



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 12:04 AM JST

PDB ID : 7V4E  
Title : Crystal Structure of VpsR display novel dimeric architecture and c-di-GMP binding: mechanistic implications in oligomerization, ATPase activity and DNA binding.  
Authors : Chakraborty, T.; Sen, U.  
Deposited on : 2021-08-12  
Resolution : 4.00 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 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 : 2.27  
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) : 2.27

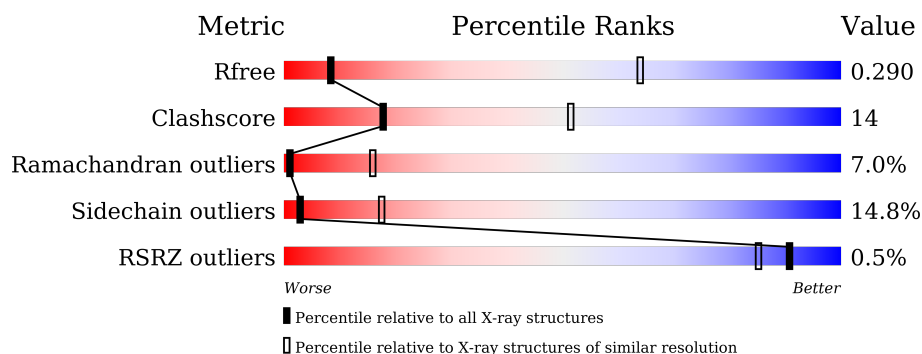
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	399	<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>55%</span> <span>30%</span> <span>8%</span> <span>• 6%</span> </div> </div>
1	D	399	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>56%</span> <span>30%</span> <span>7%</span> <span>• 6%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5974 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 VpsR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2936	1863	510	551	12			
1	D	374	Total	C	N	O	S	0	0	0
			2936	1863	510	551	12			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q9AAQ41
A	-15	HIS	-	expression tag	UNP Q9AAQ41
A	-14	HIS	-	expression tag	UNP Q9AAQ41
A	-13	HIS	-	expression tag	UNP Q9AAQ41
A	-12	HIS	-	expression tag	UNP Q9AAQ41
A	-11	HIS	-	expression tag	UNP Q9AAQ41
A	-10	SER	-	expression tag	UNP Q9AAQ41
A	-9	SER	-	expression tag	UNP Q9AAQ41
A	-8	GLY	-	expression tag	UNP Q9AAQ41
A	-7	LEU	-	expression tag	UNP Q9AAQ41
A	-6	VAL	-	expression tag	UNP Q9AAQ41
A	-5	PRO	-	expression tag	UNP Q9AAQ41
A	-4	ARG	-	expression tag	UNP Q9AAQ41
A	-3	GLY	-	expression tag	UNP Q9AAQ41
A	-2	SER	-	expression tag	UNP Q9AAQ41
A	-1	HIS	-	expression tag	UNP Q9AAQ41
A	0	MET	-	expression tag	UNP Q9AAQ41
D	-16	HIS	-	expression tag	UNP Q9AAQ41
D	-15	HIS	-	expression tag	UNP Q9AAQ41
D	-14	HIS	-	expression tag	UNP Q9AAQ41
D	-13	HIS	-	expression tag	UNP Q9AAQ41
D	-12	HIS	-	expression tag	UNP Q9AAQ41
D	-11	HIS	-	expression tag	UNP Q9AAQ41
D	-10	SER	-	expression tag	UNP Q9AAQ41
D	-9	SER	-	expression tag	UNP Q9AAQ41

*Continued on next page...*

Continued from previous page...

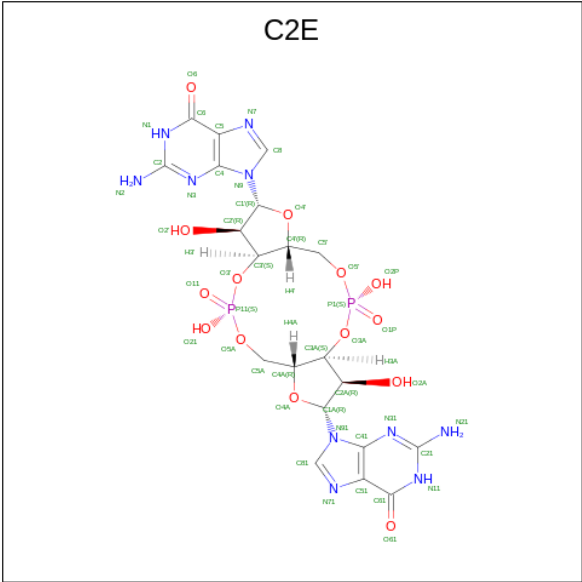
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP Q9AQ41
D	-7	LEU	-	expression tag	UNP Q9AQ41
D	-6	VAL	-	expression tag	UNP Q9AQ41
D	-5	PRO	-	expression tag	UNP Q9AQ41
D	-4	ARG	-	expression tag	UNP Q9AQ41
D	-3	GLY	-	expression tag	UNP Q9AQ41
D	-2	SER	-	expression tag	UNP Q9AQ41
D	-1	HIS	-	expression tag	UNP Q9AQ41
D	0	MET	-	expression tag	UNP Q9AQ41

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



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

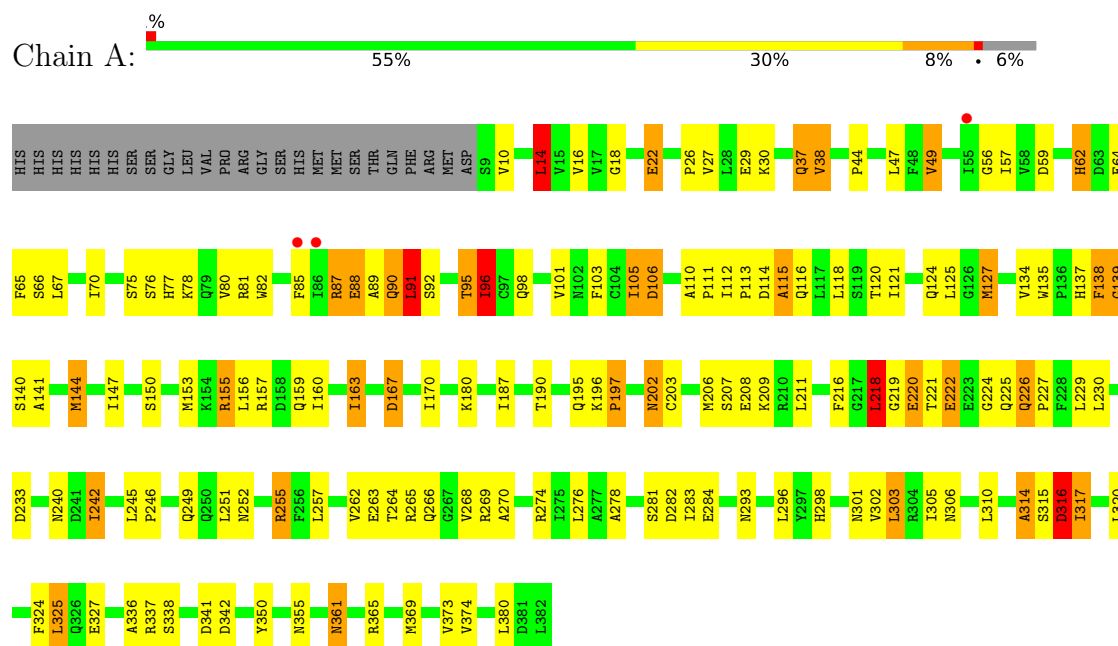
- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



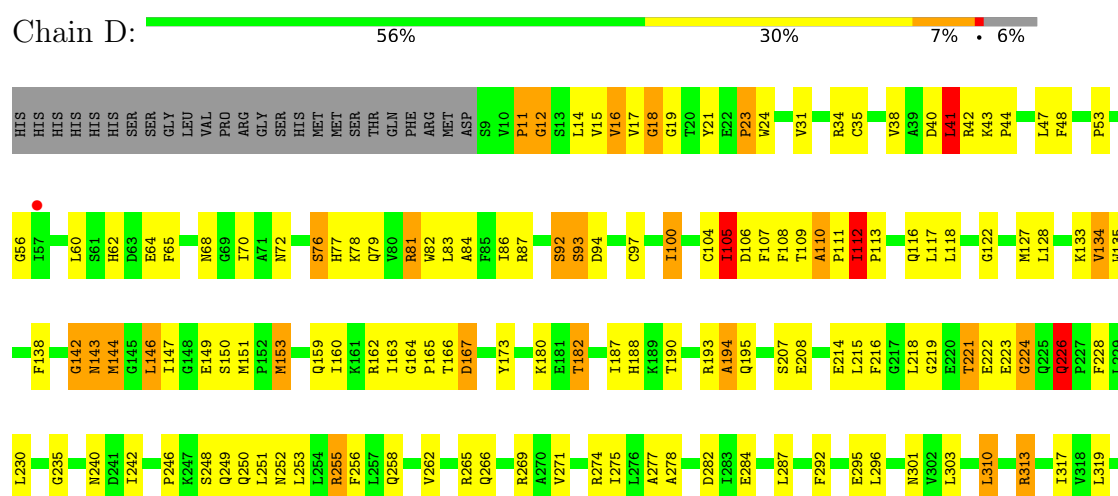
### 3 Residue-property plots [i](#)

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: VpsR



#### • Molecule 1: VpsR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.69Å 119.69Å 81.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 4.00 48.16 – 3.41	Depositor EDS
% Data completeness (in resolution range)	90.3 (48.16-4.00) 96.7 (48.16-3.41)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.241 , 0.280 0.258 , 0.290	Depositor DCC
$R_{free}$ test set	1683 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	139.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 178.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.109 for -h,-k,l 0.250 for h,-h-k,-l 0.119 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: C2E, 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	0.23	0/2990	0.48	2/4047 (0.0%)
1	D	0.24	0/2990	0.46	0/4047
All	All	0.23	0/5980	0.47	2/8094 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	14	LEU	CA-CB-CG	5.30	127.49	115.30

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	2936	0	2967	89	0
1	D	2936	0	2967	81	0
2	A	5	0	0	0	0
2	D	5	0	0	1	0
3	D	92	0	37	0	0
All	All	5974	0	5971	162	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 14.

All (162) 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:284:GLU:OE1	1:D:159:GLN:NE2	2.16	0.79
1:D:16:VAL:HG13	1:D:18:GLY:H	1.47	0.77
1:A:124:GLN:HE22	1:D:105:ILE:HD12	1.50	0.76
1:D:92:SER:O	1:D:94:ASP:N	2.22	0.72
1:A:49:VAL:HG13	1:A:78:LYS:HE2	1.70	0.72
1:D:48:PHE:HB3	1:D:78:LYS:HD2	1.70	0.71
1:A:16:VAL:HG22	1:A:18:GLY:H	1.53	0.71
1:D:104:CYS:O	1:D:106:ASP:N	2.24	0.70
1:D:142:GLY:O	1:D:144:MET:N	2.23	0.69
1:D:113:PRO:O	1:D:117:LEU:N	2.25	0.69
1:A:202:ASN:HD22	1:A:202:ASN:H	1.39	0.69
1:D:133:LYS:HD2	1:D:134:VAL:HG13	1.75	0.69
1:D:193:ARG:NH1	1:D:235:GLY:O	2.26	0.68
1:A:314:ALA:O	1:A:316:ASP:N	2.26	0.68
1:A:302:VAL:HG12	1:A:303:LEU:HD12	1.73	0.68
1:D:118:LEU:O	1:D:122:GLY:N	2.26	0.68
1:D:221:THR:OG1	1:D:222:GLU:N	2.25	0.68
1:A:240:ASN:HA	1:A:278:ALA:HB3	1.73	0.68
1:A:144:MET:SD	1:A:144:MET:N	2.67	0.66
1:D:310:LEU:HD21	1:D:355:ASN:HA	1.75	0.66
1:A:57:ILE:HG12	1:A:85:PHE:HD2	1.62	0.65
1:A:140:SER:O	1:A:157:ARG:NH2	2.30	0.64
1:D:60:LEU:N	1:D:87:ARG:O	2.29	0.63
1:A:263:GLU:HG3	1:A:268:VAL:HG22	1.81	0.62
1:A:314:ALA:O	1:A:317:ILE:HG22	2.01	0.61
1:A:207:SER:O	1:A:209:LYS:N	2.34	0.60
1:D:41:LEU:HD13	1:D:41:LEU:H	1.64	0.60
1:A:206:MET:HB3	1:A:211:LEU:HB2	1.83	0.60
1:A:113:PRO:HB2	1:A:116:GLN:HB2	1.83	0.59
1:A:77:HIS:O	1:A:81:ARG:NE	2.35	0.59
1:D:317:ILE:HD12	1:D:348:THR:HG23	1.84	0.59
1:D:100:ILE:HG23	1:D:104:CYS:HB2	1.84	0.59
1:D:160:ILE:HG23	1:D:187:ILE:HG22	1.85	0.58
1:A:150:SER:H	1:A:153:MET:HB3	1.68	0.58
1:A:160:ILE:HG23	1:A:187:ILE:HG22	1.85	0.58
1:A:26:PRO:HA	1:A:29:GLU:HB2	1.85	0.58
1:D:258:GLN:NE2	1:D:295:GLU:OE1	2.35	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD11	1:D:275:ILE:HG21	1.84	0.58
1:D:310:LEU:HD22	1:D:310:LEU:H	1.69	0.58
1:D:105:ILE:HG13	1:D:106:ASP:N	2.18	0.57
1:D:153:MET:SD	1:D:313:ARG:NH1	2.76	0.57
1:A:90:GLN:O	1:A:92:SER:N	2.38	0.57
1:A:298:HIS:HD2	1:D:76:SER:HA	1.69	0.57
1:D:16:VAL:HG13	1:D:18:GLY:N	2.18	0.57
1:A:113:PRO:O	1:A:115:ALA:N	2.31	0.56
1:D:44:PRO:HA	1:D:47:LEU:HB3	1.88	0.56
1:D:250:GLN:HE22	1:D:292:PHE:HA	1.70	0.56
1:D:301:ASN:O	1:D:301:ASN:ND2	2.39	0.55
1:D:335:GLN:HE21	1:D:371:ASP:HA	1.70	0.55
1:A:22:GLU:HB3	1:A:26:PRO:HD3	1.89	0.55
1:A:75:SER:O	1:A:77:HIS:N	2.40	0.54
1:D:230:LEU:HA	1:D:271:VAL:HG11	1.88	0.54
1:A:202:ASN:HD22	1:A:202:ASN:N	2.02	0.54
1:D:78:LYS:HA	1:D:81:ARG:HB2	1.89	0.54
1:A:373:VAL:HG13	1:A:374:VAL:HG23	1.89	0.53
1:D:221:THR:OG1	1:D:224:GLY:N	2.39	0.53
1:A:180:LYS:HD3	1:A:278:ALA:HB1	1.91	0.53
1:A:95:THR:OG1	1:A:96:ILE:N	2.41	0.53
1:A:163:ILE:HD11	1:A:303:LEU:HD13	1.90	0.53
1:D:143:ASN:O	1:D:143:ASN:ND2	2.42	0.53
1:D:240:ASN:HA	1:D:278:ALA:HB3	1.90	0.53
1:A:282:ASP:OD2	1:D:173:TYR:OH	2.25	0.53
1:A:310:LEU:H	1:A:355:ASN:HD22	1.55	0.53
1:A:139:GLY:O	1:A:157:ARG:NH1	2.42	0.52
1:D:81:ARG:H	1:D:81:ARG:HD2	1.74	0.52
1:D:163:ILE:HB	1:D:303:LEU:HD13	1.92	0.52
1:A:110:ALA:H	1:A:111:PRO:HD2	1.73	0.52
1:A:252:ASN:HA	1:A:255:ARG:HB2	1.91	0.52
1:D:226:GLN:HG2	1:D:230:LEU:HD23	1.92	0.51
1:D:11:PRO:HD2	1:D:34:ARG:H	1.76	0.51
1:A:89:ALA:O	1:A:91:LEU:N	2.33	0.51
1:D:12:GLY:HA3	1:D:35:CYS:HA	1.91	0.51
1:D:38:VAL:HG11	1:D:44:PRO:HD3	1.93	0.51
1:D:246:PRO:HG2	1:D:249:GLN:HG2	1.93	0.50
1:D:15:VAL:O	1:D:16:VAL:HB	2.12	0.50
1:A:101:VAL:HG11	1:D:166:THR:HG22	1.94	0.50
1:A:187:ILE:HD11	1:A:276:LEU:HD13	1.94	0.49
1:A:230:LEU:HD13	1:A:264:THR:HG21	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD23	1:D:296:LEU:HD21	1.94	0.49
1:A:98:GLN:HE22	1:D:134:VAL:HB	1.77	0.49
1:A:87:ARG:NH1	1:A:88:GLU:O	2.46	0.48
1:A:269:ARG:NH2	1:A:270:ALA:O	2.46	0.48
1:D:350:TYR:O	1:D:352:TRP:N	2.38	0.48
1:A:121:ILE:O	1:A:125:LEU:N	2.41	0.48
1:A:16:VAL:N	1:A:38:VAL:O	2.44	0.48
1:A:27:VAL:HG12	1:A:118:LEU:HD21	1.96	0.48
1:D:150:SER:OG	1:D:151:MET:N	2.46	0.47
1:A:134:VAL:HG13	1:A:135:TRP:HD1	1.79	0.47
1:A:156:LEU:HD12	1:A:305:ILE:HD11	1.96	0.47
1:D:251:LEU:O	1:D:255:ARG:N	2.39	0.47
1:D:341:ASP:OD1	1:D:341:ASP:N	2.35	0.47
1:D:248:SER:O	1:D:252:ASN:ND2	2.47	0.47
1:A:150:SER:HB3	1:A:316:ASP:HB2	1.97	0.47
1:A:365:ARG:O	1:A:369:MET:HG2	2.14	0.47
1:D:256:PHE:CD2	1:D:275:ILE:HD11	2.50	0.47
1:A:242:ILE:HA	1:A:245:LEU:HD13	1.97	0.47
1:A:251:LEU:O	1:A:255:ARG:N	2.47	0.47
1:D:180:LYS:NZ	2:D:501:SO4:O2	2.45	0.46
1:D:110:ALA:H	1:D:111:PRO:HD2	1.81	0.46
1:A:155:ARG:HH22	1:A:306:ASN:HB3	1.80	0.46
1:A:98:GLN:HG2	1:D:165:PRO:HB3	1.97	0.46
1:A:336:ALA:HA	1:A:373:VAL:HA	1.97	0.46
1:A:116:GLN:N	1:A:116:GLN:OE1	2.48	0.46
1:D:143:ASN:ND2	1:D:146:LEU:HD23	2.31	0.46
1:D:146:LEU:HD12	1:D:182:THR:HG23	1.98	0.46
1:A:65:PHE:CD2	1:A:70:ILE:HD11	2.52	0.45
1:D:43:LYS:N	1:D:44:PRO:HD2	2.31	0.45
1:D:65:PHE:HB3	1:D:70:ILE:HD11	1.97	0.45
1:A:127:MET:HE2	1:D:107:PHE:HD2	1.82	0.45
1:A:124:GLN:HA	1:A:127:MET:HB2	1.99	0.44
1:D:207:SER:OG	1:D:208:GLU:N	2.50	0.44
1:A:227:PRO:HG2	1:A:264:THR:HG22	1.99	0.44
1:D:16:VAL:HA	1:D:65:PHE:HZ	1.83	0.44
1:A:170:ILE:HD12	1:A:187:ILE:HD12	1.99	0.44
1:A:14:LEU:HB3	1:A:57:ILE:HB	1.99	0.44
1:A:16:VAL:HG21	1:A:59:ASP:OD2	2.18	0.44
1:A:30:LYS:HA	1:A:30:LYS:HD2	1.71	0.44
1:D:164:GLY:O	1:D:274:ARG:NH1	2.42	0.44
1:A:242:ILE:H	1:A:242:ILE:HG13	1.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HD3	1:D:108:PHE:CD2	2.54	0.43
1:D:242:ILE:HG21	1:D:277:ALA:HB1	1.99	0.43
1:A:159:GLN:OE1	1:A:305:ILE:CD1	2.66	0.43
1:D:127:MET:HB2	1:D:127:MET:HE2	1.92	0.43
1:A:229:LEU:HD13	1:A:262:VAL:HG11	2.01	0.43
1:D:143:ASN:O	1:D:146:LEU:N	2.48	0.43
1:A:167:ASP:HA	1:A:274:ARG:HD2	2.01	0.43
1:A:196:LYS:HE3	1:A:197:PRO:HD2	1.99	0.43
1:A:224:GLY:O	1:A:226:GLN:N	2.41	0.43
1:A:246:PRO:HB2	1:A:249:GLN:HG2	2.00	0.43
1:A:269:ARG:HD2	1:A:270:ALA:H	1.84	0.43
1:D:284:GLU:HA	1:D:287:LEU:HG	2.00	0.43
1:A:218:LEU:H	1:A:218:LEU:HD13	1.84	0.43
1:A:301:ASN:O	1:A:301:ASN:ND2	2.52	0.43
1:A:56:GLY:N	1:A:82:TRP:HE1	2.16	0.43
1:D:53:PRO:O	1:D:128:LEU:HD21	2.17	0.42
1:A:138:PHE:HD1	1:A:138:PHE:HA	1.65	0.42
1:D:56:GLY:H	1:D:82:TRP:HE1	1.67	0.42
1:A:293:ASN:OD1	1:A:296:LEU:N	2.46	0.42
1:D:188:HIS:O	1:D:194:ALA:HA	2.20	0.42
1:A:224:GLY:C	1:A:226:GLN:H	2.21	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.85	0.42
1:A:80:VAL:HG21	1:A:303:LEU:HD23	2.02	0.42
1:A:218:LEU:C	1:A:220:GLU:H	2.22	0.42
1:D:40:ASP:O	1:D:44:PRO:HD2	2.20	0.42
1:D:214:GLU:HG3	1:D:228:PHE:CD1	2.54	0.42
1:D:16:VAL:HA	1:D:65:PHE:CZ	2.55	0.41
1:D:82:TRP:CZ2	1:D:84:ALA:HA	2.55	0.41
1:A:14:LEU:HD11	1:A:37:GLN:HG2	2.02	0.41
1:A:44:PRO:HA	1:A:47:LEU:HB3	2.01	0.41
1:A:361:ASN:O	1:A:365:ARG:HG3	2.20	0.41
1:D:193:ARG:HH12	1:D:274:ARG:H	1.68	0.41
1:D:17:VAL:O	1:D:19:GLY:N	2.48	0.41
1:A:16:VAL:HG23	1:A:65:PHE:CE1	2.55	0.41
1:D:21:TYR:HD1	1:D:21:TYR:HA	1.75	0.41
1:A:105:ILE:HD13	1:A:106:ASP:HB2	2.02	0.41
1:A:203:CYS:HA	1:A:206:MET:HG2	2.02	0.41
1:A:218:LEU:HD23	1:A:220:GLU:HG2	2.03	0.41
1:D:16:VAL:HG11	1:D:21:TYR:HE2	1.84	0.41
1:A:81:ARG:NH2	1:A:159:GLN:NE2	2.70	0.40
1:A:218:LEU:HB2	1:A:219:GLY:H	1.59	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ILE:O	1:D:108:PHE:HB2	2.21	0.40
1:D:23:PRO:O	1:D:112:ILE:HG12	2.22	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	372/399 (93%)	283 (76%)	65 (18%)	24 (6%)	1	18
1	D	372/399 (93%)	287 (77%)	57 (15%)	28 (8%)	1	15
All	All	744/798 (93%)	570 (77%)	122 (16%)	52 (7%)	1	16

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	95	THR
1	A	208	GLU
1	A	222	GLU
1	A	315	SER
1	D	11	PRO
1	D	16	VAL
1	D	41	LEU
1	D	93	SER
1	D	105	ILE
1	D	143	ASN
1	D	215	LEU
1	A	76	SER
1	A	114	ASP
1	A	115	ALA
1	A	141	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	233	ASP
1	A	314	ALA
1	A	316	ASP
1	D	12	GLY
1	D	18	GLY
1	D	76	SER
1	D	109	THR
1	D	224	GLY
1	A	62	HIS
1	A	139	GLY
1	A	218	LEU
1	D	24	TRP
1	D	31	VAL
1	D	110	ALA
1	D	167	ASP
1	D	194	ALA
1	D	218	LEU
1	D	223	GLU
1	D	226	GLN
1	A	22	GLU
1	A	90	GLN
1	A	167	ASP
1	D	23	PRO
1	D	79	GLN
1	D	92	SER
1	D	147	ILE
1	A	66	SER
1	A	147	ILE
1	A	226	GLN
1	D	142	GLY
1	A	103	PHE
1	D	100	ILE
1	A	96	ILE
1	D	219	GLY
1	D	112	ILE
1	A	197	PRO

### 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	325/348 (93%)	273 (84%)	52 (16%)	2	15
1	D	325/348 (93%)	281 (86%)	44 (14%)	4	21
All	All	650/696 (93%)	554 (85%)	96 (15%)	3	17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	14	LEU
1	A	37	GLN
1	A	38	VAL
1	A	49	VAL
1	A	62	HIS
1	A	64	GLU
1	A	67	LEU
1	A	87	ARG
1	A	88	GLU
1	A	91	LEU
1	A	96	ILE
1	A	105	ILE
1	A	106	ASP
1	A	112	ILE
1	A	120	THR
1	A	127	MET
1	A	137	HIS
1	A	138	PHE
1	A	144	MET
1	A	155	ARG
1	A	163	ILE
1	A	190	THR
1	A	195	GLN
1	A	202	ASN
1	A	216	PHE
1	A	218	LEU
1	A	220	GLU
1	A	221	THR
1	A	222	GLU
1	A	225	GLN
1	A	242	ILE
1	A	255	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	257	LEU
1	A	265	ARG
1	A	266	GLN
1	A	281	SER
1	A	283	ILE
1	A	303	LEU
1	A	316	ASP
1	A	317	ILE
1	A	320	LEU
1	A	324	PHE
1	A	325	LEU
1	A	327	GLU
1	A	337	ARG
1	A	338	SER
1	A	341	ASP
1	A	342	ASP
1	A	350	TYR
1	A	361	ASN
1	A	380	LEU
1	D	14	LEU
1	D	41	LEU
1	D	42	ARG
1	D	62	HIS
1	D	64	GLU
1	D	68	ASN
1	D	72	ASN
1	D	77	HIS
1	D	81	ARG
1	D	83	LEU
1	D	93	SER
1	D	97	CYS
1	D	105	ILE
1	D	112	ILE
1	D	116	GLN
1	D	134	VAL
1	D	135	TRP
1	D	138	PHE
1	D	144	MET
1	D	146	LEU
1	D	149	GLU
1	D	153	MET
1	D	162	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	167	ASP
1	D	182	THR
1	D	190	THR
1	D	195	GLN
1	D	216	PHE
1	D	221	THR
1	D	226	GLN
1	D	255	ARG
1	D	262	VAL
1	D	265	ARG
1	D	266	GLN
1	D	269	ARG
1	D	282	ASP
1	D	310	LEU
1	D	313	ARG
1	D	319	LEU
1	D	341	ASP
1	D	342	ASP
1	D	361	ASN
1	D	377	GLU
1	D	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	124	GLN
1	A	195	GLN
1	A	202	ASN
1	A	225	GLN
1	A	226	GLN
1	A	298	HIS
1	A	355	ASN
1	A	362	GLN
1	D	68	ASN
1	D	79	GLN
1	D	90	GLN
1	D	195	GLN
1	D	226	GLN
1	D	240	ASN
1	D	250	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands 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	$\# Z  > 2$
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.07	0
3	C2E	D	503	-	44,52,52	5.47	30 (68%)	54,82,82	2.28	16 (29%)
3	C2E	D	502	-	44,52,52	5.47	30 (68%)	54,82,82	2.25	15 (27%)
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.05	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
3	C2E	D	503	-	-	6/22/62/62	0/6/7/7
3	C2E	D	502	-	-	8/22/62/62	0/6/7/7

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	C2E	C2'-C1'	-18.03	1.26	1.53
3	D	503	C2E	C2'-C1'	-17.90	1.26	1.53
3	D	503	C2E	C2A-C3A	-13.23	1.23	1.52
3	D	502	C2E	C2A-C3A	-13.15	1.23	1.52
3	D	503	C2E	C3'-C4'	-12.31	1.19	1.52
3	D	502	C2E	C3'-C4'	-12.09	1.20	1.52
3	D	502	C2E	C2A-C1A	9.84	1.68	1.53
3	D	503	C2E	C2A-C1A	9.73	1.68	1.53
3	D	502	C2E	C4-N3	7.34	1.47	1.35
3	D	503	C2E	C4-N3	7.33	1.47	1.35
3	D	503	C2E	O4'-C1'	7.08	1.51	1.41
3	D	502	C2E	O4'-C1'	7.07	1.50	1.41
3	D	502	C2E	C41-N31	6.96	1.46	1.35
3	D	503	C2E	O4A-C1A	-6.86	1.31	1.41
3	D	502	C2E	O4A-C1A	-6.80	1.31	1.41
3	D	503	C2E	C41-N31	6.78	1.46	1.35
3	D	502	C2E	C2'-C3'	6.57	1.67	1.52
3	D	503	C2E	C2'-C3'	6.49	1.67	1.52
3	D	502	C2E	O4'-C4'	6.38	1.59	1.45
3	D	503	C2E	O4'-C4'	6.27	1.59	1.45
3	D	503	C2E	C5-C6	6.23	1.52	1.41
3	D	503	C2E	C5A-C4A	-6.19	1.32	1.51
3	D	502	C2E	C5A-C4A	-6.19	1.32	1.51
3	D	502	C2E	C5-C6	6.10	1.51	1.41
3	D	502	C2E	C61-C51	5.55	1.50	1.41
3	D	503	C2E	C61-C51	5.51	1.50	1.41
3	D	503	C2E	C61-N11	4.73	1.41	1.33
3	D	502	C2E	C61-N11	4.69	1.41	1.33
3	D	503	C2E	C6-N1	4.68	1.41	1.33
3	D	502	C2E	C6-N1	4.47	1.40	1.33
3	D	502	C2E	C2-N1	4.47	1.43	1.35
3	D	503	C2E	C2-N1	4.43	1.43	1.35
3	D	502	C2E	C5'-C4'	3.92	1.63	1.51
3	D	503	C2E	C5'-C4'	3.90	1.63	1.51
3	D	503	C2E	C3A-C4A	3.77	1.63	1.52
3	D	502	C2E	C3A-C4A	3.76	1.63	1.52
3	D	502	C2E	C21-N11	3.72	1.42	1.35
3	D	503	C2E	C21-N11	3.72	1.42	1.35
3	D	502	C2E	O3'-C3'	3.43	1.56	1.44
3	D	503	C2E	O3'-C3'	3.27	1.56	1.44
3	D	502	C2E	O61-C61	-2.92	1.17	1.24
3	D	503	C2E	O61-C61	-2.89	1.17	1.24
3	D	503	C2E	C2-N2	2.80	1.39	1.33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	C2E	C21-N21	2.79	1.39	1.33
3	D	502	C2E	C21-N21	2.79	1.39	1.33
3	D	502	C2E	O4A-C4A	2.74	1.51	1.45
3	D	503	C2E	O4A-C4A	2.72	1.51	1.45
3	D	502	C2E	C2-N2	2.70	1.39	1.33
3	D	503	C2E	P1-O3A	2.55	1.67	1.60
3	D	502	C2E	P1-O3A	2.53	1.67	1.60
3	D	502	C2E	O3A-C3A	2.37	1.52	1.44
3	D	503	C2E	O3A-C3A	2.36	1.52	1.44
3	D	503	C2E	C21-N31	2.22	1.45	1.34
3	D	502	C2E	C21-N31	2.19	1.45	1.34
3	D	502	C2E	C2-N3	2.17	1.44	1.34
3	D	503	C2E	C2-N3	2.15	1.44	1.34
3	D	502	C2E	O2A-C2A	2.08	1.47	1.43
3	D	503	C2E	C5-C4	-2.08	1.35	1.40
3	D	503	C2E	O2A-C2A	2.04	1.47	1.43
3	D	502	C2E	C5-C4	-2.00	1.35	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	C2E	C1A-N91-C41	-8.52	111.66	126.64
3	D	503	C2E	C1A-N91-C41	-8.47	111.76	126.64
3	D	503	C2E	N3-C2-N1	-5.77	119.52	127.22
3	D	502	C2E	N31-C21-N11	-5.47	119.93	127.22
3	D	503	C2E	N31-C21-N11	-5.37	120.06	127.22
3	D	502	C2E	N3-C2-N1	-5.31	120.14	127.22
3	D	503	C2E	C2-N3-C4	4.51	120.51	115.36
3	D	502	C2E	C21-N31-C41	3.99	119.91	115.36
3	D	502	C2E	C2-N3-C4	3.94	119.85	115.36
3	D	503	C2E	C21-N31-C41	3.82	119.72	115.36
3	D	502	C2E	C3A-C2A-C1A	3.72	108.14	99.89
3	D	503	C2E	C3A-C2A-C1A	3.70	108.09	99.89
3	D	502	C2E	C3'-C2'-C1'	3.07	106.70	99.89
3	D	503	C2E	C3'-C2'-C1'	2.98	106.48	99.89
3	D	502	C2E	O21-P11-O3'	2.73	117.55	106.78
3	D	502	C2E	C5-C6-N1	-2.51	120.00	123.43
3	D	503	C2E	C61-N11-C21	2.47	119.85	115.93
3	D	502	C2E	C61-N11-C21	2.46	119.84	115.93
3	D	503	C2E	P11-O3'-C3'	-2.44	110.53	119.41
3	D	503	C2E	C51-C61-N11	-2.41	120.14	123.43
3	D	502	C2E	P1-O3A-C3A	-2.39	110.70	119.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	C2E	C2-N1-C6	2.38	119.70	115.93
3	D	503	C2E	C2-N1-C6	2.36	119.67	115.93
3	D	503	C2E	O21-P11-O3'	2.34	116.03	106.78
3	D	503	C2E	P1-O3A-C3A	-2.33	110.91	119.41
3	D	502	C2E	P11-O5A-C5A	-2.29	108.26	121.68
3	D	502	C2E	C51-C61-N11	-2.24	120.36	123.43
3	D	503	C2E	P11-O5A-C5A	-2.20	108.76	121.68
3	D	503	C2E	C5-C6-N1	-2.13	120.52	123.43
3	D	502	C2E	P11-O3'-C3'	-2.11	111.72	119.41
3	D	503	C2E	N2-C2-N1	2.07	120.47	117.25

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	C2E	C5A-O5A-P11-O3'
3	D	502	C2E	C5A-O5A-P11-O21
3	D	502	C2E	C5A-O5A-P11-O11
3	D	502	C2E	O4A-C4A-C5A-O5A
3	D	503	C2E	C5A-O5A-P11-O21
3	D	502	C2E	C3A-C4A-C5A-O5A
3	D	503	C2E	C3A-C4A-C5A-O5A
3	D	503	C2E	C5A-O5A-P11-O3'
3	D	503	C2E	O4A-C4A-C5A-O5A
3	D	502	C2E	C3A-O3A-P1-O5'
3	D	502	C2E	C5'-O5'-P1-O3A
3	D	503	C2E	C3A-O3A-P1-O5'
3	D	502	C2E	C5'-O5'-P1-O1P
3	D	503	C2E	C5A-O5A-P11-O11

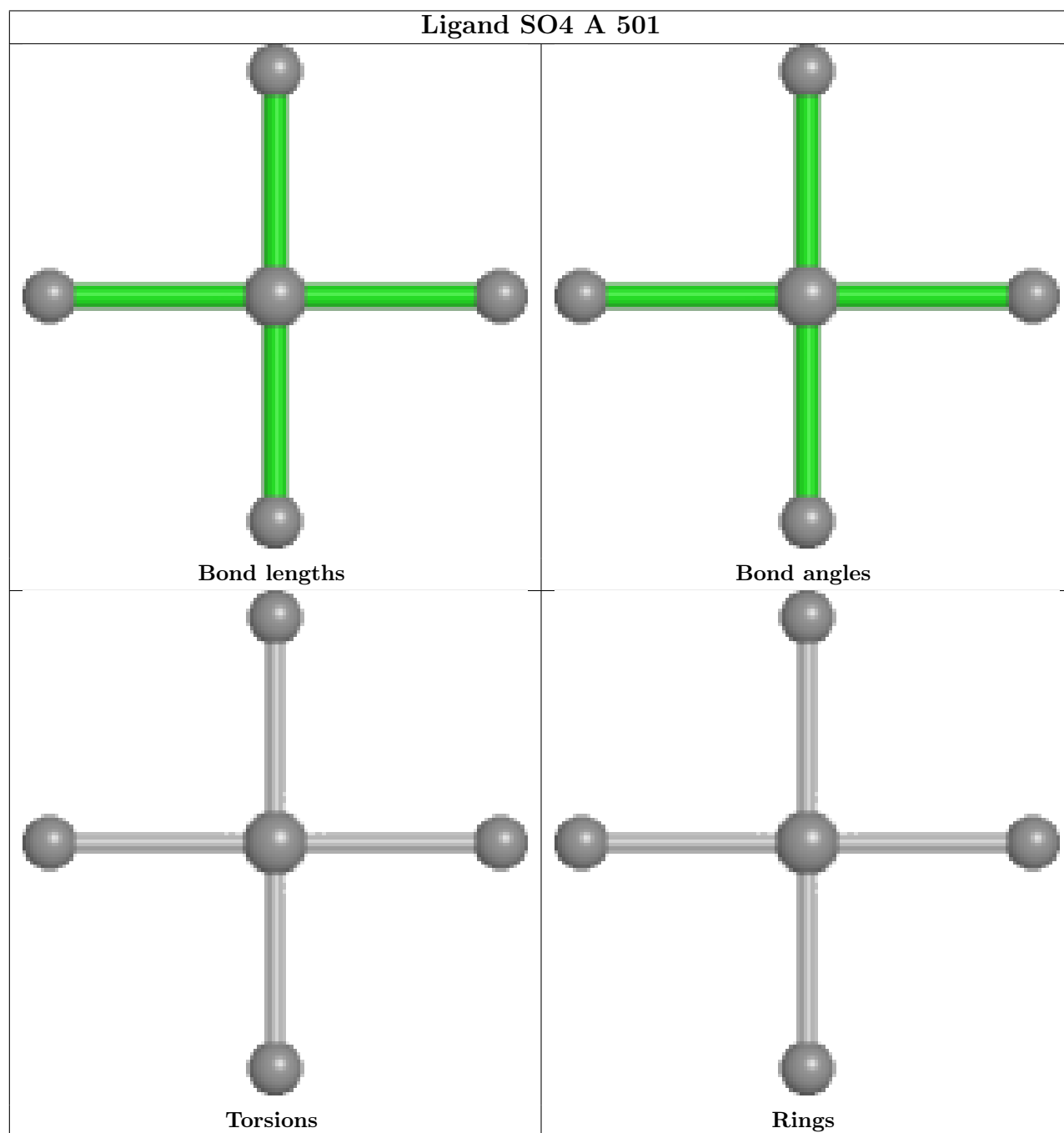
There are no ring outliers.

1 monomer is involved in 1 short contact:

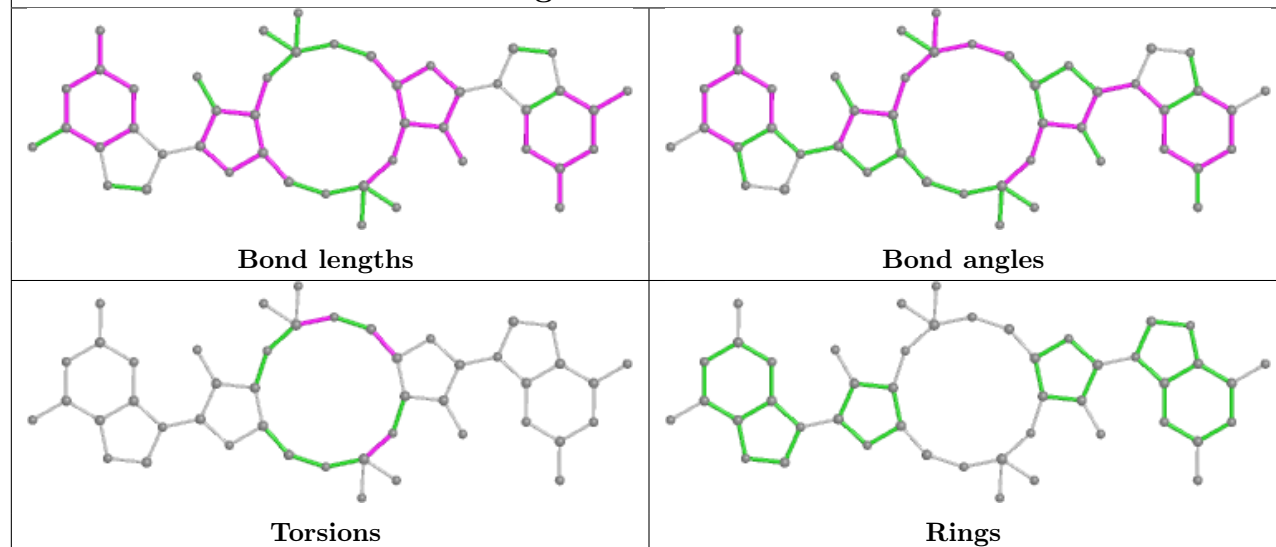
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	SO4	1	0

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

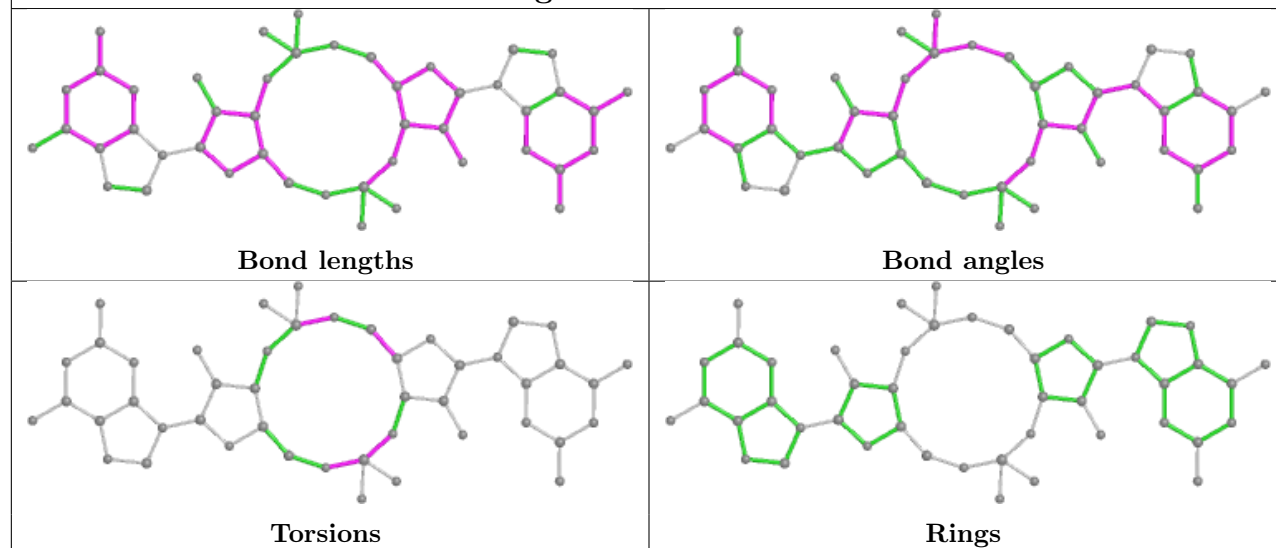
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



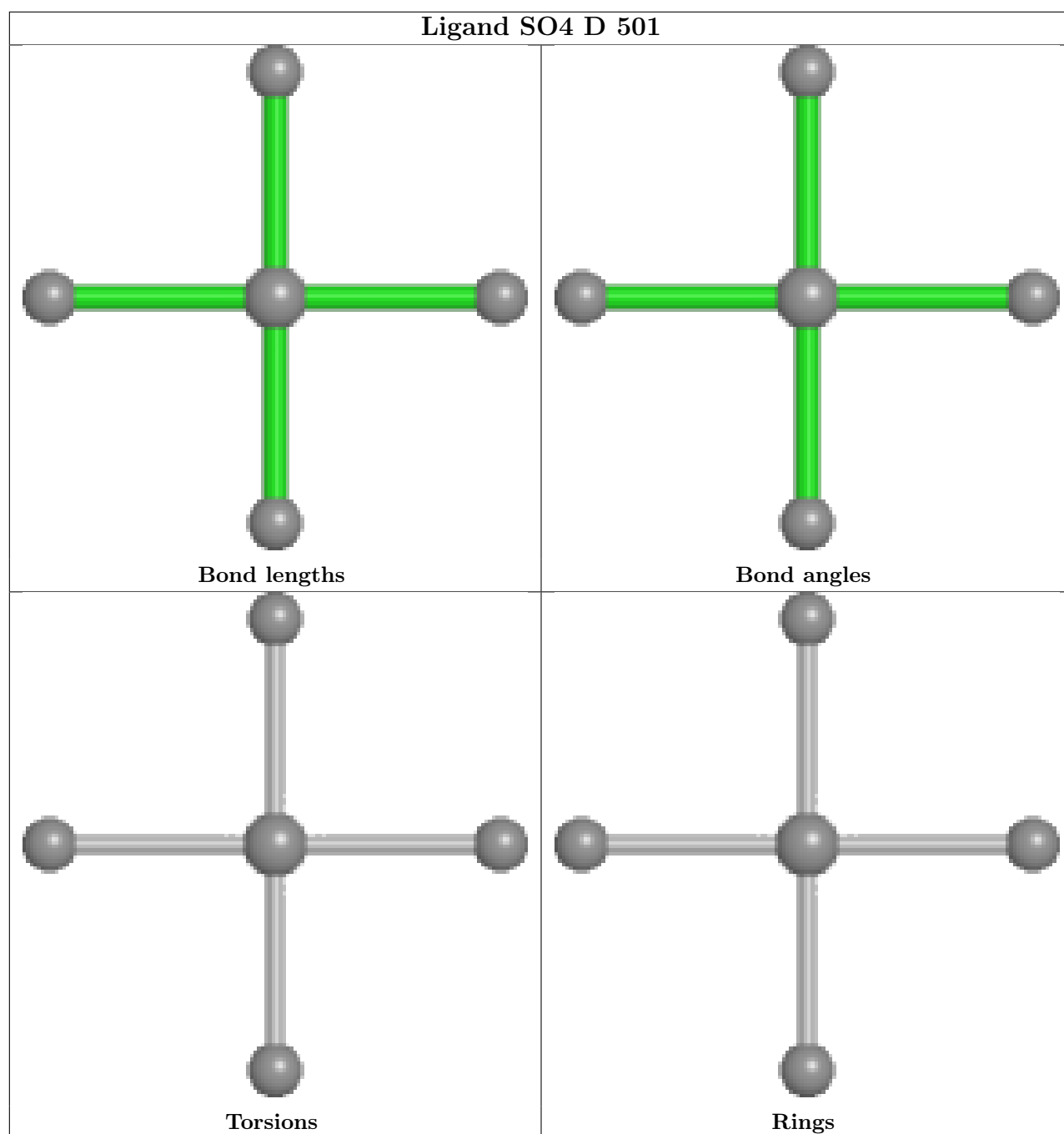
## Ligand C2E D 503



## Ligand C2E D 502







## 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	374/399 (93%)	-0.33	3 (0%) 86 79	105, 201, 237, 253	0
1	D	374/399 (93%)	-0.45	1 (0%) 94 90	94, 198, 233, 281	0
All	All	748/798 (93%)	-0.39	4 (0%) 91 85	94, 199, 235, 281	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	ILE	3.7
1	A	85	PHE	2.7
1	A	55	ILE	2.6
1	D	57	ILE	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 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
3	C2E	D	503	46/46	0.71	0.18	282,300,324,332	0

*Continued on next page...*

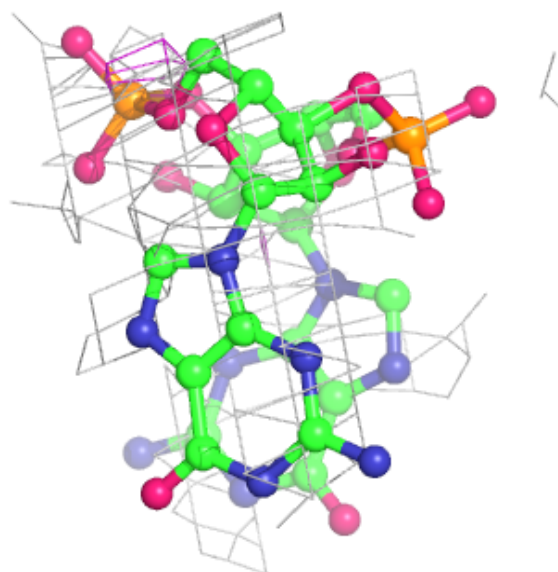
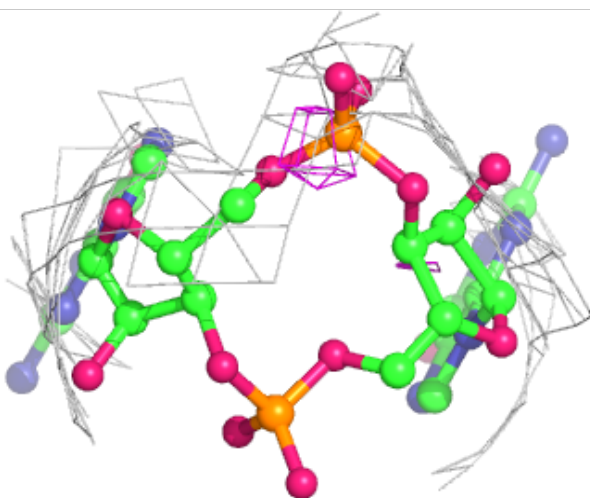
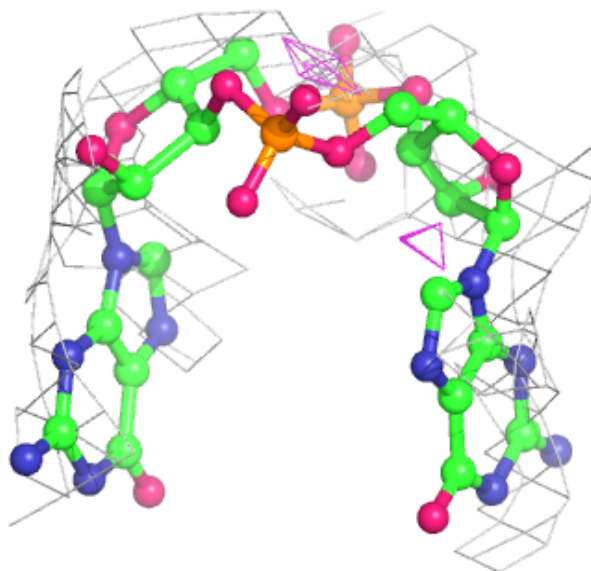
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C2E	D	502	46/46	0.76	0.15	273,296,316,319	0
2	SO4	A	501	5/5	0.91	0.29	151,153,163,179	0
2	SO4	D	501	5/5	0.92	0.25	158,163,167,177	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.

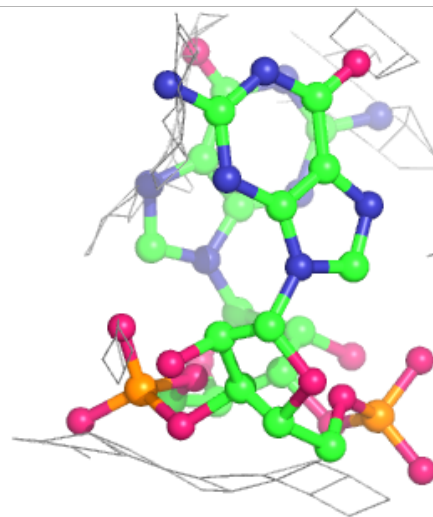
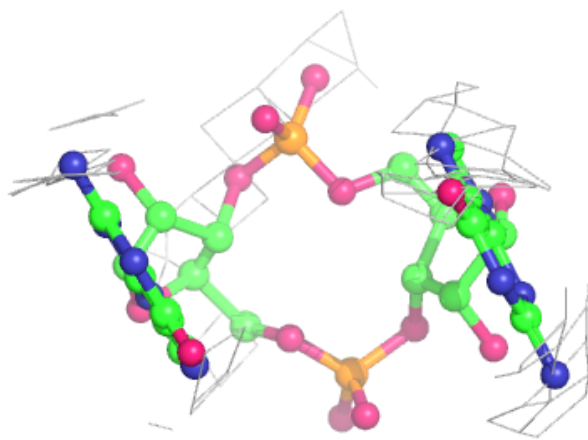
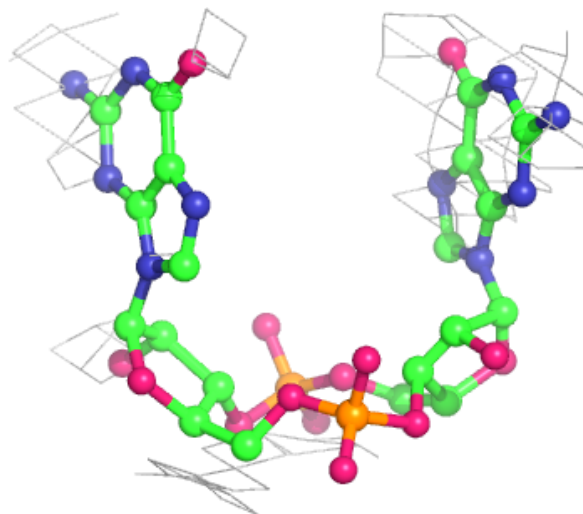
**Electron density around C2E D 503:**

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)



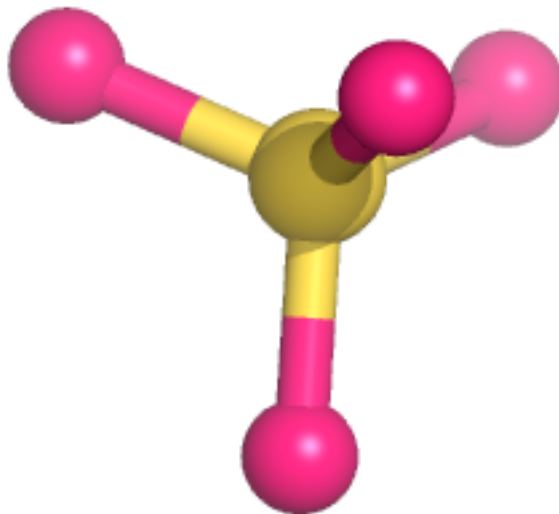
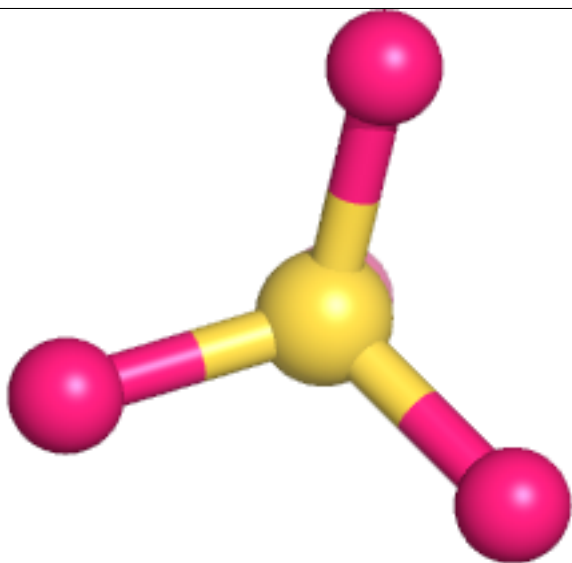
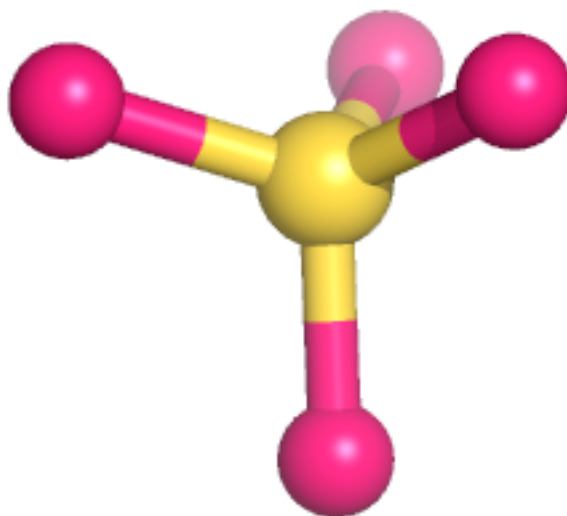
**Electron density around C2E D 502:**

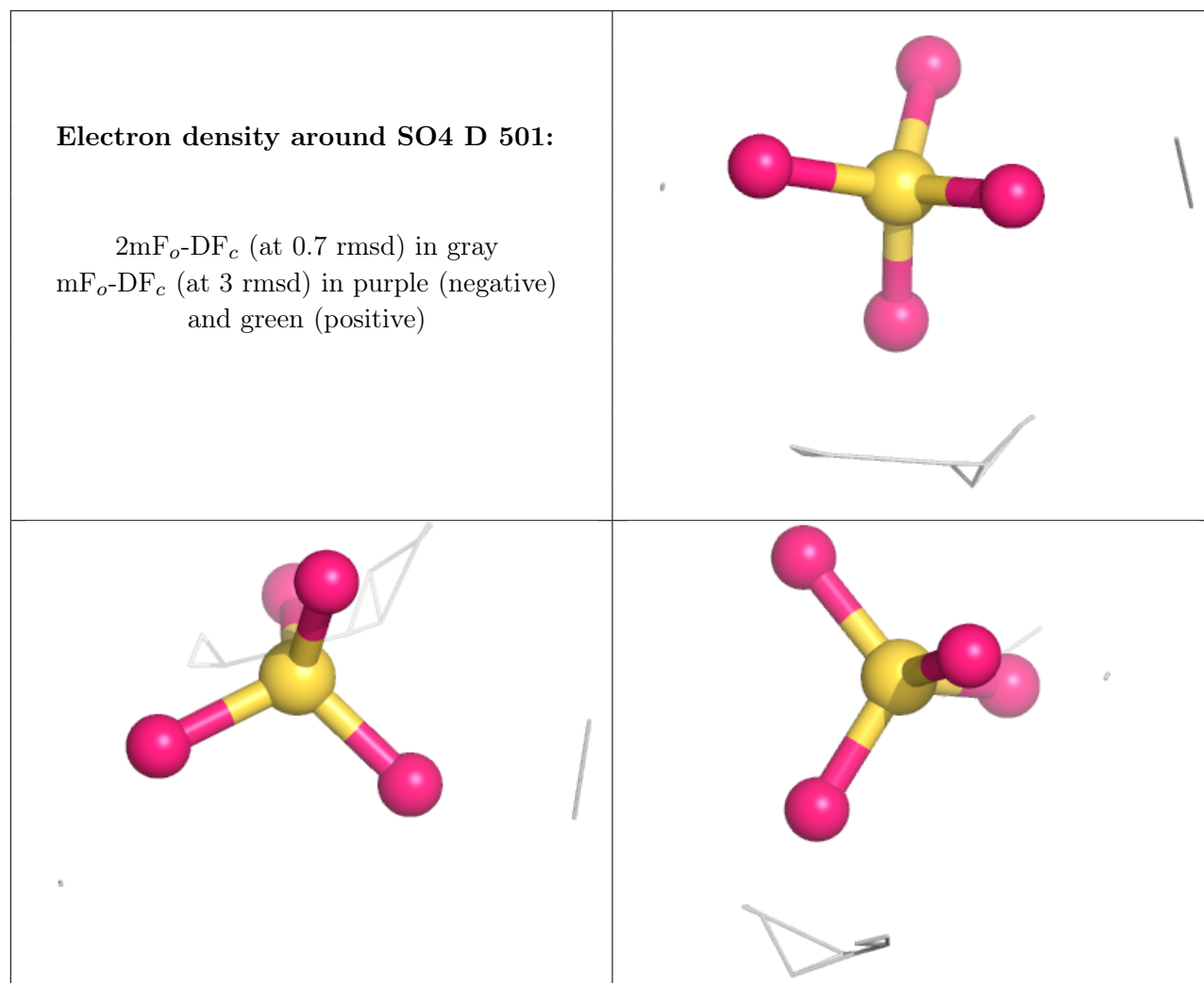
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 A 501:**

$2mF_o - DF_c$  (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.