



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:03 PM EDT

PDB ID : 2NU8
Title : C123aT Mutant of E. coli Succinyl-CoA Synthetase
Authors : Fraser, M.E.
Deposited on : 2006-11-08
Resolution : 2.15 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

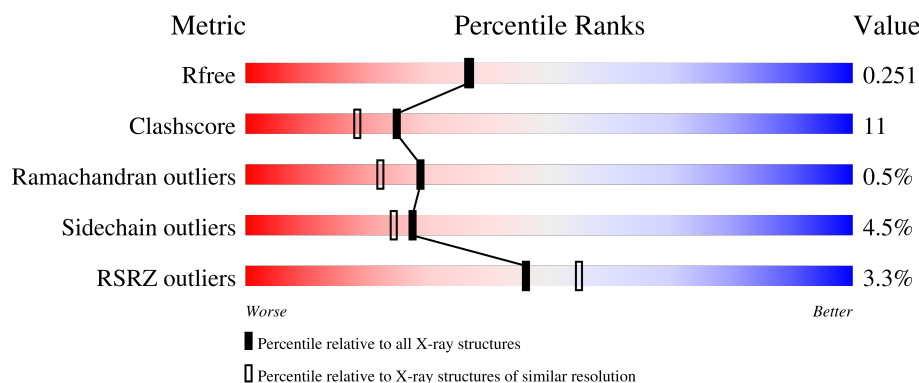
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	 79% 18% ..
1	D	288	 3% 79% 19% .
2	B	388	 2% 78% 20% .
2	E	388	 7% 73% 24% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10602 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 ligase [ADP-forming] subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2070	1314	346	400	10			
1	D	287	Total	C	N	O	S	0	0	0
			2070	1314	346	400	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	THR	CYS	engineered mutation	UNP P0AGE9
D	123	THR	CYS	engineered mutation	UNP P0AGE9

- Molecule 2 is a protein called Succinyl-CoA synthetase beta chain.

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



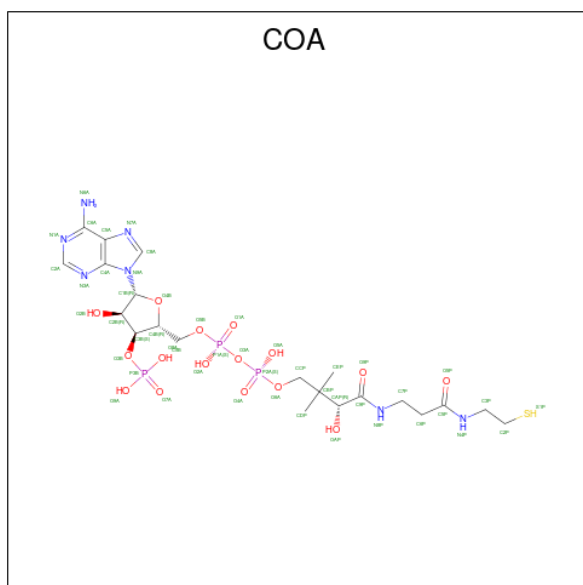
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 48 21 7 16 3 1	0	0
5	B	1	Total C N O S 18 11 2 4 1	0	0
5	D	1	Total C N O P S 48 21 7 16 3 1	0	0
5	E	1	Total C N O S 9 5 2 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

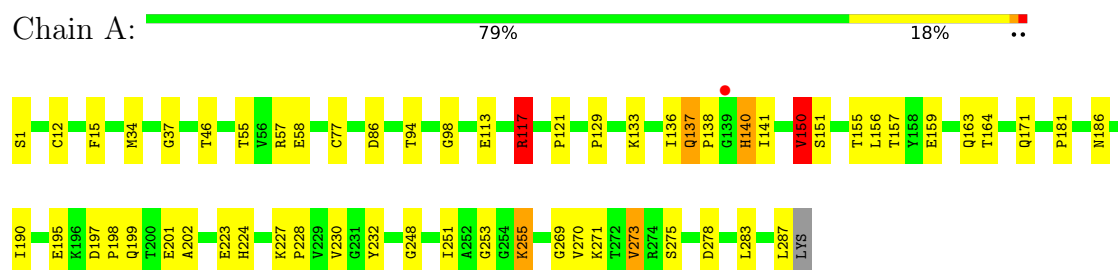
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	127	Total	O	0	0
			127	127		
7	B	156	Total	O	0	0
			156	156		
7	D	92	Total	O	0	0
			92	92		
7	E	135	Total	O	0	0
			135	135		

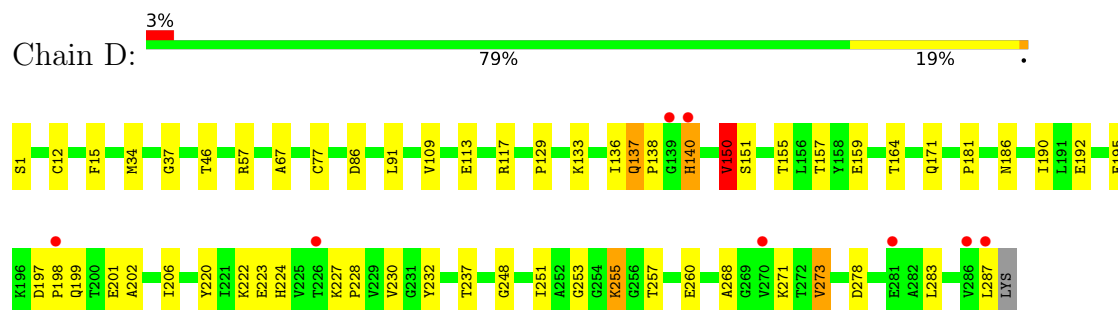
3 Residue-property plots

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.

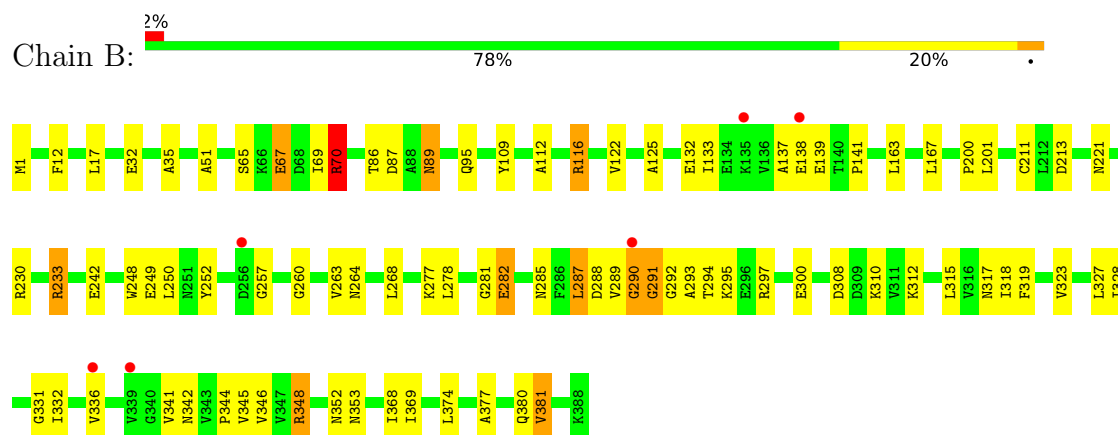
- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha



- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha



- Molecule 2: Succinyl-CoA synthetase beta chain



- Molecule 2: Succinyl-CoA synthetase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.69Å 96.69Å 385.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.97 – 2.15 42.97 – 2.11	Depositor EDS
% Data completeness (in resolution range)	91.6 (41.97-2.15) 88.5 (42.97-2.11)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.255 0.204 , 0.251	Depositor DCC
R_{free} test set	10573 reflections (11.15%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10602	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 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, PO4, SO4, GOL

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	0.82	1/2104 (0.0%)	0.86	2/2851 (0.1%)
1	D	0.78	0/2104	0.86	2/2851 (0.1%)
2	B	0.81	2/2950 (0.1%)	0.91	6/3989 (0.2%)
2	E	0.75	1/2927 (0.0%)	0.92	6/3961 (0.2%)
All	All	0.79	4/10085 (0.0%)	0.89	16/13652 (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)
2	B	211	CYS	CB-SG	7.50	1.95	1.82
1	A	77	CYS	CB-SG	-6.89	1.70	1.82
2	E	67	GLU	CG-CD	5.63	1.60	1.51
2	B	67	GLU	CG-CD	5.07	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	116	ARG	NE-CZ-NH2	-8.96	115.82	120.30
2	B	116	ARG	NE-CZ-NH2	-8.13	116.23	120.30
2	E	230	ARG	NE-CZ-NH1	7.74	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	150	VAL	CB-CA-C	-7.46	97.23	111.40
1	A	150	VAL	CB-CA-C	-7.23	97.66	111.40
2	B	116	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	B	230	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	E	201	LEU	N-CA-C	-6.24	94.15	111.00
2	B	233	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	E	230	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	E	70	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	E	203	ILE	N-CA-C	-5.61	95.87	111.00
2	B	70	ARG	NE-CZ-NH2	-5.55	117.53	120.30
2	B	201	LEU	N-CA-C	-5.43	96.35	111.00
1	A	117	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	D	77	CYS	CA-CB-SG	-5.13	104.77	114.00

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

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	2070	0	2131	46	0
1	D	2070	0	2131	40	0
2	B	2908	0	2962	70	0
2	E	2885	0	2940	82	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	E	10	0	0	0	0
5	A	48	0	32	1	0
5	B	18	0	20	4	0
5	D	48	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	9	0	9	2	0
6	A	6	0	7	3	0
7	A	127	0	0	3	0
7	B	156	0	0	2	0
7	D	92	0	0	0	0
7	E	135	0	0	3	0
All	All	10602	0	10264	220	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 11.

All (220) 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)
5:B:1325:COA:CBP	5:B:1325:COA:CAP	1.80	1.58
2:E:292:GLY:O	2:E:294:THR:HG23	1.79	0.82
1:D:223:GLU:HG2	1:D:224:HIS:CD2	2.16	0.79
1:A:202:ALA:HB2	1:A:287:LEU:HD11	1.67	0.75
1:A:181:PRO:O	2:B:116:ARG:HD3	1.87	0.75
1:A:150:VAL:HG13	1:A:190:ILE:HG21	1.70	0.74
2:B:32:GLU:OE1	2:B:70:ARG:HD2	1.88	0.74
1:A:223:GLU:HG2	1:A:224:HIS:CD2	2.23	0.73
1:A:133:LYS:NZ	1:A:137:GLN:O	2.22	0.73
2:B:137:ALA:O	2:B:141:PRO:HG3	1.87	0.73
1:D:150:VAL:HG13	1:D:190:ILE:HG21	1.70	0.73
2:E:32:GLU:OE1	2:E:70:ARG:HD2	1.89	0.73
1:D:202:ALA:HB2	1:D:287:LEU:HD11	1.69	0.72
1:A:198:PRO:HG2	7:A:1799:HOH:O	1.91	0.71
1:D:133:LYS:NZ	1:D:137:GLN:O	2.24	0.71
2:E:306:LEU:CD1	2:E:341:VAL:HG22	2.21	0.70
2:E:330:ASP:OD1	2:E:360:LYS:HD3	1.93	0.69
2:E:315:LEU:HB2	2:E:381:VAL:HG11	1.74	0.68
5:B:1325:COA:CBP	5:B:1325:COA:OAP	2.41	0.68
1:A:155:THR:HB	2:B:268:LEU:HB2	1.77	0.67
2:E:312:LYS:O	2:E:343:VAL:HB	1.94	0.67
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.77	0.65
2:E:292:GLY:O	2:E:294:THR:N	2.30	0.64
2:E:248:TRP:CD2	2:E:300:GLU:HG3	2.33	0.64
2:B:248:TRP:CD2	2:B:300:GLU:HG3	2.33	0.64
2:B:292:GLY:O	2:B:294:THR:N	2.30	0.64
2:E:248:TRP:CE2	2:E:300:GLU:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:352:ASN:O	2:E:353:ASN:HB2	1.99	0.63
2:B:70:ARG:NH2	2:E:249:GLU:OE2	2.32	0.63
2:E:287:LEU:HD12	2:E:288:ASP:N	2.14	0.62
2:B:249:GLU:OE2	2:E:70:ARG:NH2	2.33	0.61
2:B:346:VAL:HB	2:B:381:VAL:HG13	1.81	0.61
2:B:352:ASN:O	2:B:353:ASN:HB2	2.01	0.61
2:E:346:VAL:HB	2:E:381:VAL:HG13	1.82	0.61
1:A:155:THR:HG21	2:B:264:ASN:O	2.01	0.61
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.36	0.61
2:E:377:ALA:O	2:E:381:VAL:HG22	2.01	0.60
2:E:287:LEU:HD12	2:E:287:LEU:C	2.22	0.60
2:E:325:CYS:N	5:E:1325:COA:H22	2.17	0.59
1:D:181:PRO:O	2:E:116:ARG:HD3	2.01	0.59
2:E:352:ASN:HD22	5:E:1325:COA:H71	1.67	0.59
2:E:310:LYS:HE2	2:E:310:LYS:N	2.18	0.59
1:A:202:ALA:CB	1:A:287:LEU:HD11	2.33	0.58
2:E:325:CYS:HB3	2:E:349:LEU:HD13	1.85	0.58
2:B:289:VAL:O	2:B:291:GLY:N	2.37	0.58
2:B:287:LEU:C	2:B:287:LEU:HD12	2.24	0.57
1:A:15:PHE:CD2	1:A:37:GLY:HA3	2.41	0.56
2:B:287:LEU:HD12	2:B:288:ASP:N	2.19	0.56
1:D:251:ILE:HG23	1:D:255:LYS:O	2.05	0.56
2:E:306:LEU:HD11	2:E:341:VAL:HG22	1.88	0.56
2:E:312:LYS:O	2:E:344:PRO:HD2	2.05	0.56
2:B:295:LYS:HG3	2:B:331:GLY:HA2	1.88	0.56
1:A:270:VAL:HA	6:A:1700:GOL:H12	1.86	0.56
2:B:312:LYS:O	2:B:344:PRO:HD2	2.05	0.56
2:B:87:ASP:OD1	2:B:89:ASN:N	2.31	0.55
1:D:202:ALA:CB	1:D:287:LEU:HD11	2.35	0.55
2:E:250:LEU:HD21	2:E:297:ARG:CG	2.37	0.55
2:B:336:VAL:HA	2:B:341:VAL:CG2	2.37	0.55
2:B:310:LYS:HE2	2:B:310:LYS:N	2.21	0.54
1:A:269:GLY:O	6:A:1700:GOL:H12	2.06	0.54
2:B:289:VAL:O	2:B:290:GLY:C	2.46	0.54
1:D:197:ASP:O	1:D:227:LYS:NZ	2.41	0.54
1:A:253:GLY:O	1:A:255:LYS:HD2	2.07	0.54
1:D:136:ILE:CD1	5:D:1301:COA:H22	2.38	0.54
2:E:260:GLY:HA2	2:E:285:ASN:OD1	2.09	0.54
2:B:348:ARG:C	2:B:348:ARG:HD2	2.28	0.53
1:D:253:GLY:O	1:D:255:LYS:HD2	2.08	0.53
1:A:195:GLU:O	1:A:227:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:CB	2:B:268:LEU:HB2	2.39	0.53
2:B:250:LEU:HD21	2:B:297:ARG:CG	2.39	0.53
2:E:381:VAL:O	2:E:385:VAL:HG22	2.08	0.53
2:B:336:VAL:HG13	2:B:341:VAL:HB	1.91	0.53
2:E:369:ILE:HG21	2:E:380:GLN:OE1	2.09	0.53
1:D:199:GLN:O	1:D:199:GLN:HG2	2.09	0.53
2:E:382:VAL:O	2:E:385:VAL:HG23	2.08	0.53
1:D:248:GLY:O	2:E:116:ARG:NH2	2.38	0.52
1:A:251:ILE:HG23	1:A:255:LYS:O	2.09	0.52
2:B:377:ALA:O	2:B:381:VAL:HG22	2.09	0.52
2:E:230:ARG:HD2	7:E:1585:HOH:O	2.09	0.52
2:B:249:GLU:CD	2:E:70:ARG:HH22	2.14	0.51
2:E:12:PHE:HB3	2:E:17:LEU:HB2	1.92	0.51
2:E:318:ILE:HG21	2:E:328:ILE:HD13	1.92	0.51
1:A:199:GLN:O	1:A:199:GLN:HG2	2.08	0.51
1:A:137:GLN:H	1:A:137:GLN:CD	2.13	0.51
1:A:138:PRO:HB2	1:A:140:HIS:CE1	2.45	0.51
2:E:348:ARG:HD2	2:E:348:ARG:C	2.31	0.51
2:E:202:VAL:HG21	2:E:212:LEU:HD22	1.93	0.51
2:B:277:LYS:HA	2:B:281:GLY:O	2.11	0.50
2:B:332:ILE:O	2:B:336:VAL:HG23	2.11	0.50
1:A:275:SER:HB2	2:B:278:LEU:CD2	2.41	0.50
2:B:242:GLU:HG2	2:B:252:TYR:O	2.10	0.50
1:D:195:GLU:O	1:D:227:LYS:HE3	2.11	0.50
2:E:87:ASP:OD1	2:E:89:ASN:N	2.31	0.50
2:E:295:LYS:HG3	2:E:331:GLY:HA2	1.93	0.50
2:E:134:GLU:HB2	7:E:1616:HOH:O	2.11	0.50
2:B:12:PHE:HB3	2:B:17:LEU:HB2	1.94	0.50
1:A:1:SER:N	1:A:197:ASP:OD2	2.45	0.50
1:D:151:SER:HB3	1:D:157:THR:OG1	2.11	0.49
1:D:237:THR:HG23	2:E:274:ASP:OD1	2.12	0.49
2:E:312:LYS:HB2	2:E:385:VAL:HG12	1.95	0.49
2:B:323:VAL:HA	7:B:1534:HOH:O	2.11	0.49
1:A:159:GLU:OE1	2:B:348:ARG:NH2	2.46	0.49
1:A:197:ASP:O	1:A:227:LYS:NZ	2.45	0.49
2:E:36:SER:HB2	7:E:1543:HOH:O	2.13	0.49
2:B:318:ILE:HG21	2:B:328:ILE:CD1	2.43	0.49
1:D:223:GLU:HG2	1:D:224:HIS:NE2	2.27	0.49
2:E:343:VAL:HB	2:E:344:PRO:HD2	1.95	0.48
2:B:346:VAL:CG2	2:B:381:VAL:HG13	2.43	0.48
2:E:346:VAL:CG2	2:E:381:VAL:HG13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:ALA:HB1	2:E:250:LEU:HB2	1.94	0.48
2:B:308:ASP:OD1	2:B:308:ASP:C	2.50	0.48
2:E:124:MET:HA	2:E:145:HIS:O	2.14	0.48
2:B:318:ILE:HG21	2:B:328:ILE:HD13	1.96	0.48
1:D:137:GLN:CD	1:D:137:GLN:H	2.17	0.48
1:A:57:ARG:NH1	1:A:86:ASP:OD2	2.46	0.48
1:A:129:PRO:HG2	1:A:171:GLN:HB2	1.94	0.48
2:E:84:TYR:OH	2:E:132:GLU:HG3	2.14	0.48
2:B:213:ASP:HB3	7:B:1408:HOH:O	2.13	0.48
2:B:109:TYR:CE2	2:B:133:ILE:HB	2.49	0.47
2:B:260:GLY:HA2	2:B:285:ASN:OD1	2.13	0.47
1:D:192:GLU:HB2	1:D:220:TYR:OH	2.14	0.47
2:B:263:VAL:HG22	2:B:317:ASN:HB3	1.96	0.47
1:D:57:ARG:NH1	1:D:86:ASP:OD2	2.47	0.47
1:D:201:GLU:O	1:D:228:PRO:HD2	2.14	0.47
2:E:263:VAL:HG22	2:E:317:ASN:HB3	1.94	0.47
2:E:277:LYS:HA	2:E:281:GLY:O	2.13	0.47
1:D:109:VAL:HG21	2:E:151:PRO:HG2	1.97	0.47
1:D:136:ILE:HD11	5:D:1301:COA:H22	1.96	0.47
2:E:318:ILE:HG21	2:E:328:ILE:CD1	2.45	0.47
1:D:222:LYS:HB2	1:D:268:ALA:HB1	1.97	0.47
2:E:308:ASP:C	2:E:308:ASP:OD1	2.53	0.47
1:A:230:VAL:HA	1:A:271:LYS:O	2.15	0.46
2:E:67:GLU:CD	2:E:67:GLU:H	2.18	0.46
2:B:35:ALA:HB2	2:B:69:ILE:HD12	1.98	0.46
2:E:272:THR:O	2:E:275:ILE:HG22	2.15	0.46
1:A:151:SER:HB3	1:A:157:THR:OG1	2.14	0.46
2:E:1:MET:SD	2:E:233:ARG:HB2	2.56	0.46
2:E:312:LYS:HA	2:E:343:VAL:HG11	1.98	0.46
2:B:70:ARG:HH22	2:E:249:GLU:CD	2.18	0.46
2:E:29:ARG:O	2:E:32:GLU:HG2	2.16	0.46
2:B:277:LYS:NZ	2:B:282:GLU:OE2	2.43	0.45
2:E:352:ASN:O	2:E:353:ASN:CB	2.64	0.45
5:B:1325:COA:CAP	5:B:1325:COA:CCP	2.85	0.45
2:E:199:ASN:HA	2:E:200:PRO:HA	1.76	0.45
1:A:15:PHE:CG	1:A:37:GLY:HA3	2.52	0.45
1:A:181:PRO:CA	2:B:116:ARG:HD3	2.46	0.45
1:A:136:ILE:CD1	5:A:1300:COA:H22	2.47	0.45
2:B:345:VAL:O	2:B:368:ILE:HA	2.17	0.45
2:B:346:VAL:CB	2:B:381:VAL:HG13	2.46	0.45
1:D:138:PRO:HB2	1:D:140:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:312:LYS:HB2	2:E:385:VAL:CG1	2.46	0.45
1:D:155:THR:HG21	2:E:264:ASN:O	2.17	0.44
1:D:159:GLU:OE1	2:E:348:ARG:NH2	2.50	0.44
1:D:15:PHE:CD2	1:D:37:GLY:HA3	2.52	0.44
2:E:297:ARG:NH1	2:E:297:ARG:HB2	2.32	0.44
2:B:249:GLU:OE2	2:E:28:PRO:HD2	2.17	0.44
1:D:230:VAL:HA	1:D:271:LYS:O	2.16	0.44
2:E:35:ALA:HB2	2:E:69:ILE:HD12	1.98	0.44
2:E:163:LEU:O	2:E:167:LEU:HG	2.17	0.44
1:A:223:GLU:O	1:A:223:GLU:HG3	2.17	0.44
1:A:12:CYS:HB2	1:A:34:MET:HE1	2.00	0.44
1:A:181:PRO:C	2:B:116:ARG:HD3	2.35	0.44
1:A:223:GLU:HG2	1:A:224:HIS:NE2	2.31	0.44
1:D:1:SER:H2	1:D:197:ASP:CG	2.21	0.44
1:D:12:CYS:O	1:D:15:PHE:HB2	2.17	0.44
2:B:65:SER:HB2	2:B:67:GLU:OE1	2.17	0.44
2:B:369:ILE:HG21	2:B:380:GLN:OE1	2.18	0.44
1:D:67:ALA:HA	1:D:91:LEU:O	2.18	0.44
2:E:344:PRO:HB3	2:E:367:ASN:HD21	1.82	0.44
1:D:273:VAL:CG2	1:D:278:ASP:HB2	2.48	0.43
2:E:297:ARG:HB2	2:E:297:ARG:CZ	2.47	0.43
2:B:292:GLY:O	2:B:294:THR:HG23	2.18	0.43
2:B:323:VAL:HG12	2:B:327:LEU:HB2	2.00	0.43
2:B:1:MET:SD	2:B:233:ARG:HB2	2.58	0.43
2:B:139:GLU:C	2:B:141:PRO:HD3	2.39	0.43
1:D:255:LYS:HD2	1:D:255:LYS:N	2.34	0.43
1:A:117:ARG:NH2	7:A:1752:HOH:O	2.49	0.43
2:E:312:LYS:CB	2:E:385:VAL:HG12	2.48	0.43
2:E:344:PRO:HB3	2:E:367:ASN:ND2	2.34	0.43
2:B:133:ILE:HD12	2:B:133:ILE:HA	1.85	0.43
2:E:323:VAL:HG12	2:E:327:LEU:HB2	2.00	0.43
1:A:138:PRO:O	1:A:141:ILE:HG12	2.19	0.43
1:D:257:THR:OG1	1:D:260:GLU:HG3	2.18	0.42
1:A:55:THR:OG1	1:A:58:GLU:HG3	2.19	0.42
2:E:306:LEU:C	2:E:308:ASP:N	2.70	0.42
1:D:129:PRO:HG2	1:D:171:GLN:HB2	2.00	0.42
1:D:197:ASP:HA	1:D:198:PRO:HD2	1.87	0.42
2:E:20:PRO:HD3	2:E:211:CYS:O	2.19	0.42
2:B:67:GLU:H	2:B:67:GLU:CD	2.23	0.42
2:B:297:ARG:CZ	2:B:297:ARG:HB2	2.49	0.42
1:D:164:THR:HG22	1:D:283:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:ALA:HA	2:E:122:VAL:O	2.20	0.42
1:A:164:THR:HG22	1:A:283:LEU:CD1	2.50	0.41
2:E:309:ASP:HB3	2:E:310:LYS:NZ	2.35	0.41
2:E:345:VAL:O	2:E:368:ILE:HA	2.20	0.41
2:B:51:ALA:HB2	2:B:86:THR:HG22	2.03	0.41
2:E:65:SER:HB2	2:E:67:GLU:OE1	2.20	0.41
1:D:136:ILE:HD11	5:D:1301:COA:C2P	2.50	0.41
1:A:201:GLU:O	1:A:228:PRO:HD2	2.20	0.41
2:B:112:ALA:HA	2:B:122:VAL:O	2.21	0.41
2:E:268:LEU:HD12	2:E:268:LEU:HA	1.89	0.41
2:E:336:VAL:HG12	2:E:366:LEU:HD22	2.02	0.41
2:B:352:ASN:HD22	5:B:1325:COA:C7P	2.34	0.41
2:E:346:VAL:CB	2:E:381:VAL:HG13	2.47	0.41
1:A:98:GLY:O	2:B:221:ASN:HB3	2.21	0.41
1:A:248:GLY:O	2:B:116:ARG:NH2	2.48	0.41
2:B:163:LEU:O	2:B:167:LEU:HG	2.21	0.41
2:B:290:GLY:O	2:B:291:GLY:O	2.39	0.41
1:A:163:GLN:HG3	7:A:1760:HOH:O	2.21	0.41
1:A:270:VAL:HA	6:A:1700:GOL:C1	2.50	0.40
2:E:277:LYS:NZ	2:E:282:GLU:OE2	2.50	0.40
1:A:273:VAL:CG2	1:A:278:ASP:HB2	2.51	0.40
2:B:87:ASP:OD1	2:B:87:ASP:C	2.60	0.40
2:B:109:TYR:CD1	2:B:109:TYR:C	2.94	0.40
1:A:94:THR:O	1:A:121:PRO:HA	2.21	0.40
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.91	0.40
1:D:151:SER:HA	1:D:206:ILE:O	2.22	0.40
2:E:299:THR:HG23	2:E:339:VAL:HG23	2.03	0.40
2:B:109:TYR:O	2:B:125:ALA:HA	2.22	0.40
1:D:12:CYS:HB2	1:D:34:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	280 (98%)	5 (2%)	0	100	100
1	D	285/288 (99%)	276 (97%)	9 (3%)	0	100	100
2	B	386/388 (100%)	376 (97%)	6 (2%)	4 (1%)	15	9
2	E	383/388 (99%)	372 (97%)	8 (2%)	3 (1%)	19	12
All	All	1339/1352 (99%)	1304 (97%)	28 (2%)	7 (0%)	29	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	293	ALA
2	B	257	GLY
2	B	290	GLY
2	B	291	GLY
2	B	293	ALA
2	E	257	GLY
2	E	292	GLY

5.3.2 Protein sidechains ⓘ

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%)	208 (96%)	9 (4%)	30	29
1	D	217/218 (100%)	208 (96%)	9 (4%)	30	29
2	B	298/298 (100%)	285 (96%)	13 (4%)	28	25
2	E	296/298 (99%)	281 (95%)	15 (5%)	24	20
All	All	1028/1032 (100%)	982 (96%)	46 (4%)	27	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	113	GLU
1	A	117	ARG
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	140	HIS
1	A	150	VAL
1	A	186	ASN
1	A	255	LYS
1	A	273	VAL
2	B	70	ARG
2	B	89	ASN
2	B	95	GLN
2	B	132	GLU
2	B	138	GLU
2	B	200	PRO
2	B	282	GLU
2	B	287	LEU
2	B	319	PHE
2	B	342	ASN
2	B	348	ARG
2	B	374	LEU
2	B	381	VAL
1	D	46	THR
1	D	113	GLU
1	D	117	ARG
1	D	137	GLN
1	D	140	HIS
1	D	150	VAL
1	D	186	ASN
1	D	255	LYS
1	D	273	VAL
2	E	70	ARG
2	E	89	ASN
2	E	95	GLN
2	E	133	ILE
2	E	138	GLU
2	E	247	GLN
2	E	282	GLU
2	E	287	LEU
2	E	319	PHE
2	E	342	ASN
2	E	348	ARG
2	E	364	SER
2	E	374	LEU
2	E	381	VAL
2	E	385	VAL

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

Mol	Chain	Res	Type
2	B	95	GLN
2	B	244	GLN
2	B	342	ASN
2	B	352	ASN
2	E	10	GLN
2	E	95	GLN
2	E	244	GLN
2	E	342	ASN
2	E	352	ASN
2	E	367	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	$\# Z > 2$
6	GOL	A	1700	-	5,5,5	0.57	0	5,5,5	1.89	2 (40%)
4	SO4	E	1401	-	4,4,4	0.31	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1500	-	4,4,4	0.55	0	6,6,6	0.27	0
3	PO4	D	1601	-	4,4,4	1.72	1 (25%)	6,6,6	0.51	0
5	COA	B	1325	2	14,17,50	3.60	5 (35%)	19,22,75	4.72	14 (73%)
5	COA	E	1325	2	7,8,50	1.98	3 (42%)	7,8,75	1.78	1 (14%)
4	SO4	E	1501	-	4,4,4	0.45	0	6,6,6	0.24	0
3	PO4	A	1600	-	4,4,4	1.87	1 (25%)	6,6,6	0.45	0
5	COA	A	1300	-	41,50,50	0.87	2 (4%)	52,75,75	2.13	11 (21%)
5	COA	D	1301	-	41,50,50	0.92	2 (4%)	52,75,75	2.03	11 (21%)
4	SO4	B	1400	-	4,4,4	0.29	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1700	-	-	3/4/4/4	-
5	COA	B	1325	2	-	5/23/23/64	-
5	COA	E	1325	2	-	0/7/7/64	-
5	COA	A	1300	-	-	1/44/64/64	0/3/3/3
5	COA	D	1301	-	-	1/44/64/64	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1325	COA	CCP-CBP	11.16	1.60	1.53
5	B	1325	COA	C3P-N4P	4.37	1.56	1.46
5	E	1325	COA	C6P-C5P	3.77	1.58	1.51
5	B	1325	COA	C6P-C5P	2.96	1.57	1.51
5	B	1325	COA	C2P-S1P	2.88	1.90	1.80
5	B	1325	COA	CEP-CBP	2.72	1.59	1.53
3	A	1600	PO4	P-O4	-2.45	1.47	1.54
5	E	1325	COA	C3P-N4P	2.43	1.51	1.46
5	E	1325	COA	C2P-S1P	2.35	1.89	1.80
3	D	1601	PO4	P-O3	-2.22	1.47	1.54
5	A	1300	COA	C8A-N7A	-2.10	1.30	1.34
5	D	1301	COA	O6A-CCP	-2.05	1.37	1.43
5	D	1301	COA	O2B-C2B	-2.05	1.38	1.43
5	A	1300	COA	C6P-C5P	2.05	1.55	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1325	COA	C6P-C5P-N4P	9.75	132.83	116.42
5	B	1325	COA	O5P-C5P-C6P	-6.75	109.67	122.02
5	A	1300	COA	CEP-CBP-CCP	-6.72	97.27	108.23
5	B	1325	COA	C3P-N4P-C5P	6.71	135.29	122.84
5	B	1325	COA	CEP-CBP-CCP	-6.62	96.77	108.90
5	A	1300	COA	C7P-C6P-C5P	-6.57	101.42	112.36
5	D	1301	COA	C7P-C6P-C5P	-6.07	102.25	112.36
5	B	1325	COA	OAP-CAP-CBP	-6.03	96.05	110.25
5	B	1325	COA	CEP-CBP-CAP	5.78	118.84	108.82
5	D	1301	COA	C6P-C5P-N4P	5.23	125.23	116.42
5	B	1325	COA	CDP-CBP-CCP	-5.17	99.43	108.90
5	D	1301	COA	CEP-CBP-CCP	-4.96	100.14	108.23
5	D	1301	COA	O5P-C5P-C6P	-4.85	113.14	122.02
5	B	1325	COA	CDP-CBP-CAP	4.82	117.18	108.82
5	A	1300	COA	O5P-C5P-C6P	-4.52	113.76	122.02
5	A	1300	COA	C6P-C7P-N8P	-4.42	102.97	111.90
5	A	1300	COA	C6P-C5P-N4P	4.35	123.74	116.42
5	B	1325	COA	O9P-C9P-N8P	-4.29	113.79	122.99
5	A	1300	COA	CEP-CBP-CAP	4.15	116.02	108.82
5	B	1325	COA	C7P-N8P-C9P	3.73	129.24	122.59
5	E	1325	COA	C7P-C6P-C5P	3.58	119.15	112.33
5	D	1301	COA	C6P-C7P-N8P	-3.54	104.75	111.90
5	B	1325	COA	C2P-C3P-N4P	3.50	120.29	112.31
5	D	1301	COA	O3B-P3B-O7A	-3.25	96.86	109.39
5	D	1301	COA	C2P-C3P-N4P	-3.19	105.03	112.31
5	B	1325	COA	CAP-C9P-N8P	3.13	122.81	116.58
5	D	1301	COA	P2A-O3A-P1A	-2.97	122.63	132.83
5	B	1325	COA	O5P-C5P-N4P	-2.92	117.49	123.01
5	A	1300	COA	C2P-C3P-N4P	-2.86	105.78	112.31
6	A	1700	GOL	O2-C2-C1	2.74	121.19	109.12
5	A	1300	COA	P2A-O3A-P1A	-2.73	123.46	132.83
5	D	1301	COA	C3P-N4P-C5P	2.69	127.83	122.84
6	A	1700	GOL	O2-C2-C3	2.58	120.47	109.12
5	D	1301	COA	CEP-CBP-CAP	2.49	113.13	108.82
5	B	1325	COA	C6P-C7P-N8P	2.42	116.78	111.90
5	A	1300	COA	C5A-C6A-N6A	2.38	123.97	120.35
5	A	1300	COA	O3B-P3B-O7A	-2.16	101.07	109.39
5	D	1301	COA	C7P-N8P-C9P	2.07	126.29	122.59
5	A	1300	COA	C1B-N9A-C4A	-2.01	123.11	126.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

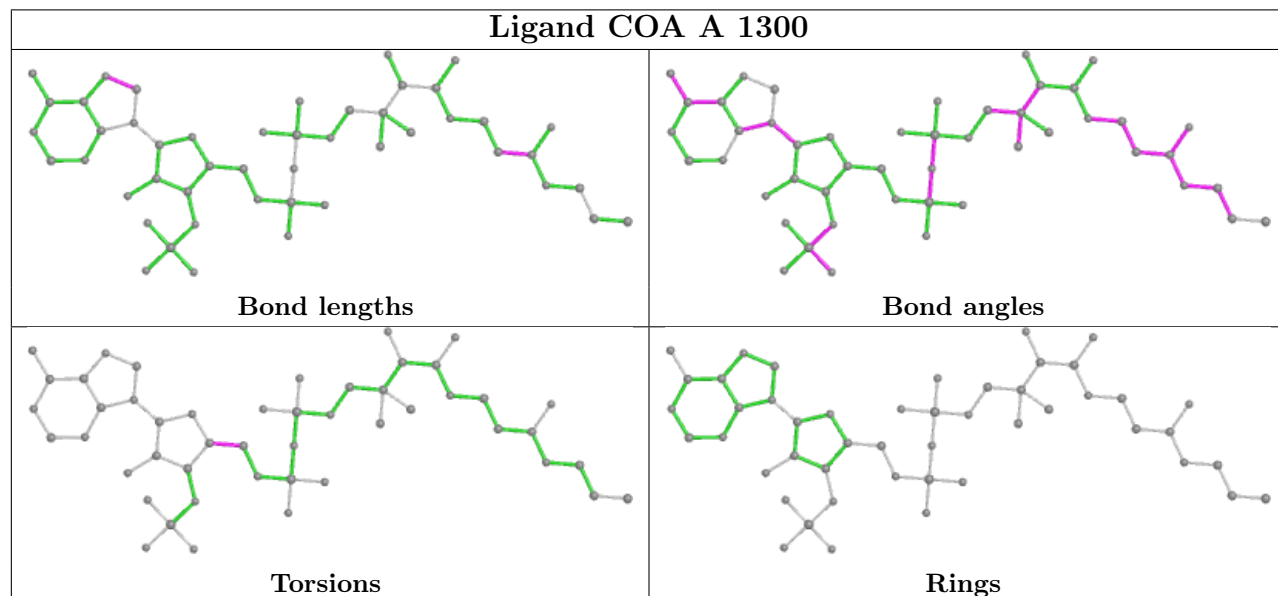
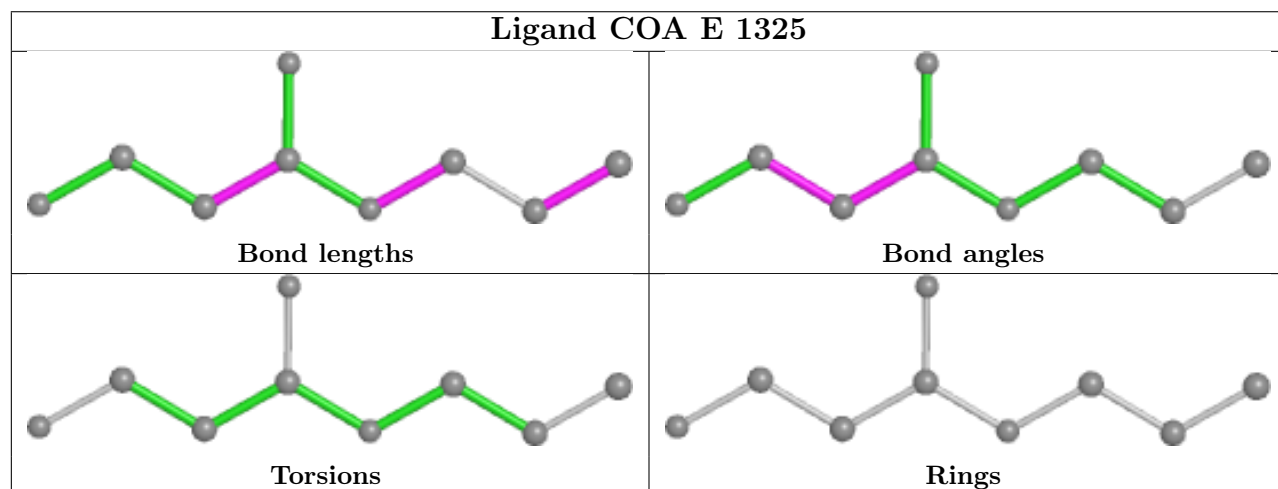
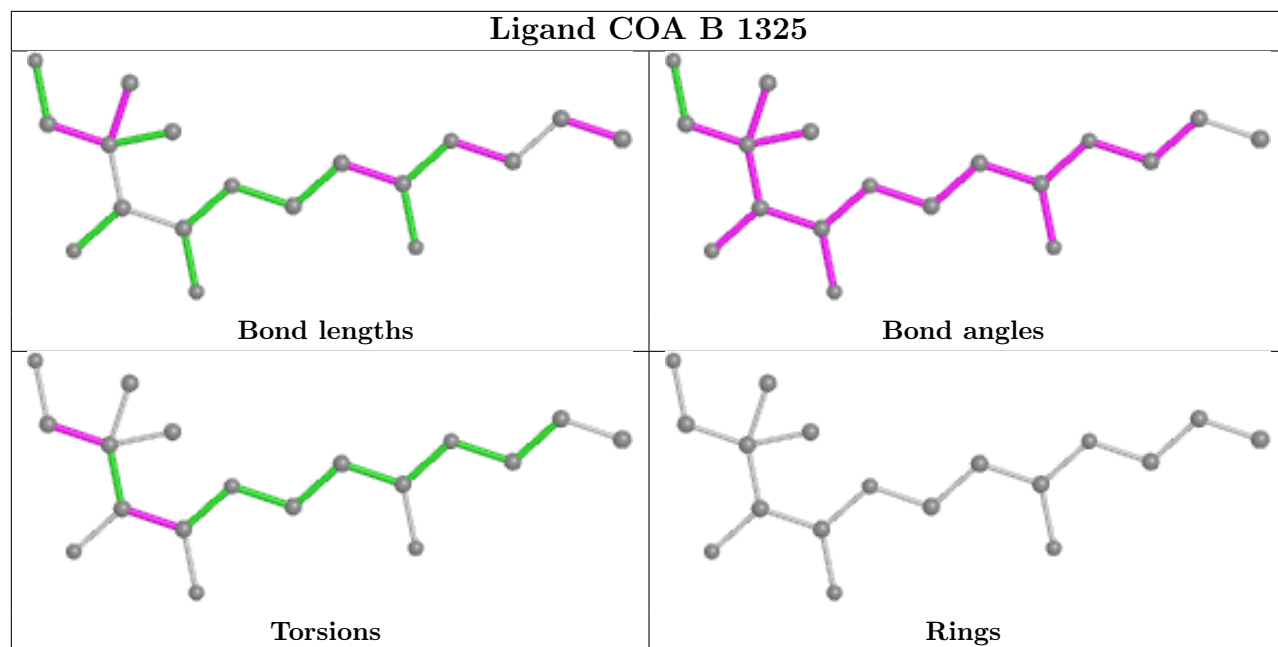
Mol	Chain	Res	Type	Atoms
5	B	1325	COA	CEP-CBP-CCP-O6A
5	B	1325	COA	O9P-C9P-CAP-CBP
5	B	1325	COA	N8P-C9P-CAP-CBP
5	B	1325	COA	O9P-C9P-CAP-OAP
6	A	1700	GOL	O1-C1-C2-C3
6	A	1700	GOL	O2-C2-C3-O3
5	B	1325	COA	N8P-C9P-CAP-OAP
6	A	1700	GOL	O1-C1-C2-O2
5	A	1300	COA	O4B-C4B-C5B-O5B
5	D	1301	COA	O4B-C4B-C5B-O5B

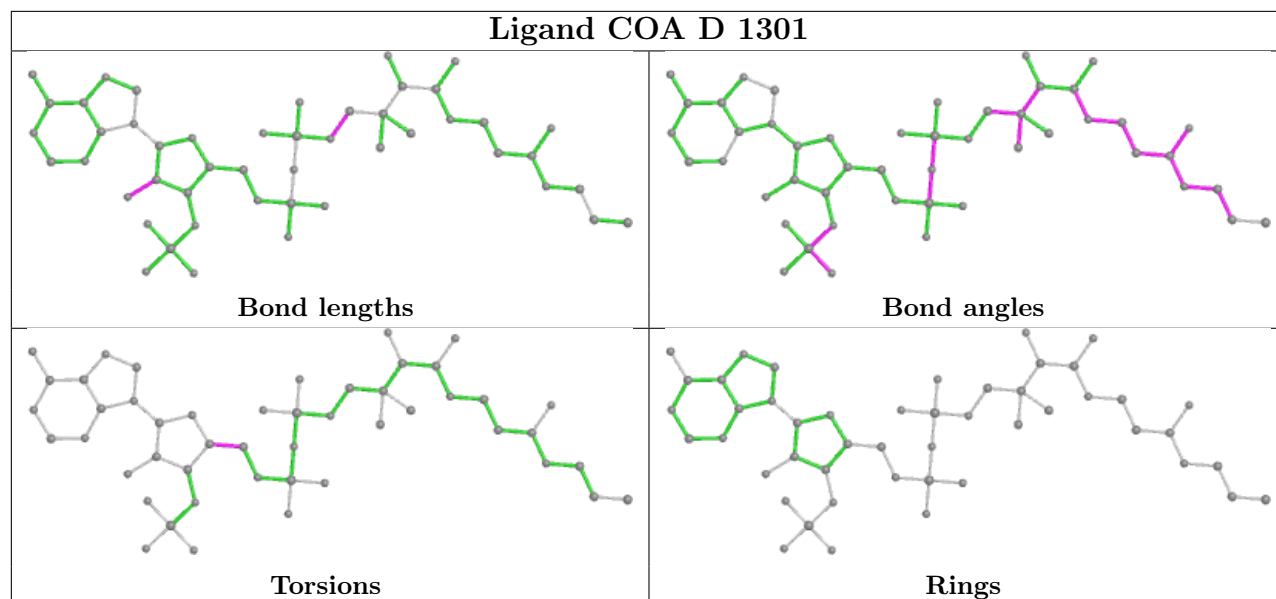
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1700	GOL	3	0
5	B	1325	COA	4	0
5	E	1325	COA	2	0
5	A	1300	COA	1	0
5	D	1301	COA	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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, 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%)	-0.09	1 (0%) 94 95	17, 27, 44, 58	0
1	D	287/288 (99%)	0.12	8 (2%) 53 62	20, 36, 52, 64	0
2	B	388/388 (100%)	-0.07	6 (1%) 73 79	16, 34, 53, 64	0
2	E	385/388 (99%)	0.17	29 (7%) 14 19	19, 36, 66, 90	0
All	All	1347/1352 (99%)	0.04	44 (3%) 46 55	16, 34, 57, 90	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	293	ALA	9.7
1	A	139	GLY	4.6
2	E	363	ASP	4.5
2	E	384	ALA	4.0
2	E	356	LEU	3.8
2	E	353	ASN	3.5
1	D	287	LEU	3.5
2	B	290	GLY	3.4
2	E	342	ASN	3.3
2	E	84	TYR	3.2
2	E	324	ARG	3.2
2	E	362	ALA	3.0
2	E	326	ASP	2.9
2	E	256	ASP	2.9
2	E	56	LYS	2.8
2	E	383	ALA	2.8
2	E	309	ASP	2.7
1	D	140	HIS	2.7
1	D	198	PRO	2.7
2	E	352	ASN	2.7
2	E	64	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	357	GLY	2.6
2	E	312	LYS	2.6
2	E	281	GLY	2.5
2	E	372	LYS	2.5
2	E	385	VAL	2.5
1	D	281	GLU	2.5
2	B	339	VAL	2.4
2	E	354	ALA	2.3
1	D	286	VAL	2.3
2	E	343	VAL	2.3
2	B	256	ASP	2.3
2	E	88	ALA	2.2
2	E	295	LYS	2.2
2	B	336	VAL	2.2
1	D	139	GLY	2.2
2	E	55	GLY	2.1
1	D	270	VAL	2.1
2	B	138	GLU	2.1
1	D	226	THR	2.1
2	E	248	TRP	2.1
2	E	327	LEU	2.0
2	E	369	ILE	2.0
2	B	135	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](#)

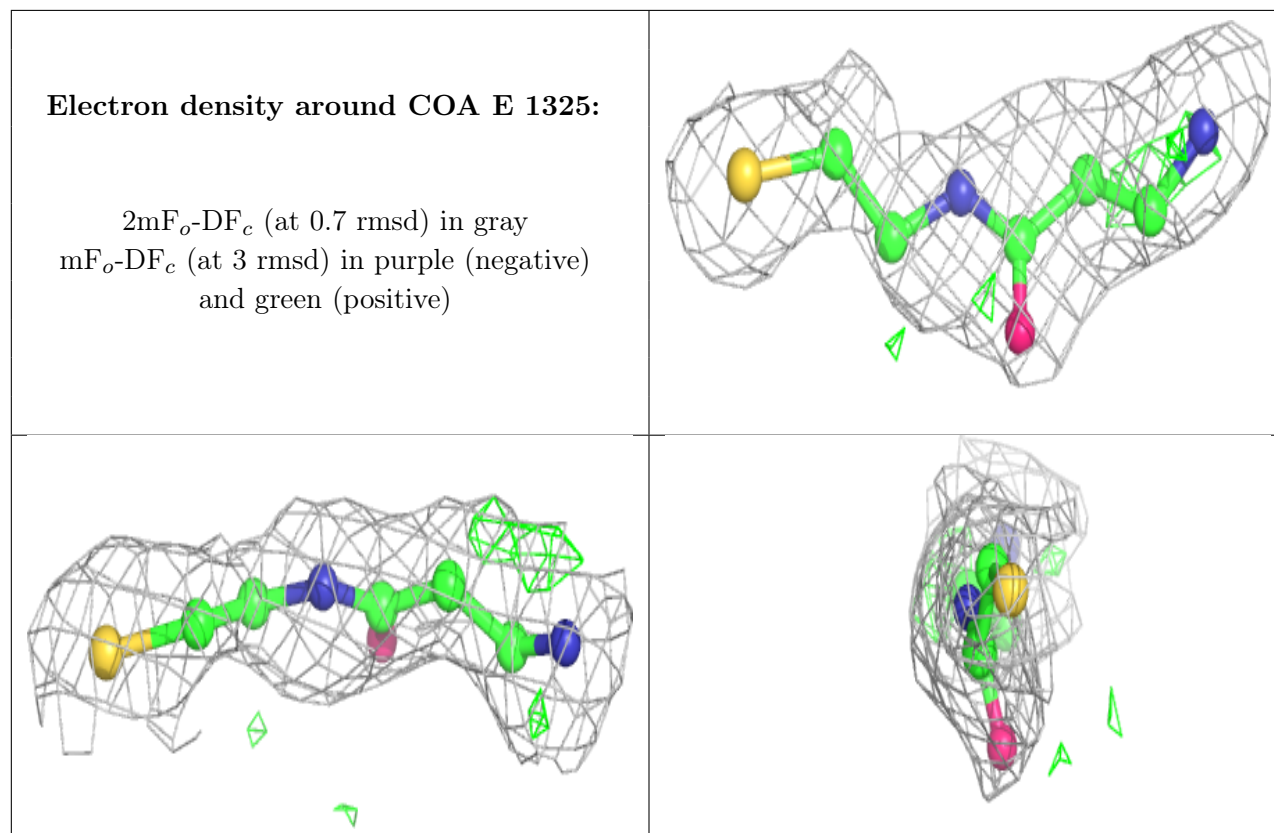
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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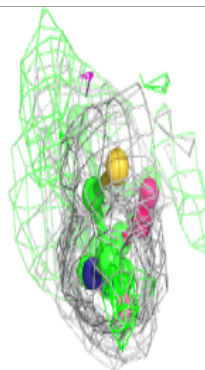
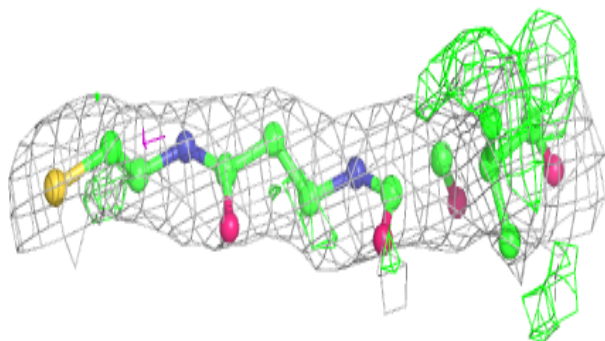
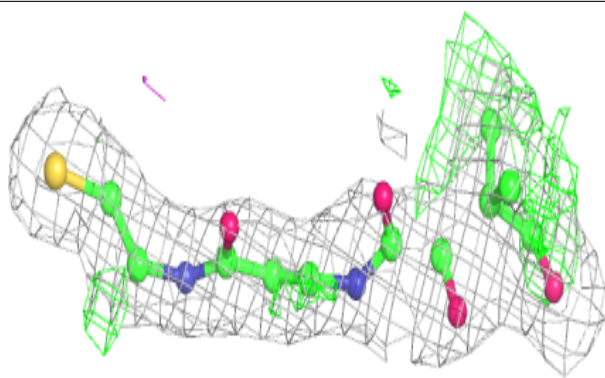
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	1700	6/6	0.53	0.34	72,72,72,72	0
5	COA	E	1325	9/48	0.76	0.19	70,72,73,73	0
5	COA	B	1325	18/48	0.77	0.21	56,64,68,69	0
4	SO4	E	1501	5/5	0.91	0.15	76,77,78,79	0
4	SO4	E	1401	5/5	0.94	0.23	23,25,27,28	5
4	SO4	A	1500	5/5	0.95	0.10	56,56,58,59	0
5	COA	D	1301	48/48	0.95	0.11	25,29,49,55	0
4	SO4	B	1400	5/5	0.95	0.17	21,24,25,25	5
5	COA	A	1300	48/48	0.95	0.11	26,29,50,53	0
3	PO4	A	1600	5/5	0.98	0.16	26,28,31,31	0
3	PO4	D	1601	5/5	0.99	0.14	30,30,30,32	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.

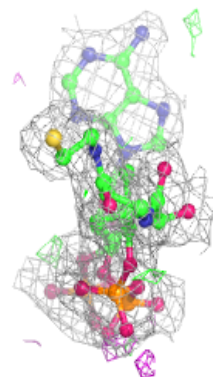
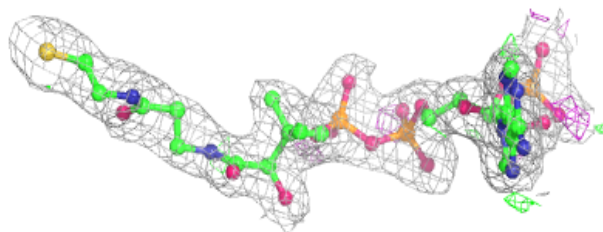
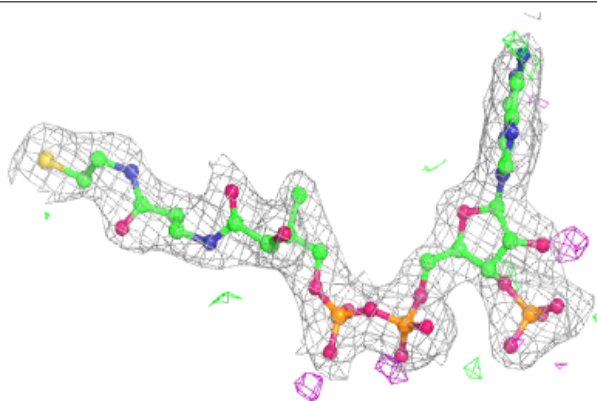


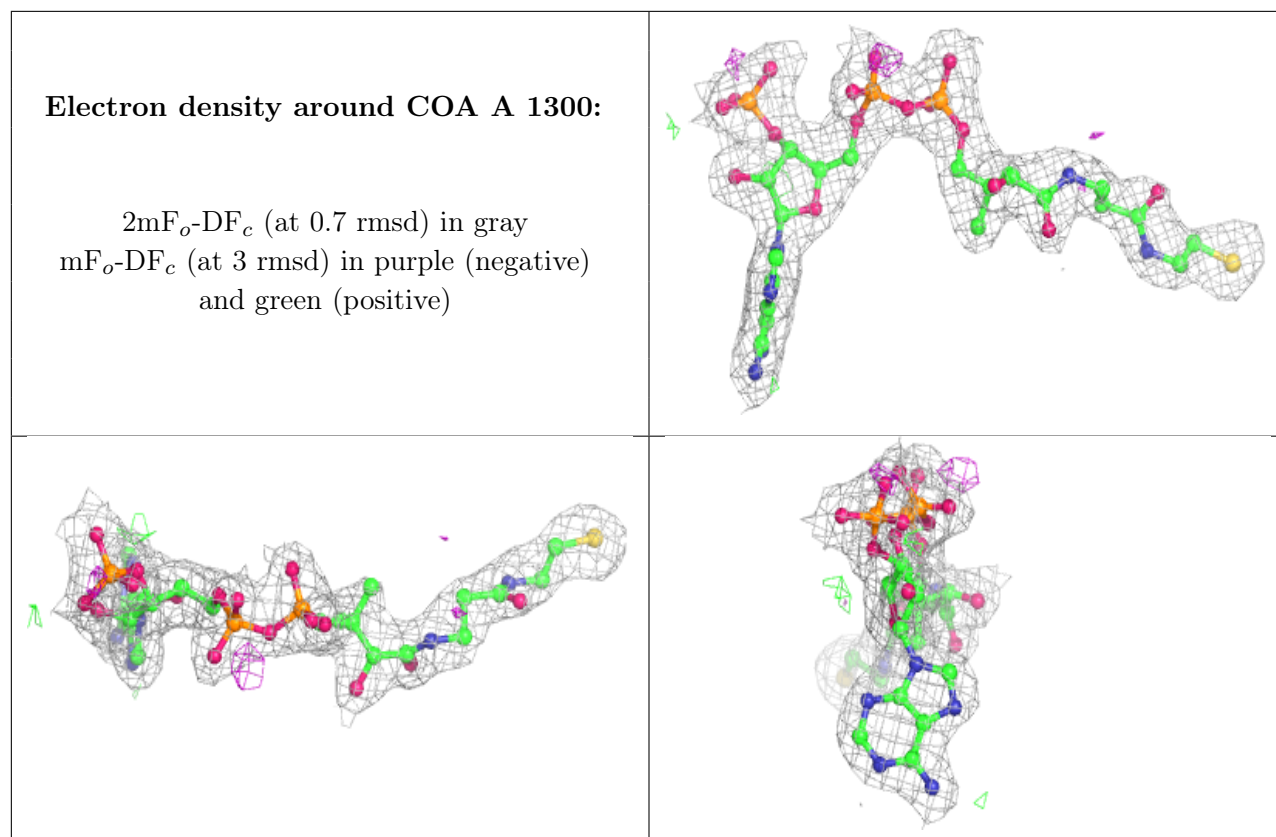
Electron density around COA B 1325:

$2mF_o-DF_c$ (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.