



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2023 – 09:11 am GMT

PDB ID : 2WKV  
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE N316D MUTANT WITH COENZYME A.  
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.  
Deposited on : 2009-06-18  
Resolution : 2.50 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.

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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

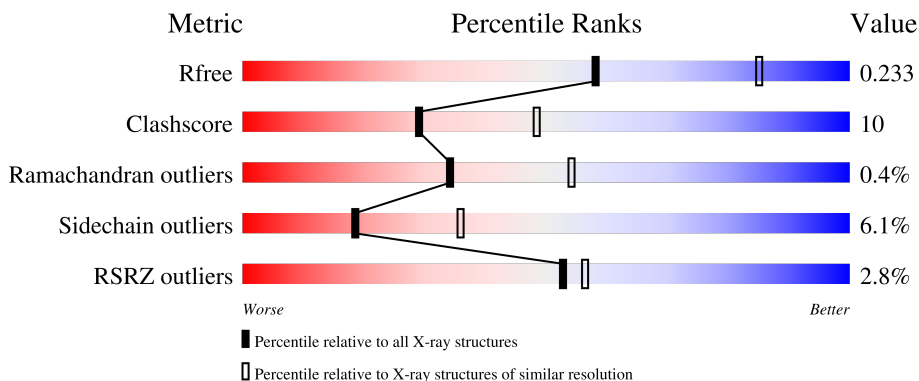
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	392	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83% 14% ..</p>
1	B	392	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 82% 16% ..</p>
1	C	392	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 73% 24% ..</p>
1	D	392	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 75% 22% ..</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1394	-	-	-	X
4	COA	B	1399	X	-	-	-
4	COA	D	1395	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12290 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 ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	2821	1751	511	538	21	0	1	0
1	B	389	2813	1746	508	538	21	0	0	0
1	C	389	2813	1746	508	538	21	0	0	0
1	D	389	2813	1746	508	538	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	316	ASP	ASN	engineered mutation	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	316	ASP	ASN	engineered mutation	UNP P07097
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	316	ASP	ASN	engineered mutation	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	316	ASP	ASN	engineered mutation	UNP P07097

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

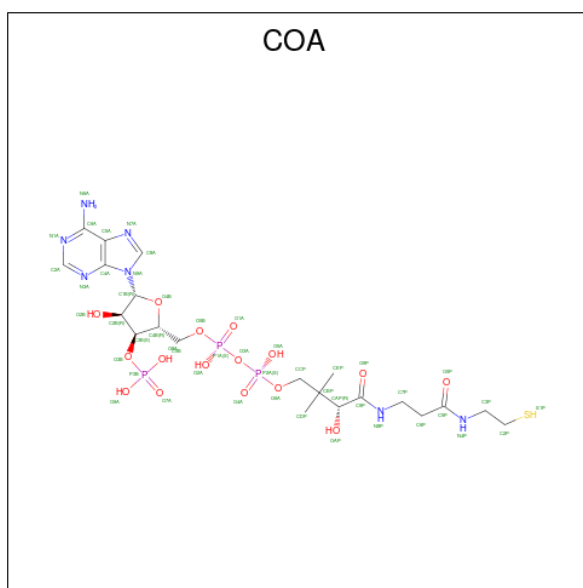


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	48	21	7	16	3	1	0	0
4	B	1	48	21	7	16	3	1	0	0
4	C	1	48	21	7	16	3	1	0	0
4	D	1	48	21	7	16	3	1	0	0

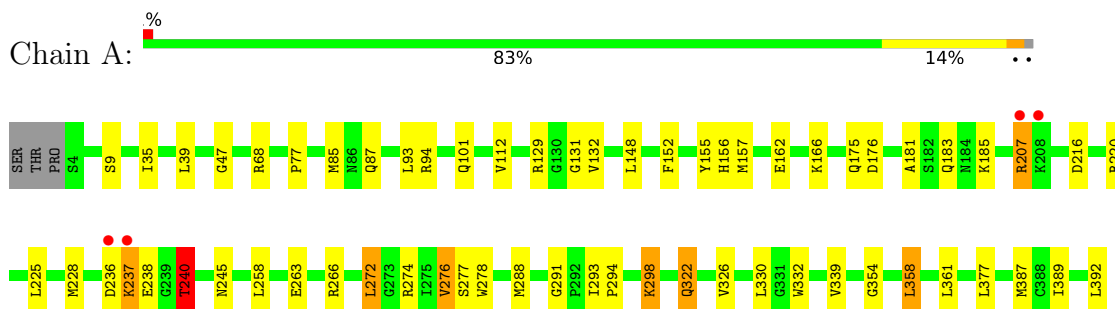
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	247	247	247	0	0
5	B	267	267	267	0	0
5	C	136	136	136	0	0
5	D	136	136	136	0	0

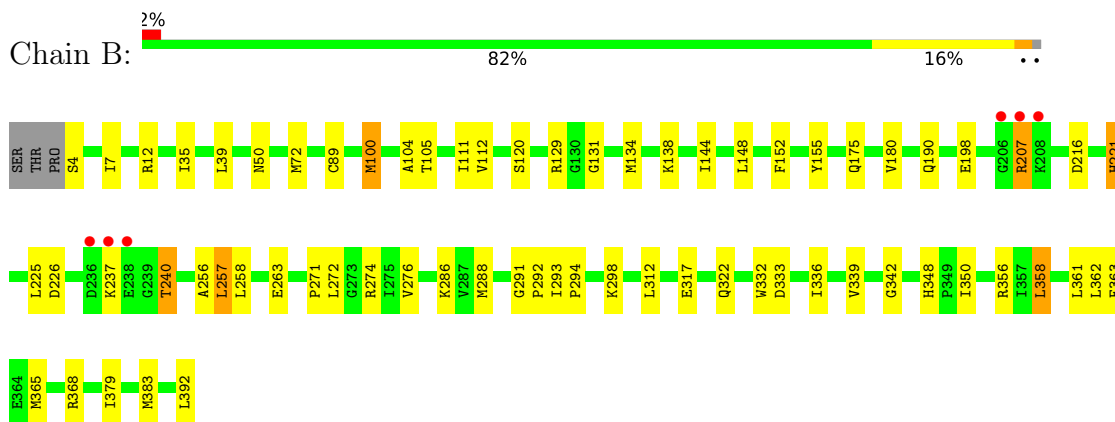
### 3 Residue-property plots [i](#)

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.

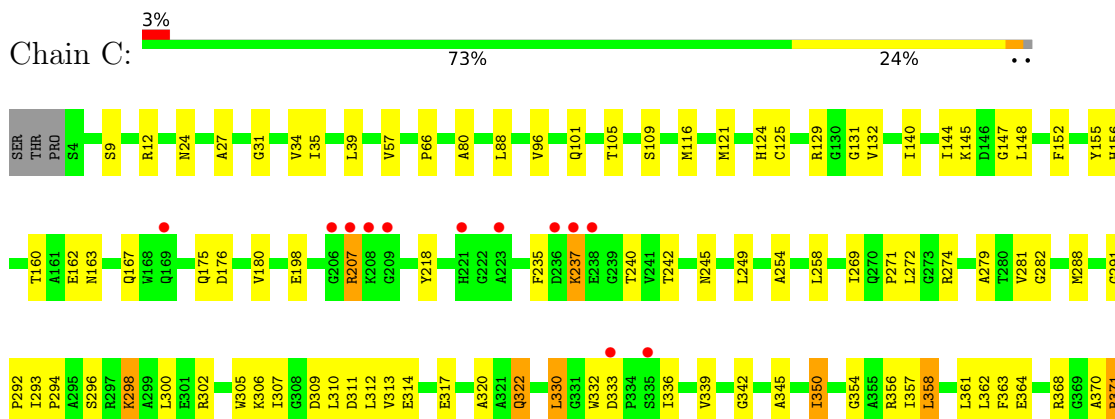
#### • Molecule 1: ACETYL-COA ACETYLTRANSFERASE

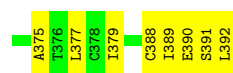


#### • Molecule 1: ACETYL-COA ACETYLTRANSFERASE

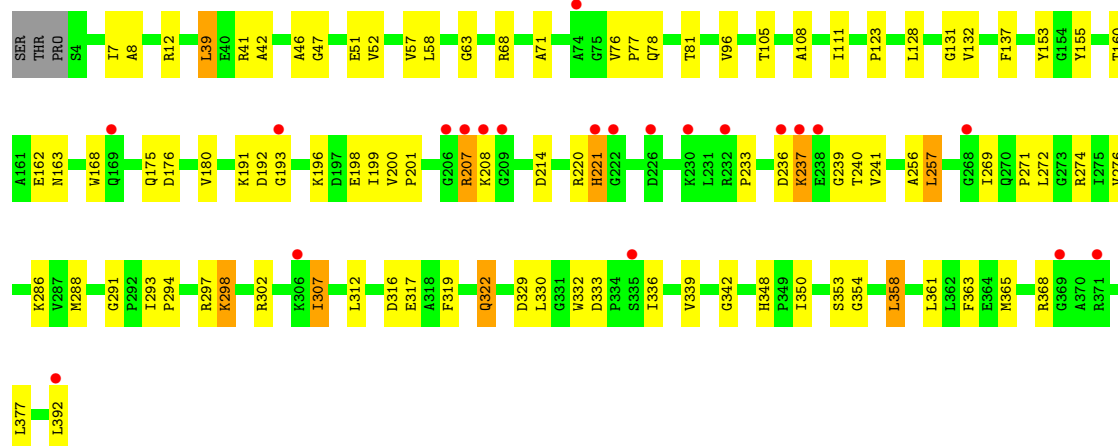
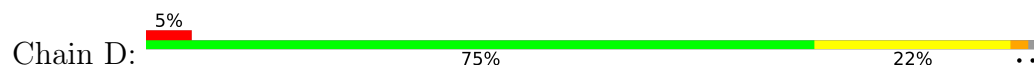


#### • Molecule 1: ACETYL-COA ACETYLTRANSFERASE





● Molecule 1: ACETYL-COA ACETYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.70Å 79.30Å 151.00Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	19.69 – 2.50 19.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.69-2.50) 99.9 (19.69-2.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.50Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.172 , 0.238 0.168 , 0.233	Depositor DCC
$R_{free}$ test set	3450 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage'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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: COA, NA, 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	0.36	0/2865	0.54	0/3867
1	B	0.36	0/2854	0.54	0/3853
1	C	0.31	0/2854	0.49	0/3853
1	D	0.30	0/2854	0.48	0/3853
All	All	0.33	0/11427	0.51	0/15426

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	2821	0	2830	56	0
1	B	2813	0	2817	43	0
1	C	2813	0	2817	68	0
1	D	2813	0	2817	64	0
2	A	15	0	0	0	0
2	B	25	0	0	2	0
2	D	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	48	0	32	1	0
4	B	48	0	30	2	0
4	C	48	0	31	2	0
4	D	48	0	29	1	0
5	A	247	0	0	6	0
5	B	267	0	0	3	0
5	C	136	0	0	3	0
5	D	136	0	0	3	0
All	All	12290	0	11403	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (220) 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:207:ARG:HD3	1:B:207:ARG:H	1.30	0.95
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.35	0.91
1:A:293:ILE:HB	1:A:294:PRO:HD3	1.59	0.85
1:D:307:ILE:HD12	1:D:307:ILE:H	1.44	0.81
1:A:207:ARG:H	1:A:207:ARG:HD3	1.47	0.79
1:A:207:ARG:HG2	1:A:207:ARG:NH1	1.98	0.76
1:B:274:ARG:HB2	1:B:392:LEU:HD21	1.67	0.74
1:C:207:ARG:H	1:C:207:ARG:HD3	1.56	0.71
1:B:226:ASP:HB3	5:B:2185:HOH:O	1.91	0.71
1:C:162:GLU:OE1	1:C:240:THR:HG22	1.90	0.71
1:C:9:SER:HA	1:C:272:LEU:HD23	1.72	0.70
1:A:387:MET:SD	5:A:2076:HOH:O	2.49	0.69
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.77	0.66
1:D:207:ARG:N	1:D:207:ARG:HD3	2.11	0.66
1:B:138:LYS:HB2	2:B:1397:SO4:O2	1.95	0.66
1:B:207:ARG:HD3	1:B:207:ARG:N	2.08	0.65
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.79	0.65
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.32	0.64
1:C:293:ILE:HB	1:C:294:PRO:HD3	1.78	0.64
1:C:88:LEU:HB2	1:C:379:ILE:HG23	1.80	0.64
1:C:9:SER:HA	1:C:272:LEU:CD2	2.29	0.62
1:A:176:ASP:HA	1:A:228:MET:HE2	1.80	0.62
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.82	0.62
1:A:225:LEU:O	1:A:225:LEU:HD23	1.99	0.61
1:D:298:LYS:O	1:D:302:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ASP:O	1:D:336:ILE:HG12	1.99	0.61
1:A:101:GLN:HG2	1:B:105:THR:HG21	1.83	0.60
1:C:314:GLU:O	1:C:375:ALA:HA	2.01	0.60
1:C:291:GLY:O	1:C:294:PRO:HD2	2.01	0.60
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.84	0.60
1:C:364:GLU:O	1:C:368:ARG:HG2	2.02	0.60
1:D:47:GLY:HA2	1:D:77:PRO:HG2	1.84	0.60
1:C:298:LYS:O	1:C:298:LYS:HD3	2.00	0.59
1:C:296:SER:O	1:C:300:LEU:HG	2.02	0.59
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.68	0.58
1:A:228:MET:CE	1:A:245:ASN:HB3	2.33	0.58
1:B:271:PRO:HG2	1:B:392:LEU:HD12	1.85	0.58
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.17	0.58
1:A:129:ARG:HD2	1:B:120:SER:O	2.04	0.57
1:D:207:ARG:HD3	1:D:207:ARG:H	1.70	0.56
1:C:176:ASP:O	1:C:180:VAL:HG23	2.05	0.56
1:D:298:LYS:O	1:D:298:LYS:HD3	2.04	0.56
1:D:354:GLY:HA2	1:D:377:LEU:HD21	1.88	0.56
1:A:35:ILE:HG12	1:A:112:VAL:HG11	1.87	0.56
1:C:274:ARG:HB2	1:C:392:LEU:HD21	1.87	0.55
1:A:129:ARG:HA	1:C:132:VAL:O	2.06	0.55
1:B:50:ASN:HB3	5:B:2047:HOH:O	2.07	0.55
1:A:93:LEU:HD11	1:A:387:MET:HE1	1.89	0.55
1:B:89:CYS:SG	1:B:348:HIS:HE1	2.29	0.55
1:A:294:PRO:HG3	5:A:2087:HOH:O	2.06	0.55
1:B:207:ARG:H	1:B:207:ARG:CD	2.11	0.54
1:A:148:LEU:O	1:A:157:MET:HG2	2.07	0.54
1:C:101:GLN:O	1:C:105:THR:HG23	2.07	0.54
1:A:216:ASP:HB3	5:A:2155:HOH:O	2.08	0.54
1:D:317:GLU:CD	1:D:342:GLY:HA3	2.27	0.54
1:D:47:GLY:HA2	1:D:77:PRO:CG	2.38	0.53
1:B:198:GLU:HB3	1:B:363:PHE:CD2	2.43	0.53
1:A:207:ARG:HH11	1:A:207:ARG:CG	2.13	0.53
1:A:276:VAL:O	1:A:277:SER:HB3	2.09	0.53
1:C:371:ARG:O	1:C:390:GLU:HA	2.08	0.53
1:D:297:ARG:CZ	1:D:330:LEU:HD23	2.38	0.53
1:C:312:LEU:HD21	1:C:364:GLU:HG3	1.90	0.52
1:A:152:PHE:CZ	1:B:72:MET:HG3	2.44	0.52
1:C:310:LEU:HD13	1:C:313:VAL:HG22	1.92	0.52
1:A:207:ARG:H	1:A:207:ARG:CD	2.15	0.52
1:A:220:ARG:HG2	5:A:2158:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ALA:O	1:A:185:LYS:HG3	2.09	0.52
1:A:132:VAL:O	1:C:129:ARG:HA	2.10	0.52
1:A:387:MET:CE	1:A:389:ILE:HD11	2.40	0.51
1:D:7:ILE:HG23	1:D:256:ALA:HB1	1.91	0.51
1:C:269:ILE:O	1:C:271:PRO:HD3	2.10	0.51
1:C:160:THR:O	1:C:163:ASN:HB2	2.11	0.51
1:C:125:CYS:HB2	1:D:123:PRO:HB2	1.93	0.51
1:D:307:ILE:H	1:D:307:ILE:CD1	2.11	0.51
1:A:266:ARG:NH1	5:A:2182:HOH:O	2.38	0.50
1:C:207:ARG:H	1:C:207:ARG:CD	2.25	0.50
1:D:198:GLU:HB3	1:D:363:PHE:CD1	2.46	0.50
1:D:269:ILE:O	1:D:271:PRO:HD3	2.10	0.50
1:A:9:SER:HA	1:A:272:LEU:HD22	1.92	0.50
1:C:339:VAL:HG11	1:C:368:ARG:NH2	2.26	0.50
1:A:387:MET:HE3	1:A:389:ILE:HD11	1.93	0.50
1:C:333:ASP:O	1:C:336:ILE:HG12	2.12	0.50
1:D:274:ARG:CB	1:D:392:LEU:HD21	2.42	0.49
1:C:24:ASN:HA	1:C:121:MET:SD	2.52	0.49
1:A:291:GLY:O	1:A:294:PRO:HD2	2.12	0.49
1:C:237:LYS:HD2	1:C:237:LYS:N	2.26	0.49
1:D:168:TRP:HH2	1:D:329:ASP:HB2	1.76	0.49
1:B:129:ARG:HA	1:D:132:VAL:O	2.12	0.49
1:C:306:LYS:O	1:C:309:ASP:HB2	2.13	0.49
1:A:183:GLN:NE2	1:A:220:ARG:HG3	2.27	0.49
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.33	0.49
1:D:316:ASP:OD2	1:D:348:HIS:CE1	2.66	0.49
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.77	0.49
1:B:100:MET:HE2	1:B:104:ALA:HB2	1.95	0.48
1:D:176:ASP:O	1:D:180:VAL:HG23	2.13	0.48
1:D:274:ARG:HB2	1:D:392:LEU:HD21	1.94	0.48
1:B:339:VAL:HG11	1:B:368:ARG:HH21	1.78	0.48
1:D:196:LYS:HE3	5:D:2076:HOH:O	2.12	0.48
1:D:271:PRO:HG2	1:D:392:LEU:HD12	1.96	0.48
4:B:1399:COA:H51A	5:B:2267:HOH:O	2.13	0.48
1:D:46:ALA:HB1	1:D:76:VAL:HA	1.95	0.48
1:A:322:GLN:O	1:A:326:VAL:HG23	2.14	0.47
1:C:152:PHE:HZ	1:D:68:ARG:HG3	1.79	0.47
1:B:293:ILE:HB	1:B:294:PRO:CD	2.45	0.47
1:D:41:ARG:HH21	1:D:200:VAL:HB	1.79	0.47
1:D:51:GLU:HB3	1:D:111:ILE:HD12	1.97	0.47
1:D:339:VAL:HG11	1:D:368:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLN:OE1	1:A:94[B]:ARG:HG2	2.15	0.47
1:B:379:ILE:HB	1:B:383:MET:HB2	1.97	0.47
1:B:7:ILE:HG23	1:B:256:ALA:HB1	1.96	0.47
1:D:312:LEU:HD23	1:D:365:MET:HG3	1.97	0.47
1:A:298:LYS:HA	1:A:298:LYS:HD3	1.81	0.46
1:D:348:HIS:CE1	1:D:353:SER:HG	2.33	0.46
1:A:183:GLN:HE21	1:A:220:ARG:HG3	1.80	0.46
1:C:66:PRO:HD2	5:C:2030:HOH:O	2.15	0.46
1:C:281:VAL:HG12	1:C:282:GLY:N	2.30	0.46
1:D:96:VAL:HG21	1:D:358:LEU:HD12	1.97	0.46
1:B:333:ASP:O	1:B:336:ILE:HG12	2.15	0.46
1:C:354:GLY:HA2	1:C:377:LEU:HD11	1.96	0.46
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.31	0.46
1:A:358:LEU:HD21	1:A:387:MET:HE3	1.98	0.46
1:D:42:ALA:CB	1:D:257:LEU:HD12	2.45	0.46
1:D:291:GLY:O	1:D:294:PRO:HD2	2.16	0.46
1:A:293:ILE:CB	1:A:294:PRO:HD3	2.40	0.45
1:C:57:VAL:HG21	1:C:350:ILE:HG22	1.98	0.45
1:D:191:LYS:C	1:D:193:GLY:H	2.20	0.45
1:C:242:THR:HG23	1:C:245:ASN:HD21	1.81	0.45
1:A:237:LYS:HE2	1:A:237:LYS:H	1.82	0.45
1:D:160:THR:O	1:D:163:ASN:HB2	2.16	0.45
1:B:100:MET:CE	1:B:104:ALA:HB2	2.46	0.45
1:D:51:GLU:HA	1:D:81:THR:O	2.16	0.45
1:D:207:ARG:NH1	1:D:208:LYS:HG3	2.32	0.44
1:D:233:PRO:HA	1:D:241:VAL:O	2.18	0.44
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.53	0.44
1:C:389:ILE:HG22	1:C:390:GLU:N	2.33	0.44
1:D:162:GLU:OE1	1:D:240:THR:HG22	2.17	0.44
1:A:47:GLY:HA2	1:A:77:PRO:HG3	1.99	0.44
1:A:156:HIS:HE1	4:A:1397:COA:H62	1.83	0.44
1:B:358:LEU:HD22	1:B:362:LEU:HD11	1.99	0.44
1:C:356:ARG:HD2	1:C:356:ARG:O	2.17	0.44
1:C:156:HIS:CD2	1:C:235:PHE:HE1	2.35	0.44
1:C:307:ILE:CD1	1:C:330:LEU:HD23	2.48	0.44
1:C:312:LEU:HD12	1:C:312:LEU:HA	1.91	0.44
1:C:322:GLN:HE21	1:C:322:GLN:HB2	1.60	0.44
1:B:111:ILE:O	1:B:257:LEU:HD23	2.17	0.44
4:C:1393:COA:O8A	4:C:1393:COA:H4B	2.18	0.44
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.83	0.44
1:B:286:LYS:HD3	2:B:1396:SO4:O4	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLN:NE2	5:D:2028:HOH:O	2.49	0.44
1:B:291:GLY:N	1:B:292:PRO:CD	2.81	0.43
1:A:68:ARG:HG3	1:B:152:PHE:HZ	1.83	0.43
1:A:93:LEU:CD1	1:A:387:MET:HE1	2.48	0.43
1:B:293:ILE:HB	1:B:294:PRO:HD3	1.99	0.43
1:C:218:TYR:CD2	1:C:345:ALA:O	2.72	0.43
1:D:128:LEU:HD21	1:D:137:PHE:CE1	2.53	0.43
1:C:358:LEU:O	1:C:362:LEU:HG	2.19	0.43
1:C:124:HIS:HA	1:C:140:ILE:O	2.18	0.43
1:A:162:GLU:O	1:A:166:LYS:HG3	2.19	0.43
1:C:357:ILE:CD1	1:C:375:ALA:HB1	2.49	0.43
1:B:358:LEU:O	1:B:362:LEU:HG	2.18	0.43
1:B:12:ARG:HD2	1:B:356:ARG:HG2	2.01	0.43
1:C:307:ILE:HD12	1:C:330:LEU:HD23	2.01	0.43
1:D:57:VAL:HG12	1:D:58:LEU:HD23	2.00	0.43
1:D:39:LEU:HD12	1:D:39:LEU:HA	1.94	0.42
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.31	0.42
1:C:307:ILE:H	1:C:307:ILE:HG12	1.72	0.42
4:D:1395:COA:O5P	4:D:1395:COA:H21	2.19	0.42
1:B:89:CYS:SG	4:B:1399:COA:H31	2.60	0.42
1:D:108:ALA:HA	5:D:2041:HOH:O	2.18	0.42
1:C:390:GLU:HG2	1:C:391:SER:O	2.18	0.42
1:B:134:MET:HE2	1:C:144:ILE:HD11	2.01	0.42
1:C:292:PRO:O	1:C:296:SER:HB2	2.20	0.42
1:D:153:TYR:CE2	1:D:286:LYS:HD3	2.55	0.42
1:A:322:GLN:HE21	1:A:322:GLN:HB2	1.72	0.42
1:B:190:GLN:OE1	1:B:221:HIS:HE1	2.03	0.42
1:C:310:LEU:HD13	1:C:313:VAL:CG2	2.50	0.42
1:C:175:GLN:HB3	1:C:320:ALA:HB3	2.02	0.42
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.83	0.41
1:A:293:ILE:HB	1:A:294:PRO:CD	2.39	0.41
1:B:317:GLU:CD	1:B:342:GLY:HA3	2.40	0.41
1:C:305:TRP:CZ3	1:C:388:CYS:HB3	2.55	0.41
1:C:27:ALA:HB1	1:C:116:MET:HG3	2.03	0.41
1:C:147:GLY:O	1:C:148:LEU:HD23	2.20	0.41
1:C:249:LEU:HD21	4:C:1393:COA:O9P	2.20	0.41
1:C:31:GLY:O	1:C:35:ILE:HG13	2.20	0.41
1:D:12:ARG:NH2	1:D:199:ILE:HD11	2.36	0.41
1:D:52:VAL:HG21	1:D:71:ALA:HB2	2.01	0.41
1:A:236:ASP:O	1:A:238:GLU:N	2.54	0.41
1:A:274:ARG:NE	5:A:2189:HOH:O	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG21	1:C:350:ILE:CG2	2.50	0.41
1:D:201:PRO:HB3	1:D:214:ASP:HB3	2.03	0.41
1:D:221:HIS:ND1	1:D:221:HIS:N	2.69	0.41
1:D:237:LYS:N	1:D:237:LYS:HD2	2.33	0.41
1:A:131:GLY:CA	1:C:131:GLY:CA	2.99	0.41
1:A:237:LYS:HE2	1:A:237:LYS:N	2.36	0.41
1:A:358:LEU:HD21	1:A:387:MET:CE	2.50	0.41
1:C:311:ASP:HB2	1:C:370:ALA:HB1	2.02	0.41
1:D:339:VAL:HG11	1:D:368:ARG:HH21	1.85	0.41
1:A:225:LEU:HD23	1:A:225:LEU:C	2.40	0.41
1:B:180:VAL:HG21	1:B:225:LEU:HA	2.03	0.41
1:B:237:LYS:N	1:B:237:LYS:HD2	2.35	0.41
1:B:274:ARG:NH2	1:B:392:LEU:HD22	2.36	0.41
1:C:101:GLN:HG2	1:D:105:THR:HG21	2.03	0.41
1:C:145:LYS:O	1:D:63:GLY:HA2	2.20	0.41
1:C:147:GLY:C	1:C:148:LEU:HD23	2.41	0.41
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.85	0.41
1:B:274:ARG:CZ	1:B:392:LEU:HD22	2.51	0.41
1:C:96:VAL:HG21	1:C:358:LEU:HD12	2.03	0.41
1:B:131:GLY:HA2	1:D:131:GLY:HA2	2.02	0.40
1:C:12:ARG:HB2	1:C:254:ALA:HB2	2.04	0.40
1:C:279:ALA:HA	5:C:2109:HOH:O	2.21	0.40
1:C:302:ARG:NH1	5:C:2109:HOH:O	2.54	0.40
1:A:392:LEU:HD13	1:A:392:LEU:HA	1.91	0.40
1:B:35:ILE:HG12	1:B:112:VAL:HG11	2.02	0.40
1:B:312:LEU:HD23	1:B:365:MET:HG3	2.02	0.40
1:D:8:ALA:O	1:D:272:LEU:HD23	2.22	0.40
1:D:319:PHE:HB2	1:D:322:GLN:HG3	2.04	0.40
1:A:94[B]:ARG:CZ	1:A:278:TRP:CH2	3.05	0.40
1:D:7:ILE:CG2	1:D:256:ALA:HB1	2.51	0.40
1:D:76:VAL:HA	1:D:77:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

## 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	388/392 (99%)	369 (95%)	18 (5%)	1 (0%)	41	61
1	B	387/392 (99%)	373 (96%)	12 (3%)	2 (0%)	29	48
1	C	387/392 (99%)	365 (94%)	20 (5%)	2 (0%)	29	48
1	D	387/392 (99%)	364 (94%)	22 (6%)	1 (0%)	41	61
All	All	1549/1568 (99%)	1471 (95%)	72 (5%)	6 (0%)	34	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	B	350	ILE
1	A	240	THR
1	B	216	ASP
1	C	80	ALA

### 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	277/279 (99%)	260 (94%)	17 (6%)	18	36
1	B	276/279 (99%)	258 (94%)	18 (6%)	17	33
1	C	276/279 (99%)	260 (94%)	16 (6%)	20	38
1	D	276/279 (99%)	260 (94%)	16 (6%)	20	38
All	All	1105/1116 (99%)	1038 (94%)	67 (6%)	18	36

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	85	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	155	TYR
1	A	207	ARG
1	A	237	LYS
1	A	240	THR
1	A	258	LEU
1	A	263	GLU
1	A	272	LEU
1	A	276	VAL
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	339	VAL
1	A	358	LEU
1	A	361	LEU
1	B	4	SER
1	B	39	LEU
1	B	100	MET
1	B	155	TYR
1	B	207	ARG
1	B	221	HIS
1	B	240	THR
1	B	257	LEU
1	B	258	LEU
1	B	263	GLU
1	B	272	LEU
1	B	276	VAL
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	358	LEU
1	B	361	LEU
1	C	34	VAL
1	C	39	LEU
1	C	109	SER
1	C	155	TYR
1	C	167	GLN
1	C	207	ARG
1	C	237	LYS
1	C	258	LEU
1	C	288	MET

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Mol	Chain	Res	Type
1	C	298	LYS
1	C	322	GLN
1	C	330	LEU
1	C	332	TRP
1	C	358	LEU
1	C	361	LEU
1	C	371	ARG
1	D	39	LEU
1	D	155	TYR
1	D	192	ASP
1	D	207	ARG
1	D	220	ARG
1	D	221	HIS
1	D	237	LYS
1	D	257	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	307	ILE
1	D	322	GLN
1	D	332	TRP
1	D	358	LEU
1	D	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	167	GLN
1	A	175	GLN
1	A	183	GLN
1	A	184	ASN
1	A	221	HIS
1	B	78	GLN
1	B	175	GLN
1	B	184	ASN
1	B	221	HIS
1	B	348	HIS
1	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	D	78	GLN

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Mol	Chain	Res	Type
1	D	175	GLN
1	D	184	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	B	1397	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	D	1393	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	1395	-	4,4,4	0.14	0	6,6,6	0.19	0
4	COA	C	1393	-	41,50,50	2.70	16 (39%)	52,75,75	1.77	10 (19%)
2	SO4	A	1394	-	4,4,4	0.14	0	6,6,6	0.06	0
4	COA	A	1397	-	41,50,50	2.71	16 (39%)	52,75,75	1.77	13 (25%)
2	SO4	B	1393	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	A	1393	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1396	-	4,4,4	0.15	0	6,6,6	0.08	0
4	COA	B	1399	-	41,50,50	2.67	18 (43%)	52,75,75	1.91	14 (26%)
2	SO4	D	1394	-	4,4,4	0.13	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	1394	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	1395	-	4,4,4	0.16	0	6,6,6	0.16	0
4	COA	D	1395	-	41,50,50	2.69	16 (39%)	52,75,75	1.83	13 (25%)

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	COA	B	1399	-	1/1/11/13	14/44/64/64	0/3/3/3
4	COA	C	1393	-	-	20/44/64/64	0/3/3/3
4	COA	A	1397	-	-	17/44/64/64	0/3/3/3
4	COA	D	1395	-	1/1/11/13	9/44/64/64	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1395	COA	C9P-N8P	6.69	1.48	1.33
4	A	1397	COA	C9P-N8P	6.64	1.48	1.33
4	C	1393	COA	C9P-N8P	6.55	1.47	1.33
4	B	1399	COA	C9P-N8P	6.43	1.47	1.33
4	C	1393	COA	C5P-N4P	6.01	1.47	1.33
4	B	1399	COA	C5P-N4P	5.92	1.46	1.33
4	A	1397	COA	C5P-N4P	5.84	1.46	1.33
4	D	1395	COA	C5P-N4P	5.84	1.46	1.33
4	A	1397	COA	C2A-N3A	5.78	1.41	1.32
4	D	1395	COA	C2A-N3A	5.69	1.41	1.32
4	C	1393	COA	C2A-N3A	5.65	1.41	1.32
4	B	1399	COA	C2A-N3A	5.63	1.41	1.32
4	A	1397	COA	C8A-N7A	5.22	1.44	1.34
4	C	1393	COA	C8A-N7A	5.15	1.43	1.34
4	D	1395	COA	C8A-N7A	5.13	1.43	1.34
4	B	1399	COA	P3B-O7A	4.74	1.65	1.50
4	B	1399	COA	C8A-N7A	4.72	1.43	1.34
4	A	1397	COA	P3B-O7A	4.69	1.65	1.50
4	D	1395	COA	P3B-O7A	4.68	1.65	1.50
4	C	1393	COA	P3B-O7A	4.68	1.65	1.50
4	D	1395	COA	O4B-C1B	4.64	1.47	1.41
4	C	1393	COA	O4B-C1B	4.56	1.47	1.41
4	A	1397	COA	O4B-C1B	4.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1393	COA	P2A-O4A	4.28	1.66	1.50
4	B	1399	COA	P2A-O4A	4.22	1.65	1.50
4	D	1395	COA	P1A-O1A	4.21	1.65	1.50
4	B	1399	COA	P1A-O1A	4.20	1.65	1.50
4	C	1393	COA	P1A-O1A	4.19	1.65	1.50
4	A	1397	COA	P1A-O1A	4.17	1.65	1.50
4	D	1395	COA	P2A-O4A	4.16	1.65	1.50
4	B	1399	COA	O4B-C1B	4.13	1.46	1.41
4	A	1397	COA	P2A-O4A	4.06	1.65	1.50
4	B	1399	COA	P3B-O3B	3.60	1.66	1.59
4	D	1395	COA	P3B-O3B	3.54	1.66	1.59
4	A	1397	COA	P3B-O3B	3.39	1.65	1.59
4	C	1393	COA	P3B-O3B	3.37	1.65	1.59
4	A	1397	COA	C6A-N6A	3.31	1.46	1.34
4	A	1397	COA	C2A-N1A	3.29	1.40	1.33
4	C	1393	COA	C6A-N6A	3.27	1.46	1.34
4	B	1399	COA	C6A-N6A	3.27	1.46	1.34
4	D	1395	COA	C6A-N6A	3.23	1.45	1.34
4	C	1393	COA	C2A-N1A	2.93	1.39	1.33
4	D	1395	COA	P3B-O8A	2.91	1.66	1.54
4	B	1399	COA	P3B-O8A	2.89	1.66	1.54
4	A	1397	COA	P3B-O8A	2.87	1.65	1.54
4	D	1395	COA	C2A-N1A	2.86	1.39	1.33
4	C	1393	COA	P3B-O8A	2.84	1.65	1.54
4	C	1393	COA	O4B-C4B	2.73	1.51	1.45
4	B	1399	COA	C2A-N1A	2.72	1.39	1.33
4	A	1397	COA	O4B-C4B	2.61	1.50	1.45
4	C	1393	COA	O9P-C9P	-2.51	1.18	1.23
4	D	1395	COA	O4B-C4B	2.51	1.50	1.45
4	B	1399	COA	O4B-C4B	2.50	1.50	1.45
4	B	1399	COA	O9P-C9P	-2.48	1.18	1.23
4	A	1397	COA	O9P-C9P	-2.44	1.18	1.23
4	D	1395	COA	O9P-C9P	-2.38	1.18	1.23
4	D	1395	COA	P1A-O5B	2.26	1.68	1.59
4	B	1399	COA	P1A-O5B	2.22	1.68	1.59
4	C	1393	COA	P1A-O5B	2.15	1.68	1.59
4	D	1395	COA	O5P-C5P	-2.10	1.19	1.23
4	C	1393	COA	P2A-O6A	2.10	1.67	1.59
4	A	1397	COA	P1A-O5B	2.09	1.67	1.59
4	A	1397	COA	O5P-C5P	-2.09	1.19	1.23
4	B	1399	COA	O5P-C5P	-2.08	1.19	1.23
4	B	1399	COA	OAP-CAP	-2.04	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1399	COA	P2A-O6A	2.03	1.67	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1399	COA	N3A-C2A-N1A	-5.69	119.78	128.68
4	C	1393	COA	N3A-C2A-N1A	-5.56	119.98	128.68
4	D	1395	COA	N3A-C2A-N1A	-5.48	120.11	128.68
4	B	1399	COA	O2B-C2B-C3B	5.18	125.89	111.17
4	A	1397	COA	N3A-C2A-N1A	-5.01	120.84	128.68
4	D	1395	COA	P2A-O3A-P1A	-4.28	118.13	132.83
4	C	1393	COA	O6A-CCP-CBP	4.27	117.42	110.55
4	A	1397	COA	O2B-C2B-C3B	4.18	123.04	111.17
4	A	1397	COA	P2A-O3A-P1A	-4.08	118.83	132.83
4	C	1393	COA	O2B-C2B-C3B	4.03	122.60	111.17
4	C	1393	COA	P2A-O3A-P1A	-3.90	119.44	132.83
4	D	1395	COA	O4B-C4B-C5B	3.87	122.10	109.37
4	B	1399	COA	O6A-CCP-CBP	3.86	116.75	110.55
4	B	1399	COA	O2B-C2B-C1B	3.75	124.71	110.85
4	D	1395	COA	O3B-C3B-C4B	3.61	123.12	110.08
4	A	1397	COA	C6P-C7P-N8P	3.53	119.02	111.90
4	B	1399	COA	C3B-C2B-C1B	3.52	107.68	99.89
4	A	1397	COA	O2B-C2B-C1B	3.47	123.65	110.85
4	B	1399	COA	P2A-O3A-P1A	-3.45	121.00	132.83
4	D	1395	COA	O3B-C3B-C2B	3.43	124.11	111.68
4	B	1399	COA	O4B-C4B-C5B	3.24	120.02	109.37
4	A	1397	COA	O6A-CCP-CBP	3.20	115.69	110.55
4	D	1395	COA	O6A-CCP-CBP	3.08	115.51	110.55
4	C	1393	COA	O2B-C2B-C1B	3.04	122.08	110.85
4	D	1395	COA	O5B-C5B-C4B	3.03	119.41	108.99
4	B	1399	COA	O5B-C5B-C4B	3.02	119.39	108.99
4	C	1393	COA	O3B-C3B-C4B	2.99	120.89	110.08
4	A	1397	COA	O3B-C3B-C4B	2.96	120.80	110.08
4	D	1395	COA	C6P-C7P-N8P	2.88	117.72	111.90
4	D	1395	COA	O2B-C2B-C3B	2.81	119.16	111.17
4	C	1393	COA	C3B-C2B-C1B	2.81	106.12	99.89
4	A	1397	COA	C3B-C2B-C1B	2.73	105.94	99.89
4	B	1399	COA	C6P-C7P-N8P	2.65	117.25	111.90
4	B	1399	COA	C2P-C3P-N4P	2.65	118.35	112.31
4	D	1395	COA	C2P-C3P-N4P	2.64	118.34	112.31
4	C	1393	COA	C7P-N8P-C9P	-2.64	117.89	122.59
4	A	1397	COA	O4B-C4B-C5B	2.61	117.97	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1399	COA	C6P-C5P-N4P	2.53	120.68	116.42
4	A	1397	COA	O5B-C5B-C4B	2.43	117.35	108.99
4	D	1395	COA	O2B-C2B-C1B	2.37	119.59	110.85
4	D	1395	COA	C3B-C2B-C1B	2.32	105.02	99.89
4	C	1393	COA	O4B-C4B-C5B	2.30	116.95	109.37
4	A	1397	COA	C7P-C6P-C5P	2.26	116.12	112.36
4	B	1399	COA	O3B-C3B-C4B	2.19	118.00	110.08
4	D	1395	COA	C2B-C3B-C4B	2.18	107.08	103.22
4	A	1397	COA	C2P-C3P-N4P	2.16	117.25	112.31
4	B	1399	COA	C5B-C4B-C3B	2.15	121.52	114.40
4	C	1393	COA	O3B-C3B-C2B	2.08	119.21	111.68
4	B	1399	COA	O5P-C5P-C6P	-2.06	118.24	122.02
4	A	1397	COA	C6P-C5P-N4P	2.04	119.86	116.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1399	COA	C2B
4	D	1395	COA	C2B

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1397	COA	C3B-O3B-P3B-O7A
4	A	1397	COA	C5B-O5B-P1A-O1A
4	A	1397	COA	C5B-O5B-P1A-O2A
4	A	1397	COA	CCP-O6A-P2A-O3A
4	A	1397	COA	CCP-O6A-P2A-O4A
4	A	1397	COA	S1P-C2P-C3P-N4P
4	B	1399	COA	C3B-O3B-P3B-O8A
4	B	1399	COA	C5B-O5B-P1A-O1A
4	B	1399	COA	CCP-O6A-P2A-O3A
4	B	1399	COA	CCP-O6A-P2A-O4A
4	B	1399	COA	CCP-O6A-P2A-O5A
4	B	1399	COA	CDP-CBP-CCP-O6A
4	B	1399	COA	CEP-CBP-CCP-O6A
4	B	1399	COA	CAP-CBP-CCP-O6A
4	C	1393	COA	C3B-O3B-P3B-O7A
4	C	1393	COA	C5B-O5B-P1A-O1A
4	C	1393	COA	C5B-O5B-P1A-O2A
4	C	1393	COA	P2A-O3A-P1A-O5B
4	C	1393	COA	CCP-O6A-P2A-O3A

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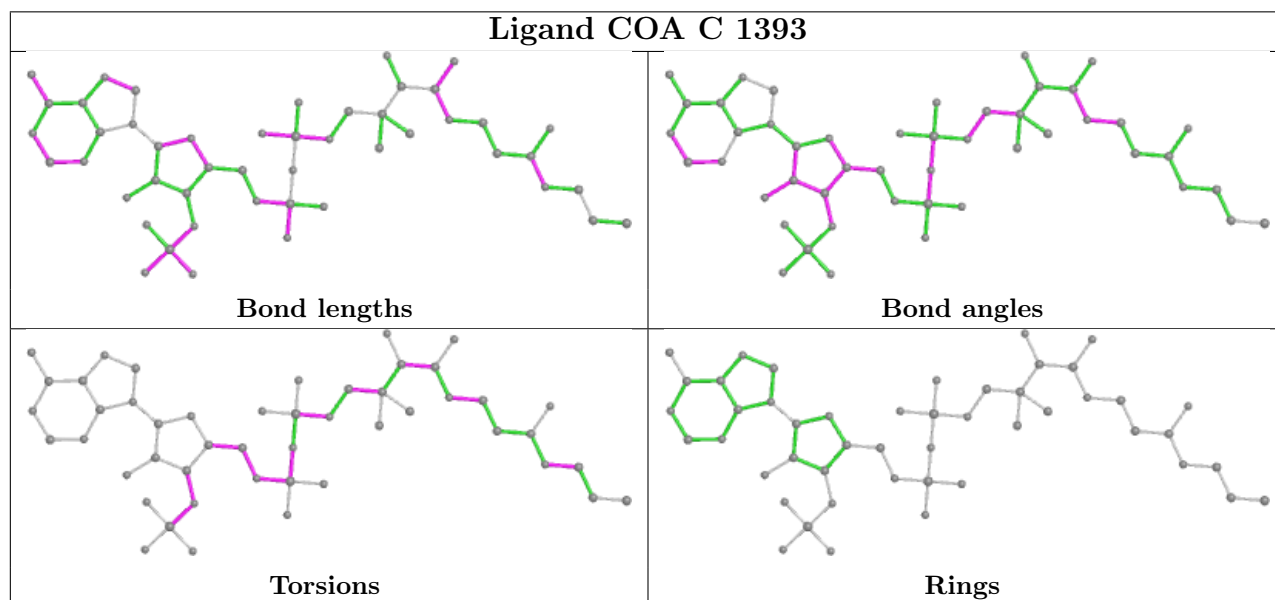
Mol	Chain	Res	Type	Atoms
4	C	1393	COA	CDP-CBP-CCP-O6A
4	C	1393	COA	CAP-CBP-CCP-O6A
4	C	1393	COA	N8P-C9P-CAP-OAP
4	D	1395	COA	C3B-C4B-C5B-O5B
4	D	1395	COA	O4B-C4B-C5B-O5B
4	D	1395	COA	C4B-C5B-O5B-P1A
4	D	1395	COA	P2A-O3A-P1A-O5B
4	D	1395	COA	CCP-O6A-P2A-O3A
4	D	1395	COA	CCP-O6A-P2A-O4A
4	D	1395	COA	C2P-C3P-N4P-C5P
4	D	1395	COA	S1P-C2P-C3P-N4P
4	A	1397	COA	C6P-C7P-N8P-C9P
4	A	1397	COA	C3B-C4B-C5B-O5B
4	A	1397	COA	O4B-C4B-C5B-O5B
4	B	1399	COA	C3B-C4B-C5B-O5B
4	C	1393	COA	C4B-C3B-O3B-P3B
4	C	1393	COA	C3B-C4B-C5B-O5B
4	C	1393	COA	O4B-C4B-C5B-O5B
4	C	1393	COA	CEP-CBP-CCP-O6A
4	C	1393	COA	C6P-C7P-N8P-C9P
4	C	1393	COA	C2B-C3B-O3B-P3B
4	C	1393	COA	C2P-C3P-N4P-C5P
4	A	1397	COA	C4B-C3B-O3B-P3B
4	A	1397	COA	P2A-O3A-P1A-O5B
4	B	1399	COA	P2A-O3A-P1A-O5B
4	B	1399	COA	O4B-C4B-C5B-O5B
4	A	1397	COA	CEP-CBP-CCP-O6A
4	B	1399	COA	C5B-O5B-P1A-O3A
4	B	1399	COA	C5B-O5B-P1A-O2A
4	C	1393	COA	CCP-O6A-P2A-O4A
4	C	1393	COA	CCP-O6A-P2A-O5A
4	D	1395	COA	CCP-O6A-P2A-O5A
4	A	1397	COA	CDP-CBP-CCP-O6A
4	A	1397	COA	C4B-C5B-O5B-P1A
4	B	1399	COA	C4B-C5B-O5B-P1A
4	C	1393	COA	O9P-C9P-CAP-OAP
4	C	1393	COA	C4B-C5B-O5B-P1A
4	A	1397	COA	C5B-O5B-P1A-O3A
4	A	1397	COA	N4P-C5P-C6P-C7P
4	C	1393	COA	C5B-O5B-P1A-O3A
4	A	1397	COA	O5P-C5P-C6P-C7P

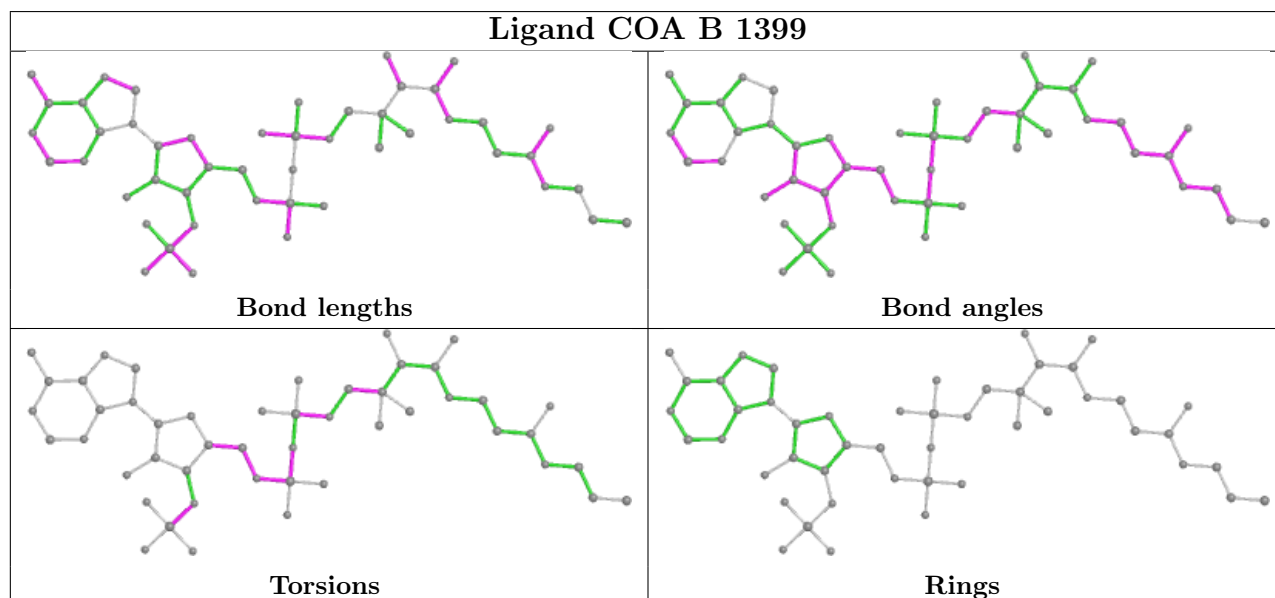
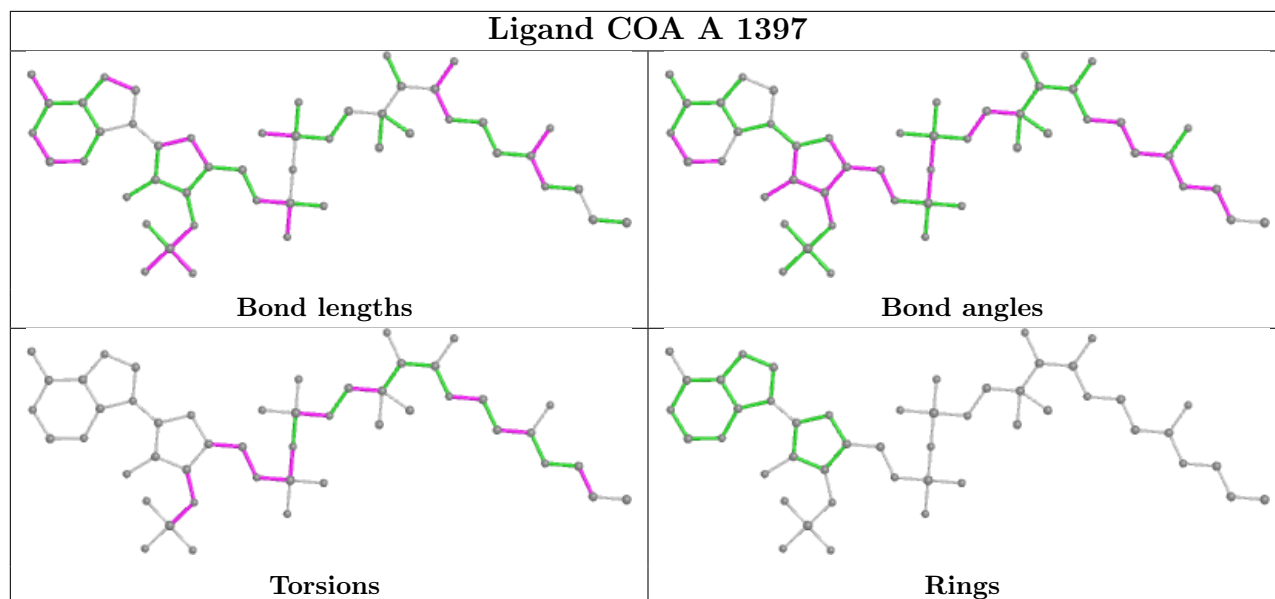
There are no ring outliers.

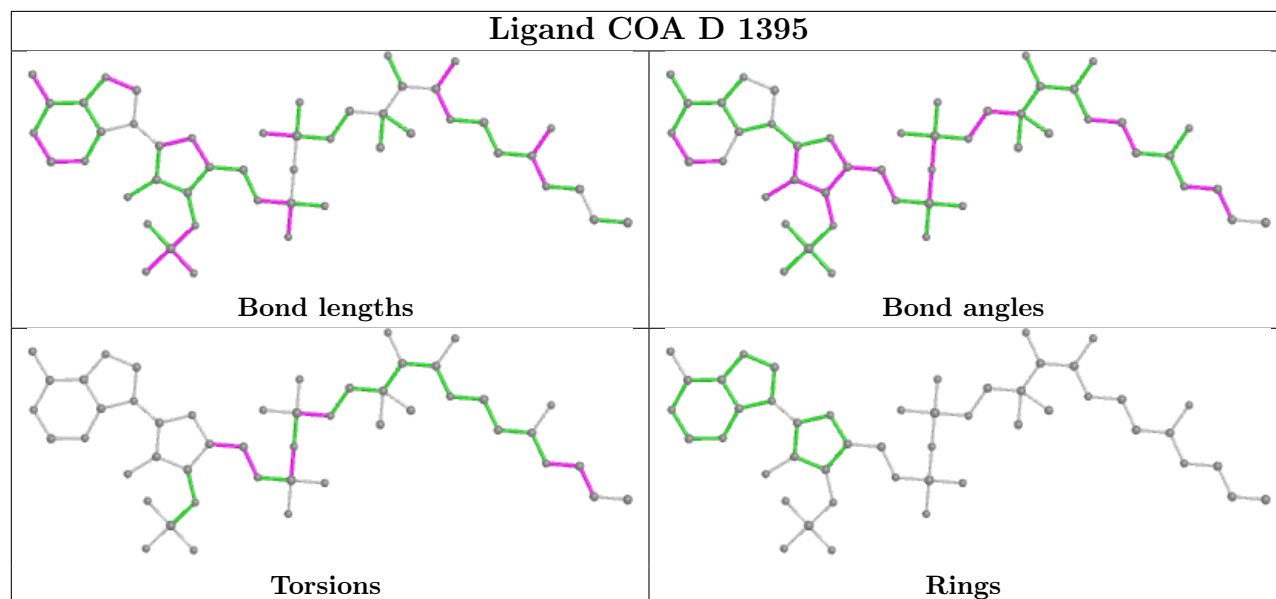
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1397	SO4	1	0
4	C	1393	COA	2	0
4	A	1397	COA	1	0
2	B	1396	SO4	1	0
4	B	1399	COA	2	0
4	D	1395	COA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	389/392 (99%)	-0.61	4 (1%) 82 84	4, 11, 34, 75	0
1	B	389/392 (99%)	-0.64	6 (1%) 73 75	4, 11, 33, 79	0
1	C	389/392 (99%)	-0.21	12 (3%) 49 52	13, 28, 51, 87	0
1	D	389/392 (99%)	-0.02	21 (5%) 25 27	8, 32, 59, 92	0
All	All	1556/1568 (99%)	-0.37	43 (2%) 53 56	4, 21, 50, 92	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207	ARG	4.5
1	C	208	LYS	4.4
1	D	207	ARG	4.4
1	A	208	LYS	4.3
1	D	208	LYS	3.9
1	C	237	LYS	3.6
1	B	208	LYS	3.5
1	B	207	ARG	3.5
1	D	221	HIS	3.4
1	D	238	GLU	3.4
1	D	206	GLY	3.4
1	C	169	GLN	3.3
1	C	209	GLY	3.3
1	D	237	LYS	3.2
1	D	222	GLY	3.2
1	A	207	ARG	3.1
1	D	169	GLN	3.1
1	D	226	ASP	3.1
1	D	268	GLY	3.1
1	D	236	ASP	3.0
1	D	232	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	237	LYS	2.9
1	B	237	LYS	2.9
1	C	236	ASP	2.9
1	C	206	GLY	2.8
1	D	74	ALA	2.7
1	C	223	ALA	2.7
1	D	209	GLY	2.6
1	D	230	LYS	2.5
1	C	238	GLU	2.5
1	D	193	GLY	2.5
1	D	335	SER	2.4
1	B	238	GLU	2.4
1	A	236	ASP	2.4
1	D	306	LYS	2.4
1	B	236	ASP	2.4
1	B	206	GLY	2.4
1	D	369	GLY	2.3
1	D	392	LEU	2.2
1	C	221	HIS	2.2
1	C	333	ASP	2.1
1	D	371	ARG	2.1
1	C	335	SER	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.

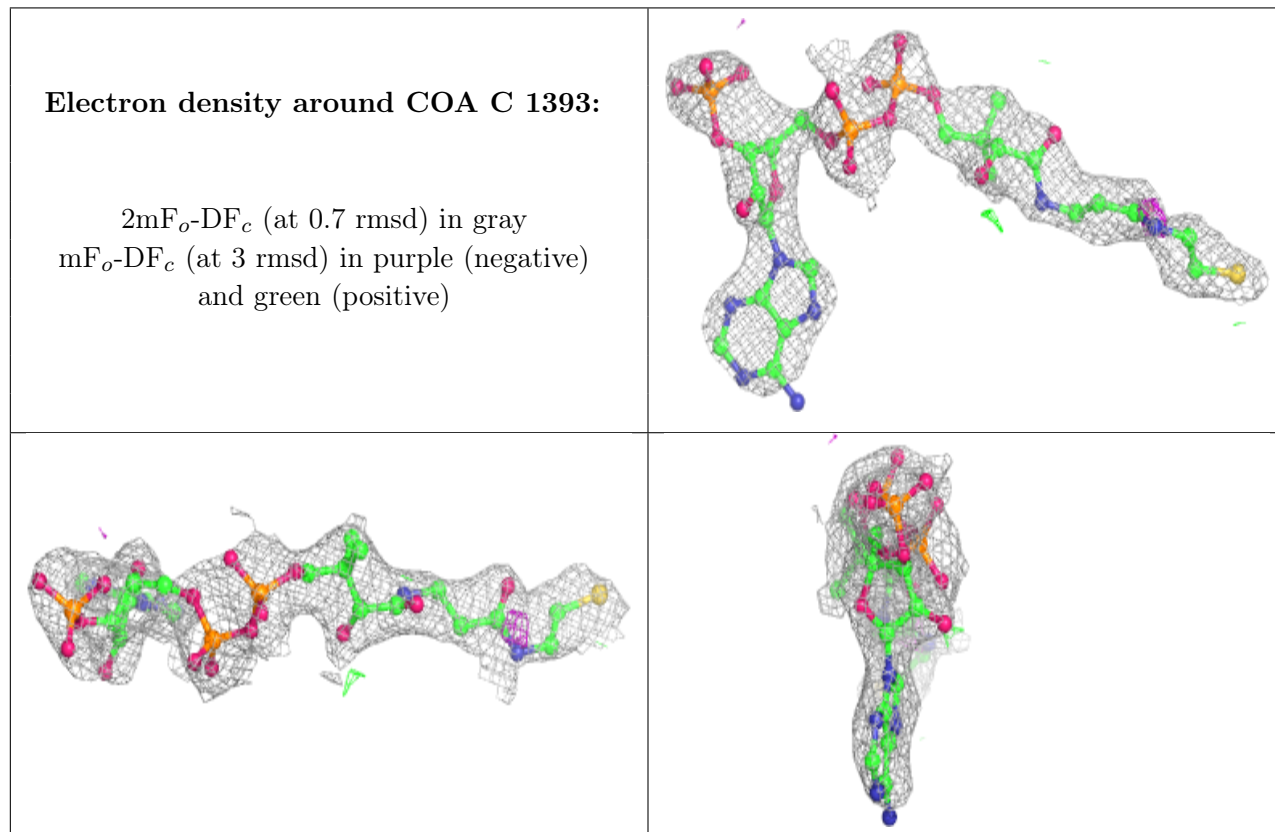
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1394	5/5	0.41	0.53	165,165,166,167	0

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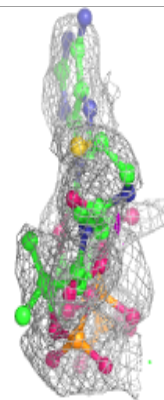
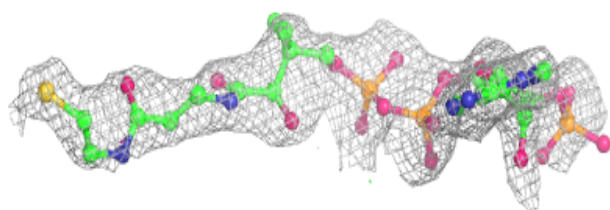
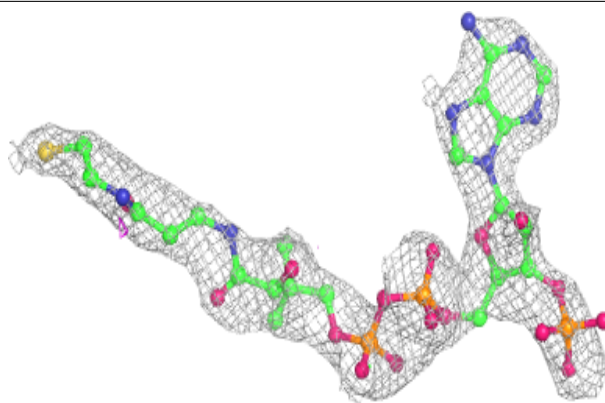
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	1394	5/5	0.84	0.30	103,104,105,108	0
2	SO4	B	1397	5/5	0.85	0.42	100,101,103,109	0
4	COA	C	1393	48/48	0.85	0.23	28,52,82,110	0
2	SO4	B	1395	5/5	0.86	0.25	66,69,76,84	0
4	COA	D	1395	48/48	0.87	0.21	35,49,101,121	0
2	SO4	B	1396	5/5	0.89	0.30	72,72,78,81	0
4	COA	B	1399	48/48	0.90	0.17	8,27,81,99	0
4	COA	A	1397	48/48	0.91	0.15	18,32,61,90	0
2	SO4	D	1393	5/5	0.95	0.29	76,77,79,82	0
2	SO4	B	1394	5/5	0.95	0.27	61,64,70,70	0
2	SO4	A	1393	5/5	0.96	0.22	60,62,66,68	0
3	NA	A	1396	1/1	0.97	0.17	22,22,22,22	0
3	NA	B	1398	1/1	0.97	0.08	30,30,30,30	0
2	SO4	B	1393	5/5	0.98	0.20	38,47,53,53	0
2	SO4	A	1395	5/5	0.99	0.21	35,37,42,44	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.

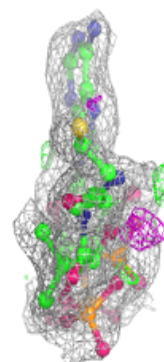
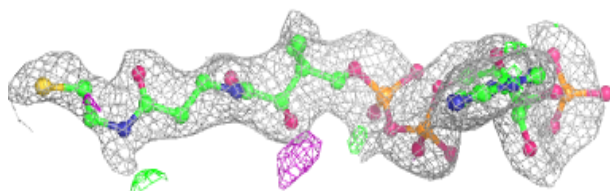
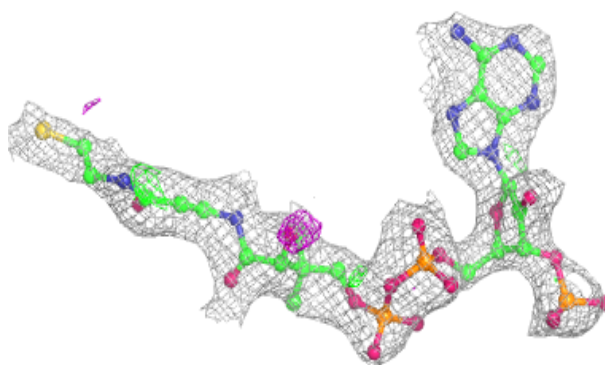


**Electron density around COA D 1395:**

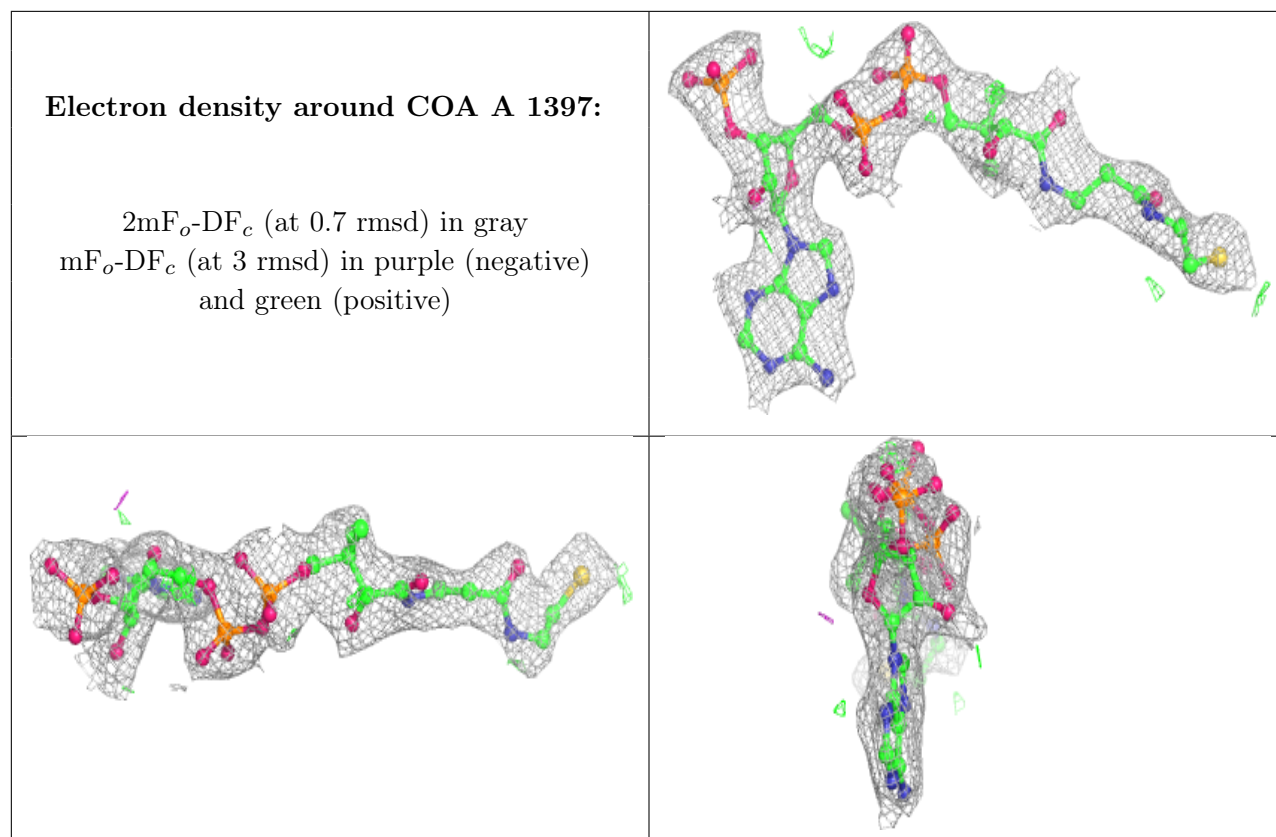
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around COA B 1399:**

$2mF_o-DF_c$  (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.