Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 03:00 AM EDT

PDB ID	:	1M3Z
Title	:	Biosynthetic thiolase, C89A mutant, complexed with acetyl coenzyme A
Authors	:	Kursula, P.; Ojala, J.; Lambeir, A.-M.; Wierenga, R.K.
Deposited on	:	2002-07-03
Resolution	:	1.87 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:

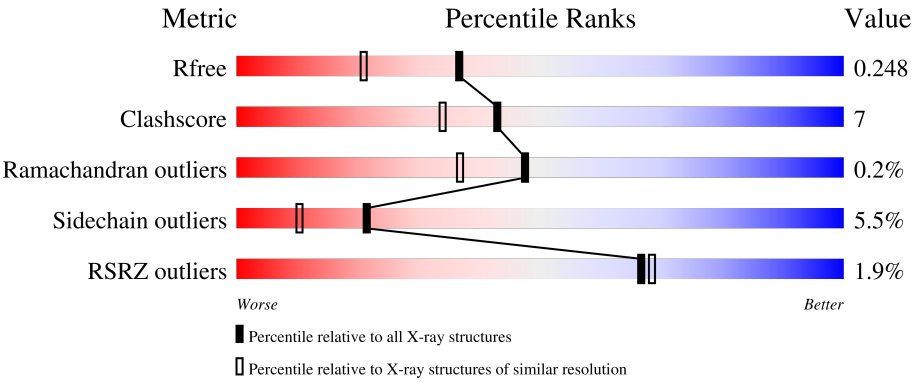
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	86% 12%
1	B	392	83% 15%
1	C	392	86% 12%
1	D	392	5% 80% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12568 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.

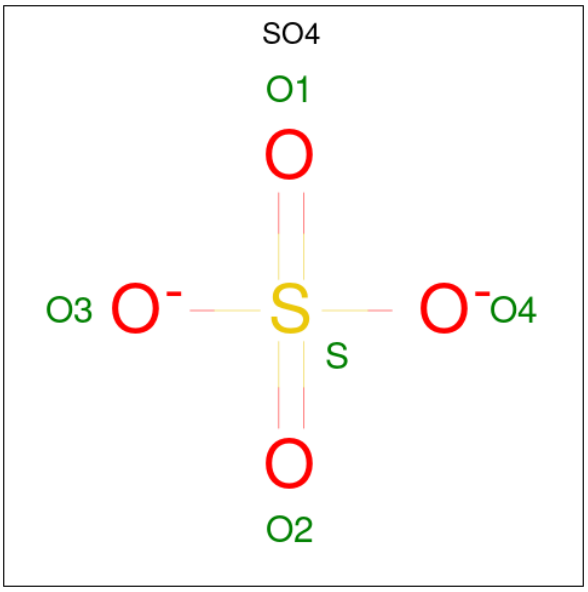
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	2	0
			2823	1753	510	540	20			
1	B	390	Total	C	N	O	S	0	2	0
			2823	1753	510	540	20			
1	C	390	Total	C	N	O	S	0	2	0
			2823	1753	510	540	20			
1	D	390	Total	C	N	O	S	0	2	0
			2823	1753	510	540	20			

There are 12 discrepancies between the modelled and reference sequences:

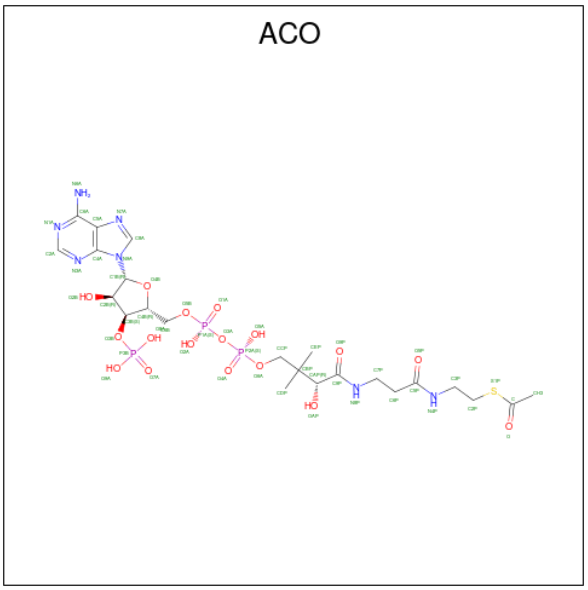
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	insertion	UNP P07097
A	89	ALA	CYS	engineered mutation	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	10	ALA	-	insertion	UNP P07097
B	89	ALA	CYS	engineered mutation	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	10	ALA	-	insertion	UNP P07097
C	89	ALA	CYS	engineered mutation	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	10	ALA	-	insertion	UNP P07097
D	89	ALA	CYS	engineered mutation	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is water.

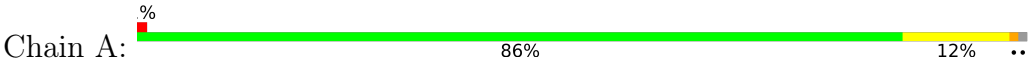
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total	O	0	0
			343	343		
4	B	346	Total	O	0	0
			346	346		
4	C	178	Total	O	0	0
			178	178		
4	D	185	Total	O	0	0
			185	185		

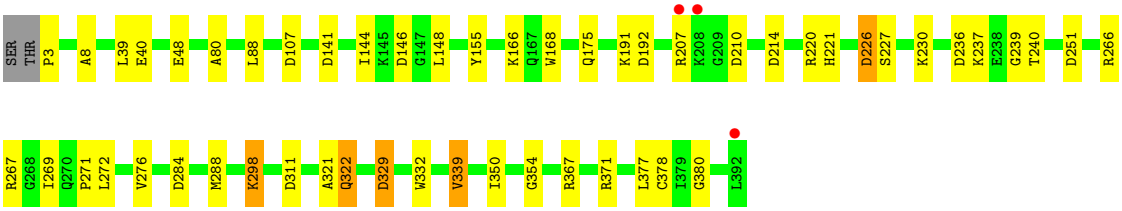
3 Residue-property plots (i)

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

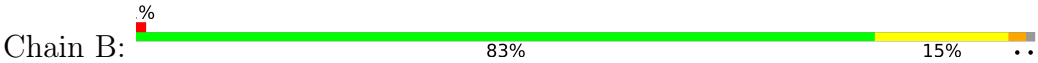
Chain A:

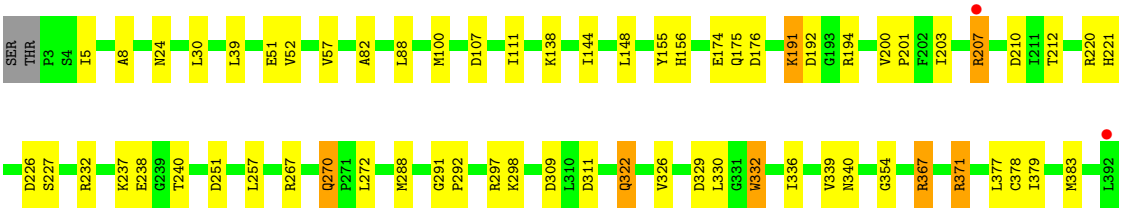




• Molecule 1: Acetyl-CoA acetyltransferase

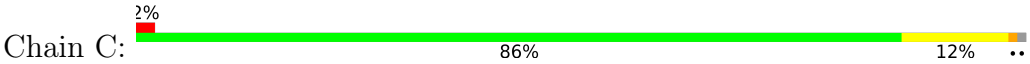
Chain B:

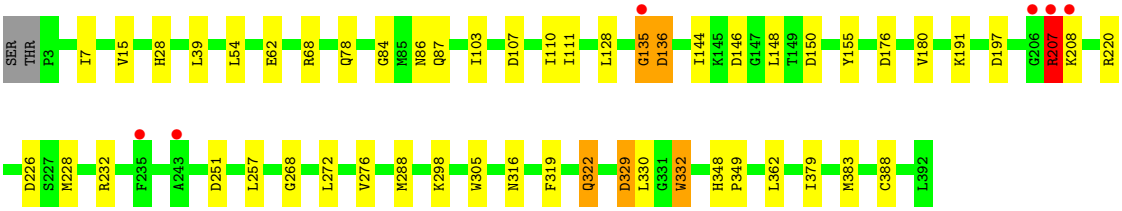




• Molecule 1: Acetyl-CoA acetyltransferase

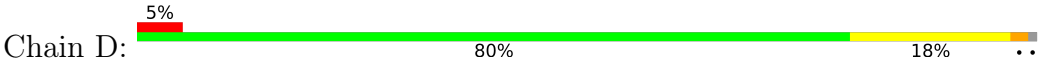
Chain C:

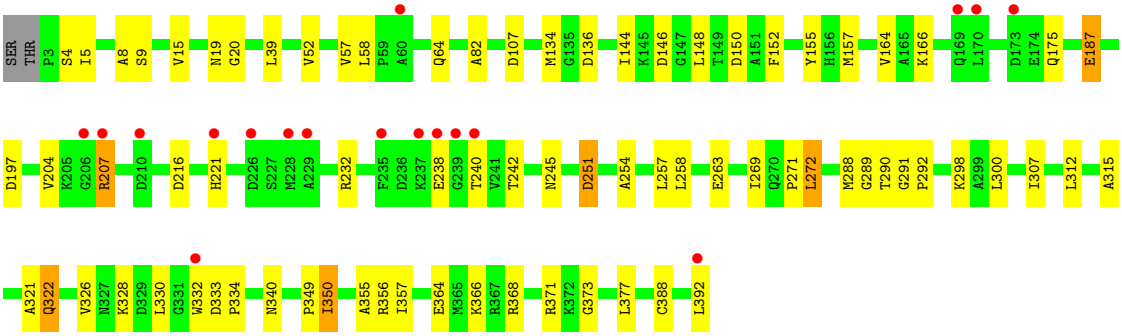




• Molecule 1: Acetyl-CoA acetyltransferase

Chain D:




SER THR P3 S4 I5 A8 S9 V15 N19 G20 L39 V52 V57 L58 P59 A60 Q64 A82 D107 M134 G135 D136 I144 K145 D146 G147 L148 T149 D150 A151 F152 Y155 H156 M157 V164 A165 K166 Q169 L170 D173 E174 Q175 E187
D197 V204 K205 G206 R207 D210 D216 H221 D226 S227 M228 A229 R232 F235 D236 K237 E238 G239 T240 V241 T242 N245 D251 A254 L257 L258 E263 I269 Q270 P271 L272 M288 G289 T290 G291 P292 K298 A299 L300 I307 L312 A315
A321 Q322 V326 N327 K328 D329 L330 G331 W332 D333 P334 N340 P349 I350 A355 R356 I357 E364 M366 K366 R367 R368 R371 K372 G373 L377 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 79.68Å 149.32Å 90.00° 92.83° 90.00°	Depositor
Resolution (Å)	20.00 – 1.87 19.78 – 1.87	Depositor EDS
% Data completeness (in resolution range)	90.9 (20.00-1.87) 78.5 (19.78-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.87Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.242 0.202 , 0.248	Depositor DCC
R_{free} test set	6848 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12568	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 4.24% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACO

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	0.87	1/2873 (0.0%)	0.98	14/3879 (0.4%)
1	B	0.87	0/2873	0.94	12/3879 (0.3%)
1	C	0.64	1/2873 (0.0%)	0.84	9/3879 (0.2%)
1	D	0.56	0/2873	0.79	6/3879 (0.2%)
All	All	0.75	2/11492 (0.0%)	0.89	41/15516 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	VAL	CB-CG2	-5.29	1.41	1.52
1	C	135	GLY	C-O	5.22	1.32	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	B	367	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	107	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	266	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	C	207	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	C	107	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	107	ASP	CB-CG-OD2	6.68	124.31	118.30
1	D	146	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	146	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	309	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	176	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	311	ASP	CB-CG-OD2	6.28	123.96	118.30
1	A	329	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	329	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	214	ASP	CB-CG-OD2	6.08	123.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	226	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	251	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	251	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	141	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	210	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	311	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	192	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	251	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	284	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	367	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	329	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	192	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	210	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	339	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	D	216	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	251	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	226	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	176	ASP	CB-CG-OD2	5.36	123.13	118.30
1	C	197	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	107	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	226	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	136	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	146	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	150	ASP	CB-CG-OD2	5.08	122.88	118.30
1	D	197	ASP	CB-CG-OD2	5.08	122.87	118.30

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	2823	0	2829	25	0
1	B	2823	0	2829	40	0
1	C	2823	0	2829	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2823	0	2829	58	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	51	0	34	6	0
3	B	51	0	34	4	0
3	C	51	0	34	1	0
3	D	51	0	34	2	0
4	A	343	0	0	12	0
4	B	346	0	0	20	0
4	C	178	0	0	13	0
4	D	185	0	0	36	0
All	All	12568	0	11452	157	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 7.

All (157) 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:332:TRP:HB2	4:B:445:HOH:O	1.59	1.02
1:D:326:VAL:HG22	4:D:4413:HOH:O	1.64	0.97
1:D:82:ALA:HB2	4:D:4563:HOH:O	1.73	0.89
1:B:340:ASN:ND2	4:B:455:HOH:O	2.05	0.89
1:D:290:THR:HA	4:D:4413:HOH:O	1.76	0.85
1:C:128:LEU:HB3	4:C:3561:HOH:O	1.77	0.82
1:B:336:ILE:HD11	4:B:445:HOH:O	1.80	0.81
1:A:3:PRO:N	4:A:9979:HOH:O	2.15	0.79
1:D:8:ALA:HA	4:D:4564:HOH:O	1.83	0.77
1:A:378:CYS:SG	3:A:1393:ACO:HH33	2.26	0.75
1:D:254:ALA:HB2	4:D:4567:HOH:O	1.90	0.72
1:C:316:ASN:HD21	1:C:348:HIS:CE1	2.08	0.71
1:D:388:CYS:SG	4:D:4523:HOH:O	2.48	0.71
1:D:19:ASN:CG	4:D:4566:HOH:O	2.29	0.70
1:D:15:VAL:HG13	4:D:4555:HOH:O	1.92	0.70
1:D:64:GLN:OE1	4:D:4408:HOH:O	2.12	0.68
1:B:57:VAL:O	4:B:9945:HOH:O	2.11	0.68
1:C:87:GLN:NE2	4:C:3503:HOH:O	2.25	0.67
1:D:392:LEU:HD21	4:D:4557:HOH:O	1.94	0.67
1:C:349:PRO:HG3	4:C:3565:HOH:O	1.94	0.66
1:C:111:ILE:HG12	4:C:3526:HOH:O	1.96	0.65
1:C:15:VAL:HG22	4:C:3565:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLY:HA2	4:C:3427:HOH:O	2.00	0.62
1:B:378:CYS:SG	3:B:2393:ACO:HH33	2.39	0.62
1:C:207:ARG:HH11	1:C:207:ARG:HG2	1.65	0.62
1:D:164:VAL:HG21	4:D:4441:HOH:O	1.98	0.62
1:C:383:MET:HB3	4:C:3503:HOH:O	2.00	0.61
1:D:269:ILE:HG22	4:D:4564:HOH:O	1.99	0.61
4:A:443:HOH:O	1:D:134:MET:SD	2.56	0.61
1:D:242:THR:HG23	1:D:245:ASN:HD21	1.65	0.61
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.15	0.59
1:D:144:ILE:HD13	1:D:148:LEU:HD12	1.83	0.59
1:C:28:HIS:ND1	1:C:62:GLU:OE2	2.34	0.59
1:D:315:ALA:HB2	4:D:4577:HOH:O	2.03	0.58
1:A:48:GLU:OE1	1:A:267:ARG:NH2	2.34	0.58
1:D:207:ARG:N	1:D:207:ARG:HD3	2.18	0.58
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.69	0.58
1:D:258:LEU:HD22	4:D:4562:HOH:O	2.05	0.57
1:C:180:VAL:HG22	1:C:228:MET:HE3	1.87	0.56
1:D:340:ASN:ND2	1:D:364:GLU:OE1	2.33	0.56
1:D:349:PRO:HG3	4:D:4555:HOH:O	2.06	0.55
3:D:4393:ACO:HH32	4:D:4497:HOH:O	2.05	0.55
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.88	0.55
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.22	0.55
1:B:100:MET:HG3	4:B:444:HOH:O	2.07	0.54
1:A:80:ALA:HB2	4:A:414:HOH:O	2.06	0.54
1:B:24:ASN:ND2	4:B:9941:HOH:O	2.10	0.54
1:C:330:LEU:HD12	1:C:332:TRP:CZ2	2.43	0.54
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.73	0.54
1:A:175:GLN:NE2	4:A:446:HOH:O	2.41	0.54
1:B:138:LYS:NZ	4:B:9984:HOH:O	2.40	0.54
3:D:4393:ACO:H4B	4:D:4554:HOH:O	2.06	0.53
1:B:322:GLN:O	1:B:326:VAL:HG23	2.08	0.53
1:D:366:LYS:HB2	4:D:4556:HOH:O	2.07	0.53
1:D:356:ARG:HG2	4:D:4567:HOH:O	2.06	0.53
4:C:3553:HOH:O	1:D:64:GLN:HG3	2.07	0.53
1:D:333:ASP:HA	4:D:4551:HOH:O	2.09	0.53
1:A:148:LEU:HD22	3:A:1393:ACO:C5P	2.39	0.53
1:A:166:LYS:NZ	4:A:9990:HOH:O	2.42	0.52
1:D:251:ASP:O	4:D:4555:HOH:O	2.19	0.52
1:A:226:ASP:CG	4:A:9836:HOH:O	2.47	0.52
1:C:207:ARG:HH11	1:C:207:ARG:CG	2.23	0.52
1:B:207:ARG:N	1:B:207:ARG:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLY:O	4:D:4473:HOH:O	2.18	0.52
1:B:371:ARG:CD	4:B:9777:HOH:O	2.58	0.51
1:A:40:GLU:HG3	4:A:9914:HOH:O	2.10	0.51
1:A:322:GLN:HB3	4:A:409:HOH:O	2.09	0.51
1:C:276:VAL:HG22	1:C:388:CYS:HB2	1.92	0.51
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.46	0.50
1:A:378:CYS:SG	3:A:1393:ACO:CH3	2.99	0.50
3:A:1393:ACO:H10	4:A:443:HOH:O	2.12	0.49
1:D:52:VAL:HB	4:D:4563:HOH:O	2.12	0.48
1:C:54:LEU:HD21	4:C:3566:HOH:O	2.12	0.48
1:D:326:VAL:HG12	1:D:330:LEU:HD12	1.95	0.48
1:B:191:LYS:NZ	4:B:398:HOH:O	2.47	0.48
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.49	0.47
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.97	0.47
1:D:321:ALA:N	4:D:4507:HOH:O	2.46	0.47
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.95	0.47
1:D:271:PRO:HA	4:D:4564:HOH:O	2.14	0.47
1:C:103:ILE:HD11	4:C:3526:HOH:O	2.15	0.47
1:D:312:LEU:HD13	1:D:368:ARG:HD2	1.97	0.47
1:D:166:LYS:HE2	4:D:4440:HOH:O	2.15	0.47
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.96	0.46
1:D:148:LEU:HD23	4:D:4561:HOH:O	2.16	0.46
1:C:329:ASP:OD1	1:C:330:LEU:HD23	2.15	0.46
1:B:174:GLU:OE1	4:B:395:HOH:O	2.20	0.46
1:B:371:ARG:HD3	4:B:9777:HOH:O	2.15	0.46
3:B:2393:ACO:H141	4:B:448:HOH:O	2.14	0.46
1:A:321:ALA:CB	4:A:446:HOH:O	2.63	0.46
1:A:8:ALA:HB1	1:A:269:ILE:HG21	1.97	0.46
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.28	0.46
1:D:322:GLN:O	1:D:326:VAL:HG23	2.16	0.46
1:A:227:SER:HB2	3:A:1393:ACO:H2A	1.98	0.46
1:B:371:ARG:HD2	4:B:9777:HOH:O	2.15	0.45
1:D:257:LEU:HD23	1:D:258:LEU:N	2.31	0.45
1:D:334:PRO:HD2	4:D:4551:HOH:O	2.15	0.45
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.99	0.45
1:C:276:VAL:CG2	1:C:388:CYS:HB2	2.47	0.45
1:C:110:ILE:CA	4:C:3526:HOH:O	2.65	0.45
1:D:271:PRO:CA	4:D:4564:HOH:O	2.64	0.45
1:B:194:ARG:HB3	4:B:455:HOH:O	2.16	0.45
1:B:297:ARG:NE	4:B:9823:HOH:O	2.50	0.45
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:GLY:HA3	4:D:4441:HOH:O	2.17	0.45
1:D:254:ALA:HB3	1:D:355:ALA:HB3	1.98	0.44
1:D:291:GLY:N	1:D:292:PRO:CD	2.80	0.44
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.81	0.44
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.81	0.44
1:B:378:CYS:O	3:B:2393:ACO:HH31	2.17	0.44
1:D:58:LEU:HD11	4:D:4494:HOH:O	2.16	0.44
1:A:354:GLY:HA2	1:A:377:LEU:HD11	2.00	0.44
1:C:180:VAL:CG2	1:C:228:MET:HE3	2.46	0.44
1:D:312:LEU:O	1:D:373:GLY:HA2	2.17	0.44
1:D:357:ILE:HD11	1:D:377:LEU:HD11	1.98	0.44
1:D:157:MET:HE1	4:D:4573:HOH:O	2.18	0.44
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.65	0.44
1:B:88:LEU:HB2	1:B:379:ILE:HG23	2.00	0.44
1:D:19:ASN:ND2	4:D:4566:HOH:O	2.48	0.43
1:C:319:PHE:O	1:C:322:GLN:HG3	2.18	0.43
3:A:1393:ACO:H142	4:A:443:HOH:O	2.18	0.43
1:D:207:ARG:HD3	1:D:207:ARG:H	1.82	0.43
1:B:51:GLU:HB3	1:B:111:ILE:CD1	2.48	0.43
1:B:8:ALA:HB3	1:B:257:LEU:HD22	2.00	0.43
1:B:156:HIS:CD2	4:B:448:HOH:O	2.71	0.43
4:C:3553:HOH:O	1:D:64:GLN:CG	2.64	0.43
1:B:379:ILE:HB	1:B:383:MET:HB2	2.01	0.43
1:D:204:VAL:HG11	4:D:4488:HOH:O	2.19	0.42
1:B:200:VAL:HA	1:B:201:PRO:HD3	1.88	0.42
1:B:270:GLN:NE2	4:B:9971:HOH:O	2.51	0.42
1:D:4:SER:C	1:D:5:ILE:HD13	2.40	0.42
1:D:150:ASP:HB2	4:D:4573:HOH:O	2.19	0.42
1:B:30:LEU:HD12	4:B:454:HOH:O	2.19	0.42
1:C:220:ARG:HD3	3:C:3393:ACO:N6A	2.34	0.42
1:B:51:GLU:HB3	1:B:111:ILE:HD13	2.02	0.42
1:B:227:SER:HG	3:B:2393:ACO:C2A	2.33	0.42
1:B:291:GLY:N	1:B:292:PRO:CD	2.82	0.42
1:C:86:ASN:ND2	4:C:3518:HOH:O	2.53	0.41
1:C:379:ILE:HB	1:C:383:MET:HB2	2.02	0.41
1:D:300:LEU:HD13	1:D:307:ILE:HG13	2.01	0.41
1:C:54:LEU:O	1:C:84:GLY:HA2	2.21	0.41
1:D:9:SER:HA	1:D:272:LEU:CD2	2.50	0.41
1:D:187:GLU:O	1:D:187:GLU:OE1	2.39	0.41
1:A:298:LYS:HE3	2:A:9722:SO4:O3	2.21	0.41
1:B:257:LEU:HD23	1:B:257:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:HB3	1:A:239:GLY:HA3	2.03	0.41
1:D:315:ALA:CB	4:D:4577:HOH:O	2.63	0.41
1:B:367:ARG:NH1	4:B:455:HOH:O	2.54	0.41
1:A:269:ILE:O	1:A:271:PRO:HD3	2.21	0.40
1:A:371:ARG:HG2	4:A:456:HOH:O	2.21	0.40
1:B:191:LYS:HG3	4:B:9877:HOH:O	2.21	0.40
1:B:354:GLY:HA2	1:B:377:LEU:HD11	2.01	0.40
1:B:52:VAL:O	1:B:82:ALA:HA	2.20	0.40
1:C:135:GLY:O	1:C:136:ASP:C	2.58	0.40
1:C:305:TRP:CZ3	1:C:388:CYS:HB3	2.55	0.40
1:A:88:LEU:HD12	1:A:380:GLY:O	2.21	0.40
1:D:356:ARG:NH2	1:D:357:ILE:HG22	2.37	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	390/392 (100%)	379 (97%)	10 (3%)	1 (0%)	41	30
1	B	390/392 (100%)	379 (97%)	11 (3%)	0	100	100
1	C	390/392 (100%)	376 (96%)	13 (3%)	1 (0%)	41	30
1	D	390/392 (100%)	374 (96%)	15 (4%)	1 (0%)	41	30
All	All	1560/1568 (100%)	1508 (97%)	49 (3%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	350	ILE
1	C	136	ASP
1	A	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	278/278 (100%)	263 (95%)	15 (5%)	22 11
1	B	278/278 (100%)	260 (94%)	18 (6%)	17 7
1	C	278/278 (100%)	265 (95%)	13 (5%)	26 14
1	D	278/278 (100%)	263 (95%)	15 (5%)	22 11
All	All	1112/1112 (100%)	1051 (94%)	61 (6%)	21 10

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	191	LYS
1	A	207	ARG
1	A	220	ARG
1	A	221	HIS
1	A	230	LYS
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	339	VAL
1	A	367	ARG
1	B	5	ILE
1	B	39	LEU
1	B	155	TYR
1	B	191	LYS
1	B	207	ARG
1	B	220	ARG
1	B	221	HIS
1	B	232	ARG
1	B	237	LYS

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Mol	Chain	Res	Type
1	B	238	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
1	B	339	VAL
1	B	371	ARG
1	C	39	LEU
1	C	78	GLN
1	C	155	TYR
1	C	191	LYS
1	C	207	ARG
1	C	208	LYS
1	C	232	ARG
1	C	257	LEU
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	D	39	LEU
1	D	155	TYR
1	D	187	GLU
1	D	207	ARG
1	D	221	HIS
1	D	232	ARG
1	D	238	GLU
1	D	263	GLU
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
1	D	371	ARG

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

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	B	78	GLN
1	B	175	GLN
1	B	184	ASN
1	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	C	316	ASN
1	C	322	GLN
1	D	78	GLN
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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	9722	-	4,4,4	0.14	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	9721	-	4,4,4	0.19	0	6,6,6	0.46	0
3	ACO	D	4393	-	45,53,53	1.42	7 (15%)	56,79,79	1.05	3 (5%)
3	ACO	C	3393	-	45,53,53	1.31	6 (13%)	56,79,79	1.01	2 (3%)
3	ACO	A	1393	-	45,53,53	1.39	4 (8%)	56,79,79	1.03	4 (7%)
3	ACO	B	2393	-	45,53,53	1.40	6 (13%)	56,79,79	1.08	6 (10%)
2	SO4	B	9719	-	4,4,4	0.17	0	6,6,6	0.32	0
2	SO4	A	9720	-	4,4,4	0.14	0	6,6,6	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACO	B	2393	-	-	10/47/67/67	0/3/3/3
3	ACO	D	4393	-	-	9/47/67/67	0/3/3/3
3	ACO	C	3393	-	-	8/47/67/67	0/3/3/3
3	ACO	A	1393	-	-	5/47/67/67	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2393	ACO	P3B-O9A	4.33	1.71	1.54
3	A	1393	ACO	P3B-O8A	4.25	1.71	1.54
3	D	4393	ACO	P3B-O8A	4.24	1.71	1.54
3	D	4393	ACO	P3B-O9A	4.22	1.71	1.54
3	C	3393	ACO	P3B-O8A	4.18	1.70	1.54
3	B	2393	ACO	P3B-O8A	4.17	1.70	1.54
3	A	1393	ACO	P3B-O9A	4.14	1.70	1.54
3	C	3393	ACO	P3B-O9A	4.13	1.70	1.54
3	B	2393	ACO	P2A-O5A	3.33	1.71	1.55
3	D	4393	ACO	P1A-O2A	3.32	1.70	1.55
3	D	4393	ACO	P2A-O5A	3.31	1.70	1.55
3	A	1393	ACO	P2A-O5A	3.31	1.70	1.55
3	C	3393	ACO	P2A-O5A	3.29	1.70	1.55
3	B	2393	ACO	P1A-O2A	3.28	1.70	1.55
3	A	1393	ACO	P1A-O2A	3.18	1.70	1.55
3	D	4393	ACO	C2A-N3A	2.23	1.35	1.32
3	D	4393	ACO	O4B-C1B	2.23	1.44	1.41
3	C	3393	ACO	C2A-N3A	2.22	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4393	ACO	C5A-C4A	2.22	1.46	1.40
3	B	2393	ACO	C5A-C4A	2.13	1.46	1.40
3	C	3393	ACO	C5A-C4A	2.11	1.46	1.40
3	B	2393	ACO	C2A-N3A	2.09	1.35	1.32
3	C	3393	ACO	P3B-O3B	2.00	1.63	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3393	ACO	N3A-C2A-N1A	-3.46	123.27	128.68
3	D	4393	ACO	N3A-C2A-N1A	-3.32	123.49	128.68
3	B	2393	ACO	N3A-C2A-N1A	-3.09	123.85	128.68
3	A	1393	ACO	N3A-C2A-N1A	-3.07	123.88	128.68
3	B	2393	ACO	P2A-O3A-P1A	-3.06	122.31	132.83
3	A	1393	ACO	P2A-O3A-P1A	-3.02	122.46	132.83
3	C	3393	ACO	CDP-CBP-CAP	2.76	113.60	108.82
3	B	2393	ACO	CDP-CBP-CAP	2.50	113.16	108.82
3	D	4393	ACO	C2A-N1A-C6A	2.44	122.92	118.75
3	A	1393	ACO	N6A-C6A-N1A	2.35	123.45	118.57
3	D	4393	ACO	C5A-C6A-N1A	-2.21	115.33	120.35
3	B	2393	ACO	C5A-C6A-N6A	2.18	123.67	120.35
3	B	2393	ACO	C2A-N1A-C6A	2.16	122.45	118.75
3	A	1393	ACO	C1B-N9A-C4A	-2.14	122.88	126.64
3	B	2393	ACO	C1B-N9A-C4A	-2.08	122.99	126.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1393	ACO	CCP-O6A-P2A-O3A
3	A	1393	ACO	CCP-O6A-P2A-O4A
3	A	1393	ACO	S1P-C2P-C3P-N4P
3	B	2393	ACO	CCP-O6A-P2A-O3A
3	C	3393	ACO	CCP-O6A-P2A-O4A
3	C	3393	ACO	N8P-C9P-CAP-OAP
3	C	3393	ACO	S1P-C2P-C3P-N4P
3	D	4393	ACO	C5B-O5B-P1A-O1A
3	D	4393	ACO	C5B-O5B-P1A-O3A
3	D	4393	ACO	CAP-CBP-CCP-O6A
3	C	3393	ACO	O9P-C9P-CAP-OAP
3	D	4393	ACO	CDP-CBP-CCP-O6A
3	D	4393	ACO	CEP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
3	C	3393	ACO	CCP-O6A-P2A-O3A
3	B	2393	ACO	CCP-O6A-P2A-O4A
3	B	2393	ACO	CCP-O6A-P2A-O5A
3	D	4393	ACO	S1P-C2P-C3P-N4P
3	B	2393	ACO	O-C-S1P-C2P
3	B	2393	ACO	P1A-O3A-P2A-O5A
3	C	3393	ACO	P1A-O3A-P2A-O5A
3	B	2393	ACO	P1A-O3A-P2A-O4A
3	C	3393	ACO	P1A-O3A-P2A-O4A
3	B	2393	ACO	O9P-C9P-CAP-OAP
3	B	2393	ACO	N8P-C9P-CAP-OAP
3	A	1393	ACO	C3B-O3B-P3B-O9A
3	C	3393	ACO	C3B-O3B-P3B-O9A
3	D	4393	ACO	P2A-O3A-P1A-O1A
3	D	4393	ACO	P2A-O3A-P1A-O2A
3	D	4393	ACO	CBP-CCP-O6A-P2A
3	B	2393	ACO	S1P-C2P-C3P-N4P
3	A	1393	ACO	O-C-S1P-C2P
3	B	2393	ACO	CH3-C-S1P-C2P

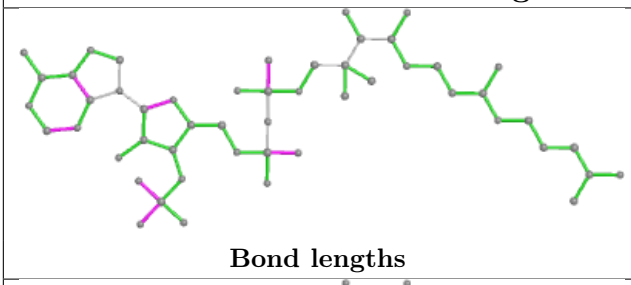
There are no ring outliers.

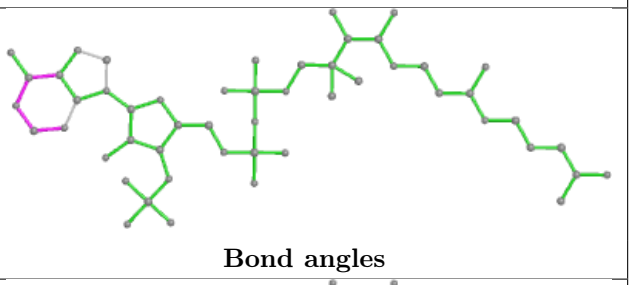
5 monomers are involved in 14 short contacts:

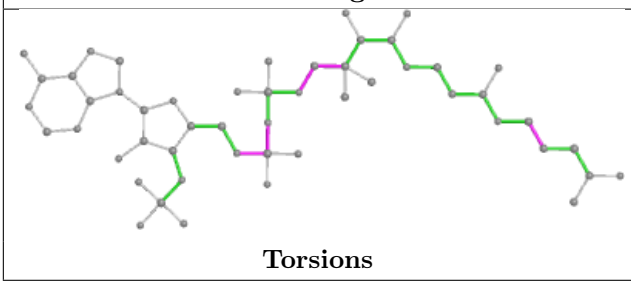
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9722	SO4	1	0
3	D	4393	ACO	2	0
3	C	3393	ACO	1	0
3	A	1393	ACO	6	0
3	B	2393	ACO	4	0

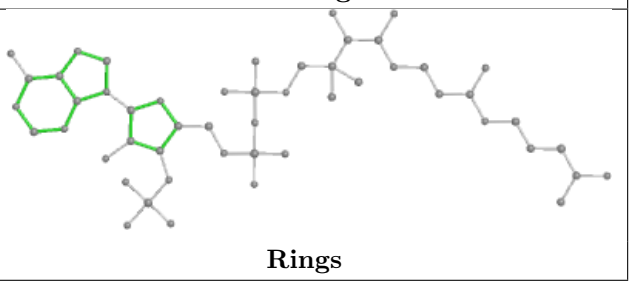
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ACO D 4393

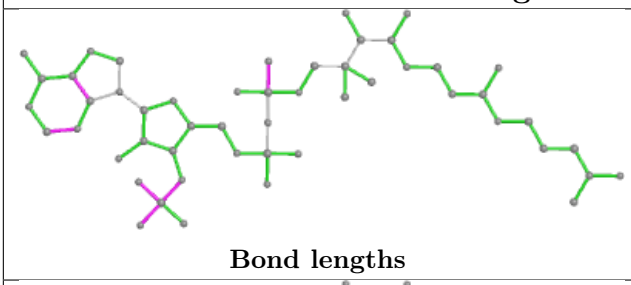

Bond lengths

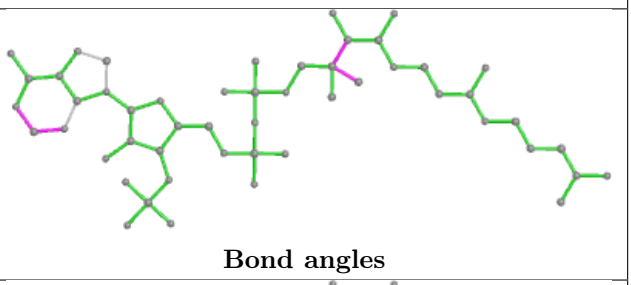

Bond angles

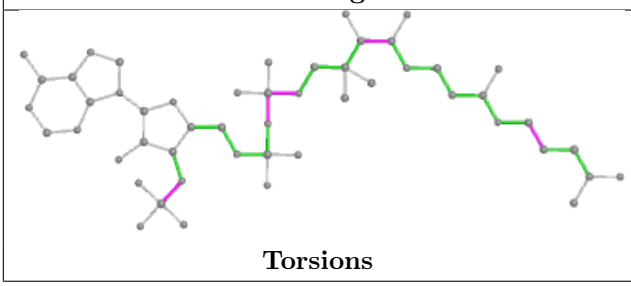

Torsions

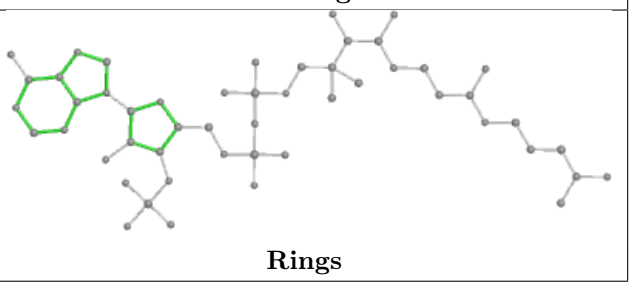

Rings

Ligand ACO C 3393

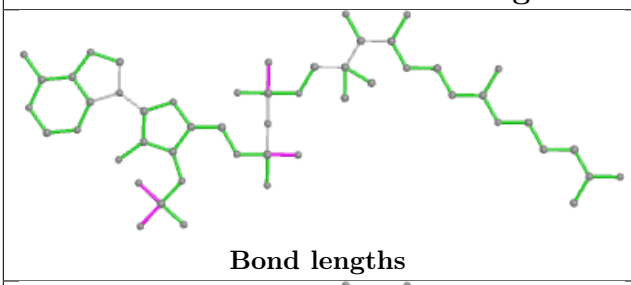

Bond lengths

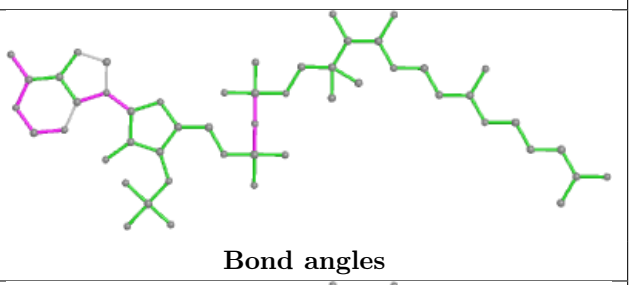

Bond angles

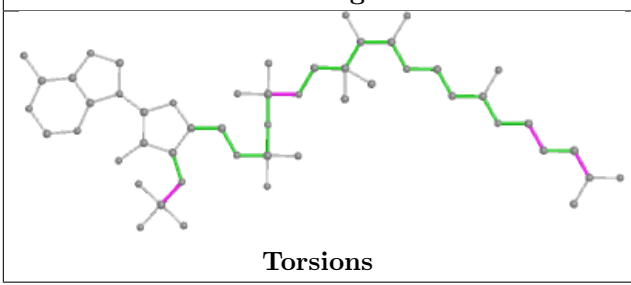

Torsions

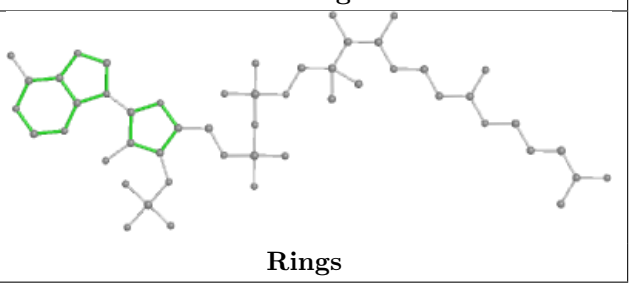

Rings

Ligand ACO A 1393

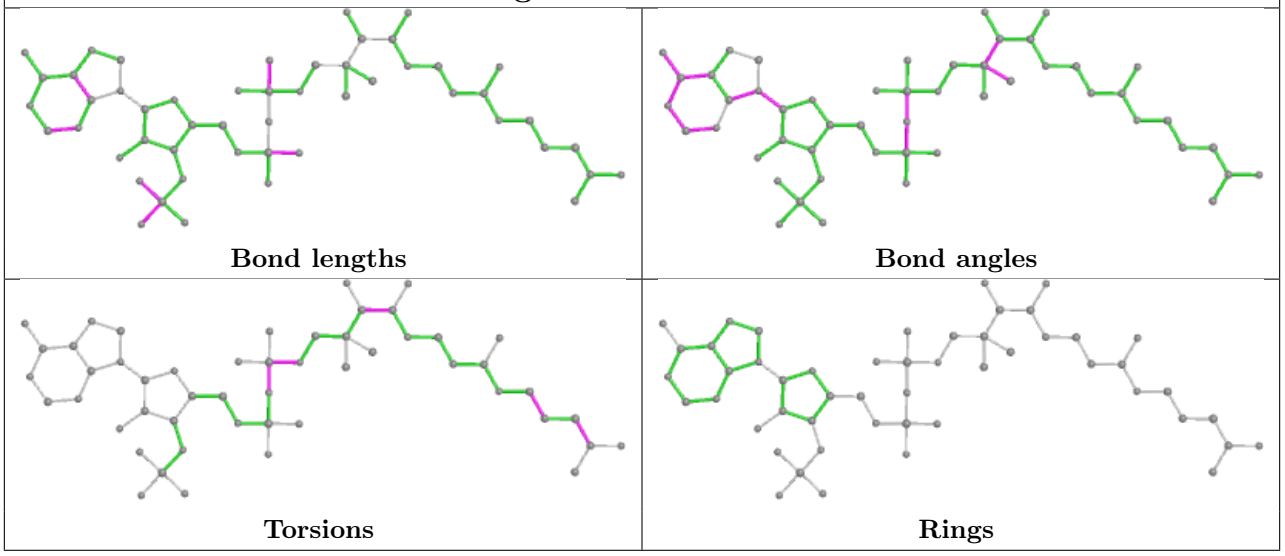

Bond lengths


Bond angles


Torsions


Rings

Ligand ACO B 2393



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	390/392 (99%)	-0.38	3 (0%)	86	87	10, 18, 32, 54	0
1	B	390/392 (99%)	-0.40	2 (0%)	91	91	9, 18, 32, 58	0
1	C	390/392 (99%)	-0.02	6 (1%)	73	75	9, 21, 33, 53	0
1	D	390/392 (99%)	0.28	18 (4%)	32	34	7, 21, 36, 52	0
All	All	1560/1568 (99%)	-0.13	29 (1%)	66	68	7, 20, 34, 58	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	LYS	4.7
1	D	206	GLY	4.7
1	D	392	LEU	4.3
1	D	173	ASP	3.9
1	B	207	ARG	3.4
1	A	392	LEU	3.4
1	D	207	ARG	3.3
1	D	228	MET	3.3
1	B	392	LEU	3.2
1	D	238	GLU	2.9
1	C	235	PHE	2.9
1	D	226	ASP	2.8
1	D	229	ALA	2.8
1	D	239	GLY	2.7
1	D	235	PHE	2.6
1	A	207	ARG	2.4
1	C	207	ARG	2.4
1	C	206	GLY	2.4
1	D	240	THR	2.4
1	C	243	ALA	2.3
1	D	210	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	60	ALA	2.3
1	D	237	LYS	2.2
1	D	170	LEU	2.2
1	C	135	GLY	2.2
1	D	221	HIS	2.1
1	C	208	LYS	2.1
1	D	169	GLN	2.1
1	D	332	TRP	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)

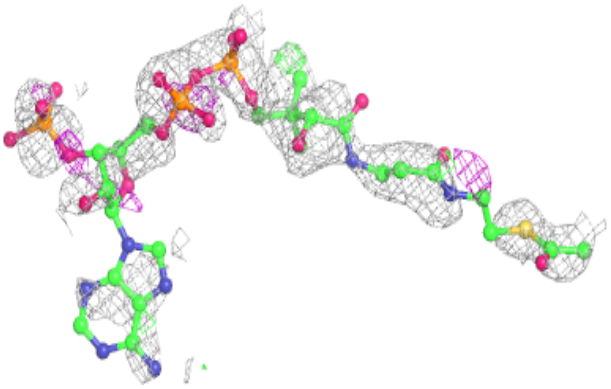
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

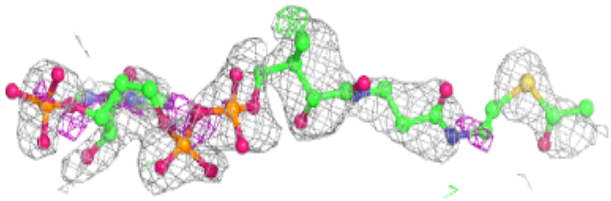
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACO	D	4393	51/51	0.60	0.35	73,94,96,97	0
3	ACO	A	1393	51/51	0.74	0.23	42,66,69,69	0
3	ACO	B	2393	51/51	0.75	0.25	54,65,71,72	0
3	ACO	C	3393	51/51	0.77	0.25	76,84,90,92	0
2	SO4	A	9722	5/5	0.92	0.12	73,73,75,76	0
2	SO4	B	9719	5/5	0.97	0.10	62,62,63,63	0
2	SO4	B	9721	5/5	0.98	0.10	50,50,53,57	0
2	SO4	A	9720	5/5	0.99	0.08	52,52,53,54	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 ACO D 4393:

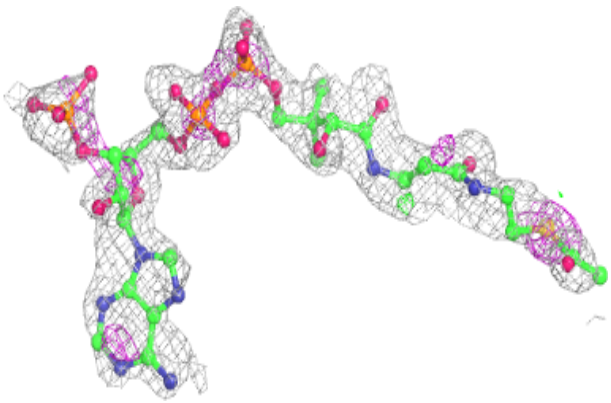
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

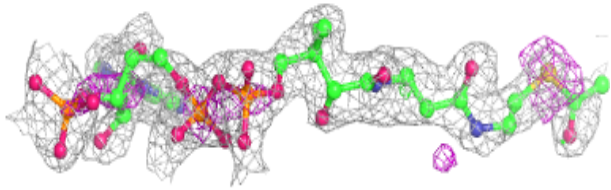




Electron density around ACO A 1393:

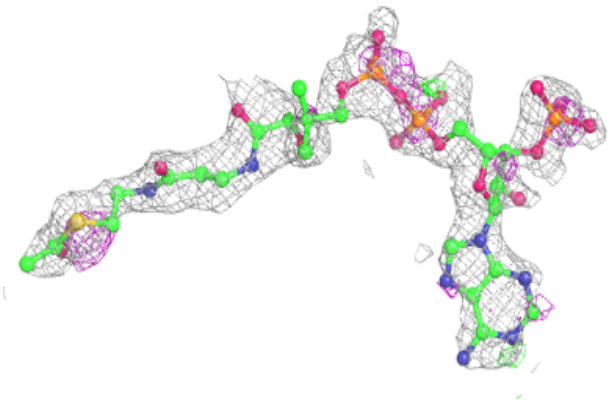
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

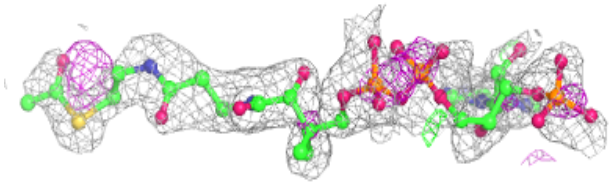




Electron density around ACO B 2393:

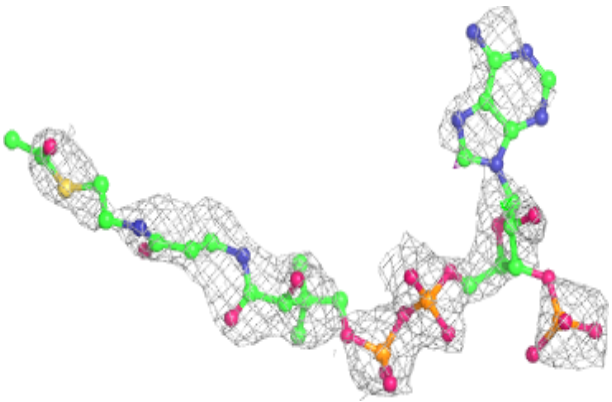
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

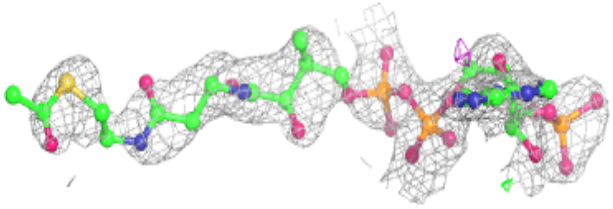


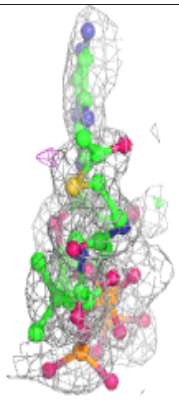


Electron density around ACO C 3393:

$2mF_o$-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.