



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:57 PM EDT

PDB ID : 1DM3  
Title : ACETYLATED BIOSYNTHETIC THIOLASE FROM ZOOGLOEA  
RAMIGERA IN COMPLEX WITH ACETYL-COA  
Authors : Modis, Y.; Wierenga, R.K.  
Deposited on : 1999-12-13  
Resolution : 2.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

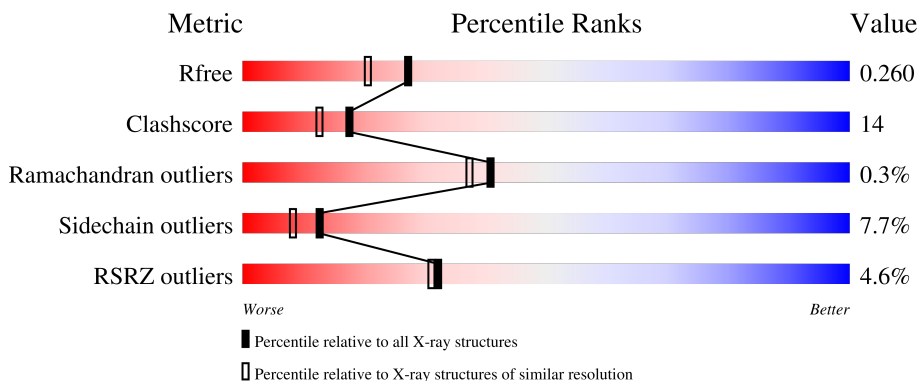
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	389	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      67%      25%      6% .</p>
1	B	389	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      69%      22%      7% .</p>
1	C	389	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">4%      72%      22%      5% .</p>
1	D	389	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">10%      67%      28%      . .</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCY	A	89	-	-	X	-
1	SCY	B	89	-	-	X	-
1	SCY	C	89	-	-	X	-
1	SCY	D	89	-	-	X	-
3	ACO	C	815	-	-	-	X
3	ACO	D	816	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12302 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 BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	2816	1748	509	538	21	0	0	0
1	B	389	2816	1748	509	538	21	0	0	0
1	C	389	2816	1748	509	538	21	0	0	0
1	D	389	2816	1748	509	538	21	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

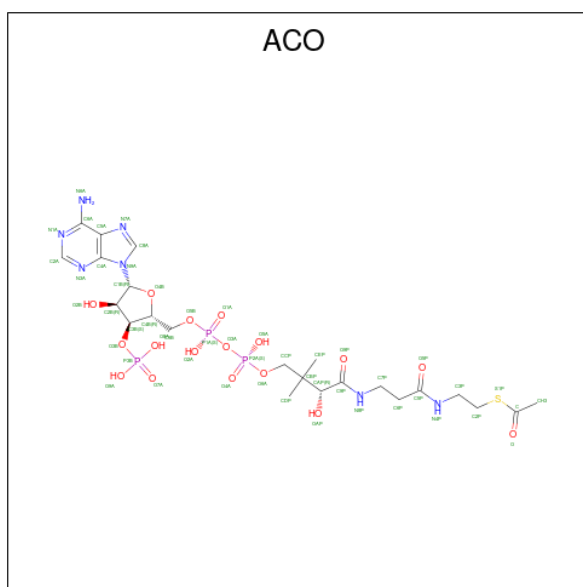
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	10	ALA	-	INSERTION	UNP P07097
D	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



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

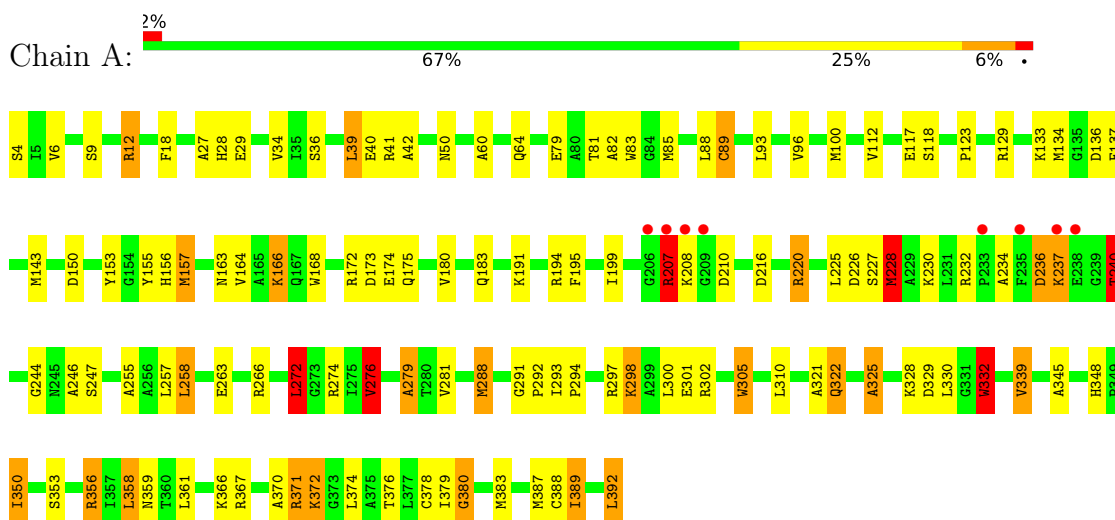
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	316	Total 316	O 316	2	0
4	B	300	Total 300	O 300	4	0
4	C	103	Total 103	O 103	1	0
4	D	85	Total 85	O 85	1	0

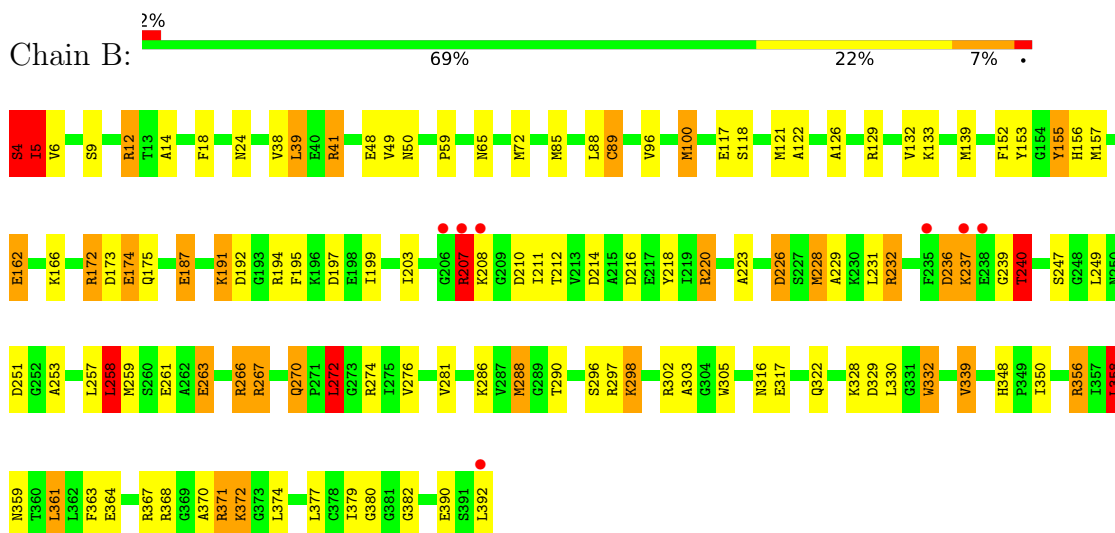
### 3 Residue-property plots

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: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89

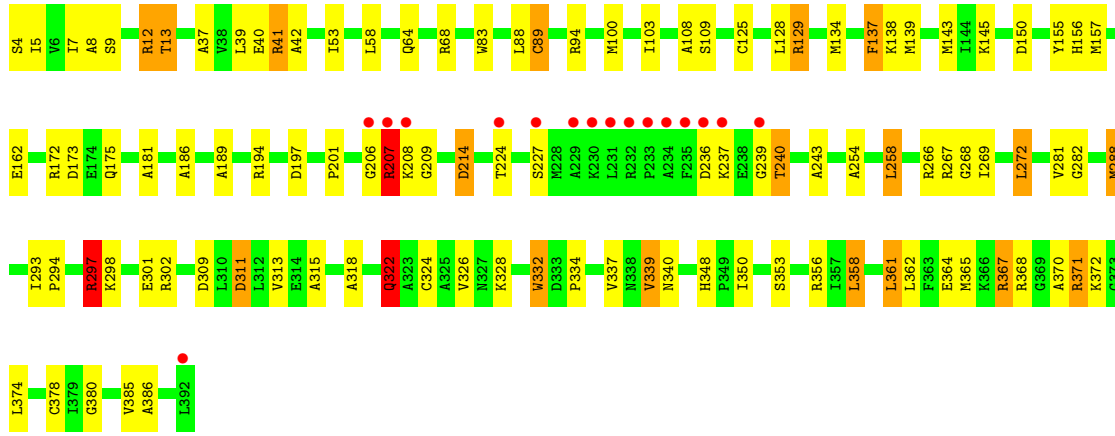


#### • Molecule 1: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89

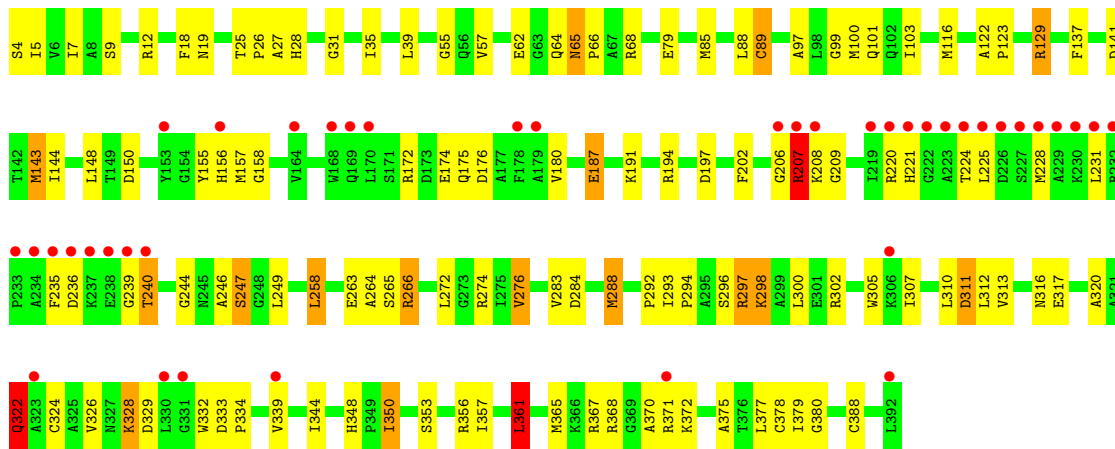


#### • Molecule 1: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89





● Molecule 1: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.38Å 78.85Å 149.73Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.82 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.00) 79.0 (49.82-1.93)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.92Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.214 , 0.256 0.223 , 0.260	Depositor DCC
$R_{free}$ test set	7058 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtrriage
Anisotropy	0.700	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, SO4, SCY

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	1.07	3/2847 (0.1%)	2.07	99/3842 (2.6%)
1	B	1.03	0/2847	2.12	107/3842 (2.8%)
1	C	0.66	0/2847	1.71	49/3842 (1.3%)
1	D	0.63	0/2847	1.56	43/3842 (1.1%)
All	All	0.87	3/11388 (0.0%)	1.88	298/15368 (1.9%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	ARG	CZ-NH2	5.30	1.40	1.33
1	A	79	GLU	CD-OE2	-5.06	1.20	1.25
1	A	79	GLU	CD-OE1	5.02	1.31	1.25

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ARG	NE-CZ-NH2	-19.89	110.36	120.30
1	C	129	ARG	NE-CZ-NH2	-18.44	111.08	120.30
1	A	228	MET	CA-CB-CG	18.43	144.63	113.30
1	B	173	ASP	CB-CG-OD2	-17.14	102.87	118.30
1	A	266	ARG	CD-NE-CZ	17.14	147.59	123.60
1	B	368	ARG	NE-CZ-NH1	-16.23	112.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	ARG	NE-CZ-NH2	-16.16	112.22	120.30
1	C	41	ARG	NE-CZ-NH2	-15.21	112.70	120.30
1	B	172	ARG	NE-CZ-NH1	-14.71	112.94	120.30
1	B	194	ARG	NE-CZ-NH2	-14.55	113.02	120.30
1	C	68	ARG	NE-CZ-NH2	-14.31	113.14	120.30
1	A	173	ASP	CB-CG-OD2	-13.92	105.77	118.30
1	D	367	ARG	NE-CZ-NH1	13.89	127.25	120.30
1	B	367	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	A	41	ARG	NE-CZ-NH1	12.87	126.73	120.30
1	B	356	ARG	NE-CZ-NH1	-12.71	113.95	120.30
1	C	129	ARG	NE-CZ-NH1	12.65	126.62	120.30
1	B	216	ASP	CB-CG-OD2	-12.47	107.08	118.30
1	B	368	ARG	NH1-CZ-NH2	12.08	132.68	119.40
1	A	356	ARG	NE-CZ-NH2	12.07	126.33	120.30
1	A	302	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	A	367	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	B	266	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	B	274	ARG	NE-CZ-NH2	11.41	126.00	120.30
1	B	302	ARG	NE-CZ-NH2	-11.25	114.68	120.30
1	A	236	ASP	CB-CG-OD1	11.17	128.35	118.30
1	B	195	PHE	CB-CG-CD2	11.13	128.59	120.80
1	C	367	ARG	NE-CZ-NH2	-11.11	114.74	120.30
1	A	274	ARG	CD-NE-CZ	10.87	138.81	123.60
1	B	216	ASP	CB-CG-OD1	10.76	127.98	118.30
1	B	267	ARG	NE-CZ-NH2	10.56	125.58	120.30
1	B	368	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	297	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	A	371	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	A	371	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	B	197	ASP	CB-CG-OD2	9.96	127.26	118.30
1	A	173	ASP	CB-CG-OD1	9.67	127.00	118.30
1	A	266	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	207	ARG	CD-NE-CZ	9.57	137.00	123.60
1	B	195	PHE	CB-CG-CD1	-9.55	114.11	120.80
1	A	339	VAL	CG1-CB-CG2	9.55	126.17	110.90
1	C	194	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	B	4	SER	CA-C-O	-9.36	100.44	120.10
1	B	153	TYR	CB-CG-CD1	-9.34	115.40	121.00
1	A	207	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	D	297	ARG	CD-NE-CZ	9.15	136.40	123.60
1	C	302	ARG	NH1-CZ-NH2	9.13	129.44	119.40
1	C	172	ARG	NE-CZ-NH2	-9.06	115.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ARG	NE-CZ-NH1	-9.03	115.78	120.30
1	C	68	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	A	172	ARG	NE-CZ-NH1	-8.99	115.81	120.30
1	D	12	ARG	CD-NE-CZ	8.99	136.18	123.60
1	D	207	ARG	CD-NE-CZ	8.86	136.01	123.60
1	C	41	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	C	12	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	B	220	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	B	363	PHE	CB-CG-CD2	-8.81	114.63	120.80
1	D	172	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	339	VAL	N-CA-CB	-8.63	92.51	111.50
1	A	228	MET	CG-SD-CE	-8.53	86.56	100.20
1	D	367	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	D	297	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	C	364	GLU	OE1-CD-OE2	-8.40	113.22	123.30
1	B	41	ARG	CD-NE-CZ	8.39	135.35	123.60
1	C	94	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	187	GLU	CG-CD-OE1	-8.35	101.61	118.30
1	B	358	LEU	CA-CB-CG	8.30	134.40	115.30
1	C	207	ARG	CD-NE-CZ	8.26	135.17	123.60
1	B	187	GLU	OE1-CD-OE2	8.19	133.13	123.30
1	A	12	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	371	ARG	CD-NE-CZ	8.12	134.96	123.60
1	B	100	MET	CG-SD-CE	-8.12	87.21	100.20
1	B	339	VAL	N-CA-CB	-8.08	93.72	111.50
1	B	356	ARG	CD-NE-CZ	8.03	134.84	123.60
1	D	313	VAL	CA-CB-CG2	7.81	122.62	110.90
1	D	172	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	C	367	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	251	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	B	370	ALA	N-CA-CB	7.66	120.82	110.10
1	A	194	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	207	ARG	CD-NE-CZ	7.51	134.12	123.60
1	B	274	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	172	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	172	ARG	NH1-CZ-NH2	7.47	127.61	119.40
1	A	226	ASP	CB-CG-OD2	7.42	124.98	118.30
1	A	129	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	D	322	GLN	CA-CB-CG	7.35	129.58	113.40
1	A	42	ALA	N-CA-CB	-7.32	99.85	110.10
1	A	150	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	D	247	SER	N-CA-CB	7.25	121.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	356	ARG	CA-CB-CG	7.23	129.30	113.40
1	A	220	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	317	GLU	OE1-CD-OE2	7.18	131.92	123.30
1	B	122	ALA	N-CA-CB	-7.17	100.07	110.10
1	D	274	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	C	348	HIS	N-CA-CB	-7.13	97.77	110.60
1	B	218	TYR	CB-CG-CD1	7.12	125.28	121.00
1	B	356	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	216	ASP	CB-CG-OD1	7.12	124.71	118.30
1	D	367	ARG	CD-NE-CZ	7.12	133.57	123.60
1	B	162	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	258	LEU	CB-CG-CD2	7.07	123.01	111.00
1	A	240	THR	N-CA-CB	-7.06	96.89	110.30
1	B	220	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	B	236	ASP	CB-CG-OD1	6.96	124.57	118.30
1	B	329	ASP	O-C-N	-6.90	111.66	122.70
1	A	325	ALA	CB-CA-C	-6.90	99.75	110.10
1	A	195	PHE	CB-CG-CD1	6.87	125.61	120.80
1	A	359	ASN	OD1-CG-ND2	6.84	137.64	121.90
1	A	266	ARG	CG-CD-NE	-6.83	97.45	111.80
1	B	214	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	129	ARG	CG-CD-NE	-6.78	97.56	111.80
1	C	267	ARG	CD-NE-CZ	6.73	133.03	123.60
1	C	339	VAL	CA-CB-CG1	6.70	120.96	110.90
1	C	139	MET	N-CA-CB	6.68	122.62	110.60
1	A	117	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	B	276	VAL	CA-CB-CG2	6.62	120.83	110.90
1	A	39	LEU	CB-CG-CD1	6.62	122.25	111.00
1	A	29	GLU	OE1-CD-OE2	-6.60	115.38	123.30
1	B	14	ALA	CB-CA-C	-6.58	100.23	110.10
1	D	356	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	305	TRP	CE3-CZ3-CH2	6.55	128.41	121.20
1	A	27	ALA	N-CA-CB	-6.49	101.01	110.10
1	B	126	ALA	N-CA-CB	6.49	119.19	110.10
1	C	4	SER	N-CA-CB	6.49	120.23	110.50
1	A	6	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	A	12	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
1	A	367	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	322	GLN	CA-CB-CG	6.43	127.56	113.40
1	D	12	ARG	CG-CD-NE	6.43	125.31	111.80
1	A	81	THR	CA-CB-CG2	-6.42	103.42	112.40
1	B	302	ARG	NH1-CZ-NH2	6.42	126.46	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	TYR	CB-CG-CD1	-6.41	117.15	121.00
1	A	157	MET	CG-SD-CE	6.39	110.43	100.20
1	C	13	THR	O-C-N	-6.38	112.48	122.70
1	C	368	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	D	329	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	153	TYR	CB-CG-CD2	6.20	124.72	121.00
1	D	141	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	231	LEU	CB-CG-CD2	-6.17	100.51	111.00
1	B	272	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	234	ALA	N-CA-CB	-6.16	101.47	110.10
1	A	279	ALA	N-CA-CB	6.15	118.72	110.10
1	B	303	ALA	CB-CA-C	-6.15	100.87	110.10
1	B	290	THR	CA-CB-CG2	-6.15	103.79	112.40
1	A	164	VAL	CG1-CB-CG2	-6.14	101.07	110.90
1	C	315	ALA	CB-CA-C	6.13	119.29	110.10
1	B	65	ASN	N-CA-CB	-6.12	99.58	110.60
1	A	100	MET	O-C-N	-6.11	112.93	122.70
1	A	60	ALA	CA-C-O	6.09	132.89	120.10
1	D	202	PHE	CB-CG-CD1	-6.09	116.54	120.80
1	C	301	GLU	OE1-CD-OE2	-6.08	116.01	123.30
1	A	272	LEU	CB-CG-CD1	6.05	121.28	111.00
1	D	356	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	12	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	152	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	B	228	MET	CA-CB-CG	5.99	123.48	113.30
1	B	72	MET	CG-SD-CE	-5.98	90.64	100.20
1	D	231	LEU	CB-CG-CD1	-5.98	100.84	111.00
1	A	64	GLN	O-C-N	5.97	132.25	122.70
1	D	79	GLU	CB-CG-CD	5.96	130.30	114.20
1	D	284	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	189	ALA	N-CA-CB	-5.95	101.77	110.10
1	A	359	ASN	CB-CG-OD1	-5.95	109.71	121.60
1	A	370	ALA	N-CA-CB	5.94	118.42	110.10
1	C	311	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	B	210	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	150	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	266	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	137	PHE	N-CA-CB	5.90	121.22	110.60
1	A	79	GLU	CG-CD-OE2	5.89	130.09	118.30
1	A	240	THR	CA-CB-CG2	5.89	120.65	112.40
1	A	118	SER	N-CA-CB	5.89	119.33	110.50
1	A	82	ALA	CB-CA-C	-5.88	101.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	181	ALA	N-CA-CB	5.88	118.33	110.10
1	B	223	ALA	N-CA-CB	-5.88	101.87	110.10
1	B	218	TYR	CG-CD2-CE2	5.84	125.97	121.30
1	B	174	GLU	OE1-CD-OE2	-5.84	116.30	123.30
1	A	4	SER	N-CA-CB	5.81	119.22	110.50
1	C	173	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	94	ARG	CD-NE-CZ	5.80	131.73	123.60
1	B	270	GLN	CB-CG-CD	5.79	126.65	111.60
1	B	261	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	B	194	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	28	HIS	N-CA-CB	5.75	120.94	110.60
1	A	210	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	363	PHE	CB-CG-CD1	5.73	124.81	120.80
1	B	367	ARG	CG-CD-NE	-5.73	99.77	111.80
1	D	129	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	6	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	D	313	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	A	367	ARG	CA-CB-CG	5.68	125.90	113.40
1	C	297	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	371	ARG	CD-NE-CZ	5.67	131.53	123.60
1	B	364	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	B	173	ASP	OD1-CG-OD2	5.64	134.02	123.30
1	B	267	ARG	CD-NE-CZ	-5.64	115.70	123.60
1	D	197	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	214	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	12	ARG	CD-NE-CZ	5.61	131.46	123.60
1	B	339	VAL	CG1-CB-CG2	5.60	119.86	110.90
1	C	318	ALA	N-CA-CB	-5.58	102.29	110.10
1	D	264	ALA	N-CA-CB	5.57	117.90	110.10
1	B	236	ASP	OD1-CG-OD2	-5.56	112.73	123.30
1	A	4	SER	CA-C-O	-5.54	108.47	120.10
1	D	68	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	332	TRP	CA-C-O	5.53	131.72	120.10
1	A	166	LYS	CA-C-O	5.53	131.72	120.10
1	B	361	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	230	LYS	N-CA-CB	-5.50	100.70	110.60
1	D	225	LEU	CD1-CG-CD2	-5.50	94.01	110.50
1	B	358	LEU	CB-CG-CD1	5.50	120.34	111.00
1	C	297	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	49	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	B	218	TYR	CZ-CE2-CD2	-5.49	114.86	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	VAL	CB-CA-C	5.49	121.82	111.40
1	B	39	LEU	CA-C-O	5.47	131.59	120.10
1	C	356	ARG	CA-CB-CG	5.47	125.44	113.40
1	A	39	LEU	N-CA-CB	-5.46	99.47	110.40
1	C	4	SER	CA-C-O	-5.46	108.63	120.10
1	A	246	ALA	CB-CA-C	-5.46	101.91	110.10
1	A	18	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	B	39	LEU	CB-CG-CD1	5.45	120.26	111.00
1	A	227	SER	O-C-N	-5.44	113.99	122.70
1	A	380	GLY	C-N-CA	-5.43	110.89	122.30
1	A	276	VAL	CG1-CB-CG2	5.43	119.58	110.90
1	B	4	SER	CA-C-N	5.42	129.13	117.20
1	C	266	ARG	CB-CA-C	-5.41	99.59	110.40
1	D	266	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	133	LYS	CD-CE-NZ	5.39	124.10	111.70
1	D	225	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	367	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	192	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	321	ALA	O-C-N	-5.37	114.11	122.70
1	A	60	ALA	O-C-N	-5.36	114.08	123.20
1	C	94	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	283	VAL	CA-CB-CG1	5.36	118.93	110.90
1	A	372	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	A	389	ILE	CA-CB-CG1	5.34	121.14	111.00
1	A	100	MET	CG-SD-CE	-5.33	91.67	100.20
1	D	129	ARG	CG-CD-NE	-5.33	100.60	111.80
1	D	137	PHE	N-CA-CB	5.33	120.20	110.60
1	B	359	ASN	O-C-N	-5.32	114.19	122.70
1	A	236	ASP	OD1-CG-OD2	-5.30	113.22	123.30
1	B	118	SER	N-CA-CB	5.30	118.44	110.50
1	B	367	ARG	O-C-N	-5.29	114.23	122.70
1	D	246	ALA	N-CA-CB	5.29	117.51	110.10
1	B	173	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	267	ARG	CB-CA-C	-5.28	99.84	110.40
1	A	137	PHE	N-CA-CB	5.28	120.10	110.60
1	A	36	SER	N-CA-CB	-5.27	102.59	110.50
1	B	281	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	A	136	ASP	CB-CG-OD1	5.26	123.04	118.30
1	D	143	MET	CA-CB-CG	5.26	122.25	113.30
1	A	392	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	372	LYS	CD-CE-NZ	-5.25	99.63	111.70
1	C	371	ARG	CD-NE-CZ	5.25	130.94	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	B	199	ILE	CG1-CB-CG2	-5.24	99.87	111.40
1	A	220	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	367	ARG	N-CA-CB	-5.22	101.20	110.60
1	B	382	GLY	O-C-N	-5.21	114.36	122.70
1	A	281	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	A	143	MET	CG-SD-CE	5.20	108.53	100.20
1	B	129	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	253	ALA	N-CA-CB	5.20	117.37	110.10
1	A	136	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	339	VAL	N-CA-CB	-5.15	100.17	111.50
1	A	4	SER	CA-C-N	5.15	128.52	117.20
1	C	150	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	C	138	LYS	O-C-N	-5.12	114.51	122.70
1	B	139	MET	N-CA-C	-5.12	97.18	111.00
1	B	226	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	240	THR	N-CA-CB	-5.12	100.58	110.30
1	D	311	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	117	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	B	229	ALA	CB-CA-C	-5.10	102.44	110.10
1	B	371	ARG	CG-CD-NE	5.09	122.50	111.80
1	B	329	ASP	CA-C-O	5.09	130.79	120.10
1	D	150	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	112	VAL	CA-CB-CG1	-5.09	103.27	110.90
1	A	383	MET	C-N-CA	5.08	132.97	122.30
1	B	12	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	361	LEU	CB-CA-C	-5.07	100.57	110.20
1	A	83	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	A	279	ALA	CB-CA-C	-5.06	102.50	110.10
1	B	191	LYS	O-C-N	-5.05	114.62	122.70
1	B	231	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	A	356	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	D	4	SER	CA-C-O	-5.04	109.52	120.10
1	C	4	SER	CA-C-N	5.04	128.28	117.20
1	B	5	ILE	CB-CA-C	-5.03	101.55	111.60
1	A	79	GLU	CG-CD-OE1	-5.02	108.26	118.30
1	A	134	MET	CA-CB-CG	5.01	121.82	113.30
1	C	4	SER	CA-CB-OG	5.01	124.73	111.20
1	A	383	MET	CA-C-O	5.00	130.61	120.10
1	A	93	LEU	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	GLY	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2816	0	2821	74	0
1	B	2816	0	2821	70	0
1	C	2816	0	2821	68	0
1	D	2816	0	2821	95	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	51	0	34	16	0
3	B	51	0	34	12	0
3	C	51	0	34	17	0
3	D	51	0	34	17	0
4	A	316	0	0	13	0
4	B	300	0	0	23	1
4	C	103	0	0	5	0
4	D	85	0	0	5	0
All	All	12302	0	11420	315	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 14.

All (315) 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:D:88:LEU:HB3	1:D:89:SCY:HE2	1.20	1.16
3:D:816:ACO:O5P	3:D:816:ACO:H21	1.33	1.14
1:B:288:MET:SD	3:B:814:ACO:HH33	1.89	1.13
1:B:247:SER:HB2	4:B:929:HOH:O	1.49	1.12
1:D:288:MET:SD	3:D:816:ACO:HH33	1.90	1.11
1:A:88:LEU:HB3	1:A:89:SCY:HE2	1.36	1.04
1:B:89:SCY:HE1	1:B:380:GLY:H	1.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:815:ACO:O5P	3:C:815:ACO:H21	1.54	1.02
1:A:247:SER:HB2	4:A:1038:HOH:O	1.58	1.01
1:B:4:SER:N	4:B:1091:HOH:O	1.90	1.01
1:A:288:MET:SD	3:A:813:ACO:HH33	2.01	1.00
1:C:288:MET:SD	3:C:815:ACO:HH33	2.03	0.99
1:B:258:LEU:HG	4:B:1030:HOH:O	1.63	0.97
3:A:813:ACO:O5P	3:A:813:ACO:H21	1.59	0.97
1:A:89:SCY:HE1	1:A:380:GLY:H	1.30	0.95
3:B:814:ACO:O5P	3:B:814:ACO:H21	1.67	0.95
1:A:89:SCY:OCD	3:A:813:ACO:HH32	1.67	0.92
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.33	0.92
1:D:89:SCY:OCD	3:D:816:ACO:HH32	1.70	0.92
1:D:88:LEU:HB3	1:D:89:SCY:CE	2.01	0.90
1:C:378:CYS:SG	3:C:815:ACO:HH31	2.12	0.89
1:C:89:SCY:HE2	1:C:89:SCY:H	1.35	0.89
1:A:288:MET:CE	3:A:813:ACO:HH33	2.05	0.87
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.40	0.86
1:D:143:MET:HE1	1:D:249:LEU:HD13	1.58	0.85
1:A:225:LEU:HG	4:A:1014:HOH:O	1.75	0.85
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.14	0.83
1:A:258:LEU:HG	4:A:861:HOH:O	1.79	0.82
1:C:378:CYS:SG	3:C:815:ACO:CH3	2.68	0.82
1:C:89:SCY:OCD	3:C:815:ACO:HH32	1.79	0.81
1:B:226:ASP:HB3	4:B:1105:HOH:O	1.81	0.78
1:A:288:MET:HE1	3:A:813:ACO:HH33	1.66	0.78
1:A:387:MET:SD	4:A:977:HOH:O	2.42	0.77
1:B:89:SCY:HE1	1:B:380:GLY:N	1.96	0.77
1:A:378:CYS:SG	3:A:813:ACO:HH31	2.26	0.76
3:C:815:ACO:O5P	3:C:815:ACO:C2P	2.27	0.75
1:D:326:VAL:HG22	4:D:869:HOH:O	1.86	0.74
1:A:387:MET:HE2	1:A:389:ILE:HD11	1.70	0.74
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.50	0.74
1:D:312:LEU:HD13	1:D:368:ARG:HD2	1.71	0.72
1:A:288:MET:SD	3:A:813:ACO:CH3	2.78	0.72
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.54	0.72
1:D:357:ILE:HD12	1:D:375:ALA:HB1	1.72	0.71
1:A:89:SCY:HE1	1:A:380:GLY:N	2.03	0.71
1:C:288:MET:CE	3:C:815:ACO:HH33	2.21	0.71
1:C:37:ALA:O	1:C:41:ARG:HG3	1.90	0.71
1:C:89:SCY:HE1	1:C:380:GLY:H	1.54	0.71
1:A:89:SCY:OCD	3:A:813:ACO:CH3	2.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.71	0.70
3:A:813:ACO:H143	4:A:846:HOH:O	1.92	0.70
1:D:89:SCY:OCD	1:D:380:GLY:N	2.24	0.70
1:A:156:HIS:HE1	3:A:813:ACO:H62	1.57	0.70
1:A:387:MET:CE	1:A:389:ILE:HD11	2.21	0.70
1:D:89:SCY:HE2	1:D:89:SCY:H	1.56	0.69
1:B:89:SCY:OCD	1:B:379:ILE:HA	1.93	0.69
1:B:288:MET:CE	3:B:814:ACO:HH33	2.23	0.68
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.07	0.68
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.76	0.68
1:D:300:LEU:HD21	1:D:310:LEU:HD11	1.76	0.67
1:D:378:CYS:O	3:D:816:ACO:HH31	1.93	0.67
3:D:816:ACO:O5P	3:D:816:ACO:C2P	2.17	0.67
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.08	0.67
1:A:279:ALA:CB	1:A:298:LYS:HG3	2.25	0.66
1:A:163:ASN:HA	1:A:166:LYS:HZ2	1.60	0.66
1:B:371:ARG:HG3	4:B:882:HOH:O	1.95	0.66
1:B:228:MET:HE2	4:B:829:HOH:O	1.96	0.66
1:B:89:SCY:OCD	3:B:814:ACO:HH32	1.97	0.65
3:D:816:ACO:O9P	3:D:816:ACO:H62	1.95	0.65
1:A:174:GLU:OE1	4:A:1040:HOH:O	2.15	0.65
1:B:157:MET:HG3	3:B:814:ACO:S1P	2.37	0.65
1:D:322:GLN:O	1:D:326:VAL:HG23	1.96	0.65
1:C:201:PRO:HB3	1:C:214:ASP:HB3	1.78	0.64
1:D:148:LEU:HD22	3:D:816:ACO:C5P	2.27	0.64
1:D:288:MET:SD	3:D:816:ACO:CH3	2.78	0.64
1:C:268:GLY:HA2	4:C:906:HOH:O	1.97	0.64
1:D:99:GLY:HA3	4:D:843:HOH:O	1.99	0.64
1:D:298:LYS:HE2	1:D:302:ARG:HG3	1.81	0.62
1:C:322:GLN:O	1:C:326:VAL:HG23	1.99	0.62
1:A:157:MET:HG3	3:A:813:ACO:S1P	2.39	0.62
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.11	0.62
1:C:89:SCY:OCD	3:C:815:ACO:CH3	2.47	0.62
1:A:50:ASN:HB3	4:A:1019:HOH:O	2.00	0.62
1:B:38:VAL:HA	4:B:998:HOH:O	2.00	0.62
1:C:207:ARG:HG2	1:C:207:ARG:HH11	1.64	0.61
1:D:89:SCY:OCD	3:D:816:ACO:CH3	2.48	0.61
3:D:816:ACO:O9P	3:D:816:ACO:C6P	2.47	0.61
1:D:88:LEU:CB	1:D:89:SCY:HE2	2.14	0.61
1:A:163:ASN:HA	1:A:166:LYS:NZ	2.15	0.61
1:D:220:ARG:HD3	3:D:816:ACO:C6A	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.16	0.59
1:B:392:LEU:HD12	4:B:943:HOH:O	2.03	0.59
1:C:89:SCY:CE	1:C:380:GLY:H	2.15	0.59
1:A:378:CYS:SG	3:A:813:ACO:CH3	2.91	0.59
1:B:372:LYS:HE3	4:B:1019:HOH:O	2.03	0.58
1:D:263:GLU:OE1	1:D:266:ARG:NH1	2.36	0.58
1:D:317:GLU:HB3	1:D:344:ILE:HG13	1.85	0.58
1:C:288:MET:HE1	3:C:815:ACO:HH33	1.85	0.58
1:D:288:MET:CE	3:D:816:ACO:HH33	2.32	0.58
1:D:244:GLY:HA2	3:D:816:ACO:N7A	2.17	0.58
1:C:88:LEU:HB3	1:C:89:SCY:CE	2.33	0.58
1:C:89:SCY:H	1:C:89:SCY:CE	2.13	0.58
1:C:89:SCY:OCD	3:C:815:ACO:C	2.52	0.57
1:B:156:HIS:HE1	3:B:814:ACO:H62	1.70	0.57
1:B:89:SCY:CD	3:B:814:ACO:HH32	2.35	0.57
1:A:89:SCY:CE	1:A:380:GLY:H	2.11	0.57
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.34	0.56
1:A:40:GLU:HG3	4:A:1098:HOH:O	2.04	0.56
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.87	0.56
1:D:143:MET:CE	1:D:249:LEU:HD22	2.36	0.56
1:D:300:LEU:HD13	1:D:307:ILE:HG13	1.88	0.56
1:A:156:HIS:CE1	3:A:813:ACO:H62	2.39	0.56
3:B:814:ACO:O5P	3:B:814:ACO:C2P	2.47	0.56
1:D:378:CYS:SG	3:D:816:ACO:HH31	2.46	0.56
3:C:815:ACO:O9P	3:C:815:ACO:H62	2.06	0.56
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.71	0.56
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.70	0.56
1:D:276:VAL:HG11	1:D:305:TRP:CZ2	2.41	0.56
1:C:293:ILE:HB	1:C:294:PRO:HD3	1.87	0.55
1:D:258:LEU:HD22	1:D:258:LEU:N	2.22	0.55
1:B:211:ILE:HD12	4:B:1110:HOH:O	2.06	0.55
1:C:313:VAL:HB	1:C:337:VAL:HG22	1.89	0.55
1:C:175:GLN:HE22	1:C:240:THR:HG23	1.72	0.55
3:B:814:ACO:H143	4:B:896:HOH:O	2.06	0.54
1:B:298:LYS:HD3	1:B:298:LYS:C	2.28	0.54
1:A:9:SER:HA	1:A:272:LEU:HD22	1.90	0.54
1:B:172:ARG:NH1	4:B:968:HOH:O	2.37	0.54
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.70	0.54
1:A:300:LEU:HD21	1:A:310:LEU:HD11	1.88	0.54
1:C:288:MET:SD	3:C:815:ACO:CH3	2.90	0.53
1:A:279:ALA:HB2	1:A:298:LYS:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:815:ACO:O9P	3:C:815:ACO:C6P	2.55	0.53
1:D:88:LEU:HD13	1:D:89:SCY:HE1	1.90	0.53
1:C:258:LEU:N	1:C:258:LEU:HD22	2.23	0.53
1:D:316:ASN:HB2	1:D:377:LEU:HG	1.91	0.52
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.45	0.52
1:D:64:GLN:O	1:D:65:ASN:C	2.48	0.52
1:D:143:MET:HE3	1:D:249:LEU:HD22	1.89	0.52
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.75	0.52
1:D:312:LEU:HD23	1:D:361:LEU:HD23	1.92	0.52
1:A:366:LYS:NZ	4:A:905:HOH:O	2.41	0.52
1:B:96:VAL:HG21	1:B:358:LEU:HD12	1.92	0.52
1:B:155:TYR:OH	1:B:286:LYS:HG2	2.09	0.52
1:B:191:LYS:NZ	1:B:191:LYS:HB3	2.25	0.52
1:A:348:HIS:CD2	3:A:813:ACO:H31	2.45	0.52
1:D:97:ALA:O	1:D:101:GLN:HG3	2.10	0.52
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.45	0.52
1:C:243:ALA:HA	3:C:815:ACO:H143	1.92	0.52
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.45	0.51
1:D:293:ILE:HG13	4:D:869:HOH:O	2.08	0.51
1:A:96:VAL:HG21	1:A:358:LEU:HD12	1.93	0.51
1:B:288:MET:SD	3:B:814:ACO:CH3	2.82	0.51
1:C:378:CYS:SG	3:C:815:ACO:HH33	2.50	0.51
1:D:293:ILE:O	1:D:297:ARG:HG3	2.09	0.51
1:D:143:MET:HE1	1:D:249:LEU:CD1	2.37	0.51
1:A:279:ALA:HB1	1:A:298:LYS:HG3	1.93	0.51
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.44	0.51
1:D:88:LEU:HB2	1:D:379:ILE:CG2	2.41	0.51
1:C:309:ASP:HB3	1:C:372:LYS:HD2	1.93	0.51
1:D:89:SCY:HE2	1:D:89:SCY:N	2.25	0.51
1:C:129:ARG:NH2	1:D:122:ALA:O	2.40	0.51
1:A:34:VAL:HG12	1:A:255:ALA:HB3	1.92	0.50
1:A:372:LYS:HE3	4:A:1010:HOH:O	2.11	0.50
1:D:156:HIS:ND1	1:D:157:MET:N	2.59	0.50
1:D:207:ARG:N	1:D:207:ARG:HD3	2.26	0.50
1:B:236:ASP:O	1:B:239:GLY:N	2.41	0.50
1:C:281:VAL:HG12	1:C:282:GLY:N	2.26	0.50
1:B:237:LYS:HB2	4:B:944:HOH:O	2.09	0.50
1:A:12:ARG:O	1:A:199:ILE:HA	2.12	0.50
1:B:348:HIS:HB2	4:B:929:HOH:O	2.12	0.50
1:B:356:ARG:HD2	1:B:356:ARG:O	2.12	0.50
1:D:187:GLU:HG3	1:D:221:HIS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HG2	1:A:208:LYS:H	1.76	0.50
1:A:89:SCY:HE2	1:A:89:SCY:H	1.77	0.49
1:A:180:VAL:CG2	1:A:228:MET:HG2	2.43	0.49
1:C:186:ALA:HA	1:C:340:ASN:O	2.12	0.49
1:B:316:ASN:HB3	4:B:833:HOH:O	2.12	0.49
1:B:390:GLU:OE2	4:B:1053:HOH:O	2.19	0.49
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.95	0.49
1:B:174:GLU:OE1	4:B:994:HOH:O	2.20	0.49
1:D:378:CYS:C	3:D:816:ACO:HH31	2.32	0.49
1:A:228:MET:HE3	4:A:934:HOH:O	2.13	0.49
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.25	0.49
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.48	0.49
1:C:12:ARG:HG3	1:C:13:THR:O	2.14	0.48
1:C:243:ALA:HA	3:C:815:ACO:CEP	2.42	0.48
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.48	0.48
1:A:174:GLU:OE2	1:A:328:LYS:NZ	2.46	0.48
1:B:162:GLU:O	1:B:166:LYS:HG3	2.13	0.48
1:C:41:ARG:NH1	1:C:197:ASP:O	2.47	0.48
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.96	0.48
1:A:298:LYS:NZ	1:A:298:LYS:HA	2.28	0.48
1:C:88:LEU:HB3	1:C:89:SCY:HE2	1.96	0.48
1:B:203:ILE:HD12	1:B:212:THR:OG1	2.13	0.48
1:D:31:GLY:O	1:D:35:ILE:HG13	2.14	0.48
1:D:305:TRP:CZ3	1:D:388:CYS:HB3	2.48	0.48
1:D:18:PHE:O	1:D:19:ASN:HB2	2.14	0.47
1:D:378:CYS:SG	3:D:816:ACO:CH3	3.03	0.47
1:B:207:ARG:HG2	1:B:208:LYS:H	1.78	0.47
1:C:8:ALA:HB1	1:C:269:ILE:HG21	1.97	0.47
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.96	0.47
1:B:328:LYS:HG3	4:B:1006:HOH:O	2.14	0.47
1:B:12:ARG:HD2	1:B:356:ARG:HG2	1.97	0.47
1:B:263:GLU:OE1	1:B:266:ARG:NH2	2.47	0.47
1:C:145:LYS:NZ	4:C:878:HOH:O	2.48	0.47
1:B:89:SCY:OCD	3:B:814:ACO:CH3	2.62	0.47
1:B:162:GLU:OE2	4:B:1057:HOH:O	2.20	0.47
1:D:311:ASP:HB2	1:D:370:ALA:HB1	1.98	0.46
1:B:88:LEU:HB3	1:B:89:SCY:HE2	1.98	0.46
1:C:227:SER:HB2	3:C:815:ACO:H2A	1.96	0.46
1:C:361:LEU:HD22	1:C:365:MET:HG3	1.98	0.46
1:C:236:ASP:HB3	1:C:239:GLY:HA3	1.98	0.46
1:D:174:GLU:OE2	1:D:328:LYS:NZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ARG:HD3	3:D:816:ACO:N6A	2.30	0.46
1:C:64:GLN:HB3	1:D:88:LEU:HD11	1.97	0.46
1:C:272:LEU:CD1	4:C:853:HOH:O	2.62	0.46
1:D:9:SER:HA	1:D:272:LEU:HD21	1.97	0.46
1:D:296:SER:O	1:D:300:LEU:HG	2.15	0.46
1:A:89:SCY:OCD	1:A:379:ILE:HA	2.15	0.46
1:B:305:TRP:CE2	1:B:372:LYS:HD3	2.51	0.46
1:C:385:VAL:HG22	1:C:386:ALA:N	2.29	0.46
1:A:371:ARG:HG3	4:A:1020:HOH:O	2.15	0.45
1:B:50:ASN:HB3	4:B:1045:HOH:O	2.16	0.45
1:B:257:LEU:HD23	1:B:258:LEU:N	2.31	0.45
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.99	0.45
1:D:66:PRO:HD2	4:D:887:HOH:O	2.15	0.45
1:C:156:HIS:ND1	1:C:157:MET:N	2.63	0.45
1:D:55:GLY:HA2	1:D:85:MET:O	2.17	0.45
1:B:48:GLU:OE1	1:B:267:ARG:NH2	2.38	0.45
1:C:206:GLY:HA3	1:C:209:GLY:O	2.17	0.45
1:D:312:LEU:HD23	1:D:361:LEU:CD2	2.46	0.45
1:A:257:LEU:C	1:A:257:LEU:HD23	2.37	0.45
3:A:813:ACO:O5P	3:A:813:ACO:C2P	2.37	0.45
1:A:374:LEU:HD21	1:A:376:THR:HB	1.99	0.44
1:B:5:ILE:HG12	1:B:100:MET:HG2	1.99	0.44
1:C:12:ARG:HA	1:C:254:ALA:HA	1.98	0.44
1:C:88:LEU:HD11	1:D:64:GLN:HB3	1.99	0.44
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.99	0.44
1:D:176:ASP:O	1:D:180:VAL:HG23	2.17	0.44
1:B:207:ARG:HD3	1:B:207:ARG:N	2.33	0.44
1:D:88:LEU:HD12	1:D:380:GLY:O	2.17	0.44
1:D:206:GLY:HA3	1:D:209:GLY:O	2.17	0.44
1:B:88:LEU:HD12	1:B:380:GLY:O	2.18	0.44
1:B:259:MET:HB2	1:B:263:GLU:HG2	1.98	0.44
1:A:191:LYS:HG3	4:A:1036:HOH:O	2.18	0.44
1:B:89:SCY:HE1	1:B:380:GLY:CA	2.47	0.44
1:D:293:ILE:HB	1:D:294:PRO:CD	2.48	0.44
1:A:291:GLY:N	1:A:292:PRO:CD	2.80	0.43
1:C:311:ASP:HB2	1:C:370:ALA:HB1	1.99	0.43
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.82	0.43
1:B:156:HIS:CE1	3:B:814:ACO:H62	2.50	0.43
1:C:89:SCY:HE1	1:C:380:GLY:N	2.28	0.43
1:D:27:ALA:HB1	1:D:116:MET:HB2	1.98	0.43
1:D:361:LEU:HD22	1:D:365:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ILE:HG21	1:A:350:ILE:HD13	1.67	0.43
1:D:293:ILE:N	1:D:294:PRO:HD2	2.33	0.43
1:D:333:ASP:HA	1:D:334:PRO:HD2	1.85	0.43
1:A:298:LYS:O	1:A:298:LYS:HD3	2.19	0.43
1:B:296:SER:HB3	1:B:374:LEU:HD11	2.00	0.43
1:B:392:LEU:HB2	4:B:943:HOH:O	2.18	0.43
1:C:207:ARG:HG2	1:C:208:LYS:H	1.84	0.43
1:D:292:PRO:HD3	1:D:378:CYS:CA	2.43	0.43
1:C:88:LEU:HB3	1:C:89:SCY:HE3	1.99	0.43
1:A:297:ARG:HG2	1:A:297:ARG:HH11	1.84	0.43
1:C:9:SER:HB3	1:C:42:ALA:HB2	2.01	0.43
1:B:232:ARG:O	4:B:937:HOH:O	2.22	0.42
1:B:298:LYS:HD3	1:B:298:LYS:O	2.18	0.42
1:D:187:GLU:OE1	1:D:191:LYS:HE2	2.19	0.42
1:C:125:CYS:HB2	1:D:123:PRO:HB2	2.01	0.42
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.54	0.42
1:C:103:ILE:HA	1:C:108:ALA:O	2.19	0.42
1:D:175:GLN:HB3	1:D:320:ALA:HB3	2.01	0.42
1:A:236:ASP:O	1:A:237:LYS:C	2.57	0.42
1:A:168:TRP:CZ3	1:A:328:LYS:HB3	2.55	0.42
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.86	0.42
1:A:293:ILE:HB	1:A:294:PRO:CD	2.50	0.42
1:A:293:ILE:HB	1:A:294:PRO:HD3	2.01	0.42
1:B:88:LEU:HB2	1:B:379:ILE:HG23	2.01	0.42
1:C:58:LEU:HD13	4:C:843:HOH:O	2.20	0.42
1:C:64:GLN:HE22	1:D:157:MET:CE	2.32	0.42
1:C:332:TRP:O	1:C:334:PRO:HD3	2.20	0.42
1:B:18:PHE:HB2	1:B:249:LEU:O	2.20	0.42
1:D:25:THR:HA	1:D:26:PRO:HD3	1.92	0.42
1:D:99:GLY:O	1:D:103:ILE:HD12	2.20	0.41
1:A:358:LEU:HD11	1:A:387:MET:CE	2.50	0.41
3:A:813:ACO:O9P	3:A:813:ACO:C6P	2.67	0.41
1:C:207:ARG:HD3	1:C:207:ARG:N	2.35	0.41
1:A:12:ARG:HD2	1:A:356:ARG:HG2	2.02	0.41
1:A:183:GLN:HA	1:A:345:ALA:HB2	2.02	0.41
1:B:236:ASP:O	1:B:237:LYS:C	2.59	0.41
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.84	0.41
1:A:358:LEU:HD11	1:A:387:MET:HE1	2.02	0.41
1:B:132:VAL:O	1:D:129:ARG:HA	2.20	0.41
1:D:247:SER:HB2	1:D:348:HIS:HB2	2.03	0.41
1:A:322:GLN:O	1:A:325:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ASN:HA	1:B:121:MET:SD	2.61	0.41
1:D:207:ARG:HG2	1:D:208:LYS:H	1.86	0.41
1:B:316:ASN:HB2	1:B:377:LEU:HG	2.03	0.41
1:D:28:HIS:ND1	1:D:62:GLU:OE2	2.46	0.41
1:D:324:CYS:O	1:D:328:LYS:HB2	2.21	0.41
1:A:85:MET:HA	1:B:85:MET:HA	2.03	0.41
1:C:143:MET:HB2	4:C:843:HOH:O	2.20	0.41
1:D:9:SER:HA	1:D:272:LEU:CD2	2.51	0.41
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.89	0.41
1:C:324:CYS:O	1:C:328:LYS:HB2	2.20	0.41
1:C:374:LEU:C	1:C:374:LEU:HD23	2.42	0.41
1:A:180:VAL:HG23	1:A:228:MET:HG2	2.02	0.40
1:C:358:LEU:HD22	1:C:362:LEU:HG	2.03	0.40
1:D:180:VAL:HG22	1:D:228:MET:HE2	2.02	0.40
1:D:89:SCY:CE	1:D:89:SCY:H	2.31	0.40
1:B:263:GLU:HB2	1:B:266:ARG:NH2	2.36	0.40
1:C:53:ILE:HD13	1:C:83:TRP:CZ2	2.56	0.40
1:A:305:TRP:CZ3	1:A:388:CYS:HB3	2.57	0.40
1:B:9:SER:HA	1:B:272:LEU:HD22	2.04	0.40
1:D:339:VAL:HG13	4:D:894:HOH:O	2.21	0.40
1:B:41:ARG:HB2	4:B:998:HOH:O	2.21	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)
4:B:965:HOH:O	4:B:1046:HOH:O[2_555]	2.19	0.01

## 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	386/389 (99%)	371 (96%)	14 (4%)	1 (0%)	41	37
1	B	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	41	37
1	C	386/389 (99%)	372 (96%)	13 (3%)	1 (0%)	41	37
1	D	386/389 (99%)	370 (96%)	14 (4%)	2 (0%)	29	23
All	All	1544/1556 (99%)	1486 (96%)	53 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ILE
1	C	350	ILE
1	D	350	ILE
1	A	350	ILE
1	D	65	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/275 (100%)	252 (92%)	23 (8%)	11	7
1	B	275/275 (100%)	253 (92%)	22 (8%)	12	7
1	C	275/275 (100%)	253 (92%)	22 (8%)	12	7
1	D	275/275 (100%)	257 (94%)	18 (6%)	17	12
All	All	1100/1100 (100%)	1015 (92%)	85 (8%)	13	8

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	123	PRO
1	A	133	LYS
1	A	155	TYR
1	A	207	ARG
1	A	220	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	228	MET
1	A	232	ARG
1	A	237	LYS
1	A	240	THR
1	A	258	LEU
1	A	263	GLU
1	A	272	LEU
1	A	276	VAL
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	339	VAL
1	A	353	SER
1	A	358	LEU
1	A	361	LEU
1	A	392	LEU
1	B	4	SER
1	B	5	ILE
1	B	39	LEU
1	B	59	PRO
1	B	155	TYR
1	B	187	GLU
1	B	207	ARG
1	B	220	ARG
1	B	232	ARG
1	B	237	LYS
1	B	240	THR
1	B	258	LEU
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	339	VAL
1	B	358	LEU
1	B	361	LEU
1	C	39	LEU
1	C	40	GLU
1	C	109	SER

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Mol	Chain	Res	Type
1	C	134	MET
1	C	155	TYR
1	C	207	ARG
1	C	224	THR
1	C	237	LYS
1	C	240	THR
1	C	258	LEU
1	C	272	LEU
1	C	288	MET
1	C	297	ARG
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	339	VAL
1	C	353	SER
1	C	358	LEU
1	C	361	LEU
1	C	367	ARG
1	C	371	ARG
1	D	39	LEU
1	D	144	ILE
1	D	155	TYR
1	D	187	GLU
1	D	207	ARG
1	D	224	THR
1	D	240	THR
1	D	258	LEU
1	D	265	SER
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
1	D	353	SER
1	D	361	LEU
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	B	78	GLN
1	B	175	GLN
1	B	184	ASN
1	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	D	175	GLN
1	D	316	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues 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
1	SCY	B	89	1	7,8,9	1.13	1 (14%)	3,9,11	4.45	3 (100%)
1	SCY	A	89	1	7,8,9	0.93	1 (14%)	3,9,11	2.48	3 (100%)
1	SCY	C	89	1	7,8,9	0.77	0	3,9,11	3.11	2 (66%)
1	SCY	D	89	1	7,8,9	0.70	0	3,9,11	3.85	2 (66%)

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
1	SCY	B	89	1	-	2/5/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	A	89	1	-	2/5/7/9	-
1	SCY	C	89	1	-	2/5/7/9	-
1	SCY	D	89	1	-	2/5/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	SCY	CB-CA	2.12	1.58	1.53
1	A	89	SCY	CB-SG	-2.05	1.76	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	SCY	OCD-CD-SG	-5.31	99.04	122.60
1	D	89	SCY	OCD-CD-CE	-5.26	101.48	123.07
1	B	89	SCY	CE-CD-SG	4.94	148.39	114.20
1	C	89	SCY	OCD-CD-CE	-4.71	103.73	123.07
1	D	89	SCY	OCD-CD-SG	4.07	140.69	122.60
1	A	89	SCY	CE-CD-SG	2.83	133.80	114.20
1	B	89	SCY	OCD-CD-CE	-2.59	112.46	123.07
1	A	89	SCY	OCD-CD-SG	-2.29	112.45	122.60
1	A	89	SCY	OCD-CD-CE	-2.27	113.74	123.07
1	C	89	SCY	OCD-CD-SG	2.20	132.35	122.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89	SCY	OCD-CD-SG-CB
1	A	89	SCY	CE-CD-SG-CB
1	C	89	SCY	OCD-CD-SG-CB
1	C	89	SCY	CE-CD-SG-CB
1	D	89	SCY	OCD-CD-SG-CB
1	D	89	SCY	CE-CD-SG-CB
1	B	89	SCY	OCD-CD-SG-CB
1	B	89	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	89	SCY	8	0
1	A	89	SCY	8	0
1	C	89	SCY	11	0
1	D	89	SCY	10	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
2	SO4	B	807	-	4,4,4	0.70	0	6,6,6	0.31	0
2	SO4	B	809	-	4,4,4	0.65	0	6,6,6	0.76	0
2	SO4	A	810	-	4,4,4	0.46	0	6,6,6	0.52	0
3	ACO	A	813	-	45,53,53	2.06	9 (20%)	56,79,79	2.23	16 (28%)
3	ACO	C	815	-	45,53,53	2.03	11 (24%)	56,79,79	2.17	16 (28%)
3	ACO	D	816	-	45,53,53	1.99	9 (20%)	56,79,79	2.03	11 (19%)
2	SO4	B	812	-	4,4,4	0.83	0	6,6,6	0.99	0
3	ACO	B	814	-	45,53,53	1.93	8 (17%)	56,79,79	2.23	19 (33%)
2	SO4	A	808	-	4,4,4	0.52	0	6,6,6	0.44	0
2	SO4	A	811	-	4,4,4	0.97	0	6,6,6	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACO	C	815	-	-	10/47/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACO	D	816	-	-	6/47/67/67	0/3/3/3
3	ACO	A	813	-	-	12/47/67/67	0/3/3/3
3	ACO	B	814	-	-	10/47/67/67	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	813	ACO	O9P-C9P	7.37	1.38	1.23
3	C	815	ACO	O9P-C9P	6.91	1.37	1.23
3	D	816	ACO	O9P-C9P	6.79	1.36	1.23
3	B	814	ACO	O9P-C9P	6.47	1.36	1.23
3	C	815	ACO	P3B-O3B	5.00	1.68	1.59
3	D	816	ACO	P3B-O3B	4.71	1.68	1.59
3	A	813	ACO	O5P-C5P	4.55	1.32	1.23
3	D	816	ACO	C3P-N4P	4.50	1.56	1.46
3	B	814	ACO	P3B-O3B	4.45	1.67	1.59
3	C	815	ACO	C3P-N4P	4.37	1.56	1.46
3	B	814	ACO	C3P-N4P	4.33	1.56	1.46
3	A	813	ACO	P3B-O3B	4.09	1.67	1.59
3	A	813	ACO	C3P-N4P	3.98	1.55	1.46
3	B	814	ACO	O5P-C5P	3.85	1.31	1.23
3	A	813	ACO	O4B-C1B	3.69	1.46	1.41
3	C	815	ACO	O4B-C1B	3.51	1.46	1.41
3	C	815	ACO	O5P-C5P	3.51	1.30	1.23
3	D	816	ACO	O4B-C1B	3.46	1.45	1.41
3	D	816	ACO	O5P-C5P	3.45	1.30	1.23
3	D	816	ACO	P3B-O7A	3.16	1.60	1.50
3	C	815	ACO	P3B-O7A	3.14	1.60	1.50
3	B	814	ACO	O4B-C4B	3.12	1.52	1.45
3	B	814	ACO	O4B-C1B	3.10	1.45	1.41
3	A	813	ACO	C2A-N1A	3.04	1.39	1.33
3	A	813	ACO	O4B-C4B	2.95	1.51	1.45
3	B	814	ACO	P3B-O7A	2.94	1.60	1.50
3	D	816	ACO	C2A-N1A	2.91	1.39	1.33
3	A	813	ACO	P3B-O7A	2.91	1.59	1.50
3	B	814	ACO	C2A-N1A	2.82	1.39	1.33
3	C	815	ACO	C2A-N1A	2.71	1.38	1.33
3	C	815	ACO	O4B-C4B	2.55	1.50	1.45
3	D	816	ACO	O4B-C4B	2.51	1.50	1.45
3	C	815	ACO	CH3-C	2.47	1.60	1.50
3	D	816	ACO	OAP-CAP	2.29	1.46	1.42
3	C	815	ACO	C6P-C5P	-2.20	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	815	ACO	OAP-CAP	2.08	1.46	1.42
3	A	813	ACO	CH3-C	-2.05	1.42	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	816	ACO	C2P-C3P-N4P	-6.90	97.92	112.42
3	A	813	ACO	C2P-C3P-N4P	-6.24	99.31	112.42
3	A	813	ACO	C6P-C5P-N4P	5.62	125.88	116.42
3	C	815	ACO	C2P-C3P-N4P	-5.49	100.88	112.42
3	B	814	ACO	O5P-C5P-C6P	-5.48	111.99	122.02
3	C	815	ACO	C3P-N4P-C5P	-5.30	113.00	122.84
3	D	816	ACO	C3P-N4P-C5P	-5.05	113.45	122.84
3	C	815	ACO	C6P-C7P-N8P	-5.04	101.72	111.90
3	B	814	ACO	C6P-C5P-N4P	5.00	124.84	116.42
3	B	814	ACO	O9P-C9P-N8P	4.78	133.25	122.99
3	C	815	ACO	O4B-C1B-C2B	-4.76	99.96	106.93
3	D	816	ACO	O4B-C1B-C2B	-4.66	100.11	106.93
3	B	814	ACO	C2P-C3P-N4P	-4.61	102.73	112.42
3	A	813	ACO	C6P-C7P-N8P	-4.60	102.61	111.90
3	D	816	ACO	CEP-CBP-CCP	-4.36	101.12	108.23
3	C	815	ACO	O6A-CCP-CBP	-4.23	103.75	110.55
3	B	814	ACO	O6A-CCP-CBP	-4.21	103.77	110.55
3	A	813	ACO	O-C-S1P	-4.21	103.91	122.60
3	C	815	ACO	CEP-CBP-CAP	4.13	115.99	108.82
3	D	816	ACO	C6P-C7P-N8P	-4.10	103.62	111.90
3	D	816	ACO	O6A-CCP-CBP	-4.06	104.02	110.55
3	A	813	ACO	O5P-C5P-C6P	-4.05	114.62	122.02
3	A	813	ACO	O6A-CCP-CBP	-4.01	104.09	110.55
3	C	815	ACO	O5P-C5P-N4P	-3.91	115.63	123.01
3	B	814	ACO	CEP-CBP-CAP	3.81	115.43	108.82
3	B	814	ACO	C6P-C7P-N8P	-3.67	104.48	111.90
3	B	814	ACO	C4A-C5A-N7A	3.67	113.22	109.40
3	A	813	ACO	O4B-C1B-C2B	-3.66	101.58	106.93
3	A	813	ACO	CEP-CBP-CAP	3.62	115.10	108.82
3	C	815	ACO	C7P-C6P-C5P	3.59	118.33	112.36
3	B	814	ACO	O4B-C1B-C2B	-3.52	101.78	106.93
3	B	814	ACO	C3P-N4P-C5P	-3.45	116.43	122.84
3	C	815	ACO	C4A-C5A-N7A	3.30	112.84	109.40
3	A	813	ACO	C4A-C5A-N7A	3.28	112.82	109.40
3	D	816	ACO	CEP-CBP-CAP	3.27	114.50	108.82
3	A	813	ACO	C5A-C6A-N1A	-3.20	113.10	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	816	ACO	C4A-C5A-N7A	3.15	112.69	109.40
3	B	814	ACO	CEP-CBP-CCP	-3.15	103.09	108.23
3	B	814	ACO	O9P-C9P-CAP	-2.96	112.02	121.06
3	C	815	ACO	C6P-C5P-N4P	2.95	121.39	116.42
3	C	815	ACO	N6A-C6A-N1A	2.89	124.58	118.57
3	A	813	ACO	C3P-N4P-C5P	-2.74	117.74	122.84
3	A	813	ACO	N6A-C6A-N1A	2.73	124.24	118.57
3	B	814	ACO	C5A-C6A-N1A	-2.65	114.36	120.35
3	A	813	ACO	C2A-N1A-C6A	2.63	123.26	118.75
3	B	814	ACO	O-C-S1P	-2.60	111.06	122.60
3	C	815	ACO	O-C-S1P	-2.59	111.09	122.60
3	C	815	ACO	CEP-CBP-CCP	-2.53	104.11	108.23
3	D	816	ACO	CDP-CBP-CCP	2.52	112.34	108.23
3	A	813	ACO	CDP-CBP-CCP	2.32	112.01	108.23
3	C	815	ACO	C7P-N8P-C9P	-2.31	118.47	122.59
3	D	816	ACO	C5A-C6A-N1A	-2.31	115.12	120.35
3	B	814	ACO	N6A-C6A-N1A	2.31	123.36	118.57
3	A	813	ACO	CH3-C-S1P	2.28	129.98	114.20
3	B	814	ACO	C7P-N8P-C9P	2.27	126.64	122.59
3	C	815	ACO	CH3-C-S1P	2.23	129.65	114.20
3	C	815	ACO	C5A-C6A-N1A	-2.23	115.31	120.35
3	B	814	ACO	C5B-C4B-C3B	2.18	121.62	114.40
3	B	814	ACO	C2P-S1P-C	2.13	112.89	101.68
3	A	813	ACO	C2P-S1P-C	2.13	112.88	101.68
3	D	816	ACO	N6A-C6A-N1A	2.01	122.75	118.57
3	B	814	ACO	CDP-CBP-CAP	2.00	112.29	108.82

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	813	ACO	C5B-O5B-P1A-O1A
3	A	813	ACO	C5B-O5B-P1A-O2A
3	A	813	ACO	CAP-C9P-N8P-C7P
3	A	813	ACO	C5P-C6P-C7P-N8P
3	A	813	ACO	C2P-C3P-N4P-C5P
3	B	814	ACO	C5B-O5B-P1A-O1A
3	B	814	ACO	C5B-O5B-P1A-O2A
3	B	814	ACO	C2P-C3P-N4P-C5P
3	C	815	ACO	C5B-O5B-P1A-O1A
3	C	815	ACO	C5B-O5B-P1A-O2A
3	C	815	ACO	C2P-C3P-N4P-C5P

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Mol	Chain	Res	Type	Atoms
3	D	816	ACO	C5B-O5B-P1A-O1A
3	D	816	ACO	C5B-O5B-P1A-O2A
3	D	816	ACO	C2P-C3P-N4P-C5P
3	B	814	ACO	C6P-C7P-N8P-C9P
3	D	816	ACO	C6P-C7P-N8P-C9P
3	A	813	ACO	C6P-C7P-N8P-C9P
3	A	813	ACO	O9P-C9P-N8P-C7P
3	C	815	ACO	CAP-C9P-N8P-C7P
3	C	815	ACO	O9P-C9P-N8P-C7P
3	C	815	ACO	C5P-C6P-C7P-N8P
3	B	814	ACO	C5B-O5B-P1A-O3A
3	B	814	ACO	O5P-C5P-C6P-C7P
3	A	813	ACO	O5P-C5P-C6P-C7P
3	A	813	ACO	S1P-C2P-C3P-N4P
3	B	814	ACO	S1P-C2P-C3P-N4P
3	C	815	ACO	C6P-C7P-N8P-C9P
3	B	814	ACO	N4P-C5P-C6P-C7P
3	A	813	ACO	N4P-C5P-C6P-C7P
3	A	813	ACO	C5B-O5B-P1A-O3A
3	C	815	ACO	C5B-O5B-P1A-O3A
3	D	816	ACO	C5B-O5B-P1A-O3A
3	A	813	ACO	CCP-O6A-P2A-O4A
3	C	815	ACO	CCP-O6A-P2A-O4A
3	D	816	ACO	CCP-O6A-P2A-O4A
3	B	814	ACO	C4B-C5B-O5B-P1A
3	C	815	ACO	S1P-C2P-C3P-N4P
3	B	814	ACO	O9P-C9P-N8P-C7P

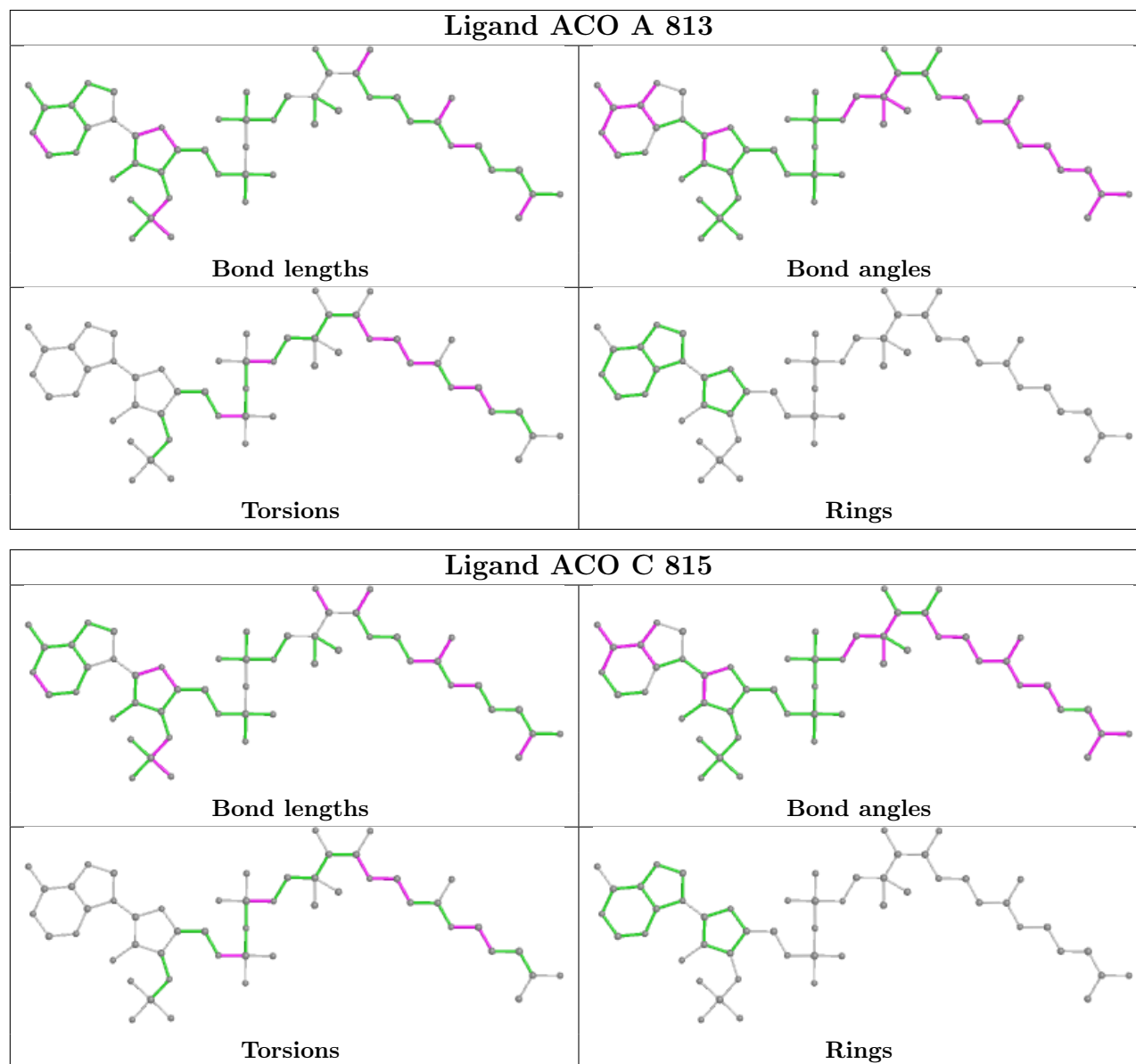
There are no ring outliers.

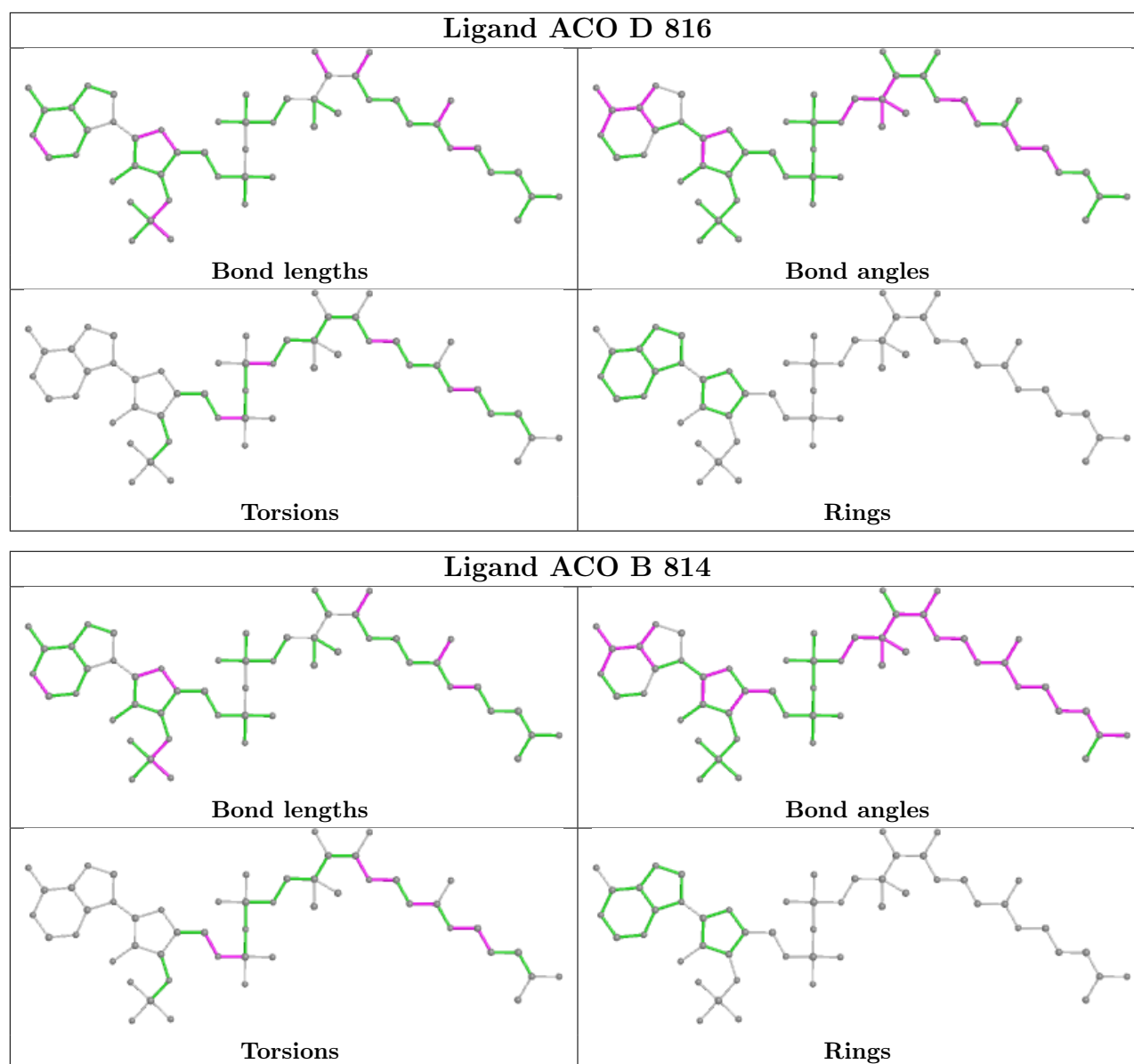
4 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	813	ACO	16	0
3	C	815	ACO	17	0
3	D	816	ACO	17	0
3	B	814	ACO	12	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, 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	388/389 (99%)	-0.57	8 (2%) 63 62	11, 18, 40, 81	0
1	B	388/389 (99%)	-0.54	7 (1%) 68 66	11, 18, 40, 88	0
1	C	388/389 (99%)	0.10	16 (4%) 37 36	22, 36, 64, 110	0
1	D	388/389 (99%)	0.55	40 (10%) 6 6	23, 41, 99, 127	0
All	All	1552/1556 (99%)	-0.12	71 (4%) 32 31	11, 31, 67, 127	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	LYS	6.6
1	D	230	LYS	6.5
1	C	237	LYS	6.2
1	D	226	ASP	5.9
1	D	235	PHE	5.8
1	C	206	GLY	5.8
1	D	231	LEU	5.8
1	D	224	THR	5.8
1	D	229	ALA	5.7
1	D	227	SER	5.6
1	D	234	ALA	5.3
1	C	227	SER	5.0
1	D	206	GLY	4.8
1	D	238	GLU	4.8
1	A	237	LYS	4.8
1	D	225	LEU	4.8
1	D	207	ARG	4.7
1	D	239	GLY	4.6
1	C	207	ARG	4.5
1	D	164	VAL	4.4
1	C	232	ARG	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	208	LYS	4.3
1	C	235	PHE	4.1
1	C	208	LYS	4.1
1	D	228	MET	3.9
1	D	392	LEU	3.9
1	D	236	ASP	3.9
1	D	170	LEU	3.8
1	B	237	LYS	3.7
1	A	206	GLY	3.7
1	C	234	ALA	3.6
1	D	232	ARG	3.6
1	B	238	GLU	3.5
1	D	156	HIS	3.5
1	B	207	ARG	3.4
1	B	208	LYS	3.4
1	D	240	THR	3.3
1	D	168	TRP	3.3
1	B	235	PHE	3.3
1	C	233	PRO	3.1
1	C	224	THR	3.0
1	D	153	TYR	3.0
1	D	330	LEU	3.0
1	B	206	GLY	2.9
1	A	235	PHE	2.8
1	D	223	ALA	2.8
1	A	207	ARG	2.8
1	D	169	GLN	2.8
1	C	239	GLY	2.7
1	D	371	ARG	2.6
1	D	220	ARG	2.6
1	D	323	ALA	2.6
1	D	233	PRO	2.6
1	D	219	ILE	2.5
1	C	392	LEU	2.5
1	D	179	ALA	2.5
1	A	208	LYS	2.5
1	C	231	LEU	2.4
1	A	233	PRO	2.4
1	C	229	ALA	2.4
1	C	230	LYS	2.3
1	D	222	GLY	2.3
1	D	178	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	331	GLY	2.2
1	B	392	LEU	2.2
1	D	339	VAL	2.2
1	A	209	GLY	2.2
1	A	238	GLU	2.2
1	C	236	ASP	2.2
1	D	221	HIS	2.1
1	D	306	LYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	SCY	C	89	9/10	0.73	0.25	29,37,57,59	0
1	SCY	D	89	9/10	0.85	0.22	33,37,55,57	0
1	SCY	A	89	9/10	0.91	0.14	13,14,28,33	0
1	SCY	B	89	9/10	0.91	0.13	13,16,29,34	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

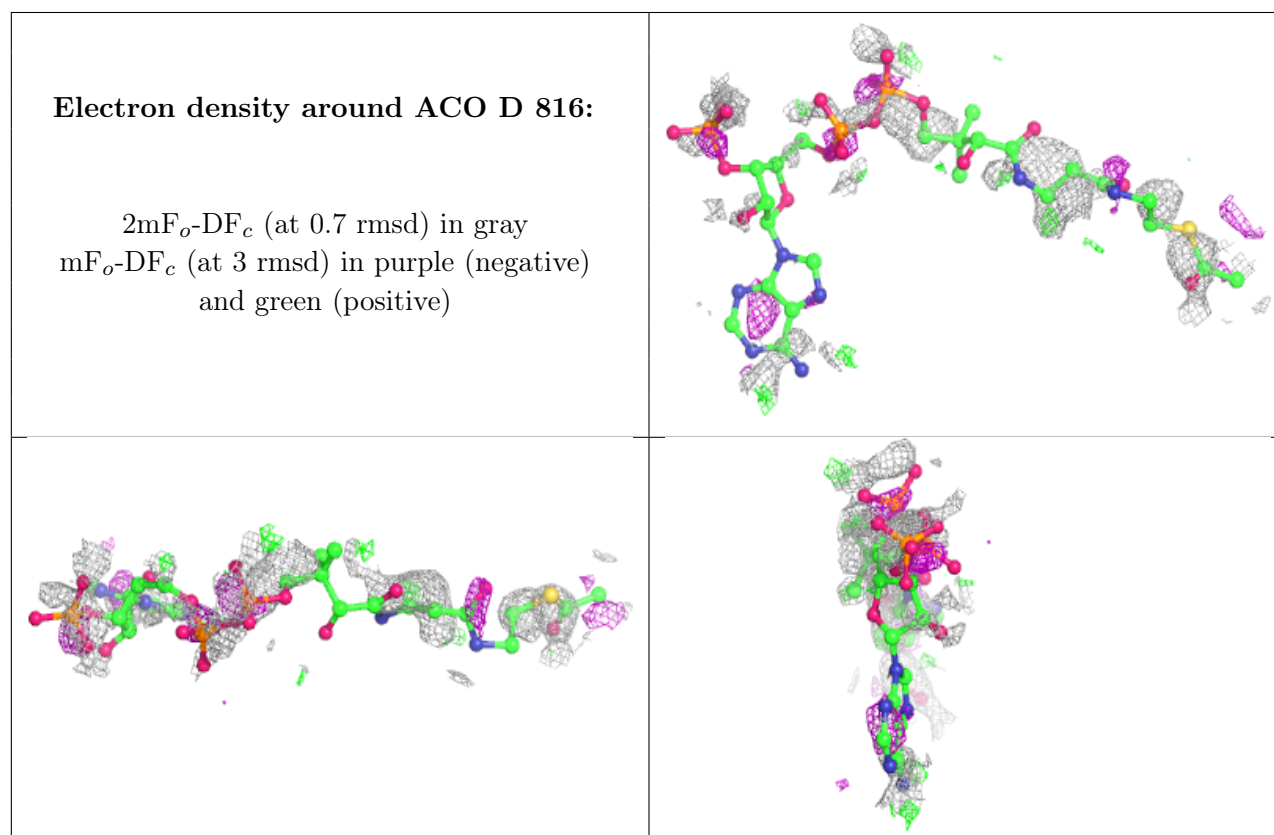
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACO	D	816	51/51	0.35	0.61	83,97,100,101	0
3	ACO	C	815	51/51	0.40	0.58	72,86,90,91	0
3	ACO	A	813	51/51	0.63	0.31	43,60,75,77	0
3	ACO	B	814	51/51	0.65	0.34	43,59,75,76	0
2	SO4	B	812	5/5	0.83	0.19	40,40,44,44	0
2	SO4	A	811	5/5	0.85	0.20	52,53,53,56	0

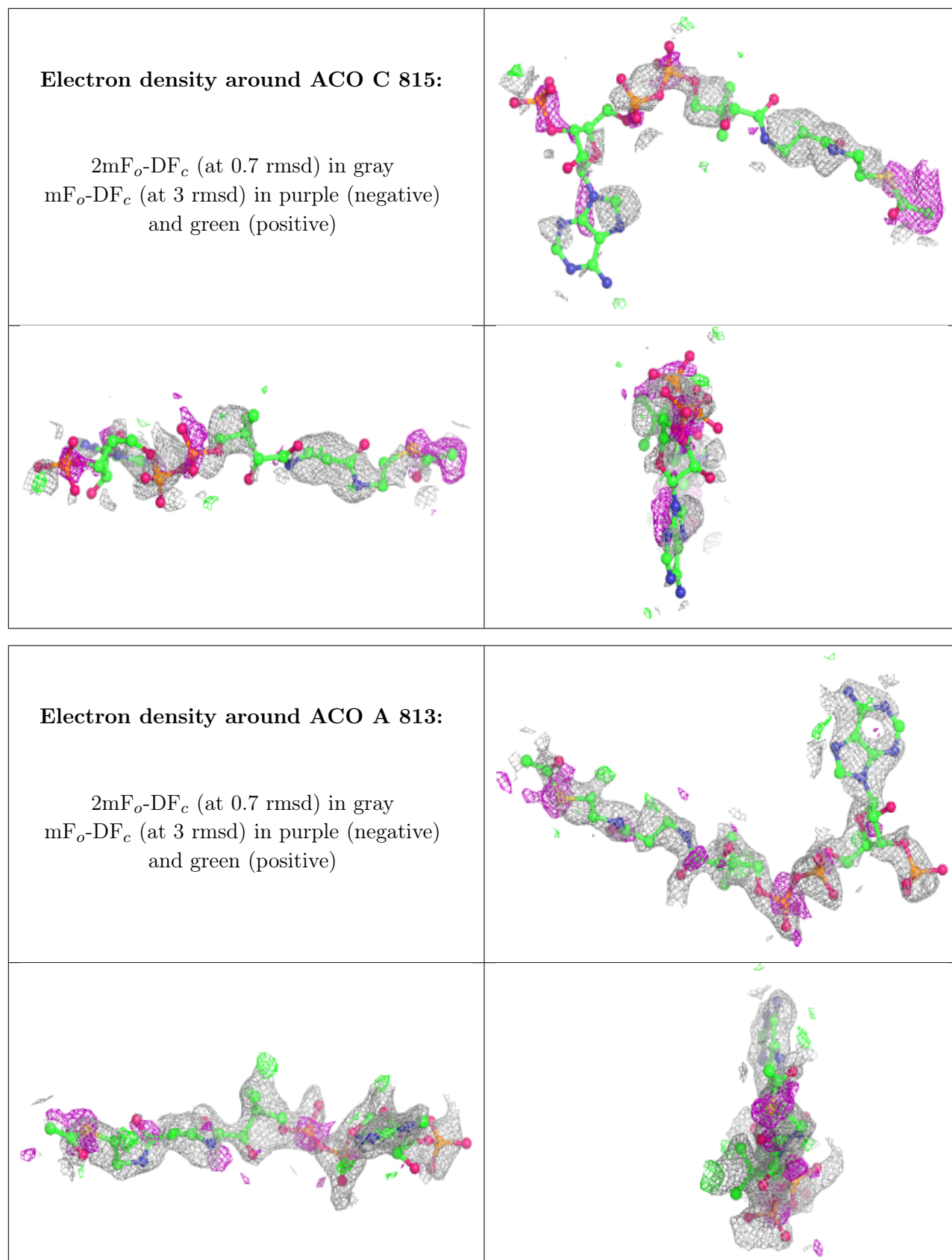
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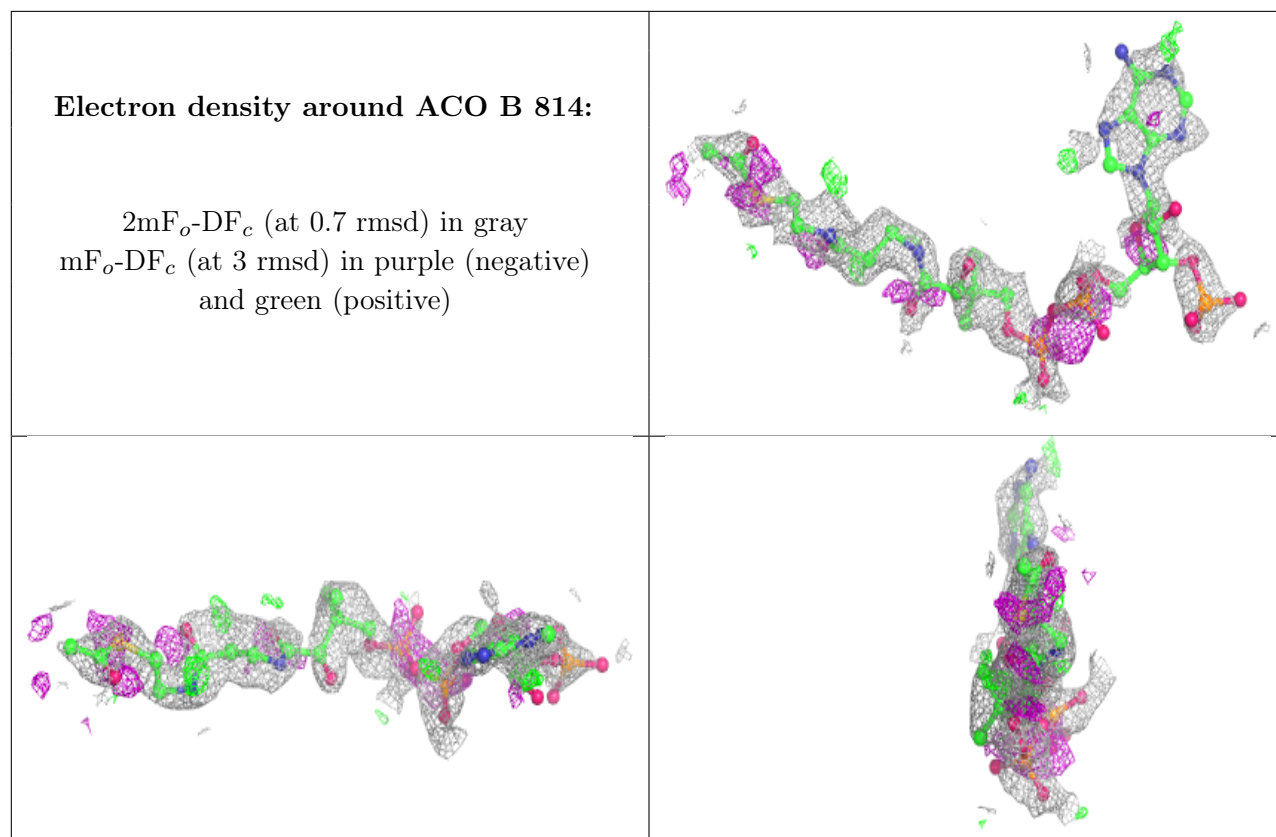
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	807	5/5	0.95	0.17	51,52,54,54	0
2	SO4	A	808	5/5	0.96	0.14	51,52,53,54	0
2	SO4	B	809	5/5	0.97	0.12	44,46,47,48	0
2	SO4	A	810	5/5	0.98	0.14	44,46,47,48	0

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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.