	0.17	51,52,55,60	0
6	SO4	B	705	5/5	0.99	0.18	47,52,58,59	0
3	FE	B	701	1/1	0.99	0.15	34,34,34,34	0
3	FE	A	702	1/1	1.00	0.15	31,31,31,31	0
6	SO4	A	708	5/5	1.00	0.18	32,35,40,43	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.

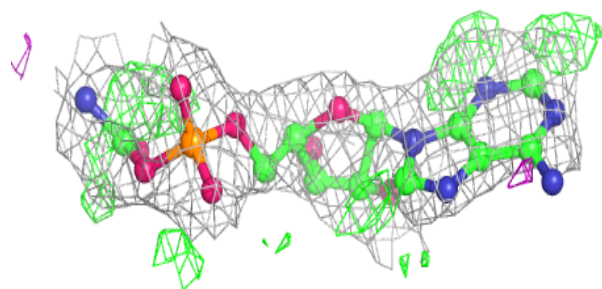
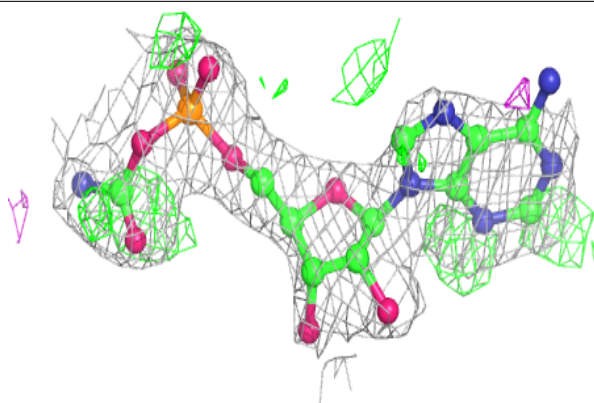
**Electron density around CA0 A 707:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA0 B 704:**

$2mF_o-DF_c$  (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.