Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 08:53 PM EDT

PDB ID	:	1JKJ
Title	:	E. coli SCS
Authors	:	Fraser, M.E.
Deposited on	:	2001-07-12
Resolution	:	2.35 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:

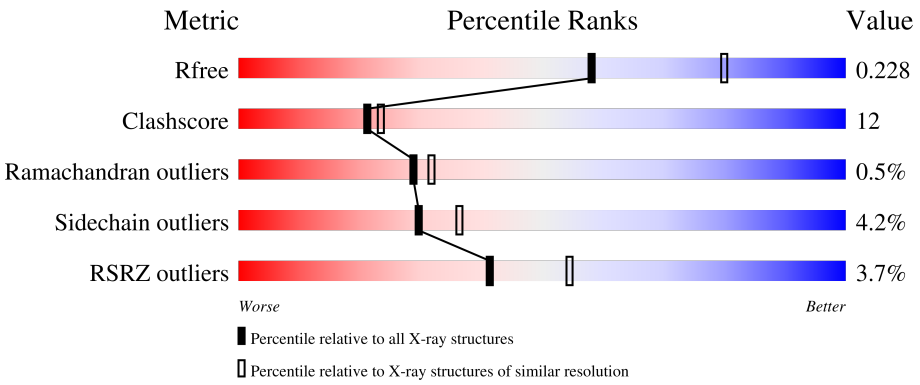
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	288	.% 79% 18% .
1	D	288	2% 76% 22% .
2	B	388	4% 74% 23% .
2	E	388	7% 76% 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
4	COA	E	1904	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10691 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.

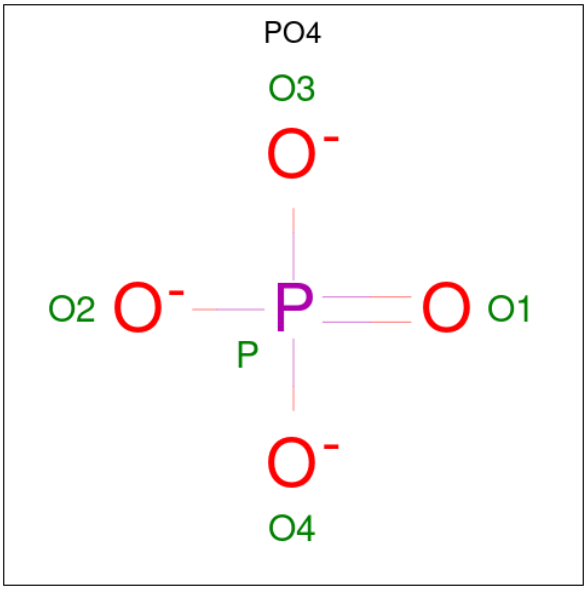
- Molecule 1 is a protein called succinyl-CoA synthetase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2069	1313	346	399	11	0	0	0
1	D	287	2069	1313	346	399	11	0	0	0

- Molecule 2 is a protein called succinyl-CoA synthetase beta subunit.

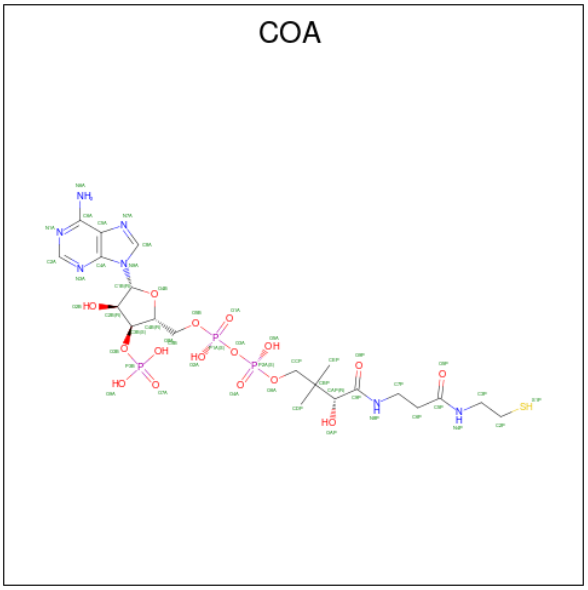
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	388	2908	1836	509	550	13	0	0	0
2	E	385	2885	1823	505	544	13	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



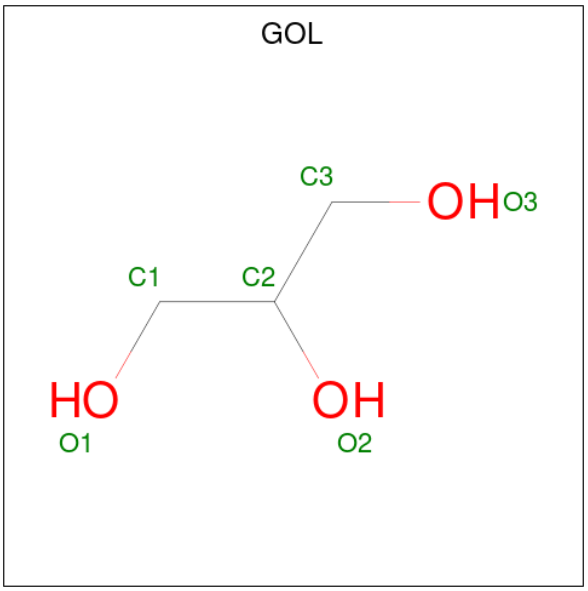
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

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



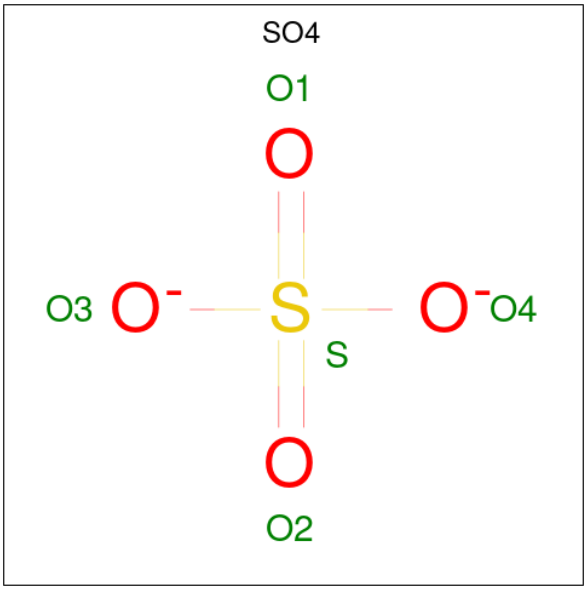
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 48 21 7 16 3 1	0	0
4	B	1	Total C N O S 27 16 7 3 1	0	0
4	D	1	Total C N O P S 48 21 7 16 3 1	0	0
4	E	1	Total C N O S 8 5 1 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	E	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	E	1	5	4	1	0	0

- Molecule 7 is water.

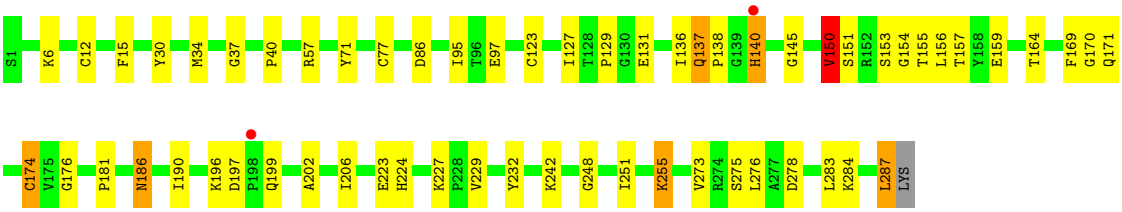
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	146	146	146	0	0
			Total	O		
7	B	191	191	191	0	0
			Total	O		
7	D	96	96	96	0	0
			Total	O		
7	E	160	160	160	0	0

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.

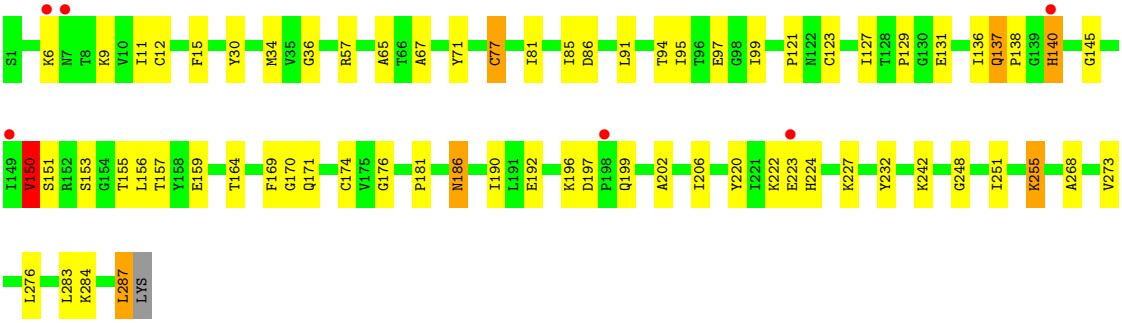
• Molecule 1: succinyl-CoA synthetase alpha subunit

Chain A:



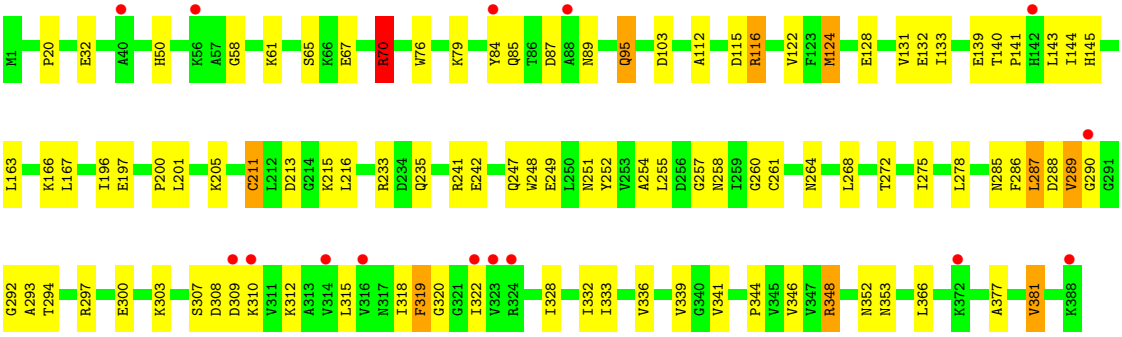
• Molecule 1: succinyl-CoA synthetase alpha subunit

Chain D:



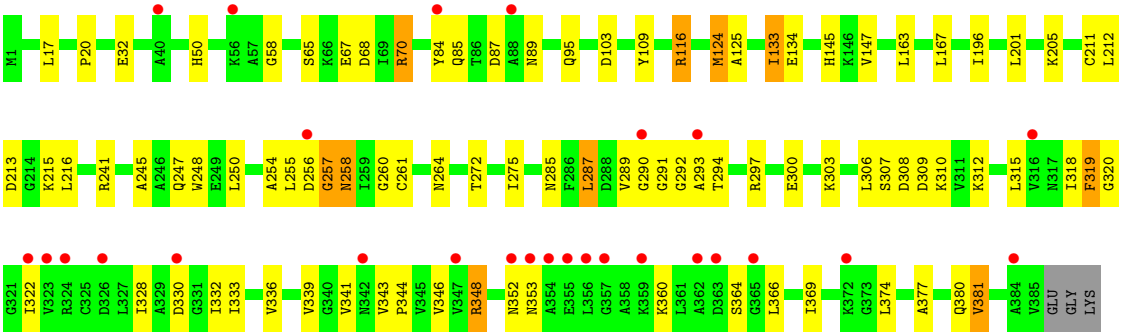
• Molecule 2: succinyl-CoA synthetase beta subunit

Chain B:



• Molecule 2: succinyl-CoA synthetase beta subunit

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.63Å 96.63Å 386.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.64 – 2.35 19.63 – 2.36	Depositor EDS
% Data completeness (in resolution range)	87.7 (19.64-2.35) 88.5 (19.63-2.36)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.35Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.238 0.185 , 0.228	Depositor DCC
R_{free} test set	1063 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10691	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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, GOL, COA, PO4

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	0.81	2/2103 (0.1%)	0.84	1/2849 (0.0%)
1	D	0.76	1/2103 (0.0%)	0.82	1/2849 (0.0%)
2	B	0.80	1/2950 (0.0%)	0.87	5/3989 (0.1%)
2	E	0.73	0/2927	0.85	3/3961 (0.1%)
All	All	0.77	4/10083 (0.0%)	0.85	10/13648 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	CYS	CB-SG	-6.24	1.71	1.82
1	A	77	CYS	CB-SG	-5.89	1.72	1.81
1	D	77	CYS	CB-SG	-5.70	1.72	1.81
2	B	211	CYS	CB-SG	5.02	1.90	1.82

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	150	VAL	CB-CA-C	-6.67	98.73	111.40
2	E	201	LEU	N-CA-C	-6.19	94.30	111.00
1	A	150	VAL	CB-CA-C	-5.81	100.37	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	116	ARG	CB-CG-CD	-5.59	97.07	111.60
2	E	116	ARG	CB-CG-CD	-5.58	97.09	111.60
2	B	201	LEU	N-CA-C	-5.56	95.98	111.00
2	B	115	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	70	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	B	286	PHE	N-CA-C	-5.09	97.25	111.00
2	E	290	GLY	N-CA-C	5.08	125.80	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	TYR	Sidechain
1	D	232	TYR	Sidechain

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	2069	0	2129	50	0
1	D	2069	0	2129	50	0
2	B	2908	0	2962	87	0
2	E	2885	0	2940	73	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	48	0	32	6	0
4	B	27	0	22	8	0
4	D	48	0	32	4	0
4	E	8	0	7	1	0
5	A	6	0	7	3	0
6	B	10	0	0	0	0
6	E	10	0	0	0	0
7	A	146	0	0	2	1
7	B	191	0	0	6	1
7	D	96	0	0	2	0
7	E	160	0	0	7	0
All	All	10691	0	10260	247	1

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 12.

All (247) 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)
2:B:124:MET:SD	2:B:124:MET:CE	2.05	1.45
2:B:320:GLY:HA2	4:B:1903:COA:H32	1.55	0.88
2:E:346:VAL:HB	2:E:381:VAL:HG13	1.61	0.83
2:E:312:LYS:O	2:E:343:VAL:HB	1.79	0.82
2:B:289:VAL:HG12	2:B:289:VAL:O	1.80	0.82
2:B:248:TRP:CD2	2:B:300:GLU:HG3	2.17	0.79
2:E:248:TRP:CD2	2:E:300:GLU:HG3	2.18	0.78
1:A:229:VAL:H	5:A:1700:GOL:H11	1.51	0.76
2:B:346:VAL:HB	2:B:381:VAL:HG13	1.66	0.76
1:D:9:LYS:HE3	7:D:1688:HOH:O	1.88	0.74
2:B:128:GLU:OE2	7:B:1958:HOH:O	2.07	0.73
1:A:57:ARG:NH1	1:A:86:ASP:OD2	2.22	0.72
2:B:352:ASN:HD22	4:B:1903:COA:H72	1.54	0.72
2:B:320:GLY:CA	4:B:1903:COA:H32	2.21	0.71
2:B:318:ILE:HG21	2:B:328:ILE:CD1	2.21	0.71
2:E:241:ARG:HH12	2:E:308:ASP:HB2	1.56	0.70
2:B:352:ASN:ND2	4:B:1903:COA:H72	2.06	0.70
2:E:68:ASP:OD2	7:E:1959:HOH:O	2.10	0.69
1:D:248:GLY:O	2:E:116:ARG:NH2	2.27	0.68
2:E:318:ILE:HG21	2:E:328:ILE:HD13	1.74	0.68
2:E:318:ILE:HG21	2:E:328:ILE:CD1	2.24	0.68
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.28	0.68
1:D:136:ILE:HD11	4:D:1301:COA:H21	1.75	0.68
2:E:248:TRP:CE2	2:E:300:GLU:HG3	2.30	0.67
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.76	0.67
1:A:248:GLY:O	2:B:116:ARG:NH2	2.27	0.67
2:B:124:MET:CE	2:B:124:MET:CB	2.73	0.67
2:B:322:ILE:HG22	4:B:1903:COA:H61A	1.61	0.66
1:A:155:THR:HG21	2:B:264:ASN:O	1.96	0.66
1:D:57:ARG:NH1	1:D:86:ASP:OD2	2.28	0.65
2:E:315:LEU:HB2	2:E:381:VAL:HG11	1.79	0.65
2:B:292:GLY:O	2:B:294:THR:N	2.27	0.64
1:D:186:ASN:HB2	7:D:1636:HOH:O	1.97	0.64
1:A:229:VAL:N	5:A:1700:GOL:H11	2.12	0.64
2:B:141:PRO:HD2	7:B:2065:HOH:O	1.97	0.64
2:E:32:GLU:OE1	2:E:70:ARG:HD2	1.98	0.64
2:E:260:GLY:HA2	2:E:285:ASN:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:289:VAL:HG12	2:E:289:VAL:O	1.98	0.62
1:A:181:PRO:O	2:B:116:ARG:HD3	1.99	0.62
2:B:318:ILE:HG21	2:B:328:ILE:HD13	1.80	0.62
2:B:213:ASP:HB3	7:B:1911:HOH:O	1.99	0.62
1:A:137:GLN:N	1:A:137:GLN:OE1	2.33	0.61
1:A:123:CYS:C	4:A:1300:COA:H22	2.21	0.61
2:E:336:VAL:HG12	2:E:366:LEU:HD22	1.82	0.60
1:A:150:VAL:HG13	1:A:190:ILE:HG21	1.83	0.60
1:D:155:THR:HG21	2:E:264:ASN:O	2.01	0.60
2:B:241:ARG:HH12	2:B:308:ASP:HB2	1.67	0.60
1:D:150:VAL:HG13	1:D:190:ILE:HG21	1.84	0.60
2:E:320:GLY:HA2	4:E:1904:COA:H32	1.83	0.60
2:B:140:THR:HB	2:B:143:LEU:HD12	1.84	0.59
2:B:348:ARG:C	2:B:348:ARG:HD2	2.22	0.59
2:E:346:VAL:CB	2:E:381:VAL:HG13	2.31	0.59
1:A:136:ILE:HD11	4:A:1300:COA:H21	1.84	0.59
2:B:352:ASN:HD22	4:B:1903:COA:C7P	2.15	0.59
2:E:343:VAL:HB	2:E:344:PRO:HD2	1.85	0.59
2:E:297:ARG:NH2	7:E:1953:HOH:O	2.36	0.58
2:E:124:MET:HA	2:E:145:HIS:O	2.03	0.58
2:E:103:ASP:HB3	2:E:205:LYS:HG3	1.85	0.58
1:D:136:ILE:CD1	4:D:1301:COA:H21	2.33	0.58
2:B:260:GLY:HA2	2:B:285:ASN:OD1	2.03	0.57
2:E:377:ALA:O	2:E:381:VAL:HG22	2.04	0.57
2:E:303:LYS:HG3	2:E:339:VAL:HG22	1.86	0.57
2:E:348:ARG:HD2	2:E:348:ARG:C	2.24	0.57
2:E:84:TYR:CE1	2:E:85:GLN:HG3	2.39	0.57
2:B:124:MET:HB2	2:B:124:MET:HE2	1.85	0.57
2:B:303:LYS:HG3	2:B:339:VAL:HG22	1.87	0.57
1:A:186:ASN:C	1:A:186:ASN:HD22	2.08	0.56
2:B:124:MET:CE	2:B:124:MET:HB2	2.35	0.56
2:E:134:GLU:HB2	7:E:2047:HOH:O	2.06	0.56
2:B:103:ASP:HB3	2:B:205:LYS:HG3	1.88	0.56
2:B:289:VAL:O	2:B:289:VAL:CG1	2.50	0.56
2:B:32:GLU:OE1	2:B:70:ARG:HD2	2.06	0.55
2:E:312:LYS:O	2:E:344:PRO:HD2	2.07	0.55
1:A:199:GLN:O	1:A:199:GLN:HG2	2.05	0.55
2:E:292:GLY:O	2:E:294:THR:HG23	2.07	0.55
1:D:223:GLU:HG2	1:D:224:HIS:CD2	2.42	0.55
1:D:196:LYS:O	1:D:196:LYS:HG2	2.06	0.54
2:E:58:GLY:HA2	7:E:2016:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:SER:HB3	1:D:157:THR:OG1	2.08	0.54
1:D:137:GLN:OE1	1:D:137:GLN:N	2.41	0.54
2:B:352:ASN:O	2:B:353:ASN:HB2	2.08	0.54
1:A:123:CYS:O	4:A:1300:COA:H22	2.08	0.54
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.43	0.54
2:B:333:ILE:HG23	2:B:366:LEU:CD1	2.38	0.54
2:E:306:LEU:CD1	2:E:341:VAL:HG22	2.37	0.54
1:A:129:PRO:HG2	1:A:171:GLN:HB2	1.90	0.53
1:A:151:SER:HB3	1:A:157:THR:OG1	2.08	0.53
1:A:202:ALA:HB2	1:A:287:LEU:HD11	1.90	0.53
1:A:12:CYS:HB2	1:A:34:MET:HE1	1.91	0.53
2:E:297:ARG:NH1	2:E:297:ARG:HB2	2.23	0.53
1:A:123:CYS:HB2	1:A:176:GLY:O	2.09	0.53
1:D:186:ASN:C	1:D:186:ASN:HD22	2.12	0.53
1:A:196:LYS:O	1:A:196:LYS:HG2	2.08	0.53
2:E:352:ASN:O	2:E:353:ASN:HB2	2.08	0.53
1:D:145:GLY:HA3	1:D:170:GLY:HA3	1.91	0.52
2:E:50:HIS:HD2	7:E:1906:HOH:O	1.93	0.52
1:D:202:ALA:HB2	1:D:287:LEU:HD11	1.91	0.52
2:E:213:ASP:HB3	7:E:2010:HOH:O	2.08	0.52
1:D:199:GLN:O	1:D:199:GLN:HG2	2.10	0.52
2:E:196:ILE:HG12	2:E:216:LEU:HD22	1.92	0.51
1:A:151:SER:HB2	1:A:206:ILE:HB	1.92	0.51
2:B:292:GLY:O	2:B:294:THR:HG23	2.11	0.51
1:D:123:CYS:HB2	1:D:176:GLY:O	2.11	0.51
2:B:87:ASP:OD1	2:B:89:ASN:N	2.31	0.51
2:B:312:LYS:O	2:B:344:PRO:HD2	2.10	0.50
2:B:336:VAL:HA	2:B:341:VAL:CG2	2.41	0.50
1:D:169:PHE:HZ	1:D:284:LYS:HA	1.76	0.50
2:E:241:ARG:HD3	2:E:307:SER:OG	2.12	0.50
2:B:124:MET:HG3	2:B:144:ILE:HG23	1.94	0.50
1:D:192:GLU:HB2	1:D:220:TYR:OH	2.12	0.50
2:E:87:ASP:OD1	2:E:89:ASN:N	2.32	0.50
2:E:289:VAL:O	2:E:289:VAL:CG1	2.59	0.50
2:B:310:LYS:HE2	2:B:310:LYS:HA	1.93	0.50
2:B:346:VAL:CB	2:B:381:VAL:HG13	2.38	0.50
2:B:251:ASN:HB2	2:B:288:ASP:HB3	1.94	0.49
2:E:215:LYS:O	2:E:216:LEU:HD23	2.12	0.49
2:B:58:GLY:HA2	7:B:1949:HOH:O	2.12	0.49
2:B:242:GLU:HG2	2:B:252:TYR:O	2.11	0.49
2:B:140:THR:CB	2:B:143:LEU:HD12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:N	1:A:131:GLU:HB3	2.27	0.49
1:D:159:GLU:OE2	2:E:319:PHE:HD2	1.94	0.49
1:D:11:ILE:HA	1:D:36:GLY:O	2.12	0.49
1:D:129:PRO:HG2	1:D:171:GLN:HB2	1.94	0.49
2:B:50:HIS:HD2	7:B:1918:HOH:O	1.96	0.49
2:B:215:LYS:O	2:B:216:LEU:HD23	2.12	0.49
1:D:67:ALA:HA	1:D:91:LEU:O	2.13	0.49
1:D:71:TYR:CE1	1:D:95:ILE:HG13	2.48	0.49
1:D:251:ILE:HG23	1:D:255:LYS:O	2.13	0.48
1:A:164:THR:HG22	1:A:283:LEU:CD1	2.44	0.48
2:B:254:ALA:C	2:B:255:LEU:HD12	2.34	0.48
2:B:333:ILE:HG23	2:B:366:LEU:HD12	1.94	0.48
2:E:133:ILE:O	2:E:133:ILE:HG12	2.14	0.48
1:A:97:GLU:HB3	4:A:1300:COA:H71	1.96	0.48
2:B:131:VAL:HG12	2:B:132:GLU:N	2.29	0.48
2:B:249:GLU:OE1	2:E:70:ARG:NH2	2.46	0.48
2:B:163:LEU:O	2:B:167:LEU:HG	2.14	0.48
2:E:330:ASP:OD1	2:E:360:LYS:HD3	2.13	0.48
1:A:275:SER:HB2	2:B:278:LEU:CD2	2.44	0.48
2:E:272:THR:O	2:E:275:ILE:HG22	2.14	0.47
2:B:249:GLU:CD	2:E:70:ARG:HH22	2.17	0.47
2:B:292:GLY:HA3	2:B:322:ILE:HD11	1.96	0.47
2:E:292:GLY:HA2	2:E:322:ILE:HD11	1.97	0.47
2:B:87:ASP:OD1	2:B:87:ASP:C	2.52	0.47
2:B:261:CYS:O	2:B:287:LEU:HB3	2.15	0.47
1:D:164:THR:HG22	1:D:283:LEU:CD1	2.45	0.47
2:E:87:ASP:OD1	2:E:87:ASP:C	2.53	0.47
2:E:346:VAL:CG2	2:E:381:VAL:HG13	2.44	0.47
1:D:12:CYS:O	1:D:15:PHE:HB2	2.15	0.47
1:D:199:GLN:O	1:D:199:GLN:CG	2.63	0.47
2:E:254:ALA:C	2:E:255:LEU:HD12	2.35	0.47
2:E:67:GLU:CD	2:E:67:GLU:H	2.18	0.47
2:B:297:ARG:NH1	2:B:297:ARG:HB2	2.29	0.46
2:E:261:CYS:O	2:E:287:LEU:HB3	2.16	0.46
1:A:229:VAL:H	5:A:1700:GOL:C1	2.25	0.46
1:D:197:ASP:O	1:D:227:LYS:NZ	2.49	0.46
2:B:112:ALA:HA	2:B:122:VAL:O	2.16	0.46
2:B:196:ILE:HG12	2:B:216:LEU:HD22	1.97	0.46
2:B:233:ARG:HD3	2:B:235:GLN:HE21	1.81	0.46
2:E:292:GLY:O	2:E:294:THR:N	2.42	0.46
1:A:12:CYS:O	1:A:15:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:H	1:A:137:GLN:CD	2.19	0.45
1:D:94:THR:O	1:D:121:PRO:HA	2.16	0.45
1:A:145:GLY:HA3	1:A:170:GLY:HA3	1.98	0.45
2:E:20:PRO:HD3	2:E:211:CYS:O	2.15	0.45
1:A:71:TYR:CE1	1:A:95:ILE:HG13	2.51	0.45
2:B:65:SER:HB2	2:B:67:GLU:OE1	2.17	0.45
1:D:123:CYS:C	4:D:1301:COA:H22	2.37	0.45
2:B:319:PHE:CD1	2:B:319:PHE:C	2.90	0.45
2:E:275:ILE:HD13	2:E:374:LEU:HG	1.98	0.45
2:E:17:LEU:N	2:E:17:LEU:HD23	2.32	0.45
1:A:138:PRO:HA	1:A:140:HIS:CE1	2.52	0.45
1:A:199:GLN:O	1:A:199:GLN:CG	2.64	0.45
2:B:145:HIS:ND1	2:B:166:LYS:HD3	2.32	0.45
2:B:322:ILE:HB	4:B:1903:COA:N6A	2.32	0.45
1:A:127:ILE:HG22	1:A:174:CYS:HB2	2.00	0.44
1:D:81:ILE:O	1:D:85:ILE:HG13	2.17	0.44
1:D:138:PRO:HA	1:D:140:HIS:CE1	2.53	0.44
2:E:328:ILE:O	2:E:332:ILE:HG13	2.17	0.44
2:B:197:GLU:HB3	2:B:215:LYS:HB3	1.99	0.44
1:A:223:GLU:HG2	1:A:224:HIS:CD2	2.52	0.44
1:D:6:LYS:N	1:D:131:GLU:HB3	2.33	0.44
1:D:151:SER:CB	1:D:157:THR:OG1	2.66	0.44
2:B:377:ALA:O	2:B:381:VAL:HG22	2.17	0.44
1:D:30:TYR:OH	1:D:129:PRO:HA	2.17	0.44
2:E:258:ASN:H	2:E:258:ASN:HD22	1.65	0.44
1:D:151:SER:HA	1:D:206:ILE:O	2.18	0.44
1:A:15:PHE:CD2	1:A:37:GLY:HA3	2.53	0.43
1:A:278:ASP:OD2	7:A:1729:HOH:O	2.21	0.43
2:E:241:ARG:CD	2:E:307:SER:OG	2.65	0.43
1:A:30:TYR:OH	1:A:129:PRO:HA	2.19	0.43
2:B:95:GLN:HE21	2:B:95:GLN:HB2	1.39	0.43
2:B:322:ILE:CG2	4:B:1903:COA:H61A	2.30	0.43
1:A:136:ILE:CD1	4:A:1300:COA:H21	2.48	0.43
1:D:159:GLU:OE1	2:E:348:ARG:NH2	2.51	0.43
1:D:127:ILE:HG22	1:D:174:CYS:HB2	1.99	0.43
2:B:61:LYS:HD3	7:B:2078:HOH:O	2.19	0.43
2:E:65:SER:HB2	2:E:67:GLU:OE1	2.18	0.43
1:D:181:PRO:O	2:E:116:ARG:HD3	2.17	0.43
1:A:154:GLY:O	1:A:157:THR:HB	2.19	0.43
2:B:139:GLU:C	2:B:141:PRO:HD3	2.39	0.43
2:B:241:ARG:HD3	2:B:307:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:CB	1:A:206:ILE:HB	2.50	0.42
1:A:169:PHE:HZ	1:A:284:LYS:HA	1.84	0.42
2:B:20:PRO:HD3	2:B:211:CYS:O	2.19	0.42
1:D:151:SER:HB2	1:D:206:ILE:HB	2.00	0.42
1:D:99:ILE:HD12	1:D:121:PRO:CB	2.50	0.42
2:E:306:LEU:HD11	2:E:341:VAL:HG22	2.02	0.42
2:B:76:TRP:O	2:B:79:LYS:HB3	2.19	0.42
1:A:151:SER:CB	1:A:157:THR:OG1	2.68	0.42
1:A:155:THR:OG1	2:B:268:LEU:HB2	2.19	0.42
2:E:285:ASN:HB3	7:E:1943:HOH:O	2.19	0.42
1:A:251:ILE:HG23	1:A:255:LYS:O	2.20	0.42
2:B:241:ARG:CD	2:B:307:SER:OG	2.67	0.42
2:B:310:LYS:HE2	2:B:310:LYS:CA	2.50	0.42
1:D:11:ILE:HG23	1:D:65:ALA:CB	2.50	0.42
1:D:138:PRO:HB2	1:D:140:HIS:ND1	2.35	0.42
2:E:256:ASP:O	2:E:257:GLY:O	2.38	0.42
1:A:155:THR:HB	2:B:268:LEU:HB2	2.01	0.42
1:A:197:ASP:O	1:A:227:LYS:NZ	2.53	0.42
2:B:133:ILE:HD12	2:B:133:ILE:HA	1.81	0.42
1:D:12:CYS:HB2	1:D:34:MET:HE1	2.02	0.41
1:A:151:SER:HA	1:A:206:ILE:O	2.20	0.41
1:A:156:LEU:CD2	1:A:276:LEU:HD22	2.50	0.41
2:E:310:LYS:HE2	2:E:310:LYS:HA	2.01	0.41
4:A:1300:COA:H2B	7:A:1817:HOH:O	2.20	0.41
2:E:32:GLU:CD	2:E:70:ARG:HH11	2.23	0.41
2:E:333:ILE:HG23	2:E:366:LEU:HD12	2.02	0.41
1:A:138:PRO:HB2	1:A:140:HIS:ND1	2.36	0.41
2:E:369:ILE:HG21	2:E:380:GLN:OE1	2.20	0.41
1:D:222:LYS:HB2	1:D:268:ALA:HB1	2.03	0.41
1:D:287:LEU:HD12	1:D:287:LEU:HA	1.89	0.41
2:B:328:ILE:O	2:B:332:ILE:HG13	2.20	0.41
1:D:255:LYS:HE2	1:D:255:LYS:HA	2.03	0.41
2:E:147:VAL:HG22	2:E:163:LEU:HD11	2.02	0.41
2:E:245:ALA:HB1	2:E:250:LEU:HB2	2.02	0.41
1:A:57:ARG:NH1	1:A:86:ASP:O	2.53	0.41
2:B:67:GLU:H	2:B:67:GLU:CD	2.24	0.41
1:D:97:GLU:HB3	4:D:1301:COA:H71	2.02	0.41
1:D:156:LEU:CD2	1:D:276:LEU:HD22	2.51	0.40
2:E:212:LEU:HA	2:E:212:LEU:HD12	1.86	0.40
1:A:159:GLU:OE1	2:B:348:ARG:NH2	2.55	0.40
2:B:124:MET:CE	2:B:124:MET:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:PHE:C	2:B:319:PHE:HD1	2.24	0.40
2:E:109:TYR:O	2:E:125:ALA:HA	2.21	0.40
2:B:272:THR:O	2:B:275:ILE:HG22	2.20	0.40
2:B:287:LEU:C	2:B:287:LEU:CD1	2.90	0.40
2:E:163:LEU:O	2:E:167:LEU:HG	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1753:HOH:O	7:B:2072:HOH:O[7_555]	2.16	0.04

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	285/288 (99%)	279 (98%)	6 (2%)	0	100	100
1	D	285/288 (99%)	275 (96%)	10 (4%)	0	100	100
2	B	386/388 (100%)	374 (97%)	8 (2%)	4 (1%)	15	15
2	E	383/388 (99%)	371 (97%)	9 (2%)	3 (1%)	19	20
All	All	1339/1352 (99%)	1299 (97%)	33 (2%)	7 (0%)	29	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	293	ALA
2	E	293	ALA
2	B	257	GLY
2	B	289	VAL
2	B	290	GLY

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Mol	Chain	Res	Type
2	E	257	GLY
2	E	291	GLY

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	217/218 (100%)	207 (95%)	10 (5%)	27	32
1	D	217/218 (100%)	207 (95%)	10 (5%)	27	32
2	B	298/298 (100%)	287 (96%)	11 (4%)	34	42
2	E	296/298 (99%)	284 (96%)	12 (4%)	30	37
All	All	1028/1032 (100%)	985 (96%)	43 (4%)	30	36

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	137	GLN
1	A	140	HIS
1	A	150	VAL
1	A	153	SER
1	A	186	ASN
1	A	242	LYS
1	A	255	LYS
1	A	273	VAL
1	A	287	LEU
2	B	70	ARG
2	B	95	GLN
2	B	124	MET
2	B	200	PRO
2	B	247	GLN
2	B	258	ASN
2	B	287	LEU
2	B	309	ASP
2	B	319	PHE

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Mol	Chain	Res	Type
2	B	348	ARG
2	B	381	VAL
1	D	77	CYS
1	D	137	GLN
1	D	140	HIS
1	D	150	VAL
1	D	153	SER
1	D	186	ASN
1	D	242	LYS
1	D	255	LYS
1	D	273	VAL
1	D	287	LEU
2	E	70	ARG
2	E	95	GLN
2	E	124	MET
2	E	133	ILE
2	E	247	GLN
2	E	258	ASN
2	E	287	LEU
2	E	309	ASP
2	E	319	PHE
2	E	348	ARG
2	E	364	SER
2	E	381	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
2	B	50	HIS
2	B	85	GLN
2	B	95	GLN
2	B	235	GLN
2	B	258	ASN
2	B	342	ASN
2	B	352	ASN
2	E	50	HIS
2	E	95	GLN
2	E	235	GLN
2	E	258	ASN
2	E	279	HIS
2	E	342	ASN

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Mol	Chain	Res	Type
2	E	353	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)

11 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	$\#\|Z\| > 2$
4	COA	D	1301	-	41,50,50	0.93	2 (4%)	52,75,75	1.74	11 (21%)
4	COA	A	1300	-	41,50,50	1.05	1 (2%)	52,75,75	1.77	9 (17%)
3	PO4	A	1600	-	4,4,4	1.42	1 (25%)	6,6,6	0.49	0
4	COA	E	1904	2	6,7,50	2.32	3 (50%)	6,7,75	3.31	5 (83%)
3	PO4	D	1601	-	4,4,4	1.52	1 (25%)	6,6,6	0.43	0
4	COA	B	1903	2	23,27,50	4.76	7 (30%)	26,36,75	3.58	12 (46%)
6	SO4	B	1500	-	4,4,4	0.52	0	6,6,6	0.41	0
6	SO4	B	1400	-	4,4,4	0.34	0	6,6,6	0.19	0
6	SO4	E	1401	-	4,4,4	0.41	0	6,6,6	0.26	0
6	SO4	E	1501	-	4,4,4	0.45	0	6,6,6	0.37	0
5	GOL	A	1700	-	5,5,5	0.53	0	5,5,5	1.87	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	D	1301	-	-	1/44/64/64	0/3/3/3
4	COA	A	1300	-	-	1/44/64/64	0/3/3/3
4	COA	E	1904	2	-	0/6/6/64	-
4	COA	B	1903	2	-	4/20/20/64	0/2/2/3
5	GOL	A	1700	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1903	COA	CBP-CAP	20.26	1.69	1.55
4	B	1903	COA	C6P-C5P	6.96	1.64	1.51
4	B	1903	COA	C3P-N4P	3.96	1.55	1.46
4	B	1903	COA	C7P-N8P	3.72	1.54	1.46
4	E	1904	COA	C6P-C5P	3.61	1.62	1.51
4	E	1904	COA	C3P-N4P	2.92	1.52	1.46
4	B	1903	COA	C2P-S1P	2.90	1.91	1.80
4	E	1904	COA	C2P-S1P	2.90	1.91	1.80
4	A	1300	COA	C6P-C5P	2.75	1.56	1.51
3	A	1600	PO4	P-O2	-2.19	1.48	1.54
4	B	1903	COA	C4A-N9A	2.11	1.38	1.34
3	D	1601	PO4	P-O2	-2.09	1.48	1.54
4	D	1301	COA	C8A-N7A	-2.04	1.31	1.34
4	D	1301	COA	C6P-C5P	2.01	1.55	1.51
4	B	1903	COA	OAP-CAP	2.00	1.46	1.42

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1903	COA	C7P-C6P-C5P	8.74	126.91	112.36
4	B	1903	COA	OAP-CAP-CBP	-8.34	94.34	109.45
4	B	1903	COA	C6P-C7P-N8P	6.59	125.20	111.90
4	D	1301	COA	C6P-C5P-N4P	6.47	127.32	116.42
4	B	1903	COA	CEP-CBP-CCP	-5.80	97.53	108.80
4	B	1903	COA	O5P-C5P-N4P	-5.49	112.66	123.01
4	A	1300	COA	O5P-C5P-C6P	-5.01	112.85	122.02
4	A	1300	COA	CDP-CBP-CAP	-4.67	100.72	108.82
4	D	1301	COA	O5P-C5P-C6P	-4.66	113.50	122.02
4	A	1300	COA	C6P-C5P-N4P	4.57	124.12	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1904	COA	C3P-N4P-C5P	4.37	130.96	122.84
4	E	1904	COA	C7P-C6P-C5P	4.22	126.70	113.30
4	E	1904	COA	C6P-C5P-N4P	4.13	120.15	115.79
4	B	1903	COA	CAP-C9P-N8P	3.93	124.40	116.58
4	A	1300	COA	CEP-CBP-CAP	3.75	115.32	108.82
4	D	1301	COA	CEP-CBP-CAP	3.74	115.31	108.82
4	B	1903	COA	C7P-N8P-C9P	3.74	129.26	122.59
4	D	1301	COA	C2P-C3P-N4P	-3.59	104.10	112.31
4	D	1301	COA	O3B-P3B-O7A	-3.31	96.63	109.39
4	A	1300	COA	O4B-C1B-C2B	-3.29	102.12	106.93
4	A	1300	COA	C2P-C3P-N4P	-3.24	104.89	112.31
4	B	1903	COA	C6P-C5P-N4P	3.22	121.84	116.42
4	A	1300	COA	P2A-O3A-P1A	-3.09	122.24	132.83
4	D	1301	COA	P2A-O3A-P1A	-3.05	122.37	132.83
4	E	1904	COA	O5P-C5P-N4P	-2.68	117.95	123.01
4	B	1903	COA	C3P-N4P-C5P	2.67	127.79	122.84
4	A	1300	COA	C5A-C6A-N6A	2.56	124.24	120.35
5	A	1700	GOL	O2-C2-C1	2.53	120.28	109.12
4	A	1300	COA	CEP-CBP-CDP	2.51	114.28	109.17
4	D	1301	COA	O4B-C1B-C2B	-2.45	103.35	106.93
5	A	1700	GOL	O2-C2-C3	2.44	119.85	109.12
4	B	1903	COA	O9P-C9P-N8P	-2.42	117.81	122.99
4	B	1903	COA	C5A-C6A-N6A	2.34	123.91	120.35
4	B	1903	COA	CDP-CBP-CAP	2.28	114.85	109.59
4	D	1301	COA	O6A-CCP-CBP	-2.26	106.92	110.55
4	E	1904	COA	C2P-C3P-N4P	2.15	117.23	112.31
4	D	1301	COA	CDP-CBP-CAP	-2.11	105.17	108.82
5	A	1700	GOL	C3-C2-C1	2.10	119.86	111.70
4	D	1301	COA	C5A-C6A-N6A	2.09	123.52	120.35
4	D	1301	COA	O5P-C5P-N4P	-2.03	119.18	123.01

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1903	COA	O9P-C9P-CAP-CBP
4	B	1903	COA	N8P-C9P-CAP-CBP
4	B	1903	COA	O9P-C9P-CAP-OAP
4	B	1903	COA	N8P-C9P-CAP-OAP
5	A	1700	GOL	O1-C1-C2-O2
5	A	1700	GOL	O2-C2-C3-O3
4	D	1301	COA	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	A	1300	COA	O4B-C4B-C5B-O5B

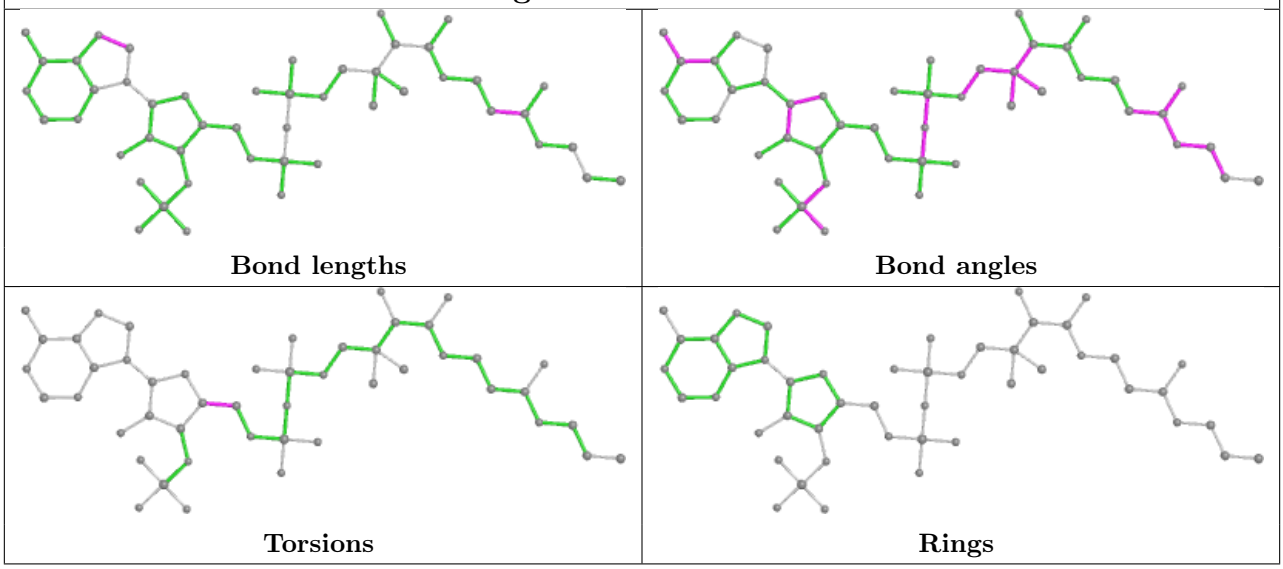
There are no ring outliers.

5 monomers are involved in 22 short contacts:

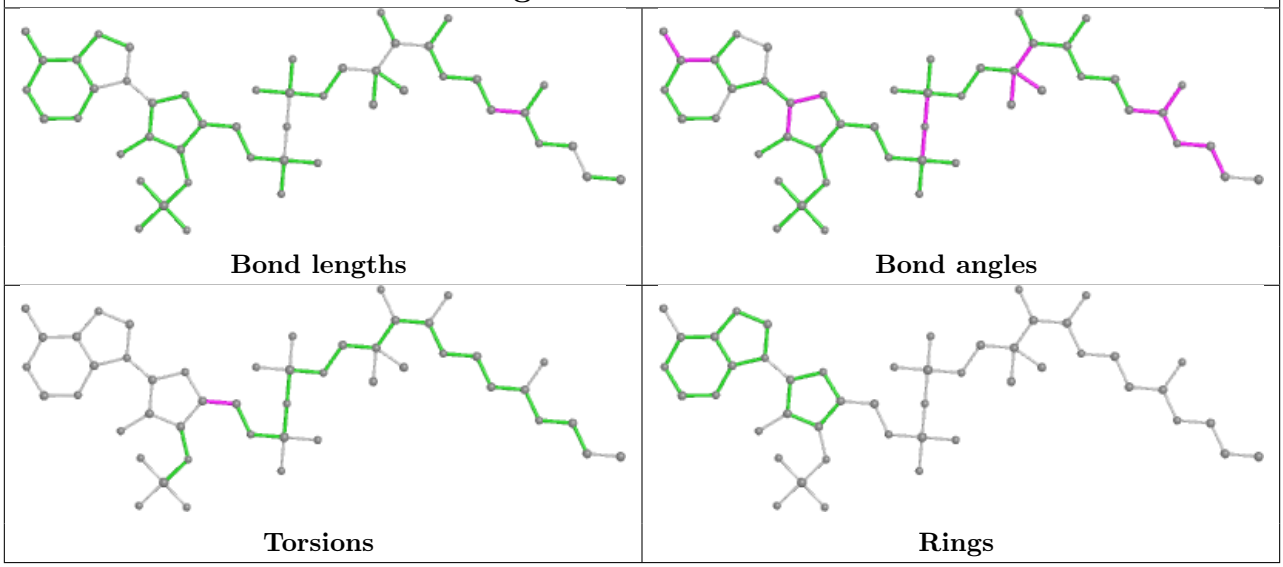
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1301	COA	4	0
4	A	1300	COA	6	0
4	E	1904	COA	1	0
4	B	1903	COA	8	0
5	A	1700	GOL	3	0

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.

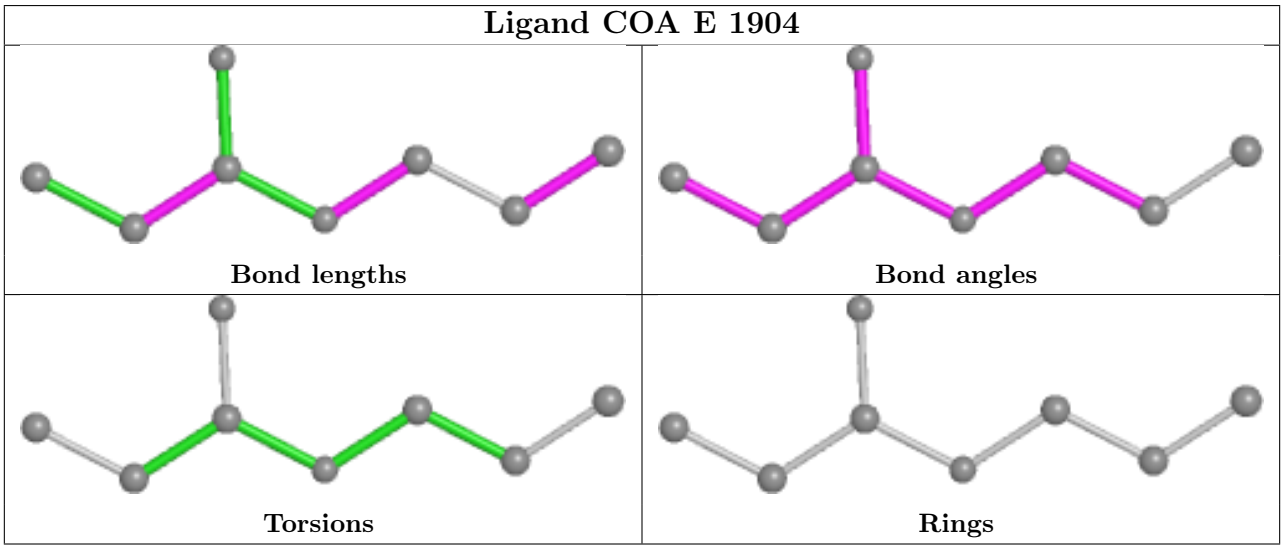
Ligand COA D 1301



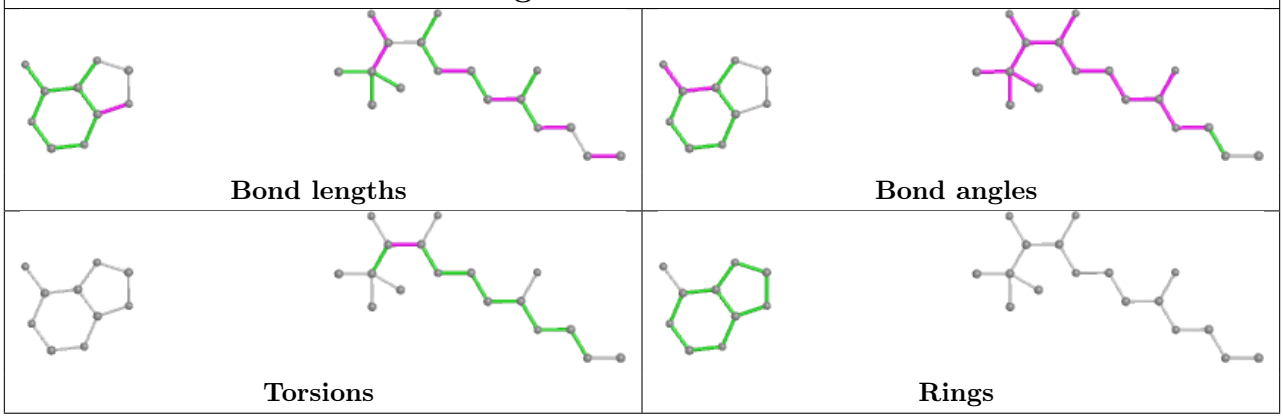
Ligand COA A 1300



Ligand COA E 1904



Ligand COA B 1903



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	287/288 (99%)	-0.26	2 (0%)	87	92	13, 26, 44, 63	0
1	D	287/288 (99%)	0.07	6 (2%)	63	74	17, 36, 57, 66	0
2	B	388/388 (100%)	-0.06	15 (3%)	39	52	14, 33, 56, 68	0
2	E	385/388 (99%)	0.19	27 (7%)	16	24	17, 36, 70, 93	0
All	All	1347/1352 (99%)	-0.00	50 (3%)	41	54	13, 33, 60, 93	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	363	ASP	5.6
2	E	88	ALA	4.7
2	E	356	LEU	4.3
2	E	324	ARG	4.3
2	E	322	ILE	4.1
2	E	352	ASN	3.9
2	E	293	ALA	3.9
2	E	372	LYS	3.9
2	E	353	ASN	3.8
2	E	84	TYR	3.7
2	B	309	ASP	3.6
2	E	323	VAL	3.4
2	E	355	GLU	3.2
1	A	140	HIS	3.1
2	E	256	ASP	3.1
2	E	342	ASN	3.0
2	E	362	ALA	2.9
1	D	7	ASN	2.8
2	B	84	TYR	2.8
1	D	198	PRO	2.8
2	E	40	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	326	ASP	2.7
2	B	322	ILE	2.7
2	E	316	VAL	2.7
2	E	56	LYS	2.6
2	B	324	ARG	2.6
2	E	357	GLY	2.6
2	B	88	ALA	2.5
2	B	142	HIS	2.4
2	E	347	VAL	2.4
1	D	149	ILE	2.4
2	B	310	LYS	2.4
2	E	384	ALA	2.3
2	B	56	LYS	2.3
2	B	290	GLY	2.3
2	B	314	VAL	2.3
2	E	290	GLY	2.3
2	B	316	VAL	2.3
2	B	372	LYS	2.3
2	E	359	LYS	2.3
2	B	323	VAL	2.2
2	B	388	LYS	2.2
1	D	140	HIS	2.2
1	D	6	LYS	2.2
2	E	354	ALA	2.2
1	A	198	PRO	2.2
2	B	40	ALA	2.1
1	D	223	GLU	2.1
2	E	330	ASP	2.0
2	E	365	GLY	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)

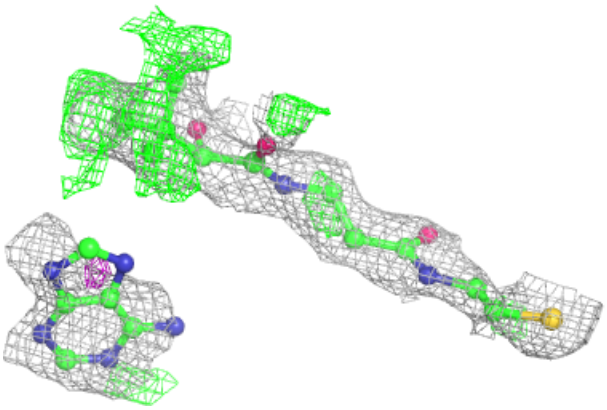
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

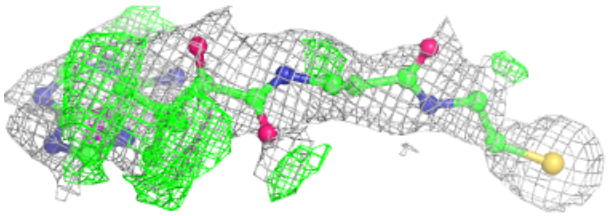
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COA	B	1903	27/48	0.64	0.25	67,79,90,90	0
4	COA	E	1904	8/48	0.70	0.23	79,82,83,83	0
5	GOL	A	1700	6/6	0.76	0.29	72,73,74,74	0
6	SO4	E	1501	5/5	0.93	0.22	65,68,68,69	0
6	SO4	E	1401	5/5	0.94	0.12	70,71,73,73	0
6	SO4	B	1400	5/5	0.94	0.15	75,75,76,76	0
6	SO4	B	1500	5/5	0.96	0.11	55,56,57,57	0
4	COA	A	1300	48/48	0.98	0.09	22,25,43,53	0
3	PO4	A	1600	5/5	0.98	0.10	30,35,37,37	0
4	COA	D	1301	48/48	0.98	0.10	18,27,44,51	0
3	PO4	D	1601	5/5	0.99	0.10	42,42,43,43	0

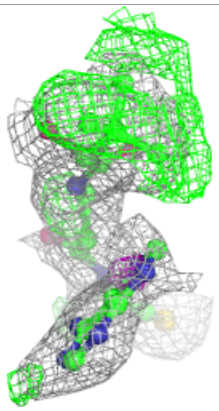
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA B 1903:

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

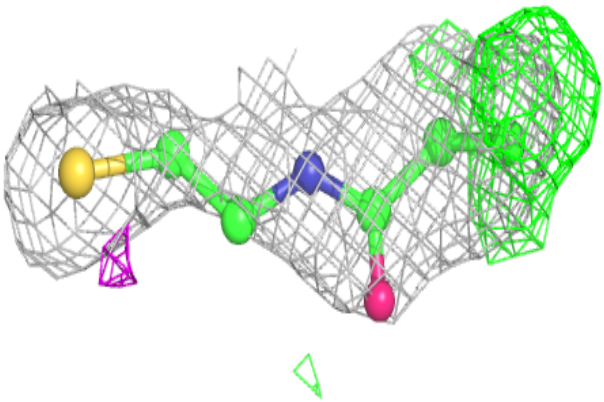


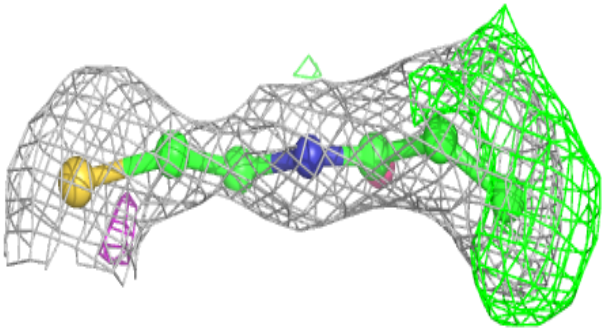


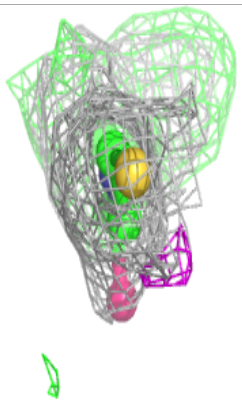


Electron density around COA E 1904:

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

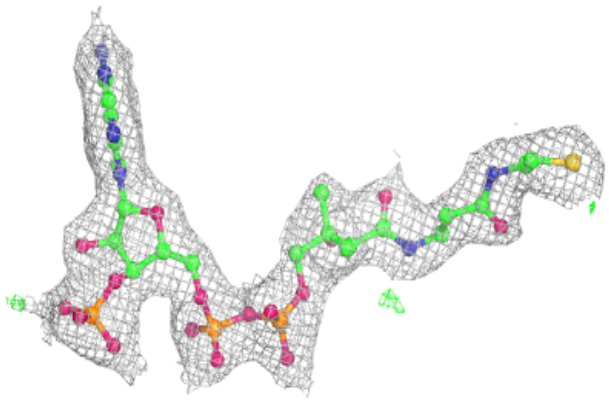


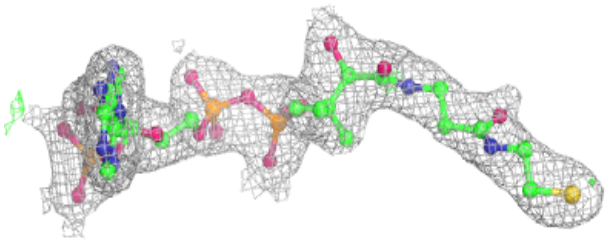


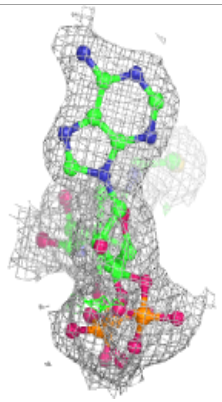


Electron density around COA A 1300:

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

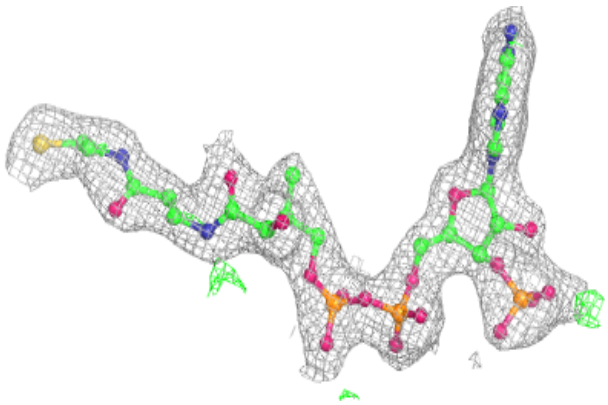


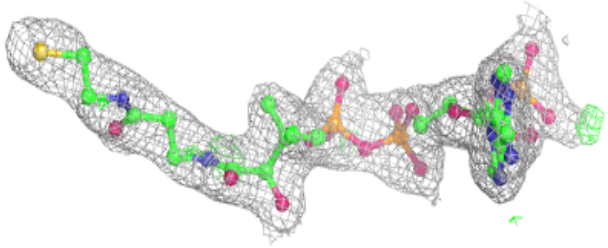


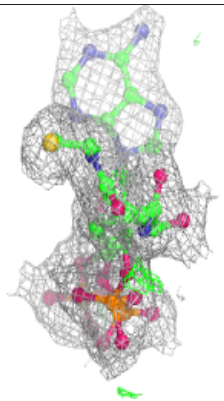


Electron density around COA D 1301:

$2mF_o$-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.