Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 03:37 pm GMT

PDB ID	:	2WKT
Title	:	BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE N316A MUTANT WITH COENZYME A.
Authors	:	Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.
Deposited on	:	2009-06-18
Resolution	:	2.00 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*
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.

The following versions of software and data (see references ⓘ) were used in the production of this report:

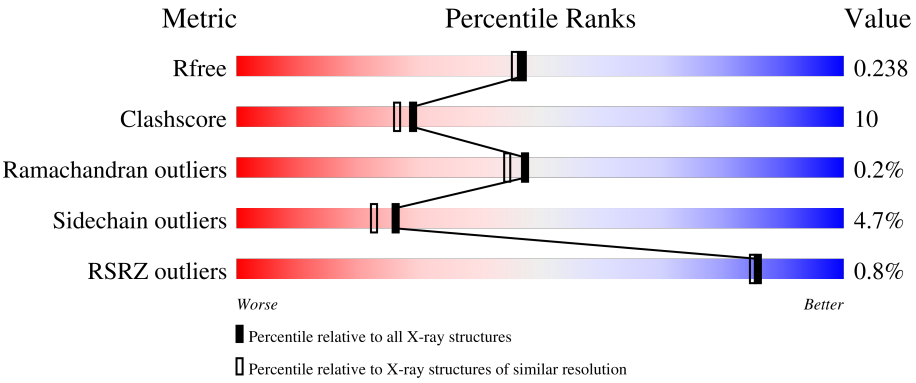
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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	84% 14%
1	B	392	87% 11%
1	D	392	77% 21%
2	C	392	77% 21%

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
5	CL	A	1396	-	-	X	X
6	COA	A	1397	X	-	-	-
6	COA	C	1394	X	-	-	-
6	COA	D	1395	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12882 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	390	Total	C	N	O	S	0	5	1
			2834	1760	508	545	21			
1	B	389	Total	C	N	O	S	0	6	0
			2841	1769	509	542	21			
1	D	389	Total	C	N	O	S	0	0	0
			2811	1745	508	537	21			

There are 6 discrepancies between the modelled and reference sequences:

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

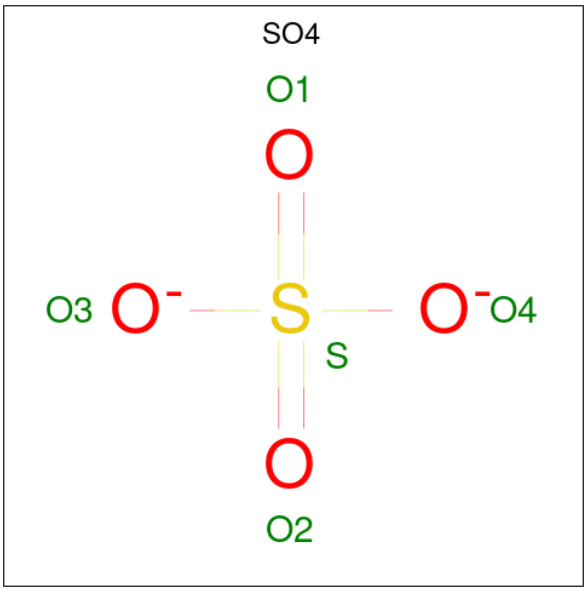
- Molecule 2 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	389	Total	C	N	O	S	0	1	0
			2813	1747	508	537	21			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	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
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

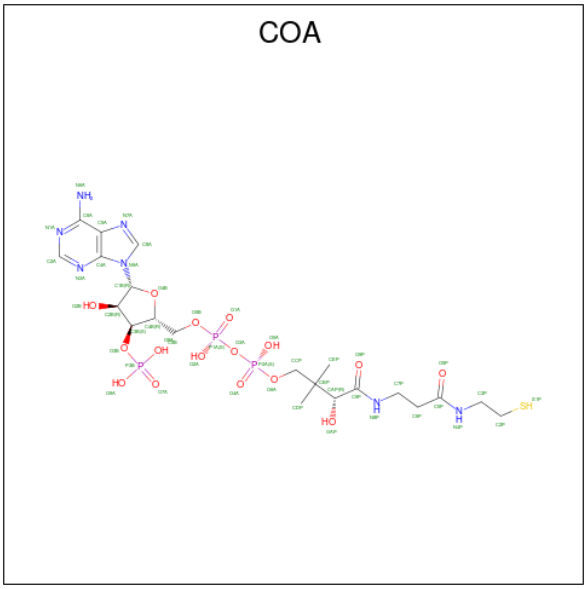
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Na 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	441	Total O 441 441	0	0

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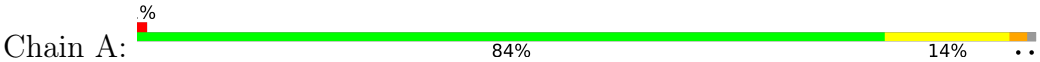
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	430	Total O 430 430	0	0
8	C	254	Total O 254 254	0	0
8	D	218	Total O 218 218	0	0

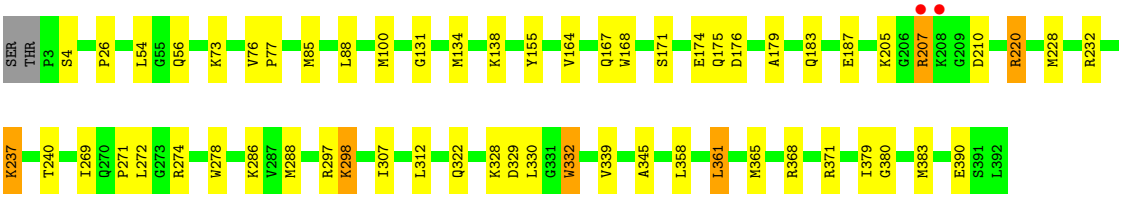
3 Residue-property plots (i)

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

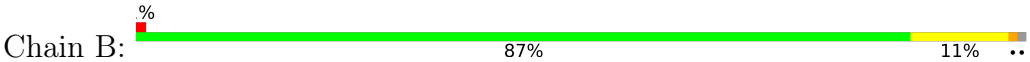
Chain A:

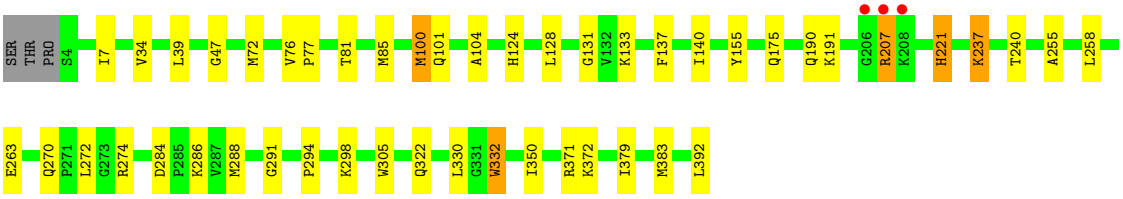




• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

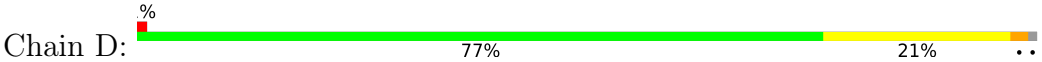
Chain B:

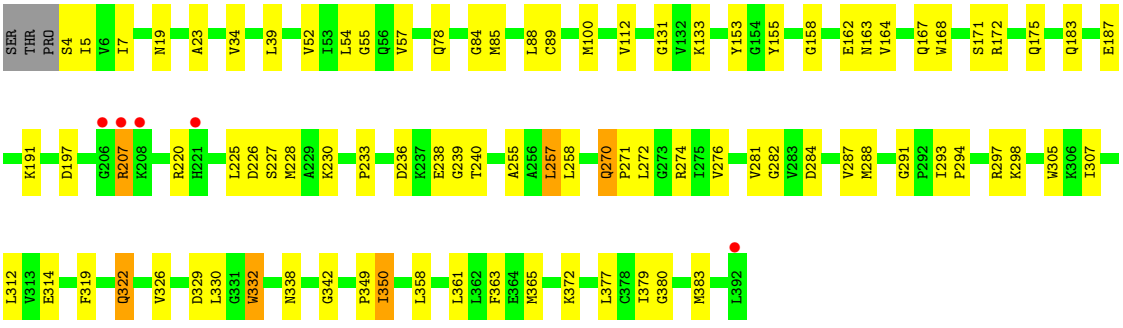




• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

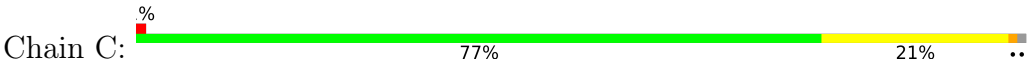
Chain D:

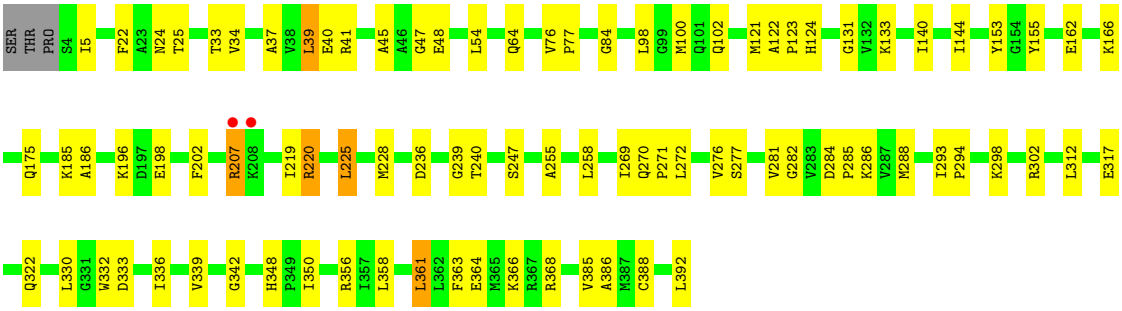




• Molecule 2: ACETYL-COA ACETYLTRANSFERASE

Chain C:




SER
THR
PRO
S4
I5
F22
A23
N24
T25
T33
V34
A37
V38
L39
E40
R41
A45
A46
G47
E48
L54
Q64
V76
P77
G84
L98
G99
M100
Q101
Q102
M121
A122
P123
H124
G131
V132
K133
I140
I144
Y153
G154
Y155
E162
K166
Q175
K185
A186
K196
D197
E198
F202
R207
K208
I219
R220
L225
M228
D236
G239
T240
S247
A255
L258
I269
Q270
P271
L272
V276
S277
V281
G282
V283
D284
P285
K286
V287
M288
I293
P294
K298
R302
L312
E317
Q322
L330
G331
W332
D333
I336
V339
G342
H348
P349
I350
R356
I357
L358
L361
L362
F363
E364
M365
K366
R367
R368
V385
A386
M387
C388
L392

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.60Å 79.20Å 148.70Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	19.63 – 2.00 19.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.63-2.00) 86.4 (19.63-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.187 , 0.236 0.188 , 0.238	Depositor DCC
R_{free} test set	6614 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12882	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K, SO4, NA, COA, CSO, CL

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	0.53	0/2882	0.65	1/3889 (0.0%)
1	B	0.54	0/2892	0.62	0/3902
1	D	0.34	0/2844	0.51	0/3838
2	C	0.36	0/2857	0.53	0/3857
All	All	0.45	0/11475	0.58	1/15486 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	361	LEU	CA-CB-CG	5.03	126.87	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	2834	0	2846	58	0
1	B	2841	0	2868	45	0
1	D	2811	0	2818	65	0
2	C	2813	0	2823	61	0
3	A	10	0	0	0	0
3	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	4	0
6	A	48	0	31	0	0
6	B	48	0	32	0	0
6	C	48	0	31	0	0
6	D	48	0	31	2	0
7	C	1	0	0	0	0
8	A	441	0	0	13	0
8	B	430	0	0	8	0
8	C	254	0	0	16	0
8	D	218	0	0	10	0
All	All	12882	0	11480	222	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 (222) 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:274:ARG:HH21	1:B:392:LEU:HD21	1.11	1.09
1:A:207:ARG:H	1:A:207:ARG:HD3	1.25	1.00
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.25	0.99
1:B:274:ARG:NH2	1:B:392:LEU:HD21	1.86	0.91
2:C:207:ARG:HD3	2:C:207:ARG:H	1.38	0.88
2:C:64:GLN:HB3	8:C:2064:HOH:O	1.73	0.88
1:D:287:VAL:HG12	8:D:2117:HOH:O	1.75	0.87
1:A:85:MET:N	5:A:1396:CL:CL	2.48	0.84
1:A:168:TRP:HZ3	1:A:329[B]:ASP:OD1	1.61	0.83
1:B:100:MET:HE1	1:B:101:GLN:HA	1.59	0.83
1:D:307:ILE:H	1:D:307:ILE:HD12	1.45	0.81
1:A:278:TRP:HD1	8:A:2348:HOH:O	1.66	0.78
1:A:207:ARG:HD3	1:A:207:ARG:N	1.99	0.77
1:A:85:MET:O	5:A:1396:CL:CL	2.40	0.76
1:B:305:TRP:CE2	1:B:372:LYS:HD3	2.21	0.76
2:C:366:LYS:HE3	8:C:2245:HOH:O	1.86	0.75
1:A:56:GLN:N	5:A:1396:CL:CL	2.57	0.75
1:B:207:ARG:HD3	1:B:207:ARG:H	1.51	0.73
1:D:172:ARG:HA	1:D:240:THR:HG23	1.68	0.73
1:D:207:ARG:HD3	1:D:207:ARG:H	1.53	0.73
1:A:168:TRP:CZ3	1:A:329[B]:ASP:OD1	2.40	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:HH2	1:A:329[B]:ASP:OD2	1.72	0.73
1:B:237:LYS:HD2	1:B:237:LYS:N	2.04	0.72
1:B:207:ARG:HG2	1:B:207:ARG:NH1	2.04	0.72
2:C:40:GLU:HB2	8:C:2038:HOH:O	1.89	0.72
1:A:274:ARG:NH1	1:A:390:GLU:OE1	2.24	0.70
2:C:312:LEU:HD23	2:C:361:LEU:HD22	1.74	0.70
1:B:100:MET:CE	1:B:104:ALA:HB2	2.23	0.68
2:C:277:SER:HB2	8:C:2198:HOH:O	1.92	0.68
1:A:339:VAL:HG11	1:A:368:ARG:NH2	2.08	0.67
1:D:342:GLY:HA3	8:D:2194:HOH:O	1.94	0.67
1:A:138:LYS:HG3	8:A:2200:HOH:O	1.95	0.67
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.06	0.67
1:D:167:GLN:HG2	8:D:2122:HOH:O	1.94	0.66
2:C:5:ILE:HG13	2:C:100:MET:HG2	1.78	0.66
1:A:164:VAL:O	1:A:168:TRP:HD1	1.79	0.65
1:A:134:MET:SD	8:D:2052:HOH:O	2.54	0.64
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.27	0.64
2:C:364:GLU:O	2:C:368:ARG:HG2	1.98	0.63
1:B:100:MET:HE2	1:B:104:ALA:HB2	1.79	0.62
2:C:270:GLN:HG2	8:C:2190:HOH:O	1.99	0.62
1:A:179:ALA:HB3	1:A:228:MET:CE	2.30	0.62
1:B:100:MET:CE	1:B:104:ALA:CB	2.77	0.62
1:B:100:MET:HE2	1:B:100:MET:O	2.00	0.61
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.65	0.61
1:D:291:GLY:O	1:D:294:PRO:HD2	2.01	0.61
1:A:176:ASP:HA	1:A:228:MET:HE1	1.82	0.60
1:D:171:SER:HB2	8:D:2127:HOH:O	1.99	0.60
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.15	0.60
1:D:227:SER:HB2	6:D:1395:COA:H2A	1.83	0.59
1:A:171:SER:OG	1:A:174[B]:GLU:HG3	2.03	0.59
1:D:175:GLN:NE2	1:D:240:THR:HG21	2.17	0.59
1:B:207:ARG:H	1:B:207:ARG:CD	2.11	0.58
1:D:284:ASP:HB3	1:D:287:VAL:HG22	1.84	0.58
8:B:2080:HOH:O	2:C:144:ILE:HG21	2.04	0.57
2:C:339:VAL:HG11	2:C:368:ARG:NH2	2.19	0.57
1:A:54:LEU:O	5:A:1396:CL:CL	2.60	0.56
1:B:47:GLY:HA2	1:B:77:PRO:HG3	1.87	0.56
1:A:164:VAL:O	1:A:168:TRP:CD1	2.58	0.56
2:C:34:VAL:HG12	2:C:255:ALA:HB3	1.87	0.56
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.36	0.56
1:B:133:LYS:HD2	8:C:2015:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:ALA:HB3	2:C:48:GLU:HG3	1.88	0.55
2:C:162:GLU:O	2:C:166:LYS:HG3	2.06	0.55
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.89	0.55
1:A:286:LYS:HE3	8:A:2354:HOH:O	2.06	0.55
1:A:207:ARG:H	1:A:207:ARG:CD	2.10	0.54
1:A:371:ARG:HG3	8:A:2420:HOH:O	2.07	0.54
1:D:314:GLU:HG2	1:D:361:LEU:HD23	1.89	0.54
2:C:175:GLN:HE22	2:C:240:THR:HG21	1.72	0.54
1:D:4:SER:N	1:D:274:ARG:HD2	2.22	0.54
2:C:247[A]:SER:OG	2:C:348:HIS:HB2	2.08	0.54
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.73	0.54
1:B:305:TRP:CZ2	1:B:372:LYS:HD3	2.42	0.54
1:A:176:ASP:HA	1:A:228:MET:CE	2.38	0.54
1:A:383:MET:SD	1:B:81:THR:HG22	2.48	0.53
1:B:207:ARG:HD3	1:B:207:ARG:N	2.23	0.53
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.43	0.53
1:D:183:GLN:OE1	1:D:220:ARG:HG2	2.09	0.52
1:A:179:ALA:HB3	1:A:228:MET:HE2	1.90	0.52
1:A:26:PRO:HG3	8:A:2011:HOH:O	2.10	0.51
1:D:271:PRO:HG2	8:D:2074:HOH:O	2.11	0.51
1:D:54:LEU:O	1:D:84:GLY:HA2	2.11	0.51
2:C:185:LYS:NZ	8:C:2142:HOH:O	2.43	0.51
1:A:307:ILE:HG13	8:A:2376:HOH:O	2.11	0.51
1:D:187:GLU:O	1:D:191:LYS:HG3	2.10	0.51
2:C:45:ALA:O	2:C:48:GLU:HG3	2.12	0.50
2:C:133:LYS:HG2	8:C:2112:HOH:O	2.12	0.49
2:C:124:HIS:HA	2:C:140:ILE:O	2.11	0.49
1:A:297:ARG:NE	8:A:2357:HOH:O	2.45	0.49
1:A:88:LEU:HD12	1:A:380:GLY:O	2.12	0.49
1:A:187:GLU:HG3	8:A:2296:HOH:O	2.12	0.49
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.48	0.48
1:B:190:GLN:OE1	1:B:221:HIS:HE1	1.96	0.48
2:C:271:PRO:HD2	2:C:392:LEU:HD12	1.95	0.48
2:C:228:MET:HE2	8:C:2174:HOH:O	2.13	0.48
8:A:2020:HOH:O	1:D:133:LYS:HE2	2.14	0.48
8:C:2064:HOH:O	1:D:88:LEU:HD11	2.14	0.48
2:C:48:GLU:HA	8:C:2045:HOH:O	2.13	0.47
2:C:186:ALA:HB1	2:C:219:ILE:HD13	1.95	0.47
1:A:383:MET:HG2	1:B:81:THR:HG22	1.96	0.47
1:D:168:TRP:HH2	1:D:329:ASP:OD1	1.98	0.47
1:D:307:ILE:H	1:D:307:ILE:CD1	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ILE:HD12	1:D:307:ILE:N	2.23	0.47
1:A:168:TRP:CH2	1:A:329[B]:ASP:CG	2.87	0.47
2:C:281:VAL:HG22	8:C:2199:HOH:O	2.13	0.47
1:D:207:ARG:H	1:D:207:ARG:CD	2.20	0.47
1:B:291:GLY:O	1:B:294:PRO:HD2	2.15	0.47
1:D:338:ASN:ND2	8:D:2194:HOH:O	2.46	0.47
1:D:197:ASP:HB3	1:D:363:PHE:CD2	2.49	0.47
1:B:207:ARG:NH1	1:B:207:ARG:CG	2.71	0.47
1:D:314:GLU:HG3	1:D:361:LEU:HB2	1.97	0.47
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.50	0.47
1:A:167:GLN:NE2	8:A:2225:HOH:O	2.48	0.46
1:A:168:TRP:CH2	1:A:329[B]:ASP:OD2	2.59	0.46
1:B:124:HIS:HA	1:B:140:ILE:O	2.16	0.46
2:C:333:ASP:O	2:C:336:ILE:HG12	2.15	0.46
1:D:226:ASP:O	1:D:230:LYS:HG3	2.15	0.46
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.96	0.46
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.51	0.46
1:D:233:PRO:HB2	1:D:236:ASP:O	2.16	0.46
1:D:281:VAL:HG12	1:D:282:GLY:N	2.30	0.46
2:C:47:GLY:HA2	2:C:77:PRO:HG2	1.98	0.46
2:C:196:LYS:HE2	2:C:196:LYS:HB3	1.57	0.46
1:B:100:MET:HE3	1:B:104:ALA:CB	2.46	0.46
1:B:100:MET:HE3	1:B:104:ALA:HB2	1.97	0.45
1:D:89:CSO:O	1:D:377:LEU:HD22	2.16	0.45
1:A:179:ALA:HB3	1:A:228:MET:HE1	1.97	0.45
1:A:328:LYS:HE3	1:A:328:LYS:HB2	1.57	0.45
2:C:207:ARG:H	2:C:207:ARG:CD	2.11	0.45
2:C:302:ARG:HD3	8:C:2198:HOH:O	2.15	0.45
1:D:55:GLY:HA2	1:D:85:MET:O	2.17	0.45
1:B:34:VAL:HG12	1:B:255:ALA:HB3	1.97	0.45
2:C:236:ASP:HB3	2:C:239:GLY:HA3	1.98	0.45
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.47	0.45
2:C:33:THR:HG1	2:C:202:PHE:HD1	1.63	0.45
1:B:7:ILE:HG12	1:B:258[A]:LEU:CD1	2.46	0.45
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.81	0.45
2:C:247[A]:SER:OG	2:C:348:HIS:CB	2.64	0.45
2:C:356:ARG:HD2	2:C:356:ARG:O	2.16	0.45
1:D:88:LEU:HD12	1:D:380:GLY:O	2.17	0.45
1:D:228:MET:HB2	1:D:228:MET:HE2	1.84	0.45
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.30	0.45
1:B:274:ARG:CZ	8:B:2325:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:LEU:HD12	2:C:225:LEU:HA	1.79	0.45
1:D:379:ILE:HB	1:D:383:MET:HB2	1.99	0.45
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.99	0.45
1:D:307:ILE:CG2	1:D:332:TRP:HB3	2.47	0.45
1:A:183:GLN:HA	1:A:345:ALA:HB2	1.99	0.44
1:D:153:TYR:HB3	1:D:155:TYR:CE2	2.53	0.44
8:B:2081:HOH:O	2:C:144:ILE:HG13	2.16	0.44
2:C:175:GLN:HE22	2:C:240:THR:CG2	2.31	0.44
1:A:205:LYS:HD3	1:A:210:ASP:OD2	2.17	0.44
1:B:191[A]:LYS:HB2	8:B:2239:HOH:O	2.16	0.44
1:B:379:ILE:HB	1:B:383:MET:HB2	1.99	0.44
1:A:383:MET:CG	1:B:81:THR:HG22	2.48	0.44
2:C:317:GLU:CD	2:C:342:GLY:HA3	2.37	0.44
1:B:284:ASP:OD1	1:B:286:LYS:HG3	2.17	0.44
2:C:293:ILE:HB	2:C:294:PRO:CD	2.47	0.44
1:B:207:ARG:NH1	8:B:2265:HOH:O	2.49	0.44
1:D:88:LEU:HB2	1:D:379:ILE:HG23	1.99	0.44
1:B:72:MET:HE3	8:B:2046:HOH:O	2.18	0.43
2:C:162:GLU:OE1	2:C:240:THR:HG22	2.18	0.43
1:D:163:ASN:HB3	8:D:2117:HOH:O	2.17	0.43
2:C:98:LEU:O	2:C:102:GLN:HG2	2.19	0.43
1:A:100:MET:HE2	8:A:2348:HOH:O	2.18	0.43
2:C:282:GLY:HA3	1:D:78:GLN:O	2.18	0.43
1:D:258:LEU:HD22	1:D:258:LEU:N	2.33	0.43
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.67	0.43
1:D:322:GLN:O	1:D:326:VAL:HG23	2.18	0.43
2:C:220:ARG:NH1	8:C:2170:HOH:O	2.52	0.43
1:B:274:ARG:HH21	1:B:392:LEU:CD2	2.03	0.43
1:A:269:ILE:O	1:A:271:PRO:HD3	2.20	0.42
2:C:153:TYR:CE2	2:C:286:LYS:HD3	2.54	0.42
2:C:202:PHE:HA	8:C:2157:HOH:O	2.19	0.42
1:D:312:LEU:HD23	1:D:365:MET:HG3	2.00	0.42
1:A:176:ASP:CB	1:A:228:MET:HE3	2.50	0.42
1:A:232:ARG:HG2	8:A:2312:HOH:O	2.19	0.42
1:B:131:GLY:HA2	1:D:131:GLY:HA2	2.01	0.42
2:C:122:ALA:HA	2:C:123:PRO:HD3	1.89	0.42
1:A:274:ARG:HH12	1:A:390:GLU:CD	2.22	0.42
2:C:220:ARG:HD2	8:C:2169:HOH:O	2.19	0.42
1:A:76:VAL:HG13	1:A:77:PRO:HD2	2.00	0.42
1:A:339:VAL:HG11	1:A:368:ARG:HH21	1.82	0.42
2:C:24:ASN:HA	2:C:121:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:VAL:HG23	8:D:2117:HOH:O	2.18	0.42
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.86	0.42
1:A:88:LEU:HB2	1:A:379:ILE:HG23	2.01	0.42
2:C:198:GLU:HB3	2:C:363:PHE:CD2	2.55	0.42
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.54	0.42
1:B:274:ARG:NH1	8:B:2326:HOH:O	2.52	0.42
2:C:22:PHE:HB3	2:C:25:THR:HB	2.02	0.42
2:C:207:ARG:HD3	2:C:207:ARG:N	2.20	0.42
2:C:269:ILE:O	2:C:271:PRO:HD3	2.18	0.42
2:C:54:LEU:O	2:C:84:GLY:HA2	2.19	0.42
1:D:19:ASN:C	1:D:23:ALA:HB2	2.40	0.42
2:C:76:VAL:HA	2:C:77:PRO:HD3	1.83	0.41
1:A:220:ARG:H	1:A:220:ARG:HG2	1.70	0.41
1:A:168:TRP:CD1	1:A:168:TRP:N	2.88	0.41
1:D:164:VAL:N	8:D:2117:HOH:O	2.52	0.41
1:B:371:ARG:NH1	8:B:2358:HOH:O	2.54	0.41
2:C:284:ASP:OD1	2:C:285:PRO:HD2	2.21	0.41
1:A:298:LYS:NZ	8:A:2360:HOH:O	2.54	0.41
1:D:293:ILE:O	1:D:297:ARG:HG3	2.21	0.41
1:D:158:GLY:HA2	1:D:319:PHE:CE2	2.56	0.41
1:D:257:LEU:HD23	1:D:258:LEU:N	2.36	0.41
1:D:326:VAL:HG12	1:D:330:LEU:HD12	2.02	0.41
1:A:131:GLY:HA2	2:C:131:GLY:HA2	2.03	0.41
2:C:385:VAL:HG22	2:C:386:ALA:N	2.34	0.41
1:D:227:SER:HB2	6:D:1395:COA:C2A	2.50	0.41
1:D:270:GLN:HA	1:D:271:PRO:HD3	1.83	0.41
1:D:349:PRO:O	1:D:350:ILE:C	2.60	0.41
1:A:85:MET:HA	1:B:85:MET:HA	2.02	0.40
2:C:356:ARG:HD2	2:C:356:ARG:C	2.42	0.40
1:D:162:GLU:OE2	1:D:239:GLY:HA3	2.22	0.40
1:A:312:LEU:HD23	1:A:365:MET:HG3	2.03	0.40
1:B:128:LEU:HD21	1:B:137:PHE:CE2	2.56	0.40
2:C:39:LEU:HD12	2:C:39:LEU:HA	1.94	0.40
2:C:276:VAL:HG22	2:C:388:CYS:O	2.22	0.40
1:B:76:VAL:HA	1:B:77:PRO:HD3	1.89	0.40
2:C:37:ALA:O	2:C:41:ARG:HG3	2.21	0.40
1:D:52:VAL:HA	1:D:112:VAL:O	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	392/392 (100%)	381 (97%)	11 (3%)	0	100	100
1	B	392/392 (100%)	378 (96%)	13 (3%)	1 (0%)	41	37
1	D	386/392 (98%)	366 (95%)	19 (5%)	1 (0%)	41	37
2	C	388/392 (99%)	373 (96%)	14 (4%)	1 (0%)	41	37
All	All	1558/1568 (99%)	1498 (96%)	57 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	350	ILE
1	B	350	ILE
2	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	279/277 (101%)	267 (96%)	12 (4%)	29	26
1	B	280/277 (101%)	267 (95%)	13 (5%)	27	23
1	D	274/277 (99%)	261 (95%)	13 (5%)	26	22
2	C	276/278 (99%)	262 (95%)	14 (5%)	24	19
All	All	1109/1109 (100%)	1057 (95%)	52 (5%)	26	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	155	TYR
1	A	207	ARG
1	A	220	ARG
1	A	237	LYS
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	100	MET
1	B	155	TYR
1	B	207	ARG
1	B	221	HIS
1	B	237	LYS
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
2	C	39	LEU
2	C	155	TYR
2	C	207	ARG
2	C	220	ARG
2	C	225	LEU
2	C	258	LEU
2	C	272	LEU
2	C	288	MET
2	C	298	LYS
2	C	322	GLN
2	C	330	LEU
2	C	332	TRP
2	C	358	LEU
2	C	361	LEU
1	D	39	LEU
1	D	207	ARG
1	D	225	LEU
1	D	238	GLU

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Mol	Chain	Res	Type
1	D	257	LEU
1	D	270	GLN
1	D	272	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	A	89	1	3,6,7	0.43	0	0,6,8	-	-
1	CSO	D	89	1	3,6,7	0.65	0	0,6,8	-	-
1	CSO	B	89	1	3,6,7	0.43	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	89	1	-	1/1/5/7	-
1	CSO	D	89	1	-	1/1/5/7	-
1	CSO	B	89	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89	CSO	N-CA-CB-SG
1	D	89	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	89	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
3	SO4	B	1394	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	A	1393	-	4,4,4	0.19	0	6,6,6	0.19	0
6	COA	C	1394	-	41,50,50	2.42	15 (36%)	52,75,75	1.75	13 (25%)
3	SO4	B	1396	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	B	1395	-	4,4,4	0.13	0	6,6,6	0.07	0
6	COA	A	1397	-	41,50,50	2.32	14 (34%)	52,75,75	1.55	10 (19%)
6	COA	D	1395	-	41,50,50	2.45	13 (31%)	52,75,75	1.66	11 (21%)
3	SO4	B	1393	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	B	1397	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	D	1393	-	4,4,4	0.15	0	6,6,6	0.05	0
6	COA	B	1398	-	41,50,50	2.50	18 (43%)	52,75,75	1.59	9 (17%)
3	SO4	A	1394	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	D	1394	-	4,4,4	0.14	0	6,6,6	0.06	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
6	COA	B	1398	-	-	14/44/64/64	0/3/3/3
6	COA	C	1394	-	1/1/11/13	10/44/64/64	0/3/3/3
6	COA	D	1395	-	2/2/11/13	12/44/64/64	0/3/3/3
6	COA	A	1397	-	2/2/11/13	6/44/64/64	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1398	COA	C9P-N8P	6.32	1.47	1.33
6	C	1394	COA	C9P-N8P	6.03	1.46	1.33
6	A	1397	COA	C9P-N8P	5.97	1.46	1.33
6	D	1395	COA	C9P-N8P	5.88	1.46	1.33
6	D	1395	COA	C5P-N4P	5.62	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1394	COA	C5P-N4P	5.34	1.45	1.33
6	A	1397	COA	C5P-N4P	5.31	1.45	1.33
6	B	1398	COA	C5P-N4P	5.20	1.45	1.33
6	C	1394	COA	O4B-C1B	4.87	1.47	1.41
6	B	1398	COA	O4B-C1B	4.76	1.47	1.41
6	B	1398	COA	P3B-O7A	4.71	1.65	1.50
6	D	1395	COA	O4B-C1B	4.71	1.47	1.41
6	C	1394	COA	P3B-O7A	4.70	1.65	1.50
6	A	1397	COA	P3B-O7A	4.68	1.65	1.50
6	D	1395	COA	P3B-O7A	4.65	1.65	1.50
6	C	1394	COA	C8A-N7A	4.31	1.42	1.34
6	B	1398	COA	C8A-N7A	4.31	1.42	1.34
6	D	1395	COA	C8A-N7A	4.17	1.42	1.34
6	B	1398	COA	P2A-O4A	4.10	1.65	1.50
6	D	1395	COA	P2A-O4A	4.08	1.65	1.50
6	C	1394	COA	P1A-O1A	4.05	1.65	1.50
6	D	1395	COA	P1A-O1A	4.00	1.65	1.50
6	A	1397	COA	C2A-N3A	3.97	1.38	1.32
6	D	1395	COA	C2A-N3A	3.96	1.38	1.32
6	B	1398	COA	P1A-O1A	3.94	1.64	1.50
6	A	1397	COA	P1A-O1A	3.93	1.64	1.50
6	A	1397	COA	C8A-N7A	3.90	1.41	1.34
6	C	1394	COA	C2A-N3A	3.74	1.38	1.32
6	A	1397	COA	O4B-C1B	3.72	1.46	1.41
6	B	1398	COA	C2A-N3A	3.63	1.37	1.32
6	B	1398	COA	C2B-C1B	-3.33	1.48	1.53
6	B	1398	COA	C6A-N6A	3.13	1.45	1.34
6	A	1397	COA	C5A-C4A	-3.10	1.32	1.40
6	D	1395	COA	C6A-N6A	3.06	1.45	1.34
6	C	1394	COA	C6A-N6A	3.03	1.45	1.34
6	A	1397	COA	C2B-C1B	-3.03	1.49	1.53
6	A	1397	COA	C6A-N6A	2.97	1.44	1.34
6	D	1395	COA	P3B-O3B	2.87	1.64	1.59
6	C	1394	COA	C5A-C4A	-2.82	1.33	1.40
6	D	1395	COA	C5A-C4A	-2.81	1.33	1.40
6	C	1394	COA	P3B-O8A	2.72	1.65	1.54
6	C	1394	COA	P3B-O3B	2.71	1.64	1.59
6	B	1398	COA	P3B-O8A	2.66	1.65	1.54
6	D	1395	COA	C2B-C1B	-2.66	1.49	1.53
6	D	1395	COA	P3B-O8A	2.66	1.65	1.54
6	C	1394	COA	C2B-C1B	-2.65	1.49	1.53
6	A	1397	COA	P3B-O8A	2.57	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1397	COA	P3B-O3B	2.51	1.64	1.59
6	C	1394	COA	O5P-C5P	-2.45	1.18	1.23
6	B	1398	COA	C2B-C3B	-2.38	1.47	1.52
6	A	1397	COA	O5P-C5P	-2.36	1.18	1.23
6	B	1398	COA	P3B-O3B	2.29	1.63	1.59
6	B	1398	COA	O9P-C9P	-2.27	1.18	1.23
6	C	1394	COA	P2A-O5A	2.26	1.65	1.55
6	B	1398	COA	C5A-C4A	-2.23	1.35	1.40
6	C	1394	COA	O4B-C4B	2.22	1.50	1.45
6	B	1398	COA	O4B-C4B	2.17	1.49	1.45
6	B	1398	COA	O5P-C5P	-2.13	1.18	1.23
6	A	1397	COA	C2B-C3B	-2.08	1.48	1.52
6	B	1398	COA	P1A-O5B	2.07	1.67	1.59

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1394	COA	N3A-C2A-N1A	-5.78	119.65	128.68
6	B	1398	COA	N3A-C2A-N1A	-5.70	119.76	128.68
6	A	1397	COA	N3A-C2A-N1A	-5.55	120.00	128.68
6	D	1395	COA	N3A-C2A-N1A	-5.53	120.03	128.68
6	D	1395	COA	P2A-O3A-P1A	-3.90	119.46	132.83
6	B	1398	COA	O2B-C2B-C3B	3.63	121.48	111.17
6	C	1394	COA	P2A-O3A-P1A	-3.41	121.11	132.83
6	C	1394	COA	O3B-C3B-C4B	3.39	122.32	110.08
6	B	1398	COA	O3B-C3B-C4B	3.37	122.27	110.08
6	C	1394	COA	O4B-C4B-C5B	3.35	120.41	109.37
6	D	1395	COA	O3B-C3B-C4B	3.32	122.09	110.08
6	A	1397	COA	P2A-O3A-P1A	-3.28	121.55	132.83
6	B	1398	COA	O2B-C2B-C1B	3.18	122.60	110.85
6	C	1394	COA	C3B-C2B-C1B	3.11	106.77	99.89
6	D	1395	COA	O5B-C5B-C4B	2.97	119.20	108.99
6	A	1397	COA	C2P-C3P-N4P	2.86	118.85	112.31
6	B	1398	COA	C2P-C3P-N4P	2.82	118.75	112.31
6	C	1394	COA	O5B-C5B-C4B	2.80	118.61	108.99
6	A	1397	COA	O2B-C2B-C3B	2.75	118.97	111.17
6	C	1394	COA	O2B-C2B-C3B	2.73	118.92	111.17
6	C	1394	COA	C3P-N4P-C5P	-2.68	117.86	122.84
6	B	1398	COA	C7P-N8P-C9P	-2.59	117.97	122.59
6	D	1395	COA	O2B-C2B-C3B	2.58	118.50	111.17
6	A	1397	COA	O2B-C2B-C1B	2.57	120.34	110.85
6	D	1395	COA	C3P-N4P-C5P	-2.57	118.07	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1397	COA	O3B-C3B-C4B	2.54	119.28	110.08
6	C	1394	COA	O2B-C2B-C1B	2.52	120.16	110.85
6	B	1398	COA	O4B-C4B-C5B	2.48	117.55	109.37
6	B	1398	COA	P2A-O3A-P1A	-2.44	124.44	132.83
6	D	1395	COA	O4B-C4B-C5B	2.44	117.39	109.37
6	A	1397	COA	O6A-CCP-CBP	2.37	114.36	110.55
6	C	1394	COA	C6P-C5P-N4P	2.33	120.35	116.42
6	C	1394	COA	O6A-CCP-CBP	2.30	114.25	110.55
6	D	1395	COA	C5B-C4B-C3B	2.27	121.92	114.40
6	C	1394	COA	C6P-C7P-N8P	2.26	116.46	111.90
6	A	1397	COA	C3B-C2B-C1B	2.20	104.77	99.89
6	A	1397	COA	C7P-C6P-C5P	2.16	115.96	112.36
6	C	1394	COA	C2P-C3P-N4P	2.12	117.14	112.31
6	D	1395	COA	O6A-CCP-CBP	2.09	113.91	110.55
6	B	1398	COA	C3B-C2B-C1B	2.09	104.53	99.89
6	D	1395	COA	C3B-C2B-C1B	2.09	104.51	99.89
6	D	1395	COA	O2B-C2B-C1B	2.09	118.56	110.85
6	A	1397	COA	OAP-CAP-CBP	2.01	114.98	110.25

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1397	COA	C2B
6	A	1397	COA	C1B
6	C	1394	COA	C2B
6	D	1395	COA	C2B
6	D	1395	COA	C3B

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1397	COA	C5B-O5B-P1A-O1A
6	A	1397	COA	CAP-CBP-CCP-O6A
6	A	1397	COA	C2P-C3P-N4P-C5P
6	B	1398	COA	C5B-O5B-P1A-O1A
6	B	1398	COA	CCP-O6A-P2A-O4A
6	B	1398	COA	C2P-C3P-N4P-C5P
6	C	1394	COA	C5B-O5B-P1A-O2A
6	C	1394	COA	C5B-O5B-P1A-O3A
6	C	1394	COA	CAP-CBP-CCP-O6A
6	C	1394	COA	C2P-C3P-N4P-C5P
6	D	1395	COA	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
6	D	1395	COA	CAP-CBP-CCP-O6A
6	D	1395	COA	N8P-C9P-CAP-OAP
6	D	1395	COA	C2P-C3P-N4P-C5P
6	B	1398	COA	C3B-C4B-C5B-O5B
6	B	1398	COA	O4B-C4B-C5B-O5B
6	C	1394	COA	C3B-C4B-C5B-O5B
6	C	1394	COA	O4B-C4B-C5B-O5B
6	D	1395	COA	C3B-C4B-C5B-O5B
6	D	1395	COA	O4B-C4B-C5B-O5B
6	B	1398	COA	C4B-C3B-O3B-P3B
6	A	1397	COA	CEP-CBP-CCP-O6A
6	A	1397	COA	CDP-CBP-CCP-O6A
6	C	1394	COA	CEP-CBP-CCP-O6A
6	D	1395	COA	CDP-CBP-CCP-O6A
6	D	1395	COA	CEP-CBP-CCP-O6A
6	C	1394	COA	C4B-C5B-O5B-P1A
6	B	1398	COA	P2A-O3A-P1A-O5B
6	C	1394	COA	P2A-O3A-P1A-O5B
6	C	1394	COA	CDP-CBP-CCP-O6A
6	B	1398	COA	C5B-O5B-P1A-O3A
6	B	1398	COA	CCP-O6A-P2A-O3A
6	D	1395	COA	CCP-O6A-P2A-O3A
6	A	1397	COA	P1A-O3A-P2A-O4A
6	B	1398	COA	C5B-O5B-P1A-O2A
6	B	1398	COA	CCP-O6A-P2A-O5A
6	D	1395	COA	CCP-O6A-P2A-O5A
6	B	1398	COA	CAP-CBP-CCP-O6A
6	B	1398	COA	CEP-CBP-CCP-O6A
6	B	1398	COA	CDP-CBP-CCP-O6A
6	D	1395	COA	C2B-C3B-O3B-P3B
6	D	1395	COA	P2A-O3A-P1A-O2A

There are no ring outliers.

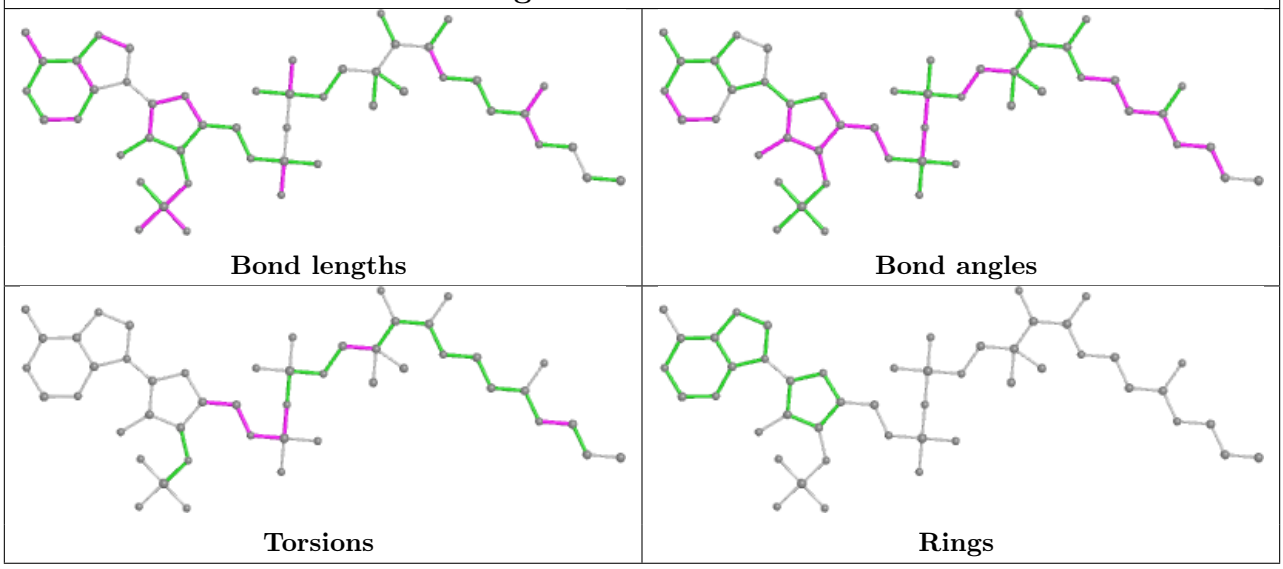
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1395	COA	2	0

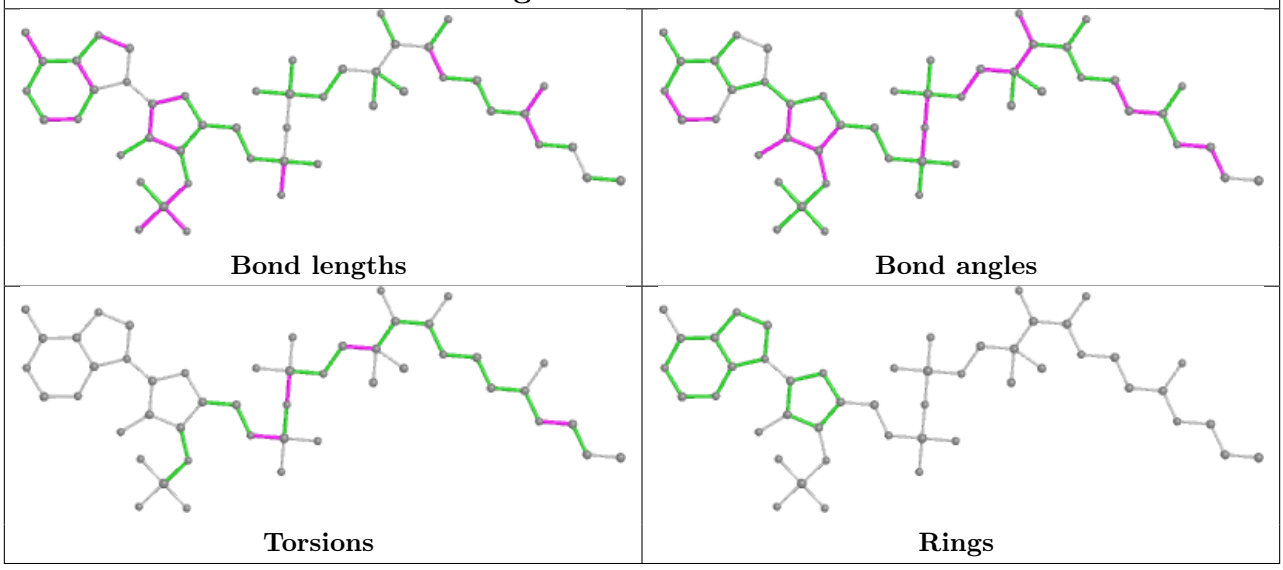
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

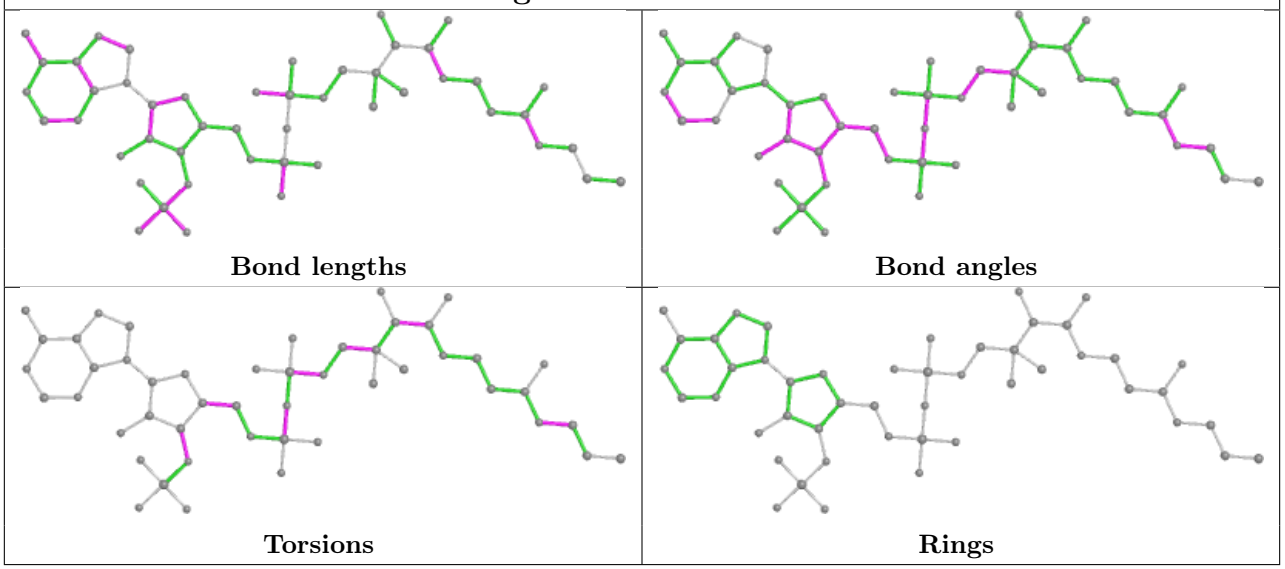
Ligand COA C 1394



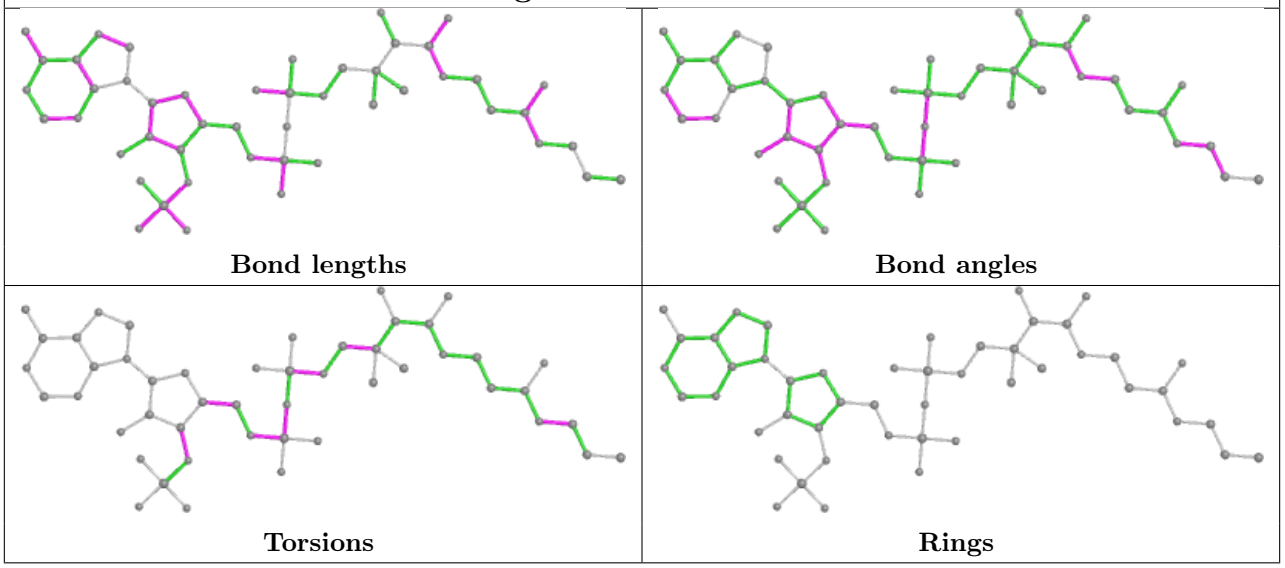
Ligand COA A 1397



Ligand COA D 1395



Ligand COA B 1398



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^{th} 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%)	-0.81	2 (0%)	91	90	3, 10, 30, 82	0
1	B	388/392 (98%)	-0.80	3 (0%)	86	85	2, 10, 28, 82	0
1	D	388/392 (98%)	-0.20	5 (1%)	77	76	15, 32, 64, 98	0
2	C	389/392 (99%)	-0.47	2 (0%)	91	90	13, 26, 45, 87	0
All	All	1554/1568 (99%)	-0.57	12 (0%)	86	85	2, 21, 48, 98	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	206	GLY	6.6
1	B	208	LYS	3.9
2	C	208	LYS	3.9
1	D	207	ARG	3.7
1	D	392	LEU	3.5
2	C	207	ARG	3.2
1	A	208	LYS	3.0
1	A	207	ARG	2.9
1	B	206	GLY	2.8
1	D	221	HIS	2.7
1	B	207	ARG	2.5
1	D	208	LYS	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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^2)	Q<0.9
1	CSO	A	89	7/8	0.95	0.08	4,9,18,31	0
1	CSO	B	89	7/8	0.96	0.07	1,6,16,34	0
1	CSO	D	89	7/8	0.96	0.09	23,28,41,59	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

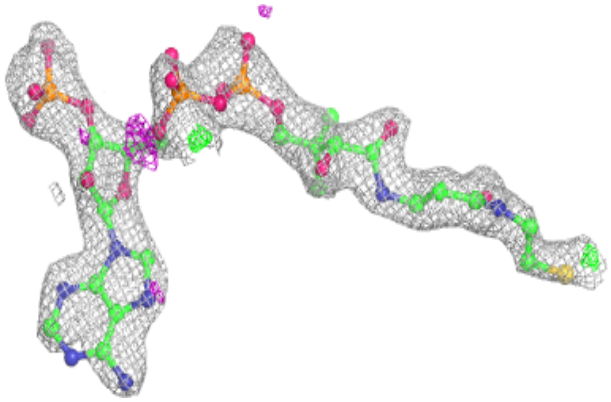
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

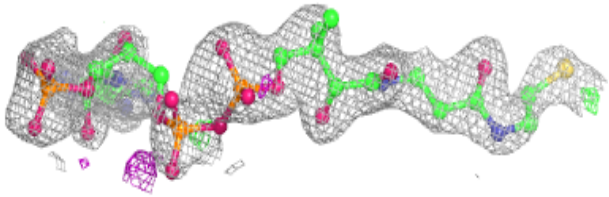
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NA	C	1393	1/1	0.56	0.38	55,55,55,55	0
3	SO4	B	1397	5/5	0.61	0.32	93,97,97,98	0
5	CL	A	1396	1/1	0.69	1.24	107,107,107,107	0
3	SO4	B	1396	5/5	0.73	0.29	153,153,154,154	0
3	SO4	D	1394	5/5	0.81	0.22	116,116,117,118	0
3	SO4	B	1395	5/5	0.88	0.20	90,91,94,95	0
3	SO4	A	1394	5/5	0.90	0.11	61,65,69,71	0
6	COA	D	1395	48/48	0.90	0.14	23,63,106,141	0
4	K	A	1395	1/1	0.90	0.11	43,43,43,43	0
6	COA	C	1394	48/48	0.92	0.11	28,45,74,101	0
6	COA	A	1397	48/48	0.94	0.10	10,25,50,103	0
6	COA	B	1398	48/48	0.96	0.08	8,22,66,84	0
3	SO4	D	1393	5/5	0.96	0.10	77,78,79,81	0
3	SO4	A	1393	5/5	0.97	0.12	43,48,52,53	0
3	SO4	B	1393	5/5	0.98	0.10	30,39,41,47	0
3	SO4	B	1394	5/5	0.99	0.08	38,38,41,41	0

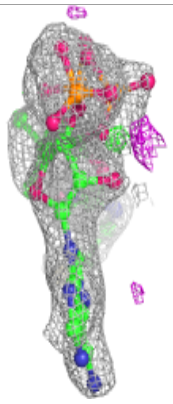
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

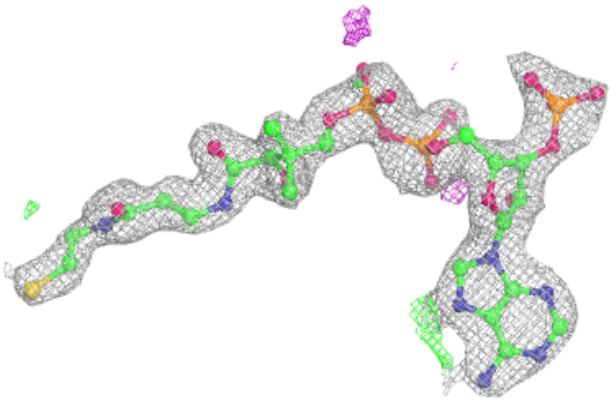


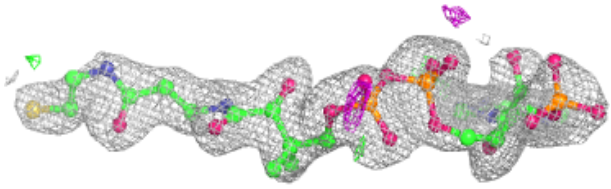


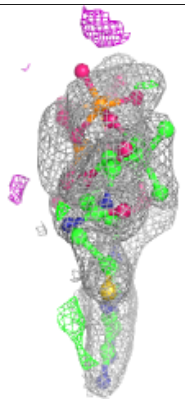


Electron density around COA C 1394:

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

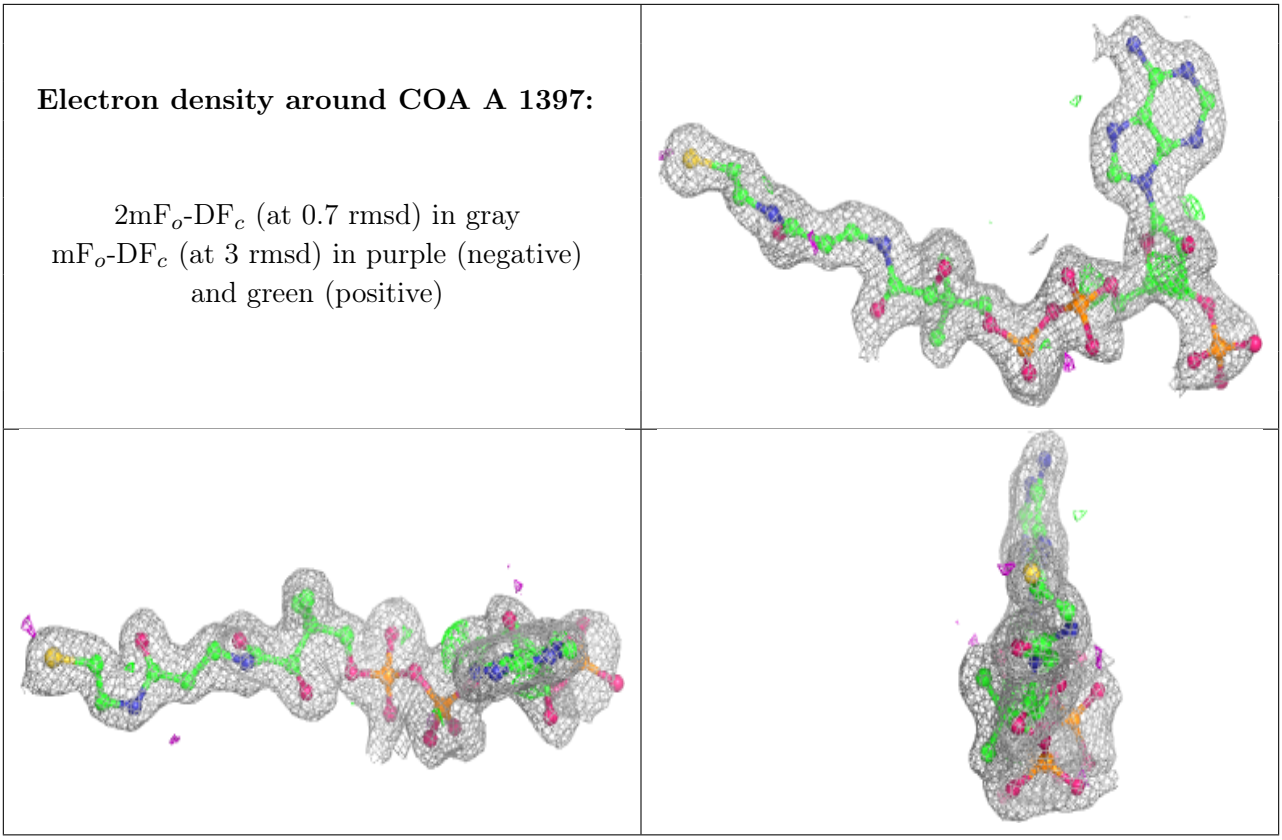






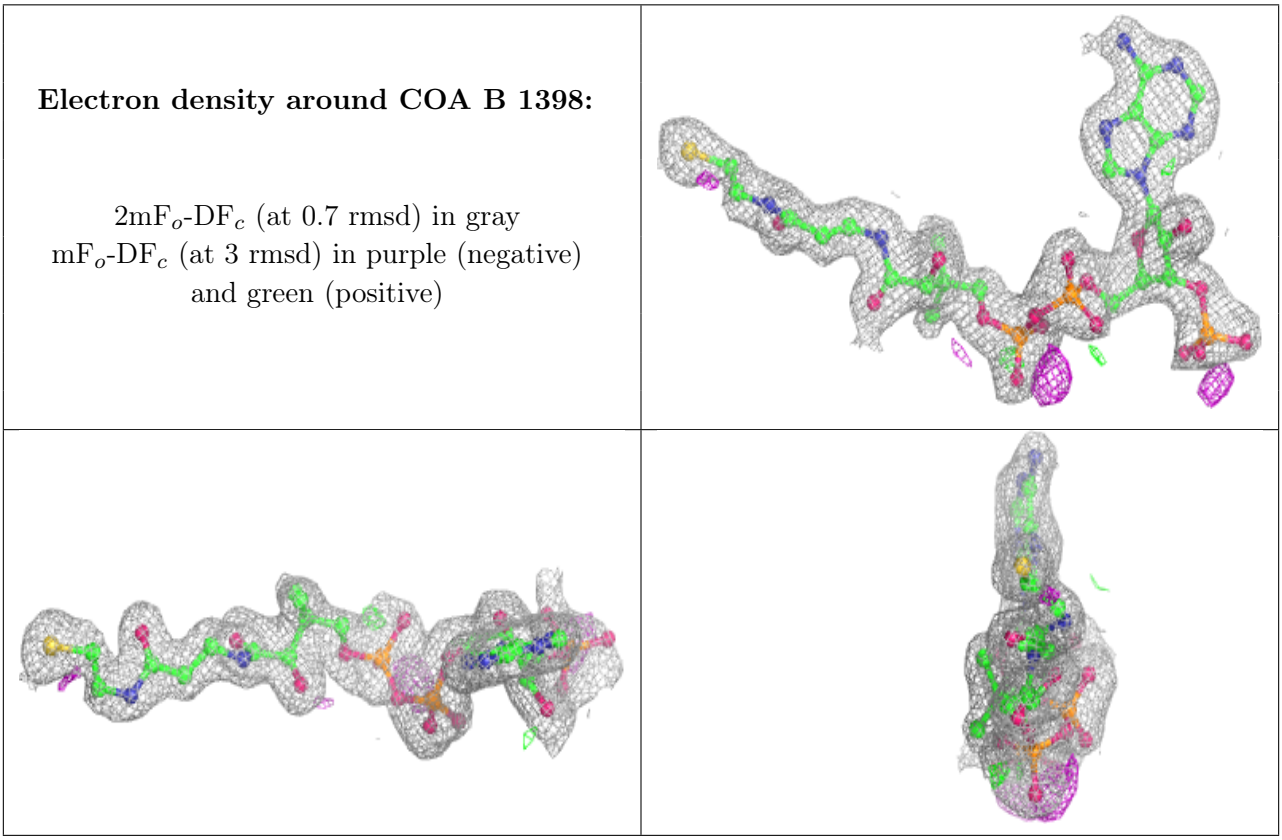
Electron density around COA A 1397:

$2mF_o$-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 1398:

$2mF_o$-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.