



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:15 pm BST

PDB ID : 2VTZ
Title : Biosynthetic thiolase from *Z. ramigera*. Complex of the C89A mutant with coenzyme A.
Authors : Kursula, P.; Merilainen, G.; Wierenga, R.K.
Deposited on : 2008-05-19
Resolution : 2.30 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

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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

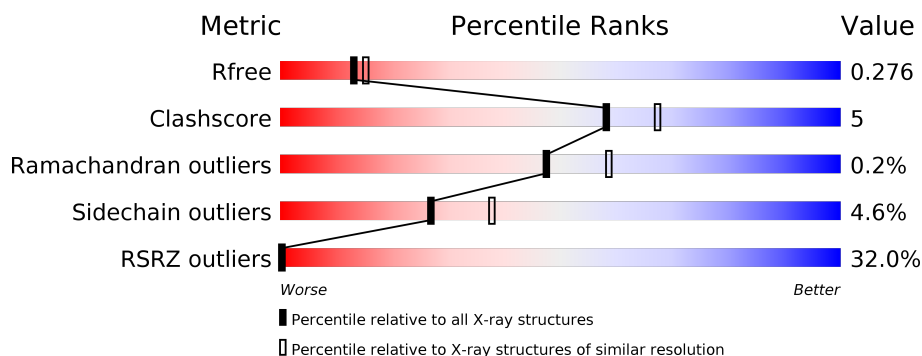
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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> <div>4%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	B	392	<div> <div>4%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	392	<div> <div>47%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	D	392	<div> <div>72%</div> <div>89%</div> <div>10%</div> <div>.</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
2	COA	C	1393	-	-	-	X
2	COA	D	1393	-	-	-	X
3	SO4	A	1396	-	-	-	X
3	SO4	B	1396	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12275 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
1	A	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			
1	B	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			
1	C	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			
1	D	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			

There are 8 discrepancies between the modelled and reference sequences:

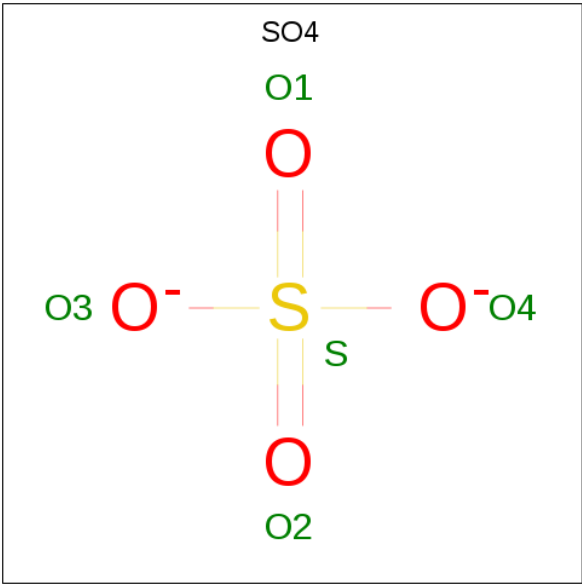
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ALA	CYS	engineered mutation	UNP P07097
B	89	ALA	CYS	engineered mutation	UNP P07097
C	89	ALA	CYS	engineered mutation	UNP P07097
D	89	ALA	CYS	engineered mutation	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

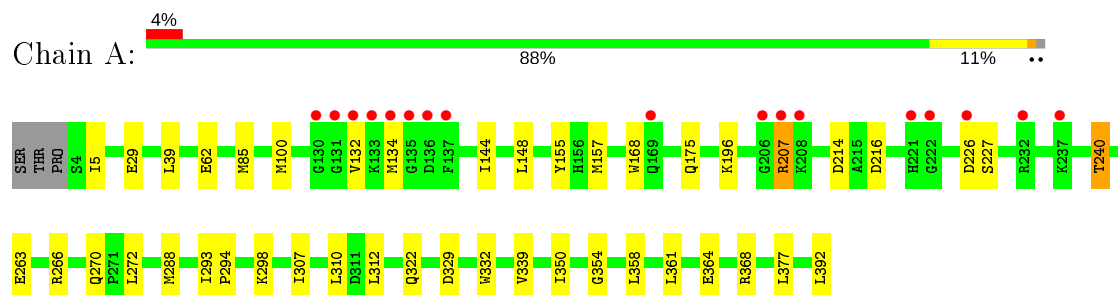
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	336	Total O 336 336	0	0
4	B	308	Total O 308 308	0	0
4	C	94	Total O 94 94	0	0
4	D	67	Total O 67 67	0	0

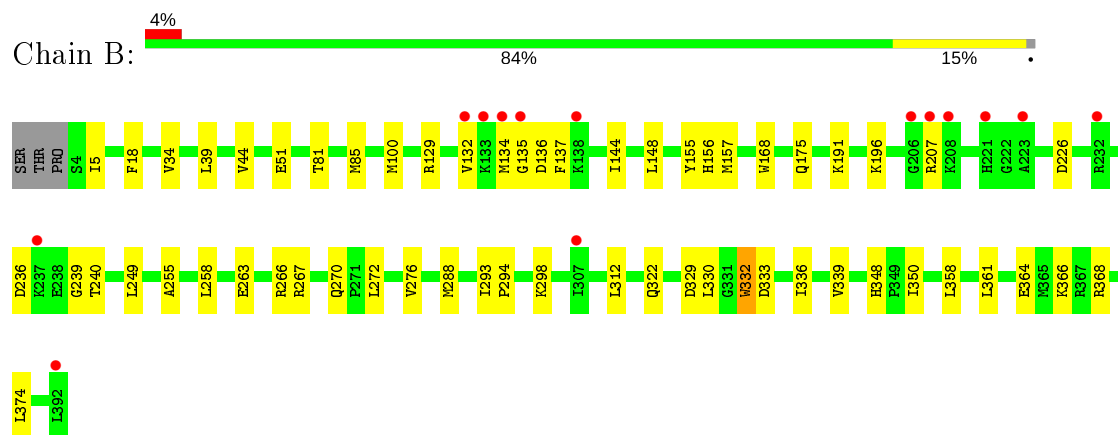
3 Residue-property plots

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.

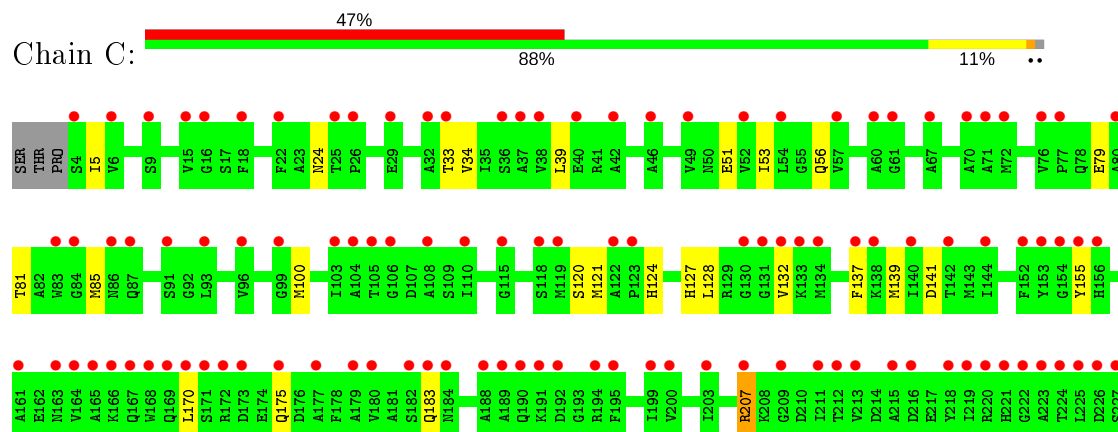
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

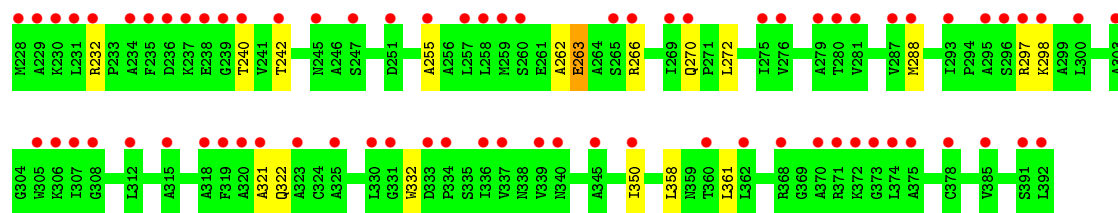


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

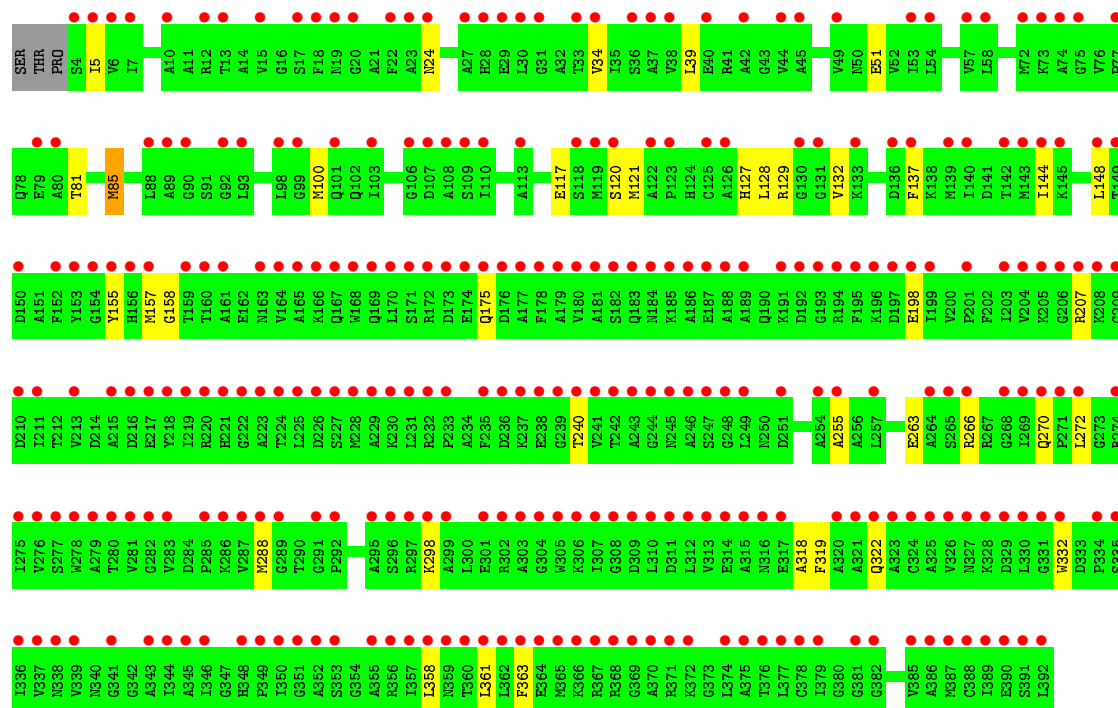
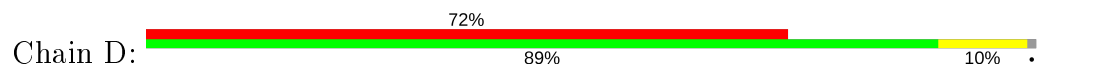


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE





● 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, α , β , γ	84.22Å 79.57Å 148.92Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.30) 81.1 (19.06-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.262 0.234 , 0.276	Depositor DCC
R_{free} test set	4262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12275	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.54	0/2853	0.64	0/3852
1	B	0.54	0/2853	0.66	0/3852
1	C	0.35	0/2853	0.51	0/3852
1	D	0.33	0/2853	0.50	0/3852
All	All	0.45	0/11412	0.58	0/15408

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	2812	0	2819	30	0
1	B	2812	0	2819	39	0
1	C	2812	0	2819	33	0
1	D	2812	0	2819	20	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	0	0
2	D	48	0	32	1	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
4	A	336	0	0	15	0
4	B	308	0	0	11	0
4	C	94	0	0	15	0
4	D	67	0	0	0	0
All	All	12275	0	11404	110	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 5.

All (110) 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:310:LEU:HD12	4:A:2275:HOH:O	1.80	0.81
1:A:310:LEU:CD1	4:A:2275:HOH:O	2.30	0.79
1:C:53:ILE:HG13	4:C:2016:HOH:O	1.85	0.76
1:A:307:ILE:HA	4:A:2275:HOH:O	1.87	0.74
1:B:44:VAL:HA	4:B:2225:HOH:O	1.93	0.67
1:A:5:ILE:HG13	1:A:100:MET:HG2	1.78	0.66
1:B:156:HIS:NE2	4:B:2136:HOH:O	2.29	0.65
1:B:226:ASP:HB3	4:B:2206:HOH:O	1.96	0.65
1:C:232:ARG:O	4:C:2066:HOH:O	2.14	0.64
1:C:33:THR:HG21	4:C:2061:HOH:O	1.98	0.64
1:A:263:GLU:HA	1:A:266:ARG:NH1	2.13	0.63
1:B:148:LEU:O	1:B:157:MET:HG2	1.99	0.62
1:D:158:GLY:HA2	1:D:319:PHE:CE2	2.35	0.61
1:A:226:ASP:HB3	4:A:2222:HOH:O	2.01	0.61
1:C:263:GLU:HA	1:C:266:ARG:NH1	2.17	0.60
1:A:196:LYS:NZ	4:A:2188:HOH:O	2.35	0.60
1:C:321:ALA:HA	4:C:2051:HOH:O	2.03	0.59
1:D:263:GLU:HA	1:D:266:ARG:NH1	2.18	0.58
2:B:1393:COA:H131	2:B:1393:COA:O9P	2.04	0.57
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.70	0.57
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.87	0.55
1:A:132:VAL:HA	4:A:2139:HOH:O	2.07	0.55
1:B:129:ARG:HA	1:D:132:VAL:O	2.07	0.55
1:A:29:GLU:HG2	4:A:2036:HOH:O	2.06	0.55
1:A:392:LEU:HG	4:A:2252:HOH:O	2.05	0.55
1:B:135:GLY:N	1:C:141:ASP:OD2	2.29	0.55
1:C:170:LEU:HB3	4:C:2051:HOH:O	2.07	0.54
1:B:196:LYS:HD2	4:B:2084:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLN:NE2	4:C:2053:HOH:O	2.39	0.53
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.23	0.52
1:C:132:VAL:HG21	1:C:137:PHE:CD1	2.45	0.52
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.92	0.52
1:A:196:LYS:HD2	4:A:2042:HOH:O	2.09	0.52
1:B:374:LEU:C	1:B:374:LEU:HD23	2.30	0.51
1:B:258:LEU:HG	4:B:2097:HOH:O	2.09	0.51
1:B:312:LEU:HD21	1:B:364:GLU:CG	2.41	0.51
1:A:214:ASP:HB2	4:A:2207:HOH:O	2.10	0.51
1:B:366:LYS:NZ	4:B:2290:HOH:O	2.39	0.50
1:C:51:GLU:C	4:C:2016:HOH:O	2.50	0.50
1:B:137:PHE:CE2	1:C:139:MET:HG3	2.46	0.50
1:A:134:MET:HA	4:A:2140:HOH:O	2.14	0.48
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.29	0.48
1:C:242:THR:HA	4:C:2066:HOH:O	2.14	0.48
1:C:262:ALA:HB3	4:C:2070:HOH:O	2.13	0.47
1:A:148:LEU:O	1:A:157:MET:HG2	2.14	0.47
1:B:137:PHE:CZ	1:C:139:MET:HG3	2.49	0.47
1:D:128:LEU:HD21	1:D:137:PHE:CE1	2.50	0.47
1:B:100:MET:HB2	4:B:2097:HOH:O	2.14	0.47
1:B:135:GLY:O	1:C:124:HIS:NE2	2.44	0.47
1:C:51:GLU:HG2	4:C:2016:HOH:O	2.14	0.47
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.80	0.46
1:D:51:GLU:HA	1:D:81:THR:O	2.16	0.46
1:B:236:ASP:O	1:B:239:GLY:N	2.48	0.46
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.51	0.46
1:B:156:HIS:CD2	4:B:2136:HOH:O	2.69	0.45
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.52	0.45
1:C:120:SER:O	1:D:127:HIS:NE2	2.48	0.45
1:D:157:MET:HG3	2:D:1393:COA:S1P	2.56	0.45
1:D:318:ALA:C	1:D:319:PHE:CD1	2.89	0.45
1:B:132:VAL:HG21	1:B:137:PHE:CD1	2.51	0.45
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.52	0.45
1:B:266:ARG:HH11	1:B:266:ARG:HG3	1.82	0.45
1:D:158:GLY:HA2	1:D:319:PHE:HE2	1.77	0.45
1:A:339:VAL:HG11	1:A:368:ARG:NH2	2.32	0.44
1:B:267:ARG:NH1	4:B:2225:HOH:O	2.50	0.44
1:B:34:VAL:HG12	1:B:255:ALA:HB3	2.00	0.44
1:B:134:MET:HA	1:D:129:ARG:NH1	2.32	0.44
1:B:18:PHE:HB2	1:B:249:LEU:O	2.18	0.44
1:A:354:GLY:HA2	1:A:377:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PHE:O	4:B:2012:HOH:O	2.21	0.43
1:C:175:GLN:CG	4:C:2051:HOH:O	2.65	0.43
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.83	0.43
1:C:85:MET:HA	1:D:85:MET:HA	1.99	0.43
1:B:136:ASP:HA	1:C:139:MET:O	2.19	0.43
1:C:79:GLU:N	1:C:79:GLU:OE1	2.51	0.43
1:C:51:GLU:HA	1:C:81:THR:O	2.18	0.43
1:A:207:ARG:N	1:A:207:ARG:HD3	2.33	0.43
1:B:5:ILE:HG13	1:B:100:MET:HG2	1.99	0.43
1:D:24:ASN:HA	1:D:121:MET:SD	2.59	0.43
1:A:293:ILE:HB	1:A:294:PRO:CD	2.49	0.43
1:D:5:ILE:HG13	1:D:100:MET:HG2	2.00	0.43
1:A:312:LEU:HD21	1:A:364:GLU:CG	2.50	0.42
1:B:134:MET:HA	1:D:129:ARG:HH12	1.84	0.42
1:D:34:VAL:HG12	1:D:255:ALA:HB3	2.01	0.42
1:C:24:ASN:HA	1:C:121:MET:SD	2.59	0.42
1:A:227:SER:OG	4:A:2221:HOH:O	2.21	0.42
1:C:207:ARG:N	1:C:207:ARG:HD3	2.35	0.42
1:C:127:HIS:NE2	1:D:120:SER:O	2.50	0.42
1:B:293:ILE:HB	1:B:294:PRO:CD	2.50	0.42
1:A:310:LEU:HG	4:A:2275:HOH:O	2.19	0.42
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.84	0.42
1:C:175:GLN:HG2	4:C:2051:HOH:O	2.20	0.42
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.85	0.42
1:C:56:GLN:N	4:C:2018:HOH:O	2.53	0.42
1:B:191:LYS:NZ	4:B:2160:HOH:O	2.42	0.42
1:B:333:ASP:O	1:B:336:ILE:HG12	2.20	0.42
1:A:62:GLU:O	1:A:62:GLU:HG2	2.20	0.41
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.55	0.41
1:C:297:ARG:HA	4:C:2079:HOH:O	2.19	0.41
1:D:144:ILE:HD13	1:D:148:LEU:HD12	2.01	0.41
1:C:5:ILE:HG13	1:C:100:MET:HG2	2.02	0.41
1:A:85:MET:HA	1:B:85:MET:HA	2.03	0.40
1:C:170:LEU:CB	4:C:2051:HOH:O	2.69	0.40
1:A:216:ASP:HB3	4:A:2309:HOH:O	2.20	0.40
1:A:310:LEU:CG	4:A:2275:HOH:O	2.65	0.40
1:D:198:GLU:HB3	1:D:363:PHE:CD2	2.56	0.40
1:A:339:VAL:HG11	1:A:368:ARG:HH21	1.86	0.40
1:B:144:ILE:HD13	1:B:148:LEU:HD12	2.02	0.40
1:B:51:GLU:HA	1:B:81:THR:O	2.22	0.40
1:B:132:VAL:O	1:D:129:ARG:HA	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	387/392 (99%)	377 (97%)	9 (2%)	1 (0%)	41	50
1	B	387/392 (99%)	376 (97%)	10 (3%)	1 (0%)	41	50
1	C	387/392 (99%)	377 (97%)	9 (2%)	1 (0%)	41	50
1	D	387/392 (99%)	377 (97%)	10 (3%)	0	100	100
All	All	1548/1568 (99%)	1507 (97%)	38 (2%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ILE
1	B	350	ILE
1	C	350	ILE

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	275/278 (99%)	263 (96%)	12 (4%)	28	39
1	B	275/278 (99%)	261 (95%)	14 (5%)	24	33
1	C	275/278 (99%)	263 (96%)	12 (4%)	28	39
1	D	275/278 (99%)	262 (95%)	13 (5%)	26	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1100/1112 (99%)	1049 (95%)	51 (5%)	27	38

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	207	ARG
1	A	240	THR
1	A	270	GLN
1	A	272	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	358	LEU
1	A	361	LEU
1	B	39	LEU
1	B	155	TYR
1	B	207	ARG
1	B	263	GLU
1	B	270	GLN
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	348	HIS
1	B	358	LEU
1	B	361	LEU
1	C	39	LEU
1	C	155	TYR
1	C	207	ARG
1	C	263	GLU
1	C	270	GLN
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	358	LEU

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Mol	Chain	Res	Type
1	C	361	LEU
1	D	39	LEU
1	D	85	MET
1	D	117	GLU
1	D	155	TYR
1	D	207	ARG
1	D	270	GLN
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	358	LEU
1	D	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	$\# Z > 2$
3	SO4	A	1395	-	4,4,4	0.17	0	6,6,6	0.21	0
2	COA	D	1393	-	41,50,50	1.72	3 (7%)	52,75,75	1.15	2 (3%)
2	COA	B	1393	-	41,50,50	1.73	3 (7%)	52,75,75	1.16	3 (5%)
2	COA	C	1393	-	41,50,50	1.72	3 (7%)	52,75,75	1.13	3 (5%)
3	SO4	B	1396	-	4,4,4	0.12	0	6,6,6	0.18	0
2	COA	A	1393	-	41,50,50	1.74	3 (7%)	52,75,75	1.21	2 (3%)
3	SO4	A	1396	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	B	1395	-	4,4,4	0.13	0	6,6,6	0.13	0
3	SO4	B	1394	-	4,4,4	0.19	0	6,6,6	0.25	0
3	SO4	A	1394	-	4,4,4	0.13	0	6,6,6	0.14	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
2	COA	D	1393	-	-	7/44/64/64	0/3/3/3
2	COA	B	1393	-	-	16/44/64/64	0/3/3/3
2	COA	C	1393	-	-	15/44/64/64	0/3/3/3
2	COA	A	1393	-	-	5/44/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1393	COA	O9P-C9P	9.15	1.41	1.23
2	C	1393	COA	O9P-C9P	9.10	1.41	1.23
2	A	1393	COA	O9P-C9P	9.08	1.41	1.23
2	B	1393	COA	O9P-C9P	8.88	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1393	COA	C2A-N3A	4.26	1.39	1.32
2	B	1393	COA	C2A-N3A	4.11	1.38	1.32
2	D	1393	COA	C2A-N3A	4.11	1.38	1.32
2	A	1393	COA	C2A-N3A	3.73	1.38	1.32
2	B	1393	COA	C2A-N1A	2.76	1.39	1.33
2	C	1393	COA	C2A-N1A	2.65	1.38	1.33
2	D	1393	COA	C2A-N1A	2.65	1.38	1.33
2	A	1393	COA	C2A-N1A	2.58	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1393	COA	N3A-C2A-N1A	-5.84	119.55	128.68
2	D	1393	COA	N3A-C2A-N1A	-5.57	119.97	128.68
2	B	1393	COA	N3A-C2A-N1A	-5.48	120.11	128.68
2	C	1393	COA	N3A-C2A-N1A	-5.40	120.24	128.68
2	D	1393	COA	P2A-O3A-P1A	-3.49	120.84	132.83
2	A	1393	COA	P2A-O3A-P1A	-3.16	121.99	132.83
2	C	1393	COA	P2A-O3A-P1A	-2.83	123.12	132.83
2	C	1393	COA	C3B-C2B-C1B	2.78	106.04	99.89
2	B	1393	COA	P2A-O3A-P1A	-2.38	124.64	132.83
2	B	1393	COA	C7P-C6P-C5P	2.11	115.87	112.36

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1393	COA	C5B-O5B-P1A-O3A
2	D	1393	COA	CAP-C9P-N8P-C7P
2	D	1393	COA	S1P-C2P-C3P-N4P
2	B	1393	COA	C5B-O5B-P1A-O1A
2	B	1393	COA	C5B-O5B-P1A-O2A
2	B	1393	COA	CCP-O6A-P2A-O3A
2	B	1393	COA	CCP-O6A-P2A-O4A
2	B	1393	COA	CCP-O6A-P2A-O5A
2	B	1393	COA	CAP-CBP-CCP-O6A
2	B	1393	COA	C5P-C6P-C7P-N8P
2	B	1393	COA	S1P-C2P-C3P-N4P
2	C	1393	COA	C5B-O5B-P1A-O1A
2	C	1393	COA	C5B-O5B-P1A-O2A
2	C	1393	COA	CCP-O6A-P2A-O4A
2	C	1393	COA	CAP-C9P-N8P-C7P

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Mol	Chain	Res	Type	Atoms
2	C	1393	COA	O9P-C9P-N8P-C7P
2	C	1393	COA	C5P-C6P-C7P-N8P
2	C	1393	COA	C6P-C5P-N4P-C3P
2	C	1393	COA	C2P-C3P-N4P-C5P
2	A	1393	COA	S1P-C2P-C3P-N4P
2	C	1393	COA	O5P-C5P-N4P-C3P
2	D	1393	COA	O9P-C9P-N8P-C7P
2	C	1393	COA	C4B-C3B-O3B-P3B
2	B	1393	COA	CDP-CBP-CCP-O6A
2	A	1393	COA	O4B-C4B-C5B-O5B
2	B	1393	COA	N8P-C9P-CAP-CBP
2	A	1393	COA	C4B-C5B-O5B-P1A
2	B	1393	COA	P2A-O3A-P1A-O5B
2	C	1393	COA	C3B-O3B-P3B-O7A
2	B	1393	COA	CEP-CBP-CCP-O6A
2	D	1393	COA	C5P-C6P-C7P-N8P
2	B	1393	COA	C5B-O5B-P1A-O3A
2	C	1393	COA	C5B-O5B-P1A-O3A
2	C	1393	COA	CCP-O6A-P2A-O3A
2	B	1393	COA	C4B-C5B-O5B-P1A
2	D	1393	COA	C5B-O5B-P1A-O2A
2	A	1393	COA	C5B-O5B-P1A-O1A
2	C	1393	COA	C2B-C3B-O3B-P3B
2	B	1393	COA	O9P-C9P-CAP-CBP
2	D	1393	COA	P2A-O3A-P1A-O1A
2	B	1393	COA	O9P-C9P-N8P-C7P
2	A	1393	COA	C5B-O5B-P1A-O3A
2	C	1393	COA	O5P-C5P-C6P-C7P

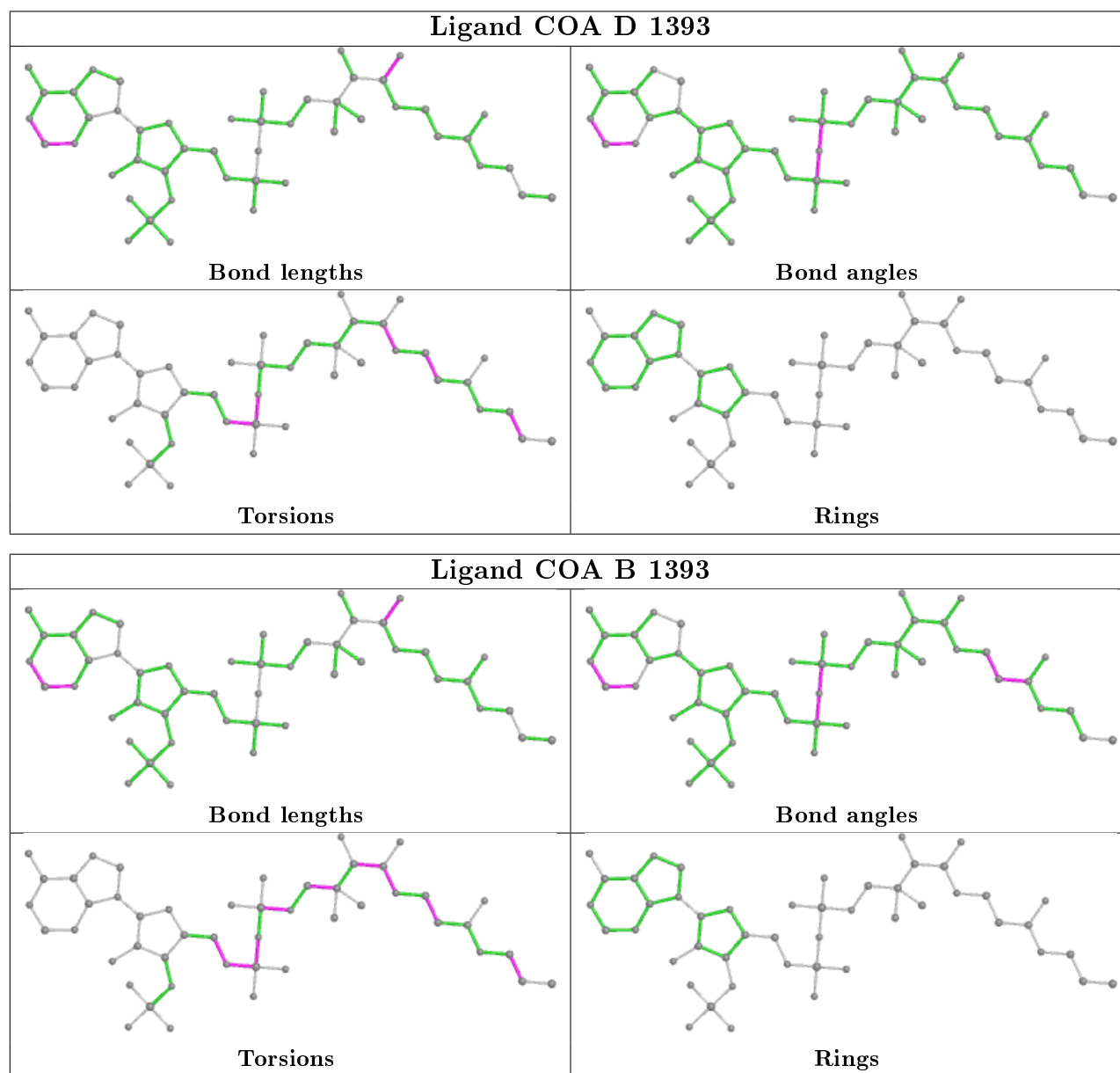
There are no ring outliers.

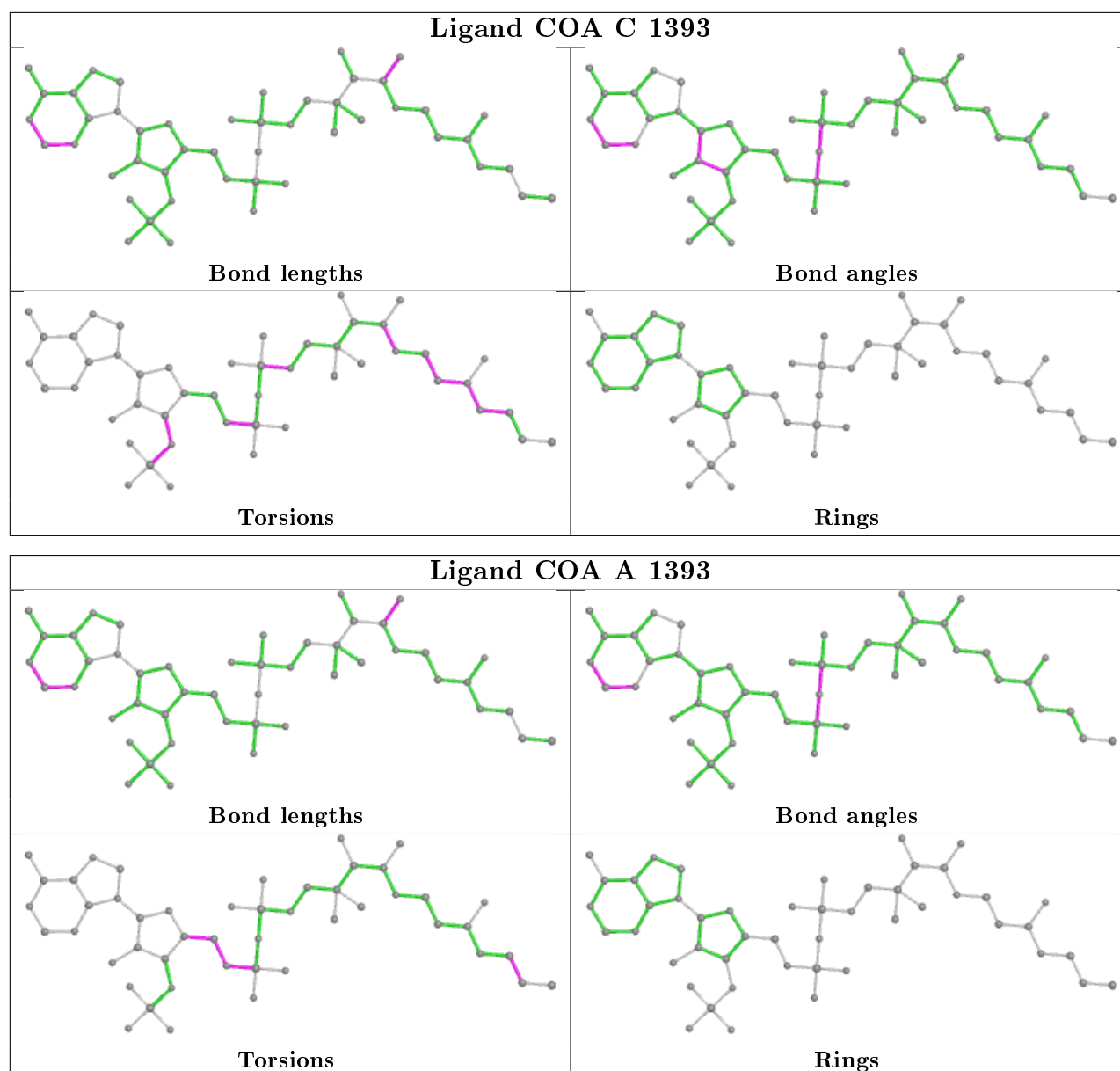
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1393	COA	1	0
2	B	1393	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	389/392 (99%)	0.42	17 (4%) 34 41	34, 39, 47, 60	0
1	B	389/392 (99%)	0.49	14 (3%) 42 49	31, 39, 47, 60	0
1	C	389/392 (99%)	2.21	185 (47%) 0 0	35, 40, 47, 56	0
1	D	389/392 (99%)	3.46	282 (72%) 0 0	36, 39, 46, 55	0
All	All	1556/1568 (99%)	1.64	498 (32%) 0 0	31, 39, 47, 60	0

All (498) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	ALA	12.5
1	D	222	GLY	12.3
1	D	238	GLU	11.8
1	D	241	VAL	11.0
1	D	170	LEU	10.8
1	D	219	ILE	10.7
1	D	231	LEU	10.0
1	D	371	ARG	9.8
1	D	331	GLY	9.8
1	D	382	GLY	9.7
1	D	323	ALA	9.5
1	D	166	LYS	8.8
1	D	228	MET	8.7
1	D	153	TYR	8.7
1	D	207	ARG	8.5
1	D	325	ALA	8.4
1	D	230	LYS	8.4
1	D	367	ARG	8.4
1	D	218	TYR	8.3
1	D	226	ASP	8.2
1	D	188	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	328	LYS	8.1
1	D	206	GLY	8.0
1	C	222	GLY	7.9
1	C	224	THR	7.8
1	D	191	LYS	7.6
1	D	224	THR	7.3
1	D	179	ALA	7.1
1	D	182	SER	7.1
1	C	223	ALA	7.1
1	D	310	LEU	7.1
1	D	165	ALA	7.0
1	D	243	ALA	7.0
1	D	205	LYS	6.9
1	D	223	ALA	6.8
1	D	269	ILE	6.8
1	D	175	GLN	6.7
1	D	237	LYS	6.7
1	D	349	PRO	6.7
1	C	80	ALA	6.6
1	D	357	ILE	6.5
1	D	232	ARG	6.5
1	A	134	MET	6.3
1	D	307	ILE	6.3
1	D	155	TYR	6.1
1	D	301	GLU	6.1
1	D	186	ALA	6.1
1	D	303	ALA	5.9
1	D	345	ALA	5.9
1	D	167	GLN	5.9
1	D	193	GLY	5.9
1	D	235	PHE	5.8
1	C	280	THR	5.8
1	C	295	ALA	5.8
1	D	377	LEU	5.8
1	C	229	ALA	5.8
1	B	134	MET	5.7
1	D	152	PHE	5.7
1	C	234	ALA	5.6
1	D	196	LYS	5.6
1	D	271	PRO	5.6
1	D	161	ALA	5.6
1	D	247	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	168	TRP	5.5
1	C	36	SER	5.5
1	D	344	ILE	5.5
1	D	178	PHE	5.4
1	D	246	ALA	5.4
1	D	326	VAL	5.4
1	D	245	ASN	5.4
1	C	131	GLY	5.4
1	C	232	ARG	5.4
1	C	269	ILE	5.3
1	D	254	ALA	5.3
1	D	160	THR	5.3
1	D	233	PRO	5.3
1	C	140	ILE	5.3
1	C	37	ALA	5.3
1	D	329	ASP	5.3
1	D	330	LEU	5.3
1	D	159	THR	5.2
1	C	156	HIS	5.2
1	D	305	TRP	5.2
1	C	227	SER	5.2
1	D	283	VAL	5.2
1	C	209	GLY	5.2
1	D	131	GLY	5.2
1	D	336	ILE	5.2
1	D	248	GLY	5.2
1	C	182	SER	5.1
1	D	164	VAL	5.1
1	D	242	THR	5.1
1	C	237	LYS	5.1
1	C	153	TYR	5.1
1	D	34	VAL	5.1
1	C	132	VAL	5.1
1	D	332	TRP	5.1
1	D	277	SER	5.0
1	A	131	GLY	5.0
1	B	135	GLY	5.0
1	D	240	THR	5.0
1	D	306	LYS	4.9
1	D	387	MET	4.9
1	C	225	LEU	4.9
1	C	226	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	368	ARG	4.9
1	D	195	PHE	4.9
1	D	37	ALA	4.8
1	D	108	ALA	4.8
1	C	266	ARG	4.8
1	D	12	ARG	4.8
1	D	192	ASP	4.8
1	C	213	VAL	4.8
1	C	211	ILE	4.8
1	D	272	LEU	4.8
1	C	391	SER	4.8
1	D	346	ILE	4.8
1	D	268	GLY	4.8
1	D	374	LEU	4.8
1	D	140	ILE	4.8
1	D	171	SER	4.7
1	D	181	ALA	4.7
1	C	110	ILE	4.7
1	D	225	LEU	4.7
1	B	208	LYS	4.7
1	D	312	LEU	4.7
1	D	220	ARG	4.6
1	D	239	GLY	4.6
1	D	211	ILE	4.6
1	C	307	ILE	4.6
1	D	177	ALA	4.6
1	C	235	PHE	4.5
1	C	238	GLU	4.5
1	D	327	ASN	4.5
1	C	230	LYS	4.5
1	C	103	ILE	4.5
1	D	372	LYS	4.5
1	D	315	ALA	4.5
1	D	370	ALA	4.4
1	B	206	GLY	4.4
1	D	176	ASP	4.4
1	C	315	ALA	4.4
1	D	221	HIS	4.3
1	D	180	VAL	4.3
1	D	19	ASN	4.3
1	C	330	LEU	4.3
1	D	358	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	33	THR	4.3
1	D	4	SER	4.3
1	D	365	MET	4.3
1	C	293	ILE	4.2
1	D	320	ALA	4.2
1	C	231	LEU	4.2
1	C	221	HIS	4.2
1	D	6	VAL	4.2
1	D	5	ILE	4.2
1	D	169	GLN	4.2
1	D	391	SER	4.2
1	D	311	ASP	4.2
1	C	212	THR	4.1
1	D	154	GLY	4.1
1	C	4	SER	4.1
1	D	119	MET	4.1
1	B	207	ARG	4.1
1	C	67	ALA	4.1
1	C	164	VAL	4.1
1	D	204	VAL	4.1
1	A	132	VAL	4.0
1	D	302	ARG	4.0
1	D	217	GLU	4.0
1	D	148	LEU	4.0
1	C	108	ALA	4.0
1	D	29	GLU	3.9
1	D	184	ASN	3.9
1	A	207	ARG	3.9
1	C	138	LYS	3.9
1	C	42	ALA	3.9
1	D	362	LEU	3.9
1	D	172	ARG	3.9
1	D	107	ASP	3.9
1	C	25	THR	3.9
1	D	24	ASN	3.9
1	D	20	GLY	3.8
1	D	281	VAL	3.8
1	D	42	ALA	3.8
1	D	321	ALA	3.8
1	C	195	PHE	3.8
1	D	189	ALA	3.8
1	D	173	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	285	PRO	3.8
1	D	157	MET	3.8
1	A	208	LYS	3.8
1	C	76	VAL	3.8
1	C	321	ALA	3.8
1	C	173	ASP	3.7
1	C	306	LYS	3.7
1	D	297	ARG	3.7
1	C	259	MET	3.7
1	A	237	LYS	3.7
1	C	104	ALA	3.7
1	C	155	TYR	3.7
1	C	207	ARG	3.7
1	D	339	VAL	3.7
1	D	187	GLU	3.6
1	D	40	GLU	3.6
1	D	361	LEU	3.6
1	C	133	LYS	3.6
1	D	295	ALA	3.6
1	D	375	ALA	3.6
1	D	183	GLN	3.6
1	D	388	CYS	3.6
1	D	279	ALA	3.5
1	D	265	SER	3.5
1	D	359	ASN	3.5
1	D	23	ALA	3.5
1	C	312	LEU	3.5
1	C	318	ALA	3.5
1	A	136	ASP	3.5
1	A	206	GLY	3.5
1	D	389	ILE	3.5
1	D	313	VAL	3.5
1	A	133	LYS	3.5
1	C	340	ASN	3.4
1	C	130	GLY	3.4
1	D	156	HIS	3.4
1	D	199	ILE	3.4
1	D	392	LEU	3.4
1	D	338	ASN	3.4
1	D	308	GLY	3.4
1	C	236	ASP	3.4
1	C	122	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	88	LEU	3.4
1	D	291	GLY	3.4
1	C	296	SER	3.4
1	D	30	LEU	3.4
1	C	152	PHE	3.3
1	D	350	ILE	3.3
1	C	52	VAL	3.3
1	B	133	LYS	3.3
1	C	169	GLN	3.3
1	D	49	VAL	3.3
1	C	303	ALA	3.3
1	D	366	LYS	3.3
1	D	18	PHE	3.3
1	D	110	ILE	3.3
1	D	360	THR	3.3
1	D	106	GLY	3.3
1	D	355	ALA	3.3
1	C	392	LEU	3.3
1	D	227	SER	3.3
1	D	369	GLY	3.2
1	A	135	GLY	3.2
1	D	236	ASP	3.2
1	D	93	LEU	3.2
1	D	7	ILE	3.2
1	D	92	GLY	3.2
1	C	49	VAL	3.2
1	D	314	GLU	3.2
1	D	264	ALA	3.2
1	C	26	PRO	3.2
1	C	219	ILE	3.2
1	D	15	VAL	3.2
1	D	125	CYS	3.2
1	D	216	ASP	3.2
1	D	274	ARG	3.2
1	D	203	ILE	3.1
1	D	79	GLU	3.1
1	C	323	ALA	3.1
1	C	167	GLN	3.1
1	C	93	LEU	3.1
1	D	215	ALA	3.1
1	D	385	VAL	3.1
1	D	120	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	105	THR	3.1
1	D	364	GLU	3.1
1	D	197	ASP	3.1
1	D	210	ASP	3.1
1	D	213	VAL	3.1
1	D	133	LYS	3.1
1	D	54	LEU	3.1
1	C	40	GLU	3.1
1	D	103	ILE	3.1
1	D	390	GLU	3.1
1	D	255	ALA	3.1
1	D	343	ALA	3.1
1	D	363	PHE	3.0
1	D	378	CYS	3.0
1	D	163	ASN	3.0
1	D	335	SER	3.0
1	C	220	ARG	3.0
1	C	288	MET	3.0
1	C	372	LYS	3.0
1	D	352	ALA	3.0
1	D	282	GLY	3.0
1	D	289	GLY	3.0
1	D	10	ALA	3.0
1	D	376	THR	3.0
1	D	143	MET	3.0
1	C	297	ARG	3.0
1	A	226	ASP	3.0
1	C	333	ASP	3.0
1	D	109	SER	2.9
1	D	145	LYS	2.9
1	C	287	VAL	2.9
1	D	142	THR	2.9
1	C	375	ALA	2.9
1	C	334	PRO	2.9
1	D	201	PRO	2.9
1	B	132	VAL	2.9
1	C	180	VAL	2.9
1	D	113	ALA	2.9
1	A	130	GLY	2.9
1	C	245	ASN	2.9
1	C	298	LYS	2.9
1	B	223	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	334	PRO	2.9
1	C	265	SER	2.8
1	C	84	GLY	2.8
1	C	166	LYS	2.8
1	D	337	VAL	2.8
1	D	74	ALA	2.8
1	B	221	HIS	2.8
1	C	137	PHE	2.8
1	D	185	LYS	2.8
1	D	244	GLY	2.8
1	C	203	ILE	2.8
1	D	137	PHE	2.8
1	C	165	ALA	2.8
1	D	80	ALA	2.8
1	D	249	LEU	2.8
1	C	188	ALA	2.8
1	C	61	GLY	2.8
1	C	374	LEU	2.8
1	D	288	MET	2.8
1	D	126	ALA	2.7
1	D	198	GLU	2.7
1	C	192	ASP	2.7
1	C	200	VAL	2.7
1	D	194	ARG	2.7
1	C	336	ILE	2.7
1	D	270	GLN	2.7
1	C	15	VAL	2.7
1	C	83	TRP	2.7
1	C	172	ARG	2.7
1	C	371	ARG	2.7
1	C	373	GLY	2.7
1	C	215	ALA	2.7
1	C	305	TRP	2.7
1	D	17	SER	2.7
1	D	123	PRO	2.7
1	D	44	VAL	2.7
1	C	260	SER	2.7
1	D	276	VAL	2.7
1	D	324	CYS	2.6
1	C	9	SER	2.6
1	D	57	VAL	2.6
1	D	90	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	171	SER	2.6
1	C	16	GLY	2.6
1	B	237	LYS	2.6
1	D	150	ASP	2.6
1	C	54	LEU	2.6
1	C	123	PRO	2.6
1	C	60	ALA	2.6
1	C	175	GLN	2.6
1	D	98	LEU	2.6
1	D	257	LEU	2.6
1	D	348	HIS	2.6
1	C	46	ALA	2.6
1	C	71	ALA	2.6
1	C	87	GLN	2.6
1	D	118	SER	2.6
1	D	149	THR	2.6
1	C	99	GLY	2.6
1	D	27	ALA	2.6
1	C	184	ASN	2.6
1	C	199	ILE	2.6
1	C	275	ILE	2.6
1	D	33	THR	2.5
1	C	168	TRP	2.5
1	D	286	LYS	2.5
1	A	232	ARG	2.5
1	C	194	ARG	2.5
1	C	370	ALA	2.5
1	C	270	GLN	2.5
1	D	251	ASP	2.5
1	C	96	VAL	2.5
1	C	218	TYR	2.5
1	D	386	ALA	2.5
1	C	57	VAL	2.5
1	D	22	PHE	2.5
1	D	287	VAL	2.5
1	C	216	ASP	2.5
1	C	38	VAL	2.5
1	C	319	PHE	2.5
1	D	38	VAL	2.5
1	C	154	GLY	2.4
1	C	170	LEU	2.4
1	D	122	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	183	GLN	2.4
1	D	28	HIS	2.4
1	D	296	SER	2.4
1	C	106	GLY	2.4
1	C	91	SER	2.4
1	C	239	GLY	2.4
1	D	75	GLY	2.4
1	C	368	ARG	2.4
1	D	379	ILE	2.4
1	B	392	LEU	2.4
1	D	31	GLY	2.4
1	C	385	VAL	2.4
1	D	136	ASP	2.4
1	C	251	ASP	2.3
1	C	179	ALA	2.3
1	C	325	ALA	2.3
1	D	322	GLN	2.3
1	C	70	ALA	2.3
1	C	177	ALA	2.3
1	C	189	ALA	2.3
1	C	240	THR	2.3
1	D	278	TRP	2.3
1	D	280	THR	2.3
1	D	298	LYS	2.3
1	C	190	GLN	2.3
1	B	232	ARG	2.3
1	D	275	ILE	2.3
1	C	345	ALA	2.3
1	C	242	THR	2.3
1	C	228	MET	2.3
1	D	45	ALA	2.3
1	D	58	LEU	2.3
1	D	353	SER	2.3
1	D	381	GLY	2.3
1	C	18	PHE	2.3
1	D	316	ASN	2.3
1	C	320	ALA	2.3
1	D	53	ILE	2.3
1	C	360	THR	2.2
1	D	13	THR	2.2
1	C	362	LEU	2.2
1	C	276	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	307	ILE	2.2
1	C	29	GLU	2.2
1	C	77	PRO	2.2
1	D	292	PRO	2.2
1	C	281	VAL	2.2
1	D	208	LYS	2.2
1	C	247	SER	2.2
1	C	115	GLY	2.2
1	D	99	GLY	2.2
1	D	130	GLY	2.2
1	D	351	GLY	2.2
1	C	32	ALA	2.2
1	C	72	MET	2.2
1	C	118	SER	2.2
1	C	255	ALA	2.2
1	D	299	ALA	2.2
1	D	209	GLY	2.2
1	D	341	GLY	2.2
1	D	139	MET	2.2
1	C	22	PHE	2.1
1	C	279	ALA	2.1
1	D	89	ALA	2.1
1	D	144	ILE	2.1
1	C	257	LEU	2.1
1	C	300	LEU	2.1
1	C	339	VAL	2.1
1	D	36	SER	2.1
1	D	174	GLU	2.1
1	C	142	THR	2.1
1	A	169	GLN	2.1
1	C	163	ASN	2.1
1	A	222	GLY	2.1
1	D	304	GLY	2.1
1	D	317	GLU	2.1
1	C	134	MET	2.1
1	C	161	ALA	2.1
1	C	337	VAL	2.1
1	C	86	ASN	2.1
1	C	331	GLY	2.1
1	B	138	LYS	2.1
1	D	73	LYS	2.1
1	D	77	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	221	HIS	2.1
1	D	266	ARG	2.1
1	D	309	ASP	2.0
1	C	119	MET	2.0
1	C	6	VAL	2.0
1	A	137	PHE	2.0
1	C	191	LYS	2.0
1	C	258	LEU	2.0
1	D	72	MET	2.0
1	C	308	GLY	2.0
1	D	101	GLN	2.0
1	C	378	CYS	2.0
1	C	144	ILE	2.0
1	C	350	ILE	2.0
1	D	356	ARG	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 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, 95th 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.

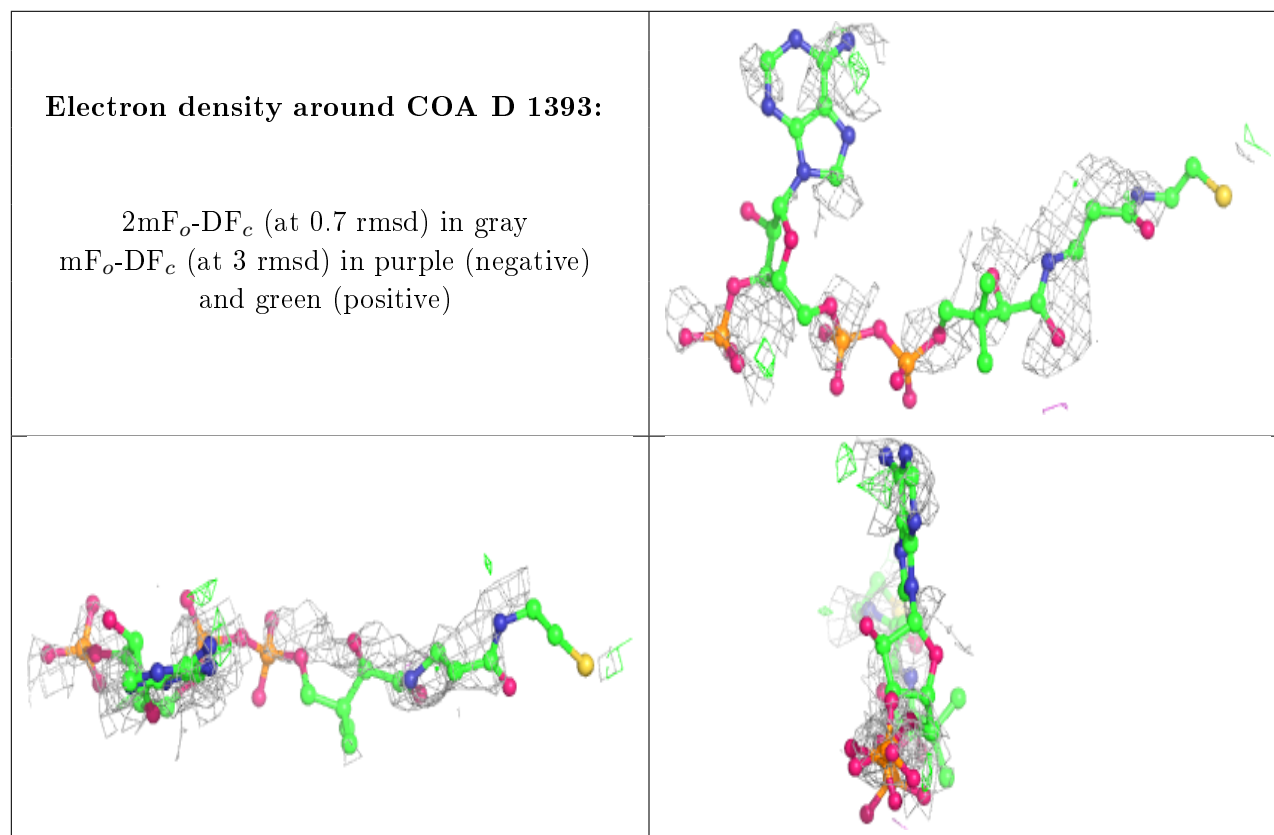
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	COA	D	1393	48/48	0.22	0.66	72,72,75,76	0
2	COA	C	1393	48/48	0.56	0.40	67,69,70,71	0
2	COA	B	1393	48/48	0.76	0.31	46,72,77,78	0
3	SO4	B	1396	5/5	0.77	0.46	86,86,87,87	0
3	SO4	A	1396	5/5	0.77	0.46	81,82,82,83	0
2	COA	A	1393	48/48	0.79	0.27	50,68,76,77	0
3	SO4	A	1395	5/5	0.81	0.39	67,67,68,69	0
3	SO4	B	1394	5/5	0.91	0.24	59,59,60,60	0

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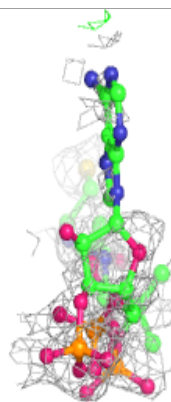
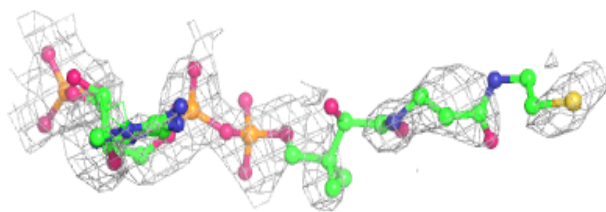
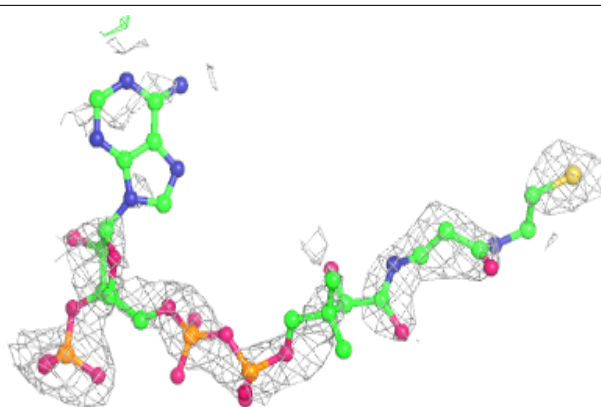
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	1394	5/5	0.96	0.17	44,44,45,46	0
3	SO4	B	1395	5/5	0.98	0.23	44,44,45,46	0

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.

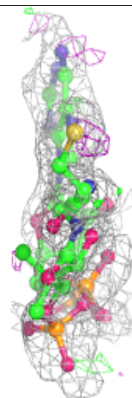
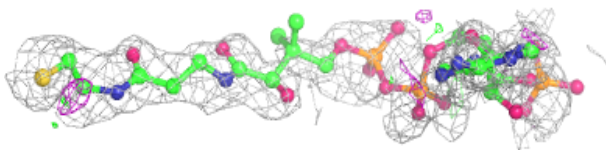
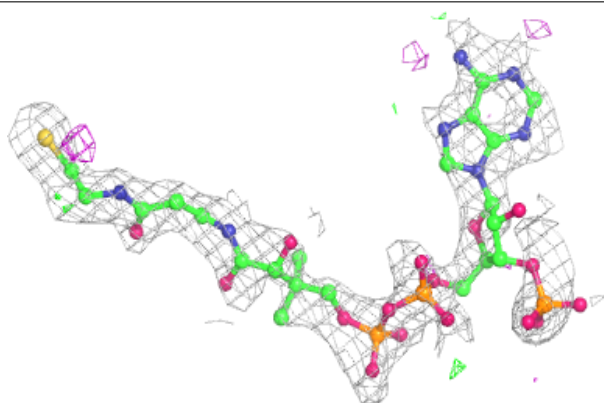


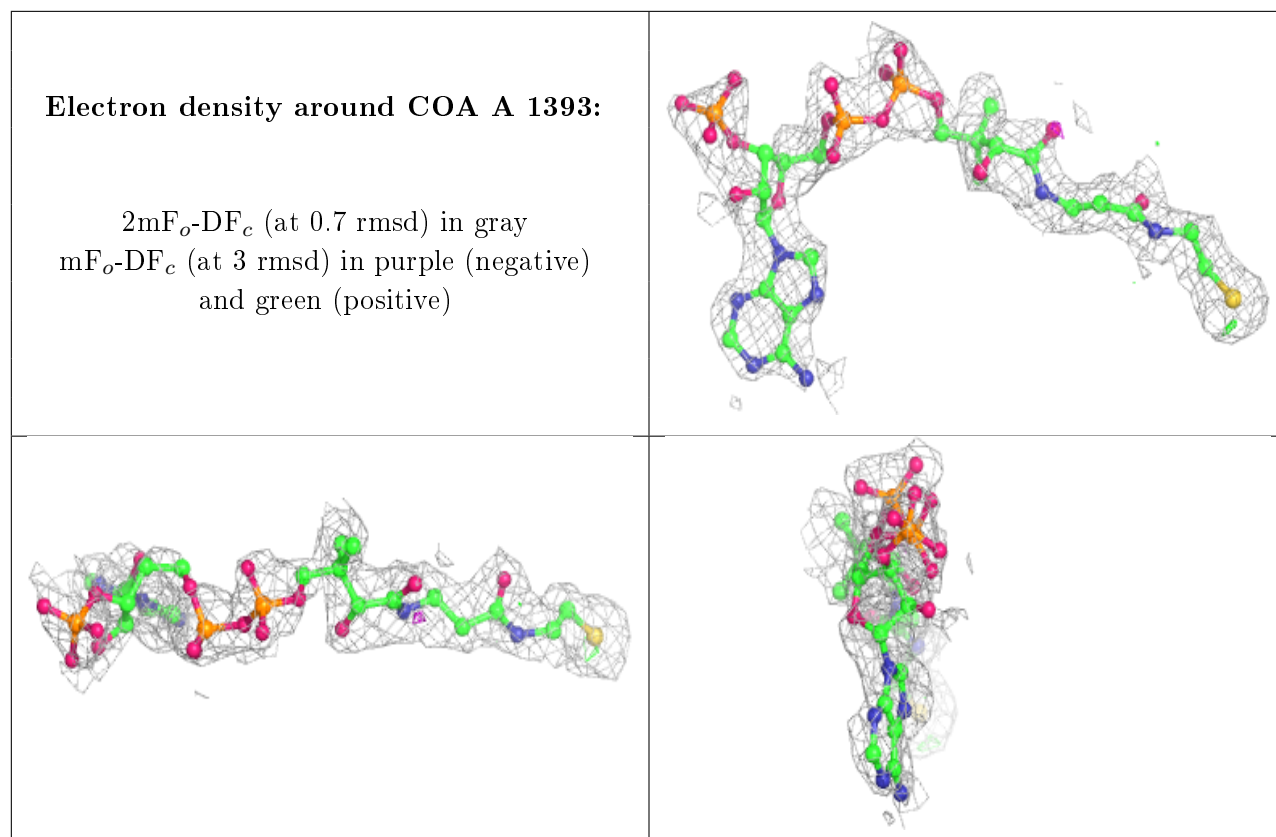
Electron density around COA C 1393:

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

**Electron density around COA B 1393:**

$2mF_o-DF_c$ (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.