



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:12 AM UTC

PDB ID : 4DPM / pdb_00004dpm
Title : Structure of malonyl-coenzyme A reductase from crenarchaeota in complex with CoA
Authors : Demmer, U.; Warkentin, E.; Srivastava, A.; Kockelkorn, D.; Fuchs, G.; Ermler, U.
Deposited on : 2012-02-13
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

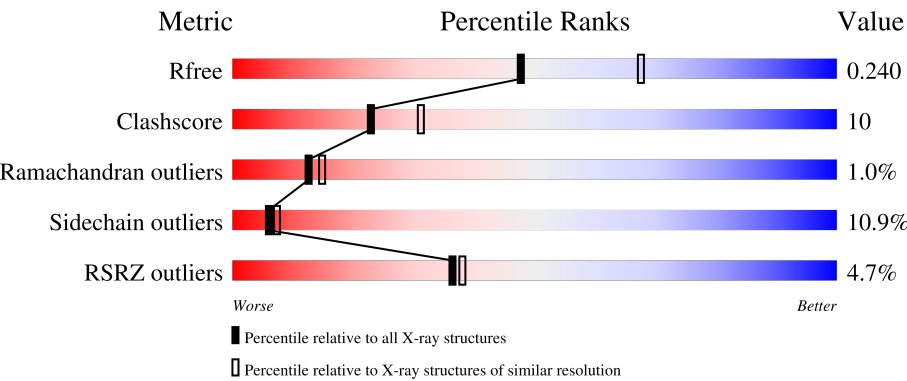
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	359	39%48%10%..
1	B	359	46%43%8%..
1	C	359	4% 70%25%..
1	D	359	19% 71%24%..

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Mol	Chain	Length	Quality of chain
1	E	359	2% 70% 25% • •
1	F	359	3% 72% 23% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17284 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 Malonyl-CoA/succinyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	B	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	C	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	D	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	E	353	Total	C	N	O	S	0	0	0
			2732	1753	462	509	8			
1	F	353	Total	C	N	O	S	0	0	0
			2732	1753	462	509	8			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

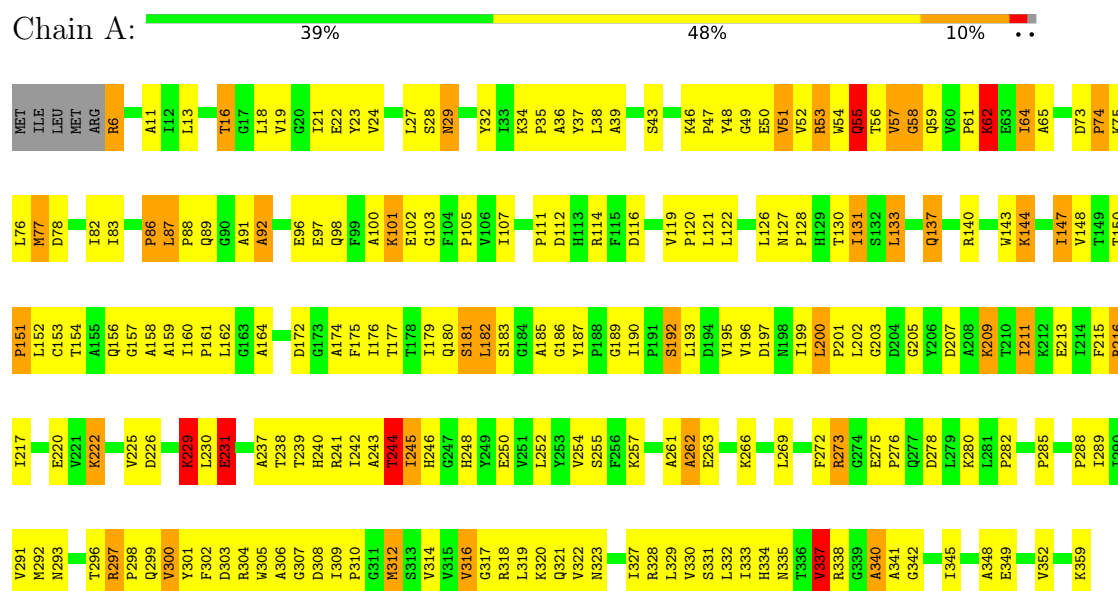
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	172	Total	O	0	0
			172	172		
4	C	59	Total	O	0	0
			59	59		
4	D	57	Total	O	0	0
			57	57		
4	E	52	Total	O	0	0
			52	52		
4	F	30	Total	O	0	0
			30	30		

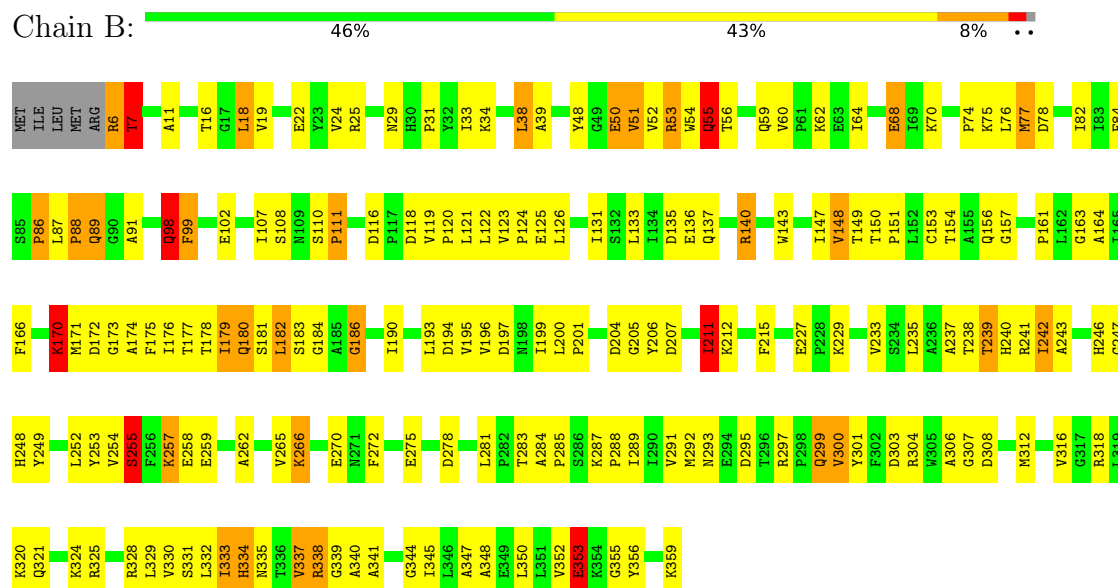
3 Residue-property plots

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: Malonyl-CoA/succinyl-CoA reductase



• Molecule 1: Malonyl-CoA/succinyl-CoA reductase



Chain C:

4% 70% 25%

MET ILE LEU MET ARG R6 I7 L8 K9 L13 H30 K34 Y37 K41 G42 S43 V51 V52 R53 W54 Q55 K62 E63 I64 I165 K167 W176 M77 D78 D79 V80 S85 P86 L87 P88 Q89 E96 F97 Q98 F99 A100 P111 D112 H113 R114 F115 V119 P120 I121

L122 L126 H129 T130 I131 S132 E136 Q137 R138 K139 R140 W143 K144 G145 F146 I147 V148 C153 T154 A158 A159 I160 P161 A164 I165 F166 K167 F175 Q180 I190 P191 S192 V196 I199 L200 P201 K209 T210 I211 K212 R215 R216 K222 R223 P228 K229 L230 E231 L235 H240 Y249 L252 K257 E258 E259 A262 E263 K264 V265 K266 E267 R273 K280 T283 K287 P288 E294 R297 P298 D308 I309 W312 R318 L319 K320 Q321 V322 R328 L329 V330 I333 V337 R338 I345 K353 K359

Chain D:

19% 71% 24%

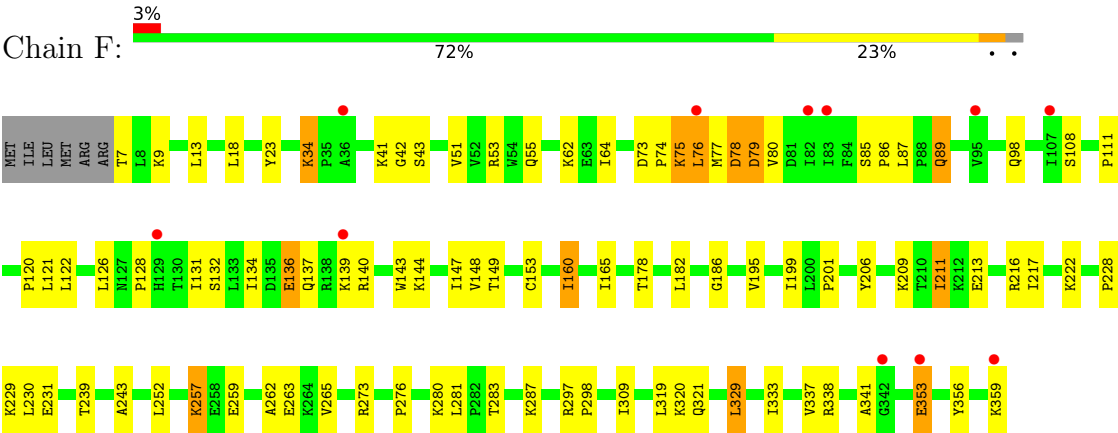
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Chain E:

2% 70% 25%

MET ILE LEU MET ARG ARG T7 L8 K9 L13 L18 Y23 K34 Y37 L38 A39 G40 K41 G42 S43 Y48 V51 V52 R53 W54 Q55 K62 E63 I64 M67 D73 P74 K75 L76 M77 D78 D79 V80 S85 P86 L87 P88 Q89 V95 S110 P111 R112 D118 V119 L120 L121 L122 L126 N127 P128 H129 T130 S132 E136 Q137 R138 R139 R140 V143 K144 G145 F146 I147 V148 I160 K167 I179 G186 Y187 P188 G189 I190 V195 I199 L200 P201 K209 T210 K212 E213 R216 T217 K222 R223 W224 V225 R226

● Molecule 1: Malonyl-CoA/succinyl-CoA reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.63Å 137.62Å 362.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.9 (30.00-2.30) 87.9 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.198 , 0.247 (Not available) , 0.240	Depositor DCC
R_{free} test set	6243 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17284	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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, MG

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	2.63	178/2804 (6.3%)	1.97	81/3808 (2.1%)
1	B	2.41	145/2804 (5.2%)	1.86	63/3808 (1.7%)
1	C	1.14	3/2804 (0.1%)	1.14	2/3808 (0.1%)
1	D	0.99	4/2804 (0.1%)	1.07	2/3808 (0.1%)
1	E	1.07	5/2793 (0.2%)	1.11	5/3794 (0.1%)
1	F	0.88	1/2793 (0.0%)	1.03	2/3794 (0.1%)
All	All	1.68	336/16802 (2.0%)	1.42	155/22820 (0.7%)

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 (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	SER	C-O	13.11	1.39	1.24
1	A	238	THR	CA-C	-11.39	1.39	1.52
1	A	333	ILE	CA-C	10.56	1.66	1.52
1	A	245	ILE	C-O	10.35	1.35	1.23
1	B	39	ALA	CA-CB	-10.30	1.36	1.53
1	A	329	LEU	C-O	9.87	1.36	1.23
1	A	200	LEU	CG-CD1	9.86	1.85	1.52
1	A	310	PRO	N-CA	9.83	1.59	1.47
1	A	38	LEU	N-CA	9.79	1.60	1.46
1	A	246	HIS	C-O	9.71	1.36	1.23
1	B	123	VAL	CA-C	9.62	1.61	1.52
1	A	330	VAL	C-O	9.25	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	ILE	CA-CB	9.24	1.67	1.54
1	A	176	ILE	N-CA	9.21	1.56	1.46
1	B	353	GLU	CB-CG	9.12	1.79	1.52
1	B	333	ILE	C-O	9.06	1.33	1.24
1	B	126	LEU	CA-C	-9.01	1.41	1.52
1	B	238	THR	N-CA	-8.89	1.35	1.46
1	A	57	VAL	CA-CB	8.82	1.64	1.54
1	B	204	ASP	C-O	8.75	1.34	1.24
1	B	243	ALA	CA-C	8.73	1.65	1.53
1	A	199	ILE	CA-CB	-8.59	1.42	1.54
1	A	243	ALA	CA-C	8.54	1.64	1.53
1	A	187	TYR	C-O	-8.51	1.11	1.25
1	A	53	ARG	CG-CD	8.46	1.77	1.52
1	B	246	HIS	C-O	8.40	1.34	1.23
1	A	332	LEU	N-CA	8.38	1.56	1.46
1	A	338	ARG	C-O	8.38	1.33	1.24
1	A	112	ASP	C-O	8.29	1.33	1.24
1	A	19	VAL	CA-C	8.29	1.63	1.52
1	B	91	ALA	CA-C	8.26	1.64	1.52
1	A	205	GLY	N-CA	8.22	1.57	1.45
1	A	240	HIS	C-O	8.17	1.34	1.23
1	A	158	ALA	CA-C	8.16	1.63	1.52
1	A	306	ALA	CA-CB	8.15	1.66	1.53
1	B	249	TYR	CA-CB	-8.14	1.41	1.53
1	B	237	ALA	C-O	-8.11	1.14	1.23
1	B	233	VAL	CA-CB	8.04	1.65	1.54
1	B	289	ILE	CA-CB	8.04	1.64	1.53
1	B	82	ILE	C-O	7.99	1.31	1.24
1	B	54	TRP	CA-CB	7.98	1.62	1.52
1	A	333	ILE	C-O	7.98	1.33	1.24
1	A	150	THR	CA-C	7.93	1.63	1.52
1	B	211	ILE	CA-CB	7.91	1.63	1.54
1	A	348	ALA	CA-C	7.84	1.62	1.52
1	A	86	PRO	C-O	-7.82	1.13	1.24
1	A	222	LYS	N-CA	7.73	1.55	1.46
1	A	130	THR	CA-CB	7.71	1.67	1.53
1	A	62	LYS	N-CA	7.68	1.56	1.46
1	A	241	ARG	CZ-NH1	7.67	1.43	1.32
1	B	347	ALA	N-CA	7.66	1.55	1.46
1	A	154	THR	CA-CB	7.65	1.65	1.53
1	B	339	GLY	C-O	7.64	1.33	1.23
1	A	159	ALA	C-O	-7.63	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLY	C-O	7.57	1.33	1.23
1	B	284	ALA	C-O	-7.52	1.15	1.24
1	A	111	PRO	CA-CB	7.51	1.66	1.53
1	A	199	ILE	C-O	7.51	1.31	1.24
1	A	22	GLU	CA-C	7.50	1.63	1.52
1	A	348	ALA	C-O	-7.48	1.15	1.24
1	A	335	ASN	CA-C	-7.48	1.42	1.52
1	A	157	GLY	N-CA	7.48	1.55	1.45
1	A	254	VAL	CA-CB	7.45	1.63	1.54
1	B	181	SER	N-CA	7.44	1.54	1.45
1	B	190	ILE	N-CA	-7.44	1.37	1.46
1	B	18	LEU	C-O	7.37	1.33	1.24
1	B	241	ARG	C-O	7.37	1.33	1.23
1	B	88	PRO	CA-CB	7.35	1.63	1.53
1	A	186	GLY	C-O	7.35	1.33	1.24
1	A	302	PHE	CE1-CZ	7.32	1.60	1.38
1	B	212	LYS	CA-C	7.27	1.62	1.52
1	B	29	ASN	CB-CG	7.26	1.70	1.52
1	B	88	PRO	CG-CD	7.24	1.75	1.50
1	B	25	ARG	NE-CZ	7.24	1.41	1.33
1	B	254	VAL	CA-C	-7.23	1.43	1.52
1	A	291	VAL	N-CA	-7.22	1.37	1.46
1	A	244	THR	C-O	7.22	1.32	1.23
1	B	289	ILE	C-O	-7.22	1.16	1.24
1	A	197	ASP	CG-OD2	7.22	1.39	1.25
1	B	84	PHE	CA-C	7.20	1.61	1.52
1	A	147	ILE	CA-CB	7.20	1.62	1.54
1	A	203	GLY	C-O	7.15	1.31	1.24
1	A	211	ILE	N-CA	7.14	1.55	1.46
1	A	255	SER	CB-OG	-7.14	1.27	1.42
1	A	312	MET	SD-CE	7.12	1.97	1.79
1	B	241	ARG	CZ-NH1	7.07	1.42	1.32
1	A	193	LEU	N-CA	7.05	1.55	1.46
1	A	230	LEU	CA-C	7.03	1.61	1.52
1	A	308	ASP	C-O	-7.02	1.15	1.24
1	B	272	PHE	C-O	-7.01	1.15	1.23
1	A	197	ASP	CB-CG	7.01	1.69	1.52
1	B	53	ARG	CG-CD	7.01	1.73	1.52
1	A	151	PRO	C-O	6.99	1.32	1.23
1	A	190	ILE	N-CA	-6.96	1.38	1.46
1	B	38	LEU	N-CA	6.96	1.55	1.46
1	E	211	ILE	CA-CB	6.92	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLU	CA-CB	-6.92	1.42	1.53
1	A	27	LEU	C-O	-6.90	1.15	1.24
1	A	269	LEU	C-O	6.86	1.32	1.24
1	A	37	TYR	C-O	6.85	1.31	1.23
1	B	347	ALA	CA-CB	6.85	1.64	1.53
1	A	345	ILE	N-CA	-6.85	1.39	1.46
1	A	92	ALA	N-CA	-6.84	1.37	1.46
1	A	156	GLN	N-CA	6.82	1.55	1.46
1	A	309	ILE	C-O	6.78	1.30	1.23
1	A	174	ALA	CA-CB	6.78	1.65	1.53
1	D	221	VAL	CA-CB	6.76	1.61	1.53
1	A	36	ALA	CA-CB	6.72	1.63	1.53
1	B	248	HIS	C-O	6.70	1.31	1.24
1	A	91	ALA	CA-C	6.70	1.61	1.52
1	A	162	LEU	C-O	6.68	1.32	1.24
1	A	114	ARG	CZ-NH1	6.67	1.42	1.32
1	A	338	ARG	C-N	6.65	1.41	1.33
1	A	238	THR	CA-CB	6.64	1.63	1.53
1	A	32	TYR	CA-C	6.63	1.60	1.52
1	B	205	GLY	C-O	6.63	1.31	1.23
1	B	341	ALA	CA-C	6.59	1.61	1.52
1	A	266	LYS	CA-C	6.56	1.61	1.52
1	B	22	GLU	CA-C	6.54	1.61	1.52
1	A	202	LEU	CA-C	-6.52	1.44	1.52
1	A	231	GLU	C-O	-6.50	1.15	1.24
1	A	242	ILE	CA-CB	-6.48	1.45	1.54
1	A	122	LEU	CA-CB	6.46	1.62	1.53
1	B	108	SER	N-CA	-6.46	1.38	1.46
1	B	150	THR	CA-C	6.43	1.61	1.52
1	B	255	SER	CB-OG	-6.42	1.29	1.42
1	B	318	ARG	NE-CZ	6.42	1.40	1.33
1	B	239	THR	C-O	6.42	1.32	1.23
1	B	197	ASP	CG-OD2	6.42	1.37	1.25
1	A	304	ARG	NE-CZ	6.38	1.40	1.33
1	A	179	ILE	N-CA	-6.38	1.37	1.46
1	B	238	THR	CA-CB	6.38	1.62	1.53
1	A	21	ILE	CA-CB	6.37	1.62	1.54
1	B	292	MET	C-O	6.37	1.31	1.23
1	B	335	ASN	CA-CB	6.36	1.63	1.53
1	E	48	TYR	C-O	-6.35	1.16	1.24
1	B	345	ILE	C-O	6.35	1.31	1.24
1	A	300	VAL	N-CA	-6.34	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	GLU	C-O	-6.32	1.18	1.24
1	A	180	GLN	C-O	6.31	1.31	1.23
1	B	148	VAL	C-O	6.30	1.30	1.24
1	B	166	PHE	C-O	6.29	1.32	1.24
1	A	190	ILE	C-O	6.29	1.32	1.24
1	B	7	THR	CA-C	6.27	1.60	1.52
1	B	52	VAL	N-CA	-6.26	1.38	1.46
1	B	306	ALA	CA-CB	6.25	1.63	1.53
1	A	101	LYS	C-O	-6.25	1.16	1.24
1	B	175	PHE	CA-C	-6.25	1.45	1.53
1	A	35	PRO	CG-CD	6.24	1.72	1.50
1	A	207	ASP	CG-OD1	6.24	1.37	1.25
1	A	161	PRO	CA-CB	6.21	1.63	1.53
1	E	179	ILE	N-CA	-6.19	1.39	1.46
1	B	174	ALA	CA-CB	6.18	1.66	1.53
1	A	215	PHE	C-O	-6.17	1.16	1.24
1	A	197	ASP	CG-OD1	6.16	1.37	1.25
1	B	265	VAL	N-CA	-6.16	1.39	1.46
1	B	11	ALA	CA-CB	-6.15	1.44	1.53
1	A	328	ARG	CZ-NH1	6.14	1.41	1.32
1	A	180	GLN	CA-C	6.14	1.60	1.52
1	A	340	ALA	N-CA	6.14	1.54	1.46
1	B	304	ARG	CB-CG	6.13	1.70	1.52
1	B	55	GLN	CA-CB	6.13	1.62	1.53
1	A	164	ALA	CA-C	-6.13	1.44	1.52
1	A	318	ARG	NE-CZ	6.13	1.39	1.33
1	B	176	ILE	CA-CB	6.11	1.62	1.54
1	C	190	ILE	CA-C	6.11	1.57	1.53
1	A	54	TRP	CA-CB	6.08	1.60	1.52
1	B	194	ASP	CA-C	-6.07	1.44	1.52
1	A	52	VAL	CA-CB	6.06	1.60	1.54
1	B	180	GLN	C-O	6.04	1.31	1.23
1	B	177	THR	C-O	6.04	1.30	1.24
1	B	266	LYS	N-CA	-6.04	1.39	1.46
1	A	177	THR	CA-CB	6.00	1.65	1.53
1	A	248	HIS	C-N	5.98	1.41	1.33
1	A	335	ASN	CA-CB	5.96	1.63	1.53
1	B	206	TYR	C-O	-5.95	1.16	1.24
1	B	98	GLN	CG-CD	5.95	1.67	1.52
1	B	242	ILE	N-CA	-5.91	1.39	1.46
1	B	340	ALA	CA-CB	5.91	1.63	1.53
1	B	304	ARG	NE-CZ	5.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	THR	C-O	-5.89	1.18	1.24
1	A	289	ILE	N-CA	-5.88	1.38	1.46
1	B	200	LEU	N-CA	5.88	1.53	1.46
1	B	247	GLY	CA-C	5.88	1.60	1.51
1	B	183	SER	CA-CB	5.88	1.63	1.53
1	A	61	PRO	N-CA	5.87	1.54	1.47
1	A	328	ARG	CA-C	5.87	1.59	1.52
1	A	302	PHE	C-O	-5.86	1.16	1.24
1	A	179	ILE	C-O	5.84	1.30	1.24
1	B	334	HIS	N-CA	-5.84	1.39	1.46
1	B	82	ILE	N-CA	-5.83	1.39	1.46
1	B	328	ARG	CD-NE	5.82	1.54	1.46
1	A	330	VAL	CA-CB	5.82	1.64	1.54
1	B	186	GLY	C-O	5.82	1.34	1.24
1	A	103	GLY	N-CA	5.82	1.53	1.45
1	B	123	VAL	CA-CB	-5.81	1.49	1.54
1	B	297	ARG	C-O	5.79	1.29	1.24
1	A	11	ALA	CA-CB	-5.79	1.44	1.53
1	A	341	ALA	C-O	-5.78	1.17	1.24
1	B	170	LYS	CD-CE	5.78	1.69	1.52
1	A	243	ALA	CA-CB	5.78	1.60	1.52
1	B	56	THR	C-O	5.77	1.30	1.23
1	B	281	LEU	N-CA	5.77	1.54	1.46
1	A	97	GLU	N-CA	-5.76	1.39	1.46
1	B	240	HIS	C-O	5.75	1.30	1.23
1	B	118	ASP	CB-CG	5.74	1.66	1.52
1	B	126	LEU	C-O	-5.73	1.15	1.23
1	B	211	ILE	N-CA	-5.72	1.40	1.46
1	B	350	LEU	N-CA	-5.71	1.39	1.46
1	B	215	PHE	CG-CD1	5.71	1.50	1.38
1	B	352	VAL	CA-C	5.70	1.59	1.52
1	A	148	VAL	CA-CB	-5.70	1.47	1.54
1	A	293	ASN	N-CA	-5.68	1.38	1.46
1	A	107	ILE	CA-C	5.67	1.59	1.52
1	B	179	ILE	CA-C	-5.66	1.48	1.53
1	B	116	ASP	CA-C	5.66	1.59	1.53
1	A	137	GLN	N-CA	5.66	1.53	1.46
1	B	33	ILE	C-O	-5.66	1.18	1.24
1	A	307	GLY	C-O	5.66	1.31	1.23
1	A	182	LEU	C-O	5.65	1.31	1.24
1	A	144	LYS	C-O	5.64	1.31	1.24
1	A	245	ILE	CA-CB	5.64	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	ARG	CA-CB	5.64	1.61	1.53
1	A	215	PHE	N-CA	-5.64	1.39	1.46
1	B	229	LYS	CA-C	5.63	1.60	1.52
1	B	328	ARG	CG-CD	5.63	1.69	1.52
1	A	238	THR	CB-CG2	5.63	1.71	1.52
1	B	133	LEU	C-O	-5.63	1.16	1.24
1	B	297	ARG	CZ-NH1	5.61	1.40	1.32
1	A	105	PRO	C-O	5.61	1.29	1.23
1	A	291	VAL	CA-CB	-5.61	1.47	1.54
1	A	312	MET	CA-CB	5.61	1.62	1.53
1	B	161	PRO	CA-C	5.60	1.60	1.52
1	A	92	ALA	CA-CB	-5.58	1.44	1.53
1	A	293	ASN	C-O	-5.56	1.16	1.24
1	A	252	LEU	N-CA	5.56	1.52	1.46
1	A	107	ILE	C-O	5.55	1.30	1.24
1	B	338	ARG	C-O	5.55	1.30	1.24
1	B	182	LEU	N-CA	5.54	1.53	1.46
1	B	337	VAL	N-CA	5.52	1.53	1.46
1	F	160	ILE	CA-CB	5.52	1.57	1.54
1	B	184	GLY	CA-C	5.51	1.59	1.51
1	C	235	LEU	N-CA	5.51	1.52	1.46
1	B	299	GLN	N-CA	-5.51	1.39	1.46
1	A	303	ASP	CA-CB	5.50	1.62	1.54
1	E	190	ILE	CA-C	5.50	1.57	1.53
1	A	185	ALA	CA-C	-5.49	1.45	1.52
1	B	257	LYS	N-CA	-5.47	1.39	1.46
1	B	297	ARG	NE-CZ	5.47	1.39	1.33
1	B	149	THR	CA-C	-5.46	1.46	1.52
1	D	262	ALA	CA-CB	5.46	1.61	1.53
1	B	119	VAL	CA-CB	5.45	1.61	1.54
1	B	25	ARG	CZ-NH2	5.44	1.40	1.33
1	A	24	VAL	C-O	5.44	1.30	1.24
1	B	154	THR	CA-C	5.43	1.60	1.52
1	B	178	THR	N-CA	-5.43	1.39	1.45
1	B	99	PHE	CA-C	5.42	1.59	1.52
1	A	250	GLU	CA-C	-5.42	1.46	1.52
1	B	50	GLU	N-CA	-5.42	1.38	1.46
1	B	31	PRO	CG-CD	5.41	1.69	1.50
1	B	172	ASP	CA-C	5.41	1.59	1.52
1	A	220	GLU	C-O	-5.38	1.16	1.24
1	A	56	THR	C-O	5.38	1.29	1.23
1	A	302	PHE	CG-CD2	5.38	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	GLY	C-O	5.37	1.29	1.23
1	A	303	ASP	C-O	-5.37	1.17	1.24
1	B	243	ALA	CA-CB	5.37	1.59	1.52
1	B	183	SER	CA-C	-5.36	1.45	1.52
1	A	187	TYR	CD2-CE2	5.36	1.54	1.38
1	A	46	LYS	C-O	-5.35	1.18	1.24
1	A	59	GLN	CD-OE1	5.35	1.33	1.23
1	A	229	LYS	CD-CE	5.35	1.68	1.52
1	B	300	VAL	CB-CG2	5.35	1.70	1.52
1	A	114	ARG	C-O	-5.35	1.17	1.24
1	B	193	LEU	CA-C	5.34	1.60	1.52
1	B	353	GLU	CG-CD	-5.34	1.38	1.52
1	A	242	ILE	CG1-CD1	5.33	1.72	1.51
1	A	337	VAL	CA-CB	5.33	1.61	1.54
1	B	275	GLU	CD-OE2	5.31	1.35	1.25
1	E	37	TYR	CA-C	5.31	1.58	1.52
1	B	330	VAL	C-O	5.30	1.29	1.24
1	B	193	LEU	N-CA	5.29	1.53	1.46
1	B	39	ALA	CA-C	5.27	1.60	1.53
1	B	356	TYR	CA-C	5.26	1.60	1.52
1	A	189	GLY	CA-C	5.25	1.59	1.51
1	A	54	TRP	CA-C	-5.25	1.47	1.53
1	A	183	SER	N-CA	5.24	1.53	1.46
1	D	160	ILE	CA-CB	5.24	1.56	1.54
1	A	83	ILE	C-O	5.24	1.29	1.24
1	A	175	PHE	CA-C	-5.23	1.46	1.52
1	A	195	VAL	CA-CB	5.23	1.61	1.54
1	B	333	ILE	CA-CB	-5.22	1.47	1.55
1	C	160	ILE	CA-C	5.21	1.58	1.52
1	B	86	PRO	C-O	-5.20	1.17	1.24
1	A	148	VAL	C-N	5.19	1.41	1.33
1	A	345	ILE	C-O	5.19	1.29	1.24
1	A	189	GLY	N-CA	5.18	1.52	1.45
1	A	18	LEU	N-CA	-5.17	1.39	1.46
1	A	327	ILE	C-O	5.17	1.29	1.23
1	B	131	ILE	CB-CG1	5.17	1.63	1.53
1	B	205	GLY	N-CA	5.17	1.52	1.45
1	A	172	ASP	CA-C	5.16	1.59	1.52
1	A	88	PRO	CA-CB	5.16	1.60	1.53
1	B	278	ASP	C-O	-5.16	1.17	1.24
1	B	98	GLN	CA-CB	5.16	1.61	1.53
1	B	190	ILE	CA-C	5.16	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	ASP	N-CA	5.16	1.52	1.46
1	B	98	GLN	C-O	-5.15	1.17	1.24
1	A	201	PRO	C-O	5.14	1.30	1.23
1	D	211	ILE	CA-CB	5.13	1.61	1.54
1	B	190	ILE	C-O	-5.13	1.18	1.24
1	A	181	SER	CA-C	-5.13	1.45	1.53
1	A	333	ILE	CG1-CD1	5.12	1.71	1.51
1	A	262	ALA	C-O	-5.12	1.17	1.24
1	A	349	GLU	N-CA	-5.11	1.40	1.46
1	B	348	ALA	C-O	-5.11	1.18	1.24
1	A	100	ALA	CA-CB	-5.09	1.45	1.53
1	A	55	GLN	C-O	5.08	1.31	1.23
1	A	230	LEU	C-O	-5.08	1.18	1.24
1	A	182	LEU	CG-CD2	5.06	1.69	1.52
1	B	201	PRO	CA-C	-5.06	1.46	1.52
1	B	331	SER	CA-C	-5.06	1.46	1.52
1	A	58	GLY	N-CA	5.05	1.53	1.45
1	A	319	LEU	C-O	-5.04	1.17	1.23
1	B	253	TYR	CA-CB	5.04	1.60	1.53
1	A	338	ARG	CD-NE	5.04	1.53	1.46
1	A	160	ILE	CA-CB	5.03	1.60	1.54
1	A	323	ASN	N-CA	5.02	1.53	1.46
1	A	278	ASP	C-O	-5.02	1.18	1.24
1	A	207	ASP	CB-CG	5.01	1.64	1.52
1	B	355	GLY	CA-C	5.01	1.58	1.51
1	A	213	GLU	C-O	5.01	1.29	1.24
1	A	197	ASP	C-O	5.01	1.30	1.23
1	B	124	PRO	C-O	-5.00	1.17	1.24
1	A	296	THR	N-CA	5.00	1.51	1.46
1	B	176	ILE	CB-CG2	-5.00	1.36	1.52

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ILE	N-CA-C	-12.98	96.85	111.00
1	B	19	VAL	N-CA-C	-10.82	101.39	111.67
1	A	255	SER	N-CA-CB	-10.42	93.64	110.63
1	A	179	ILE	N-CA-CB	-9.65	100.86	112.35
1	A	225	VAL	N-CA-C	-9.01	97.82	108.82
1	B	328	ARG	NE-CZ-NH2	8.93	127.23	119.20
1	B	301	TYR	N-CA-C	-8.74	101.83	111.36
1	A	164	ALA	N-CA-C	-8.23	102.39	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	LEU	CB-CA-C	-8.10	98.80	110.13
1	A	28	SER	N-CA-C	-7.96	103.29	113.16
1	B	211	ILE	CA-CB-CG2	7.71	123.61	110.50
1	B	353	GLU	CB-CG-CD	-7.58	99.71	112.60
1	A	248	HIS	CA-C-O	-7.45	112.13	120.32
1	E	112	ASP	N-CA-C	7.32	118.90	111.07
1	A	211	ILE	CA-CB-CG2	7.27	122.85	110.50
1	A	48	TYR	N-CA-C	-7.23	103.48	111.36
1	A	114	ARG	NE-CZ-NH2	-7.14	112.77	119.20
1	B	295	ASP	N-CA-C	-7.11	104.60	113.20
1	B	22	GLU	N-CA-C	-7.04	103.03	111.69
1	A	126	LEU	CA-C-N	-6.99	115.15	122.28
1	A	126	LEU	C-N-CA	-6.99	115.15	122.28
1	B	353	GLU	CG-CD-OE1	-6.86	102.61	118.40
1	A	23	TYR	N-CA-C	-6.85	103.82	111.28
1	B	126	LEU	CA-C-N	-6.84	115.23	122.89
1	B	126	LEU	C-N-CA	-6.84	115.23	122.89
1	A	211	ILE	N-CA-CB	-6.83	99.15	110.56
1	A	307	GLY	N-CA-C	-6.75	105.54	111.95
1	B	297	ARG	CD-NE-CZ	-6.71	115.00	124.40
1	B	195	VAL	CB-CA-C	-6.67	100.36	111.29
1	A	309	ILE	CA-C-N	-6.63	112.93	119.76
1	A	309	ILE	C-N-CA	-6.63	112.93	119.76
1	A	133	LEU	N-CA-C	-6.55	105.11	113.23
1	A	43	SER	N-CA-C	6.50	121.04	111.87
1	F	122	LEU	N-CA-C	6.50	119.32	108.73
1	A	292	MET	CG-SD-CE	-6.47	86.67	100.90
1	D	122	LEU	N-CA-C	6.46	119.25	108.20
1	B	207	ASP	N-CA-C	-6.45	104.25	111.28
1	A	89	GLN	N-CA-C	6.40	119.31	110.35
1	A	239	THR	N-CA-C	6.40	120.12	109.95
1	A	201	PRO	CB-CA-C	-6.38	100.92	110.17
1	A	301	TYR	N-CA-C	-6.37	104.42	111.36
1	B	348	ALA	N-CA-C	-6.36	104.42	111.36
1	A	22	GLU	N-CA-C	-6.34	104.25	112.23
1	A	175	PHE	CA-C-N	-6.26	112.74	122.69
1	A	175	PHE	C-N-CA	-6.26	112.74	122.69
1	C	122	LEU	N-CA-C	6.19	118.78	108.20
1	B	255	SER	N-CA-CB	-6.18	100.55	110.63
1	A	177	THR	N-CA-CB	-6.14	100.17	110.80
1	C	112	ASP	N-CA-C	6.14	117.97	111.28
1	B	201	PRO	N-CA-C	-6.11	102.28	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	SER	N-CA-C	-6.10	100.95	110.17
1	B	292	MET	CG-SD-CE	-6.09	87.51	100.90
1	B	199	ILE	N-CA-C	-6.08	99.40	108.46
1	B	255	SER	N-CA-C	6.07	119.95	110.17
1	A	352	VAL	N-CA-C	-6.07	104.59	110.72
1	B	285	PRO	CB-CA-C	-6.06	103.47	111.23
1	B	111	PRO	N-CA-C	-6.02	106.14	114.27
1	A	16	THR	N-CA-C	5.96	120.41	113.20
1	B	18	LEU	N-CA-C	5.94	119.35	111.75
1	B	303	ASP	CA-C-N	-5.93	110.01	121.58
1	B	303	ASP	C-N-CA	-5.93	110.01	121.58
1	A	49	GLY	CA-C-N	-5.92	111.04	122.06
1	A	49	GLY	C-N-CA	-5.92	111.04	122.06
1	A	285	PRO	CB-CA-C	-5.91	103.24	110.98
1	A	112	ASP	CA-C-N	-5.90	113.21	122.65
1	A	112	ASP	C-N-CA	-5.90	113.21	122.65
1	B	332	LEU	N-CA-C	-5.90	98.46	108.26
1	B	255	SER	CA-CB-OG	-5.89	99.32	111.10
1	B	156	GLN	N-CA-C	5.88	117.69	111.28
1	D	112	ASP	N-CA-C	5.88	117.69	111.28
1	B	89	GLN	CB-CA-C	-5.86	99.26	109.64
1	B	180	GLN	N-CA-C	5.85	119.18	110.52
1	A	342	GLY	CA-C-N	5.85	126.58	120.03
1	A	342	GLY	C-N-CA	5.85	126.58	120.03
1	A	297	ARG	O-C-N	5.79	125.42	121.71
1	A	87	LEU	N-CA-C	5.78	118.52	110.20
1	B	124	PRO	N-CA-C	-5.77	105.51	113.53
1	A	216	ARG	N-CA-C	-5.76	104.60	111.69
1	B	157	GLY	N-CA-C	-5.76	105.70	113.24
1	A	201	PRO	CA-C-N	-5.75	113.12	122.26
1	A	201	PRO	C-N-CA	-5.75	113.12	122.26
1	A	332	LEU	N-CA-C	-5.75	98.92	108.34
1	A	314	VAL	CA-C-N	-5.73	115.70	122.93
1	A	314	VAL	C-N-CA	-5.73	115.70	122.93
1	B	135	ASP	N-CA-C	5.72	117.32	111.14
1	A	273	ARG	CB-CA-C	-5.71	99.70	110.16
1	B	50	GLU	CA-C-N	-5.66	115.67	122.35
1	B	50	GLU	C-N-CA	-5.66	115.67	122.35
1	E	122	LEU	N-CA-C	5.64	117.92	108.73
1	A	303	ASP	N-CA-C	-5.59	105.06	113.89
1	B	201	PRO	CA-C-O	-5.58	115.21	122.12
1	B	181	SER	CA-CB-OG	-5.57	99.97	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	GLN	N-CA-C	-5.56	105.22	112.23
1	B	215	PHE	CA-C-N	-5.56	112.40	120.29
1	B	215	PHE	C-N-CA	-5.56	112.40	120.29
1	B	307	GLY	CA-C-O	-5.55	118.40	122.23
1	B	211	ILE	N-CA-CB	-5.55	104.35	110.51
1	B	183	SER	N-CA-C	-5.53	105.80	112.54
1	A	11	ALA	N-CA-C	-5.52	100.18	109.07
1	B	344	GLY	N-CA-C	-5.52	105.71	112.77
1	A	328	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	82	ILE	CA-C-N	-5.50	116.37	123.19
1	A	82	ILE	C-N-CA	-5.50	116.37	123.19
1	B	163	GLY	N-CA-C	-5.49	106.13	112.50
1	A	161	PRO	CB-CA-C	-5.47	103.60	112.62
1	B	110	SER	CB-CA-C	-5.46	100.69	109.37
1	A	244	THR	N-CA-C	-5.46	101.96	110.42
1	A	215	PHE	N-CA-C	-5.45	105.50	111.82
1	B	122	LEU	N-CA-C	5.43	117.37	108.52
1	A	205	GLY	N-CA-C	-5.42	100.33	113.18
1	A	120	PRO	CA-C-N	5.42	131.31	123.13
1	A	120	PRO	C-N-CA	5.42	131.31	123.13
1	B	52	VAL	N-CA-C	5.40	117.40	109.63
1	A	182	LEU	N-CA-CB	-5.38	102.05	110.44
1	B	178	THR	CA-CB-CG2	5.38	119.64	110.50
1	B	200	LEU	CB-CG-CD2	-5.37	94.58	110.70
1	A	182	LEU	CD1-CG-CD2	-5.36	99.00	110.80
1	B	194	ASP	CA-C-N	-5.36	112.32	121.97
1	B	194	ASP	C-N-CA	-5.36	112.32	121.97
1	A	130	THR	N-CA-C	-5.35	106.75	113.28
1	B	339	GLY	N-CA-C	-5.31	108.36	115.32
1	A	29	ASN	N-CA-C	5.30	119.05	112.59
1	A	47	PRO	N-CA-C	-5.29	103.52	111.57
1	A	285	PRO	CA-C-O	-5.29	115.21	121.67
1	A	288	PRO	N-CA-C	-5.29	107.24	113.86
1	B	77	MET	CG-SD-CE	-5.29	89.26	100.90
1	A	92	ALA	N-CA-C	-5.29	105.18	111.69
1	B	89	GLN	CB-CG-CD	-5.28	103.62	112.60
1	A	292	MET	CB-CG-SD	-5.28	96.86	112.70
1	E	80	VAL	N-CA-C	5.28	116.57	108.71
1	B	107	ILE	N-CA-C	-5.26	100.17	107.80
1	A	257	LYS	CB-CA-C	-5.22	99.39	110.31
1	E	195	VAL	N-CA-C	5.21	118.73	113.47
1	B	287	LYS	CA-C-N	-5.21	114.25	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LYS	C-N-CA	-5.21	114.25	119.56
1	A	245	ILE	CA-C-N	-5.21	114.42	122.59
1	A	245	ILE	C-N-CA	-5.21	114.42	122.59
1	A	77	MET	CG-SD-CE	-5.19	89.49	100.90
1	B	164	ALA	N-CA-C	-5.16	105.83	111.82
1	E	110	SER	N-CA-C	5.14	117.75	110.24
1	B	266	LYS	N-CA-C	-5.14	104.94	111.11
1	A	150	THR	CA-C-N	-5.13	115.28	120.31
1	A	150	THR	C-N-CA	-5.13	115.28	120.31
1	A	196	VAL	CA-CB-CG2	-5.11	101.71	110.40
1	B	171	MET	CB-CA-C	-5.09	102.62	110.26
1	B	211	ILE	CB-CA-C	5.09	118.39	111.88
1	A	190	ILE	N-CA-CB	-5.08	104.10	111.21
1	A	332	LEU	O-C-N	-5.08	117.33	123.27
1	B	308	ASP	N-CA-C	-5.08	106.60	112.89
1	F	195	VAL	N-CA-C	5.06	118.58	113.47
1	A	291	VAL	CA-C-N	-5.05	114.05	122.64
1	A	291	VAL	C-N-CA	-5.05	114.05	122.64
1	A	322	VAL	CB-CA-C	-5.05	105.30	111.92
1	B	59	GLN	N-CA-C	-5.05	101.62	109.24
1	A	305	TRP	N-CA-C	-5.01	105.89	112.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ALA	Mainchain

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	2743	0	2799	61	0
1	B	2743	0	2799	60	0
1	C	2743	0	2799	65	1
1	D	2743	0	2799	53	0
1	E	2732	0	2786	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2732	0	2786	47	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	2	0
3	C	48	0	32	1	0
3	D	48	0	32	4	0
3	E	48	0	32	1	0
3	F	48	0	32	3	0
4	A	184	0	0	13	0
4	B	172	0	0	5	0
4	C	59	0	0	20	0
4	D	57	0	0	14	0
4	E	52	0	0	10	0
4	F	30	0	0	12	0
All	All	17284	0	16960	349	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 10.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:CD	1:A:53:ARG:CG	1.77	1.61
1:B:353:GLU:CG	1:B:353:GLU:CB	1.79	1.58
1:A:200:LEU:CD1	1:A:200:LEU:CG	1.85	1.54
1:B:88:PRO:CD	1:B:88:PRO:CG	1.75	1.51
1:C:223:ARG:HA	4:C:656:HOH:O	1.19	1.29
1:F:134:ILE:HG22	4:F:613:HOH:O	1.22	1.28
1:A:231:GLU:HG3	4:A:733:HOH:O	1.41	1.16
1:E:223:ARG:HA	4:E:643:HOH:O	1.41	1.15
1:C:100:ALA:HB2	4:C:655:HOH:O	1.54	1.07
1:F:34:LYS:HG2	4:F:628:HOH:O	1.52	1.06
1:B:353:GLU:HB2	1:B:353:GLU:OE1	1.60	1.02
1:A:262:ALA:H	1:A:321:GLN:HE22	1.07	1.00
1:C:6:ARG:HA	1:C:6:ARG:NH1	1.77	0.99
1:B:353:GLU:CB	1:B:353:GLU:OE1	2.10	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ARG:HA	1:C:6:ARG:HH11	1.28	0.94
1:C:267:GLU:HG3	4:C:650:HOH:O	1.67	0.93
1:B:353:GLU:CB	1:B:353:GLU:CD	2.44	0.90
1:B:353:GLU:C	1:B:353:GLU:HG3	1.95	0.89
1:F:206:TYR:HA	4:F:627:HOH:O	1.70	0.89
1:C:13:LEU:HD12	1:C:85:SER:HB2	1.57	0.86
1:E:252:LEU:HB2	1:E:329:LEU:CD2	2.06	0.85
1:B:353:GLU:CG	1:B:353:GLU:C	2.49	0.84
1:A:262:ALA:H	1:A:321:GLN:NE2	1.75	0.84
1:C:252:LEU:HB2	1:C:329:LEU:CD2	2.08	0.84
1:B:68:GLU:HG2	4:B:741:HOH:O	1.80	0.81
1:C:167:LYS:HA	4:C:656:HOH:O	1.81	0.81
1:A:137:GLN:HE22	1:A:147:ILE:H	1.26	0.81
1:F:34:LYS:CG	4:F:628:HOH:O	2.18	0.80
1:D:353:GLU:HA	4:D:654:HOH:O	1.81	0.80
1:C:294:GLU:HB3	4:C:638:HOH:O	1.82	0.80
1:C:137:GLN:HE21	1:C:143:TRP:HE1	1.31	0.79
1:F:252:LEU:HB2	1:F:329:LEU:CD2	2.13	0.79
1:B:6:ARG:HD2	1:B:7:THR:N	1.98	0.78
1:B:6:ARG:CD	1:B:7:THR:H	1.96	0.78
1:D:252:LEU:HB2	1:D:329:LEU:CD2	2.12	0.78
1:B:137:GLN:HE22	1:B:147:ILE:H	1.32	0.77
1:D:6:ARG:HH11	1:D:6:ARG:N	1.83	0.76
1:C:252:LEU:HB2	1:C:329:LEU:HD23	1.67	0.75
1:D:262:ALA:H	1:D:321:GLN:HE22	1.33	0.74
1:A:53:ARG:CD	1:A:53:ARG:CB	2.65	0.73
1:D:230:LEU:HD23	4:D:611:HOH:O	1.87	0.73
1:E:129:HIS:CD2	1:E:222:LYS:HZ1	2.06	0.73
1:A:53:ARG:CG	1:A:53:ARG:NE	2.51	0.73
1:B:353:GLU:CG	1:B:353:GLU:CA	2.67	0.72
1:A:6:ARG:CZ	1:A:6:ARG:HB3	2.20	0.71
1:B:53:ARG:HE	1:B:55:GLN:NE2	1.89	0.71
1:C:294:GLU:HA	4:C:618:HOH:O	1.92	0.70
1:F:153:CYS:SG	3:F:402:COA:S1P	2.89	0.70
1:C:120:PRO:HA	4:C:643:HOH:O	1.91	0.69
1:B:353:GLU:HG3	1:B:353:GLU:O	1.91	0.69
1:B:6:ARG:HD2	1:B:7:THR:H	1.53	0.69
1:A:262:ALA:N	1:A:321:GLN:HE22	1.86	0.69
1:D:352:VAL:HG12	4:D:654:HOH:O	1.94	0.68
1:E:252:LEU:HB2	1:E:329:LEU:HD23	1.73	0.68
1:C:89:GLN:HG2	1:C:111:PRO:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:GLN:HE21	1:F:143:TRP:HE1	1.40	0.68
1:C:100:ALA:CA	4:C:655:HOH:O	2.42	0.68
1:E:167:LYS:HA	4:E:643:HOH:O	1.92	0.67
1:A:53:ARG:HH21	1:A:55:GLN:HE22	1.39	0.67
1:F:252:LEU:HB2	1:F:329:LEU:HD23	1.76	0.67
1:E:225:VAL:HG22	4:E:649:HOH:O	1.94	0.66
1:E:226:ASP:HB2	4:E:608:HOH:O	1.96	0.66
1:A:53:ARG:HD2	4:A:707:HOH:O	1.96	0.66
1:C:262:ALA:H	1:C:321:GLN:HE22	1.41	0.66
1:E:223:ARG:HB2	4:E:646:HOH:O	1.95	0.66
1:E:262:ALA:H	1:E:321:GLN:HE22	1.42	0.66
1:A:53:ARG:HB2	4:A:707:HOH:O	1.95	0.65
1:B:6:ARG:NH1	4:B:768:HOH:O	2.30	0.65
1:A:229:LYS:HD3	1:A:229:LYS:N	2.12	0.65
1:F:120:PRO:HG2	1:F:148:VAL:HG22	1.77	0.65
1:C:153:CYS:HG	3:C:402:COA:HS1	0.69	0.65
1:E:89:GLN:HG2	1:E:111:PRO:HG2	1.79	0.65
1:B:137:GLN:HE21	1:B:143:TRP:HE1	1.41	0.65
1:E:129:HIS:CD2	1:E:222:LYS:NZ	2.65	0.64
3:E:402:COA:O5P	3:E:402:COA:H22	1.98	0.64
1:B:18:LEU:HD12	1:B:186:GLY:HA2	1.81	0.63
1:E:295:ASP:OD2	4:E:645:HOH:O	2.15	0.63
1:D:137:GLN:HE21	1:D:143:TRP:HE1	1.46	0.63
1:B:262:ALA:H	1:B:321:GLN:HE22	1.45	0.62
1:A:226:ASP:HB2	4:A:776:HOH:O	1.98	0.62
1:A:200:LEU:CD1	1:A:200:LEU:CD2	2.78	0.62
1:C:13:LEU:HD12	1:C:85:SER:CB	2.29	0.62
1:F:18:LEU:HD12	1:F:186:GLY:HA2	1.80	0.62
1:C:120:PRO:HG2	1:C:148:VAL:HG22	1.82	0.61
1:F:262:ALA:H	1:F:321:GLN:HE22	1.46	0.61
1:E:137:GLN:HE21	1:E:143:TRP:HE1	1.48	0.61
1:F:42:GLY:CA	4:F:624:HOH:O	2.47	0.61
1:B:153:CYS:SG	3:B:402:COA:S1P	2.97	0.61
1:F:42:GLY:N	4:F:624:HOH:O	2.34	0.61
1:D:120:PRO:HG2	1:D:148:VAL:HG22	1.80	0.61
1:D:252:LEU:HB2	1:D:329:LEU:HD23	1.82	0.60
1:C:318:ARG:HA	4:C:602:HOH:O	2.00	0.60
1:C:267:GLU:CA	4:C:650:HOH:O	2.49	0.60
1:C:228:PRO:HG3	1:C:257:LYS:HD2	1.84	0.60
1:D:135:ASP:HA	4:D:610:HOH:O	2.01	0.60
1:A:272:PHE:O	1:A:273:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ALA:H	1:D:321:GLN:NE2	1.99	0.60
3:B:402:COA:H10	4:B:743:HOH:O	2.01	0.60
1:A:92:ALA:O	1:A:96:GLU:HG3	2.02	0.59
1:D:143:TRP:HA	4:D:645:HOH:O	2.01	0.59
1:F:131:ILE:C	4:F:629:HOH:O	2.46	0.59
1:B:259:GLU:HG3	1:B:324:LYS:HB3	1.83	0.59
1:A:74:PRO:HB3	1:A:102:GLU:HG3	1.85	0.59
1:B:120:PRO:HG2	1:B:148:VAL:HG22	1.83	0.59
1:A:16:THR:HG21	1:A:51:VAL:HG22	1.85	0.58
1:D:70:LYS:HG2	4:D:607:HOH:O	2.03	0.57
1:A:6:ARG:CZ	1:A:6:ARG:CB	2.81	0.57
1:A:151:PRO:CG	1:A:217:ILE:HD11	2.34	0.57
1:C:267:GLU:N	4:C:650:HOH:O	2.36	0.57
1:D:126:LEU:HD11	1:D:160:ILE:HA	1.86	0.57
1:C:138:ARG:HH21	1:C:146:PHE:HD2	1.52	0.57
1:A:200:LEU:CD1	1:A:200:LEU:CB	2.77	0.57
1:E:120:PRO:HG2	1:E:148:VAL:HG22	1.86	0.56
1:B:24:VAL:HG13	1:B:64:ILE:HG13	1.87	0.56
1:B:74:PRO:HB2	1:B:102:GLU:HG3	1.86	0.56
1:C:137:GLN:NE2	1:C:143:TRP:HE1	2.00	0.56
1:A:50:GLU:OE1	4:A:772:HOH:O	2.18	0.56
1:D:228:PRO:HG3	1:D:257:LYS:HD2	1.89	0.55
1:C:89:GLN:CG	1:C:111:PRO:HG2	2.37	0.55
1:B:137:GLN:HE22	1:B:147:ILE:N	2.04	0.55
1:C:53:ARG:HH11	1:C:53:ARG:HG3	1.72	0.55
1:C:129:HIS:ND1	4:C:601:HOH:O	2.31	0.55
1:D:137:GLN:HE22	1:D:147:ILE:H	1.56	0.54
1:A:245:ILE:HD11	1:B:196:VAL:HG12	1.88	0.54
1:F:132:SER:N	4:F:629:HOH:O	2.41	0.54
1:E:228:PRO:HG3	1:E:257:LYS:HD2	1.90	0.54
1:D:75:LYS:HE3	4:D:656:HOH:O	2.07	0.53
1:C:262:ALA:H	1:C:321:GLN:NE2	2.03	0.53
1:F:262:ALA:H	1:F:321:GLN:NE2	2.06	0.53
1:E:121:LEU:HD23	1:E:216:ARG:HG2	1.89	0.53
1:A:6:ARG:N	4:A:684:HOH:O	2.41	0.53
1:B:16:THR:HG21	1:B:51:VAL:HG22	1.90	0.53
1:B:60:VAL:HG23	4:B:716:HOH:O	2.08	0.53
1:A:127:ASN:N	1:A:128:PRO:CD	2.71	0.53
1:F:228:PRO:HG3	1:F:257:LYS:HD2	1.91	0.52
1:E:262:ALA:H	1:E:321:GLN:NE2	2.08	0.52
1:D:77:MET:O	1:D:80:VAL:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:O	1:E:283:THR:HG22	2.10	0.52
1:B:6:ARG:CD	1:B:7:THR:N	2.65	0.52
1:C:154:THR:HG21	1:C:180:GLN:NE2	2.25	0.52
1:E:167:LYS:HG3	4:E:643:HOH:O	2.09	0.52
1:D:27:LEU:HD21	1:D:345:ILE:HG12	1.92	0.52
1:F:132:SER:HA	4:F:629:HOH:O	2.09	0.52
1:F:206:TYR:CA	4:F:627:HOH:O	2.42	0.52
1:D:213:GLU:O	1:D:217:ILE:HG13	2.10	0.51
1:D:18:LEU:HD12	1:D:186:GLY:HA2	1.92	0.51
1:F:128:PRO:O	1:F:131:ILE:HG12	2.11	0.51
1:E:126:LEU:HD11	1:E:160:ILE:HA	1.93	0.51
1:D:202:LEU:HD22	4:D:634:HOH:O	2.11	0.51
1:E:118:ASP:HA	4:E:644:HOH:O	2.10	0.51
1:B:77:MET:HE1	1:B:99:PHE:HZ	1.74	0.51
1:C:121:LEU:HD23	1:C:216:ARG:HG2	1.92	0.51
1:E:53:ARG:HE	1:E:55:GLN:NE2	2.09	0.51
1:C:119:VAL:O	1:C:216:ARG:NH2	2.42	0.50
1:D:280:LYS:HB3	4:D:652:HOH:O	2.11	0.50
1:C:37:TYR:CE2	1:C:77:MET:HE2	2.47	0.50
1:C:136:GLU:O	1:C:140:ARG:HB2	2.11	0.50
1:D:38:LEU:O	4:D:651:HOH:O	2.18	0.50
1:B:334:HIS:CE1	1:B:337:VAL:HG23	2.46	0.50
1:D:13:LEU:HD12	1:D:85:SER:HB2	1.94	0.50
1:E:329:LEU:HD23	1:E:329:LEU:C	2.37	0.50
1:B:53:ARG:NE	1:B:55:GLN:NE2	2.59	0.49
1:B:266:LYS:NZ	1:B:293:ASN:ND2	2.59	0.49
1:E:89:GLN:CG	1:E:111:PRO:HG2	2.42	0.49
1:B:53:ARG:HH21	1:B:55:GLN:HE22	1.60	0.49
1:B:262:ALA:H	1:B:321:GLN:NE2	2.10	0.49
1:B:125:GLU:N	1:B:125:GLU:OE1	2.44	0.49
1:A:137:GLN:HE21	1:A:143:TRP:HE1	1.59	0.49
1:B:136:GLU:O	1:B:140:ARG:HG3	2.12	0.49
1:F:333:ILE:HD11	1:F:338:ARG:HG3	1.94	0.49
1:D:127:ASN:HB2	1:D:130:THR:HG23	1.94	0.49
1:A:76:LEU:HD13	4:A:769:HOH:O	2.13	0.49
1:E:18:LEU:HD12	1:E:186:GLY:HA2	1.95	0.49
1:A:98:GLN:HG2	4:A:710:HOH:O	2.13	0.49
1:C:77:MET:O	1:C:80:VAL:N	2.42	0.49
1:F:53:ARG:HG3	4:F:622:HOH:O	2.13	0.48
1:A:152:LEU:O	1:A:153:CYS:C	2.56	0.48
1:B:53:ARG:HE	1:B:55:GLN:HE21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ALA:CB	4:C:655:HOH:O	2.24	0.48
1:D:153:CYS:SG	3:D:402:COA:S1P	3.05	0.48
1:E:137:GLN:HE22	1:E:147:ILE:H	1.61	0.48
1:A:73:ASP:H	1:A:77:MET:CE	2.26	0.48
1:B:288:PRO:HD2	4:B:629:HOH:O	2.12	0.48
1:C:115:PHE:CZ	1:C:212:LYS:HD3	2.48	0.48
1:A:359:LYS:HE2	4:A:730:HOH:O	2.13	0.48
1:E:199:ILE:O	1:E:201:PRO:HD3	2.14	0.47
1:F:137:GLN:NE2	1:F:143:TRP:HE1	2.10	0.47
1:B:179:ILE:HG22	1:B:242:ILE:HG12	1.95	0.47
1:A:297:ARG:HB3	1:A:298:PRO:HA	1.95	0.47
1:C:53:ARG:HE	1:C:55:GLN:HE21	1.62	0.47
1:F:182:LEU:HD11	1:F:243:ALA:HA	1.96	0.47
1:E:13:LEU:HD12	1:E:85:SER:HB2	1.96	0.47
1:C:280:LYS:HA	4:C:619:HOH:O	2.14	0.47
1:E:53:ARG:HG3	1:E:53:ARG:HH11	1.79	0.47
1:F:13:LEU:HD12	1:F:85:SER:HB2	1.97	0.47
1:A:73:ASP:O	1:A:77:MET:HE3	2.15	0.47
1:A:121:LEU:HD23	1:A:216:ARG:HD3	1.97	0.47
1:C:252:LEU:HB2	1:C:329:LEU:HD21	1.94	0.47
1:D:138:ARG:HH21	1:D:146:PHE:HD2	1.61	0.47
1:C:308:ASP:HA	4:C:625:HOH:O	2.15	0.47
1:E:128:PRO:O	1:E:131:ILE:HG12	2.15	0.47
1:F:108:SER:HB3	1:F:149:THR:HG22	1.97	0.47
1:A:16:THR:OG1	3:A:402:COA:O8A	2.30	0.46
1:C:53:ARG:HE	1:C:55:GLN:NE2	2.12	0.46
1:D:128:PRO:O	1:D:131:ILE:HG12	2.15	0.46
1:A:116:ASP:HB2	1:A:119:VAL:HG23	1.97	0.46
1:A:121:LEU:CD2	1:A:216:ARG:HD3	2.45	0.46
1:F:89:GLN:HG2	1:F:111:PRO:HG2	1.98	0.46
1:B:137:GLN:NE2	1:B:147:ILE:H	2.08	0.46
1:B:173:GLY:H	1:B:255:SER:HB3	1.81	0.46
1:A:334:HIS:CE1	1:A:337:VAL:HG23	2.51	0.46
1:F:121:LEU:HD23	1:F:216:ARG:HG2	1.96	0.46
1:C:333:ILE:HD11	1:C:338:ARG:HG3	1.97	0.46
1:D:28:SER:HB3	4:D:628:HOH:O	2.15	0.46
1:B:252:LEU:HD12	1:B:252:LEU:N	2.31	0.46
1:A:116:ASP:HB2	1:A:119:VAL:CG2	2.46	0.46
1:A:275:GLU:N	1:A:276:PRO:CD	2.79	0.45
1:E:333:ILE:HD11	1:E:338:ARG:HG3	1.98	0.45
1:F:77:MET:O	1:F:80:VAL:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HB2	1:A:101:LYS:HE3	1.69	0.45
1:D:297:ARG:HB3	1:D:298:PRO:HA	1.98	0.45
1:F:75:LYS:H	1:F:75:LYS:HG2	1.55	0.45
1:A:229:LYS:HD3	1:A:229:LYS:H	1.81	0.45
1:D:9:LYS:HG3	1:D:36:ALA:CB	2.45	0.45
1:D:53:ARG:HG3	1:D:53:ARG:HH11	1.82	0.45
1:D:89:GLN:HE21	1:D:89:GLN:HB3	1.44	0.45
1:B:34:LYS:HE2	1:B:34:LYS:HA	1.98	0.45
1:D:77:MET:C	1:D:79:ASP:H	2.25	0.45
1:D:154:THR:HG21	1:D:180:GLN:NE2	2.32	0.45
1:F:211:ILE:HD12	1:F:211:ILE:HA	1.70	0.45
1:D:121:LEU:HD23	1:D:216:ARG:HG2	1.99	0.45
1:E:213:GLU:O	1:E:217:ILE:HG13	2.17	0.45
1:C:137:GLN:HE22	1:C:147:ILE:H	1.63	0.45
1:F:199:ILE:O	1:F:201:PRO:HD3	2.16	0.44
1:B:333:ILE:HD11	1:B:338:ARG:HG3	1.98	0.44
1:C:297:ARG:HB3	1:C:298:PRO:HA	1.99	0.44
1:F:77:MET:C	1:F:79:ASP:H	2.25	0.44
1:B:170:LYS:HA	1:B:227:GLU:O	2.17	0.44
1:F:73:ASP:HA	1:F:74:PRO:HD2	1.83	0.44
1:A:13:LEU:HA	1:A:39:ALA:HB3	2.00	0.44
1:E:89:GLN:HE21	1:E:89:GLN:HB3	1.40	0.44
1:F:276:PRO:HB3	1:F:281:LEU:HD12	2.00	0.44
1:C:283:THR:HG22	1:C:283:THR:O	2.18	0.44
1:D:252:LEU:HB2	1:D:329:LEU:HD21	1.97	0.44
1:C:192:SER:O	1:C:196:VAL:HG23	2.18	0.44
1:C:267:GLU:HA	4:C:650:HOH:O	2.14	0.44
1:E:67:MET:HE3	4:E:614:HOH:O	2.17	0.44
1:A:74:PRO:CB	1:A:102:GLU:HG3	2.47	0.43
1:D:355:GLY:HA2	4:D:637:HOH:O	2.17	0.43
1:A:131:ILE:C	1:A:133:LEU:H	2.26	0.43
1:A:181:SER:HA	1:A:244:THR:OG1	2.17	0.43
1:A:209:LYS:NZ	4:A:727:HOH:O	2.51	0.43
1:D:207:ASP:OD2	4:D:632:HOH:O	2.21	0.43
1:A:57:VAL:HG22	1:A:58:GLY:N	2.34	0.43
1:E:138:ARG:HH21	1:E:146:PHE:HD2	1.65	0.43
1:D:180:GLN:HB3	1:D:248:HIS:CE1	2.53	0.43
1:E:275:GLU:N	1:E:276:PRO:CD	2.81	0.43
1:F:23:TYR:CZ	1:F:341:ALA:HA	2.54	0.43
1:A:261:ALA:HA	1:A:321:GLN:HE22	1.84	0.43
1:A:316:VAL:HA	1:A:331:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLU:N	4:C:632:HOH:O	2.51	0.43
1:C:322:VAL:HA	4:C:604:HOH:O	2.18	0.43
1:A:128:PRO:HG3	4:A:708:HOH:O	2.18	0.43
1:E:13:LEU:HA	1:E:39:ALA:HB3	2.01	0.43
1:E:266:LYS:NZ	1:E:293:ASN:ND2	2.67	0.43
1:B:258:GLU:O	1:B:259:GLU:C	2.61	0.43
1:E:329:LEU:HD23	1:E:329:LEU:O	2.18	0.43
1:A:62:LYS:H	1:A:62:LYS:HG2	1.58	0.42
1:A:64:ILE:O	1:A:65:ALA:C	2.61	0.42
1:F:126:LEU:HD11	1:F:160:ILE:HA	2.01	0.42
1:F:137:GLN:HE22	1:F:147:ILE:H	1.65	0.42
1:F:297:ARG:HB3	1:F:298:PRO:HA	1.99	0.42
1:B:74:PRO:HG2	1:B:98:GLN:HG3	2.01	0.42
1:A:229:LYS:HE3	4:A:704:HOH:O	2.18	0.42
1:A:312:MET:HE3	1:A:312:MET:HB3	1.63	0.42
1:B:89:GLN:HG2	1:B:111:PRO:HG3	2.01	0.42
1:D:329:LEU:HD23	1:D:329:LEU:C	2.45	0.42
1:E:95:VAL:HG23	4:E:641:HOH:O	2.18	0.42
3:A:402:COA:H22	4:A:630:HOH:O	2.19	0.42
1:B:270:GLU:HG3	1:B:291:VAL:HG21	2.02	0.42
1:D:19:VAL:HG23	3:D:402:COA:H132	2.02	0.42
1:E:87:LEU:HA	1:E:87:LEU:HD12	1.79	0.42
1:C:77:MET:C	1:C:79:ASP:H	2.28	0.42
1:F:165:ILE:HG12	1:F:265:VAL:HG13	2.02	0.42
1:C:158:ALA:O	1:C:161:PRO:HD2	2.20	0.42
1:B:283:THR:O	1:B:283:THR:HG22	2.20	0.42
1:F:356:TYR:CE2	4:F:629:HOH:O	2.56	0.42
1:E:77:MET:C	1:E:79:ASP:N	2.78	0.42
1:B:211:ILE:HG13	1:B:235:LEU:HB3	2.01	0.41
1:C:199:ILE:O	1:C:201:PRO:HD3	2.20	0.41
1:D:127:ASN:HB2	1:D:130:THR:CG2	2.50	0.41
1:E:211:ILE:HD12	1:E:211:ILE:HA	1.80	0.41
1:C:328:ARG:HD2	1:C:329:LEU:N	2.36	0.41
1:E:211:ILE:HD11	1:E:236:ALA:C	2.45	0.41
1:F:283:THR:HG22	1:F:283:THR:O	2.20	0.41
1:C:77:MET:O	1:C:79:ASP:N	2.53	0.41
1:D:316:VAL:HA	1:D:330:VAL:O	2.20	0.41
1:B:180:GLN:NE2	1:B:239:THR:HB	2.35	0.41
3:D:402:COA:H122	4:D:635:HOH:O	2.20	0.41
1:F:77:MET:C	1:F:79:ASP:N	2.78	0.41
1:F:136:GLU:O	1:F:140:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:GLU:O	1:F:217:ILE:HG13	2.21	0.41
1:C:180:GLN:HG3	1:C:240:HIS:O	2.21	0.41
1:C:287:LYS:HA	1:C:288:PRO:HD2	1.91	0.41
1:C:308:ASP:CA	4:C:625:HOH:O	2.68	0.41
1:E:73:ASP:HA	1:E:74:PRO:HD2	1.85	0.41
1:E:137:GLN:NE2	1:E:143:TRP:HE1	2.16	0.41
1:F:178:THR:OG1	1:F:239:THR:HA	2.21	0.41
1:D:77:MET:C	1:D:79:ASP:N	2.78	0.41
1:E:23:TYR:CZ	1:E:341:ALA:HA	2.55	0.41
1:E:73:ASP:OD1	1:E:75:LYS:HG2	2.21	0.41
1:D:252:LEU:HD12	1:D:252:LEU:N	2.36	0.41
3:D:402:COA:O5P	3:D:402:COA:H22	2.20	0.41
1:A:182:LEU:HG	1:A:244:THR:O	2.21	0.41
1:A:192:SER:HB2	1:B:182:LEU:HD13	2.03	0.41
1:C:96:GLU:OE1	1:C:113:HIS:HD2	2.03	0.41
1:C:119:VAL:HA	1:C:120:PRO:HD3	1.90	0.41
3:F:402:COA:O5P	3:F:402:COA:H22	2.20	0.41
1:B:88:PRO:O	1:B:89:GLN:C	2.64	0.41
1:B:337:VAL:O	1:B:338:ARG:C	2.63	0.41
1:C:126:LEU:HD11	1:C:160:ILE:HA	2.02	0.41
1:D:276:PRO:HB3	1:D:281:LEU:HD12	2.01	0.41
1:E:136:GLU:O	1:E:140:ARG:HB2	2.21	0.41
1:A:53:ARG:HE	1:A:55:GLN:NE2	2.19	0.40
1:B:312:MET:HE3	1:B:312:MET:HB3	2.00	0.40
1:C:309:ILE:O	1:C:312:MET:HB2	2.21	0.40
1:D:182:LEU:HD11	1:D:243:ALA:HA	2.04	0.40
1:E:13:LEU:HD12	1:E:85:SER:CB	2.50	0.40
1:E:252:LEU:HB2	1:E:329:LEU:HD21	1.99	0.40
1:D:187:TYR:HA	1:D:188:PRO:C	2.46	0.40
1:E:77:MET:C	1:E:79:ASP:H	2.30	0.40
1:E:119:VAL:HA	1:E:120:PRO:HD3	1.93	0.40
1:F:53:ARG:HG3	1:F:53:ARG:HH11	1.86	0.40
1:B:38:LEU:HD13	1:B:48:TYR:CD1	2.56	0.40
1:C:30:HIS:HA	4:C:631:HOH:O	2.21	0.40
1:D:136:GLU:O	1:D:140:ARG:HB2	2.21	0.40
1:E:75:LYS:HG2	1:E:75:LYS:H	1.60	0.40
1:E:77:MET:O	1:E:79:ASP:N	2.53	0.40
1:E:187:TYR:HA	1:E:188:PRO:C	2.47	0.40
1:A:299:GLN:O	1:A:300:VAL:C	2.62	0.40
1:B:121:LEU:HD11	1:B:151:PRO:HA	2.03	0.40
1:C:53:ARG:HH21	1:C:55:GLN:HE22	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ILE:HG12	1:C:265:VAL:HG13	2.04	0.40
1:D:13:LEU:HA	1:D:39:ALA:HB3	2.02	0.40
1:D:275:GLU:N	1:D:276:PRO:CD	2.84	0.40
1:E:37:TYR:CE2	1:E:77:MET:HE2	2.57	0.40
1:E:53:ARG:HE	1:E:55:GLN:HE21	1.67	0.40
3:F:402:COA:O1A	3:F:402:COA:O4A	2.39	0.40
1:B:299:GLN:O	1:B:300:VAL:C	2.62	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:C:9:LYS:NZ	1:F:353:GLU:OE2[3_555]	2.01	0.19

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	352/359 (98%)	333 (95%)	15 (4%)	4 (1%)	11	13
1	B	352/359 (98%)	332 (94%)	17 (5%)	3 (1%)	14	17
1	C	352/359 (98%)	334 (95%)	14 (4%)	4 (1%)	11	13
1	D	352/359 (98%)	334 (95%)	15 (4%)	3 (1%)	14	17
1	E	351/359 (98%)	334 (95%)	14 (4%)	3 (1%)	14	17
1	F	351/359 (98%)	335 (95%)	12 (3%)	4 (1%)	11	13
All	All	2110/2154 (98%)	2002 (95%)	87 (4%)	21 (1%)	12	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	76	LEU

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Mol	Chain	Res	Type
1	A	86	PRO
1	D	76	LEU
1	F	76	LEU
1	A	231	GLU
1	C	76	LEU
1	C	86	PRO
1	D	86	PRO
1	D	337	VAL
1	F	337	VAL
1	A	340	ALA
1	B	75	LYS
1	B	170	LYS
1	C	337	VAL
1	F	86	PRO
1	B	86	PRO
1	F	78	ASP
1	E	337	VAL
1	A	337	VAL
1	C	211	ILE
1	E	86	PRO

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	297/302 (98%)	272 (92%)	25 (8%)	10	14
1	B	297/302 (98%)	274 (92%)	23 (8%)	12	16
1	C	297/302 (98%)	260 (88%)	37 (12%)	4	5
1	D	297/302 (98%)	260 (88%)	37 (12%)	4	5
1	E	296/302 (98%)	261 (88%)	35 (12%)	5	6
1	F	296/302 (98%)	259 (88%)	37 (12%)	4	5
All	All	1780/1812 (98%)	1586 (89%)	194 (11%)	6	7

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	29	ASN
1	A	34	LYS
1	A	51	VAL
1	A	55	GLN
1	A	62	LYS
1	A	64	ILE
1	A	74	PRO
1	A	75	LYS
1	A	78	ASP
1	A	87	LEU
1	A	131	ILE
1	A	140	ARG
1	A	144	LYS
1	A	209	LYS
1	A	211	ILE
1	A	222	LYS
1	A	229	LYS
1	A	231	GLU
1	A	244	THR
1	A	263	GLU
1	A	280	LYS
1	A	282	PRO
1	A	316	VAL
1	A	320	LYS
1	B	6	ARG
1	B	7	THR
1	B	50	GLU
1	B	51	VAL
1	B	55	GLN
1	B	62	LYS
1	B	68	GLU
1	B	70	LYS
1	B	76	LEU
1	B	78	ASP
1	B	87	LEU
1	B	98	GLN
1	B	140	ARG
1	B	170	LYS
1	B	211	ILE
1	B	255	SER
1	B	257	LYS
1	B	316	VAL

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Mol	Chain	Res	Type
1	B	320	LYS
1	B	325	ARG
1	B	329	LEU
1	B	353	GLU
1	B	359	LYS
1	C	7	THR
1	C	9	LYS
1	C	34	LYS
1	C	41	LYS
1	C	43	SER
1	C	51	VAL
1	C	55	GLN
1	C	62	LYS
1	C	64	ILE
1	C	75	LYS
1	C	76	LEU
1	C	79	ASP
1	C	87	LEU
1	C	89	GLN
1	C	98	GLN
1	C	132	SER
1	C	136	GLU
1	C	139	LYS
1	C	144	LYS
1	C	209	LYS
1	C	211	ILE
1	C	222	LYS
1	C	229	LYS
1	C	230	LEU
1	C	231	GLU
1	C	257	LYS
1	C	259	GLU
1	C	263	GLU
1	C	273	ARG
1	C	280	LYS
1	C	287	LYS
1	C	319	LEU
1	C	320	LYS
1	C	329	LEU
1	C	330	VAL
1	C	353	GLU
1	C	359	LYS

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Mol	Chain	Res	Type
1	D	6	ARG
1	D	7	THR
1	D	9	LYS
1	D	34	LYS
1	D	41	LYS
1	D	43	SER
1	D	51	VAL
1	D	55	GLN
1	D	62	LYS
1	D	64	ILE
1	D	75	LYS
1	D	76	LEU
1	D	78	ASP
1	D	79	ASP
1	D	87	LEU
1	D	89	GLN
1	D	98	GLN
1	D	132	SER
1	D	136	GLU
1	D	139	LYS
1	D	144	LYS
1	D	209	LYS
1	D	211	ILE
1	D	219	SER
1	D	222	LYS
1	D	229	LYS
1	D	231	GLU
1	D	257	LYS
1	D	263	GLU
1	D	273	ARG
1	D	280	LYS
1	D	287	LYS
1	D	319	LEU
1	D	320	LYS
1	D	329	LEU
1	D	353	GLU
1	D	359	LYS
1	E	7	THR
1	E	9	LYS
1	E	34	LYS
1	E	41	LYS
1	E	43	SER

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Mol	Chain	Res	Type
1	E	51	VAL
1	E	55	GLN
1	E	62	LYS
1	E	64	ILE
1	E	75	LYS
1	E	76	LEU
1	E	78	ASP
1	E	79	ASP
1	E	87	LEU
1	E	89	GLN
1	E	132	SER
1	E	136	GLU
1	E	139	LYS
1	E	144	LYS
1	E	209	LYS
1	E	211	ILE
1	E	222	LYS
1	E	229	LYS
1	E	230	LEU
1	E	231	GLU
1	E	257	LYS
1	E	263	GLU
1	E	273	ARG
1	E	280	LYS
1	E	287	LYS
1	E	319	LEU
1	E	320	LYS
1	E	329	LEU
1	E	353	GLU
1	E	359	LYS
1	F	7	THR
1	F	9	LYS
1	F	34	LYS
1	F	41	LYS
1	F	43	SER
1	F	51	VAL
1	F	55	GLN
1	F	62	LYS
1	F	64	ILE
1	F	75	LYS
1	F	76	LEU
1	F	78	ASP

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Mol	Chain	Res	Type
1	F	79	ASP
1	F	87	LEU
1	F	89	GLN
1	F	98	GLN
1	F	136	GLU
1	F	139	LYS
1	F	144	LYS
1	F	209	LYS
1	F	211	ILE
1	F	222	LYS
1	F	229	LYS
1	F	230	LEU
1	F	231	GLU
1	F	257	LYS
1	F	259	GLU
1	F	263	GLU
1	F	273	ARG
1	F	280	LYS
1	F	287	LYS
1	F	309	ILE
1	F	319	LEU
1	F	320	LYS
1	F	329	LEU
1	F	353	GLU
1	F	359	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	98	GLN
1	A	137	GLN
1	A	293	ASN
1	A	321	GLN
1	B	55	GLN
1	B	129	HIS
1	B	137	GLN
1	B	180	GLN
1	B	293	ASN
1	B	321	GLN
1	C	55	GLN
1	C	89	GLN

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Mol	Chain	Res	Type
1	C	109	ASN
1	C	129	HIS
1	C	137	GLN
1	C	156	GLN
1	C	180	GLN
1	C	293	ASN
1	C	321	GLN
1	D	55	GLN
1	D	89	GLN
1	D	129	HIS
1	D	137	GLN
1	D	180	GLN
1	D	248	HIS
1	D	293	ASN
1	D	321	GLN
1	E	55	GLN
1	E	89	GLN
1	E	109	ASN
1	E	129	HIS
1	E	137	GLN
1	E	293	ASN
1	E	321	GLN
1	F	55	GLN
1	F	89	GLN
1	F	109	ASN
1	F	129	HIS
1	F	137	GLN
1	F	180	GLN
1	F	248	HIS
1	F	293	ASN
1	F	321	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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
3	COA	F	402	2	47,50,50	0.89	1 (2%)	69,75,75	2.04	15 (21%)
3	COA	D	402	2	47,50,50	1.12	3 (6%)	69,75,75	1.85	14 (20%)
3	COA	B	402	2	47,50,50	1.75	8 (17%)	69,75,75	3.47	36 (52%)
3	COA	E	402	2	47,50,50	1.04	6 (12%)	69,75,75	2.07	17 (24%)
3	COA	C	402	2	47,50,50	1.06	5 (10%)	69,75,75	2.19	16 (23%)
3	COA	A	402	2	47,50,50	2.43	14 (29%)	69,75,75	3.22	30 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	F	402	2	-	2/48/64/64	0/3/3/3
3	COA	D	402	2	-	4/48/64/64	0/3/3/3
3	COA	B	402	2	-	11/48/64/64	0/3/3/3
3	COA	E	402	2	-	8/48/64/64	0/3/3/3
3	COA	C	402	2	-	5/48/64/64	0/3/3/3
3	COA	A	402	2	-	7/48/64/64	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	COA	P1A-O3A	-8.84	1.50	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	COA	P1A-O3A	-7.62	1.51	1.59
3	A	402	COA	P2A-O3A	6.50	1.66	1.59
3	A	402	COA	CCP-CBP	5.48	1.61	1.52
3	A	402	COA	C5A-N7A	-4.57	1.30	1.39
3	A	402	COA	C4A-N9A	-3.54	1.30	1.37
3	B	402	COA	C5A-C6A	3.22	1.50	1.41
3	D	402	COA	P2A-O3A	3.15	1.62	1.59
3	A	402	COA	C9P-N8P	3.13	1.41	1.33
3	D	402	COA	C5A-C6A	3.05	1.49	1.41
3	B	402	COA	C8A-N7A	3.01	1.37	1.31
3	F	402	COA	C5A-C6A	2.86	1.49	1.41
3	D	402	COA	P1A-O3A	2.85	1.62	1.59
3	A	402	COA	OAP-CAP	2.81	1.47	1.42
3	B	402	COA	CEP-CBP	2.78	1.59	1.53
3	A	402	COA	C8A-N7A	2.71	1.36	1.31
3	E	402	COA	C5A-C6A	2.54	1.48	1.41
3	A	402	COA	C7P-C6P	2.45	1.59	1.51
3	B	402	COA	C5P-N4P	2.44	1.39	1.33
3	E	402	COA	P3B-O3B	-2.43	1.55	1.59
3	E	402	COA	C5A-N7A	-2.40	1.34	1.39
3	C	402	COA	C5A-C6A	2.37	1.47	1.41
3	C	402	COA	OAP-CAP	2.36	1.46	1.42
3	A	402	COA	O6A-CCP	-2.33	1.36	1.43
3	B	402	COA	C4A-N9A	-2.33	1.32	1.37
3	E	402	COA	C4A-N9A	-2.32	1.32	1.37
3	C	402	COA	C5A-N7A	-2.27	1.34	1.39
3	E	402	COA	C8A-N7A	2.27	1.36	1.31
3	B	402	COA	C2A-N1A	-2.22	1.30	1.33
3	A	402	COA	O5P-C5P	2.17	1.27	1.23
3	A	402	COA	O4B-C1B	-2.17	1.37	1.42
3	A	402	COA	P3B-O9A	-2.15	1.46	1.54
3	A	402	COA	C8A-N9A	-2.13	1.33	1.37
3	C	402	COA	C8A-N9A	-2.08	1.34	1.37
3	B	402	COA	OAP-CAP	2.04	1.45	1.42
3	C	402	COA	C4A-N9A	-2.00	1.33	1.37
3	E	402	COA	C4A-N3A	2.00	1.38	1.34

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	C7P-N8P-C9P	8.54	137.89	122.55
3	B	402	COA	CDP-CBP-CAP	8.36	123.03	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	C6P-C7P-N8P	-7.51	96.02	112.00
3	B	402	COA	O5A-P2A-O3A	7.38	127.22	107.27
3	A	402	COA	CDP-CBP-CCP	7.35	120.36	108.22
3	B	402	COA	CEP-CBP-CCP	7.18	120.08	108.22
3	C	402	COA	CDP-CBP-CCP	-7.11	96.48	108.22
3	B	402	COA	O5P-C5P-C6P	-7.00	109.33	122.02
3	F	402	COA	C6P-C7P-N8P	-6.95	97.20	112.00
3	E	402	COA	C6P-C7P-N8P	-6.86	97.41	112.00
3	C	402	COA	C6P-C7P-N8P	-6.72	97.71	112.00
3	A	402	COA	O6A-CCP-CBP	-6.65	99.86	110.55
3	B	402	COA	CDP-CBP-CCP	6.64	119.18	108.22
3	B	402	COA	CEP-CBP-CAP	6.62	120.05	108.77
3	A	402	COA	CEP-CBP-CCP	6.60	119.12	108.22
3	B	402	COA	CEP-CBP-CDP	-6.50	96.25	109.20
3	A	402	COA	O9A-P3B-O8A	6.02	130.39	107.80
3	D	402	COA	C6P-C7P-N8P	-5.96	99.32	112.00
3	A	402	COA	CEP-CBP-CDP	-5.87	97.50	109.20
3	A	402	COA	N3A-C2A-N1A	-5.80	119.80	128.58
3	A	402	COA	C5A-C4A-N9A	5.80	112.13	105.81
3	B	402	COA	O2A-P1A-O3A	5.46	122.03	107.27
3	A	402	COA	O4B-C1B-N9A	5.38	118.43	108.09
3	B	402	COA	C6P-C5P-N4P	5.27	125.95	116.34
3	F	402	COA	C5A-C4A-N3A	-5.27	119.45	126.72
3	D	402	COA	C5A-C4A-N3A	-5.25	119.48	126.72
3	A	402	COA	CEP-CBP-CAP	5.20	117.62	108.77
3	B	402	COA	C5A-C4A-N3A	-5.19	119.57	126.72
3	E	402	COA	C5A-C4A-N3A	-5.19	119.58	126.72
3	C	402	COA	CEP-CBP-CCP	5.17	116.76	108.22
3	A	402	COA	C2P-C3P-N4P	-5.14	100.65	112.31
3	B	402	COA	O3A-P1A-O1A	-5.07	95.46	110.70
3	B	402	COA	C2A-N3A-C4A	5.05	124.17	111.83
3	A	402	COA	P3B-O3B-C3B	5.01	136.82	123.43
3	C	402	COA	C5A-C4A-N3A	-5.00	119.83	126.72
3	B	402	COA	O9A-P3B-O8A	4.92	126.25	107.80
3	D	402	COA	N3A-C2A-N1A	-4.90	121.17	128.58
3	F	402	COA	N3A-C2A-N1A	-4.89	121.18	128.58
3	C	402	COA	C7P-N8P-C9P	4.60	130.82	122.55
3	B	402	COA	N3A-C2A-N1A	-4.55	121.69	128.58
3	A	402	COA	OAP-CAP-CBP	-4.55	99.63	110.18
3	B	402	COA	C7P-C6P-C5P	4.52	119.93	112.39
3	F	402	COA	C2A-N3A-C4A	4.43	122.65	111.83
3	E	402	COA	C2P-C3P-N4P	-4.37	102.39	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	COA	N3A-C2A-N1A	-4.36	121.99	128.58
3	D	402	COA	C2A-N3A-C4A	4.28	122.28	111.83
3	D	402	COA	C2P-C3P-N4P	-4.24	102.67	112.31
3	F	402	COA	N3A-C4A-N9A	4.21	134.32	127.17
3	A	402	COA	O2A-P1A-O3A	4.19	118.59	107.27
3	E	402	COA	CDP-CBP-CCP	-4.16	101.36	108.22
3	B	402	COA	O6A-CCP-CBP	-4.16	103.86	110.55
3	A	402	COA	C2A-N3A-C4A	4.15	121.97	111.83
3	C	402	COA	N3A-C2A-N1A	-4.14	122.32	128.58
3	F	402	COA	N9A-C8A-N7A	-4.09	108.13	113.94
3	A	402	COA	C5A-C4A-N3A	-4.00	121.21	126.72
3	B	402	COA	O4B-C4B-C3B	3.98	113.31	104.92
3	B	402	COA	C3P-N4P-C5P	3.96	130.19	122.82
3	E	402	COA	C2A-N3A-C4A	3.92	121.41	111.83
3	D	402	COA	N3A-C4A-N9A	3.91	133.82	127.17
3	C	402	COA	N9A-C8A-N7A	-3.91	108.38	113.94
3	B	402	COA	P3B-O3B-C3B	3.90	133.86	123.43
3	F	402	COA	O4B-C1B-N9A	3.90	115.58	108.09
3	E	402	COA	N3A-C4A-N9A	3.89	133.79	127.17
3	A	402	COA	C6P-C7P-N8P	-3.85	103.80	112.00
3	F	402	COA	C2P-C3P-N4P	-3.84	103.60	112.31
3	F	402	COA	C4A-N9A-C8A	3.83	109.76	105.74
3	A	402	COA	CDP-CBP-CAP	3.83	115.29	108.77
3	A	402	COA	O5B-C5B-C4B	-3.73	96.30	108.99
3	B	402	COA	C5A-C4A-N9A	3.72	109.86	105.81
3	C	402	COA	C2A-N3A-C4A	3.69	120.84	111.83
3	E	402	COA	N9A-C8A-N7A	-3.69	108.71	113.94
3	E	402	COA	C7P-N8P-C9P	3.66	129.13	122.55
3	A	402	COA	C4A-C5A-N7A	-3.62	106.45	110.58
3	E	402	COA	O5P-C5P-C6P	-3.61	115.47	122.02
3	C	402	COA	C2P-C3P-N4P	-3.59	104.16	112.31
3	B	402	COA	O6A-P2A-O4A	-3.56	94.82	108.94
3	E	402	COA	CDP-CBP-CAP	3.49	114.71	108.77
3	E	402	COA	C4A-N9A-C8A	3.37	109.27	105.74
3	A	402	COA	O5A-P2A-O3A	3.34	116.31	107.27
3	C	402	COA	N3A-C4A-N9A	3.34	132.84	127.17
3	B	402	COA	O4B-C1B-N9A	3.31	114.45	108.09
3	A	402	COA	O9P-C9P-N8P	3.27	129.91	122.98
3	D	402	COA	N9A-C8A-N7A	-3.18	109.43	113.94
3	C	402	COA	C4A-N9A-C8A	3.15	109.05	105.74
3	C	402	COA	C4A-C5A-N7A	-3.12	107.01	110.58
3	C	402	COA	C5A-N7A-C8A	3.04	108.22	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	O5B-P1A-O1A	-3.02	96.97	108.94
3	D	402	COA	O4B-C1B-N9A	2.99	113.84	108.09
3	E	402	COA	O4B-C1B-N9A	2.95	113.75	108.09
3	B	402	COA	C7P-N8P-C9P	2.88	127.71	122.55
3	B	402	COA	C5B-C4B-C3B	-2.81	105.02	114.38
3	B	402	COA	C2B-C1B-N9A	-2.78	106.39	113.30
3	D	402	COA	C4A-N9A-C8A	2.77	108.64	105.74
3	B	402	COA	P1A-O5B-C5B	-2.75	105.59	121.35
3	C	402	COA	C7P-C6P-C5P	2.71	116.90	112.39
3	D	402	COA	O6A-CCP-CBP	2.69	114.88	110.55
3	A	402	COA	O3A-P1A-O1A	-2.68	102.64	110.70
3	F	402	COA	C5A-N7A-C8A	2.64	107.60	103.45
3	A	402	COA	O2B-C2B-C1B	2.64	119.18	110.10
3	B	402	COA	O2A-P1A-O5B	2.62	119.42	107.57
3	B	402	COA	O5B-C5B-C4B	2.60	117.84	108.99
3	D	402	COA	O5P-C5P-C6P	-2.58	117.34	122.02
3	F	402	COA	O6A-CCP-CBP	2.57	114.68	110.55
3	E	402	COA	CEP-CBP-CCP	2.56	112.45	108.22
3	B	402	COA	C2B-C3B-C4B	-2.55	98.78	103.24
3	C	402	COA	CDP-CBP-CAP	2.51	113.05	108.77
3	A	402	COA	O5A-P2A-O6A	-2.44	96.52	107.57
3	B	402	COA	C4B-O4B-C1B	-2.43	104.11	109.47
3	C	402	COA	CEP-CBP-CDP	2.43	114.04	109.20
3	A	402	COA	O4B-C4B-C5B	-2.41	101.61	109.33
3	F	402	COA	CDP-CBP-CCP	-2.34	104.36	108.22
3	B	402	COA	O3B-C3B-C2B	-2.28	103.49	111.68
3	F	402	COA	CEP-CBP-CCP	2.27	111.98	108.22
3	A	402	COA	C1B-N9A-C8A	2.26	132.11	127.09
3	E	402	COA	C6P-C5P-N4P	2.25	120.44	116.34
3	D	402	COA	C7P-N8P-C9P	2.23	126.54	122.55
3	A	402	COA	C5B-C4B-C3B	2.21	121.75	114.38
3	F	402	COA	C7P-N8P-C9P	2.19	126.48	122.55
3	B	402	COA	O2B-C2B-C1B	2.18	117.62	110.10
3	D	402	COA	C5A-N7A-C8A	2.16	106.85	103.45
3	E	402	COA	O3B-C3B-C2B	-2.15	103.96	111.68
3	B	402	COA	O9A-P3B-O7A	-2.12	102.57	110.83
3	A	402	COA	C3P-N4P-C5P	2.11	126.76	122.82
3	D	402	COA	O8A-P3B-O7A	2.07	118.91	110.83
3	B	402	COA	O5B-P1A-O1A	2.07	117.13	108.94
3	E	402	COA	C5A-N7A-C8A	2.06	106.69	103.45
3	B	402	COA	N9A-C8A-N7A	-2.01	111.08	113.94
3	F	402	COA	C4A-C5A-N7A	-2.01	108.28	110.58

There are no chirality outliers.

All (37) torsion outliers are listed below:

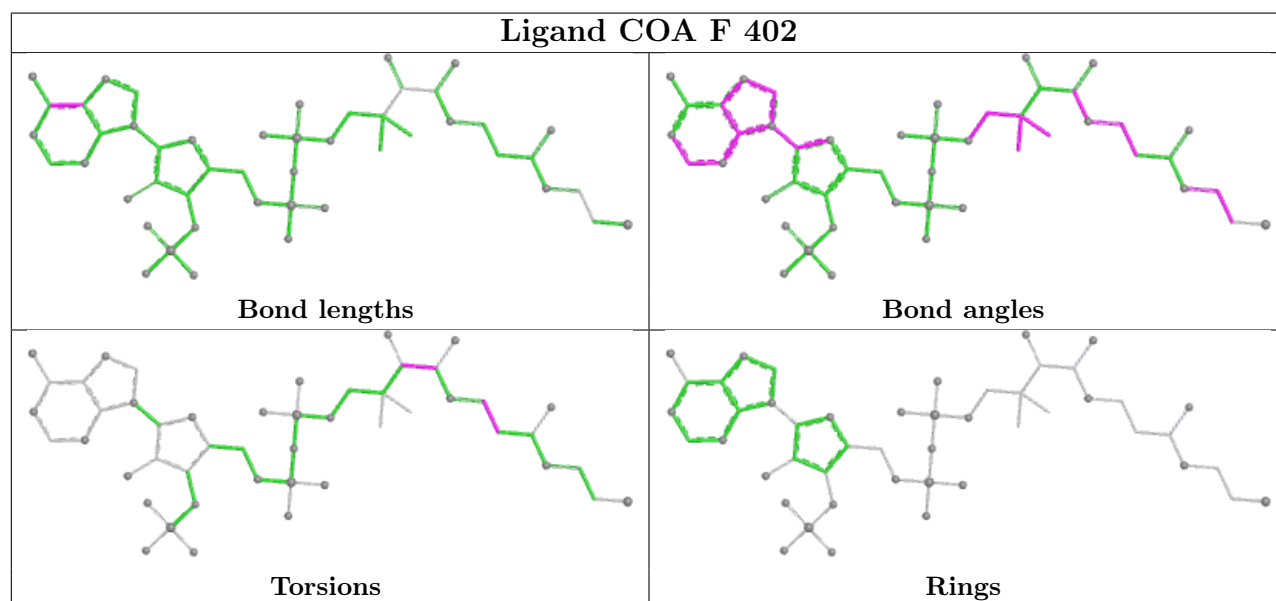
Mol	Chain	Res	Type	Atoms
3	A	402	COA	C5B-O5B-P1A-O1A
3	A	402	COA	C5B-O5B-P1A-O3A
3	B	402	COA	O4B-C4B-C5B-O5B
3	B	402	COA	C5B-O5B-P1A-O1A
3	B	402	COA	C5B-O5B-P1A-O2A
3	B	402	COA	C5B-O5B-P1A-O3A
3	B	402	COA	C2P-C3P-N4P-C5P
3	C	402	COA	N8P-C9P-CAP-OAP
3	D	402	COA	N8P-C9P-CAP-OAP
3	E	402	COA	N8P-C9P-CAP-OAP
3	E	402	COA	C2P-C3P-N4P-C5P
3	B	402	COA	O5P-C5P-C6P-C7P
3	B	402	COA	N4P-C5P-C6P-C7P
3	B	402	COA	C3B-C4B-C5B-O5B
3	C	402	COA	C5P-C6P-C7P-N8P
3	D	402	COA	C5P-C6P-C7P-N8P
3	F	402	COA	C5P-C6P-C7P-N8P
3	B	402	COA	C3B-O3B-P3B-O8A
3	E	402	COA	C5P-C6P-C7P-N8P
3	D	402	COA	O9P-C9P-CAP-OAP
3	B	402	COA	CDP-CBP-CCP-O6A
3	A	402	COA	C5B-O5B-P1A-O2A
3	B	402	COA	CCP-O6A-P2A-O4A
3	A	402	COA	C3B-O3B-P3B-O8A
3	C	402	COA	O9P-C9P-CAP-OAP
3	E	402	COA	O9P-C9P-CAP-OAP
3	E	402	COA	O4B-C4B-C5B-O5B
3	E	402	COA	N4P-C5P-C6P-C7P
3	A	402	COA	C2B-C1B-N9A-C8A
3	A	402	COA	C3B-O3B-P3B-O9A
3	C	402	COA	C3B-O3B-P3B-O9A
3	D	402	COA	C3B-O3B-P3B-O9A
3	C	402	COA	O5P-C5P-C6P-C7P
3	E	402	COA	O5P-C5P-C6P-C7P
3	E	402	COA	C3B-C4B-C5B-O5B
3	F	402	COA	N8P-C9P-CAP-OAP
3	A	402	COA	P1A-O3A-P2A-O5A

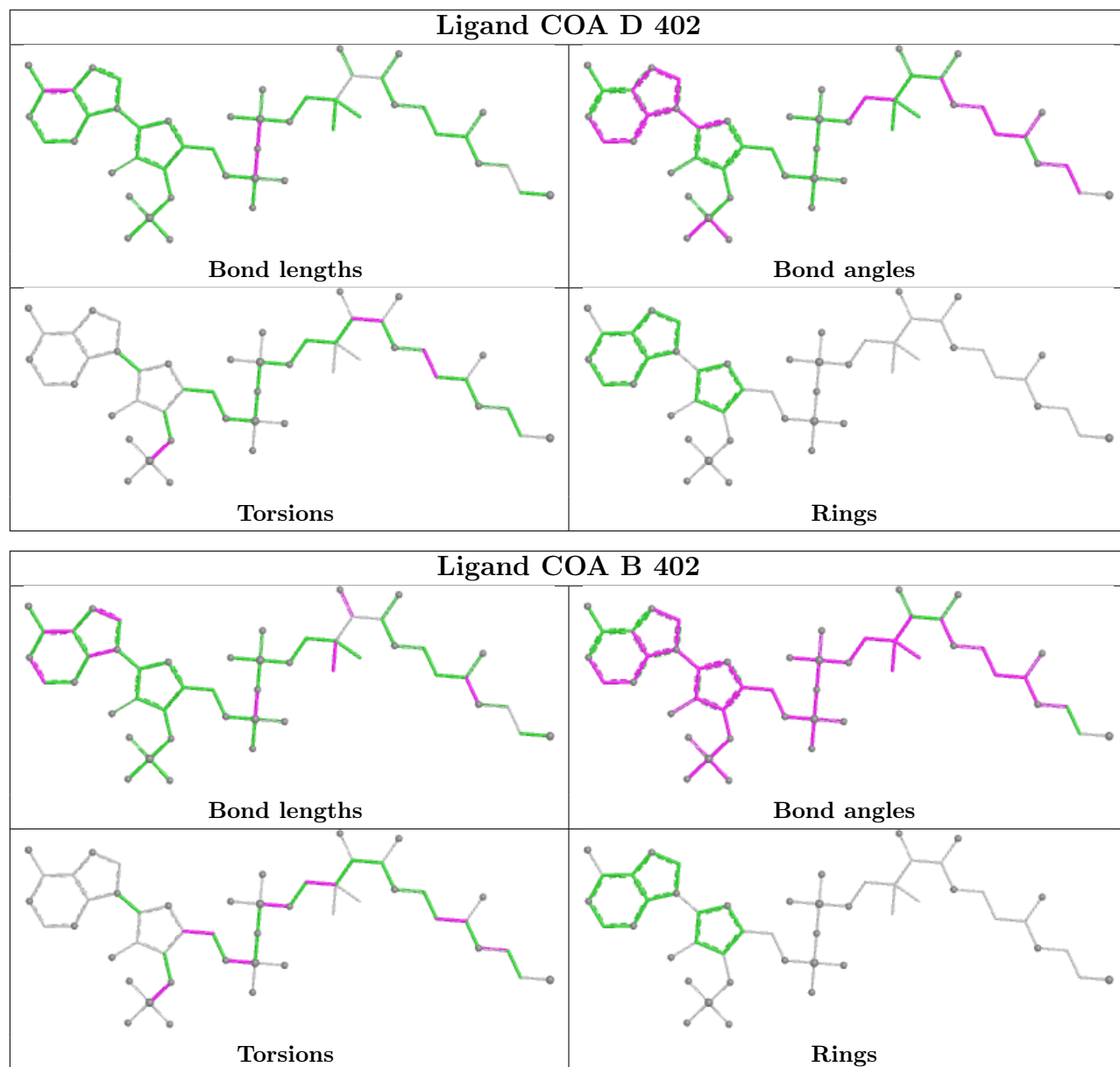
There are no ring outliers.

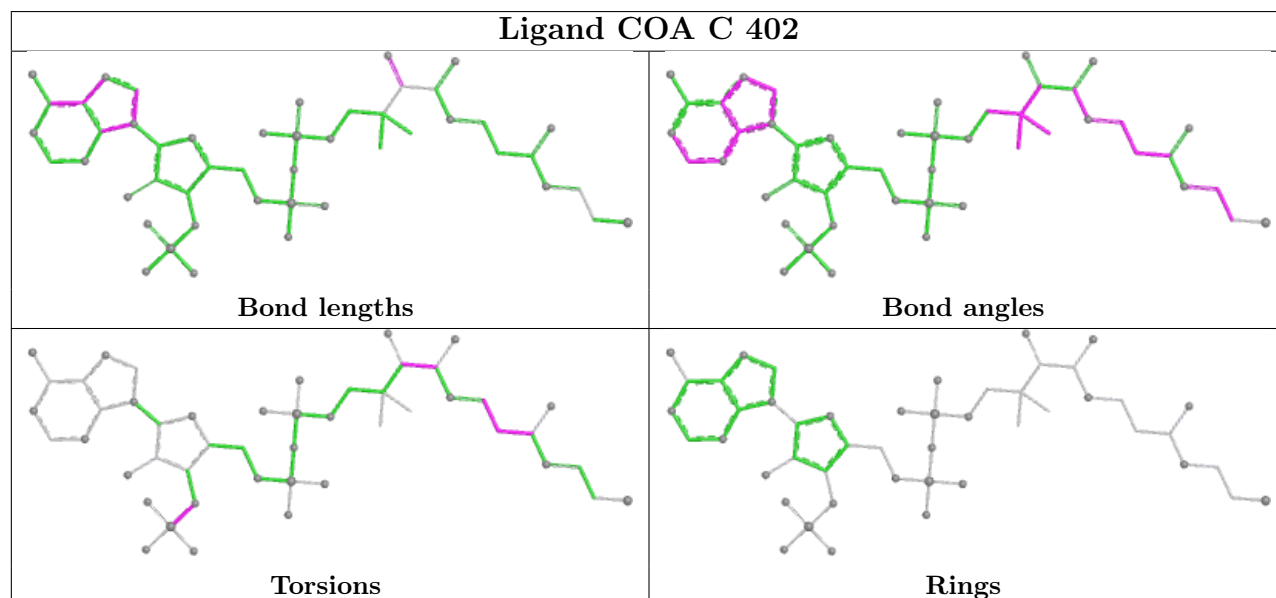
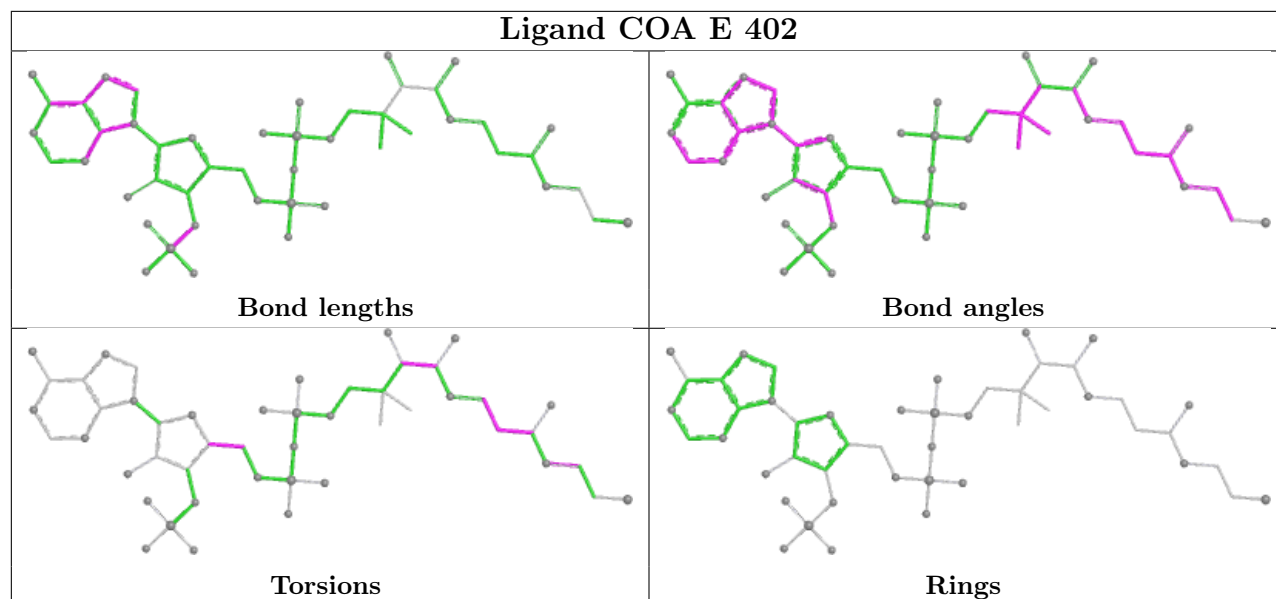
6 monomers are involved in 13 short contacts:

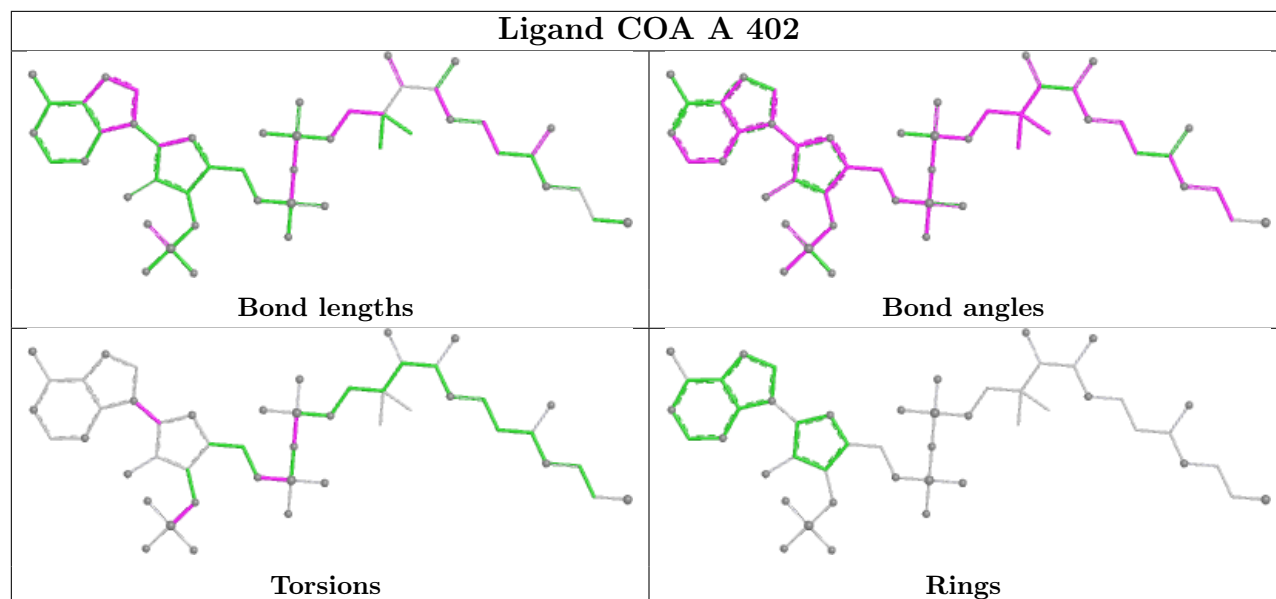
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	COA	3	0
3	D	402	COA	4	0
3	B	402	COA	2	0
3	E	402	COA	1	0
3	C	402	COA	1	0
3	A	402	COA	2	0

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	354/359 (98%)	-0.91	0	100	100	11, 29, 59, 105	0
1	B	354/359 (98%)	-0.86	0	100	100	14, 34, 63, 94	0
1	C	354/359 (98%)	0.51	13 (3%)	45	48	53, 87, 132, 173	0
1	D	354/359 (98%)	1.23	68 (19%)	3	3	64, 116, 187, 220	0
1	E	353/359 (98%)	0.44	8 (2%)	61	63	53, 98, 162, 193	0
1	F	353/359 (98%)	0.55	11 (3%)	51	53	61, 114, 181, 216	0
All	All	2122/2154 (98%)	0.16	100 (4%)	36	38	11, 84, 164, 220	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	LEU	4.5
1	D	139	LYS	4.4
1	C	359	LYS	4.3
1	E	7	THR	3.8
1	D	82	ILE	3.7
1	D	218	LEU	3.6
1	D	214	ILE	3.2
1	D	147	ILE	3.1
1	D	359	LYS	3.1
1	F	359	LYS	3.1
1	D	18	LEU	3.1
1	D	44	VAL	3.0
1	D	72	THR	3.0
1	E	76	LEU	3.0
1	D	129	HIS	3.0
1	F	82	ILE	3.0
1	E	359	LYS	2.9
1	D	14	GLY	2.8
1	D	184	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	76	LEU	2.8
1	D	76	LEU	2.8
1	D	225	VAL	2.8
1	D	351	LEU	2.7
1	D	84	PHE	2.7
1	D	175	PHE	2.7
1	D	33	ILE	2.7
1	F	342	GLY	2.7
1	D	101	LYS	2.7
1	D	121	LEU	2.7
1	F	139	LYS	2.6
1	C	140	ARG	2.6
1	D	140	ARG	2.6
1	D	19	VAL	2.6
1	D	322	VAL	2.6
1	D	83	ILE	2.6
1	D	357	ILE	2.6
1	D	126	LEU	2.6
1	D	94	PRO	2.6
1	D	60	VAL	2.5
1	D	11	ALA	2.5
1	D	95	VAL	2.5
1	D	343	GLY	2.5
1	F	353	GLU	2.4
1	C	345	ILE	2.4
1	D	67	MET	2.4
1	D	35	PRO	2.4
1	D	99	PHE	2.4
1	E	272	PHE	2.4
1	D	151	PRO	2.4
1	D	347	ALA	2.4
1	D	144	LYS	2.4
1	F	83	ILE	2.4
1	F	107	ILE	2.4
1	D	133	LEU	2.4
1	D	36	ALA	2.4
1	C	175	PHE	2.4
1	D	106	VAL	2.4
1	E	217	ILE	2.4
1	C	129	HIS	2.3
1	D	13	LEU	2.3
1	D	87	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	320	LYS	2.3
1	D	71	PRO	2.3
1	D	173	GLY	2.3
1	D	64	ILE	2.3
1	D	117	PRO	2.3
1	D	233	VAL	2.3
1	D	75	LYS	2.3
1	D	350	LEU	2.3
1	C	249	TYR	2.3
1	D	10	ALA	2.3
1	D	148	VAL	2.3
1	F	95	VAL	2.3
1	C	131	ILE	2.2
1	D	211	ILE	2.2
1	C	230	LEU	2.2
1	D	78	ASP	2.2
1	D	54	TRP	2.2
1	C	76	LEU	2.2
1	C	215	PHE	2.2
1	C	139	LYS	2.2
1	C	164	ALA	2.2
1	D	12	ILE	2.2
1	D	155	ALA	2.2
1	D	22	GLU	2.1
1	D	107	ILE	2.1
1	E	230	LEU	2.1
1	E	129	HIS	2.1
1	F	129	HIS	2.1
1	F	36	ALA	2.1
1	D	237	ALA	2.1
1	D	326	MET	2.1
1	D	27	LEU	2.1
1	D	224	ASN	2.1
1	D	37	TYR	2.1
1	D	146	PHE	2.1
1	D	122	LEU	2.0
1	E	350	LEU	2.0
1	D	221	VAL	2.0
1	D	190	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

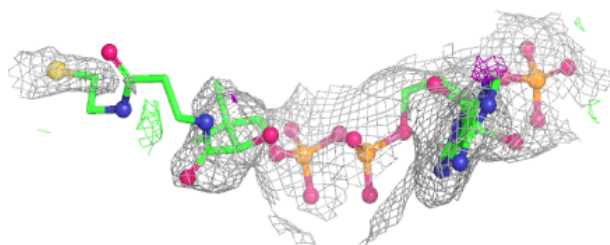
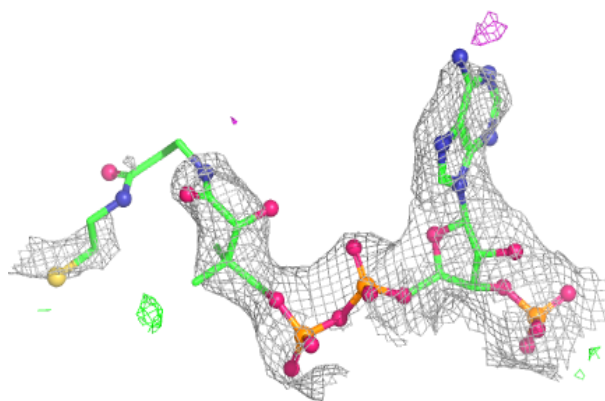
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	D	401	1/1	0.46	0.13	125,125,125,125	0
2	MG	F	401	1/1	0.60	0.20	127,127,127,127	0
2	MG	C	401	1/1	0.86	0.08	75,75,75,75	0
3	COA	D	402	48/48	0.89	0.11	120,144,169,175	0
2	MG	A	401	1/1	0.90	0.08	52,52,52,52	0
3	COA	F	402	48/48	0.90	0.10	133,144,156,160	0
2	MG	E	401	1/1	0.93	0.05	78,78,78,78	0
2	MG	B	401	1/1	0.93	0.05	48,48,48,48	0
3	COA	E	402	48/48	0.96	0.07	63,73,97,106	0
3	COA	C	402	48/48	0.97	0.07	63,69,100,108	0
3	COA	A	402	48/48	0.97	0.07	31,40,58,72	0
3	COA	B	402	48/48	0.98	0.06	31,43,61,70	0

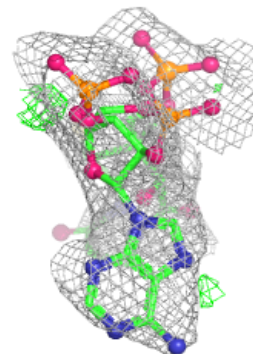
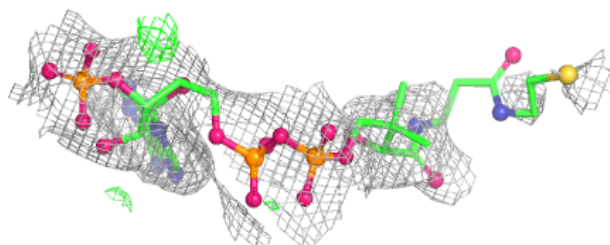
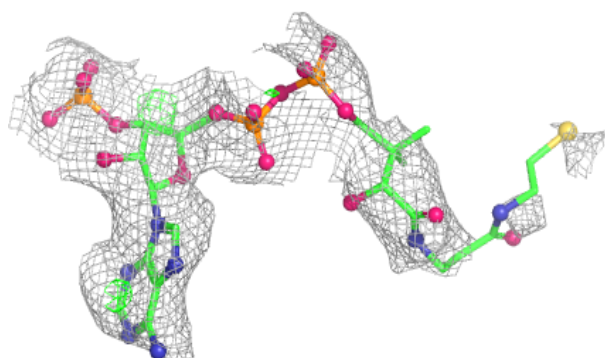
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 402:

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

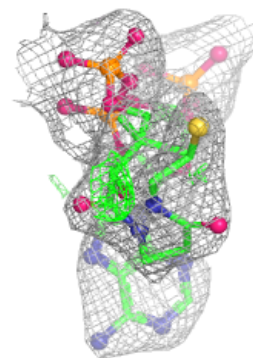
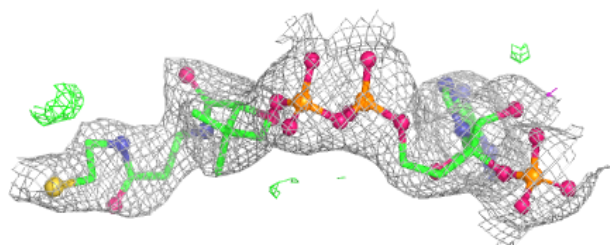
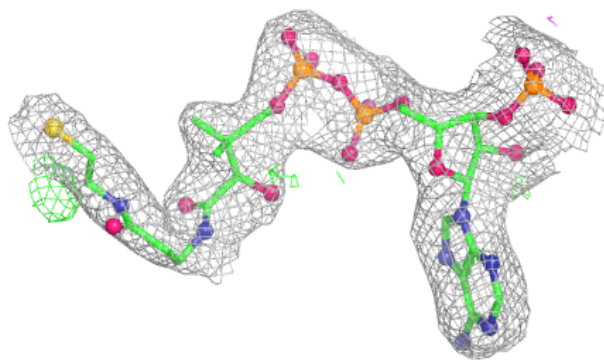
**Electron density around COA F 402:**

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

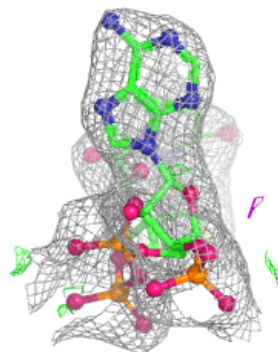
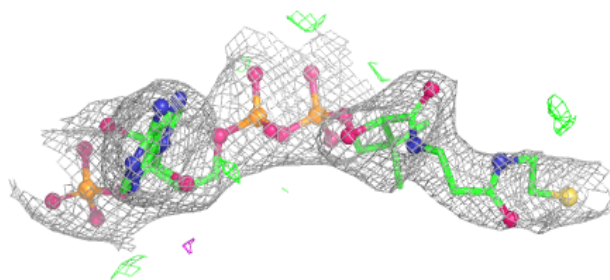
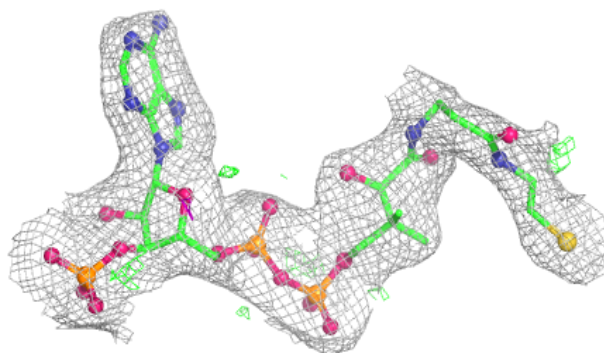


Electron density around COA E 402:

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

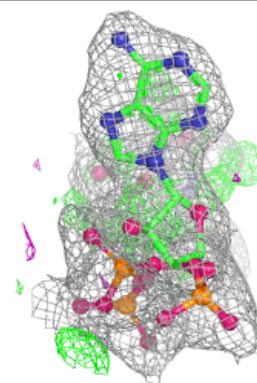
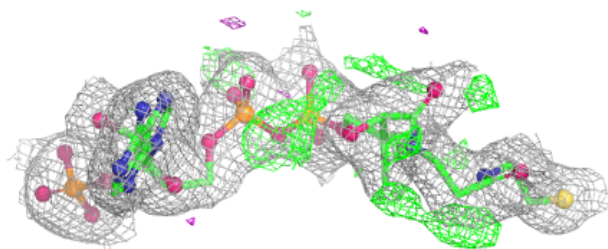
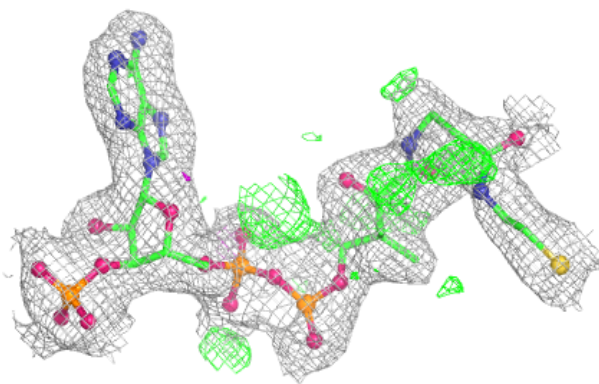
**Electron density around COA C 402:**

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

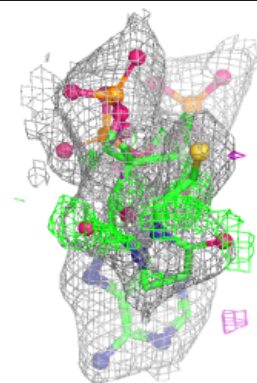
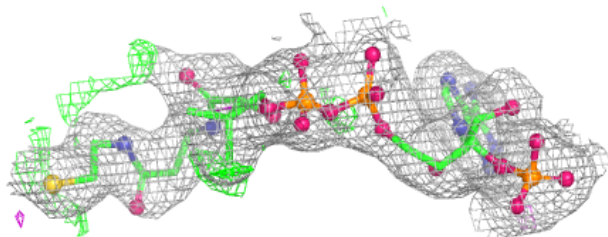
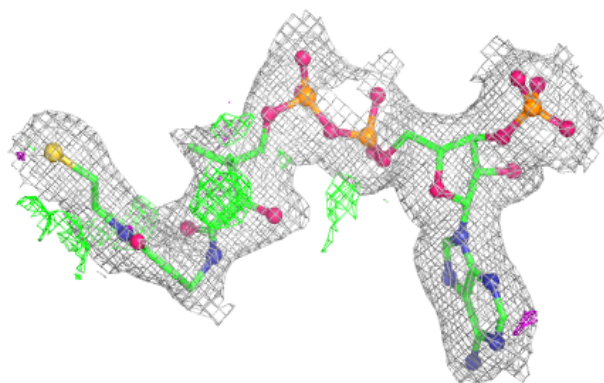


Electron density around COA A 402:

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

**Electron density around COA B 402:**

$2mF_o-DF_c$ (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.