Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 04:57 pm GMT

PDB ID	:	2VSS
Title	:	Wild-type Hydroxycinnamoyl-CoA hydratase lyase in complex with acetyl-CoA and vanillin
Authors	:	Bennett, J.P.; Bertin, L.M.; Brzozowski, A.M.; Walton, N.J.; Grogan, G.
Deposited on	:	2008-04-29
Resolution	:	2.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

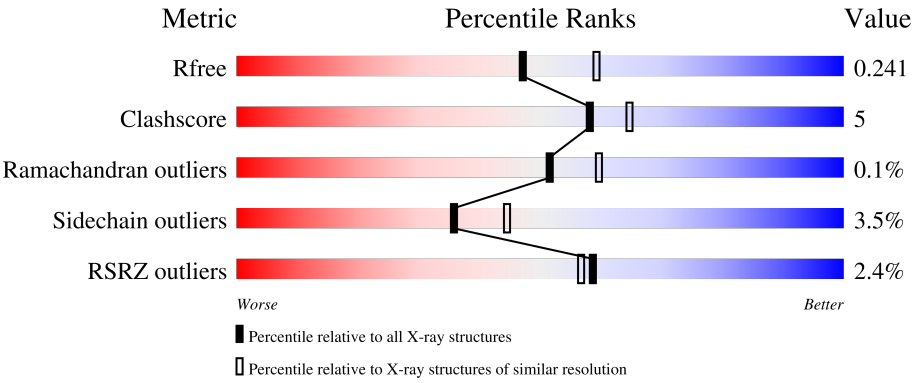
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	276	2% 76% 9% • 13%
1	B	276	4% 77% 9% • 10%
1	C	276	3% 70% 14% • 14%
1	D	276	81% 7% • 11%
2	E	276	2% 78% 8% • 13%

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Mol	Chain	Length	Quality of chain
3	F	276	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	V55	D	1250	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11928 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 P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	1	1
			1847	1170	320	344	13			
1	B	248	Total	C	N	O	S	0	0	1
			1943	1233	336	362	12			
1	C	236	Total	C	N	O	S	0	1	1
			1821	1151	319	339	12			
1	D	246	Total	C	N	O	S	0	2	0
			1957	1242	342	361	12			

- Molecule 2 is a protein called P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	241	Total	C	N	O	S	0	1	1
			1887	1199	325	350	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	TYR	TRP	conflict	UNP O69762

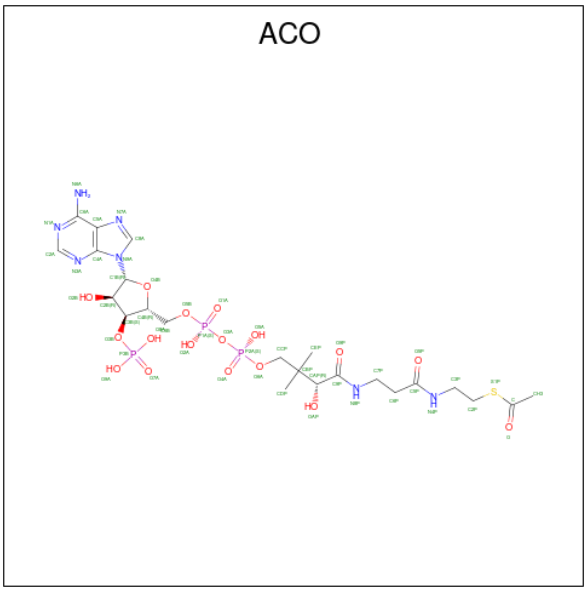
- Molecule 3 is a protein called P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	247	Total	C	N	O	S	0	1	1
			1942	1234	337	359	12			

There is a discrepancy between the modelled and reference sequences:

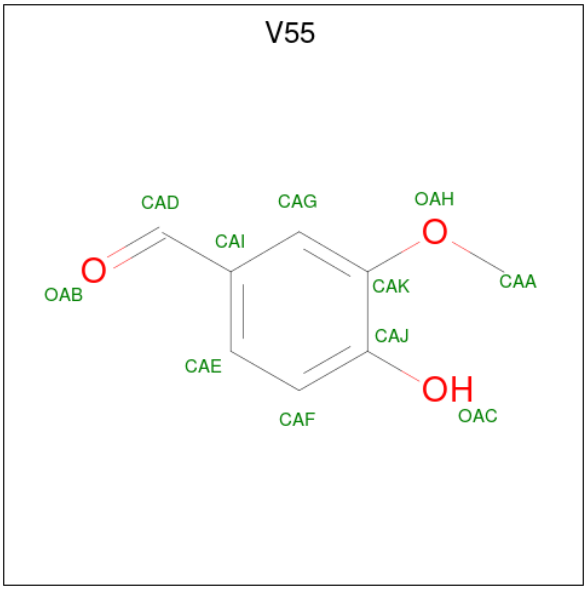
Chain	Residue	Modelled	Actual	Comment	Reference
F	29	ARG	LYS	conflict	UNP O69762

- Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



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

- Molecule 5 is 4-hydroxy-3-methoxybenzaldehyde (three-letter code: V55) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 11 8 3	0	0

- Molecule 6 is water.

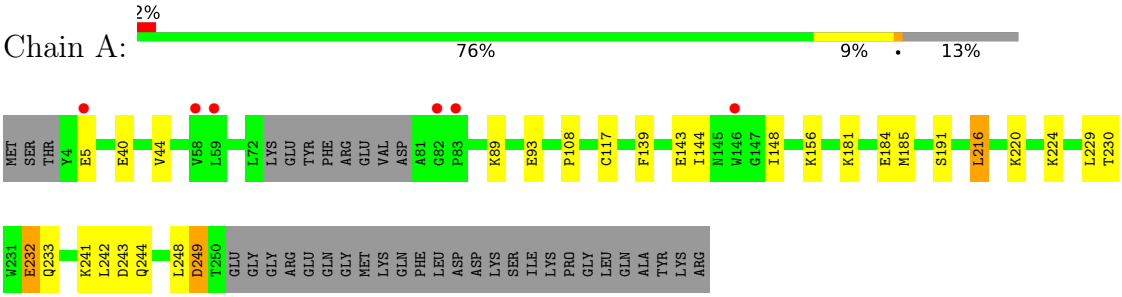
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0
6	B	60	Total O 60 60	0	0
6	C	38	Total O 38 38	0	0
6	D	60	Total O 60 60	0	0
6	E	61	Total O 61 61	0	0
6	F	62	Total O 62 62	0	0

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.

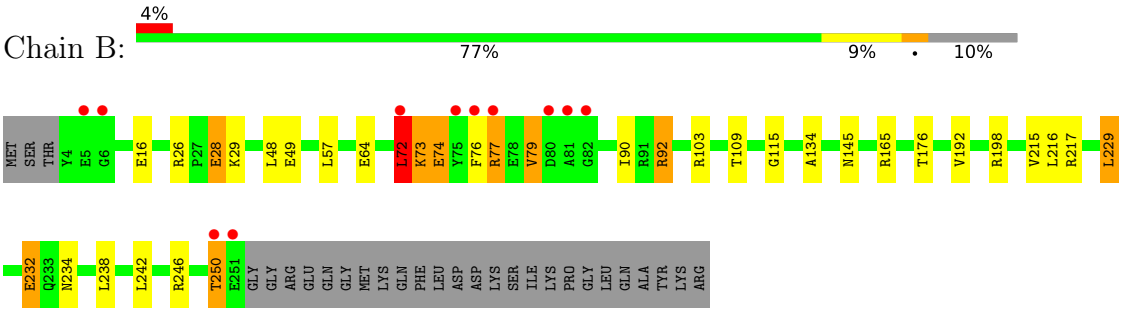
• Molecule 1: P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE

Chain A:



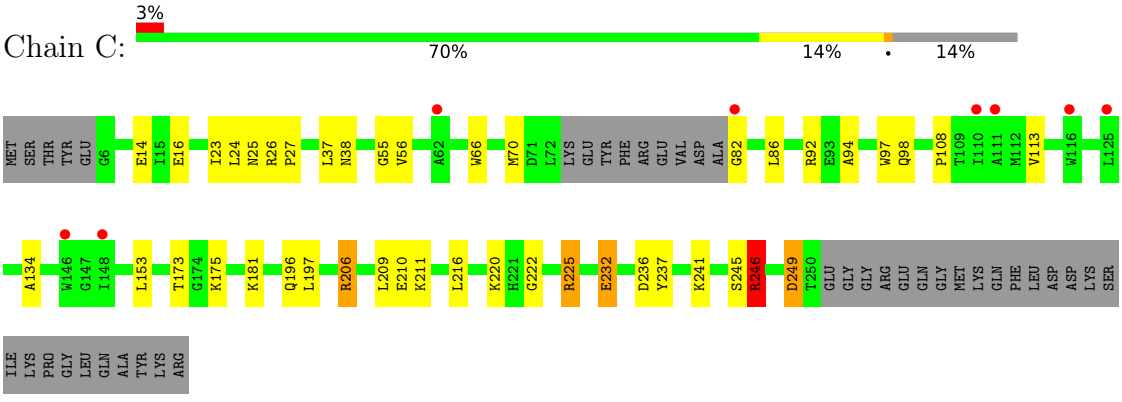
• Molecule 1: P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE

Chain B:



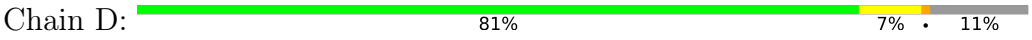
• Molecule 1: P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE

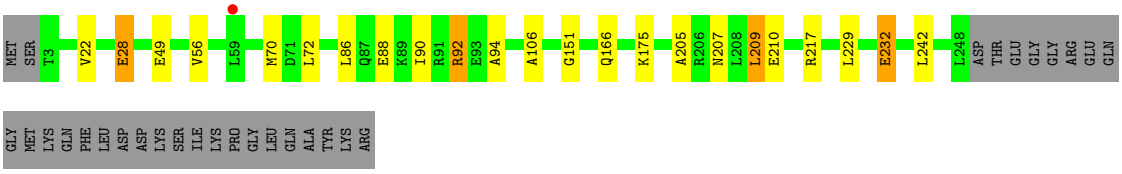
Chain C:



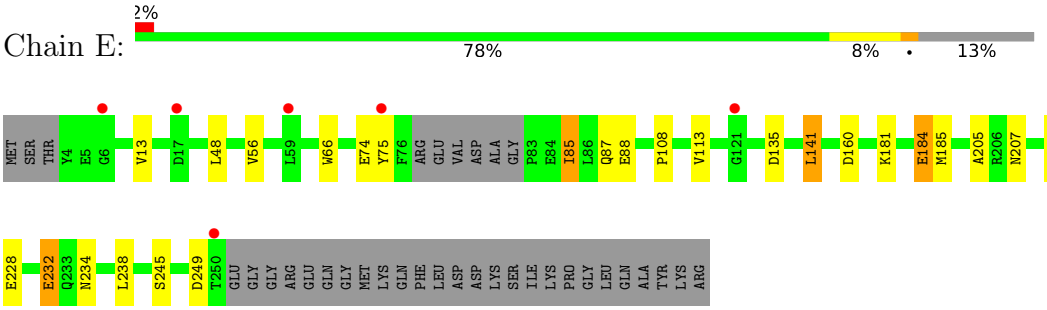
• Molecule 1: P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE

Chain D:

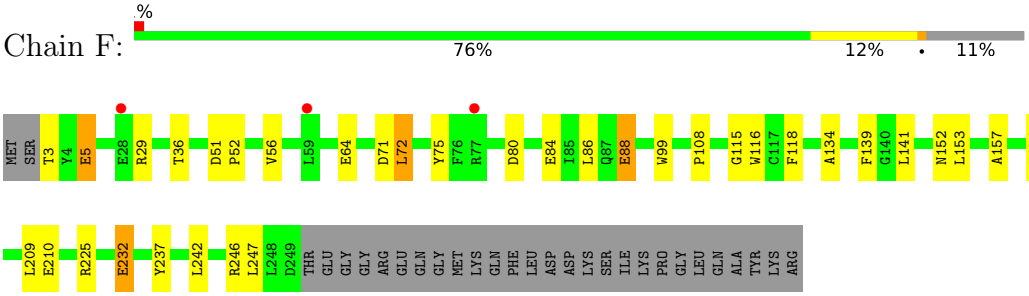




• Molecule 2: P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE



• Molecule 3: P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.22Å 130.59Å 144.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.13 – 2.22 24.74 – 2.22	Depositor EDS
% Data completeness (in resolution range)	91.5 (97.13-2.22) 91.6 (24.74-2.22)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.183 , 0.242 0.182 , 0.241	Depositor DCC
R_{free} test set	3933 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11928	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: ACO, V55

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	0.94	2/1881 (0.1%)	0.88	1/2545 (0.0%)
1	B	1.11	4/1982 (0.2%)	1.00	7/2684 (0.3%)
1	C	1.03	4/1854 (0.2%)	0.95	7/2510 (0.3%)
1	D	1.13	4/1996 (0.2%)	0.96	4/2701 (0.1%)
2	E	1.17	5/1924 (0.3%)	0.94	3/2603 (0.1%)
3	F	1.14	6/1981 (0.3%)	0.95	2/2683 (0.1%)
All	All	1.09	25/11618 (0.2%)	0.95	24/15726 (0.2%)

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	232	GLU	CG-CD	8.85	1.65	1.51
1	D	232	GLU	CG-CD	6.96	1.62	1.51
2	E	232	GLU	CD-OE1	6.84	1.33	1.25
1	D	232	GLU	CD-OE1	6.31	1.32	1.25
1	C	232	GLU	CG-CD	6.25	1.61	1.51
1	C	237	TYR	CD1-CE1	6.24	1.48	1.39
3	F	80	ASP	CB-CG	6.24	1.64	1.51
1	B	232	GLU	CG-CD	6.20	1.61	1.51
3	F	232	GLU	CG-CD	6.18	1.61	1.51
1	D	232	GLU	CB-CG	6.11	1.63	1.52
3	F	210	GLU	CG-CD	5.84	1.60	1.51
1	B	232	GLU	CD-OE1	5.82	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	GLU	CD-OE1	5.64	1.31	1.25
1	B	28	GLU	CB-CG	5.63	1.62	1.52
1	A	232	GLU	CG-CD	5.57	1.60	1.51
1	B	28	GLU	CG-CD	5.48	1.60	1.51
2	E	184	GLU	CG-CD	5.46	1.60	1.51
2	E	210	GLU	CG-CD	5.44	1.60	1.51
3	F	88	GLU	CG-CD	5.42	1.60	1.51
1	D	22	VAL	CB-CG1	5.40	1.64	1.52
3	F	232	GLU	CD-OE1	5.36	1.31	1.25
1	A	232	GLU	CD-OE1	5.30	1.31	1.25
2	E	228	GLU	CB-CG	5.24	1.62	1.52
1	C	16	GLU	CB-CG	5.14	1.61	1.52
3	F	157	ALA	CA-CB	5.06	1.63	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	92	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	D	92	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	C	92	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	D	92	ARG	NE-CZ-NH1	8.23	124.42	120.30
3	F	242	LEU	CA-CB-CG	8.13	133.99	115.30
1	C	225	ARG	CG-CD-NE	-7.82	95.38	111.80
1	B	165	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	242	LEU	CA-CB-CG	7.40	132.32	115.30
1	B	165	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	92	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	C	246	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	E	135	ASP	CB-CG-OD1	6.54	124.19	118.30
1	D	242	LEU	CA-CB-CG	6.26	129.69	115.30
1	C	92	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	C	225	ARG	CB-CA-C	-6.01	98.37	110.40
1	D	28	GLU	CB-CA-C	-5.92	98.56	110.40
3	F	72	LEU	CA-CB-CG	5.87	128.81	115.30
1	C	236	ASP	CB-CG-OD1	5.86	123.58	118.30
2	E	141	LEU	CA-CB-CG	5.71	128.43	115.30
2	E	160	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	225	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	242	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	72	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	26	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	LEU	Peptide

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	1847	0	1830	21	0
1	B	1943	0	1931	22	1
1	C	1821	0	1811	23	0
1	D	1957	0	1955	19	0
2	E	1887	0	1870	14	0
3	F	1942	0	1936	21	1
4	B	51	0	34	0	0
4	D	51	0	34	6	0
4	E	51	0	34	0	0
4	F	51	0	34	2	0
5	D	11	0	7	6	0
6	A	35	0	0	1	0
6	B	60	0	0	2	0
6	C	38	0	0	2	0
6	D	60	0	0	2	0
6	E	61	0	0	1	0
6	F	62	0	0	1	0
All	All	11928	0	11476	111	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 5.

All (111) 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)
4:F:1249:ACO:C	4:F:1249:ACO:S1P	2.02	1.46
4:D:1249:ACO:C	4:D:1249:ACO:S1P	2.06	1.41
1:B:232:GLU:HG2	3:F:232:GLU:HG2	1.28	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:HG2	1:D:232:GLU:HG2	1.36	1.06
1:C:232:GLU:HG2	2:E:232:GLU:HG2	1.28	1.06
1:C:94:ALA:O	1:C:98:GLN:HG3	1.69	0.93
1:B:232:GLU:HG2	3:F:232:GLU:CG	2.03	0.88
1:C:246:ARG:HH11	1:C:246:ARG:HB3	1.39	0.87
3:F:99:TRP:HE1	3:F:152:ASN:HD21	1.24	0.85
1:A:232:GLU:HG2	1:D:232:GLU:CG	2.08	0.82
1:D:56:VAL:HG23	1:D:209:LEU:HD13	1.61	0.82
1:B:49:GLU:OE2	1:D:92:ARG:NH2	2.15	0.80
1:C:232:GLU:CG	2:E:232:GLU:HG2	2.13	0.76
2:E:108:PRO:HG3	2:E:216:LEU:HD13	1.68	0.76
4:D:1249:ACO:HH31	5:D:1250:V55:CAD	2.16	0.76
3:F:3:THR:OG1	3:F:5:GLU:HB2	1.87	0.74
2:E:108:PRO:HG3	2:E:216:LEU:CD1	2.18	0.73
1:B:217:ARG:NH1	1:D:88:GLU:OE1	2.24	0.70
1:A:89:LYS:O	1:A:93:GLU:HG3	1.91	0.70
1:D:56:VAL:HG23	1:D:209:LEU:CD1	2.24	0.67
1:B:198:ARG:HD2	6:B:2039:HOH:O	1.94	0.67
1:C:245[B]:SER:O	1:C:249:ASP:HB3	1.95	0.66
1:B:145:ASN:OD1	1:C:211:LYS:NZ	2.29	0.64
2:E:75:TYR:OH	2:E:87:GLN:HG3	1.99	0.63
1:C:25:ASN:C	1:C:27:PRO:HD3	2.19	0.62
1:D:106:ALA:O	1:D:217[B]:ARG:HD3	2.00	0.62
1:C:56:VAL:HG22	1:C:108:PRO:HG2	1.80	0.61
1:D:70:MET:SD	5:D:1250:V55:HAA3	2.40	0.61
1:D:175:LYS:NZ	6:D:2044:HOH:O	2.32	0.61
1:C:246:ARG:HH11	1:C:246:ARG:CB	2.11	0.60
1:A:181:LYS:HG3	1:A:185[B]:MET:CE	2.31	0.60
1:A:241:LYS:NZ	1:A:244:GLN:HE22	2.00	0.59
1:D:151:GLY:HA3	5:D:1250:V55:CAE	2.32	0.59
1:C:245[A]:SER:O	1:C:249:ASP:HB3	2.01	0.58
3:F:99:TRP:HE1	3:F:152:ASN:ND2	2.00	0.57
1:A:5:GLU:HG3	6:A:2003:HOH:O	2.03	0.57
1:D:166:GLN:NE2	6:D:2042:HOH:O	2.37	0.57
2:E:184:GLU:HB3	6:E:2033:HOH:O	2.05	0.57
1:B:79:VAL:HG23	1:B:90:ILE:HD12	1.88	0.55
1:A:230:THR:H	1:A:233:GLN:HE21	1.53	0.55
1:D:205:ALA:O	1:D:209:LEU:HD22	2.08	0.53
1:B:92:ARG:NH2	1:D:49:GLU:OE2	2.37	0.53
1:D:56:VAL:CG2	1:D:209:LEU:HD13	2.34	0.52
1:D:86:LEU:O	1:D:90:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:225:ARG:HG2	3:F:237:TYR:CZ	2.46	0.51
1:A:108:PRO:HG3	1:A:216:LEU:CD1	2.40	0.51
1:C:134:ALA:HB2	1:C:197:LEU:HD22	1.93	0.51
2:E:181:LYS:HG3	2:E:185[B]:MET:CE	2.40	0.51
3:F:134:ALA:HA	3:F:192:VAL:O	2.11	0.51
3:F:152:ASN:HD22	3:F:153:LEU:H	1.59	0.51
1:C:66:TRP:CD1	1:C:113:VAL:HA	2.45	0.50
1:A:156:LYS:NZ	1:B:229:LEU:O	2.43	0.50
1:A:243:ASP:O	3:F:247:LEU:HD22	2.12	0.50
1:B:64:GLU:O	1:B:115:GLY:HA3	2.11	0.49
1:A:241:LYS:HZ2	1:A:244:GLN:HE22	1.60	0.49
3:F:56:VAL:HG23	3:F:209:LEU:HG	1.94	0.48
4:D:1249:ACO:S1P	4:D:1249:ACO:CH3	2.96	0.48
4:D:1249:ACO:CH3	5:D:1250:V55:OAB	2.61	0.48
3:F:116:TRP:HB3	3:F:118:PHE:HE1	1.78	0.48
1:C:222:GLY:HA3	6:C:2030:HOH:O	2.13	0.47
3:F:116:TRP:HB3	3:F:118:PHE:CE1	2.49	0.47
1:C:24:LEU:HD22	1:C:37:LEU:HD11	1.95	0.47
1:B:49:GLU:CD	1:D:92:ARG:HH22	2.16	0.47
3:F:84:GLU:OE2	3:F:88:GLU:CG	2.63	0.47
1:C:249:ASP:OD1	1:C:249:ASP:O	2.32	0.47
1:A:220:LYS:O	1:A:224:LYS:HG3	2.15	0.47
1:A:143:GLU:HB3	1:A:148:ILE:O	2.15	0.46
1:A:117:CYS:O	1:A:139:PHE:HA	2.15	0.46
1:C:55:GLY:HA3	1:C:209:LEU:CD2	2.46	0.46
2:E:75:TYR:CD2	2:E:75:TYR:C	2.88	0.46
2:E:66:TRP:CD1	2:E:113:VAL:HA	2.51	0.46
1:B:29:LYS:HD3	1:B:29:LYS:HA	1.79	0.46
2:E:245:SER:O	2:E:249:ASP:HB3	2.16	0.46
1:B:72:LEU:HD23	1:B:73:LYS:N	2.31	0.46
1:B:74:GLU:HA	1:B:77:ARG:HB3	1.97	0.45
2:E:56:VAL:HG11	2:E:205:ALA:HB1	1.98	0.45
1:D:94:ALA:HB1	5:D:1250:V55:HAA1	1.98	0.45
3:F:206:ARG:HD3	6:F:2006:HOH:O	2.15	0.45
1:A:181:LYS:HG3	1:A:185[B]:MET:HE3	1.97	0.45
1:B:232:GLU:HG2	3:F:232:GLU:CB	2.47	0.44
4:D:1249:ACO:HH33	5:D:1250:V55:OAB	2.17	0.44
1:A:108:PRO:HG3	1:A:216:LEU:HD13	1.97	0.44
1:B:57:LEU:HB2	1:B:109:THR:HG22	2.00	0.44
1:C:206:ARG:NH2	6:C:2025:HOH:O	2.50	0.44
4:D:1249:ACO:C	4:D:1249:ACO:C2P	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLU:HG3	1:C:23:ILE:HD11	2.00	0.44
1:A:230:THR:H	1:A:233:GLN:NE2	2.15	0.43
1:C:38:ASN:HA	1:C:97:TRP:CD1	2.53	0.43
2:E:234:ASN:O	2:E:238:LEU:HB2	2.17	0.43
1:B:134:ALA:HA	1:B:192:VAL:O	2.18	0.43
3:F:64:GLU:O	3:F:115:GLY:HA3	2.19	0.43
1:C:26:ARG:N	1:C:27:PRO:HD3	2.34	0.43
2:E:85:ILE:O	2:E:88:GLU:HB2	2.19	0.43
3:F:139:PHE:O	3:F:176:THR:HA	2.19	0.43
1:C:241:LYS:HA	1:C:241:LYS:HD2	1.84	0.43
3:F:29:ARG:HA	4:F:1249:ACO:O4B	2.20	0.42
3:F:71:ASP:O	3:F:75:TYR:HB3	2.20	0.42
1:B:234:ASN:HB3	1:B:238:LEU:HD12	2.01	0.42
2:E:13:VAL:HG11	2:E:48:LEU:HD21	2.02	0.42
1:A:241:LYS:HA	1:A:241:LYS:HD2	1.81	0.42
1:D:207:ASN:O	1:D:210:GLU:HB2	2.20	0.42
3:F:51:ASP:HA	3:F:52:PRO:HD2	1.94	0.41
3:F:56:VAL:HG22	3:F:108:PRO:HG2	2.02	0.41
1:A:144:ILE:HD12	1:B:215:VAL:HG12	2.01	0.41
1:A:40:GLU:O	1:A:44:VAL:HG23	2.20	0.41
1:C:173:THR:OG1	1:C:175:LYS:HG3	2.20	0.41
1:B:103:ARG:HD3	6:B:2018:HOH:O	2.20	0.41
1:A:232:GLU:HG2	1:D:232:GLU:CB	2.49	0.41
1:C:82:GLY:HA3	1:C:86:LEU:HD23	2.03	0.41
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.84	0.40
1:B:246:ARG:HH11	1:B:246:ARG:HD2	1.76	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)
1:B:16:GLU:OE2	3:F:36:THR:OG1[3_544]	2.14	0.06

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	236/276 (86%)	225 (95%)	10 (4%)	1 (0%)	34 37
1	B	246/276 (89%)	239 (97%)	6 (2%)	1 (0%)	34 37
1	C	233/276 (84%)	225 (97%)	8 (3%)	0	100 100
1	D	246/276 (89%)	234 (95%)	12 (5%)	0	100 100
2	E	238/276 (86%)	229 (96%)	9 (4%)	0	100 100
3	F	246/276 (89%)	236 (96%)	10 (4%)	0	100 100
All	All	1445/1656 (87%)	1388 (96%)	55 (4%)	2 (0%)	51 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASP
1	B	250	THR

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	190/227 (84%)	185 (97%)	5 (3%)	46 57
1	B	202/227 (89%)	191 (95%)	11 (5%)	22 25
1	C	188/227 (83%)	177 (94%)	11 (6%)	19 22
1	D	203/227 (89%)	199 (98%)	4 (2%)	55 67
2	E	195/227 (86%)	190 (97%)	5 (3%)	46 57
3	F	201/227 (88%)	196 (98%)	5 (2%)	47 58
All	All	1179/1362 (87%)	1138 (96%)	41 (4%)	36 44

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	191	SER
1	A	216	LEU
1	A	229	LEU
1	A	249	ASP
1	B	28	GLU
1	B	72	LEU
1	B	73	LYS
1	B	74	GLU
1	B	76	PHE
1	B	77	ARG
1	B	79	VAL
1	B	176	THR
1	B	216	LEU
1	B	229	LEU
1	B	250	THR
1	C	70	MET
1	C	153	LEU
1	C	181	LYS
1	C	196	GLN
1	C	206	ARG
1	C	210	GLU
1	C	216	LEU
1	C	220	LYS
1	C	225	ARG
1	C	246	ARG
1	C	249	ASP
1	D	28	GLU
1	D	72	LEU
1	D	209	LEU
1	D	229	LEU
2	E	74	GLU
2	E	85	ILE
2	E	141	LEU
2	E	207	ASN
2	E	216	LEU
3	F	5	GLU
3	F	72	LEU
3	F	86	LEU
3	F	141	LEU
3	F	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	50	GLN
1	A	87	GLN
1	A	98	GLN
1	A	166	GLN
1	A	207	ASN
1	A	233	GLN
1	A	244	GLN
1	B	25	ASN
1	B	87	GLN
1	B	207	ASN
1	C	166	GLN
1	C	207	ASN
1	D	25	ASN
1	D	166	GLN
2	E	25	ASN
2	E	50	GLN
3	F	152	ASN
3	F	207	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

5 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	ACO	F	1249	-	45,53,53	1.64	7 (15%)	56,79,79	2.25	14 (25%)
5	V55	D	1250	-	11,11,11	1.10	0	14,14,14	1.71	5 (35%)
4	ACO	B	1251	-	45,53,53	1.22	5 (11%)	56,79,79	1.61	11 (19%)
4	ACO	D	1249	-	45,53,53	1.68	4 (8%)	56,79,79	1.60	11 (19%)
4	ACO	E	1250	-	45,53,53	1.59	7 (15%)	56,79,79	1.81	13 (23%)

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	ACO	F	1249	-	-	12/47/67/67	0/3/3/3
5	V55	D	1250	-	-	0/4/4/4	0/1/1/1
4	ACO	B	1251	-	-	3/47/67/67	0/3/3/3
4	ACO	D	1249	-	-	1/47/67/67	0/3/3/3
4	ACO	E	1250	-	-	8/47/67/67	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1249	ACO	O4B-C1B	6.37	1.50	1.41
4	D	1249	ACO	C-S1P	5.27	2.06	1.75
4	F	1249	ACO	O4B-C1B	4.94	1.48	1.41
4	F	1249	ACO	C-S1P	4.59	2.02	1.75
4	E	1250	ACO	P3B-O3B	4.55	1.67	1.59
4	E	1250	ACO	P1A-O1A	4.44	1.66	1.50
4	F	1249	ACO	P3B-O3B	4.06	1.67	1.59
4	B	1251	ACO	P1A-O1A	3.71	1.64	1.50
4	D	1249	ACO	OAP-CAP	3.52	1.48	1.42
4	F	1249	ACO	C2B-C1B	-3.27	1.48	1.53
4	E	1250	ACO	O4B-C4B	3.09	1.51	1.45
4	F	1249	ACO	C7P-C6P	3.02	1.61	1.51
4	D	1249	ACO	P3B-O7A	2.93	1.60	1.50
4	B	1251	ACO	P3B-O7A	2.79	1.59	1.50
4	B	1251	ACO	C-S1P	2.75	1.91	1.75
4	B	1251	ACO	P2A-O4A	2.67	1.60	1.50
4	F	1249	ACO	C7P-N8P	2.63	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1250	ACO	P2A-O4A	2.56	1.60	1.50
4	B	1251	ACO	O4B-C1B	2.47	1.44	1.41
4	E	1250	ACO	O4B-C1B	2.44	1.44	1.41
4	E	1250	ACO	C7P-N8P	2.28	1.51	1.46
4	E	1250	ACO	CH3-C	2.22	1.59	1.50
4	F	1249	ACO	P3B-O7A	2.01	1.57	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1249	ACO	C7P-N8P-C9P	-10.41	104.02	122.59
4	E	1250	ACO	C3P-N4P-C5P	6.08	134.13	122.84
4	F	1249	ACO	N3A-C2A-N1A	-5.49	120.10	128.68
4	B	1251	ACO	N3A-C2A-N1A	-5.46	120.14	128.68
4	D	1249	ACO	O4B-C1B-C2B	-4.69	100.07	106.93
4	E	1250	ACO	N3A-C2A-N1A	-4.66	121.39	128.68
4	E	1250	ACO	C6P-C5P-N4P	4.57	124.12	116.42
4	D	1249	ACO	N3A-C2A-N1A	-4.19	122.13	128.68
4	F	1249	ACO	C4A-C5A-N7A	-3.69	105.55	109.40
4	F	1249	ACO	O9P-C9P-N8P	-3.69	115.07	122.99
4	F	1249	ACO	CAP-C9P-N8P	3.56	123.66	116.58
4	F	1249	ACO	O3B-P3B-O7A	-3.55	95.70	109.39
4	B	1251	ACO	O4B-C1B-C2B	-3.53	101.76	106.93
4	F	1249	ACO	O9A-P3B-O8A	3.38	120.57	107.64
5	D	1250	V55	CAE-CAF-CAJ	-3.20	117.21	120.50
4	D	1249	ACO	C4A-C5A-N7A	-3.13	106.14	109.40
4	B	1251	ACO	P2A-O3A-P1A	-3.04	122.38	132.83
4	F	1249	ACO	C5A-C6A-N6A	3.02	124.93	120.35
4	D	1249	ACO	O-C-S1P	3.00	135.92	122.60
4	E	1250	ACO	C7P-C6P-C5P	-2.93	107.47	112.36
4	D	1249	ACO	O3B-P3B-O7A	-2.91	98.15	109.39
4	F	1249	ACO	O-C-CH3	-2.91	111.14	123.07
4	E	1250	ACO	C4A-C5A-N7A	-2.82	106.46	109.40
4	B	1251	ACO	C6P-C7P-N8P	-2.77	106.31	111.90
4	F	1249	ACO	C2A-N1A-C6A	2.77	123.48	118.75
4	D	1249	ACO	CEP-CBP-CAP	2.72	113.53	108.82
4	D	1249	ACO	OAP-CAP-CBP	2.71	116.63	110.25
4	E	1250	ACO	O5P-C5P-N4P	-2.71	117.90	123.01
4	E	1250	ACO	P2A-O3A-P1A	-2.66	123.70	132.83
4	D	1249	ACO	O-C-CH3	-2.62	112.30	123.07
4	D	1249	ACO	O4B-C4B-C5B	-2.62	100.75	109.37
4	D	1249	ACO	C5A-C6A-N6A	2.37	123.95	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1250	ACO	C2P-C3P-N4P	-2.34	107.49	112.42
4	E	1250	ACO	O3B-P3B-O7A	-2.29	100.55	109.39
4	B	1251	ACO	O9A-P3B-O7A	2.28	119.59	110.68
4	E	1250	ACO	O4B-C1B-C2B	-2.25	103.64	106.93
5	D	1250	V55	OAH-CAK-CAJ	2.24	117.82	114.57
4	F	1249	ACO	CEP-CBP-CDP	2.24	113.73	109.17
4	B	1251	ACO	CDP-CBP-CAP	2.24	112.70	108.82
4	D	1249	ACO	O9A-P3B-O7A	2.23	119.43	110.68
4	B	1251	ACO	O9A-P3B-O8A	2.22	116.13	107.64
4	E	1250	ACO	O5P-C5P-C6P	-2.21	117.97	122.02
5	D	1250	V55	CAI-CAG-CAK	-2.21	117.18	120.17
5	D	1250	V55	OAH-CAK-CAG	-2.21	120.32	124.12
4	B	1251	ACO	C1B-N9A-C4A	-2.21	122.76	126.64
4	B	1251	ACO	C4A-C5A-N7A	-2.17	107.14	109.40
5	D	1250	V55	OAB-CAD-CAI	-2.14	117.66	124.59
4	F	1249	ACO	C1B-N9A-C4A	-2.09	122.96	126.64
4	E	1250	ACO	CDP-CBP-CCP	-2.08	104.84	108.23
4	E	1250	ACO	O-C-S1P	-2.07	113.39	122.60
4	B	1251	ACO	OAP-CAP-CBP	-2.06	105.41	110.25
4	B	1251	ACO	O6A-CCP-CBP	-2.03	107.28	110.55
4	F	1249	ACO	C2P-C3P-N4P	-2.03	108.16	112.42
4	F	1249	ACO	CDP-CBP-CCP	-2.02	104.94	108.23

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1251	ACO	C3B-O3B-P3B-O7A
4	E	1250	ACO	C3B-O3B-P3B-O7A
4	E	1250	ACO	S1P-C2P-C3P-N4P
4	F	1249	ACO	C5B-O5B-P1A-O2A
4	F	1249	ACO	C5B-O5B-P1A-O3A
4	F	1249	ACO	CCP-O6A-P2A-O4A
4	F	1249	ACO	CAP-CBP-CCP-O6A
4	E	1250	ACO	C6P-C5P-N4P-C3P
4	E	1250	ACO	O5P-C5P-N4P-C3P
4	F	1249	ACO	CEP-CBP-CCP-O6A
4	F	1249	ACO	C3B-C4B-C5B-O5B
4	B	1251	ACO	O-C-S1P-C2P
4	B	1251	ACO	CH3-C-S1P-C2P
4	E	1250	ACO	O-C-S1P-C2P
4	E	1250	ACO	CH3-C-S1P-C2P

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Mol	Chain	Res	Type	Atoms
4	F	1249	ACO	O4B-C4B-C5B-O5B
4	F	1249	ACO	CDP-CBP-CCP-O6A
4	E	1250	ACO	C5P-C6P-C7P-N8P
4	F	1249	ACO	C5P-C6P-C7P-N8P
4	D	1249	ACO	C3B-O3B-P3B-O8A
4	F	1249	ACO	CCP-O6A-P2A-O3A
4	F	1249	ACO	C5B-O5B-P1A-O1A
4	F	1249	ACO	CCP-O6A-P2A-O5A
4	E	1250	ACO	C3P-C2P-S1P-C

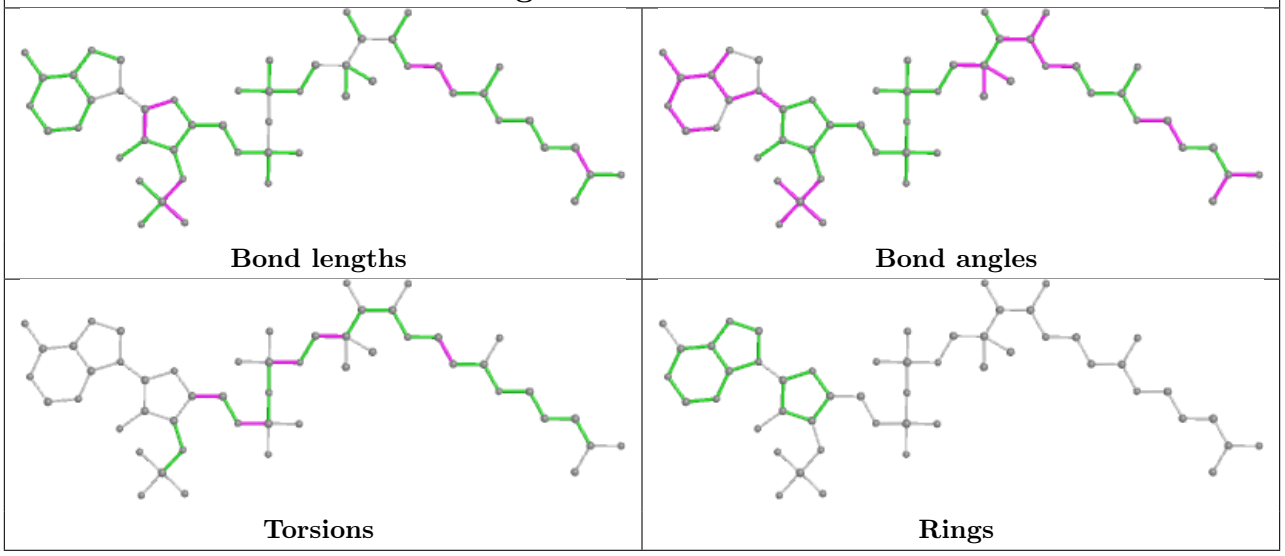
There are no ring outliers.

3 monomers are involved in 11 short contacts:

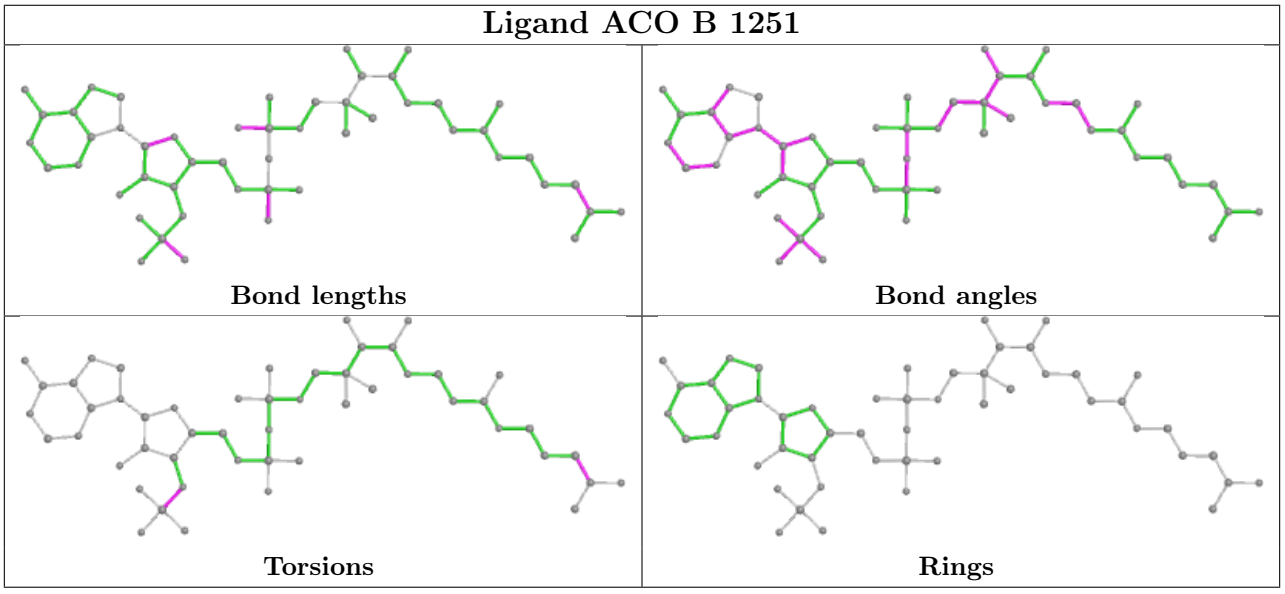
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1249	ACO	2	0
5	D	1250	V55	6	0
4	D	1249	ACO	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

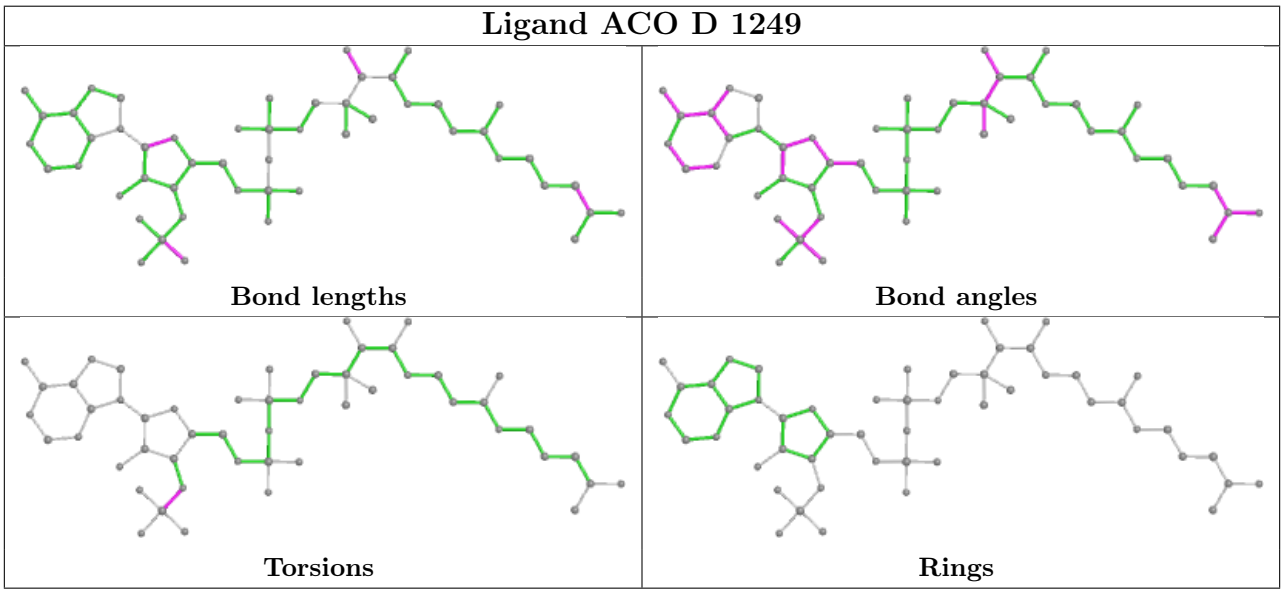
Ligand ACO F 1249



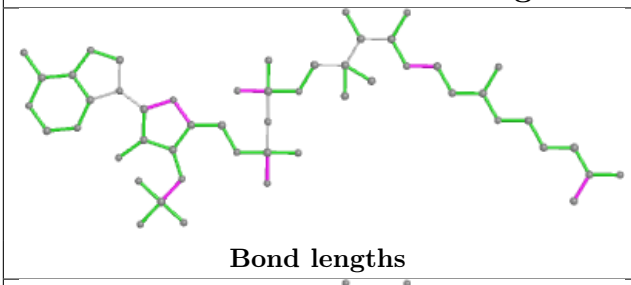
Ligand ACO B 1251



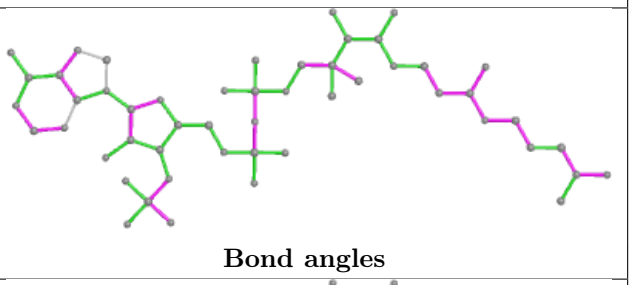
Ligand ACO D 1249



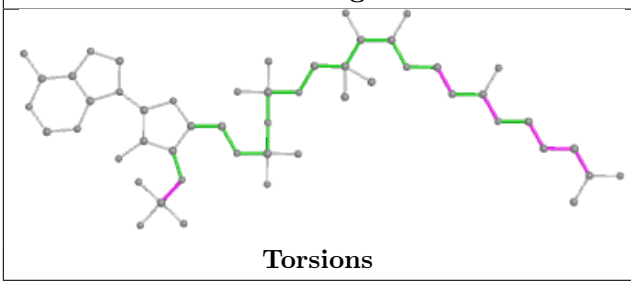
Ligand ACO E 1250



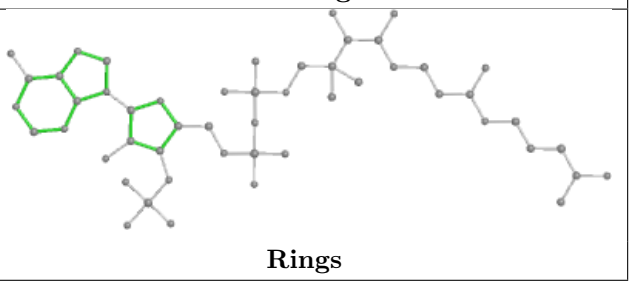
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	239/276 (86%)	-0.08	6 (2%)	57	55	31, 44, 56, 66	0
1	B	248/276 (89%)	-0.29	11 (4%)	34	32	27, 33, 51, 64	3 (1%)
1	C	236/276 (85%)	0.03	8 (3%)	45	43	29, 45, 54, 60	0
1	D	246/276 (89%)	-0.41	1 (0%)	92	92	25, 32, 45, 54	3 (1%)
2	E	241/276 (87%)	-0.38	6 (2%)	57	55	25, 33, 47, 61	1 (0%)
3	F	247/276 (89%)	-0.35	3 (1%)	79	77	24, 35, 45, 55	1 (0%)
All	All	1457/1656 (87%)	-0.25	35 (2%)	59	57	24, 36, 52, 66	8 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	GLU	6.4
1	A	82	GLY	5.6
2	E	75	TYR	4.8
1	B	81	ALA	4.6
1	B	76	PHE	3.8
1	C	146	TRP	3.6
1	A	5	GLU	3.1
1	B	6	GLY	3.1
1	C	111	ALA	3.0
1	B	82	GLY	3.0
1	C	116	TRP	3.0
1	B	80	ASP	2.9
2	E	250	THR	2.8
1	B	75	TYR	2.8
1	C	62	ALA	2.8
1	A	59	LEU	2.7
1	B	250	THR	2.6
1	B	5	GLU	2.6
1	C	82	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	125	LEU	2.6
1	A	58	VAL	2.6
3	F	59	LEU	2.5
2	E	59	LEU	2.5
3	F	77	ARG	2.4
1	B	72	LEU	2.4
2	E	121	GLY	2.4
1	C	148	ILE	2.4
1	A	146	TRP	2.4
1	A	83	PRO	2.3
1	D	59	LEU	2.3
3	F	28	GLU	2.2
2	E	17	ASP	2.2
2	E	6	GLY	2.1
1	B	77	ARG	2.0
1	C	110	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

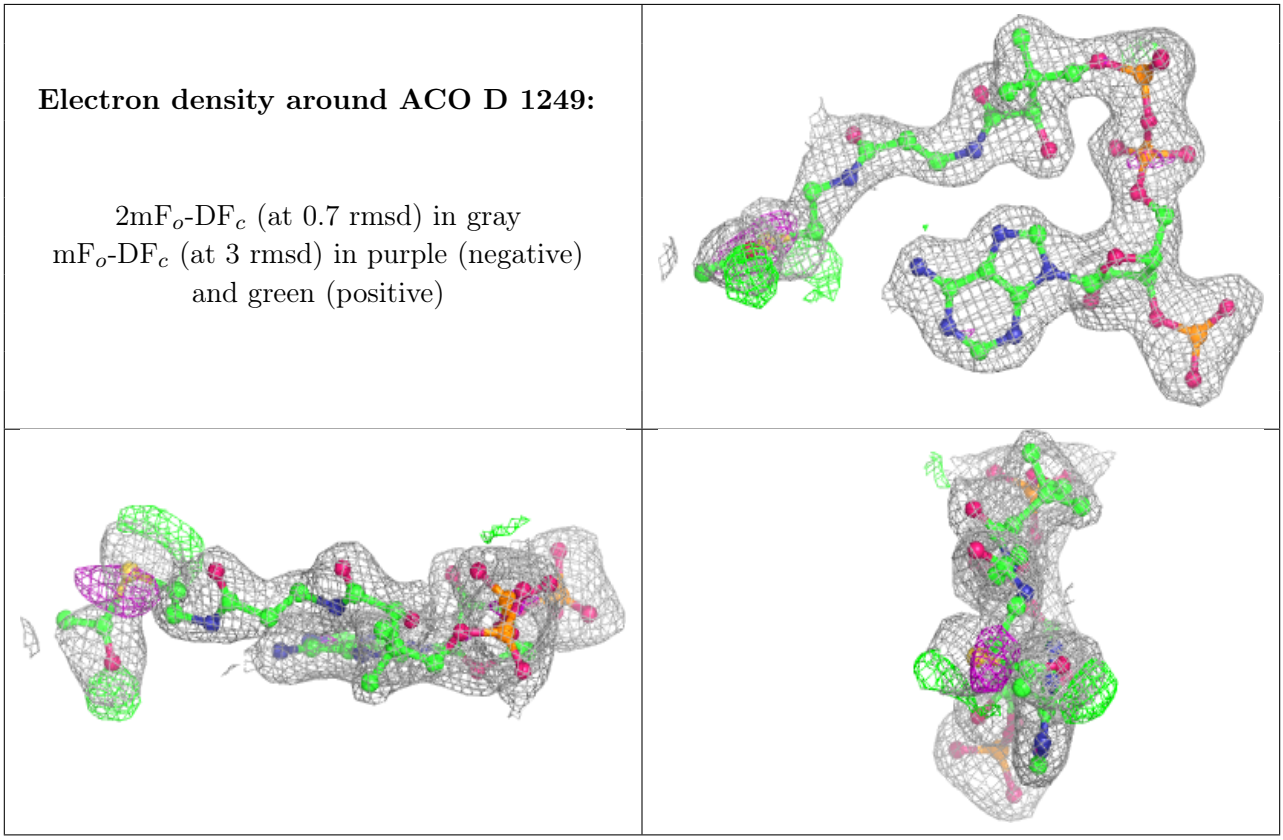
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACO	D	1249	51/51	0.94	0.17	32,40,52,62	0
4	ACO	F	1249	51/51	0.94	0.18	38,44,52,66	0
5	V55	D	1250	11/11	0.95	0.16	35,40,41,43	3
4	ACO	B	1251	51/51	0.96	0.17	37,44,65,68	0
4	ACO	E	1250	51/51	0.96	0.17	37,44,68,73	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

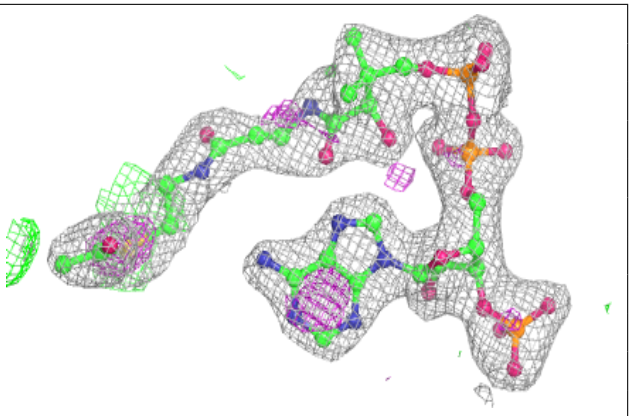
Electron density around ACO D 1249:

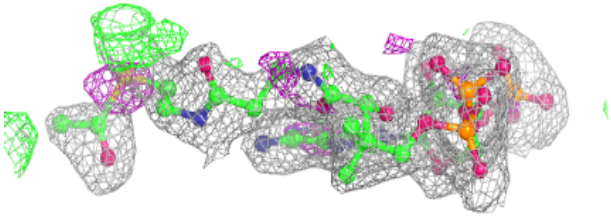
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

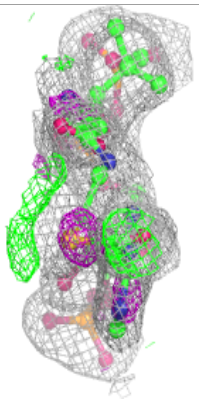


Electron density around ACO F 1249:

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

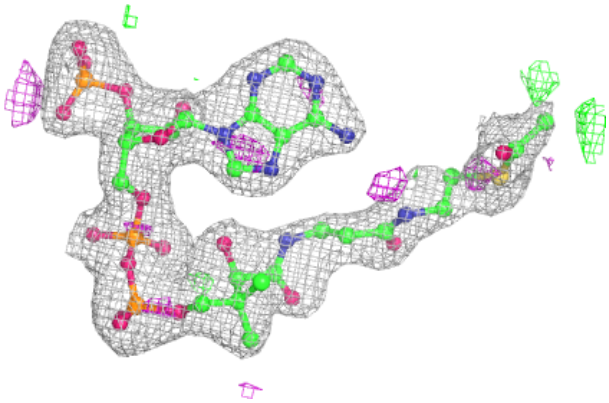


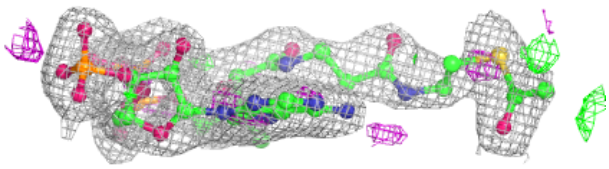


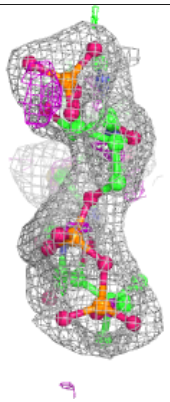


Electron density around ACO B 1251:

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

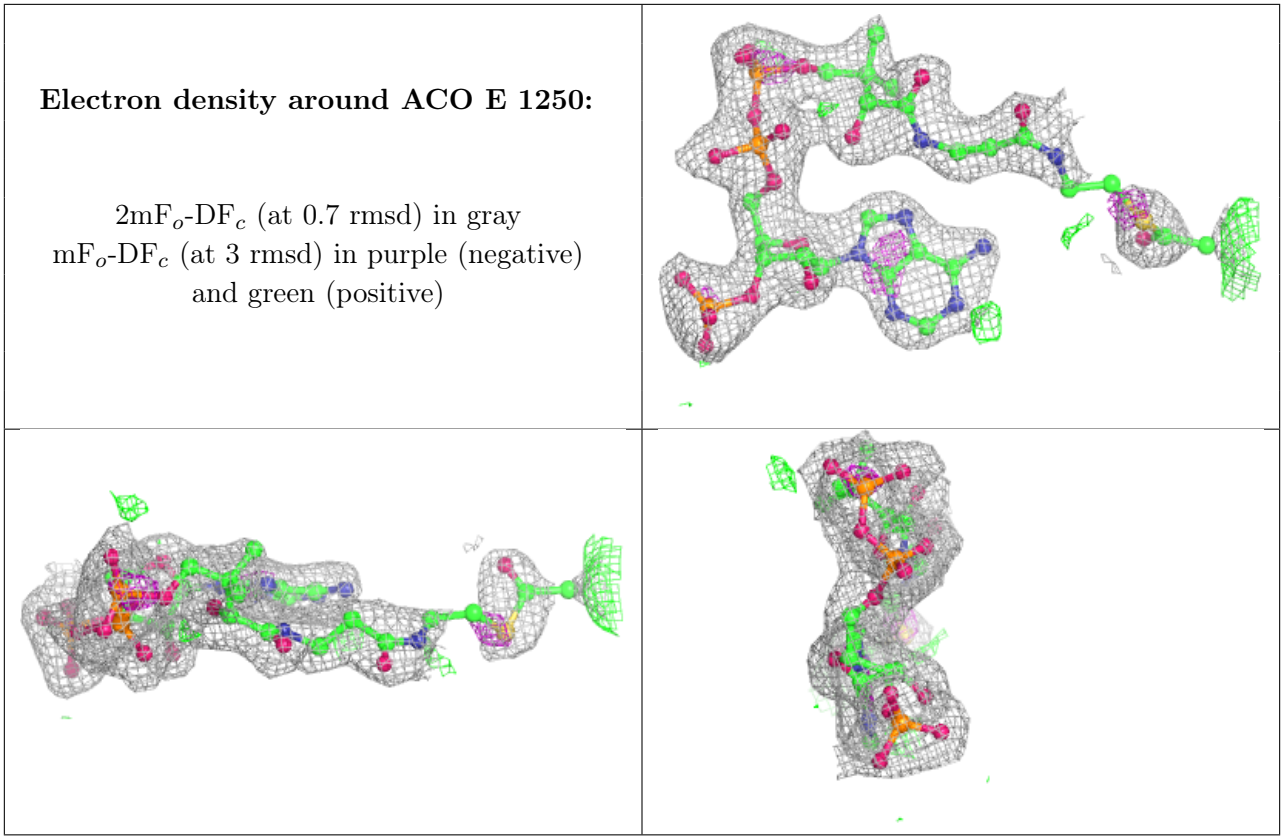






Electron density around ACO E 1250:

$2mF_o$-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.