Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 07:48 PM EDT

PDB ID	:	3UBM
Title	:	Formyl-CoA:oxalate CoA-transferase from Acetobacter aceti
Authors	:	Starks, C.M.; Mullins, E.A.; Kappock, T.J.
Deposited on	:	2011-10-24
Resolution	:	1.99 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 (i) 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 (i)) were used in the production of this report:

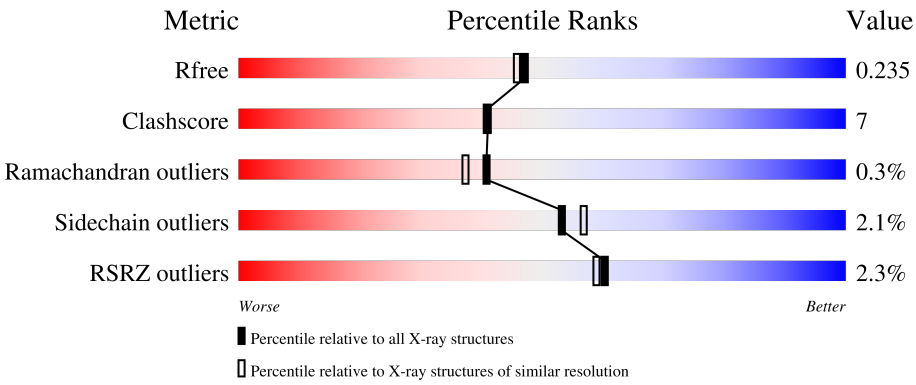
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.99 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	456	2% 79% 14% 6%
1	B	456	% 81% 12% • 6%
1	C	456	4% 80% 14% 6%
1	D	456	% 81% 13% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14381 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 Formyl-CoA:oxalate CoA-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	3293	2084	569	625	15	0	0	0
1	B	430	3307	2091	572	629	15	0	0	0
1	C	429	3299	2087	570	627	15	0	0	0
1	D	430	3307	2091	572	629	15	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A9X6P7
A	-18	GLY	-	expression tag	UNP A9X6P7
A	-17	SER	-	expression tag	UNP A9X6P7
A	-16	SER	-	expression tag	UNP A9X6P7
A	-15	HIS	-	expression tag	UNP A9X6P7
A	-14	HIS	-	expression tag	UNP A9X6P7
A	-13	HIS	-	expression tag	UNP A9X6P7
A	-12	HIS	-	expression tag	UNP A9X6P7
A	-11	HIS	-	expression tag	UNP A9X6P7
A	-10	HIS	-	expression tag	UNP A9X6P7
A	-9	SER	-	expression tag	UNP A9X6P7
A	-8	SER	-	expression tag	UNP A9X6P7
A	-7	GLY	-	expression tag	UNP A9X6P7
A	-6	LEU	-	expression tag	UNP A9X6P7
A	-5	VAL	-	expression tag	UNP A9X6P7
A	-4	PRO	-	expression tag	UNP A9X6P7
A	-3	ARG	-	expression tag	UNP A9X6P7
A	-2	GLY	-	expression tag	UNP A9X6P7
A	-1	SER	-	expression tag	UNP A9X6P7
A	0	HIS	-	expression tag	UNP A9X6P7
B	-19	MET	-	expression tag	UNP A9X6P7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A9X6P7
B	-17	SER	-	expression tag	UNP A9X6P7
B	-16	SER	-	expression tag	UNP A9X6P7
B	-15	HIS	-	expression tag	UNP A9X6P7
B	-14	HIS	-	expression tag	UNP A9X6P7
B	-13	HIS	-	expression tag	UNP A9X6P7
B	-12	HIS	-	expression tag	UNP A9X6P7
B	-11	HIS	-	expression tag	UNP A9X6P7
B	-10	HIS	-	expression tag	UNP A9X6P7
B	-9	SER	-	expression tag	UNP A9X6P7
B	-8	SER	-	expression tag	UNP A9X6P7
B	-7	GLY	-	expression tag	UNP A9X6P7
B	-6	LEU	-	expression tag	UNP A9X6P7
B	-5	VAL	-	expression tag	UNP A9X6P7
B	-4	PRO	-	expression tag	UNP A9X6P7
B	-3	ARG	-	expression tag	UNP A9X6P7
B	-2	GLY	-	expression tag	UNP A9X6P7
B	-1	SER	-	expression tag	UNP A9X6P7
B	0	HIS	-	expression tag	UNP A9X6P7
C	-19	MET	-	expression tag	UNP A9X6P7
C	-18	GLY	-	expression tag	UNP A9X6P7
C	-17	SER	-	expression tag	UNP A9X6P7
C	-16	SER	-	expression tag	UNP A9X6P7
C	-15	HIS	-	expression tag	UNP A9X6P7
C	-14	HIS	-	expression tag	UNP A9X6P7
C	-13	HIS	-	expression tag	UNP A9X6P7
C	-12	HIS	-	expression tag	UNP A9X6P7
C	-11	HIS	-	expression tag	UNP A9X6P7
C	-10	HIS	-	expression tag	UNP A9X6P7
C	-9	SER	-	expression tag	UNP A9X6P7
C	-8	SER	-	expression tag	UNP A9X6P7
C	-7	GLY	-	expression tag	UNP A9X6P7
C	-6	LEU	-	expression tag	UNP A9X6P7
C	-5	VAL	-	expression tag	UNP A9X6P7
C	-4	PRO	-	expression tag	UNP A9X6P7
C	-3	ARG	-	expression tag	UNP A9X6P7
C	-2	GLY	-	expression tag	UNP A9X6P7
C	-1	SER	-	expression tag	UNP A9X6P7
C	0	HIS	-	expression tag	UNP A9X6P7
D	-19	MET	-	expression tag	UNP A9X6P7
D	-18	GLY	-	expression tag	UNP A9X6P7
D	-17	SER	-	expression tag	UNP A9X6P7

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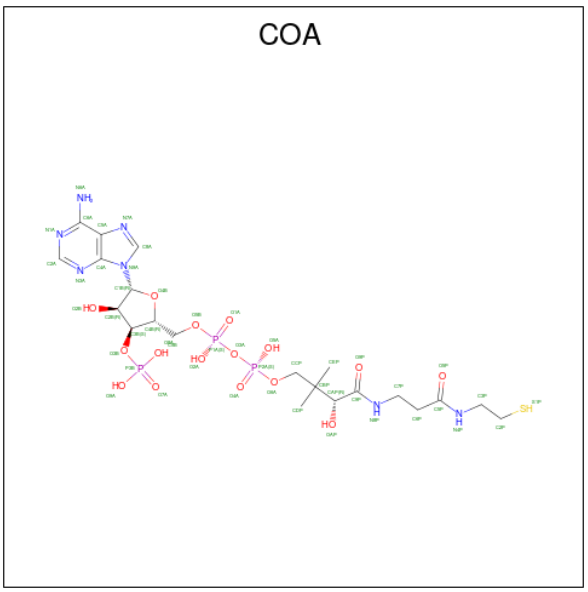
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A9X6P7
D	-15	HIS	-	expression tag	UNP A9X6P7
D	-14	HIS	-	expression tag	UNP A9X6P7
D	-13	HIS	-	expression tag	UNP A9X6P7
D	-12	HIS	-	expression tag	UNP A9X6P7
D	-11	HIS	-	expression tag	UNP A9X6P7
D	-10	HIS	-	expression tag	UNP A9X6P7
D	-9	SER	-	expression tag	UNP A9X6P7
D	-8	SER	-	expression tag	UNP A9X6P7
D	-7	GLY	-	expression tag	UNP A9X6P7
D	-6	LEU	-	expression tag	UNP A9X6P7
D	-5	VAL	-	expression tag	UNP A9X6P7
D	-4	PRO	-	expression tag	UNP A9X6P7
D	-3	ARG	-	expression tag	UNP A9X6P7
D	-2	GLY	-	expression tag	UNP A9X6P7
D	-1	SER	-	expression tag	UNP A9X6P7
D	0	HIS	-	expression tag	UNP A9X6P7

- 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
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0
2	B	1	48	21	7	16	3	1	0	0
2	C	1	48	21	7	16	3	1	0	0

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

- Molecule 3 is water.

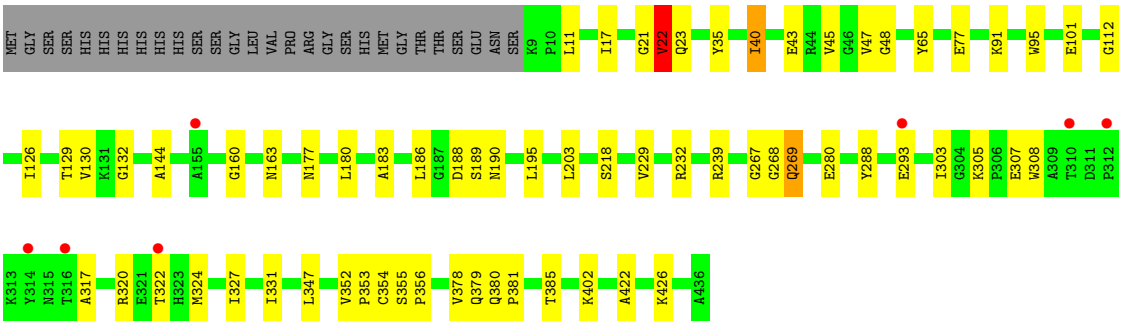
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	251	251	251	0	0
			Total	O		
3	B	228	228	228	0	0
			Total	O		
3	C	251	251	251	0	0
			Total	O		
3	D	253	253	253	0	0

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.

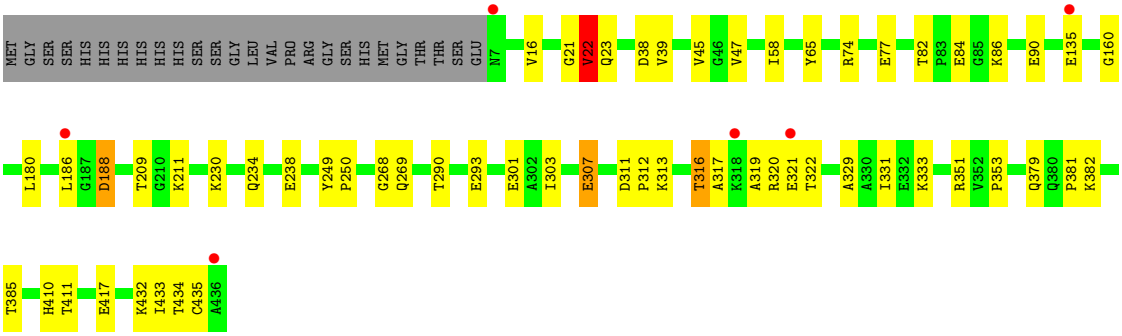
• Molecule 1: Formyl-CoA:oxalate CoA-transferase

Chain A:



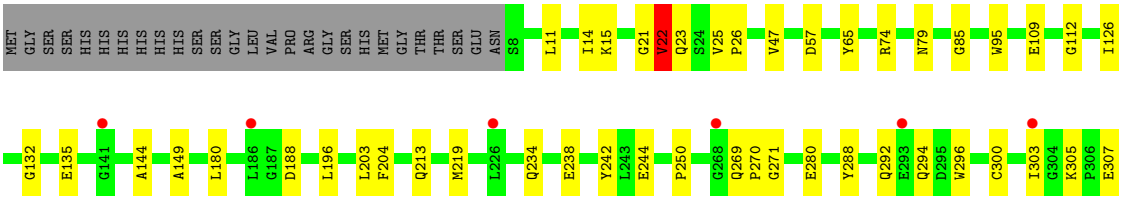
• Molecule 1: Formyl-CoA:oxalate CoA-transferase

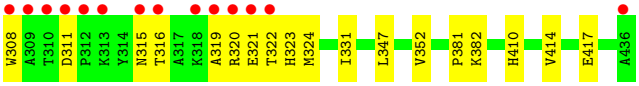
Chain B:



• Molecule 1: Formyl-CoA:oxalate CoA-transferase

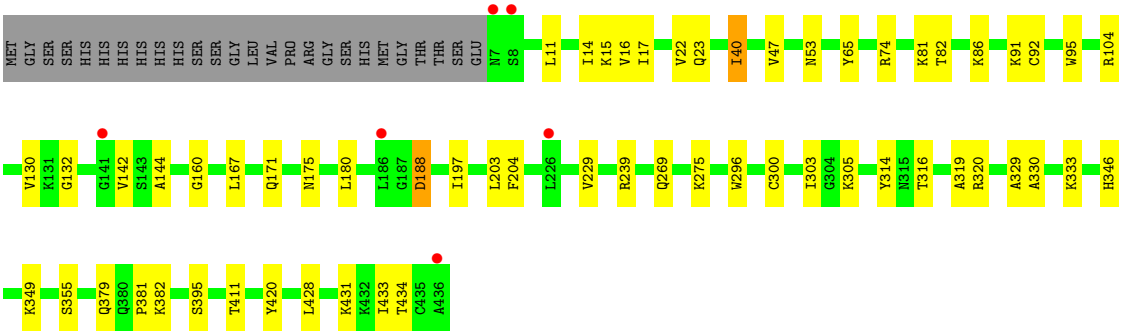
Chain C:





• Molecule 1: Formyl-CoA:oxalate CoA-transferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.16Å 121.61Å 161.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.64 – 1.99 39.64 – 1.99	Depositor EDS
% Data completeness (in resolution range)	88.4 (39.64-1.99) 88.4 (39.64-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.196 , 0.242 0.190 , 0.235	Depositor DCC
R_{free} test set	5889 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14381	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: COA

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	0.38	0/3366	0.53	0/4564
1	B	0.36	0/3380	0.51	0/4583
1	C	0.37	0/3372	0.52	0/4572
1	D	0.36	0/3380	0.52	0/4583
All	All	0.37	0/13498	0.52	0/18302

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	3293	0	3257	56	0
1	B	3307	0	3268	50	0
1	C	3299	0	3262	50	0
1	D	3307	0	3268	51	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	251	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	228	0	0	3	0
3	C	251	0	0	6	0
3	D	253	0	0	7	0
All	All	14381	0	13183	188	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 (188) 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:D:330:ALA:HA	1:D:333:LYS:HD2	1.44	0.95
1:C:320:ARG:O	1:C:322:THR:N	1.99	0.95
1:C:303:ILE:HD11	1:C:331:ILE:HG12	1.51	0.92
1:C:320:ARG:C	1:C:322:THR:H	1.78	0.87
1:C:204:PHE:CE2	1:D:14:ILE:HD11	2.09	0.87
1:A:379:GLN:HG3	3:A:741:HOH:O	1.74	0.86
1:A:17:ILE:HG12	1:A:40:ILE:HD11	1.59	0.85
1:C:112:GLY:O	3:C:569:HOH:O	1.94	0.85
1:C:347:LEU:HB3	1:C:352:VAL:CG2	2.08	0.83
1:B:411:THR:HG21	1:B:434:THR:HG23	1.62	0.81
1:D:316:THR:HG23	1:D:319:ALA:H	1.44	0.81
1:D:142:VAL:O	3:D:947:HOH:O	1.98	0.81
1:A:347:LEU:HB3	1:A:352:VAL:CG2	2.12	0.79
1:D:74:ARG:HD3	3:D:728:HOH:O	1.83	0.78
1:D:329:ALA:O	1:D:333:LYS:HG3	1.86	0.75
1:D:330:ALA:HA	1:D:333:LYS:CD	2.16	0.74
1:D:11:LEU:HA	1:D:14:ILE:HD12	1.71	0.73
1:B:188:ASP:OD1	2:B:2004:COA:S1P	2.44	0.73
1:B:23:GLN:HB3	1:B:188:ASP:OD2	1.89	0.73
1:A:422:ALA:O	1:A:426:LYS:HD3	1.90	0.72
1:B:268:GLY:O	1:B:269:GLN:NE2	2.20	0.72
1:C:320:ARG:O	1:C:323:HIS:N	2.15	0.71
1:D:40:ILE:HD12	1:D:95:TRP:CZ3	2.26	0.71
1:C:74:ARG:HD3	3:C:467:HOH:O	1.90	0.70
1:A:40:ILE:HD12	1:A:95:TRP:CZ3	2.27	0.70
1:C:316:THR:HG23	1:C:319:ALA:H	1.55	0.69
1:A:23:GLN:HB2	1:A:188:ASP:CG	2.13	0.69
1:D:175:ASN:OD1	3:D:837:HOH:O	2.13	0.67
1:D:17:ILE:HD13	1:D:40:ILE:HD11	1.75	0.67
1:A:101:GLU:OE1	1:A:129:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ILE:HD12	1:D:95:TRP:CH2	2.31	0.66
1:B:411:THR:HG21	1:B:434:THR:CG2	2.26	0.65
1:A:160:GLY:HA2	1:B:180:LEU:HD21	1.78	0.65
1:A:23:GLN:HB2	1:A:188:ASP:OD2	1.97	0.65
1:C:347:LEU:HB3	1:C:352:VAL:HG22	1.79	0.64
1:B:313:LYS:O	1:B:313:LYS:HG2	1.98	0.64
1:A:11:LEU:HD12	1:A:35:TYR:HB2	1.78	0.64
1:A:305:LYS:HD2	1:A:308:TRP:CZ2	2.33	0.64
1:B:434:THR:HG22	1:B:434:THR:O	1.98	0.63
1:B:290:THR:HB	1:B:353:PRO:HG2	1.81	0.62
1:B:329:ALA:O	1:B:333:LYS:HG3	1.99	0.62
1:D:346:HIS:O	1:D:349:LYS:HG2	1.98	0.62
1:A:347:LEU:HB3	1:A:352:VAL:HG22	1.81	0.61
1:C:204:PHE:HE2	1:D:14:ILE:HD11	1.65	0.61
1:B:434:THR:CG2	1:B:434:THR:O	2.49	0.61
1:C:23:GLN:HB2	1:C:188:ASP:CG	2.22	0.60
1:B:45:VAL:HA	1:B:77:GLU:HG2	1.83	0.60
1:B:316:THR:HG23	1:B:319:ALA:HB3	1.83	0.60
1:C:180:LEU:HD22	1:D:180:LEU:HD23	1.83	0.60
1:B:379:GLN:OE1	1:B:385:THR:HG22	2.02	0.59
1:B:250:PRO:HG3	1:B:322:THR:HG23	1.84	0.59
1:D:81:LYS:HE2	3:D:543:HOH:O	2.03	0.59
1:B:74:ARG:NH2	1:B:417:GLU:OE2	2.36	0.58
1:D:23:GLN:HB3	1:D:188:ASP:OD2	2.03	0.58
1:A:40:ILE:HD12	1:A:95:TRP:CH2	2.38	0.58
1:B:38:ASP:OD1	3:B:606:HOH:O	2.17	0.58
1:D:91:LYS:HD2	1:D:420:TYR:CE1	2.39	0.57
1:C:14:ILE:HD11	1:D:204:PHE:HE2	1.69	0.57
1:D:17:ILE:CD1	1:D:40:ILE:HD11	2.34	0.57
1:D:428:LEU:HD23	1:D:433:ILE:HD13	1.86	0.57
1:C:180:LEU:CD2	1:D:180:LEU:HD23	2.35	0.57
1:D:17:ILE:HD11	1:D:92:CYS:HB3	1.85	0.57
1:A:45:VAL:HA	1:A:77:GLU:HG2	1.85	0.57
1:C:180:LEU:HD21	1:D:160:GLY:HA2	1.87	0.56
1:C:381:PRO:O	1:C:382:LYS:HB2	2.05	0.56
1:A:324:MET:HA	1:A:324:MET:CE	2.36	0.56
1:B:211:LYS:HE3	3:B:663:HOH:O	2.06	0.56
1:C:57:ASP:OD2	1:D:239:ARG:HD2	2.06	0.56
1:C:320:ARG:C	1:C:322:THR:N	2.48	0.55
1:A:180:LEU:HD23	1:B:180:LEU:HD23	1.89	0.55
1:C:250:PRO:HG3	1:C:322:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ILE:H	1:D:40:ILE:HD13	1.72	0.54
1:D:303:ILE:CG2	1:D:303:ILE:O	2.55	0.54
1:A:47:VAL:HG22	3:A:458:HOH:O	2.06	0.54
1:A:267:GLY:N	3:A:872:HOH:O	2.40	0.54
1:B:86:LYS:O	1:B:90:GLU:HG3	2.08	0.53
1:C:14:ILE:HD11	1:D:204:PHE:CE2	2.43	0.53
1:A:324:MET:HE1	1:A:327:ILE:HG13	1.89	0.53
1:D:40:ILE:CD1	1:D:95:TRP:CZ3	2.91	0.53
1:A:112:GLY:O	3:A:515:HOH:O	2.19	0.53
1:A:180:LEU:CD2	1:B:180:LEU:HD23	2.38	0.53
1:B:16:VAL:HB	1:B:39:VAL:HG22	1.91	0.52
1:C:213:GLN:HB2	1:D:395:SER:OG	2.09	0.52
1:D:11:LEU:CA	1:D:14:ILE:HD12	2.38	0.52
1:A:320:ARG:HB3	1:A:324:MET:CE	2.39	0.52
1:C:47:VAL:HG22	3:C:727:HOH:O	2.08	0.52
1:D:16:VAL:O	1:D:40:ILE:HD13	2.09	0.52
1:B:316:THR:HG23	1:B:319:ALA:CB	2.39	0.52
1:C:15:LYS:HD2	3:C:445:HOH:O	2.10	0.51
1:B:84:GLU:CB	1:B:433:ILE:HD13	2.41	0.51
1:C:196:LEU:HD23	1:D:197:ILE:HD13	1.93	0.51
1:C:269:GLN:OE1	1:C:292:GLN:HG2	2.10	0.51
1:A:132:GLY:HA3	1:A:144:ALA:HB2	1.93	0.51
1:C:132:GLY:HA3	1:C:144:ALA:HB2	1.92	0.51
1:C:242:TYR:HE1	1:C:244:GLU:HG3	1.75	0.50
1:A:324:MET:HA	1:A:324:MET:HE2	1.93	0.50
1:D:303:ILE:HG22	1:D:305:LYS:HG2	1.93	0.50
1:B:303:ILE:HG21	1:B:331:ILE:HG12	1.94	0.49
1:C:25:VAL:HB	1:C:26:PRO:HD3	1.94	0.49
1:A:17:ILE:HA	1:A:40:ILE:HD13	1.94	0.49
1:A:126:ILE:CD1	1:A:203:LEU:HA	2.42	0.49
1:A:186:LEU:HD21	1:B:186:LEU:HD21	1.95	0.49
1:B:84:GLU:HB2	1:B:433:ILE:HD13	1.93	0.49
1:A:402:LYS:HB2	1:A:402:LYS:HE3	1.58	0.49
1:C:352:VAL:HG23	1:C:352:VAL:O	2.12	0.48
1:D:104:ARG:NE	2:D:2003:COA:O9A	2.40	0.48
1:A:239:ARG:CZ	1:B:58:ILE:HD11	2.42	0.48
1:A:320:ARG:HB3	1:A:324:MET:HE3	1.94	0.48
1:B:249:TYR:HE2	1:B:321:GLU:OE2	1.96	0.48
1:B:250:PRO:CG	1:B:322:THR:HG23	2.43	0.48
1:C:271:GLY:HA3	1:C:288:TYR:OH	2.14	0.47
1:B:381:PRO:O	1:B:382:LYS:HB2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:VAL:HG21	3:C:729:HOH:O	2.14	0.47
1:A:293:GLU:HG2	1:A:317:ALA:HB2	1.97	0.47
1:A:305:LYS:HD2	1:A:308:TRP:CE2	2.49	0.47
1:A:379:GLN:NE2	3:A:590:HOH:O	2.48	0.47
1:B:322:THR:O	1:B:322:THR:HG22	2.15	0.47
1:B:432:LYS:HD3	1:B:435:CYS:SG	2.55	0.47
1:B:293:GLU:HA	1:B:320:ARG:HH21	1.79	0.47
1:D:431:LYS:HB2	1:D:433:ILE:HD12	1.97	0.46
1:D:275:LYS:NZ	3:D:482:HOH:O	2.48	0.46
1:C:74:ARG:NH2	1:C:417:GLU:OE2	2.46	0.46
1:C:79:ASN:O	1:C:85:GLY:HA3	2.15	0.46
1:B:82:THR:O	1:B:86:LYS:HG3	2.15	0.46
1:B:351:ARG:HH21	1:C:109:GLU:HG2	1.80	0.46
1:B:234:GLN:O	1:B:238:GLU:HG3	2.16	0.46
1:D:15:LYS:HB3	1:D:95:TRP:CH2	2.52	0.45
1:C:305:LYS:HD3	1:C:308:TRP:CE2	2.51	0.45
1:C:11:LEU:HA	1:C:14:ILE:HD13	1.97	0.45
1:D:47:VAL:HG22	3:D:576:HOH:O	2.15	0.45
1:A:303:ILE:HG21	1:A:331:ILE:HG12	1.99	0.45
1:C:270:PRO:HG2	1:C:324:MET:CE	2.47	0.45
1:A:126:ILE:HD11	1:A:203:LEU:HA	1.98	0.45
1:D:47:VAL:HG23	1:D:53:ASN:ND2	2.32	0.45
1:A:21:GLY:C	1:A:22:VAL:HG23	2.38	0.45
1:A:268:GLY:O	1:A:269:GLN:HG3	2.16	0.45
1:A:347:LEU:HD22	1:A:352:VAL:HG21	1.98	0.45
1:C:74:ARG:CD	3:C:467:HOH:O	2.59	0.45
1:D:229:VAL:HG22	3:D:544:HOH:O	2.17	0.45
1:B:74:ARG:HB3	1:B:410:HIS:CG	2.52	0.45
1:C:234:GLN:O	1:C:238:GLU:HG3	2.17	0.45
1:B:307:GLU:H	1:B:307:GLU:HG3	1.26	0.45
1:A:378:VAL:O	1:A:385:THR:HA	2.17	0.44
1:B:249:TYR:HA	1:B:250:PRO:HA	1.84	0.44
1:C:352:VAL:CG2	1:C:352:VAL:O	2.65	0.44
1:D:14:ILE:HD13	1:D:203:LEU:HD21	2.00	0.44
1:A:163:ASN:OD1	1:A:177:ASN:HB2	2.18	0.44
1:C:15:LYS:HD3	1:C:95:TRP:CE2	2.52	0.44
1:A:180:LEU:HD21	1:B:160:GLY:HA2	2.00	0.44
1:C:126:ILE:CD1	1:C:203:LEU:HA	2.48	0.44
1:C:269:GLN:HA	1:C:270:PRO:HD3	1.78	0.44
1:A:324:MET:HE1	1:A:327:ILE:CG1	2.48	0.44
1:B:209:THR:OG1	1:B:211:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:HB3	1:A:48:GLY:HA2	1.99	0.43
1:A:352:VAL:HA	1:A:353:PRO:HD3	1.86	0.43
1:A:180:LEU:CD2	1:B:180:LEU:CD2	2.97	0.43
1:C:410:HIS:O	1:C:414:VAL:HG23	2.19	0.42
1:D:305:LYS:HZ1	1:D:330:ALA:CB	2.32	0.42
1:A:229:VAL:O	1:A:232:ARG:HB3	2.20	0.42
1:D:381:PRO:O	1:D:382:LYS:HB2	2.19	0.42
1:A:355:SER:OG	1:A:356:PRO:HD2	2.20	0.42
1:B:301:GLU:OE2	3:B:973:HOH:O	2.22	0.42
1:D:411:THR:HG21	1:D:434:THR:HB	2.01	0.42
1:A:288:TYR:O	1:A:354:CYS:HA	2.19	0.42
1:A:186:LEU:O	1:A:190:ASN:HB3	2.19	0.42
1:D:82:THR:O	1:D:86:LYS:HG3	2.19	0.42
1:A:380:GLN:HA	1:A:381:PRO:HD3	1.95	0.41
1:B:311:ASP:OD2	1:B:312:PRO:HD2	2.20	0.41
1:A:40:ILE:CD1	1:A:95:TRP:CZ3	3.02	0.41
1:A:183:ALA:HB1	1:B:230:LYS:HE3	2.01	0.41
1:C:21:GLY:C	1:C:22:VAL:HG23	2.41	0.41
1:A:324:MET:CE	1:A:327:ILE:HG13	2.50	0.41
1:B:316:THR:O	1:B:317:ALA:C	2.59	0.41
1:D:296:TRP:CE2	1:D:300:CYS:SG	3.13	0.41
1:A:280:GLU:H	1:A:280:GLU:CD	2.24	0.41
1:B:74:ARG:HH22	1:B:417:GLU:CD	2.22	0.41
1:D:296:TRP:CZ2	1:D:314:TYR:HB3	2.55	0.41
1:A:130:VAL:HG23	1:A:195:LEU:HD22	2.03	0.41
1:A:347:LEU:O	1:A:352:VAL:HG22	2.21	0.41
1:B:21:GLY:C	1:B:22:VAL:HG23	2.41	0.41
1:D:314:TYR:O	1:D:320:ARG:HG3	2.21	0.41
1:B:23:GLN:HB3	1:B:188:ASP:HB3	2.03	0.41
1:C:296:TRP:CE2	1:C:300:CYS:SG	3.14	0.41
1:C:149:ALA:HB2	1:C:219:MET:HE2	2.03	0.40
1:C:311:ASP:O	1:C:315:ASN:HB3	2.21	0.40
1:D:167:LEU:HA	1:D:171:GLN:OE1	2.21	0.40
1:D:132:GLY:HA3	1:D:144:ALA:HB2	2.02	0.40
1:C:270:PRO:HG2	1:C:324:MET:HE3	2.02	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	426/456 (93%)	413 (97%)	12 (3%)	1 (0%)	47	44
1	B	428/456 (94%)	413 (96%)	14 (3%)	1 (0%)	47	44
1	C	427/456 (94%)	412 (96%)	13 (3%)	2 (0%)	29	23
1	D	428/456 (94%)	418 (98%)	9 (2%)	1 (0%)	47	44
All	All	1709/1824 (94%)	1656 (97%)	48 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	321	GLU
1	A	22	VAL
1	C	22	VAL
1	B	22	VAL
1	D	22	VAL

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	342/366 (93%)	333 (97%)	9 (3%)	46	48
1	B	344/366 (94%)	337 (98%)	7 (2%)	55	58
1	C	343/366 (94%)	337 (98%)	6 (2%)	60	65
1	D	344/366 (94%)	337 (98%)	7 (2%)	55	58
All	All	1373/1464 (94%)	1344 (98%)	29 (2%)	53	57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	40	ILE
1	A	65	TYR
1	A	91	LYS
1	A	189	SER
1	A	218	SER
1	A	269	GLN
1	A	307	GLU
1	A	322	THR
1	B	22	VAL
1	B	47	VAL
1	B	65	TYR
1	B	135	GLU
1	B	188	ASP
1	B	307	GLU
1	B	316	THR
1	C	22	VAL
1	C	65	TYR
1	C	135	GLU
1	C	280	GLU
1	C	294	GLN
1	C	307	GLU
1	D	40	ILE
1	D	65	TYR
1	D	130	VAL
1	D	188	ASP
1	D	269	GLN
1	D	355	SER
1	D	379	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	379	GLN
1	B	23	GLN
1	B	175	ASN
1	D	379	GLN

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	COA	B	2004	-	41,50,50	1.75	5 (12%)	52,75,75	1.47	10 (19%)
2	COA	C	2002	-	41,50,50	1.74	7 (17%)	52,75,75	1.37	7 (13%)
2	COA	D	2003	-	41,50,50	1.75	6 (14%)	52,75,75	1.50	11 (21%)
2	COA	A	2001	-	41,50,50	1.69	5 (12%)	52,75,75	1.51	9 (17%)

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	B	2004	-	-	6/44/64/64	0/3/3/3
2	COA	C	2002	-	-	4/44/64/64	0/3/3/3
2	COA	D	2003	-	-	8/44/64/64	0/3/3/3
2	COA	A	2001	-	-	6/44/64/64	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2004	COA	C9P-N8P	5.65	1.45	1.33
2	C	2002	COA	C9P-N8P	5.54	1.45	1.33
2	D	2003	COA	C9P-N8P	5.50	1.45	1.33
2	A	2001	COA	C9P-N8P	5.34	1.45	1.33
2	C	2002	COA	C5P-N4P	5.18	1.45	1.33
2	D	2003	COA	C5P-N4P	5.04	1.44	1.33
2	B	2004	COA	C5P-N4P	5.00	1.44	1.33
2	A	2001	COA	C5P-N4P	4.69	1.44	1.33
2	D	2003	COA	C2B-C3B	-4.62	1.42	1.52
2	A	2001	COA	C2B-C3B	-4.50	1.42	1.52
2	C	2002	COA	C2B-C3B	-4.33	1.43	1.52
2	B	2004	COA	C2B-C3B	-4.32	1.43	1.52
2	B	2004	COA	C6A-N6A	3.22	1.45	1.34
2	C	2002	COA	C6A-N6A	3.06	1.45	1.34
2	A	2001	COA	C6A-N6A	2.99	1.44	1.34
2	D	2003	COA	C6A-N6A	2.89	1.44	1.34
2	D	2003	COA	C2B-C1B	-2.80	1.49	1.53
2	B	2004	COA	C2B-C1B	-2.63	1.49	1.53
2	A	2001	COA	C2B-C1B	-2.63	1.49	1.53
2	C	2002	COA	C2B-C1B	-2.42	1.50	1.53
2	C	2002	COA	O4B-C1B	-2.02	1.38	1.41
2	C	2002	COA	O6A-CCP	-2.02	1.37	1.43
2	D	2003	COA	C3B-C4B	-2.01	1.47	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2002	COA	N3A-C2A-N1A	-4.92	120.99	128.68
2	A	2001	COA	N3A-C2A-N1A	-4.49	121.67	128.68
2	B	2004	COA	O6A-CCP-CBP	4.35	117.54	110.55
2	B	2004	COA	N3A-C2A-N1A	-4.24	122.05	128.68
2	D	2003	COA	O6A-CCP-CBP	4.18	117.26	110.55
2	D	2003	COA	N3A-C2A-N1A	-4.12	122.23	128.68
2	A	2001	COA	O6A-CCP-CBP	3.62	116.36	110.55
2	D	2003	COA	O4B-C1B-C2B	-3.26	102.17	106.93
2	C	2002	COA	C1B-N9A-C4A	-3.20	121.01	126.64
2	C	2002	COA	O4B-C1B-C2B	-3.15	102.32	106.93
2	B	2004	COA	O4B-C1B-C2B	-3.00	102.54	106.93
2	A	2001	COA	C6P-C7P-N8P	2.96	117.87	111.90
2	A	2001	COA	C1B-N9A-C4A	-2.83	121.67	126.64
2	D	2003	COA	C4A-C5A-N7A	-2.76	106.52	109.40
2	C	2002	COA	CEP-CBP-CCP	2.69	112.62	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2003	COA	O5B-C5B-C4B	2.69	118.24	108.99
2	A	2001	COA	O5P-C5P-N4P	-2.67	117.97	123.01
2	D	2003	COA	C6P-C7P-N8P	2.65	117.25	111.90
2	B	2004	COA	P2A-O3A-P1A	-2.52	124.16	132.83
2	B	2004	COA	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	2001	COA	C7P-N8P-C9P	-2.44	118.24	122.59
2	B	2004	COA	O5B-C5B-C4B	2.43	117.34	108.99
2	A	2001	COA	O4B-C1B-C2B	-2.39	103.43	106.93
2	B	2004	COA	C6P-C7P-N8P	2.30	116.54	111.90
2	D	2003	COA	C1B-N9A-C4A	-2.28	122.63	126.64
2	D	2003	COA	O9P-C9P-N8P	-2.24	118.17	122.99
2	B	2004	COA	C1B-N9A-C4A	-2.22	122.74	126.64
2	C	2002	COA	P2A-O3A-P1A	-2.21	125.25	132.83
2	D	2003	COA	P2A-O3A-P1A	-2.20	125.26	132.83
2	A	2001	COA	O9P-C9P-N8P	-2.20	118.28	122.99
2	B	2004	COA	C6P-C5P-N4P	2.16	120.06	116.42
2	A	2001	COA	C3P-N4P-C5P	-2.15	118.85	122.84
2	C	2002	COA	C6P-C7P-N8P	2.14	116.21	111.90
2	B	2004	COA	CDP-CBP-CCP	2.12	111.70	108.23
2	D	2003	COA	C6P-C5P-N4P	2.10	119.95	116.42
2	D	2003	COA	O5P-C5P-N4P	-2.04	119.16	123.01
2	C	2002	COA	C4A-C5A-N7A	-2.02	107.29	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	COA	C3B-O3B-P3B-O7A
2	A	2001	COA	C5B-O5B-P1A-O1A
2	A	2001	COA	C5P-C6P-C7P-N8P
2	B	2004	COA	C3B-O3B-P3B-O7A
2	B	2004	COA	C5B-O5B-P1A-O1A
2	B	2004	COA	C5P-C6P-C7P-N8P
2	C	2002	COA	C3B-O3B-P3B-O7A
2	C	2002	COA	C5B-O5B-P1A-O1A
2	D	2003	COA	C3B-O3B-P3B-O7A
2	D	2003	COA	C5B-O5B-P1A-O1A
2	D	2003	COA	C5P-C6P-C7P-N8P
2	D	2003	COA	S1P-C2P-C3P-N4P
2	B	2004	COA	CDP-CBP-CCP-O6A
2	D	2003	COA	CDP-CBP-CCP-O6A
2	B	2004	COA	CEP-CBP-CCP-O6A

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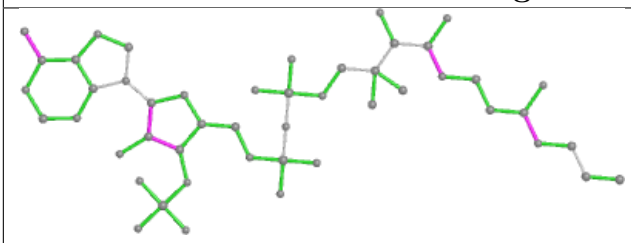
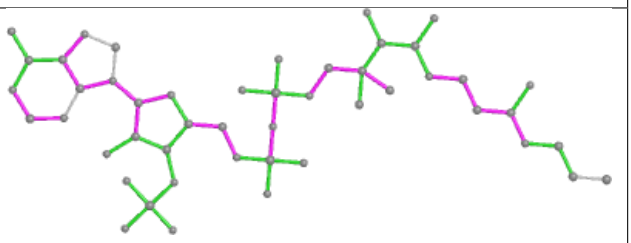
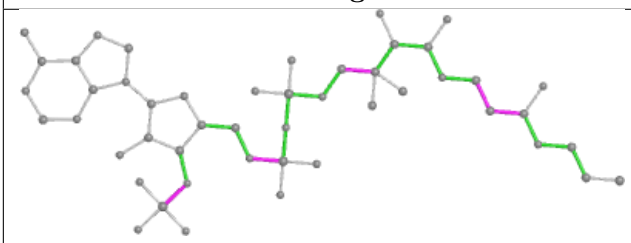
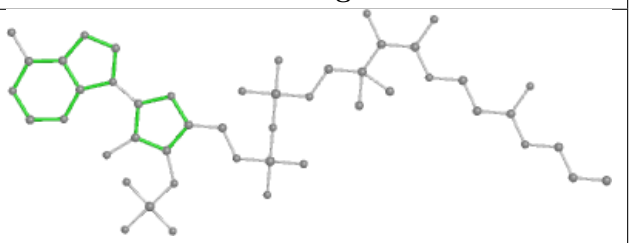
Mol	Chain	Res	Type	Atoms
2	A	2001	COA	CCP-O6A-P2A-O3A
2	C	2002	COA	CCP-O6A-P2A-O3A
2	C	2002	COA	CCP-O6A-P2A-O4A
2	D	2003	COA	CEP-CBP-CCP-O6A
2	D	2003	COA	O5P-C5P-C6P-C7P
2	B	2004	COA	O5P-C5P-C6P-C7P
2	A	2001	COA	O5P-C5P-C6P-C7P
2	A	2001	COA	CCP-O6A-P2A-O4A
2	D	2003	COA	N4P-C5P-C6P-C7P

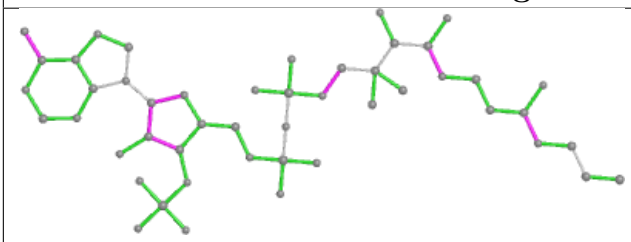
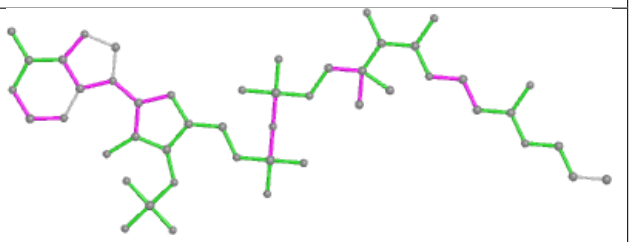
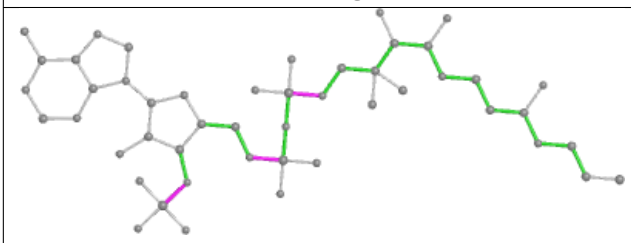
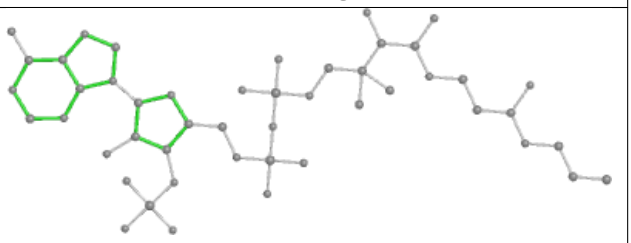
There are no ring outliers.

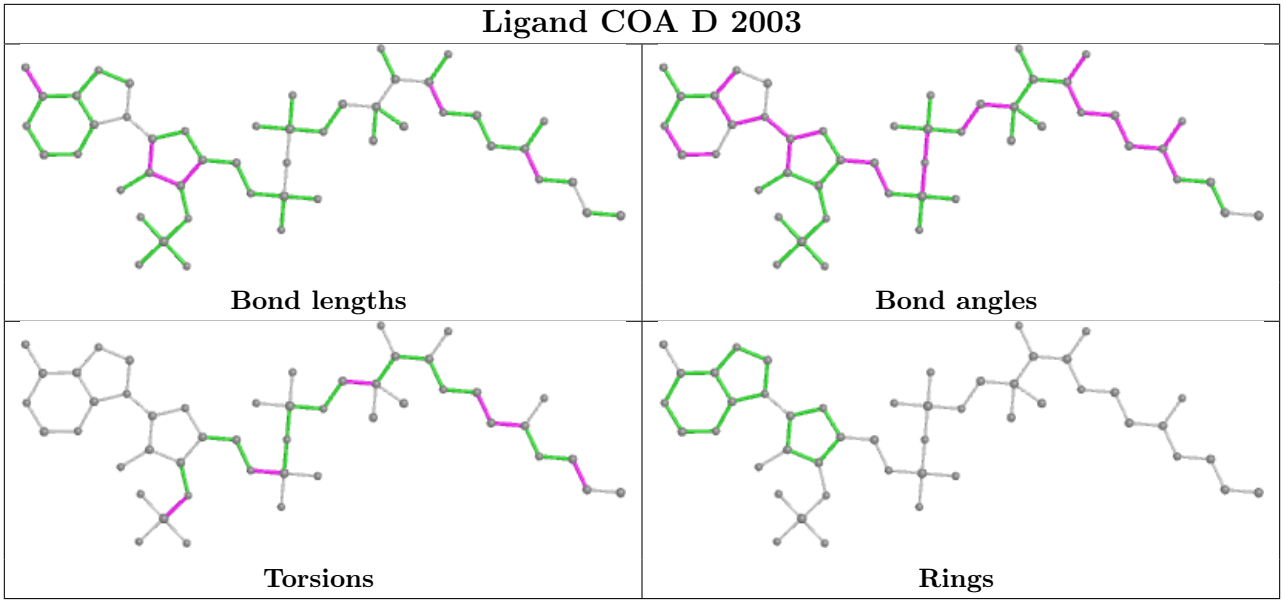
2 monomers are involved in 2 short contacts:

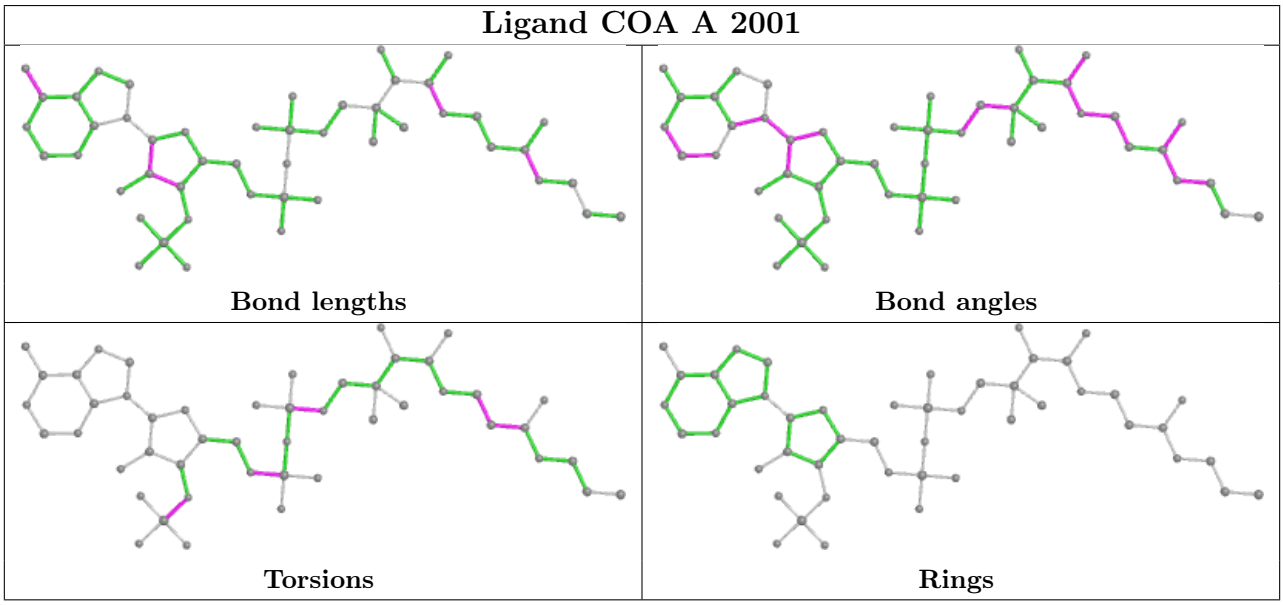
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2004	COA	1	0
2	D	2003	COA	1	0

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 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 B 2004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand COA C 2002	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	428/456 (93%)	-0.14	7 (1%)	72	70	12, 20, 42, 55	0
1	B	430/456 (94%)	-0.17	6 (1%)	75	74	12, 22, 42, 61	0
1	C	429/456 (94%)	-0.07	20 (4%)	31	30	11, 19, 47, 63	0
1	D	430/456 (94%)	-0.22	6 (1%)	75	74	12, 20, 35, 55	0
All	All	1717/1824 (94%)	-0.15	39 (2%)	60	59	11, 21, 40, 63	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	THR	5.6
1	C	312	PRO	4.7
1	C	310	THR	4.5
1	A	310	THR	3.6
1	C	309	ALA	3.5
1	C	268	GLY	3.3
1	A	316	THR	3.3
1	A	322	THR	3.2
1	C	436	ALA	3.2
1	D	7	ASN	3.2
1	C	226	LEU	3.0
1	C	313	LYS	3.0
1	C	315	ASN	3.0
1	D	141	GLY	3.0
1	A	312	PRO	2.9
1	B	436	ALA	2.9
1	C	293	GLU	2.8
1	B	321	GLU	2.7
1	D	8	SER	2.7
1	D	186	LEU	2.6
1	B	7	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	319	ALA	2.5
1	C	308	TRP	2.5
1	C	141	GLY	2.4
1	A	293	GLU	2.4
1	C	186	LEU	2.4
1	B	186	LEU	2.3
1	C	320	ARG	2.3
1	C	322	THR	2.3
1	A	314	TYR	2.2
1	C	311	ASP	2.2
1	B	318	LYS	2.2
1	C	321	GLU	2.2
1	C	303	ILE	2.1
1	B	135	GLU	2.1
1	D	226	LEU	2.1
1	A	155	ALA	2.0
1	D	436	ALA	2.0
1	C	318	LYS	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)

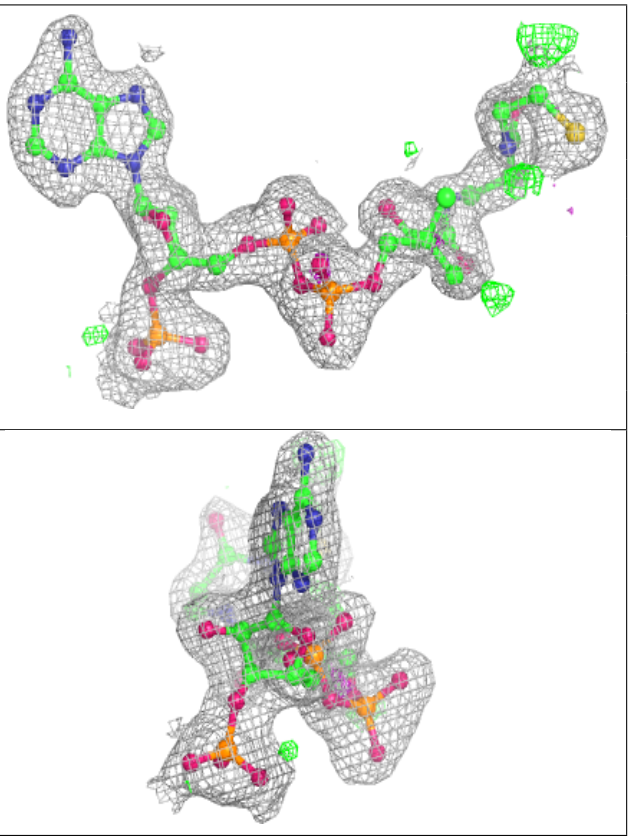
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

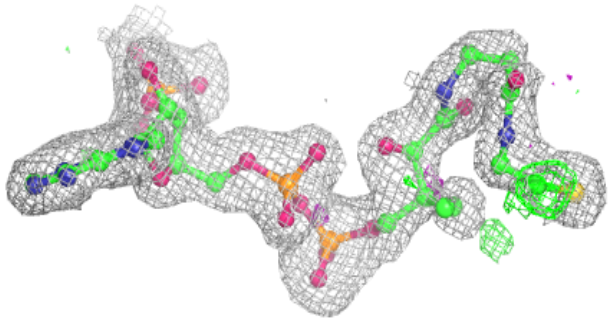
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	COA	D	2003	48/48	0.95	0.09	21,31,42,47	0
2	COA	B	2004	48/48	0.96	0.09	22,28,43,47	0
2	COA	C	2002	48/48	0.97	0.08	12,23,32,48	0
2	COA	A	2001	48/48	0.97	0.08	16,23,35,45	0

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 2003:

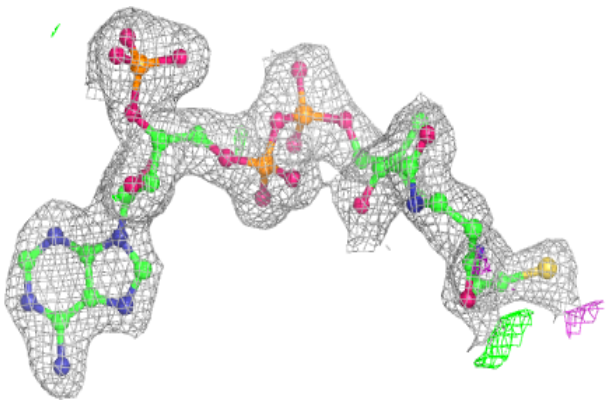
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

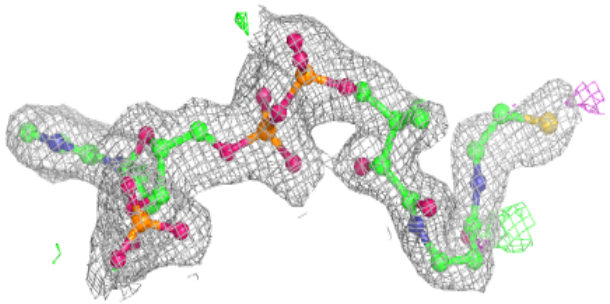


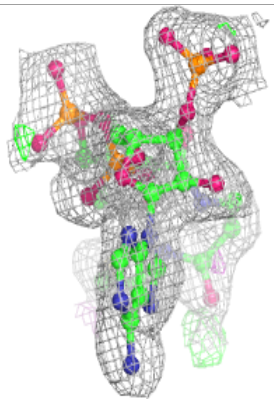


Electron density around COA B 2004:

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

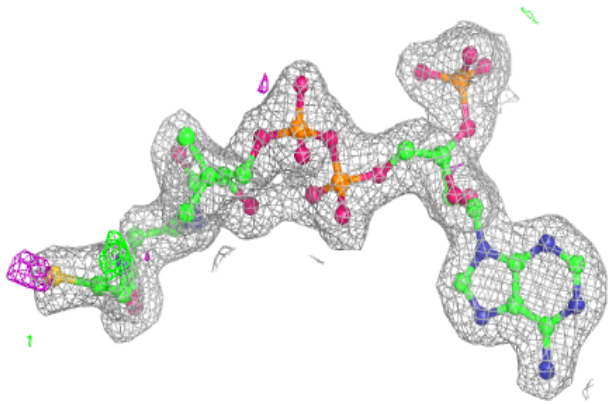


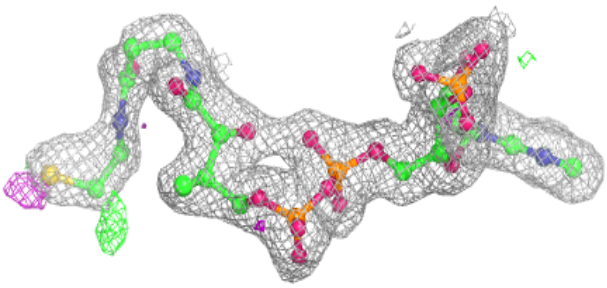


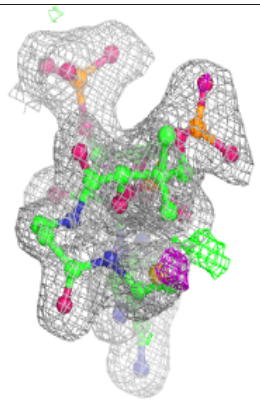


Electron density around COA C 2002:

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

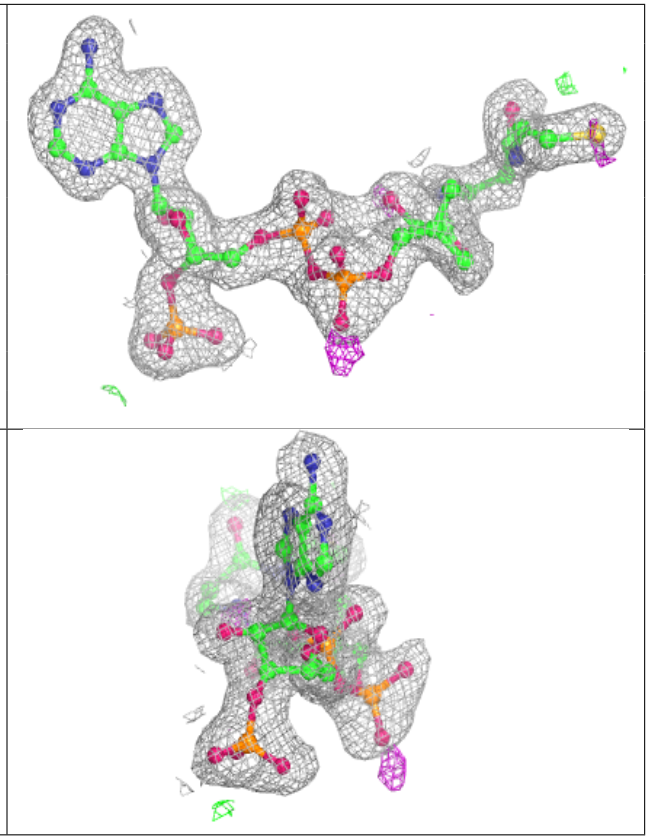






Electron density around COA A 2001:

$2mF_o$-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.