



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:38 pm BST

PDB ID : 2REQ  
Title : METHYLMALONYL-COA MUTASE, NON-PRODUCTIVE COA COMPLEX, IN OPEN CONFORMATION REPRESENTING SUBSTRATE-FREE STATE  
Authors : Evans, P.R.; Mancia, F.  
Deposited on : 1997-09-22  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

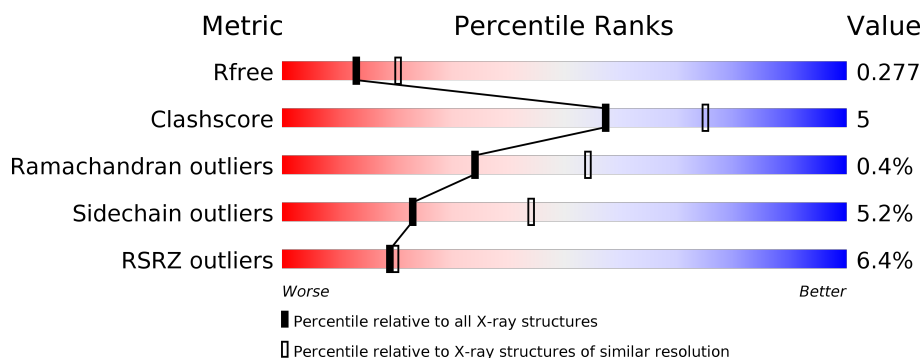
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	727	
1	C	727	
2	B	637	
2	D	637	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21240 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 METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5564	3518	965	1057	24			
1	C	725	Total	C	N	O	S	0	0	0
			5564	3518	965	1057	24			

- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4616	2912	795	896	13			
2	D	619	Total	C	N	O	S	0	0	0
			4616	2912	795	896	13			

There are 6 discrepancies between the modelled and reference sequences:

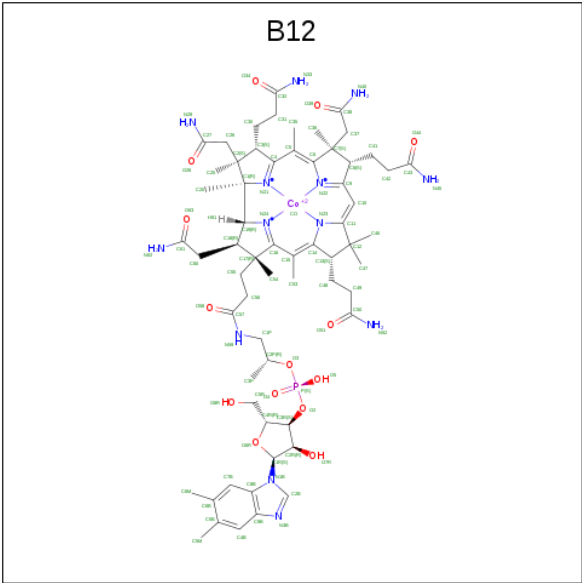
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0
			91	62	1	13	14	1	
4	C	1	Total	C	Co	N	O	P	0
			91	62	1	13	14	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0
5	B	112	Total 112	O 112	0	0
5	C	201	Total 201	O 201	0	0
5	D	117	Total 117	O 117	0	0

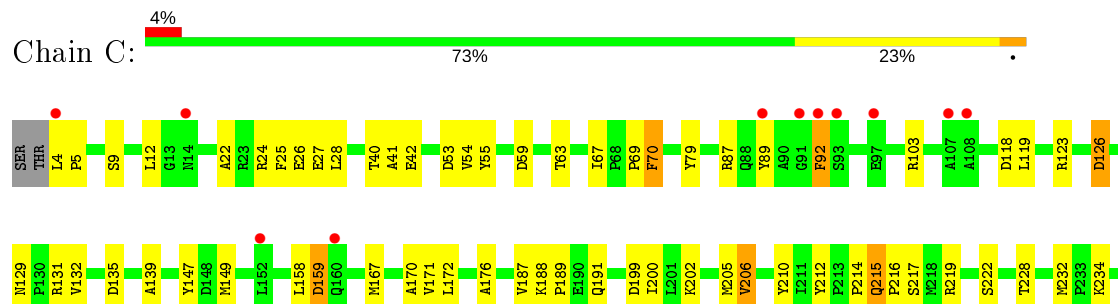
### 3 Residue-property plots

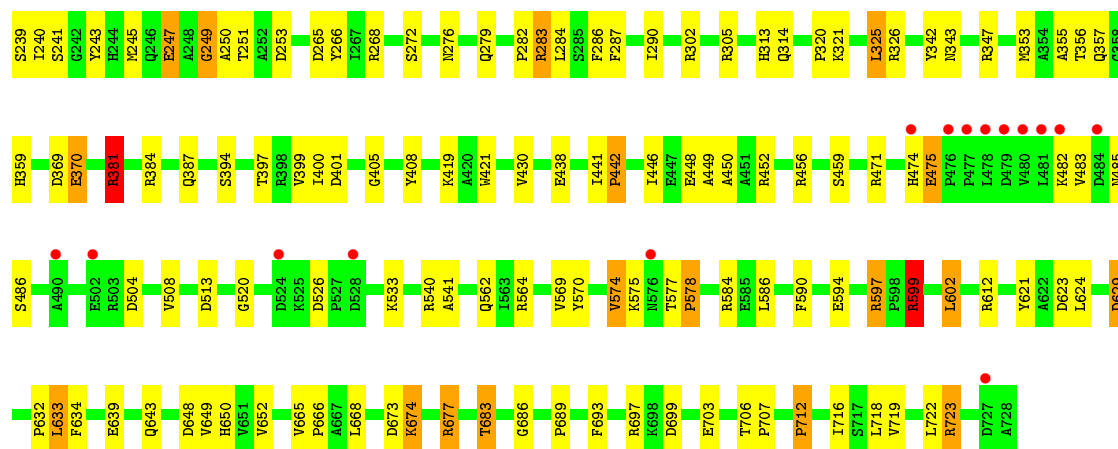
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: METHYLMALONYL-COA MUTASE

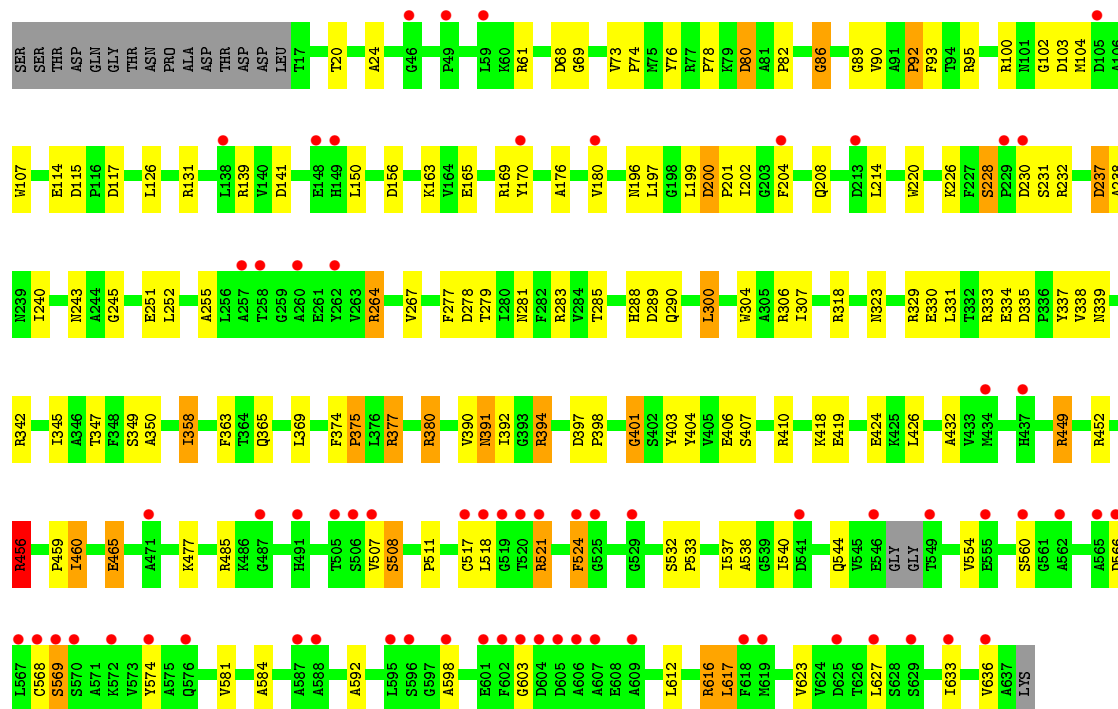
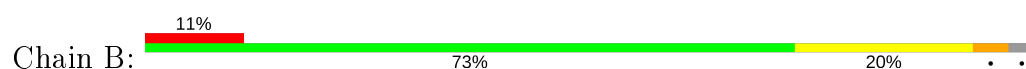


#### • Molecule 1: METHYLMALONYL-COA MUTASE

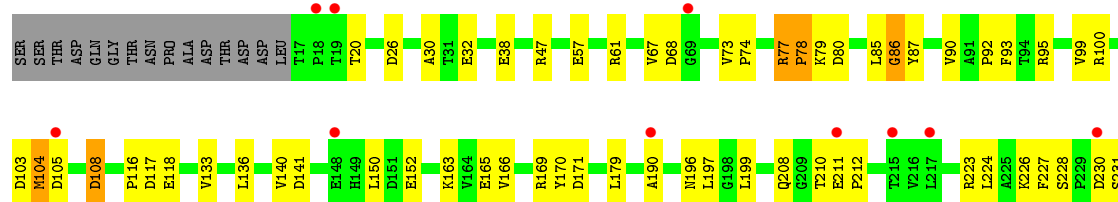


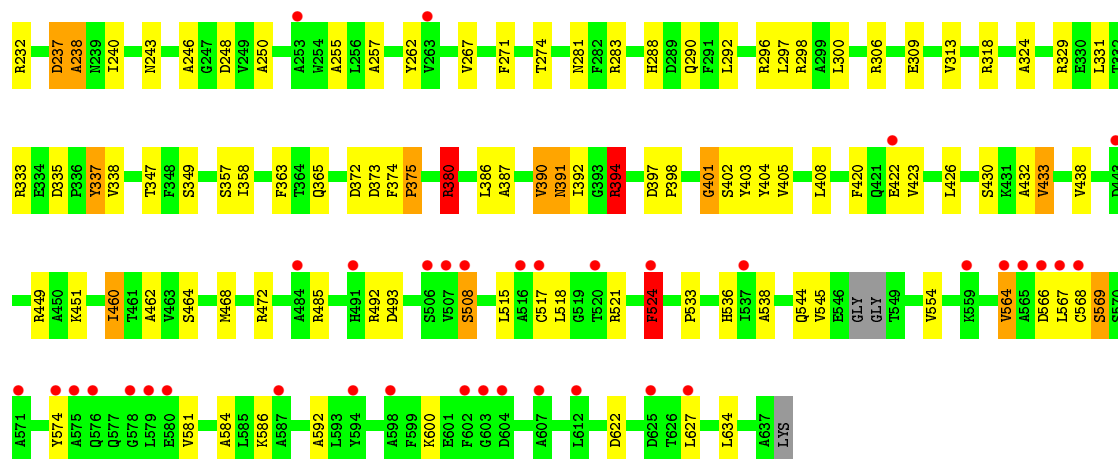


• Molecule 2: METHYLMALONYL-COA MUTASE



• Molecule 2: METHYLMALONYL-COA MUTASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.95Å 162.06Å 104.20Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 99.8 (19.98-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.259 , 0.325 0.224 , 0.277	Depositor DCC
$R_{free}$ test set	4538 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, B12

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	0.65	0/5680	1.86	123/7715 (1.6%)
1	C	0.68	0/5680	1.95	131/7715 (1.7%)
2	B	0.60	0/4706	1.77	88/6414 (1.4%)
2	D	0.57	0/4706	1.74	90/6414 (1.4%)
All	All	0.63	0/20772	1.84	432/28258 (1.5%)

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	19
1	C	0	23
2	B	0	18
2	D	0	10
All	All	0	70

There are no bond length outliers.

All (432) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	ARG	CD-NE-CZ	21.55	153.77	123.60
1	C	384	ARG	NE-CZ-NH2	-19.09	110.76	120.30
2	B	283	ARG	NE-CZ-NH1	16.99	128.79	120.30
2	B	264	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	C	540	ARG	NE-CZ-NH2	16.69	128.65	120.30
1	A	540	ARG	CD-NE-CZ	15.78	145.69	123.60
1	C	597	ARG	NE-CZ-NH1	15.26	127.93	120.30
1	A	458	ASP	CB-CG-OD1	15.14	131.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	ARG	NE-CZ-NH2	-14.78	112.91	120.30
2	B	61	ARG	NE-CZ-NH2	-14.27	113.17	120.30
1	A	452	ARG	NE-CZ-NH2	-14.01	113.30	120.30
2	B	456	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	C	584	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	C	123	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	C	283	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	C	584	ARG	CD-NE-CZ	12.03	140.44	123.60
1	C	79	TYR	CB-CG-CD2	-11.91	113.85	121.00
1	C	456	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	C	504	ASP	CB-CG-OD1	11.67	128.80	118.30
2	D	472	ARG	NE-CZ-NH2	-11.57	114.52	120.30
2	B	318	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	C	283	ARG	CD-NE-CZ	11.06	139.09	123.60
1	C	253	ASP	CB-CG-OD1	10.85	128.07	118.30
2	D	296	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	C	621	TYR	CB-CG-CD1	10.69	127.42	121.00
1	A	340	ASP	CB-CG-OD1	10.68	127.91	118.30
2	B	61	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	A	305	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	596	ARG	NE-CZ-NH1	10.54	125.57	120.30
2	D	318	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	C	621	TYR	CB-CG-CD2	-10.45	114.73	121.00
1	A	456	ARG	NE-CZ-NH2	-10.39	115.11	120.30
2	B	404	TYR	CB-CG-CD1	9.98	126.99	121.00
2	D	61	ARG	NE-CZ-NH1	9.94	125.27	120.30
2	D	380	ARG	CD-NE-CZ	9.86	137.40	123.60
1	A	370	GLU	CA-CB-CG	9.68	134.70	113.40
2	D	95	ARG	CG-CD-NE	9.57	131.90	111.80
1	A	633	LEU	O-C-N	-9.47	107.55	122.70
1	C	540	ARG	NE-CZ-NH1	-9.45	115.57	120.30
1	C	268	ARG	NE-CZ-NH2	-9.37	115.61	120.30
2	D	298	ARG	NE-CZ-NH2	9.34	124.97	120.30
2	D	333	ARG	CD-NE-CZ	9.30	136.62	123.60
1	C	612	ARG	NE-CZ-NH2	-9.27	115.67	120.30
2	D	80	ASP	CB-CG-OD2	9.10	126.49	118.30
2	B	329	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	A	283	ARG	CD-NE-CZ	9.04	136.26	123.60
2	B	95	ARG	CG-CD-NE	8.93	130.55	111.80
1	A	597	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	C	79	TYR	CB-CG-CD1	8.76	126.26	121.00
1	C	55	TYR	CB-CG-CD1	8.73	126.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	597	ARG	CD-NE-CZ	8.73	135.82	123.60
2	D	77	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	456	ARG	NE-CZ-NH1	8.69	124.64	120.30
2	B	283	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	232	MET	CA-CB-CG	8.61	127.94	113.30
1	C	590	PHE	CB-CG-CD1	8.50	126.75	120.80
1	A	621	TYR	CB-CG-CD2	-8.47	115.92	121.00
2	D	566	ASP	CB-CG-OD1	8.42	125.88	118.30
2	D	394	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	621	TYR	CB-CG-CD1	8.36	126.02	121.00
2	B	92	PRO	O-C-N	-8.33	109.38	122.70
1	C	243	TYR	CB-CG-CD2	8.24	125.94	121.00
1	C	633	LEU	O-C-N	-8.23	109.53	122.70
2	B	200	ASP	CB-CG-OD1	8.20	125.68	118.30
2	B	397	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	297	GLU	OE1-CD-OE2	-8.13	113.55	123.30
1	A	53	ASP	CB-CG-OD1	8.01	125.51	118.30
1	C	147	TYR	CB-CG-CD1	7.95	125.77	121.00
1	C	232	MET	CA-CB-CG	7.91	126.75	113.30
2	D	329	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	C	693	PHE	CB-CG-CD1	7.87	126.31	120.80
2	D	61	ARG	CD-NE-CZ	7.85	134.59	123.60
1	A	456	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	41	ALA	C-N-CA	7.79	141.19	121.70
2	B	460	ILE	CB-CA-C	7.77	127.14	111.60
2	B	115	ASP	CB-CG-OD1	7.76	125.29	118.30
2	D	90	VAL	CA-CB-CG2	7.76	122.54	110.90
1	A	693	PHE	CB-CG-CD1	7.72	126.21	120.80
1	A	384	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	D	262	TYR	CB-CG-CD1	7.69	125.61	121.00
2	B	452	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	677	ARG	CA-CB-CG	7.66	130.26	113.40
2	B	86	GLY	O-C-N	-7.66	110.45	122.70
1	C	59	ASP	CB-CG-OD2	7.66	125.19	118.30
2	B	456	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	55	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	D	485	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	326	ARG	NE-CZ-NH2	7.57	124.08	120.30
2	B	68	ASP	CB-CG-OD1	7.57	125.11	118.30
2	B	338	VAL	O-C-N	-7.53	110.65	122.70
1	A	559	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	A	584	ARG	CD-NE-CZ	7.47	134.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	264	ARG	NH1-CZ-NH2	7.44	127.58	119.40
1	C	199	ASP	CB-CG-OD1	7.42	124.98	118.30
1	C	206	VAL	CA-CB-CG1	7.37	121.96	110.90
2	D	337	TYR	O-C-N	-7.36	110.92	122.70
1	A	219	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	A	597	ARG	CD-NE-CZ	7.32	133.85	123.60
2	B	390	VAL	O-C-N	-7.32	110.98	122.70
2	B	100	ARG	CD-NE-CZ	7.32	133.84	123.60
1	A	302	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	570	TYR	CB-CG-CD1	-7.29	116.62	121.00
1	A	118	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	612	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	B	403	TYR	CB-CG-CD2	-7.26	116.65	121.00
1	C	189	PRO	C-N-CA	7.25	139.84	121.70
1	A	612	ARG	CD-NE-CZ	7.25	133.75	123.60
1	C	648	ASP	CB-CG-OD1	7.23	124.81	118.30
2	D	61	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	452	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	325	LEU	CA-CB-CG	7.16	131.77	115.30
1	A	693	PHE	CB-CG-CD2	-7.11	115.82	120.80
1	C	693	PHE	CB-CG-CD2	-7.11	115.82	120.80
2	B	78	PRO	O-C-N	-7.07	111.39	122.70
1	C	24	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	B	566	ASP	CB-CG-OD1	7.04	124.64	118.30
2	D	449	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	540	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	256	MET	CA-CB-CG	7.01	125.21	113.30
2	D	262	TYR	CB-CG-CD2	-6.96	116.82	121.00
2	D	248	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	405	GLY	O-C-N	-6.93	111.61	122.70
1	A	540	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	258	TYR	CB-CG-CD1	6.91	125.14	121.00
2	B	237	ASP	CB-CG-OD1	6.88	124.49	118.30
2	D	390	VAL	O-C-N	-6.87	111.71	122.70
1	C	370	GLU	CA-CB-CG	6.87	128.51	113.40
1	A	408	TYR	CB-CG-CD1	6.86	125.12	121.00
1	A	461	ARG	NE-CZ-NH2	-6.85	116.87	120.30
2	B	404	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	199	ASP	CB-CG-OD1	6.84	124.45	118.30
1	C	397	THR	O-C-N	-6.83	111.77	122.70
1	C	79	TYR	O-C-N	-6.83	111.77	122.70
1	C	384	ARG	NH1-CZ-NH2	6.82	126.90	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	TYR	CB-CG-CD1	6.81	125.08	121.00
1	C	302	ARG	CD-NE-CZ	6.79	133.11	123.60
2	D	460	ILE	CB-CA-C	6.79	125.17	111.60
1	A	147	TYR	CB-CG-CD1	6.77	125.06	121.00
1	A	225	PHE	CB-CG-CD1	6.76	125.53	120.80
1	C	597	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	6	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	558	ARG	CD-NE-CZ	6.73	133.02	123.60
2	B	449	ARG	CD-NE-CZ	6.71	132.99	123.60
1	C	677	ARG	CA-CB-CG	6.70	128.15	113.40
1	A	131	ARG	NE-CZ-NH1	6.69	123.65	120.30
2	B	95	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	212	TYR	CB-CG-CD2	6.68	125.01	121.00
2	D	380	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	B	401	GLY	O-C-N	-6.67	112.02	122.70
2	D	78	PRO	O-C-N	-6.64	112.08	122.70
1	A	559	TYR	CB-CG-CD1	6.61	124.97	121.00
2	B	616	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	471	ARG	NE-CZ-NH2	6.60	123.60	120.30
2	D	108	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	103	ARG	CD-NE-CZ	6.58	132.81	123.60
1	C	369	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	528	ASP	C-N-CA	6.56	138.10	121.70
1	A	411	GLU	O-C-N	-6.53	112.26	122.70
1	A	225	PHE	CB-CG-CD2	-6.51	116.24	120.80
1	A	564	ARG	CA-CB-CG	6.50	127.70	113.40
1	A	79	TYR	CB-CG-CD2	-6.49	117.11	121.00
2	B	80	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	347	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	B	104	MET	C-N-CA	6.46	137.85	121.70
1	C	302	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	A	356	THR	O-C-N	-6.44	112.40	122.70
2	D	493	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	42	GLU	O-C-N	-6.37	112.50	122.70
1	A	623	ASP	CB-CG-OD1	6.36	124.02	118.30
1	C	219	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	420	ALA	N-CA-CB	6.35	119.00	110.10
2	D	600	LYS	C-N-CA	6.35	137.57	121.70
2	B	335	ASP	CA-CB-CG	6.35	127.36	113.40
1	C	305	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	243	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	456	ARG	CD-NE-CZ	6.33	132.46	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	86	GLY	O-C-N	-6.33	112.58	122.70
1	C	666	PRO	N-CA-CB	6.32	110.88	103.30
1	C	103	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	B	485	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	C	287	PHE	CB-CG-CD1	6.30	125.21	120.80
2	D	404	TYR	CB-CG-CD1	6.26	124.76	121.00
2	B	278	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	228	THR	CA-C-N	6.26	130.97	117.20
1	C	343	ASN	CA-C-N	6.26	130.96	117.20
1	C	159	ASP	CB-CG-OD1	6.25	123.93	118.30
1	C	89	TYR	CB-CG-CD1	6.23	124.74	121.00
1	A	385	ASN	N-CA-CB	6.22	121.80	110.60
1	A	79	TYR	O-C-N	-6.22	112.75	122.70
1	C	135	ASP	CB-CG-OD1	-6.22	112.71	118.30
1	C	520	GLY	O-C-N	-6.19	112.79	122.70
2	B	90	VAL	CA-CB-CG2	6.18	120.18	110.90
2	D	574	TYR	CB-CG-CD1	6.18	124.71	121.00
1	C	683	THR	N-CA-CB	6.17	122.02	110.30
2	B	131	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	699	ASP	CB-CG-OD1	6.15	123.84	118.30
2	D	472	ARG	NH1-CZ-NH2	6.14	126.16	119.40
1	A	101	PHE	CB-CG-CD1	6.14	125.10	120.80
1	A	23	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	C	210	TYR	CB-CG-CD2	-6.13	117.32	121.00
2	D	397	ASP	CB-CG-OD1	6.13	123.81	118.30
1	C	41	ALA	O-C-N	-6.12	112.91	122.70
1	A	59	ASP	CB-CG-OD1	6.11	123.80	118.30
2	B	398	PRO	N-CA-CB	6.11	110.63	103.30
1	C	408	TYR	CB-CG-CD1	6.10	124.66	121.00
1	C	126	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	C	639	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	683	THR	N-CA-CB	6.06	121.82	110.30
2	B	403	TYR	CB-CG-CD1	6.06	124.64	121.00
1	C	599	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	612	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	B	349	SER	O-C-N	-6.01	113.08	122.70
1	C	623	ASP	O-C-N	-6.01	113.08	122.70
1	A	358	GLY	CA-C-O	6.00	131.39	120.60
2	B	89	GLY	C-N-CA	5.99	136.67	121.70
2	D	403	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	C	87	ARG	CD-NE-CZ	5.97	131.96	123.60
2	D	536	HIS	O-C-N	-5.97	113.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	TYR	CB-CG-CD1	5.96	124.58	121.00
1	A	60	TRP	O-C-N	-5.96	113.16	122.70
1	A	52	GLU	O-C-N	-5.96	113.17	122.70
2	D	283	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	B	459	PRO	N-CA-CB	5.93	110.41	103.30
2	B	363	PHE	C-N-CA	5.92	136.51	121.70
1	C	210	TYR	CB-CG-CD1	5.92	124.55	121.00
1	C	578	PRO	C-N-CA	5.92	136.49	121.70
2	D	85	LEU	C-N-CA	-5.91	109.88	122.30
1	C	623	ASP	C-N-CA	5.91	136.47	121.70
2	D	373	ASP	CB-CG-OD1	5.91	123.61	118.30
2	D	401	GLY	O-C-N	-5.90	113.26	122.70
1	C	442	PRO	N-CA-CB	5.89	110.37	103.30
1	A	255	GLU	OE1-CD-OE2	-5.88	116.24	123.30
2	B	283	ARG	CD-NE-CZ	5.88	131.83	123.60
2	B	333	ARG	CD-NE-CZ	5.88	131.83	123.60
1	C	381	ARG	CA-CB-CG	5.88	126.33	113.40
2	D	380	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	D	47	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	320	PRO	O-C-N	-5.86	113.33	122.70
2	D	100	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	B	350	ALA	CB-CA-C	5.84	118.86	110.10
1	A	558	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	233	PRO	N-CA-CB	5.83	110.30	103.30
1	A	326	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	C	320	PRO	C-N-CA	5.82	136.25	121.70
1	C	272	SER	O-C-N	-5.82	113.39	122.70
2	D	26	ASP	O-C-N	-5.82	113.39	122.70
2	D	79	LYS	C-N-CA	5.82	136.25	121.70
1	C	541	ALA	O-C-N	-5.82	113.39	122.70
1	C	639	GLU	CG-CD-OE1	5.80	129.91	118.30
1	C	697	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	B	335	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	131	ARG	NE-CZ-NH2	5.79	123.20	120.30
2	B	521	ARG	CD-NE-CZ	5.79	131.71	123.60
2	D	533	PRO	N-CA-CB	5.79	110.25	103.30
2	B	90	VAL	CB-CA-C	-5.78	100.42	111.40
1	A	249	GLY	CA-C-O	-5.75	110.26	120.60
2	D	492	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	B	169	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	D	380	ARG	NH1-CZ-NH2	-5.74	113.09	119.40
2	D	420	PHE	CA-CB-CG	5.73	127.66	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	PHE	C-N-CA	5.73	136.02	121.70
1	A	251	THR	CA-CB-CG2	-5.72	104.39	112.40
1	A	513	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	314	GLN	C-N-CA	5.70	135.96	121.70
1	A	527	PRO	N-CA-CB	5.70	110.14	103.30
1	A	287	PHE	CB-CG-CD1	5.69	124.78	120.80
1	C	384	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	87	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	147	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	C	634	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	D	93	PHE	O-C-N	-5.66	113.64	122.70
1	C	633	LEU	C-N-CA	5.65	135.82	121.70
2	D	524	PHE	CB-CG-CD1	5.64	124.75	120.80
1	A	228	THR	CA-C-N	5.63	129.59	117.20
1	C	347	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	266	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	522	PRO	N-CA-CB	5.62	110.05	103.30
1	A	678	PRO	N-CA-CB	5.61	110.03	103.30
1	C	400	ILE	C-N-CA	5.61	135.71	121.70
1	C	63	THR	O-C-N	-5.60	113.74	122.70
2	B	86	GLY	C-N-CA	5.59	135.68	121.70
2	D	349	SER	O-C-N	-5.59	113.75	122.70
2	D	78	PRO	C-N-CA	5.59	135.68	121.70
1	A	384	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	249	GLY	CA-C-O	-5.59	110.54	120.60
1	A	120	PRO	N-CA-CB	5.59	110.00	103.30
1	A	699	ASP	CB-CG-OD1	5.58	123.33	118.30
1	C	712	PRO	O-C-N	-5.58	113.77	122.70
1	C	170	ALA	C-N-CA	5.58	135.65	121.70
2	D	283	ARG	CD-NE-CZ	5.57	131.40	123.60
2	B	117	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	699	ASP	CA-CB-CG	5.57	125.66	113.40
1	A	674	LYS	C-N-CA	5.56	135.61	121.70
2	D	404	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	A	584	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	189	PRO	C-N-CA	5.56	135.60	121.70
1	A	442	PRO	N-CA-CB	5.55	109.96	103.30
2	D	283	ARG	N-CA-CB	5.54	120.58	110.60
1	A	412	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	C	508	VAL	CB-CA-C	-5.54	100.88	111.40
2	D	238	ALA	O-C-N	-5.53	113.85	122.70
2	B	232	ARG	CD-NE-CZ	5.52	131.32	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	633	LEU	C-N-CA	5.51	135.47	121.70
2	B	24	ALA	O-C-N	-5.51	113.84	123.20
1	A	369	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	398	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	114	SER	CB-CA-C	-5.48	99.69	110.10
2	B	449	ARG	NE-CZ-NH1	-5.48	117.56	120.30
2	D	68	ASP	CB-CG-OD1	5.48	123.23	118.30
2	D	104	MET	C-N-CA	5.47	135.39	121.70
2	D	375	PRO	O-C-N	-5.47	113.94	122.70
1	A	42	GLU	C-N-CA	5.47	135.38	121.70
2	D	26	ASP	C-N-CA	5.47	135.38	121.70
2	B	318	ARG	NH1-CZ-NH2	5.47	125.42	119.40
1	C	513	ASP	O-C-N	-5.46	113.97	122.70
1	C	131	ARG	O-C-N	-5.46	113.97	122.70
1	C	689	PRO	N-CA-CB	5.46	109.85	103.30
2	D	398	PRO	O-C-N	-5.45	113.98	122.70
1	C	370	GLU	N-CA-CB	-5.45	100.80	110.60
2	D	338	VAL	O-C-N	-5.45	113.99	122.70
1	C	564	ARG	CA-CB-CG	5.44	125.37	113.40
2	B	358	ILE	CB-CG1-CD1	5.44	129.13	113.90
1	C	69	PRO	O-C-N	-5.43	114.01	122.70
1	A	571	SER	O-C-N	-5.43	114.02	122.70
2	D	171	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	333	GLY	C-N-CA	5.42	135.26	121.70
2	B	617	LEU	CA-CB-CG	5.42	127.77	115.30
2	D	86	GLY	CA-C-O	5.42	130.35	120.60
1	A	189	PRO	N-CA-CB	5.41	109.79	103.30
2	B	410	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	297	GLU	O-C-N	-5.38	114.09	122.70
1	C	176	ALA	CB-CA-C	-5.38	102.03	110.10
1	A	410	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	C	147	TYR	CB-CG-CD2	-5.36	117.78	121.00
2	D	363	PHE	C-N-CA	5.35	135.07	121.70
2	D	394	ARG	NH1-CZ-NH2	5.35	125.28	119.40
2	B	69	GLY	N-CA-C	5.34	126.44	113.10
1	A	358	GLY	O-C-N	-5.33	114.16	122.70
2	B	380	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	15	ALA	N-CA-CB	-5.33	102.64	110.10
2	B	169	ARG	CD-NE-CZ	5.32	131.05	123.60
1	C	723	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	D	169	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	76	TYR	CB-CG-CD1	-5.31	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	304	TRP	CA-CB-CG	5.31	123.79	113.70
2	B	90	VAL	CG1-CB-CG2	-5.30	102.42	110.90
2	B	524	PHE	CB-CG-CD1	5.29	124.50	120.80
1	C	325	LEU	CB-CG-CD1	5.29	119.98	111.00
1	C	673	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	123	ARG	C-N-CA	5.27	133.37	122.30
1	A	461	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	342	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	D	86	GLY	C-N-CA	5.27	134.87	121.70
2	D	117	ASP	CB-CG-OD1	5.26	123.03	118.30
2	B	524	PHE	CA-CB-CG	5.25	126.51	113.90
1	A	42	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	C	421	TRP	C-N-CA	5.25	133.32	122.30
1	C	430	VAL	CA-C-N	5.24	126.68	116.20
2	D	462	ALA	C-N-CA	5.23	134.78	121.70
2	D	38	GLU	OE1-CD-OE2	-5.23	117.02	123.30
2	B	307	ILE	O-C-N	-5.22	114.33	123.20
1	C	314	GLN	C-N-CA	5.22	134.74	121.70
2	D	390	VAL	CA-CB-CG2	5.21	118.72	110.90
1	C	70	PHE	CA-CB-CG	5.21	126.41	113.90
1	A	321	LYS	O-C-N	-5.21	114.37	122.70
1	A	584	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	401	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	674	LYS	O-C-N	-5.21	114.37	122.70
1	A	135	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	B	306	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	D	92	PRO	O-C-N	-5.20	114.38	122.70
2	B	243	ASN	O-C-N	-5.20	114.39	122.70
2	D	390	VAL	CG1-CB-CG2	-5.19	102.60	110.90
2	D	586	LYS	C-N-CA	5.19	134.68	121.70
1	C	314	GLN	O-C-N	-5.18	114.41	122.70
1	C	624	LEU	C-N-CA	5.18	133.17	122.30
1	C	286	PHE	CB-CG-CD1	5.17	124.42	120.80
1	A	633	LEU	CA-C-O	5.17	130.96	120.10
2	D	243	ASN	O-C-N	-5.17	114.43	122.70
1	C	228	THR	CA-CB-CG2	-5.17	105.16	112.40
2	D	380	ARG	O-C-N	-5.16	114.45	122.70
2	B	264	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	320	PRO	N-CA-CB	5.15	109.48	103.30
2	B	375	PRO	N-CA-CB	5.15	109.48	103.30
1	C	54	VAL	O-C-N	-5.15	114.47	122.70
2	B	406	GLU	OE1-CD-OE2	-5.14	117.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TYR	CB-CG-CD1	-5.14	117.91	121.00
2	B	78	PRO	C-N-CA	5.14	134.55	121.70
1	A	63	THR	O-C-N	-5.14	114.48	122.70
1	C	629	ASP	CB-CG-OD2	-5.13	113.69	118.30
2	B	574	TYR	CB-CG-CD1	5.12	124.07	121.00
2	B	333	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	D	524	PHE	CA-CB-CG	5.11	126.17	113.90
1	A	79	TYR	CB-CG-CD1	5.11	124.07	121.00
2	B	20	THR	O-C-N	-5.11	114.53	122.70
1	A	228	THR	O-C-N	-5.11	114.53	122.70
2	D	296	ARG	NH1-CZ-NH2	5.11	125.02	119.40
2	B	419	GLU	O-C-N	-5.11	114.53	122.70
2	D	309	GLU	O-C-N	-5.10	114.54	122.70
2	B	78	PRO	N-CA-CB	5.09	109.41	103.30
1	C	674	LYS	O-C-N	-5.09	114.55	122.70
1	C	222	SER	CB-CA-C	-5.08	100.44	110.10
2	B	424	GLU	O-C-N	-5.07	114.58	122.70
2	D	116	PRO	N-CA-CB	5.07	109.39	103.30
1	A	599	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	419	LYS	O-C-N	-5.07	114.59	122.70
1	C	381	ARG	CB-CA-C	5.07	120.54	110.40
1	A	537	ASP	O-C-N	-5.07	114.59	122.70
1	C	247	GLU	C-N-CA	5.06	134.36	121.70
1	C	92	PHE	CA-C-O	5.06	130.73	120.10
1	A	452	ARG	NH1-CZ-NH2	5.06	124.96	119.40
2	D	32	GLU	C-N-CA	5.06	134.34	121.70
1	A	426	GLU	CG-CD-OE1	5.05	128.41	118.30
1	A	434	ALA	CA-C-N	5.05	128.32	117.20
1	C	399	VAL	CG1-CB-CG2	-5.05	102.81	110.90
2	B	330	GLU	CA-C-O	-5.05	109.49	120.10
1	A	514	LYS	CA-CB-CG	5.05	124.51	113.40
1	C	353	MET	CG-SD-CE	5.05	108.28	100.20
2	D	78	PRO	CA-C-N	5.04	128.29	117.20
2	B	338	VAL	CA-C-N	5.04	128.29	117.20
1	A	263	GLY	C-N-CA	5.04	134.30	121.70
1	A	70	PHE	CA-CB-CG	5.03	125.97	113.90
2	D	622	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	570	TYR	CB-CG-CD1	-5.03	117.98	121.00
2	D	20	THR	N-CA-CB	5.03	119.85	110.30
1	C	53	ASP	O-C-N	-5.02	114.66	122.70
2	B	465	GLU	N-CA-CB	5.02	119.63	110.60
2	D	422	GLU	O-C-N	-5.01	114.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	136	LEU	CA-CB-CG	5.01	126.82	115.30
2	D	248	ASP	OD1-CG-OD2	-5.00	113.79	123.30
2	B	377	ARG	CD-NE-CZ	5.00	130.60	123.60
2	B	232	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Mainchain
1	A	167	MET	Mainchain
1	A	20	ASP	Mainchain
1	A	313	HIS	Mainchain
1	A	342	TYR	Mainchain
1	A	376	THR	Mainchain
1	A	387	GLN	Mainchain
1	A	40	THR	Mainchain
1	A	405	GLY	Mainchain
1	A	409	VAL	Mainchain
1	A	588	GLU	Mainchain
1	A	625	GLY	Mainchain
1	A	627	ASP	Mainchain
1	A	665	VAL	Mainchain
1	A	672	LEU	Mainchain
1	A	677	ARG	Mainchain
1	A	697	ARG	Mainchain
1	A	70	PHE	Mainchain
1	A	723	ARG	Mainchain
2	B	103	ASP	Mainchain
2	B	204	PHE	Mainchain
2	B	220	TRP	Mainchain
2	B	228	SER	Mainchain
2	B	231	SER	Mainchain
2	B	277	PHE	Mainchain
2	B	334	GLU	Mainchain
2	B	337	TYR	Mainchain
2	B	339	ASN	Mainchain
2	B	380	ARG	Mainchain
2	B	391	ASN	Mainchain
2	B	394	ARG	Mainchain
2	B	401	GLY	Mainchain
2	B	418	LYS	Mainchain

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Mol	Chain	Res	Type	Group
2	B	456	ARG	Mainchain
2	B	465	GLU	Mainchain
2	B	82	PRO	Mainchain
2	B	86	GLY	Mainchain
1	C	126	ASP	Mainchain
1	C	158	LEU	Mainchain
1	C	167	MET	Mainchain
1	C	172	LEU	Mainchain
1	C	205	MET	Mainchain
1	C	215	GLN	Mainchain
1	C	27	GLU	Mainchain
1	C	313	HIS	Mainchain
1	C	342	TYR	Mainchain
1	C	356	THR	Mainchain
1	C	381	ARG	Mainchain
1	C	387	GLN	Mainchain
1	C	394	SER	Mainchain
1	C	40	THR	Mainchain
1	C	405	GLY	Mainchain
1	C	526	ASP	Mainchain
1	C	633	LEU	Mainchain
1	C	665	VAL	Mainchain
1	C	674	LYS	Mainchain
1	C	677	ARG	Mainchain
1	C	70	PHE	Mainchain
1	C	712	PRO	Mainchain
1	C	723	ARG	Mainchain
2	D	231	SER	Mainchain
2	D	237	ASP	Mainchain
2	D	324	ALA	Mainchain
2	D	337	TYR	Mainchain
2	D	380	ARG	Mainchain
2	D	387	ALA	Mainchain
2	D	391	ASN	Mainchain
2	D	394	ARG	Mainchain
2	D	401	GLY	Mainchain
2	D	86	GLY	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	5564	0	5472	42	0
1	C	5564	0	5472	45	0
2	B	4616	0	4428	47	0
2	D	4616	0	4428	49	0
3	A	31	0	11	1	0
3	C	31	0	11	1	0
4	A	91	0	88	19	0
4	C	91	0	88	12	0
5	A	206	0	0	1	0
5	B	112	0	0	0	0
5	C	201	0	0	0	0
5	D	117	0	0	0	0
All	All	21240	0	19998	200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (200) 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:A:800:B12:H362	4:A:800:B12:H351	1.22	1.11
4:C:800:B12:H362	4:C:800:B12:H351	1.17	1.09
4:A:800:B12:H531	4:A:800:B12:H552	1.09	1.09
4:A:800:B12:C53	4:A:800:B12:H552	1.98	0.93
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.21	0.88
4:C:800:B12:C35	4:C:800:B12:H362	2.02	0.88
4:A:800:B12:H351	4:A:800:B12:C36	2.04	0.87
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.24	0.85
4:C:800:B12:C36	4:C:800:B12:H351	1.96	0.85
4:A:800:B12:C55	4:A:800:B12:H531	2.01	0.84
4:A:800:B12:H362	4:A:800:B12:C35	2.05	0.83
4:A:800:B12:H312	4:A:800:B12:C25	2.11	0.81
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.30	0.78
4:A:800:B12:H253	4:A:800:B12:H312	1.65	0.77
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.70	0.74
4:C:800:B12:H531	4:C:800:B12:H552	1.67	0.74
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.73	0.71
2:B:281:ASN:ND2	2:B:323:ASN:HD21	1.92	0.68
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:GLU:HB3	4:C:800:B12:H532	1.77	0.67
2:D:402:SER:HB3	2:D:405:VAL:HB	1.77	0.66
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.78	0.66
2:D:391:ASN:ND2	2:D:394:ARG:HH21	1.94	0.65
4:A:800:B12:H302	4:A:800:B12:H353	1.78	0.65
1:A:662:LEU:HD21	1:A:692:ASP:HB3	1.78	0.65
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.45	0.65
2:D:391:ASN:HD21	2:D:394:ARG:HH21	1.46	0.63
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.81	0.61
1:C:706:THR:HB	1:C:707:PRO:CD	2.30	0.61
2:D:165:GLU:HB2	2:D:196:ASN:HB2	1.81	0.61
1:C:448:GLU:HG2	1:C:569:VAL:HG21	1.83	0.60
1:C:602:LEU:HD21	4:C:800:B12:HM52	1.84	0.60
4:C:800:B12:H531	4:C:800:B12:C55	2.32	0.60
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.84	0.60
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.52	0.57
2:D:237:ASP:HB3	2:D:240:ILE:HD12	1.85	0.57
1:A:359:HIS:CE1	1:A:401:ASP:H	2.23	0.57
1:A:247:GLU:HB3	4:A:800:B12:H532	1.85	0.57
1:C:706:THR:HB	1:C:707:PRO:HD2	1.86	0.57
4:A:800:B12:C31	4:A:800:B12:C25	2.82	0.56
1:A:353:MET:HE3	2:B:345:ILE:HG13	1.87	0.56
1:A:196:ILE:HG22	1:A:235:TRP:HE1	1.70	0.56
1:C:577:THR:HB	1:C:578:PRO:HD2	1.88	0.56
1:C:129:ASN:HB3	1:C:132:VAL:HG22	1.87	0.56
2:B:165:GLU:HB2	2:B:196:ASN:HB2	1.88	0.56
1:C:250:ALA:HB2	1:C:446:ILE:HG12	1.88	0.55
1:A:214:PRO:HG2	1:A:438:GLU:HG3	1.89	0.55
1:C:206:VAL:HG11	1:C:245:MET:HA	1.89	0.54
4:C:800:B12:H262	4:C:800:B12:H601	1.89	0.54
1:A:172:LEU:HB2	1:A:173:PRO:HD3	1.90	0.54
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.90	0.54
2:B:201:PRO:HB2	2:B:214:LEU:HD12	1.91	0.53
1:C:650:HIS:HB3	1:C:722:LEU:HD11	1.90	0.53
2:D:77:ARG:HB3	2:D:78:PRO:HD2	1.89	0.53
2:D:518:LEU:HD11	2:D:581:VAL:HG11	1.90	0.53
2:D:166:VAL:HG13	2:D:179:LEU:HD22	1.88	0.53
1:A:441:ILE:HB	1:A:442:PRO:CD	2.38	0.53
2:B:568:CYS:O	2:B:569:SER:HB2	2.09	0.53
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.91	0.53
1:C:599:ARG:HG2	1:C:649:VAL:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:GLN:NE2	2:D:290:GLN:HE22	2.02	0.52
4:A:800:B12:O28	4:A:800:B12:H3	2.10	0.51
2:D:433:VAL:HG23	2:D:438:VAL:HG21	1.92	0.51
1:C:282:PRO:HB3	1:C:321:LYS:HD2	1.93	0.51
1:A:336:LEU:HD22	1:A:344:ASN:HB3	1.93	0.51
2:B:532:SER:HB2	2:B:533:PRO:HD3	1.92	0.51
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.93	0.51
1:C:441:ILE:HB	1:C:442:PRO:CD	2.39	0.51
2:D:108:ASP:HB3	2:D:357:SER:HA	1.93	0.50
2:D:212:PRO:HG2	2:D:430:SER:HB3	1.92	0.50
2:D:208:GLN:HB2	2:D:210:THR:HG23	1.94	0.50
2:B:518:LEU:HD21	2:B:581:VAL:HG21	1.94	0.50
1:A:602:LEU:HD13	1:A:618:ALA:HA	1.92	0.50
2:B:245:GLY:HA2	2:B:449:ARG:HH12	1.77	0.50
1:C:67:ILE:HG21	2:D:30:ALA:HB2	1.93	0.50
1:A:95:ALA:HB1	1:A:151:GLU:HG2	1.93	0.49
4:A:800:B12:C35	4:A:800:B12:C36	2.77	0.49
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.03	0.49
2:D:197:LEU:HD11	2:D:224:LEU:HD13	1.94	0.49
4:A:800:B12:H251	4:A:800:B12:H312	1.92	0.49
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.95	0.49
2:D:515:LEU:HB2	2:D:544:GLN:HB3	1.94	0.49
1:C:188:LYS:HB2	1:C:191:GLN:NE2	2.28	0.49
1:A:240:ILE:HD11	1:A:284:LEU:HD22	1.94	0.49
1:C:118:ASP:HA	1:C:139:ALA:HB3	1.95	0.49
4:A:800:B12:O7R	4:A:800:B12:H2B	2.13	0.48
2:B:426:LEU:HD11	2:B:432:ALA:HB2	1.95	0.48
2:B:511:PRO:HB2	2:B:540:ILE:HG12	1.95	0.48
2:B:598:ALA:HA	2:B:616:ARG:HH11	1.77	0.48
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.96	0.48
2:B:331:LEU:HD13	2:B:365:GLN:HB3	1.96	0.48
1:C:240:ILE:HD11	1:C:284:LEU:HD22	1.96	0.48
1:A:706:THR:HB	1:A:707:PRO:CD	2.44	0.47
1:C:12:LEU:HD12	2:D:306:ARG:HG2	1.97	0.47
1:C:359:HIS:CE1	1:C:401:ASP:H	2.31	0.47
4:C:800:B12:C35	4:C:800:B12:C36	2.73	0.47
2:B:126:LEU:HD22	2:B:156:ASP:HB3	1.96	0.47
1:C:683:THR:HG22	1:C:703:GLU:HB2	1.97	0.47
1:A:4:LEU:HD21	2:B:267:VAL:HG11	1.97	0.47
1:A:129:ASN:HB3	1:A:132:VAL:HG22	1.97	0.47
1:A:632:PRO:HG2	1:A:635:GLN:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.97	0.47
1:A:282:PRO:HB3	1:A:321:LYS:HD2	1.97	0.46
1:A:683:THR:HG22	1:A:703:GLU:HB2	1.98	0.46
4:A:800:B12:H492	4:A:800:B12:C47	2.46	0.46
1:A:448:GLU:HG2	1:A:569:VAL:HG21	1.98	0.46
1:A:390:LEU:HA	1:A:394:SER:HB3	1.98	0.46
1:C:632:PRO:HD2	1:C:643:GLN:HE22	1.80	0.45
2:D:232:ARG:HG3	2:D:281:ASN:ND2	2.30	0.45
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.98	0.45
3:C:801:COA:H8A	3:C:801:COA:O4A	2.15	0.45
2:D:274:THR:HA	2:D:313:VAL:HG13	1.97	0.45
1:A:600:ILE:HG13	1:A:651:VAL:HG13	1.98	0.45
2:B:114:GLU:HG2	2:B:139:ARG:HB2	1.98	0.45
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.97	0.45
1:C:686:GLY:O	1:C:707:PRO:HD3	2.17	0.45
1:A:541:ALA:O	1:A:542:MET:HB2	2.16	0.45
2:B:238:ALA:HB2	2:B:255:ALA:HB2	1.98	0.45
1:C:574:VAL:O	1:C:575:LYS:HB2	2.16	0.45
2:D:426:LEU:HD11	2:D:432:ALA:HB2	1.99	0.45
1:A:504:ASP:O	1:A:508:VAL:HG23	2.16	0.45
1:C:215:GLN:HB2	1:C:216:PRO:HD3	1.98	0.45
2:D:170:TYR:HA	2:D:208:GLN:NE2	2.32	0.45
2:D:257:ALA:HB1	2:D:423:VAL:HG11	1.99	0.45
1:C:251:THR:HG23	1:C:449:ALA:HB1	1.99	0.45
1:A:63:THR:HB	5:A:808:HOH:O	2.17	0.44
2:D:538:ALA:HB2	2:D:627:LEU:HD13	1.98	0.44
2:D:238:ALA:HB2	2:D:255:ALA:HB2	2.00	0.44
2:B:369:LEU:HB2	2:B:477:LYS:HB2	1.98	0.44
4:A:800:B12:O39	4:A:800:B12:H8	2.18	0.44
2:B:107:TRP:HH2	2:B:392:ILE:HD11	1.83	0.44
1:A:188:LYS:HB3	1:A:189:PRO:HD2	2.00	0.44
2:B:290:GLN:HE21	2:B:345:ILE:HD11	1.83	0.43
2:D:267:VAL:HA	2:D:271:PHE:O	2.19	0.43
1:A:336:LEU:HD11	1:A:366:ASN:HB3	2.00	0.43
1:A:480:VAL:HG21	1:A:689:PRO:HB3	1.99	0.43
2:B:170:TYR:HA	2:B:208:GLN:NE2	2.33	0.43
2:B:518:LEU:HD11	2:B:581:VAL:HG11	2.00	0.43
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.53	0.43
1:A:394:SER:O	2:B:289:ASP:HA	2.18	0.43
2:B:92:PRO:O	2:B:93:PHE:HB2	2.18	0.43
1:C:474:HIS:O	1:C:475:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:LEU:HD23	2:D:408:LEU:HD21	2.00	0.43
2:B:281:ASN:HD22	2:B:323:ASN:ND2	2.00	0.43
2:B:80:ASP:HB3	2:B:407:SER:HB2	1.99	0.43
2:B:592:ALA:HB2	2:B:633:ILE:HD13	2.01	0.43
2:B:73:VAL:HB	2:B:74:PRO:HD2	2.00	0.43
1:C:586:LEU:HB3	1:C:719:VAL:HG11	2.00	0.43
2:D:568:CYS:O	2:D:569:SER:HB2	2.18	0.43
1:A:706:THR:HB	1:A:707:PRO:HD2	2.01	0.43
1:C:214:PRO:HG2	1:C:438:GLU:HG3	2.01	0.42
4:C:800:B12:H251	4:C:800:B12:H312	2.01	0.42
2:D:133:VAL:HG23	2:D:380:ARG:HD3	2.00	0.42
1:A:399:VAL:O	1:A:402:PRO:HD3	2.19	0.42
2:B:176:ALA:O	2:B:180:VAL:HG22	2.19	0.42
2:B:202:ILE:HG13	2:B:214:LEU:HD11	2.01	0.42
1:C:25:PHE:HB2	2:D:87:TYR:HB3	2.00	0.42
2:B:538:ALA:HB2	2:B:627:LEU:HD13	2.02	0.42
1:C:22:ALA:O	1:C:26:GLU:HG3	2.19	0.42
4:A:800:B12:C2B	4:A:800:B12:O7R	2.67	0.42
3:A:801:COA:H8A	3:A:801:COA:O4A	2.18	0.42
1:C:441:ILE:N	1:C:442:PRO:HD2	2.35	0.42
4:C:800:B12:O39	4:C:800:B12:H8	2.19	0.42
1:A:4:LEU:HD13	2:B:264:ARG:HG2	2.01	0.42
1:A:472:LEU:HD21	2:B:377:ARG:NE	2.34	0.42
1:C:159:ASP:HB3	1:C:187:VAL:HG13	2.01	0.42
2:D:331:LEU:HD13	2:D:365:GLN:HB3	2.02	0.42
1:A:313:HIS:HB2	1:A:323:MET:SD	2.59	0.42
2:D:118:GLU:HG3	2:D:152:GLU:HG2	2.01	0.42
2:D:564:VAL:HG13	2:D:592:ALA:HB3	2.02	0.41
1:C:200:ILE:HG12	1:C:217:SER:HB3	2.02	0.41
1:A:256:MET:HE2	1:A:420:ALA:HB3	2.02	0.41
1:C:652:VAL:HG11	1:C:668:LEU:HD21	2.03	0.41
2:B:200:ASP:N	2:B:201:PRO:HD3	2.36	0.41
2:D:103:ASP:HB3	2:D:105:ASP:OD1	2.20	0.41
2:D:517:CYS:HB2	2:D:545:VAL:O	2.20	0.41
1:A:665:VAL:N	1:A:666:PRO:HD2	2.36	0.41
1:C:249:GLY:HA3	1:C:450:ALA:HB2	2.02	0.41
2:D:390:VAL:HG12	2:D:392:ILE:HG23	2.02	0.41
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.99	0.41
2:D:386:LEU:HD23	2:D:390:VAL:HG21	2.02	0.41
4:A:800:B12:H482	4:A:800:B12:H533	2.03	0.41
2:B:252:LEU:HD12	2:B:300:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HD21	2:D:267:VAL:HG11	2.02	0.41
1:A:171:VAL:HG11	1:A:198:ASN:ND2	2.36	0.41
2:B:554:VAL:HG21	2:B:584:ALA:HB1	2.03	0.41
4:C:800:B12:H312	4:C:800:B12:C25	2.51	0.41
1:C:459:SER:HA	1:C:577:THR:HG21	2.02	0.40
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.50	0.40
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.56	0.40
2:D:554:VAL:HG21	2:D:584:ALA:HB1	2.01	0.40
1:C:586:LEU:HD12	1:C:716:ILE:HG23	2.04	0.40
1:A:684:VAL:HG11	1:A:696:LEU:HD13	2.01	0.40
2:B:507:VAL:HB	2:B:636:VAL:HG13	2.02	0.40
2:B:537:ILE:HD13	2:B:623:VAL:HG21	2.02	0.40
1:C:28:LEU:HB3	2:D:99:VAL:HG21	2.03	0.40
1:A:550:ASP:O	1:A:554:LYS:HG2	2.21	0.40
2:B:102:GLY:O	2:B:394:ARG:HD3	2.22	0.40
1:A:652:VAL:HG11	1:A:668:LEU:HD21	2.03	0.40
2:D:190:ALA:O	2:D:227:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	723/727 (99%)	682 (94%)	36 (5%)	5 (1%)	22	39
1	C	723/727 (99%)	688 (95%)	33 (5%)	2 (0%)	41	61
2	B	615/637 (96%)	569 (92%)	43 (7%)	3 (0%)	29	48
2	D	615/637 (96%)	576 (94%)	38 (6%)	1 (0%)	47	68
All	All	2676/2728 (98%)	2515 (94%)	150 (6%)	11 (0%)	34	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	SER
1	A	10	VAL
1	A	486	SER
1	A	542	MET
1	A	575	LYS
2	B	569	SER
1	C	475	GLU
2	D	508	SER
1	A	475	GLU
2	B	508	SER
2	B	603	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/590 (97%)	541 (95%)	30 (5%)	22	43
1	C	571/590 (97%)	544 (95%)	27 (5%)	26	49
2	B	457/509 (90%)	438 (96%)	19 (4%)	30	54
2	D	457/509 (90%)	427 (93%)	30 (7%)	16	32
All	All	2056/2198 (94%)	1950 (95%)	106 (5%)	23	44

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	PHE
1	A	119	LEU
1	A	131	ARG
1	A	150	ARG
1	A	161	MET
1	A	198	ASN
1	A	234	LYS
1	A	239	SER
1	A	265	ASP
1	A	276	ASN
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	283	ARG
1	A	325	LEU
1	A	326	ARG
1	A	335	SER
1	A	365	THR
1	A	370	GLU
1	A	381	ARG
1	A	406	SER
1	A	482	LYS
1	A	483	VAL
1	A	485	ASN
1	A	498	LYS
1	A	503	ARG
1	A	533	LYS
1	A	562	GLN
1	A	564	ARG
1	A	574	VAL
1	A	602	LEU
1	A	725	SER
2	B	141	ASP
2	B	150	LEU
2	B	163	LYS
2	B	199	LEU
2	B	226	LYS
2	B	228	SER
2	B	230	ASP
2	B	279	THR
2	B	285	THR
2	B	288	HIS
2	B	300	LEU
2	B	456	ARG
2	B	460	ILE
2	B	508	SER
2	B	521	ARG
2	B	544	GLN
2	B	560	SER
2	B	612	LEU
2	B	617	LEU
1	C	9	SER
1	C	92	PHE
1	C	119	LEU
1	C	149	MET

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Mol	Chain	Res	Type
1	C	171	VAL
1	C	202	LYS
1	C	234	LYS
1	C	239	SER
1	C	241	SER
1	C	265	ASP
1	C	276	ASN
1	C	279	GLN
1	C	283	ARG
1	C	325	LEU
1	C	370	GLU
1	C	381	ARG
1	C	482	LYS
1	C	483	VAL
1	C	485	ASN
1	C	533	LYS
1	C	562	GLN
1	C	574	VAL
1	C	594	GLU
1	C	597	ARG
1	C	599	ARG
1	C	602	LEU
1	C	629	ASP
2	D	57	GLU
2	D	67	VAL
2	D	104	MET
2	D	140	VAL
2	D	141	ASP
2	D	150	LEU
2	D	163	LYS
2	D	199	LEU
2	D	211	GLU
2	D	223	ARG
2	D	226	LYS
2	D	228	SER
2	D	230	ASP
2	D	288	HIS
2	D	297	LEU
2	D	300	LEU
2	D	335	ASP
2	D	372	ASP
2	D	433	VAL

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Mol	Chain	Res	Type
2	D	451	LYS
2	D	460	ILE
2	D	464	SER
2	D	468	MET
2	D	508	SER
2	D	521	ARG
2	D	524	PHE
2	D	564	VAL
2	D	567	LEU
2	D	569	SER
2	D	634	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	246	GLN
1	A	359	HIS
1	A	385	ASN
1	A	485	ASN
1	A	635	GLN
1	A	643	GLN
2	B	239	ASN
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	391	ASN
1	C	198	ASN
1	C	246	GLN
1	C	359	HIS
1	C	385	ASN
1	C	485	ASN
1	C	576	ASN
1	C	635	GLN
1	C	643	GLN
2	D	239	ASN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN
2	D	391	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	B12	C	800	1	80,101,101	1.34	5 (6%)	101,166,166	1.73	25 (24%)
3	COA	A	801	-	28,33,50	0.93	0	35,52,75	1.08	3 (8%)
3	COA	C	801	-	28,33,50	0.82	0	35,52,75	1.01	2 (5%)
4	B12	A	800	1	80,101,101	1.21	5 (6%)	101,166,166	1.75	22 (21%)

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	B12	C	800	1	-	1/51/223/223	0/3/11/11
3	COA	A	801	-	-	6/17/37/64	0/3/3/3
3	COA	C	801	-	-	6/17/37/64	0/3/3/3
4	B12	A	800	1	-	5/51/223/223	0/3/11/11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	800	B12	CO-N24	-6.58	1.72	1.89
4	A	800	B12	CO-N21	-5.32	1.76	1.89
4	C	800	B12	CO-N23	-4.05	1.74	1.94
4	A	800	B12	O6R-C1R	-3.27	1.36	1.41
4	C	800	B12	CO-N21	-3.23	1.81	1.89
4	A	800	B12	C11-C10	-2.79	1.36	1.40
4	C	800	B12	C11-C10	-2.69	1.36	1.40
4	A	800	B12	C54-C17	2.40	1.59	1.55
4	C	800	B12	C54-C17	2.31	1.59	1.55
4	A	800	B12	C2-C3	-2.15	1.54	1.58

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	B12	C16-C15-C14	-4.91	116.61	124.27
4	C	800	B12	C2-C1-C19	-4.39	111.68	118.60
4	A	800	B12	C7B-C8B-C9B	4.38	124.87	120.54
4	C	800	B12	C55-C17-C16	4.22	123.97	109.92
4	A	800	B12	C6-C5-C4	-4.08	117.91	124.27
4	A	800	B12	O58-C57-C56	-3.88	114.92	122.02
4	A	800	B12	C2-C1-C19	-3.60	112.92	118.60
4	A	800	B12	C55-C17-C18	3.57	118.04	111.14
4	C	800	B12	C25-C2-C1	3.54	119.06	113.80
4	C	800	B12	O28-C27-N29	-3.53	112.85	122.50
4	C	800	B12	C20-C1-C2	3.52	119.14	113.32
4	C	800	B12	C2-C3-C4	3.51	105.35	101.67
4	C	800	B12	C16-C15-C14	-3.51	118.80	124.27
4	C	800	B12	C1-C19-C18	-3.48	116.16	121.93
4	A	800	B12	C36-C7-C37	3.45	116.71	110.83
4	C	800	B12	C7B-C8B-C9B	3.37	123.88	120.54
4	A	800	B12	C2P-C1P-N59	-3.22	108.19	112.93
4	A	800	B12	O28-C27-N29	-3.22	113.72	122.50
4	C	800	B12	C48-C13-C12	-3.18	107.75	116.59
4	A	800	B12	C26-C2-C3	-3.13	101.72	107.47
4	A	800	B12	O51-C50-C49	-3.09	111.98	121.07
4	A	800	B12	C4B-C9B-C8B	-3.09	117.94	121.10
4	A	800	B12	C3-C4-C5	-3.08	120.50	131.68
4	A	800	B12	C13-C14-C15	-3.06	120.58	131.68
4	C	800	B12	C13-C14-C15	-3.03	120.68	131.68
4	C	800	B12	C1P-N59-C57	-3.01	116.14	122.69
3	A	801	COA	O4B-C1B-C2B	-2.92	102.66	106.93
4	C	800	B12	C6-C5-C4	-2.86	119.81	124.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	COA	C5A-C6A-N6A	2.84	124.67	120.35
3	A	801	COA	C5A-C6A-N6A	2.72	124.49	120.35
4	A	800	B12	C49-C50-N52	2.65	124.77	116.51
4	C	800	B12	C1-C2-C3	-2.65	98.26	101.59
4	C	800	B12	C8-C9-N22	2.58	114.35	111.12
4	C	800	B12	C19-C1-N21	-2.56	99.54	102.16
4	C	800	B12	C9-C10-C11	-2.55	122.01	130.91
4	C	800	B12	C30-C3-C2	-2.54	113.75	119.13
4	C	800	B12	C12-C11-C10	-2.41	120.56	124.64
3	C	801	COA	O5A-P2A-O4A	2.38	120.00	110.68
4	C	800	B12	C4B-C9B-C8B	-2.37	118.67	121.10
3	A	801	COA	O5A-P2A-O4A	2.30	119.69	110.68
4	A	800	B12	C3P-C2P-C1P	2.23	115.72	111.39
4	C	800	B12	C36-C7-C37	2.22	114.62	110.83
4	A	800	B12	C55-C56-C57	-2.21	106.41	111.23
4	A	800	B12	C26-C27-N29	2.21	123.52	116.52
4	A	800	B12	C41-C8-C7	-2.18	108.19	114.08
4	C	800	B12	C3-C4-C5	-2.14	123.93	131.68
4	A	800	B12	C48-C49-C50	-2.14	105.34	112.59
4	C	800	B12	C30-C31-C32	-2.14	105.35	112.59
4	C	800	B12	O44-C43-N45	-2.12	116.70	122.50
4	A	800	B12	C55-C17-C16	2.08	116.84	109.92
4	C	800	B12	O34-C32-C31	-2.07	114.99	121.07
4	A	800	B12	C20-C1-C2	2.00	116.63	113.32

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	B12	C16-C17-C55-C56
4	A	800	B12	C18-C17-C55-C56
3	A	801	COA	C3B-C4B-C5B-O5B
3	A	801	COA	O4B-C4B-C5B-O5B
3	C	801	COA	C3B-C4B-C5B-O5B
4	A	800	B12	C2-C3-C30-C31
3	C	801	COA	O4B-C4B-C5B-O5B
4	C	800	B12	C2P-O3-P-O2
4	A	800	B12	N59-C1P-C2P-O3
3	C	801	COA	P2A-O3A-P1A-O2A
4	A	800	B12	N59-C1P-C2P-C3P
3	A	801	COA	P2A-O3A-P1A-O2A
3	A	801	COA	C3B-O3B-P3B-O7A

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Mol	Chain	Res	Type	Atoms
3	C	801	COA	C3B-O3B-P3B-O7A
3	A	801	COA	C3B-O3B-P3B-O8A
3	C	801	COA	C3B-O3B-P3B-O8A
3	A	801	COA	P2A-O3A-P1A-O1A
3	C	801	COA	P2A-O3A-P1A-O1A

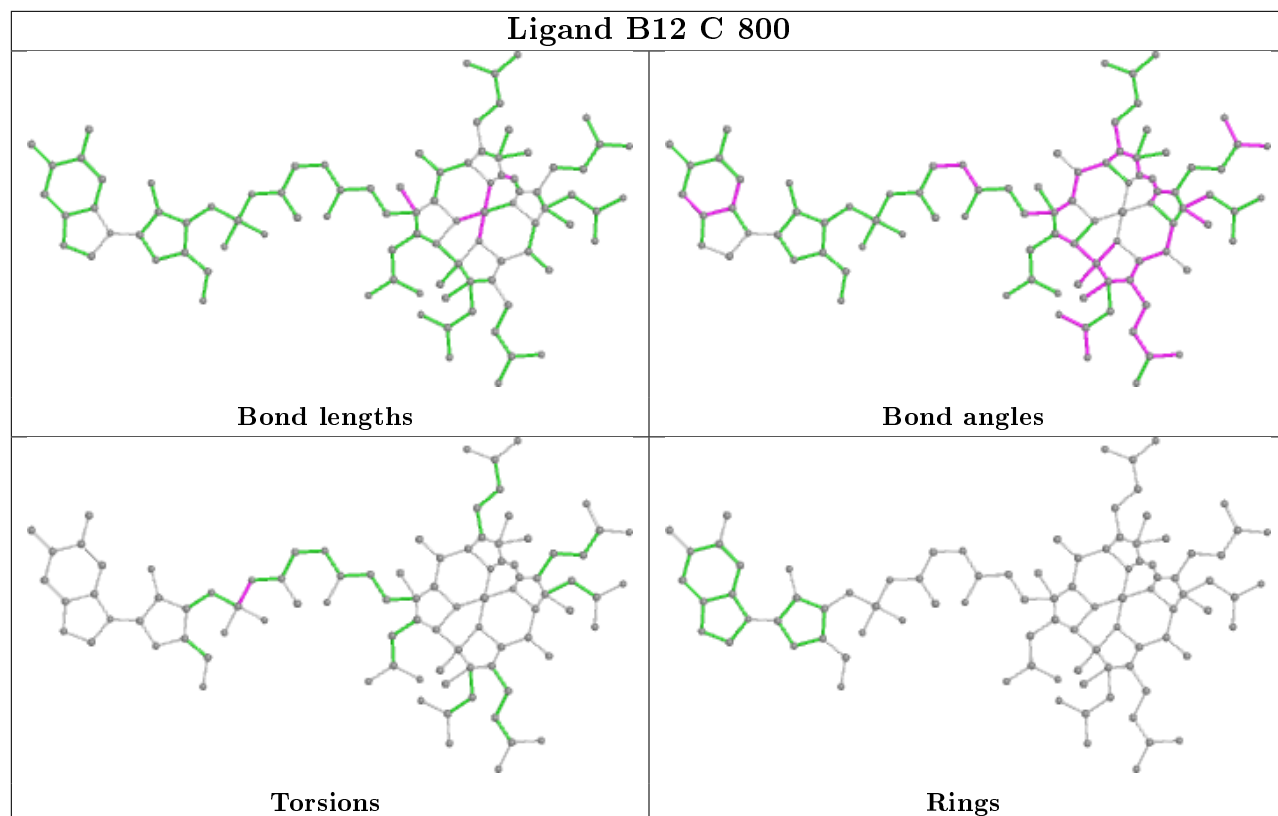
There are no ring outliers.

4 monomers are involved in 33 short contacts:

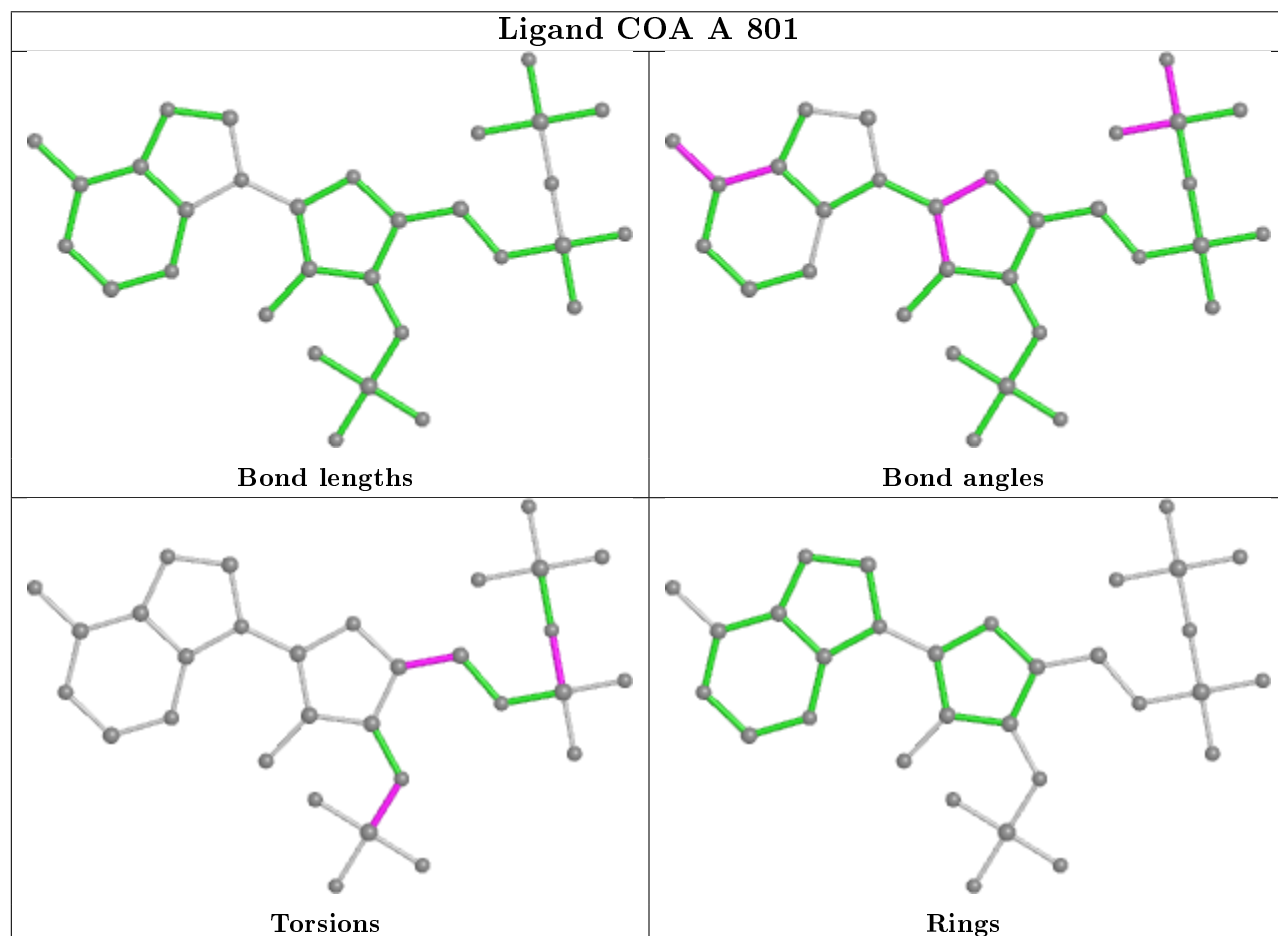
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	800	B12	12	0
3	A	801	COA	1	0
3	C	801	COA	1	0
4	A	800	B12	19	0

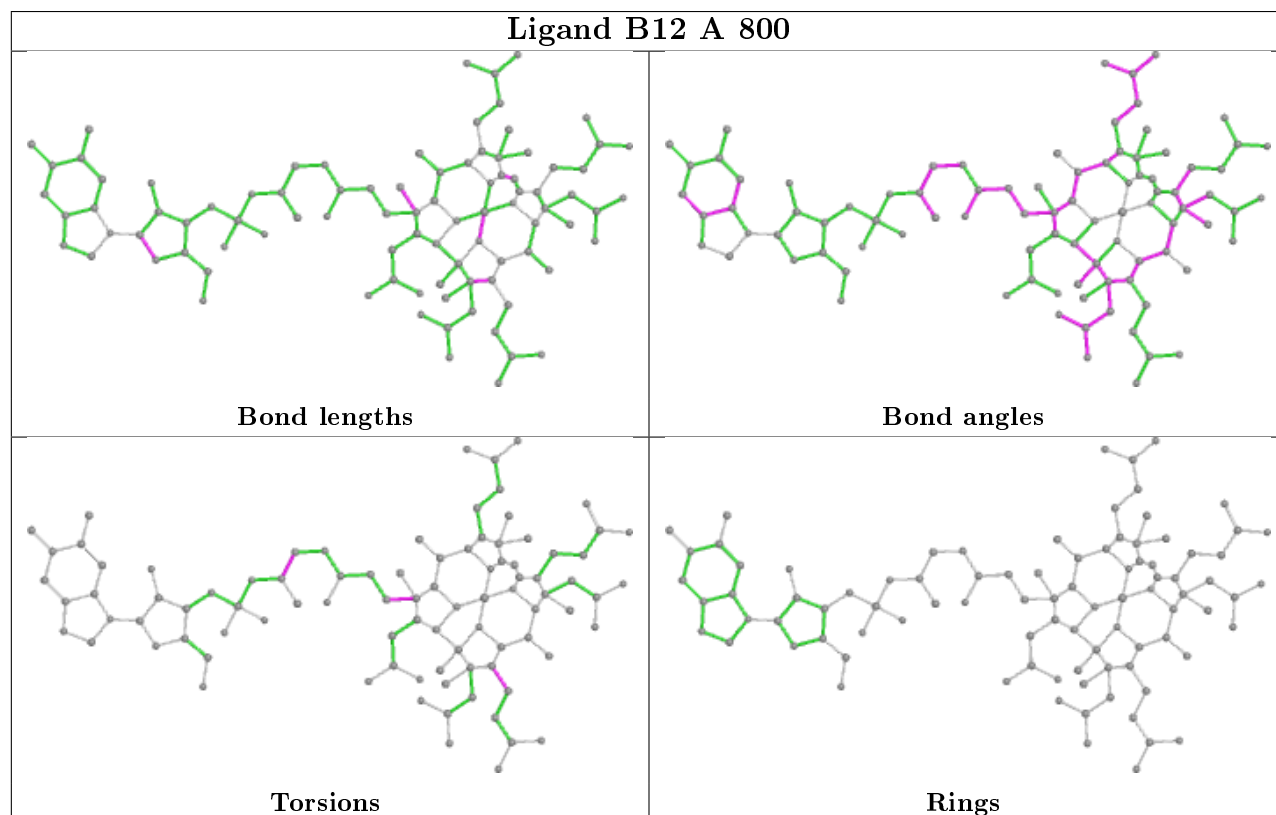
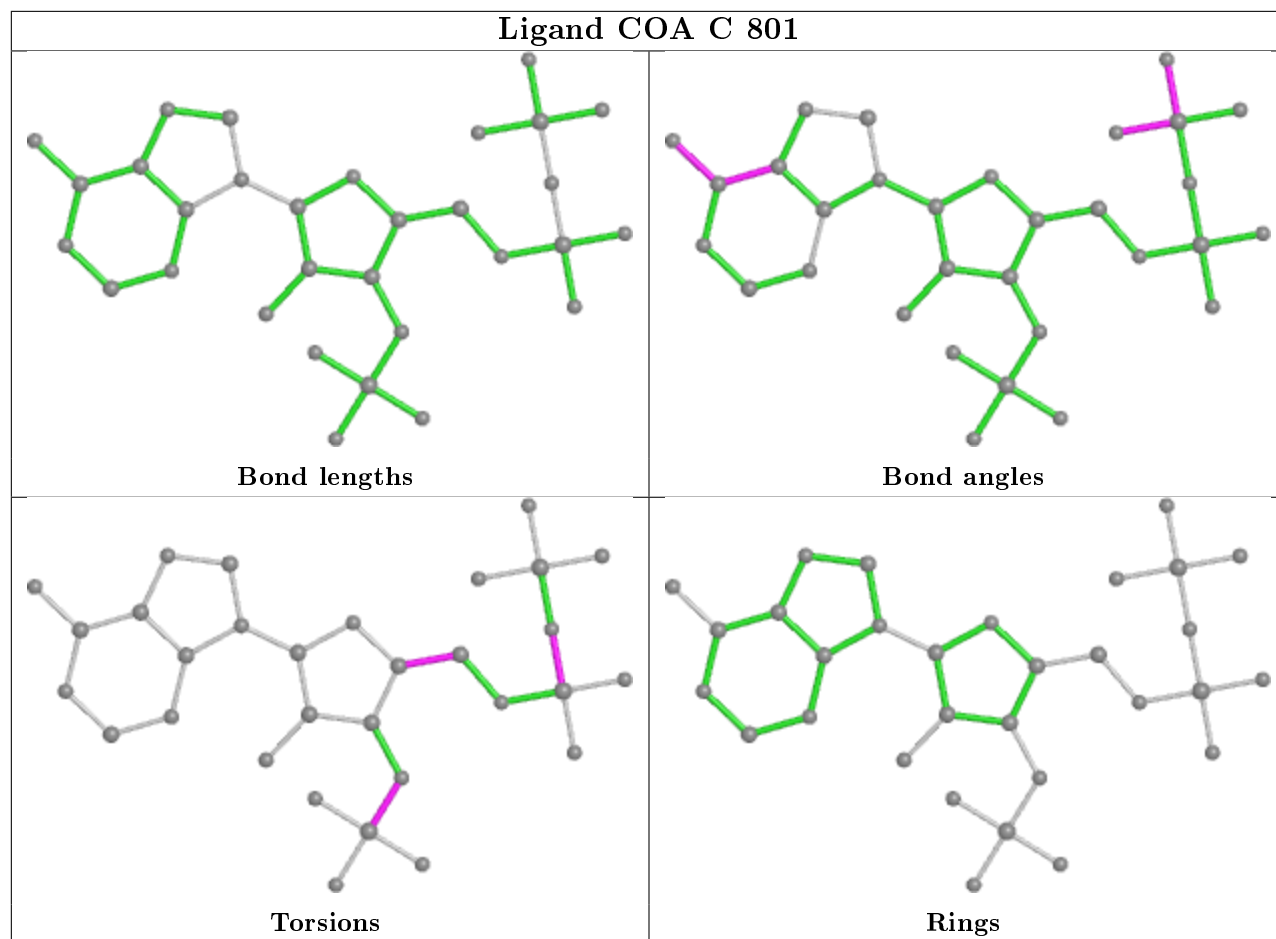
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand B12 C 800



## Ligand COA A 801





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	725/727 (99%)	0.08	30 (4%) 37 40	18, 35, 68, 125	0
1	C	725/727 (99%)	0.11	26 (3%) 42 46	14, 34, 68, 125	0
2	B	619/637 (97%)	0.58	68 (10%) 5 5	19, 51, 99, 129	0
2	D	619/637 (97%)	0.45	47 (7%) 13 14	19, 52, 99, 130	0
All	All	2688/2728 (98%)	0.29	171 (6%) 19 20	14, 42, 87, 130	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	519	GLY	6.9
2	D	568	CYS	6.3
1	C	474	HIS	5.9
1	A	92	PHE	5.9
2	B	574	TYR	5.8
2	B	520	THR	5.7
2	B	607	ALA	5.4
2	D	603	GLY	5.3
1	A	477	PRO	5.2
1	C	107	ALA	5.0
2	B	566	ASP	4.6
2	B	588	ALA	4.5
2	B	525	GLY	4.3
2	B	568	CYS	4.3
2	D	507	VAL	4.2
2	B	567	LEU	4.2
1	C	160	GLN	4.1
2	D	567	LEU	4.1
1	A	107	ALA	4.1
2	D	604	ASP	4.1
1	C	92	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	604	ASP	4.0
2	D	517	CYS	3.9
2	D	508	SER	3.8
2	B	49	PRO	3.8
1	C	479	ASP	3.7
2	D	574	TYR	3.6
2	B	603	GLY	3.6
2	D	524	PHE	3.6
1	A	474	HIS	3.6
1	C	481	LEU	3.6
2	B	619	MET	3.6
1	C	478	LEU	3.6
2	B	529	GLY	3.5
1	C	108	ALA	3.5
1	C	477	PRO	3.5
1	A	484	ASP	3.5
2	B	605	ASP	3.5
2	B	505	THR	3.5
2	B	569	SER	3.5
1	C	528	ASP	3.5
2	B	587	ALA	3.4
2	D	520	THR	3.4
2	B	565	ALA	3.4
2	B	230	ASP	3.3
2	B	491	HIS	3.3
2	D	579	LEU	3.3
1	A	476	PRO	3.3
2	D	566	ASP	3.3
1	A	501	ALA	3.2
2	B	598	ALA	3.2
2	D	576	GLN	3.2
2	B	618	PHE	3.2
2	B	105	ASP	3.1
2	B	602	PHE	3.1
1	A	109	GLY	3.1
2	B	572	LYS	3.1
1	A	505	PRO	3.1
2	D	105	ASP	3.1
2	B	570	SER	3.0
2	B	549	THR	3.0
2	B	601	GLU	3.0
2	D	594	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	627	LEU	3.0
2	B	258	THR	2.9
2	D	565	ALA	2.9
2	D	575	ALA	2.9
1	A	482	LYS	2.9
2	D	587	ALA	2.8
1	A	374	LEU	2.8
1	A	504	ASP	2.8
2	B	625	ASP	2.8
2	B	59	LEU	2.8
1	A	528	ASP	2.8
1	A	108	ALA	2.8
2	D	506	SER	2.7
2	D	211	GLU	2.7
2	D	69	GLY	2.7
2	D	215	THR	2.7
2	D	598	ALA	2.7
1	C	484	ASP	2.7
2	D	580	GLU	2.6
2	D	612	LEU	2.6
2	D	627	LEU	2.6
2	D	602	PHE	2.6
1	A	130	PRO	2.6
2	B	595	LEU	2.6
1	A	138	MET	2.6
2	B	149	HIS	2.6
2	D	571	ALA	2.5
2	D	564	VAL	2.5
2	B	518	LEU	2.5
2	D	217	LEU	2.5
2	B	606	ALA	2.5
2	D	607	ALA	2.5
2	D	578	GLY	2.5
1	C	490	ALA	2.5
1	A	460	GLY	2.5
2	B	633	ILE	2.5
1	A	565	THR	2.5
2	B	170	TYR	2.4
1	C	93	SER	2.4
2	B	506	SER	2.4
1	C	89	TYR	2.4
1	A	728	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	19	THR	2.4
2	B	507	VAL	2.4
2	B	204	PHE	2.4
2	D	516	ALA	2.4
2	D	230	ASP	2.4
2	B	562	ALA	2.4
2	B	636	VAL	2.4
2	B	541	ASP	2.4
2	B	609	ALA	2.4
2	B	555	GLU	2.4
1	C	480	VAL	2.3
2	D	484	ALA	2.3
1	C	91	GLY	2.3
1	A	479	ASP	2.3
1	C	482	LYS	2.3
2	B	180	VAL	2.3
1	A	274	GLY	2.3
1	C	576	ASN	2.3
2	B	46	GLY	2.3
2	D	559	LYS	2.3
1	C	476	PRO	2.3
1	C	14	ASN	2.3
2	B	596	SER	2.3
2	D	491	HIS	2.3
1	A	103	ARG	2.2
2	B	517	CYS	2.2
1	C	502	GLU	2.2
2	B	546	GLU	2.2
2	D	537	ILE	2.2
2	B	521	ARG	2.2
2	B	229	PRO	2.2
2	B	262	TYR	2.2
2	B	576	GLN	2.2
2	D	625	ASP	2.2
1	A	105	ASN	2.2
1	A	575	LYS	2.2
2	D	422	GLU	2.2
2	B	260	ALA	2.2
2	D	253	ALA	2.2
1	C	524	ASP	2.1
1	C	97	GLU	2.1
2	B	148	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	434	MET	2.1
2	D	443	ASP	2.1
2	B	437	HIS	2.1
2	B	560	SER	2.1
1	C	4	LEU	2.1
1	A	486	SER	2.1
1	C	727	ASP	2.1
2	B	487	GLY	2.1
2	D	18	PRO	2.1
1	A	4	LEU	2.1
2	B	471	ALA	2.1
2	D	263	VAL	2.1
2	D	148	GLU	2.1
2	B	213	ASP	2.1
1	A	481	LEU	2.1
1	C	152	LEU	2.1
2	B	138	LEU	2.1
2	B	629	SER	2.1
1	A	91	GLY	2.1
2	D	190	ALA	2.0
1	A	694	ASP	2.0
2	B	257	ALA	2.0
1	A	158	LEU	2.0
2	B	524	PHE	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](#)

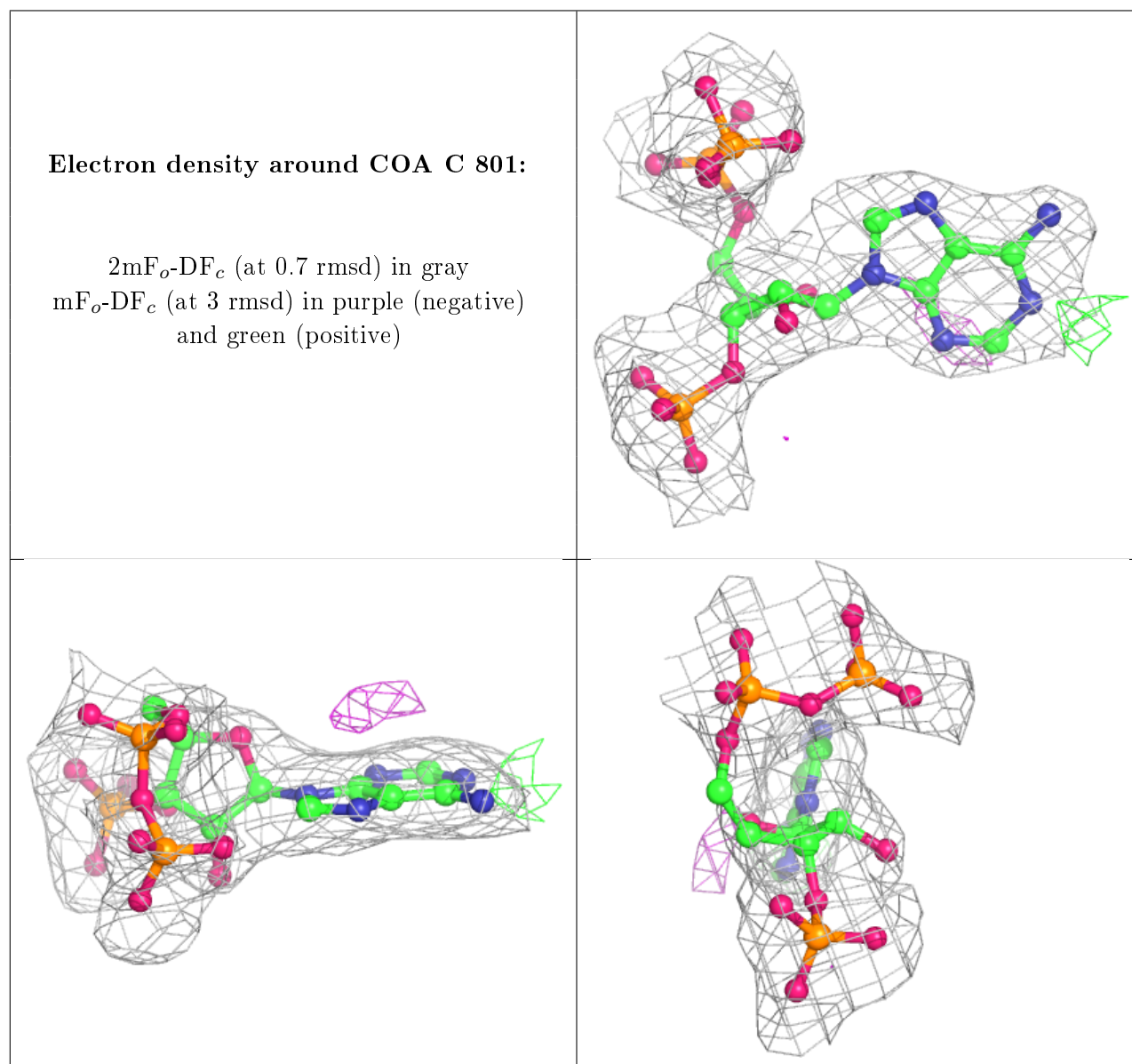
There are no carbohydrates in this entry.

## 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<sup>th</sup> 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.

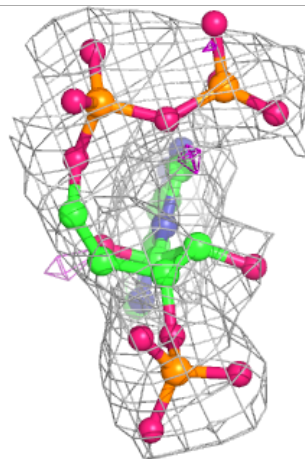
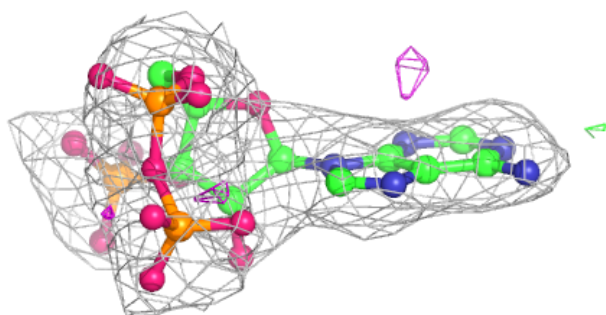
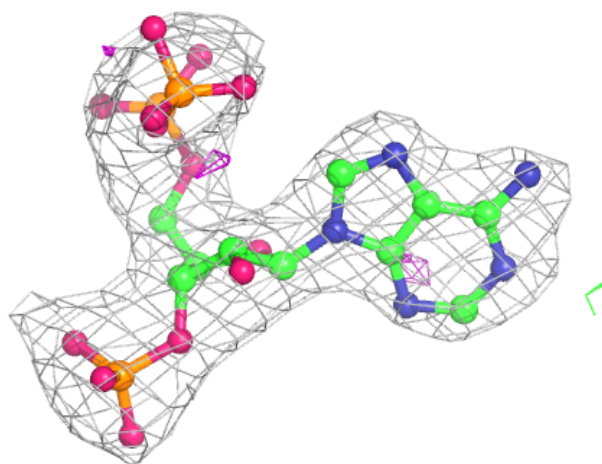
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	COA	C	801	31/48	0.83	0.22	43,77,100,101	0
3	COA	A	801	31/48	0.86	0.27	48,79,100,101	0
4	B12	A	800	91/91	0.96	0.12	14,27,39,45	0
4	B12	C	800	91/91	0.97	0.12	9,22,33,41	0

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.



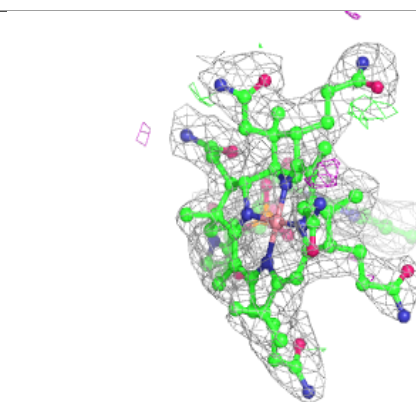
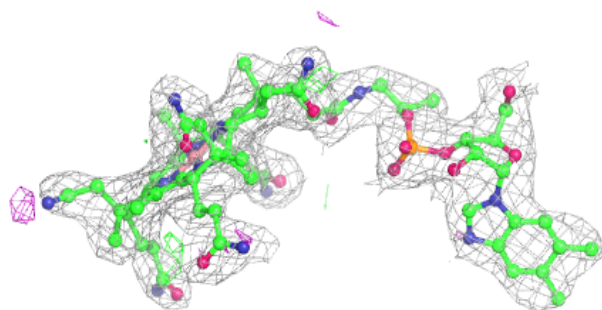
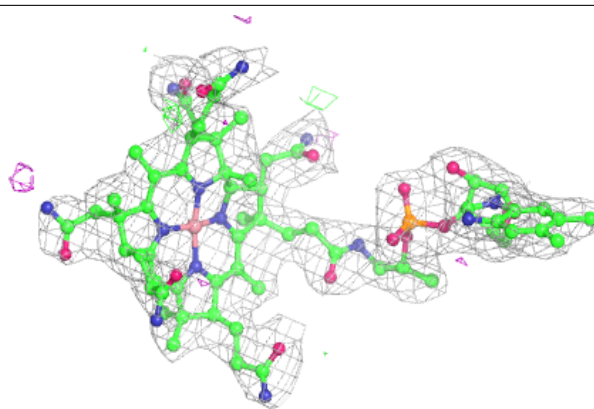
**Electron density around COA A 801:**

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

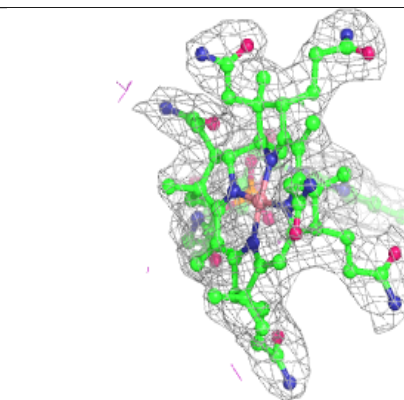
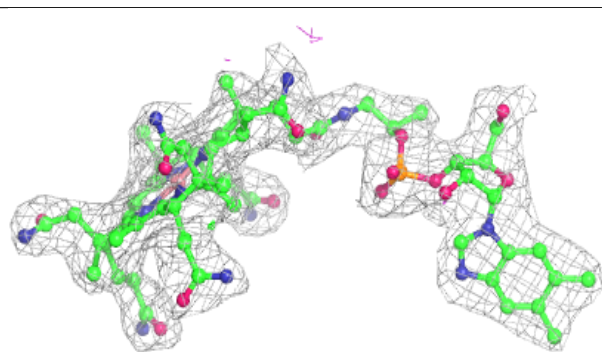
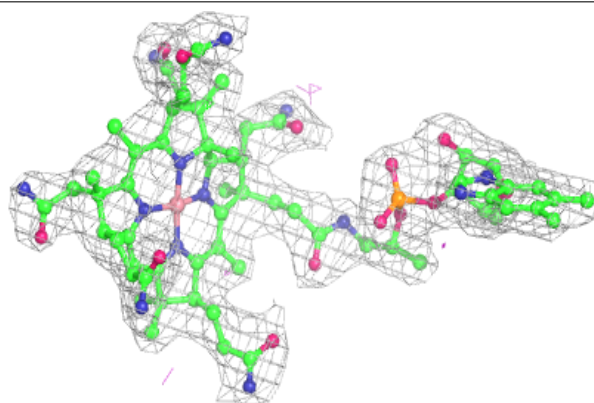


**Electron density around B12 A 800:**

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

**Electron density around B12 C 800:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.