



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:17 am BST

PDB ID : 5IU0  
Title : Rubisco from Arabidopsis thaliana  
Authors : Valegaard, K.; Hasse, D.; Gunn, L.; Andersson, I.  
Deposited on : 2016-03-17  
Resolution : 1.50 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

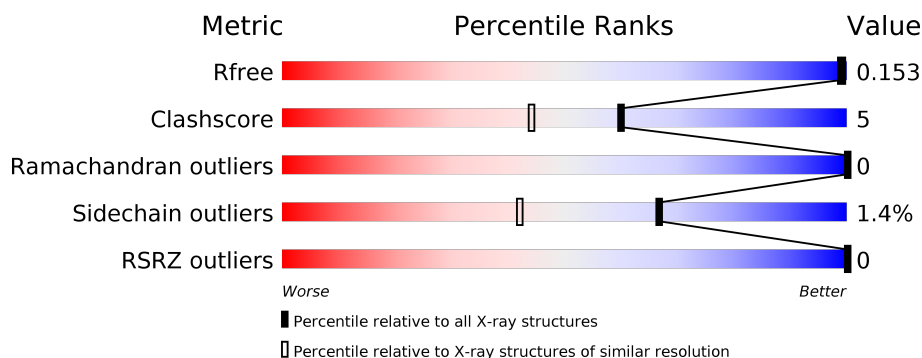
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	479	<div> <div>86%</div> <div>10%</div> <div>•</div> </div>
1	B	479	<div> <div>86%</div> <div>11%</div> <div>•</div> </div>
2	I	181	<div> <div>61%</div> <div>7%</div> <div>32%</div> </div>
2	J	181	<div> <div>59%</div> <div>8%</div> <div>•</div> <div>32%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	509	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10407 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3622	2305	630	671	16			
1	B	463	Total	C	N	O	S	0	0	0
			3622	2305	630	671	16			

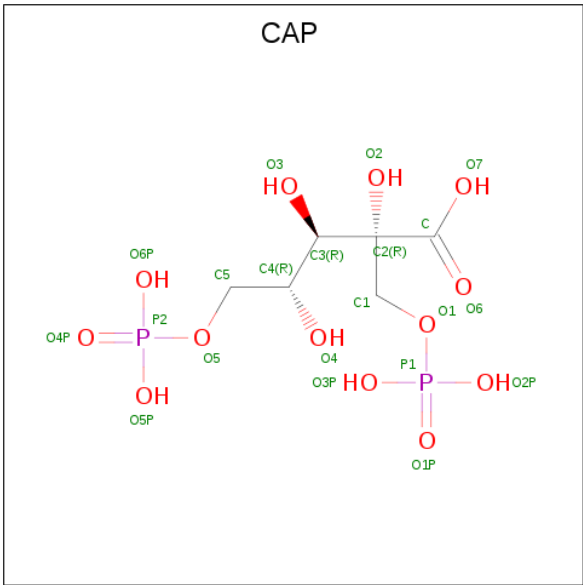
- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain 1B, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	123	Total	C	N	O	S	0	0	0
			1025	675	163	181	6			
2	I	123	Total	C	N	O	S	0	0	0
			1025	675	163	181	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

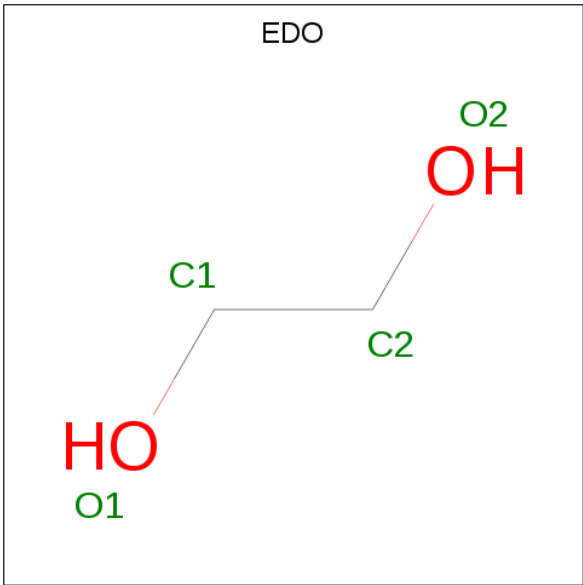
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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

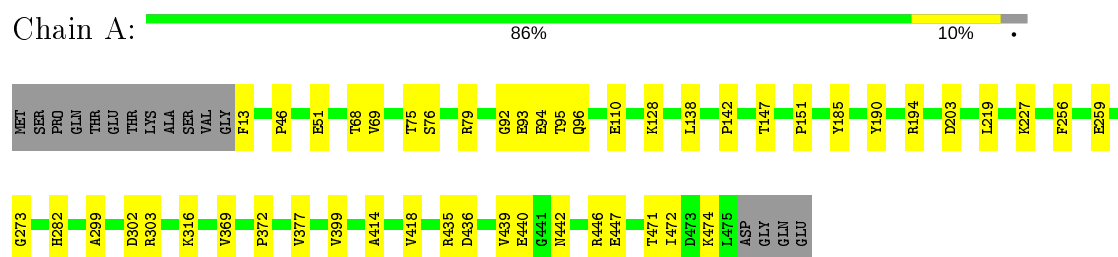
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	373	Total O 373 373	0	0
6	B	374	Total O 374 374	0	0
6	J	126	Total O 126 126	0	0
6	I	144	Total O 144 144	0	0

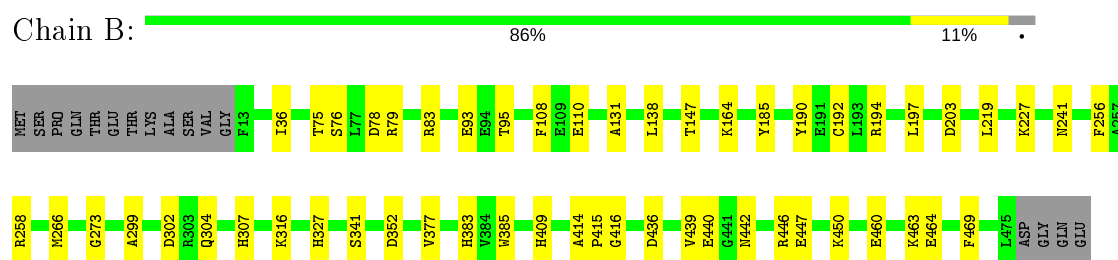
### 3 Residue-property plots

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.

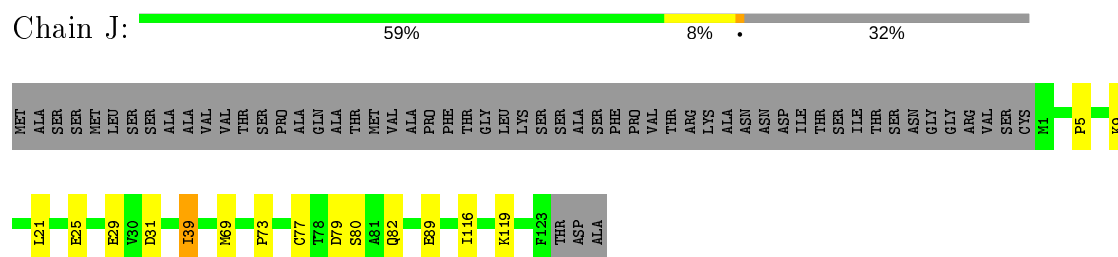
- Molecule 1: Ribulose biphosphate carboxylase large chain



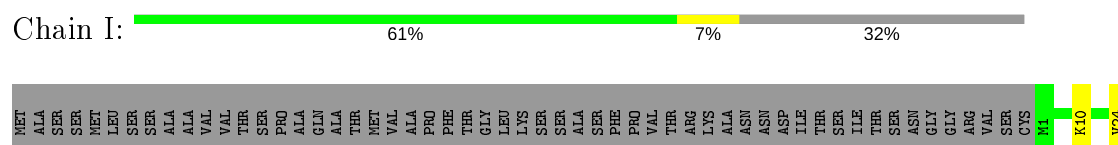
- Molecule 1: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose biphosphate carboxylase small chain 1B, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain 1B, chloroplastic







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.86Å 111.86Å 197.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 1.50 49.43 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.43-1.50) 99.6 (49.43-1.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.50Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.136 , 0.152 0.137 , 0.153	Depositor DCC
$R_{free}$ test set	9636 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for -h,k,-l	Depositor
Outliers	0 of 192721 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: MG, CAP, EDO, KCX

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	0.35	0/3701	0.55	0/5022
1	B	0.36	0/3701	0.56	0/5022
2	I	0.38	0/1059	0.55	0/1436
2	J	0.39	0/1059	0.57	0/1436
All	All	0.36	0/9520	0.55	0/12916

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 [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	3622	0	3535	37	0
1	B	3622	0	3535	34	0
2	I	1025	0	1006	9	0
2	J	1025	0	1006	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	8	0	0
4	B	21	0	8	0	0
5	A	32	0	48	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	12	0	18	0	0
5	I	8	0	12	3	0
6	A	373	0	0	9	2
6	B	374	0	0	4	5
6	I	144	0	0	3	1
6	J	126	0	0	2	1
All	All	10407	0	9176	85	5

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 5.

All (85) 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)
5:A:508:EDO:H22	1:B:304:GLN:HG3	1.60	0.82
1:A:69:VAL:H	5:A:509:EDO:H22	1.44	0.82
1:A:472:ILE:HD11	1:B:131:ALA:HA	1.61	0.82
2:J:31:ASP:OD1	2:J:80:SER:OG	1.99	0.80
1:B:83:ARG:NH1	6:B:601:HOH:O	2.11	0.76
1:A:440:GLU:OE1	6:A:601:HOH:O	2.05	0.73
1:A:436:ASP:HB3	1:A:439:VAL:HG12	1.71	0.71
1:A:259:GLU:OE1	6:A:602:HOH:O	2.11	0.67
1:A:13:PHE:N	6:A:607:HOH:O	2.28	0.66
1:A:92:GLY:O	6:A:603:HOH:O	2.13	0.66
2:J:69:MET:O	6:J:201:HOH:O	2.14	0.65
2:I:65:ARG:HD2	5:I:202:EDO:H22	1.80	0.64
1:B:460:GLU:OE1	1:B:463:LYS:NZ	2.31	0.63
5:A:508:EDO:H12	1:B:307:HIS:HB3	1.81	0.62
1:A:93:GLU:HG2	1:A:96:GLN:HB3	1.83	0.61
1:B:447:GLU:HA	1:B:450:LYS:HE2	1.83	0.60
2:J:89:GLU:OE1	6:J:202:HOH:O	2.17	0.59
1:B:447:GLU:O	1:B:450:LYS:HG2	2.03	0.58
1:A:94:GLU:HG2	1:A:95:THR:HG23	1.86	0.57
1:A:93:GLU:CG	1:A:96:GLN:HB3	2.34	0.57
1:B:219:LEU:HD13	1:B:256:PHE:HZ	1.70	0.57
1:B:436:ASP:HB3	1:B:439:VAL:HG22	1.86	0.56
1:B:442:ASN:HB3	1:B:446:ARG:NH1	2.20	0.56
1:A:471:THR:HB	1:A:474:LYS:HE2	1.89	0.55
1:A:282:HIS:CE1	5:A:503:EDO:H22	2.41	0.55
2:I:35:ARG:NH2	6:I:309:HOH:O	2.40	0.54
1:A:46:PRO:O	6:A:604:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD13	1:A:256:PHE:HZ	1.75	0.51
2:I:65:ARG:HB2	5:I:202:EDO:H12	1.92	0.51
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.45	0.51
1:A:303:ARG:NH2	1:A:472:ILE:HD12	2.25	0.51
1:B:83:ARG:NH2	6:B:610:HOH:O	2.39	0.51
2:I:79:ASP:HB3	2:I:82:GLN:HG3	1.92	0.50
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.47	0.50
1:B:76:SER:HB3	1:B:79:ARG:HG2	1.94	0.50
1:A:190:TYR:CZ	1:A:194:ARG:HD3	2.47	0.50
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.48	0.49
1:B:138:LEU:O	1:B:316:LYS:NZ	2.39	0.49
1:A:68:THR:HA	5:A:509:EDO:H22	1.94	0.49
1:B:439:VAL:HG23	1:B:440:GLU:HG3	1.94	0.49
1:B:352:ASP:OD2	6:B:602:HOH:O	2.20	0.48
1:A:435:ARG:NH2	1:A:447:GLU:OE1	2.34	0.48
1:B:192:CYS:HB3	1:B:197:LEU:HD12	1.94	0.48
1:B:442:ASN:HB3	1:B:446:ARG:HH12	1.78	0.48
1:A:282:HIS:HE1	5:A:503:EDO:H22	1.78	0.48
2:J:25:GLU:O	2:J:29:GLU:HG2	2.13	0.47
1:A:142:PRO:HB3	1:A:369:VAL:HG11	1.95	0.47
1:B:327:HIS:HA	1:B:377:VAL:HB	1.96	0.47
2:I:74:LEU:HD12	2:I:83:VAL:HG22	1.97	0.47
1:A:377:VAL:HG22	1:A:399:VAL:HB	1.97	0.46
2:J:79:ASP:HB3	2:J:82:GLN:HG3	1.97	0.46
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.97	0.45
2:J:5:PRO:HB2	2:J:9:LYS:HG3	1.99	0.45
1:B:190:TYR:CZ	1:B:194:ARG:HD3	2.52	0.45
1:A:69:VAL:N	5:A:509:EDO:H22	2.23	0.45
2:I:119:LYS:NZ	6:I:305:HOH:O	2.32	0.44
2:J:116:ILE:HG21	2:J:119:LYS:HE2	2.00	0.44
1:A:13:PHE:N	6:A:628:HOH:O	2.49	0.44
6:A:847:HOH:O	2:I:10:LYS:HE3	2.17	0.44
2:J:39:ILE:HD11	2:J:73:PRO:CB	2.48	0.44
1:A:474:LYS:NZ	6:A:606:HOH:O	2.23	0.43
1:A:128:LYS:HB3	1:B:469:PHE:CD2	2.54	0.43
2:I:89:GLU:OE1	6:I:301:HOH:O	2.21	0.43
1:A:51:GLU:OE1	6:A:605:HOH:O	2.21	0.43
1:B:36:ILE:HD13	1:B:108:PHE:CE2	2.54	0.42
1:A:299:ALA:HA	1:A:302:ASP:OD1	2.19	0.42
1:B:299:ALA:HA	1:B:302:ASP:OD1	2.20	0.42
1:B:409:HIS:CD2	1:B:416:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LYS:HG3	1:B:464:GLU:HG2	2.00	0.42
1:B:75:THR:OG1	1:B:76:SER:N	2.46	0.41
1:A:69:VAL:HG22	5:A:509:EDO:H21	2.03	0.41
1:A:138:LEU:O	1:A:316:LYS:NZ	2.46	0.41
5:A:508:EDO:H11	1:B:304:GLN:HB2	2.01	0.41
1:B:414:ALA:HB3	1:B:415:PRO:HD3	2.02	0.41
1:A:414:ALA:O	1:A:418:VAL:HG23	2.21	0.41
1:B:241:ASN:HA	1:B:266:MET:HG3	2.02	0.41
1:B:78:ASP:O	1:B:83:ARG:NH2	2.54	0.41
1:A:110:GLU:HB3	1:A:147:THR:HB	2.03	0.40
2:I:65:ARG:CB	5:I:202:EDO:H12	2.51	0.40
1:A:442:ASN:O	1:A:446:ARG:HG3	2.20	0.40
1:A:151:PRO:HD2	1:A:372:PRO:HD2	2.03	0.40
1:A:76:SER:HB3	1:A:79:ARG:HG2	2.03	0.40
1:B:164:LYS:HE3	6:B:734:HOH:O	2.22	0.40
1:A:75:THR:OG1	1:A:76:SER:N	2.52	0.40
1:B:110:GLU:HB3	1:B:147:THR:HB	2.02	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:639:HOH:O	6:B:877:HOH:O[3_655]	1.93	0.27
6:B:615:HOH:O	6:J:201:HOH:O[4_565]	1.96	0.24
6:A:910:HOH:O	6:B:809:HOH:O[4_565]	2.04	0.16
6:B:915:HOH:O	6:I:350:HOH:O[6_555]	2.08	0.12
6:A:858:HOH:O	6:B:949:HOH:O[4_565]	2.17	0.03

## 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	460/479 (96%)	443 (96%)	17 (4%)	0	100	100
1	B	460/479 (96%)	443 (96%)	17 (4%)	0	100	100
2	I	121/181 (67%)	116 (96%)	5 (4%)	0	100	100
2	J	121/181 (67%)	115 (95%)	6 (5%)	0	100	100
All	All	1162/1320 (88%)	1117 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/388 (97%)	373 (100%)	2 (0%)	88	78
1	B	375/388 (97%)	369 (98%)	6 (2%)	62	36
2	I	111/157 (71%)	108 (97%)	3 (3%)	44	15
2	J	111/157 (71%)	108 (97%)	3 (3%)	44	15
All	All	972/1090 (89%)	958 (99%)	14 (1%)	67	42

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	TYR
1	A	203	ASP
1	B	93	GLU
1	B	95	THR
1	B	185	TYR
1	B	203	ASP
1	B	258	ARG
1	B	341	SER
2	J	21	LEU
2	J	39	ILE
2	J	77	CYS
2	I	24	VAL
2	I	110	VAL

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Mol	Chain	Res	Type
2	I	116	ILE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	KCX	B	201	1,3	7,11,12	0.51	0	4,12,14	0.28	0
1	KCX	A	201	1,3	7,11,12	0.57	0	4,12,14	0.49	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
1	KCX	B	201	1,3	-	0/7/10/12	-
1	KCX	A	201	1,3	-	0/7/10/12	-

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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	CAP	A	502	3	15,20,20	0.87	0	20,31,31	0.76	0
5	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.10	0
5	EDO	A	505	-	3,3,3	0.47	0	2,2,2	0.17	0
4	CAP	B	502	3	15,20,20	0.84	0	20,31,31	0.84	0
5	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.18	0
5	EDO	A	508	-	3,3,3	0.41	0	2,2,2	0.40	0
5	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.24	0
5	EDO	A	506	-	3,3,3	0.37	0	2,2,2	0.29	0
5	EDO	A	509	-	3,3,3	0.42	0	2,2,2	0.57	0
5	EDO	I	202	-	3,3,3	0.56	0	2,2,2	0.35	0
5	EDO	I	201	-	3,3,3	0.45	0	2,2,2	0.22	0
5	EDO	B	505	-	3,3,3	0.51	0	2,2,2	0.21	0
5	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.30	0
5	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.13	0
5	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.25	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	CAP	A	502	3	-	4/23/29/29	-
5	EDO	A	504	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	505	-	-	0/1/1/1	-
4	CAP	B	502	3	-	5/23/29/29	-
5	EDO	B	504	-	-	0/1/1/1	-
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	B	503	-	-	0/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	I	202	-	-	1/1/1/1	-
5	EDO	I	201	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	CAP	C2-C3-C4-O4
4	A	502	CAP	O3-C3-C4-O4
4	B	502	CAP	C2-C3-C4-O4
4	B	502	CAP	O3-C3-C4-O4
5	A	509	EDO	O1-C1-C2-O2
4	A	502	CAP	O2-C2-C3-C4
4	B	502	CAP	O2-C2-C3-C4
4	B	502	CAP	C2-C3-C4-C5
5	I	202	EDO	O1-C1-C2-O2
4	B	502	CAP	C5-O5-P2-O4P
5	A	506	EDO	O1-C1-C2-O2
4	A	502	CAP	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 12 short contacts:

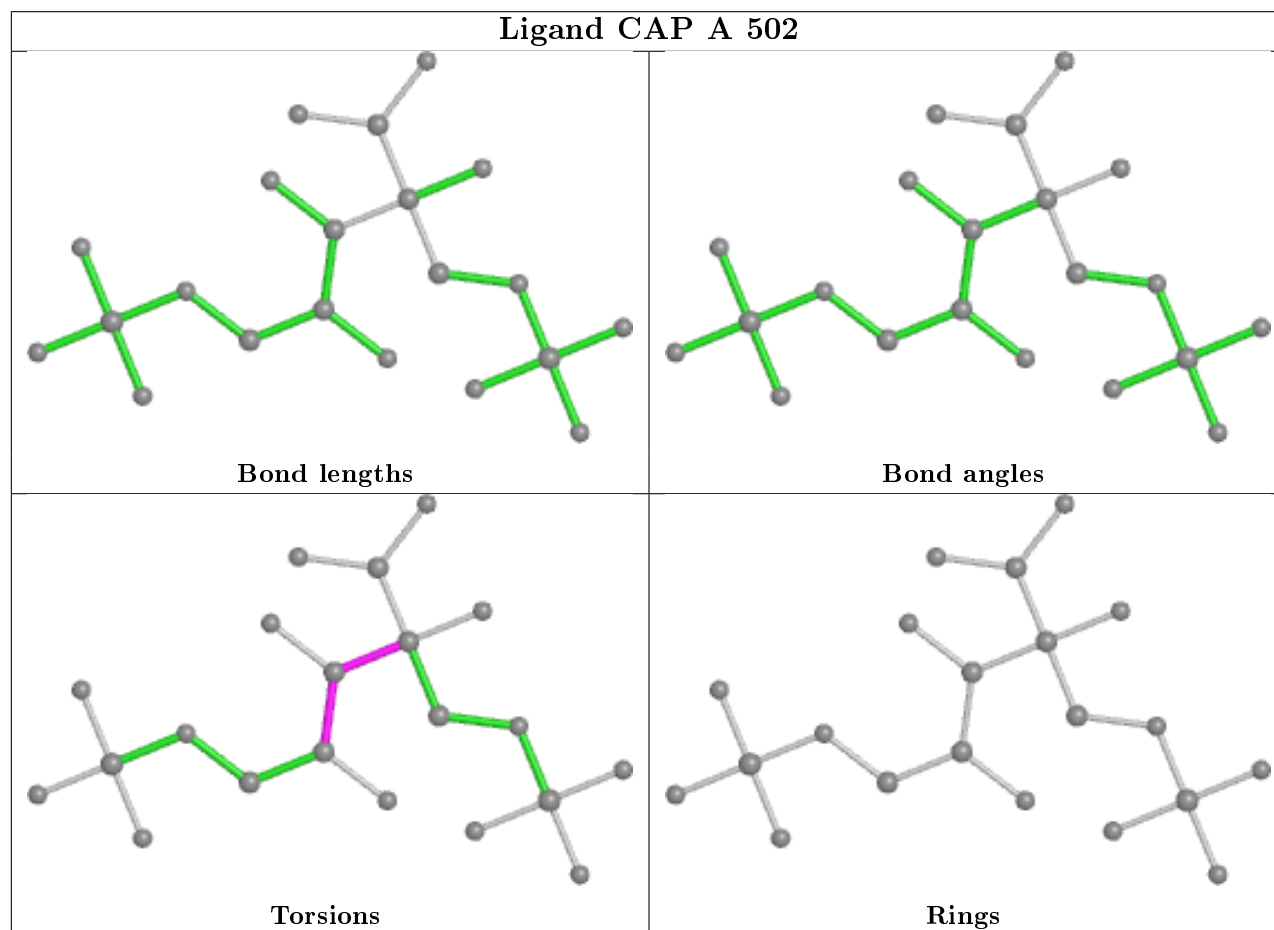
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	EDO	3	0
5	A	509	EDO	4	0
5	I	202	EDO	3	0

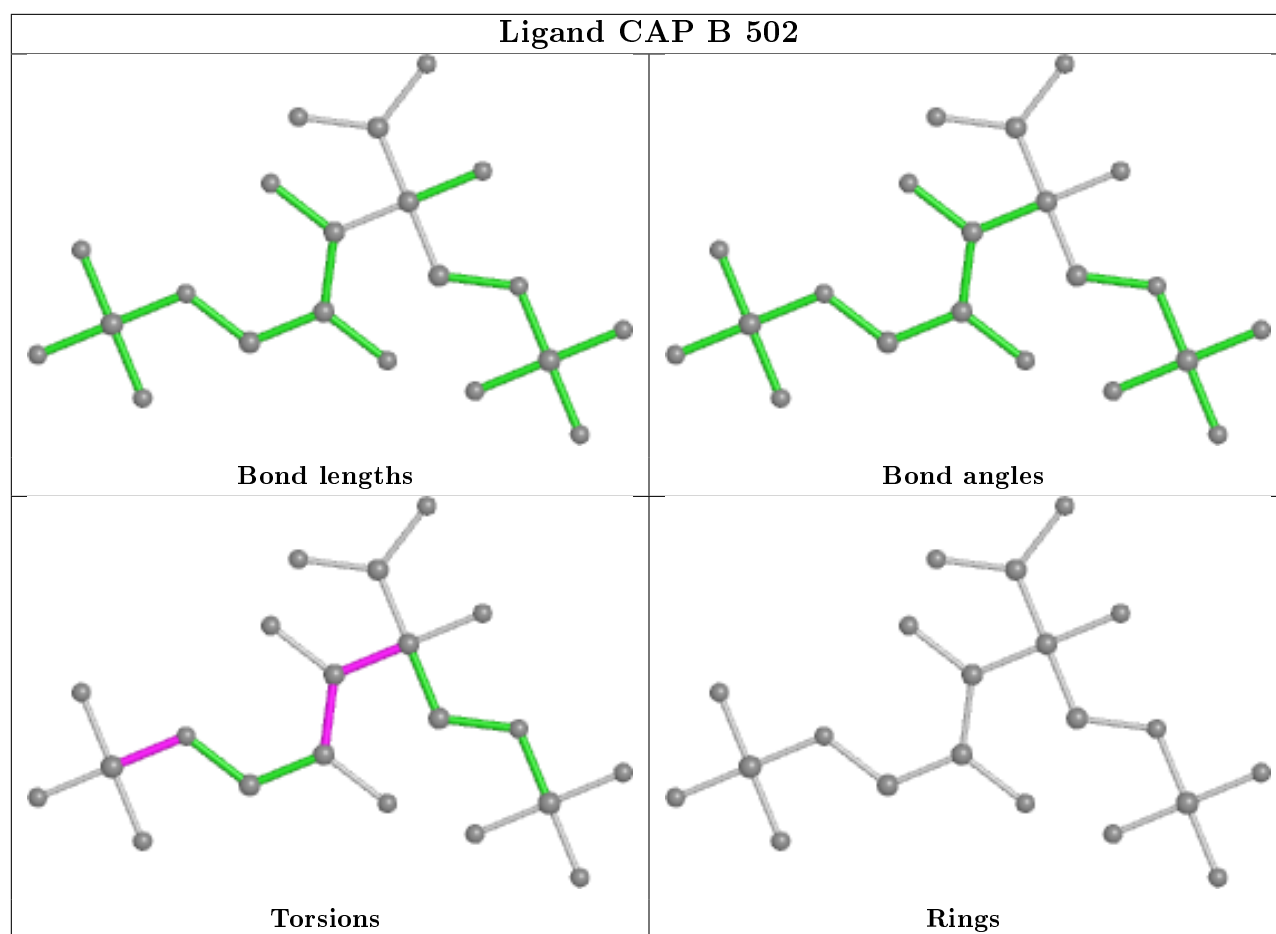
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	EDO	2	0

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 [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	462/479 (96%)	-0.95	0 100 100	10, 14, 23, 30	0
1	B	462/479 (96%)	-0.93	0 100 100	10, 15, 23, 31	0
2	I	123/181 (67%)	-0.90	0 100 100	11, 18, 25, 36	0
2	J	123/181 (67%)	-0.79	0 100 100	13, 20, 27, 35	0
All	All	1170/1320 (88%)	-0.92	0 100 100	10, 15, 24, 36	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	B	201	12/13	0.99	0.05	11,12,13,13	0
1	KCX	A	201	12/13	0.99	0.04	11,11,12,13	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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

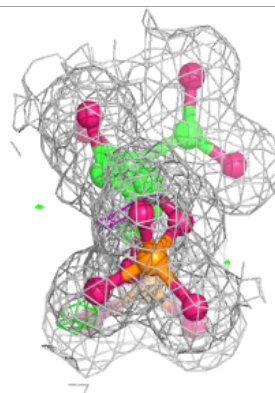
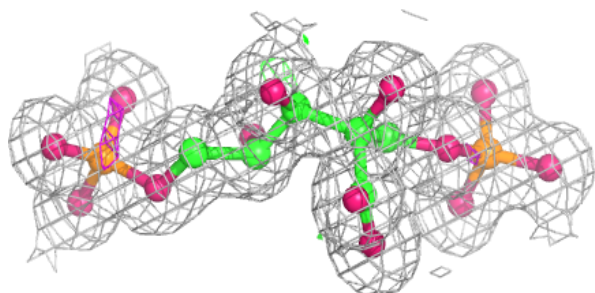
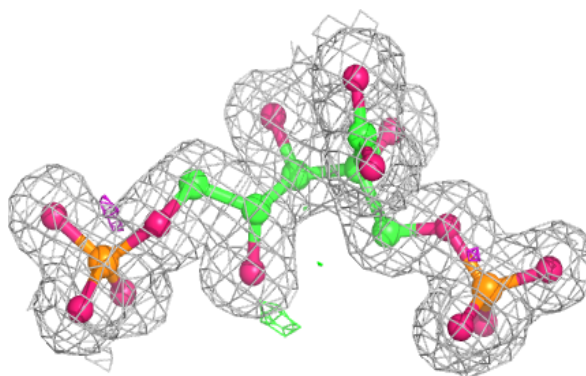
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	I	202	4/4	0.89	0.17	16,16,17,20	0
5	EDO	A	509	4/4	0.94	0.11	17,17,19,21	0
5	EDO	A	508	4/4	0.96	0.12	18,19,19,20	0
5	EDO	A	506	4/4	0.98	0.05	17,18,19,20	0
5	EDO	B	504	4/4	0.98	0.05	16,17,17,19	0
5	EDO	B	503	4/4	0.98	0.05	17,17,17,18	0
5	EDO	A	504	4/4	0.98	0.05	14,15,15,17	0
5	EDO	I	201	4/4	0.98	0.08	17,17,18,18	0
5	EDO	B	505	4/4	0.98	0.06	17,18,18,19	0
5	EDO	A	503	4/4	0.98	0.13	15,16,18,19	0
4	CAP	B	502	21/21	0.99	0.04	13,13,14,15	0
5	EDO	A	510	4/4	0.99	0.06	16,17,17,17	0
5	EDO	A	507	4/4	0.99	0.06	13,14,14,14	0
5	EDO	A	505	4/4	0.99	0.05	15,15,16,16	0
4	CAP	A	502	21/21	1.00	0.04	12,13,13,14	0
3	MG	A	501	1/1	1.00	0.06	13,13,13,13	0
3	MG	B	501	1/1	1.00	0.06	14,14,14,14	0

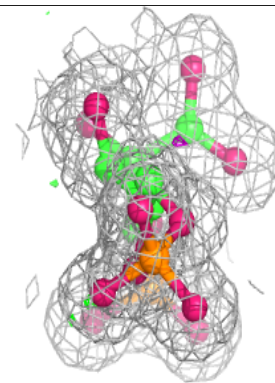
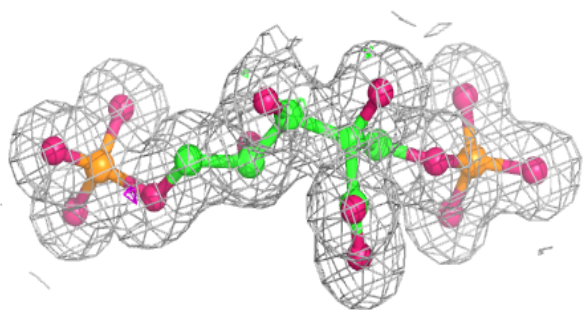
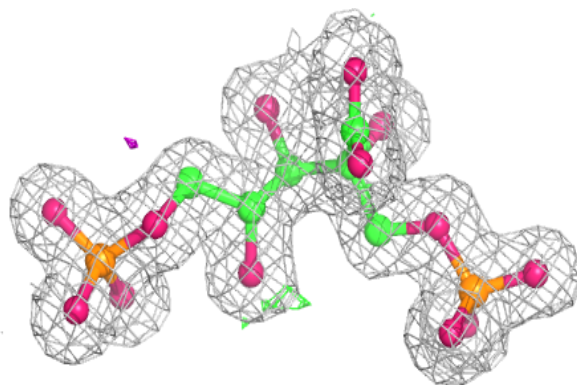
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CAP B 502:**

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

**Electron density around CAP A 502:**

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



## 6.5 Other polymers

There are no such residues in this entry.