



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2021 – 02:40 am GMT

PDB ID : 6ZNG  
Title : MaeB full-length acetyl-CoA bound state  
Authors : Lovering, A.L.; Harding, C.J.  
Deposited on : 2020-07-06  
Resolution : 2.72 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:

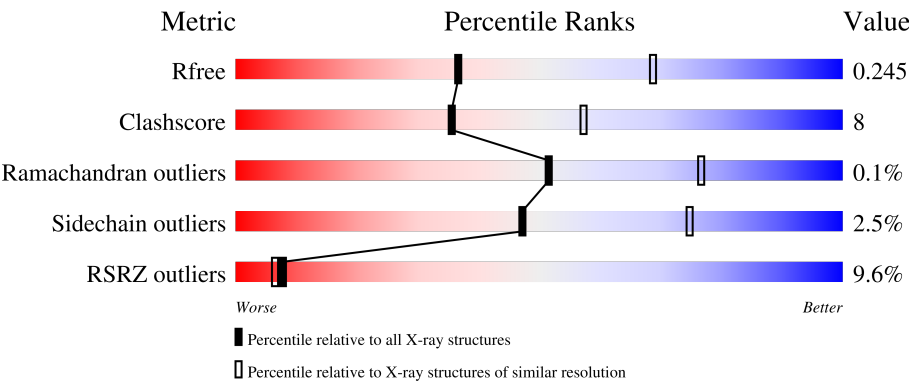
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17.1

# 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 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	791	<div><div>29%</div><div><div></div><div>70%</div><div>24%</div><div>• 5%</div></div></div>
1	B	791	<div><div>15%</div><div><div></div><div>75%</div><div>18%</div><div>• 5%</div></div></div>
1	C	791	<div><div>2%</div><div><div></div><div>80%</div><div>14%</div><div>• 5%</div></div></div>
1	D	791	<div><div>%</div><div><div></div><div>80%</div><div>15%</div><div>• 5%</div></div></div>
1	E	791	<div><div>3%</div><div><div></div><div>79%</div><div>15%</div><div>• 5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	791	<div> <div>5%</div> <div>75%</div> <div>19%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 34603 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 NADP-dependent malate dehydrogenase, Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	0	0
			5708	3626	978	1076	28			
1	B	748	Total	C	N	O	S	3	1	0
			5704	3624	977	1075	28			
1	C	750	Total	C	N	O	S	0	0	0
			5714	3629	979	1078	28			
1	D	750	Total	C	N	O	S	0	1	0
			5721	3633	982	1078	28			
1	E	751	Total	C	N	O	S	0	0	0
			5716	3631	981	1076	28			
1	F	753	Total	C	N	O	S	0	0	0
			5734	3641	986	1079	28			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q6MM14
A	-9	GLY	-	expression tag	UNP Q6MM14
A	-8	SER	-	expression tag	UNP Q6MM14
A	-7	SER	-	expression tag	UNP Q6MM14
A	-6	HIS	-	expression tag	UNP Q6MM14
A	-5	HIS	-	expression tag	UNP Q6MM14
A	-4	HIS	-	expression tag	UNP Q6MM14
A	-3	HIS	-	expression tag	UNP Q6MM14
A	-2	HIS	-	expression tag	UNP Q6MM14
A	-1	HIS	-	expression tag	UNP Q6MM14
A	0	SER	-	expression tag	UNP Q6MM14
A	121	ASP	-	linker	UNP Q6MM14
A	122	ILE	-	linker	UNP Q6MM14
A	123	GLU	-	linker	UNP Q6MM14
A	124	VAL	-	linker	UNP Q6MM14
B	-10	MET	-	initiating methionine	UNP Q6MM14

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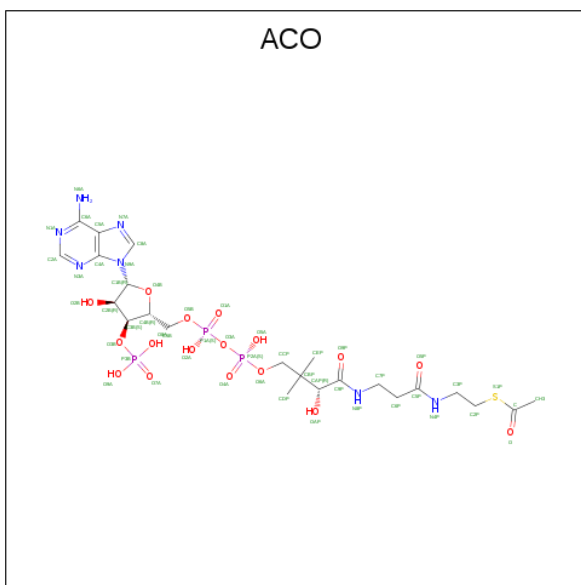
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP Q6MM14
B	-8	SER	-	expression tag	UNP Q6MM14
B	-7	SER	-	expression tag	UNP Q6MM14
B	-6	HIS	-	expression tag	UNP Q6MM14
B	-5	HIS	-	expression tag	UNP Q6MM14
B	-4	HIS	-	expression tag	UNP Q6MM14
B	-3	HIS	-	expression tag	UNP Q6MM14
B	-2	HIS	-	expression tag	UNP Q6MM14
B	-1	HIS	-	expression tag	UNP Q6MM14
B	0	SER	-	expression tag	UNP Q6MM14
B	121	ASP	-	linker	UNP Q6MM14
B	122	ILE	-	linker	UNP Q6MM14
B	123	GLU	-	linker	UNP Q6MM14
B	124	VAL	-	linker	UNP Q6MM14
C	-10	MET	-	initiating methionine	UNP Q6MM14
C	-9	GLY	-	expression tag	UNP Q6MM14
C	-8	SER	-	expression tag	UNP Q6MM14
C	-7	SER	-	expression tag	UNP Q6MM14
C	-6	HIS	-	expression tag	UNP Q6MM14
C	-5	HIS	-	expression tag	UNP Q6MM14
C	-4	HIS	-	expression tag	UNP Q6MM14
C	-3	HIS	-	expression tag	UNP Q6MM14
C	-2	HIS	-	expression tag	UNP Q6MM14
C	-1	HIS	-	expression tag	UNP Q6MM14
C	0	SER	-	expression tag	UNP Q6MM14
C	121	ASP	-	linker	UNP Q6MM14
C	122	ILE	-	linker	UNP Q6MM14
C	123	GLU	-	linker	UNP Q6MM14
C	124	VAL	-	linker	UNP Q6MM14
D	-10	MET	-	initiating methionine	UNP Q6MM14
D	-9	GLY	-	expression tag	UNP Q6MM14
D	-8	SER	-	expression tag	UNP Q6MM14
D	-7	SER	-	expression tag	UNP Q6MM14
D	-6	HIS	-	expression tag	UNP Q6MM14
D	-5	HIS	-	expression tag	UNP Q6MM14
D	-4	HIS	-	expression tag	UNP Q6MM14
D	-3	HIS	-	expression tag	UNP Q6MM14
D	-2	HIS	-	expression tag	UNP Q6MM14
D	-1	HIS	-	expression tag	UNP Q6MM14
D	0	SER	-	expression tag	UNP Q6MM14
D	121	ASP	-	linker	UNP Q6MM14
D	122	ILE	-	linker	UNP Q6MM14

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Chain	Residue	Modelled	Actual	Comment	Reference
D	123	GLU	-	linker	UNP Q6MM14
D	124	VAL	-	linker	UNP Q6MM14
E	-10	MET	-	initiating methionine	UNP Q6MM14
E	-9	GLY	-	expression tag	UNP Q6MM14
E	-8	SER	-	expression tag	UNP Q6MM14
E	-7	SER	-	expression tag	UNP Q6MM14
E	-6	HIS	-	expression tag	UNP Q6MM14
E	-5	HIS	-	expression tag	UNP Q6MM14
E	-4	HIS	-	expression tag	UNP Q6MM14
E	-3	HIS	-	expression tag	UNP Q6MM14
E	-2	HIS	-	expression tag	UNP Q6MM14
E	-1	HIS	-	expression tag	UNP Q6MM14
E	0	SER	-	expression tag	UNP Q6MM14
E	121	ASP	-	linker	UNP Q6MM14
E	122	ILE	-	linker	UNP Q6MM14
E	123	GLU	-	linker	UNP Q6MM14
E	124	VAL	-	linker	UNP Q6MM14
F	-10	MET	-	initiating methionine	UNP Q6MM14
F	-9	GLY	-	expression tag	UNP Q6MM14
F	-8	SER	-	expression tag	UNP Q6MM14
F	-7	SER	-	expression tag	UNP Q6MM14
F	-6	HIS	-	expression tag	UNP Q6MM14
F	-5	HIS	-	expression tag	UNP Q6MM14
F	-4	HIS	-	expression tag	UNP Q6MM14
F	-3	HIS	-	expression tag	UNP Q6MM14
F	-2	HIS	-	expression tag	UNP Q6MM14
F	-1	HIS	-	expression tag	UNP Q6MM14
F	0	SER	-	expression tag	UNP Q6MM14
F	121	ASP	-	linker	UNP Q6MM14
F	122	ILE	-	linker	UNP Q6MM14
F	123	GLU	-	linker	UNP Q6MM14
F	124	VAL	-	linker	UNP Q6MM14

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).

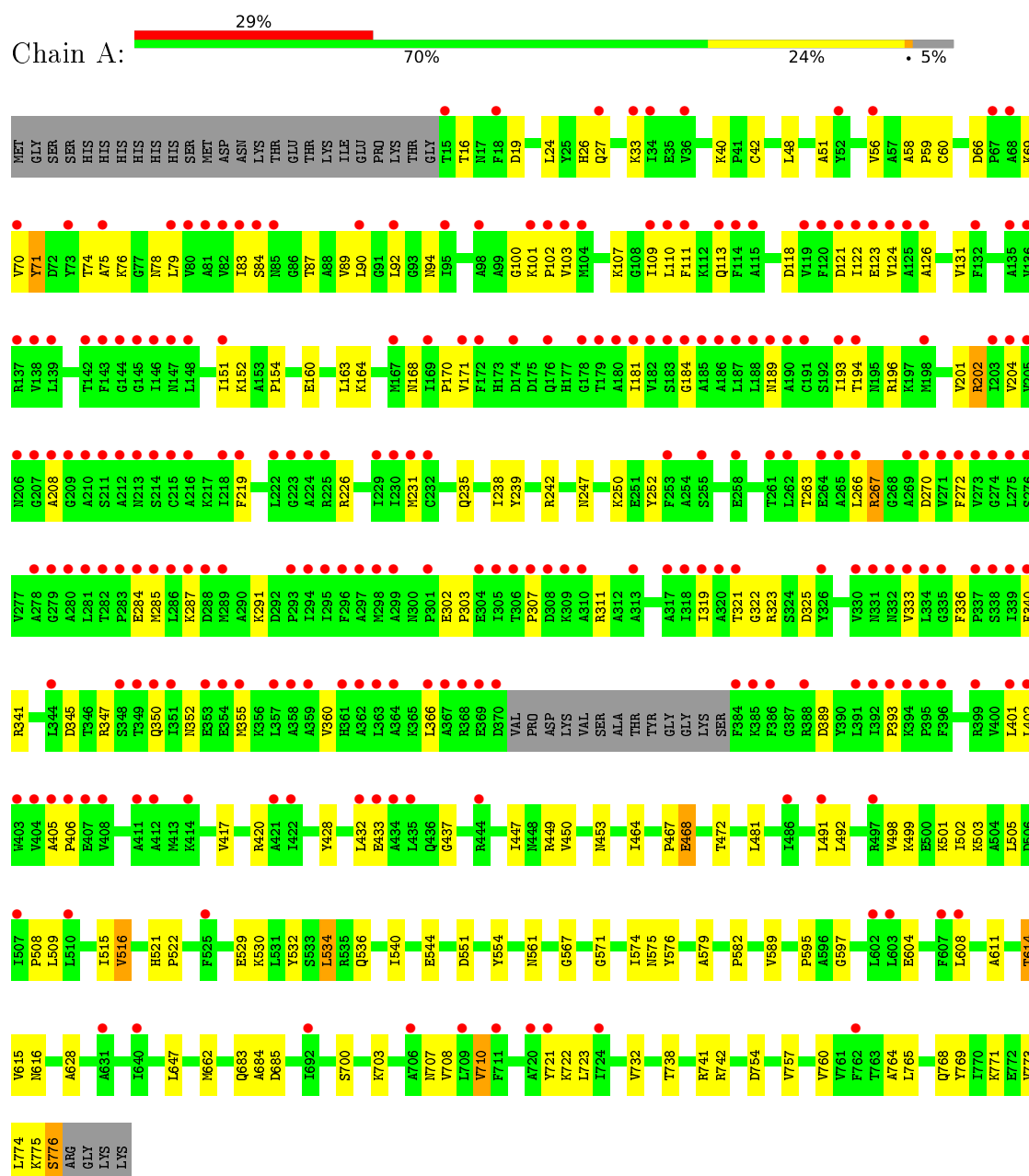


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
2	B	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
2	C	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
2	D	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
2	E	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
2	F	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADP-dependent malate dehydrogenase, Malate dehydrogenase

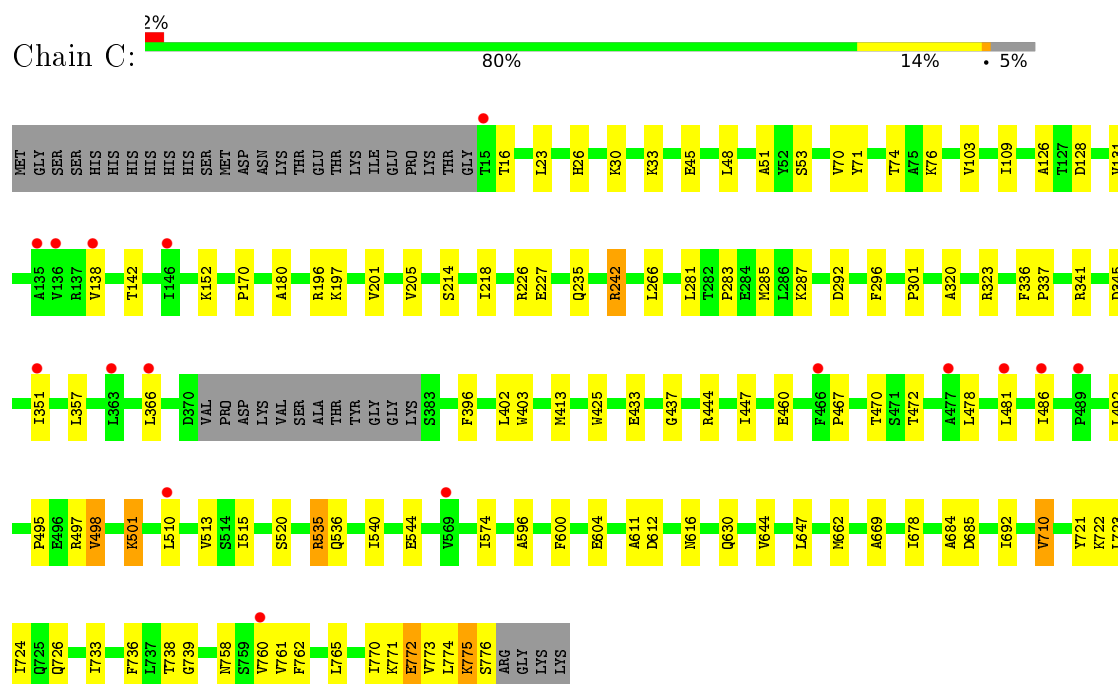


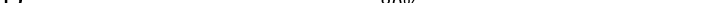


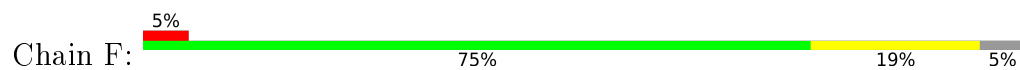
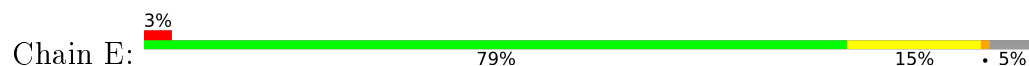
Chain B:

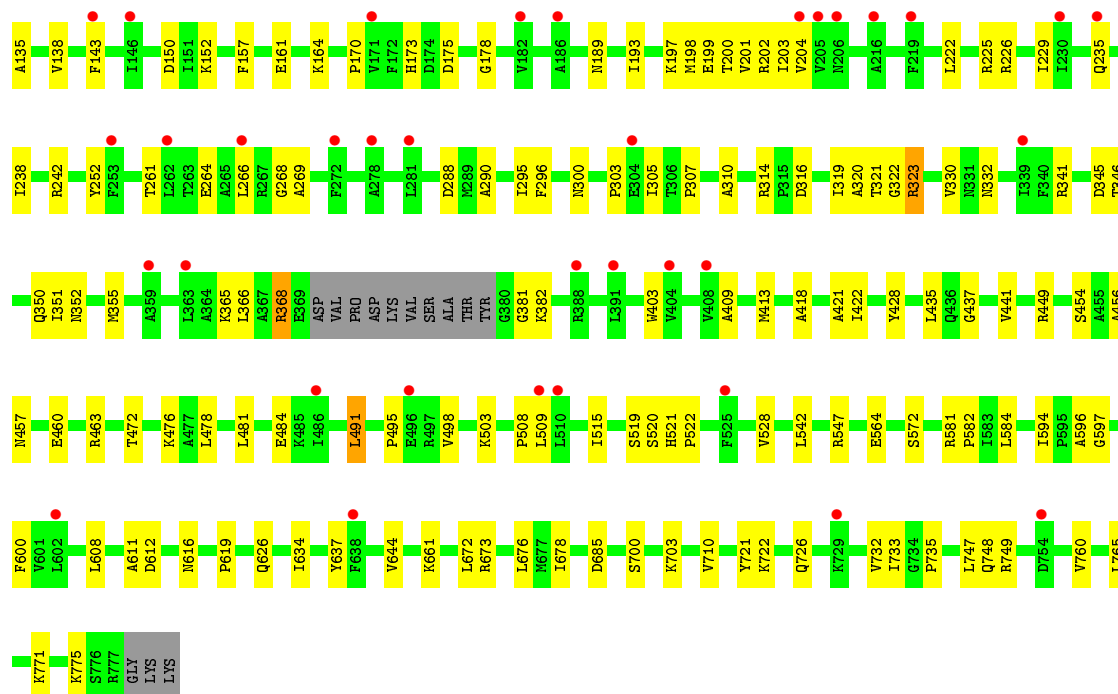


Chain C:



- Chain D:  80% 15% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	250.42Å 144.79Å 171.14Å 90.00° 100.61° 90.00°	Depositor
Resolution (Å)	109.38 – 2.72 123.07 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (109.38-2.72) 99.3 (123.07-2.72)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.73Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, $R_{free}$	0.190 , 0.230 0.217 , 0.245	Depositor DCC
$R_{free}$ test set	7980 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34603	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

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	0.41	0/5808	0.63	1/7864 (0.0%)
1	B	0.44	0/5807	0.65	0/7863
1	C	0.59	0/5814	0.70	1/7872 (0.0%)
1	D	0.61	0/5824	0.72	0/7885
1	E	0.53	0/5816	0.68	1/7872 (0.0%)
1	F	0.55	0/5834	0.70	0/7896
All	All	0.53	0/34903	0.68	3/47252 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	LEU	CA-CB-CG	10.57	139.60	115.30
1	E	175	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	242	ARG	NE-CZ-NH2	-5.66	117.47	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5708	0	5811	142	0
1	B	5704	0	5809	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5714	0	5816	97	0
1	D	5721	0	5827	88	0
1	E	5716	0	5824	80	0
1	F	5734	0	5844	101	0
2	A	51	0	34	3	0
2	B	51	0	34	4	0
2	C	51	0	34	4	0
2	D	51	0	34	5	0
2	E	51	0	34	4	0
2	F	51	0	34	6	0
All	All	34603	0	35135	567	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 8.

All (567) 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)
2:D:801:ACO:O4B	2:D:801:ACO:C1B	1.64	1.24
2:C:801:ACO:O4B	2:C:801:ACO:C1B	1.63	1.18
2:E:801:ACO:O4B	2:E:801:ACO:C1B	1.63	1.18
2:A:801:ACO:O4B	2:A:801:ACO:C1B	1.64	1.16
2:F:801:ACO:O4B	2:F:801:ACO:C1B	1.64	1.15
2:B:801:ACO:O4B	2:B:801:ACO:C1B	1.64	1.13
1:F:352:ASN:H	1:F:355:MET:HE3	1.30	0.94
1:C:74:THR:HG22	1:C:76:LYS:H	1.34	0.92
1:A:66:ASP:HB3	1:A:69:LYS:HE2	1.52	0.91
1:C:402:LEU:HD21	1:C:433:GLU:HG3	1.58	0.85
2:E:801:ACO:H8A	2:E:801:ACO:H52A	1.58	0.84
1:F:748:GLN:HB3	2:F:801:ACO:HH31	1.59	0.83
1:D:235:GLN:HB2	1:D:242:ARG:HH21	1.42	0.82
1:A:773:VAL:O	1:A:776:SER:HB3	1.79	0.82
1:D:78:ASN:OD1	1:D:341:ARG:NH2	2.16	0.79
1:A:196:ARG:NH2	1:A:291:LYS:O	2.17	0.77
1:B:352:ASN:H	1:B:355:MET:HE3	1.47	0.77
1:E:321:THR:HG22	1:E:323:ARG:H	1.51	0.75
1:F:305:ILE:HD13	1:F:310:ALA:HB2	1.69	0.74
1:C:770:ILE:O	1:C:773:VAL:HG12	1.88	0.74
1:D:26:HIS:NE2	1:D:33:LYS:HE3	2.04	0.73
1:C:180:ALA:HB1	1:C:218:ILE:HD11	1.69	0.72
1:E:700:SER:O	1:E:703:LYS:NZ	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ASP:HB3	1:F:131:VAL:HG12	1.70	0.71
1:A:126:ALA:HB2	1:B:138:VAL:HG21	1.72	0.71
1:F:307:PRO:HA	1:F:319:ILE:HD13	1.71	0.70
1:B:83:ILE:HG12	1:B:122:ILE:HB	1.74	0.69
1:F:226:ARG:NH2	1:F:252:TYR:O	2.26	0.69
1:B:614:THR:HG22	1:B:615:VAL:HG23	1.74	0.68
1:A:16:THR:HA	1:A:19:ASP:HB2	1.75	0.68
1:A:771:LYS:O	1:A:774:LEU:HB2	1.92	0.68
1:B:282:THR:HG22	1:B:285:MET:HG3	1.74	0.68
1:A:508:PRO:HD2	1:A:509:LEU:HD12	1.76	0.68
1:F:300:ASN:ND2	1:F:323:ARG:HH22	1.93	0.67
1:A:530:LYS:O	1:A:534:LEU:HD23	1.93	0.67
1:B:235:GLN:HB2	1:B:242:ARG:HH22	1.58	0.67
1:A:352:ASN:H	1:A:355:MET:HE3	1.58	0.67
1:C:70:VAL:O	1:C:74:THR:HB	1.93	0.67
1:C:497:ARG:HH12	1:F:519:SER:HB3	1.60	0.67
1:A:453:ASN:CB	1:A:768:GLN:OE1	2.43	0.67
1:E:138:VAL:HG21	1:F:126:ALA:HB2	1.76	0.67
1:A:498:VAL:HG11	1:A:515:ILE:HG21	1.78	0.66
1:A:26:HIS:NE2	1:A:33:LYS:HE3	2.11	0.66
1:B:306:THR:HG23	1:B:309:LYS:H	1.61	0.66
1:B:350:GLN:HE21	1:B:352:ASN:HB3	1.61	0.66
1:C:30:LYS:O	1:D:40:LYS:NZ	2.28	0.66
1:C:109:ILE:HD12	1:D:38:SER:HB3	1.76	0.66
1:A:131:VAL:HG21	1:B:137:ARG:NH1	2.12	0.65
1:A:501:LYS:HE2	1:A:505:LEU:HD11	1.76	0.65
1:A:42:CYS:O	1:B:113:GLN:NE2	2.30	0.65
1:A:311:ARG:NH2	1:A:389:ASP:OD1	2.30	0.65
1:B:301:PRO:O	1:B:323:ARG:NH2	2.30	0.65
1:E:33:LYS:NZ	1:F:51:ALA:O	2.29	0.65
1:C:692:ILE:HD13	1:D:750:THR:CG2	2.27	0.65
1:A:33:LYS:NZ	1:A:102:PRO:O	2.29	0.64
1:F:472:THR:HG22	1:F:476:LYS:HE2	1.80	0.64
1:A:614:THR:HG22	1:A:615:VAL:HG23	1.79	0.64
1:A:164:LYS:HG2	1:A:171:VAL:HB	1.79	0.64
1:C:26:HIS:NE2	1:C:33:LYS:HE3	2.12	0.64
2:B:801:ACO:H52A	2:B:801:ACO:H8A	1.79	0.64
1:D:170:PRO:HB3	1:D:351:ILE:HG13	1.79	0.64
1:E:263:THR:HG22	1:E:285:MET:CE	2.28	0.63
1:A:307:PRO:HA	1:A:319:ILE:HD13	1.81	0.63
1:D:341:ARG:NH1	1:D:345:ASP:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:THR:HG23	1:E:285:MET:HG2	1.80	0.63
1:B:673:ARG:HG2	1:B:676:LEU:HD22	1.80	0.63
1:E:307:PRO:HA	1:E:319:ILE:HD13	1.81	0.63
1:C:74:THR:HG21	1:D:101:LYS:HD3	1.79	0.63
1:C:773:VAL:HG13	1:C:774:LEU:N	2.13	0.63
1:F:268:GLY:N	1:F:288:ASP:O	2.29	0.63
1:F:198:MET:HA	1:F:201:VAL:HG23	1.79	0.63
1:B:67:PRO:O	1:B:70:VAL:HG12	1.98	0.63
1:F:463:ARG:NH1	1:F:564:GLU:O	2.32	0.63
1:E:42:CYS:HA	1:E:47:ASP:HB3	1.81	0.62
1:B:748:GLN:HB3	2:B:801:ACO:HH31	1.82	0.62
1:F:235:GLN:HB2	1:F:242:ARG:NH2	2.15	0.62
1:E:661:LYS:HE3	1:E:662:MET:CE	2.30	0.62
1:B:196:ARG:NH2	1:B:291:LYS:O	2.32	0.62
1:B:366:LEU:HD12	1:B:403:TRP:CG	2.35	0.62
1:A:170:PRO:HA	1:A:350:GLN:HA	1.82	0.61
1:B:108:GLY:CA	1:B:119:VAL:HG21	2.30	0.61
1:D:128:ASP:HB3	1:D:131:VAL:HG22	1.82	0.61
1:B:449:ARG:HA	1:B:452:GLN:HG2	1.82	0.61
1:D:126:ALA:HB1	1:D:131:VAL:HG23	1.82	0.61
1:B:208:ALA:HB2	1:B:233:ASP:HB3	1.83	0.61
1:E:108:GLY:HA2	1:E:119:VAL:HG21	1.82	0.61
1:F:303:PRO:HB3	1:F:321:THR:HG23	1.82	0.61
1:A:154:PRO:HG3	1:A:247:ASN:HD22	1.66	0.60
1:A:616:ASN:OD1	2:A:801:ACO:N6A	2.34	0.60
1:D:300:ASN:OD1	1:D:323:ARG:NH2	2.34	0.60
1:E:108:GLY:CA	1:E:119:VAL:HG21	2.31	0.60
1:A:499:LYS:HA	1:A:502:ILE:HG12	1.84	0.60
1:C:770:ILE:O	1:C:773:VAL:CG1	2.49	0.60
1:E:282:THR:OG1	1:E:284:GLU:OE1	2.18	0.60
1:D:616:ASN:OD1	2:D:801:ACO:N6A	2.34	0.60
1:B:170:PRO:HB3	1:B:351:ILE:HG13	1.81	0.60
1:D:283:PRO:O	1:D:287:LYS:HG3	2.02	0.60
1:A:597:GLY:HA3	1:A:614:THR:HB	1.83	0.60
1:E:189:ASN:O	1:E:193:ILE:HD12	2.02	0.60
1:F:463:ARG:HH12	1:F:564:GLU:C	2.04	0.60
1:C:536:GLN:HA	1:C:540:ILE:O	2.02	0.59
1:F:413:MET:HE1	1:F:422:ILE:H	1.65	0.59
1:C:772:GLU:OE1	1:C:775:LYS:NZ	2.30	0.59
1:D:242:ARG:NH1	1:D:246:MET:SD	2.75	0.59
1:B:498:VAL:HG11	1:B:515:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:771:LYS:HG2	1:F:775:LYS:HE2	1.84	0.59
1:A:184:GLY:HA2	1:A:219:PHE:HE1	1.68	0.59
1:C:460:GLU:OE2	1:C:771:LYS:NZ	2.31	0.59
1:F:611:ALA:O	1:F:710:VAL:HA	2.03	0.59
1:A:447:ILE:O	1:A:450:VAL:HG12	2.03	0.58
1:A:131:VAL:HG21	1:B:137:ARG:HH11	1.68	0.58
1:A:71:TYR:CD1	1:A:347:ARG:HD2	2.39	0.58
1:E:662:MET:HE3	1:E:712:PRO:HA	1.85	0.58
1:B:366:LEU:HD22	1:B:393:PRO:HG3	1.84	0.58
1:D:116:GLY:HA3	1:D:435:LEU:HD22	1.85	0.58
1:E:306:THR:HG23	1:E:309:LYS:H	1.68	0.58
1:B:597:GLY:HA3	1:B:614:THR:HB	1.86	0.57
1:D:773:VAL:O	1:D:776:SER:HB3	2.04	0.57
1:F:202:ARG:NH1	1:F:268:GLY:O	2.37	0.57
1:C:283:PRO:O	1:C:287:LYS:HG2	2.03	0.57
1:F:261:THR:HG23	1:F:264:GLU:H	1.68	0.57
2:C:801:ACO:H8A	2:C:801:ACO:H52A	1.85	0.57
1:A:71:TYR:OH	1:A:420:ARG:NH1	2.31	0.57
1:C:170:PRO:HB3	1:C:351:ILE:HG13	1.87	0.57
1:B:164:LYS:HG2	1:B:171:VAL:HB	1.86	0.57
1:C:235:GLN:HB3	1:C:242:ARG:HH22	1.68	0.56
1:D:26:HIS:CD2	1:D:33:LYS:HE3	2.39	0.56
1:A:341:ARG:NH1	1:A:345:ASP:OD1	2.38	0.56
1:A:71:TYR:CG	1:A:347:ARG:HD2	2.41	0.56
1:A:154:PRO:HG3	1:A:247:ASN:ND2	2.20	0.56
1:E:128:ASP:HB3	1:E:131:VAL:HG22	1.87	0.56
1:A:284:GLU:HA	1:A:287:LYS:HG3	1.88	0.56
1:A:24:LEU:HA	1:A:27:GLN:HG2	1.88	0.56
1:D:413:MET:HE1	1:D:425:TRP:HZ2	1.71	0.56
1:C:180:ALA:CB	1:C:218:ILE:HD11	2.36	0.56
1:C:447:ILE:HG23	1:C:486:ILE:HD11	1.89	0.56
1:A:66:ASP:HB3	1:A:69:LYS:CE	2.31	0.55
1:A:226:ARG:NH2	1:A:252:TYR:O	2.39	0.55
1:D:596:ALA:HB1	1:D:612:ASP:HB2	1.88	0.55
1:F:126:ALA:HB1	1:F:131:VAL:HG13	1.88	0.55
1:A:468:GLU:OE1	1:A:571:GLY:N	2.35	0.55
1:B:557:ALA:HA	1:B:568:MET:CE	2.36	0.55
1:C:126:ALA:HB1	1:C:131:VAL:HG23	1.87	0.55
1:E:397:ASP:HB3	1:E:400:VAL:HG23	1.88	0.55
1:C:196:ARG:NH2	1:C:292:ASP:O	2.36	0.55
1:A:321:THR:HG22	1:A:323:ARG:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ALA:HB2	1:F:138:VAL:HG21	1.89	0.55
1:A:647:LEU:O	1:A:662:MET:HG3	2.07	0.55
1:A:402:LEU:HD21	1:A:433:GLU:HG3	1.89	0.55
1:E:498:VAL:HG11	1:E:515:ILE:HG21	1.88	0.55
1:A:33:LYS:HB3	1:A:109:ILE:HD11	1.87	0.54
1:B:197:LYS:O	1:B:200:THR:HG22	2.06	0.54
1:C:535:ARG:NH2	2:C:801:ACO:O9A	2.41	0.54
1:D:282:THR:HG22	1:D:284:GLU:H	1.70	0.54
1:F:197:LYS:O	1:F:200:THR:HG22	2.07	0.54
1:E:494:TYR:HD2	1:E:497:ARG:HD3	1.71	0.54
1:F:56:VAL:O	1:F:59:PRO:HD2	2.08	0.54
1:F:202:ARG:HH12	1:F:269:ALA:HA	1.71	0.54
1:A:323:ARG:NH2	1:A:325:ASP:OD1	2.40	0.54
1:A:481:LEU:HG	1:A:757:VAL:HG12	1.90	0.54
1:D:189:ASN:OD1	1:D:368:ARG:HD2	2.08	0.54
1:A:194:THR:O	1:A:194:THR:HG22	2.08	0.54
1:C:413:MET:HE1	1:C:425:TRP:HZ2	1.72	0.54
1:E:554:TYR:CE1	1:E:582:PRO:HB3	2.42	0.54
1:A:449:ARG:HD2	1:A:765:LEU:HD21	1.89	0.54
1:D:508:PRO:HD2	1:D:509:LEU:HD12	1.89	0.54
1:A:201:VAL:HG13	1:A:270:ASP:HB2	1.90	0.54
1:A:40:LYS:NZ	1:B:30:LYS:O	2.40	0.54
1:A:453:ASN:HB2	1:A:768:GLN:OE1	2.07	0.54
2:A:801:ACO:H8A	2:A:801:ACO:H52A	1.88	0.54
1:C:214:SER:O	1:C:218:ILE:HG12	2.07	0.54
1:A:589:VAL:HG11	1:A:595:PRO:HD3	1.89	0.54
1:C:472:THR:HG22	1:C:501:LYS:HE2	1.89	0.54
1:B:589:VAL:HG11	1:B:595:PRO:HD3	1.90	0.53
1:F:321:THR:HG22	1:F:322:GLY:N	2.24	0.53
1:A:90:LEU:HB2	1:A:92:LEU:HD13	1.90	0.53
1:A:754:ASP:HA	1:A:757:VAL:HG22	1.91	0.53
1:E:170:PRO:HB3	1:E:351:ILE:HG13	1.91	0.53
1:E:296:PHE:CD1	1:E:320:ALA:HB3	2.44	0.53
1:F:295:ILE:HG21	1:F:305:ILE:HD11	1.88	0.53
1:B:128:ASP:HB3	1:B:131:VAL:HG12	1.89	0.53
1:E:263:THR:HG22	1:E:285:MET:HE2	1.90	0.53
1:A:123:GLU:N	1:B:142:THR:OG1	2.38	0.53
1:B:211:SER:OG	1:B:275:LEU:HD13	2.09	0.53
1:C:413:MET:HE1	1:C:425:TRP:CZ2	2.44	0.53
1:D:217:LYS:O	1:D:220:ILE:HG13	2.08	0.53
1:B:248:LYS:HD3	1:B:249:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:748:GLN:HB3	2:E:801:ACO:HH31	1.92	0.52
1:B:134:ASN:OD1	1:B:137:ARG:NH2	2.43	0.52
1:D:760:VAL:HA	1:D:763:THR:HG23	1.91	0.52
1:E:424:ASP:HB3	1:E:427:GLN:HB3	1.91	0.52
1:C:600:PHE:HB2	1:C:733:ILE:CG1	2.39	0.52
1:B:447:ILE:O	1:B:450:VAL:HG12	2.10	0.52
1:D:137:ARG:NH1	1:D:162:ARG:HH21	2.07	0.52
1:B:271:VAL:HG22	1:B:294:ILE:HB	1.92	0.52
1:E:164:LYS:HG2	1:E:171:VAL:HB	1.91	0.51
1:E:321:THR:HG22	1:E:323:ARG:N	2.23	0.51
1:D:770:ILE:HA	1:D:773:VAL:HG12	1.92	0.51
1:E:37:ILE:HD13	1:F:37:ILE:HD13	1.92	0.51
1:A:101:LYS:HE3	1:A:121:ASP:OD2	2.10	0.51
1:C:722:LYS:HE3	1:D:685:ASP:OD2	2.10	0.51
1:B:301:PRO:C	1:B:323:ARG:HH21	2.13	0.51
1:D:413:MET:HE1	1:D:425:TRP:CZ2	2.45	0.51
1:D:447:ILE:HG23	1:D:486:ILE:HD11	1.93	0.51
1:B:66:ASP:HB2	1:B:69:LYS:HE2	1.92	0.51
1:F:198:MET:HA	1:F:201:VAL:CG2	2.41	0.51
1:F:199:GLU:HG3	1:F:225:ARG:HG3	1.92	0.51
1:C:281:LEU:HD12	1:C:285:MET:HE2	1.93	0.51
1:D:737:LEU:H	1:D:745:ASN:HD22	1.57	0.51
1:D:301:PRO:O	1:D:323:ARG:NE	2.44	0.51
1:B:238:ILE:HG22	1:B:254:ALA:HA	1.93	0.51
1:D:499:LYS:O	1:D:503:LYS:HG3	2.11	0.51
1:C:596:ALA:HB1	1:C:612:ASP:HB2	1.92	0.50
1:E:467:PRO:HA	1:E:492:LEU:HB2	1.92	0.50
1:C:574:ILE:HG21	1:F:547:ARG:HD2	1.93	0.50
1:D:437:GLY:HA3	1:D:604:GLU:O	2.10	0.50
1:F:596:ALA:HB1	1:F:612:ASP:HB2	1.93	0.50
1:A:611:ALA:O	1:A:710:VAL:HA	2.12	0.50
1:E:722:LYS:HE3	1:F:685:ASP:OD1	2.12	0.50
1:F:95:ILE:HD12	1:F:99:ALA:HB3	1.92	0.50
1:A:78:ASN:ND2	1:A:118:ASP:OD1	2.44	0.50
1:A:208:ALA:HB1	1:A:250:LYS:HE2	1.93	0.50
1:A:536:GLN:HA	1:A:540:ILE:O	2.12	0.50
1:B:677:MET:CE	1:B:703:LYS:H	2.25	0.50
1:C:235:GLN:CB	1:C:242:ARG:HH22	2.24	0.50
1:F:58:ALA:HB3	1:F:59:PRO:HD3	1.92	0.50
1:A:437:GLY:HA3	1:A:604:GLU:O	2.11	0.50
1:B:194:THR:HG22	1:B:194:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HD12	1:B:403:TRP:CD1	2.46	0.50
1:C:74:THR:HG22	1:C:76:LYS:N	2.16	0.50
1:E:257:THR:O	1:E:260:ARG:NH1	2.44	0.49
1:E:661:LYS:HE3	1:E:662:MET:HE2	1.93	0.49
1:E:685:ASP:OD1	1:F:722:LYS:HD3	2.12	0.49
1:F:616:ASN:OD1	2:F:801:ACO:N6A	2.45	0.49
1:A:160:GLU:O	1:A:164:LYS:HG3	2.13	0.49
1:A:769:TYR:CD1	1:A:769:TYR:C	2.85	0.49
1:B:198:MET:O	1:B:201:VAL:HG12	2.12	0.49
1:E:524:TYR:O	1:E:527:PHE:HB2	2.12	0.49
1:C:738:THR:HG22	1:C:739:GLY:N	2.28	0.49
1:E:321:THR:HG22	1:E:322:GLY:N	2.27	0.49
1:A:491:LEU:HB2	1:A:515:ILE:HG12	1.95	0.49
1:A:266:LEU:HD21	1:A:272:PHE:CD1	2.48	0.49
1:B:605:ASP:OD2	1:B:605:ASP:N	2.38	0.49
1:E:478:LEU:HD11	1:E:491:LEU:HD21	1.95	0.49
1:F:76:LYS:NZ	1:F:143:PHE:O	2.37	0.49
1:F:296:PHE:CD1	1:F:320:ALA:HB3	2.48	0.49
1:F:409:ALA:O	1:F:413:MET:HG2	2.13	0.49
1:A:100:GLY:O	1:A:103:VAL:HG22	2.13	0.49
1:C:341:ARG:NH1	1:C:345:ASP:OD1	2.46	0.49
1:A:401:LEU:CD2	1:A:432:LEU:HB3	2.42	0.49
1:B:208:ALA:HB1	1:B:250:LYS:HD2	1.94	0.49
1:B:469:GLY:HA2	1:B:491:LEU:HD22	1.95	0.49
1:B:677:MET:HE3	1:B:702:LEU:HD12	1.95	0.49
1:C:142:THR:O	1:D:101:LYS:NZ	2.38	0.49
1:E:554:TYR:CZ	1:E:582:PRO:HB3	2.48	0.49
1:F:700:SER:O	1:F:703:LYS:HE3	2.13	0.49
1:D:614:THR:HG22	2:D:801:ACO:HH33	1.95	0.49
1:D:737:LEU:H	1:D:745:ASN:ND2	2.11	0.49
1:F:478:LEU:CD1	1:F:491:LEU:HD11	2.42	0.49
1:F:498:VAL:HG13	1:F:515:ILE:HD13	1.94	0.49
1:A:574:ILE:HG23	1:A:579:ALA:HB2	1.95	0.48
1:C:510:LEU:HD22	1:C:513:VAL:HG21	1.95	0.48
1:A:502:ILE:HG13	1:A:503:LYS:N	2.28	0.48
1:A:574:ILE:HD12	1:D:544:GLU:HG2	1.95	0.48
1:A:684:ALA:HB1	1:B:723:LEU:HG	1.96	0.48
1:B:204:VAL:HG11	1:B:266:LEU:HD12	1.96	0.48
1:F:413:MET:HE2	1:F:421:ALA:HA	1.96	0.48
1:B:673:ARG:CG	1:B:676:LEU:HD22	2.43	0.48
1:C:630:GLN:HB3	1:C:738:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:LEU:HD13	1:D:724:ILE:HD11	1.94	0.48
1:E:413:MET:HE1	1:E:425:TRP:CZ2	2.48	0.48
1:F:673:ARG:HG2	1:F:676:LEU:HD12	1.96	0.48
1:A:401:LEU:HD23	1:A:432:LEU:HB3	1.95	0.48
1:B:95:ILE:HD12	1:B:99:ALA:HB3	1.96	0.48
1:A:700:SER:O	1:A:703:LYS:HE3	2.14	0.48
1:B:219:PHE:HE2	1:B:273:VAL:HG21	1.78	0.48
1:C:301:PRO:HA	1:C:323:ARG:HH21	1.79	0.48
1:E:496:GLU:O	1:E:500:GLU:HG3	2.14	0.48
1:F:198:MET:HE1	1:F:222:LEU:HB3	1.96	0.48
1:A:84:SER:HA	1:A:151:ILE:HD11	1.94	0.48
1:A:204:VAL:HG11	1:A:266:LEU:HD12	1.96	0.48
1:C:138:VAL:HG21	1:D:126:ALA:HB2	1.94	0.48
1:D:481:LEU:HD13	1:D:760:VAL:HG11	1.96	0.48
1:F:157:PHE:O	1:F:161:GLU:HG3	2.14	0.48
1:A:109:ILE:O	1:A:113:GLN:HG2	2.13	0.48
1:A:402:LEU:HD21	1:A:433:GLU:CG	2.44	0.48
1:A:492:LEU:HD23	1:A:516:VAL:HG13	1.95	0.48
1:B:101:LYS:HG3	1:B:123:GLU:CD	2.34	0.48
1:B:240:LYS:HD2	1:B:251:GLU:OE2	2.14	0.48
1:C:128:ASP:HB3	1:C:131:VAL:HG22	1.96	0.48
1:B:544:GLU:HG2	1:E:574:ILE:HD13	1.96	0.47
1:D:239:TYR:CE2	1:D:242:ARG:HD2	2.49	0.47
1:D:673:ARG:HG2	1:D:676:LEU:HD12	1.95	0.47
1:B:472:THR:HB	1:B:505:LEU:HD11	1.95	0.47
1:A:554:TYR:CZ	1:A:582:PRO:HB3	2.49	0.47
1:B:160:GLU:O	1:B:164:LYS:HG3	2.14	0.47
1:A:685:ASP:OD1	1:B:722:LYS:HD3	2.14	0.47
1:B:510:LEU:O	1:B:513:VAL:HG22	2.15	0.47
1:C:197:LYS:O	1:C:201:VAL:HG23	2.14	0.47
1:D:287:LYS:HA	1:D:314:ARG:HD2	1.96	0.47
1:D:495:PRO:HA	1:D:515:ILE:HG21	1.97	0.47
1:D:600:PHE:O	1:D:732:VAL:HA	2.15	0.47
1:A:467:PRO:HA	1:A:492:LEU:HB2	1.96	0.47
1:F:204:VAL:HG11	1:F:266:LEU:HD12	1.97	0.47
1:F:203:ILE:HB	1:F:229:ILE:HG12	1.96	0.47
1:A:561:ASN:OD1	1:A:741:ARG:NH2	2.48	0.46
1:C:611:ALA:O	1:C:710:VAL:HA	2.15	0.46
1:D:744:ALA:O	1:D:745:ASN:ND2	2.48	0.46
1:F:508:PRO:HD2	1:F:509:LEU:HD12	1.96	0.46
1:E:741:ARG:NH1	1:E:742:ARG:HH22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:VAL:HA	1:F:150:ASP:OD2	2.14	0.46
1:F:382:LYS:HD2	1:F:456:ALA:HB3	1.95	0.46
1:F:189:ASN:O	1:F:193:ILE:HD12	2.14	0.46
1:D:221:ALA:HB1	1:D:357:LEU:HD11	1.97	0.46
1:D:284:GLU:N	1:D:284:GLU:OE1	2.47	0.46
1:E:656:GLU:OE1	1:E:660:ARG:NE	2.49	0.46
1:F:316:ASP:N	1:F:316:ASP:OD1	2.46	0.46
1:F:600:PHE:HB2	1:F:733:ILE:CG1	2.45	0.46
1:A:70:VAL:O	1:A:74:THR:HB	2.16	0.46
1:C:685:ASP:OD2	1:D:722:LYS:HD3	2.16	0.46
2:D:801:ACO:C5B	2:D:801:ACO:H8A	2.46	0.46
1:E:754:ASP:O	1:E:757:VAL:HG22	2.15	0.46
1:A:774:LEU:O	1:A:776:SER:N	2.49	0.46
1:B:202:ARG:O	1:B:270:ASP:N	2.48	0.46
1:C:770:ILE:HA	1:C:773:VAL:HG12	1.97	0.46
1:E:196:ARG:NH2	1:E:292:ASP:O	2.30	0.46
1:F:323:ARG:HH11	1:F:323:ARG:HA	1.81	0.46
1:A:453:ASN:ND2	1:A:768:GLN:OE1	2.45	0.46
1:B:80:VAL:O	1:B:119:VAL:HA	2.16	0.46
1:B:108:GLY:HA3	1:B:119:VAL:HG21	1.97	0.46
1:C:266:LEU:HD22	1:C:285:MET:HB3	1.97	0.46
1:A:235:GLN:HB2	1:A:242:ARG:HH21	1.80	0.46
1:C:771:LYS:HG2	1:C:775:LYS:HE2	1.98	0.46
1:E:559:MET:HG2	1:E:564:GLU:HB2	1.97	0.46
1:E:525:PHE:O	1:E:528:VAL:HG22	2.16	0.46
1:A:51:ALA:O	1:B:33:LYS:NZ	2.46	0.45
1:B:287:LYS:HA	1:B:314:ARG:HD2	1.98	0.45
1:A:263:THR:HA	1:A:267:ARG:HH21	1.82	0.45
1:A:683:GLN:NE2	2:B:801:ACO:H21	2.31	0.45
1:A:722:LYS:HE3	1:B:685:ASP:OD1	2.16	0.45
1:C:180:ALA:C	1:C:218:ILE:HD11	2.36	0.45
1:F:341:ARG:NH1	1:F:345:ASP:OD1	2.48	0.45
1:D:589:VAL:HG11	1:D:595:PRO:HD3	1.99	0.45
1:E:110:LEU:HD23	1:E:333:VAL:HG23	1.98	0.45
1:E:336:PHE:CG	1:E:337:PRO:HD3	2.52	0.45
1:A:263:THR:HG22	1:A:285:MET:HG2	1.98	0.45
1:C:103:VAL:HG23	1:D:60:CYS:SG	2.57	0.45
1:C:684:ALA:HB2	1:D:719:ILE:HG23	1.98	0.45
1:C:685:ASP:CG	1:D:722:LYS:HD3	2.37	0.45
1:E:89:VAL:HA	1:E:150:ASP:OD2	2.16	0.45
1:A:70:VAL:HG13	1:A:76:LYS:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:OE2	1:D:749:ARG:NH1	2.47	0.45
1:C:470:THR:O	1:C:501:LYS:HD3	2.17	0.45
1:E:472:THR:HG22	1:E:501:LYS:NZ	2.31	0.45
1:E:574:ILE:HG22	1:E:579:ALA:HB2	1.98	0.45
1:F:321:THR:HG22	1:F:323:ARG:H	1.81	0.45
1:B:557:ALA:HA	1:B:568:MET:HE1	1.99	0.45
1:F:202:ARG:NH1	1:F:269:ALA:HA	2.32	0.45
1:A:89:VAL:HG13	1:A:103:VAL:HG21	1.98	0.45
1:D:198:MET:O	1:D:201:VAL:HG12	2.17	0.45
1:E:103:VAL:HG13	1:F:60:CYS:SG	2.56	0.45
1:F:503:LYS:HA	1:F:503:LYS:HD3	1.60	0.45
1:C:235:GLN:HB3	1:C:242:ARG:NH2	2.30	0.45
1:C:644:VAL:HB	1:C:678:ILE:HG23	1.98	0.45
1:D:561:ASN:OD1	1:D:741:ARG:NH2	2.50	0.45
1:A:83:ILE:HG12	1:A:122:ILE:HB	1.99	0.44
1:C:51:ALA:O	1:D:33:LYS:HE2	2.16	0.44
1:F:135:ALA:O	1:F:138:VAL:HG12	2.18	0.44
1:A:124:VAL:HG13	1:B:138:VAL:HG13	1.97	0.44
1:A:267:ARG:HD3	1:A:267:ARG:HA	1.42	0.44
1:B:561:ASN:HB2	1:B:587:ILE:HD13	1.98	0.44
1:C:71:TYR:CZ	1:C:76:LYS:HD3	2.51	0.44
1:C:722:LYS:HE3	1:D:685:ASP:CG	2.37	0.44
1:C:724:ILE:HD11	1:D:723:LEU:HD13	1.99	0.44
1:B:576:TYR:OH	1:B:614:THR:HG21	2.17	0.44
1:A:202:ARG:H	1:A:202:ARG:HG2	1.60	0.44
1:A:576:TYR:OH	1:A:614:THR:HG21	2.17	0.44
1:A:742:ARG:HA	1:A:742:ARG:HD3	1.85	0.44
1:B:126:ALA:HB1	1:B:131:VAL:HG13	1.99	0.44
1:B:437:GLY:HA3	1:B:604:GLU:O	2.18	0.44
1:B:494:TYR:O	1:B:498:VAL:HG12	2.17	0.44
1:B:723:LEU:HD23	1:B:723:LEU:HA	1.80	0.44
1:C:647:LEU:O	1:C:662:MET:HG3	2.16	0.44
1:C:773:VAL:CG1	1:C:774:LEU:N	2.79	0.44
1:D:173:HIS:NE2	1:D:175:ASP:HB2	2.33	0.44
1:F:321:THR:HG22	1:F:322:GLY:H	1.81	0.44
1:A:405:ALA:HB3	1:A:406:PRO:HD3	1.99	0.44
1:B:368:ARG:HG2	1:B:386:PHE:CZ	2.53	0.44
1:A:498:VAL:CG1	1:A:515:ILE:HD13	2.48	0.44
1:A:551:ASP:OD1	1:D:547:ARG:NH2	2.51	0.44
1:A:722:LYS:HE3	1:B:685:ASP:CG	2.38	0.44
1:B:770:ILE:HA	1:B:773:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:PRO:HA	1:C:492:LEU:HB2	1.99	0.44
1:D:753:VAL:HG23	1:D:754:ASP:N	2.33	0.44
1:F:345:ASP:OD2	1:F:428:TYR:OH	2.21	0.44
1:A:764:ALA:O	1:A:768:GLN:HG3	2.17	0.44
1:B:600:PHE:HB2	1:B:733:ILE:CG1	2.48	0.44
1:E:536:GLN:HA	1:E:540:ILE:O	2.17	0.44
1:E:135:ALA:O	1:E:138:VAL:HG12	2.18	0.44
1:A:56:VAL:O	1:A:59:PRO:HD2	2.18	0.44
1:E:465:VAL:HG21	1:E:559:MET:HE3	2.00	0.44
1:F:584:LEU:HB3	2:F:801:ACO:O4B	2.17	0.44
1:A:58:ALA:HB3	1:A:59:PRO:HD3	1.99	0.43
1:A:231:MET:HB2	1:A:238:ILE:HB	2.00	0.43
1:A:453:ASN:HB3	1:A:768:GLN:OE1	2.18	0.43
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.90	0.43
1:D:164:LYS:HG2	1:D:171:VAL:HB	1.98	0.43
1:D:559:MET:HG2	1:D:564:GLU:HB2	1.99	0.43
1:E:95:ILE:HD12	1:E:99:ALA:HB3	2.00	0.43
1:B:341:ARG:HE	1:B:341:ARG:HA	1.83	0.43
1:C:774:LEU:O	1:C:776:SER:N	2.50	0.43
1:C:776:SER:O	1:C:776:SER:OG	2.34	0.43
1:D:282:THR:HG22	1:D:284:GLU:OE1	2.18	0.43
1:E:498:VAL:HG13	1:E:515:ILE:HD13	2.00	0.43
1:E:685:ASP:HA	1:F:726:GLN:HG3	2.00	0.43
1:F:735:PRO:HG3	2:F:801:ACO:HH33	2.00	0.43
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.80	0.43
1:F:116:GLY:HA3	1:F:435:LEU:HD22	2.00	0.43
1:A:774:LEU:C	1:A:776:SER:N	2.72	0.43
1:B:105:GLU:O	1:B:109:ILE:HD12	2.19	0.43
1:E:478:LEU:CD1	1:E:491:LEU:HD21	2.48	0.43
1:E:589:VAL:HG11	1:E:595:PRO:HD3	1.98	0.43
1:F:238:ILE:HA	1:F:242:ARG:HH11	1.84	0.43
1:A:464:ILE:HA	1:A:567:GLY:O	2.19	0.43
1:C:357:LEU:HA	1:C:357:LEU:HD23	1.77	0.43
1:E:95:ILE:HD12	1:E:99:ALA:CB	2.49	0.43
1:E:45:GLU:HG3	1:E:46:LYS:N	2.33	0.43
1:A:189:ASN:O	1:A:193:ILE:HG22	2.19	0.43
1:D:478:LEU:HD23	1:D:478:LEU:HA	1.93	0.43
1:E:259:ALA:O	1:E:260:ARG:HD2	2.18	0.43
1:F:498:VAL:HG11	1:F:515:ILE:HG21	1.99	0.43
1:A:498:VAL:O	1:A:502:ILE:HG23	2.19	0.43
1:A:87:THR:HA	1:A:94:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:LEU:HA	1:D:696:LEU:HD23	1.80	0.43
1:B:467:PRO:HA	1:B:492:LEU:HB2	2.01	0.42
1:C:218:ILE:HG21	1:C:218:ILE:HD13	1.67	0.42
1:A:111:PHE:CE1	1:A:336:PHE:HD1	2.36	0.42
1:A:333:VAL:HA	1:A:336:PHE:CE2	2.54	0.42
1:A:521:HIS:CG	1:A:522:PRO:HD2	2.53	0.42
1:B:217:LYS:O	1:B:220:ILE:HG13	2.18	0.42
1:B:350:GLN:NE2	1:B:352:ASN:HB3	2.31	0.42
1:A:336:PHE:O	1:A:340:PHE:HD2	2.03	0.42
1:A:428:TYR:CE2	1:A:432:LEU:HD11	2.53	0.42
1:B:463:ARG:HH12	1:B:564:GLU:C	2.23	0.42
1:C:366:LEU:HD13	1:C:403:TRP:CE2	2.55	0.42
1:C:774:LEU:C	1:C:776:SER:N	2.73	0.42
1:F:542:LEU:HA	1:F:542:LEU:HD23	1.80	0.42
1:A:126:ALA:HB2	1:B:138:VAL:CG2	2.43	0.42
1:F:173:HIS:NE2	1:F:175:ASP:HB2	2.34	0.42
1:F:202:ARG:HH12	1:F:268:GLY:C	2.23	0.42
1:B:189:ASN:O	1:B:193:ILE:HD12	2.19	0.42
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.81	0.42
1:C:616:ASN:OD1	2:C:801:ACO:N6A	2.53	0.42
1:E:126:ALA:HB1	1:E:131:VAL:HG23	2.02	0.42
1:E:413:MET:HE1	1:E:425:TRP:HZ2	1.85	0.42
1:F:178:GLY:HA3	1:F:332:ASN:OD1	2.19	0.42
1:A:722:LYS:HE3	1:B:685:ASP:OD2	2.20	0.42
1:C:33:LYS:HE2	1:D:51:ALA:O	2.19	0.42
1:C:323:ARG:HA	1:C:323:ARG:HD3	1.89	0.42
1:A:321:THR:HG22	1:A:322:GLY:N	2.34	0.42
1:C:33:LYS:O	1:D:38:SER:HA	2.19	0.42
1:C:45:GLU:HG2	1:D:396:PHE:CE2	2.54	0.42
1:C:227:GLU:H	1:C:227:GLU:CD	2.23	0.42
1:C:396:PHE:CD2	1:C:444:ARG:HD3	2.54	0.42
1:F:437:GLY:O	1:F:441:VAL:HG22	2.19	0.42
1:A:60:CYS:SG	1:B:103:VAL:HG23	2.59	0.42
1:A:574:ILE:HG13	1:A:575:ASN:N	2.35	0.42
1:C:772:GLU:CD	1:C:775:LYS:NZ	2.73	0.42
1:F:366:LEU:HD13	1:F:403:TRP:CE2	2.54	0.42
1:C:765:LEU:HD12	1:C:765:LEU:HA	1.95	0.42
1:D:336:PHE:CG	1:D:337:PRO:HD3	2.55	0.42
1:D:357:LEU:HD23	1:D:357:LEU:HA	1.93	0.42
1:F:457:ASN:O	1:F:460:GLU:OE1	2.37	0.42
1:B:560:VAL:HG21	1:B:568:MET:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:THR:HG22	1:D:750:THR:O	2.20	0.42
1:A:107:LYS:O	1:A:110:LEU:HB2	2.20	0.41
1:B:600:PHE:HB2	1:B:733:ILE:HG12	2.01	0.41
1:C:336:PHE:CG	1:C:337:PRO:HD3	2.55	0.41
1:C:726:GLN:HG3	1:D:685:ASP:HA	2.02	0.41
1:F:634:ILE:O	1:F:637:TYR:HB3	2.20	0.41
1:F:644:VAL:HB	1:F:678:ILE:HG23	2.02	0.41
1:F:748:GLN:CB	2:F:801:ACO:HH31	2.39	0.41
1:A:247:ASN:OD1	1:A:247:ASN:N	2.53	0.41
1:A:366:LEU:HD22	1:A:393:PRO:HG3	2.02	0.41
1:A:481:LEU:HD13	1:A:760:VAL:HG11	2.02	0.41
1:C:33:LYS:HE2	1:D:51:ALA:HA	2.02	0.41
1:C:437:GLY:HA3	1:C:604:GLU:O	2.20	0.41
1:D:314:ARG:NH2	1:D:316:ASP:OD2	2.48	0.41
1:E:33:LYS:HB3	1:E:109:ILE:HD11	2.02	0.41
1:F:495:PRO:HA	1:F:515:ILE:HG21	2.02	0.41
1:F:594:ILE:HG22	1:F:626:GLN:HG3	2.03	0.41
1:B:235:GLN:CB	1:B:242:ARG:HH22	2.29	0.41
1:C:138:VAL:HG13	1:D:124:VAL:HG13	2.01	0.41
1:F:597:GLY:O	1:F:612:ASP:HA	2.20	0.41
1:A:181:ILE:HG23	1:A:360:VAL:CG2	2.50	0.41
1:B:352:ASN:N	1:B:355:MET:HE3	2.25	0.41
1:C:478:LEU:HD23	1:C:478:LEU:HA	1.91	0.41
1:D:79:LEU:HD12	1:D:79:LEU:HA	1.77	0.41
1:E:80:VAL:O	1:E:119:VAL:HG12	2.21	0.41
1:E:101:LYS:HB3	1:E:102:PRO:HD3	2.02	0.41
1:F:128:ASP:HB3	1:F:131:VAL:CG1	2.44	0.41
1:F:290:ALA:O	1:F:314:ARG:NH1	2.53	0.41
1:A:529:GLU:O	1:A:532:TYR:HB3	2.20	0.41
1:B:213:ASN:HA	1:B:253:PHE:HE2	1.85	0.41
1:D:521:HIS:CG	1:D:522:PRO:HD2	2.55	0.41
1:E:615:VAL:HG23	2:E:801:ACO:H143	2.03	0.41
1:F:765:LEU:HA	1:F:765:LEU:HD23	1.79	0.41
1:A:498:VAL:HG13	1:A:515:ILE:HD13	2.03	0.41
1:B:400:VAL:HG23	1:B:401:LEU:N	2.36	0.41
1:C:481:LEU:HD13	1:C:760:VAL:HG11	2.03	0.41
1:D:723:LEU:O	1:D:727:ILE:HG12	2.19	0.41
1:E:202:ARG:NH1	1:E:228:ASN:HA	2.35	0.41
1:F:619:PRO:O	1:F:661:LYS:HD2	2.21	0.41
1:B:268:GLY:N	1:B:288:ASP:O	2.42	0.41
1:C:296:PHE:CD1	1:C:320:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:PRO:HA	1:C:515:ILE:HG21	2.03	0.41
1:C:498:VAL:HG22	1:C:515:ILE:HD13	2.03	0.41
1:D:110:LEU:HD23	1:D:110:LEU:HA	1.84	0.41
1:D:355:MET:O	1:D:358:ALA:HB3	2.20	0.41
1:F:521:HIS:CG	1:F:522:PRO:HD2	2.55	0.41
1:B:111:PHE:CE2	1:B:336:PHE:HD1	2.38	0.41
1:B:137:ARG:HA	1:B:167:MET:SD	2.61	0.41
1:C:669:ALA:HB1	1:C:678:ILE:HD13	2.03	0.41
1:E:45:GLU:OE1	1:F:484:GLU:HG3	2.20	0.41
1:E:596:ALA:HB1	1:E:612:ASP:HB2	2.03	0.41
1:E:669:ALA:HB1	1:E:678:ILE:HD13	2.02	0.41
1:F:170:PRO:HB3	1:F:351:ILE:HG13	2.03	0.41
1:A:48:LEU:HA	1:A:48:LEU:HD23	1.85	0.41
1:A:70:VAL:HG13	1:A:76:LYS:HD2	2.03	0.41
1:A:355:MET:CE	1:A:417:VAL:HG21	2.51	0.41
1:C:736:PHE:CE2	1:C:762:PHE:HB2	2.56	0.41
1:C:770:ILE:HA	1:C:773:VAL:CG1	2.50	0.41
1:D:702:LEU:HD21	1:D:706:ALA:HB2	2.02	0.41
1:E:71:TYR:HB3	1:E:347:ARG:CZ	2.50	0.41
1:E:486:ILE:HD13	1:E:486:ILE:HA	1.93	0.41
1:E:634:ILE:O	1:E:637:TYR:HB3	2.20	0.41
1:F:449:ARG:HG3	1:F:449:ARG:HH11	1.85	0.41
1:A:71:TYR:HH	1:A:420:ARG:HH11	1.62	0.41
1:A:74:THR:HG22	1:A:75:ALA:N	2.35	0.41
1:A:628:ALA:HB2	1:A:710:VAL:HG11	2.03	0.41
1:B:87:THR:HB	1:B:152:LYS:HB3	2.03	0.41
1:C:226:ARG:HG2	1:C:226:ARG:HH11	1.86	0.41
1:D:33:LYS:NZ	1:D:102:PRO:O	2.54	0.41
1:E:495:PRO:HD3	1:E:517:HIS:HB2	2.03	0.41
1:F:481:LEU:HD13	1:F:760:VAL:HG11	2.02	0.41
1:A:33:LYS:HE2	1:B:51:ALA:O	2.22	0.40
1:A:608:LEU:HD23	1:A:707:ASN:HA	2.01	0.40
1:C:758:ASN:O	1:C:761:VAL:HB	2.21	0.40
1:D:576:TYR:CD2	2:D:801:ACO:HH32	2.56	0.40
1:E:170:PRO:HA	1:E:350:GLN:HA	2.02	0.40
1:F:572:SER:HB3	1:F:747:LEU:HD12	2.03	0.40
1:A:765:LEU:HD12	1:A:765:LEU:HA	1.81	0.40
1:E:478:LEU:HA	1:E:481:LEU:HB2	2.04	0.40
1:A:302:GLU:HA	1:A:303:PRO:HD3	1.82	0.40
1:B:594:ILE:HG22	1:B:626:GLN:HG3	2.04	0.40
1:D:651:ASN:HB3	1:D:697:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:THR:HB	1:F:418:ALA:HB1	2.03	0.40
1:A:347:ARG:HE	1:A:347:ARG:HB3	1.69	0.40
1:A:595:PRO:HA	1:A:738:THR:O	2.21	0.40
1:C:544:GLU:OE1	1:F:749:ARG:NH1	2.55	0.40
1:F:413:MET:HA	1:F:418:ALA:HB3	2.03	0.40
1:B:71:TYR:HB3	1:B:347:ARG:CZ	2.51	0.40
1:B:460:GLU:OE1	1:B:460:GLU:N	2.50	0.40
1:D:591:LYS:O	1:D:592:GLU:HB2	2.21	0.40
1:F:350:GLN:O	1:F:355:MET:HE1	2.22	0.40
1:F:365:LYS:HA	1:F:368:ARG:HH11	1.86	0.40
1:F:581:ARG:HB3	1:F:582:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 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	745/791 (94%)	724 (97%)	20 (3%)	1 (0%)	51	77
1	B	745/791 (94%)	725 (97%)	20 (3%)	0	100	100
1	C	746/791 (94%)	726 (97%)	19 (2%)	1 (0%)	51	77
1	D	747/791 (94%)	729 (98%)	18 (2%)	0	100	100
1	E	747/791 (94%)	727 (97%)	20 (3%)	0	100	100
1	F	749/791 (95%)	730 (98%)	18 (2%)	1 (0%)	51	77
All	All	4479/4746 (94%)	4361 (97%)	115 (3%)	3 (0%)	51	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	775	LYS

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Mol	Chain	Res	Type
1	A	775	LYS
1	F	381	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	606/642 (94%)	589 (97%)	17 (3%)	43	71
1	B	606/642 (94%)	590 (97%)	16 (3%)	46	73
1	C	607/642 (94%)	596 (98%)	11 (2%)	59	82
1	D	608/642 (95%)	594 (98%)	14 (2%)	50	77
1	E	606/642 (94%)	588 (97%)	18 (3%)	41	69
1	F	608/642 (95%)	593 (98%)	15 (2%)	47	75
All	All	3641/3852 (94%)	3550 (98%)	91 (2%)	47	75

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	79	LEU
1	A	152	LYS
1	A	163	LEU
1	A	168	ASN
1	A	202	ARG
1	A	239	TYR
1	A	267	ARG
1	A	468	GLU
1	A	472	THR
1	A	516	VAL
1	A	614	THR
1	A	708	VAL
1	A	710	VAL
1	A	721	TYR
1	A	732	VAL

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Mol	Chain	Res	Type
1	A	776	SER
1	B	27	GLN
1	B	66	ASP
1	B	70	VAL
1	B	127	THR
1	B	146	ILE
1	B	250	LYS
1	B	282	THR
1	B	472	THR
1	B	542	LEU
1	B	568	MET
1	B	614	THR
1	B	693	MET
1	B	721	TYR
1	B	729	LYS
1	B	732	VAL
1	B	749	ARG
1	C	16	THR
1	C	53	SER
1	C	152	LYS
1	C	205	VAL
1	C	498	VAL
1	C	501	LYS
1	C	520	SER
1	C	535	ARG
1	C	710	VAL
1	C	721	TYR
1	C	772	GLU
1	D	107	LYS
1	D	127	THR
1	D	205	VAL
1	D	214	SER
1	D	323	ARG
1	D	330	VAL
1	D	341	ARG
1	D	384	PHE
1	D	520	SER
1	D	533	SER
1	D	721	TYR
1	D	732	VAL
1	D	763	THR
1	D	772	GLU

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Mol	Chain	Res	Type
1	E	53	SER
1	E	119	VAL
1	E	152	LYS
1	E	204	VAL
1	E	205	VAL
1	E	260	ARG
1	E	282	THR
1	E	325	ASP
1	E	403	TRP
1	E	472	THR
1	E	533	SER
1	E	572	SER
1	E	574	ILE
1	E	615	VAL
1	E	693	MET
1	E	721	TYR
1	E	749	ARG
1	E	754	ASP
1	F	124	VAL
1	F	127	THR
1	F	152	LYS
1	F	164	LYS
1	F	323	ARG
1	F	330	VAL
1	F	368	ARG
1	F	454	SER
1	F	491	LEU
1	F	520	SER
1	F	528	VAL
1	F	608	LEU
1	F	672	LEU
1	F	721	TYR
1	F	732	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	ASN
1	A	725	GLN
1	B	113	GLN
1	B	350	GLN
1	C	28	GLN

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Mol	Chain	Res	Type
1	D	452	GLN
1	D	745	ASN
1	E	350	GLN
1	F	300	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

6 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	ACO	F	801	-	45,53,53	4.07	17 (37%)	56,79,79	2.03	10 (17%)
2	ACO	B	801	-	45,53,53	3.97	17 (37%)	56,79,79	2.22	11 (19%)
2	ACO	A	801	-	45,53,53	3.96	16 (35%)	56,79,79	2.38	10 (17%)
2	ACO	C	801	-	45,53,53	3.95	16 (35%)	56,79,79	2.31	11 (19%)
2	ACO	E	801	-	45,53,53	3.97	17 (37%)	56,79,79	2.61	16 (28%)
2	ACO	D	801	-	45,53,53	4.11	15 (33%)	56,79,79	2.39	15 (26%)

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
2	ACO	F	801	-	-	14/47/67/67	0/3/3/3
2	ACO	B	801	-	-	17/47/67/67	0/3/3/3
2	ACO	A	801	-	-	13/47/67/67	0/3/3/3
2	ACO	C	801	-	-	15/47/67/67	0/3/3/3
2	ACO	E	801	-	-	20/47/67/67	0/3/3/3
2	ACO	D	801	-	-	19/47/67/67	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	ACO	O4B-C1B	17.04	1.64	1.41
2	A	801	ACO	O4B-C1B	16.74	1.64	1.41
2	B	801	ACO	O4B-C1B	16.69	1.64	1.41
2	F	801	ACO	O4B-C1B	16.54	1.64	1.41
2	C	801	ACO	O4B-C1B	16.31	1.63	1.41
2	E	801	ACO	O4B-C1B	16.08	1.63	1.41
2	F	801	ACO	C2B-C1B	-13.65	1.33	1.53
2	D	801	ACO	C2B-C1B	-13.26	1.33	1.53
2	E	801	ACO	C2B-C1B	-12.98	1.34	1.53
2	A	801	ACO	C2B-C1B	-12.73	1.34	1.53
2	C	801	ACO	C2B-C1B	-12.63	1.34	1.53
2	B	801	ACO	C2B-C1B	-12.58	1.34	1.53
2	C	801	ACO	C9P-N8P	6.96	1.48	1.33
2	E	801	ACO	O4B-C4B	-6.81	1.29	1.45
2	F	801	ACO	C5P-N4P	6.55	1.48	1.33
2	F	801	ACO	C9P-N8P	6.52	1.47	1.33
2	D	801	ACO	O4B-C4B	-6.51	1.30	1.45
2	B	801	ACO	O4B-C4B	-6.36	1.30	1.45
2	D	801	ACO	C5P-N4P	6.25	1.47	1.33
2	E	801	ACO	C9P-N8P	6.24	1.47	1.33
2	A	801	ACO	O4B-C4B	-6.21	1.31	1.45
2	B	801	ACO	C9P-N8P	6.07	1.46	1.33
2	D	801	ACO	C9P-N8P	6.03	1.46	1.33
2	F	801	ACO	O4B-C4B	-5.99	1.31	1.45
2	C	801	ACO	O4B-C4B	-5.85	1.31	1.45
2	A	801	ACO	C9P-N8P	5.74	1.46	1.33
2	B	801	ACO	C5P-N4P	5.67	1.46	1.33
2	C	801	ACO	C5P-N4P	5.62	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ACO	C5P-N4P	5.49	1.45	1.33
2	E	801	ACO	C6A-N6A	5.34	1.53	1.34
2	E	801	ACO	C5P-N4P	5.30	1.45	1.33
2	F	801	ACO	C6A-N6A	5.23	1.53	1.34
2	B	801	ACO	C6A-N6A	5.20	1.53	1.34
2	D	801	ACO	C6A-N6A	5.07	1.52	1.34
2	A	801	ACO	C6A-N6A	5.06	1.52	1.34
2	C	801	ACO	C6A-N6A	5.01	1.52	1.34
2	C	801	ACO	P3B-O3B	5.01	1.68	1.59
2	B	801	ACO	P3B-O3B	4.96	1.68	1.59
2	D	801	ACO	P3B-O3B	4.76	1.68	1.59
2	A	801	ACO	P3B-O3B	4.72	1.68	1.59
2	D	801	ACO	C2A-N3A	4.41	1.39	1.32
2	E	801	ACO	P3B-O3B	4.26	1.67	1.59
2	F	801	ACO	C6P-C5P	4.25	1.59	1.51
2	F	801	ACO	P3B-O3B	4.09	1.67	1.59
2	D	801	ACO	C6P-C5P	4.08	1.59	1.51
2	C	801	ACO	P1A-O5B	3.96	1.75	1.59
2	A	801	ACO	P1A-O5B	3.91	1.75	1.59
2	E	801	ACO	P1A-O5B	3.87	1.74	1.59
2	E	801	ACO	C2A-N3A	3.84	1.38	1.32
2	F	801	ACO	P1A-O5B	3.83	1.74	1.59
2	B	801	ACO	P1A-O5B	3.79	1.74	1.59
2	D	801	ACO	P1A-O5B	3.75	1.74	1.59
2	B	801	ACO	C6P-C5P	3.69	1.58	1.51
2	A	801	ACO	C2A-N3A	3.65	1.38	1.32
2	E	801	ACO	C6P-C5P	3.62	1.58	1.51
2	F	801	ACO	C2A-N3A	3.60	1.37	1.32
2	B	801	ACO	C2A-N3A	3.53	1.37	1.32
2	D	801	ACO	C7P-C6P	3.49	1.62	1.51
2	C	801	ACO	C7P-C6P	3.43	1.62	1.51
2	F	801	ACO	C7P-C6P	3.41	1.62	1.51
2	A	801	ACO	C6P-C5P	3.33	1.57	1.51
2	B	801	ACO	C7P-C6P	3.20	1.61	1.51
2	E	801	ACO	C7P-C6P	3.13	1.61	1.51
2	C	801	ACO	C2A-N3A	3.12	1.37	1.32
2	C	801	ACO	O5P-C5P	-3.06	1.17	1.23
2	C	801	ACO	C6P-C5P	3.03	1.57	1.51
2	D	801	ACO	P2A-O6A	2.99	1.71	1.59
2	A	801	ACO	C7P-C6P	2.98	1.60	1.51
2	C	801	ACO	P2A-O6A	2.95	1.71	1.59
2	E	801	ACO	P2A-O6A	2.95	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	ACO	P2A-O6A	2.94	1.71	1.59
2	A	801	ACO	C5A-C4A	-2.90	1.33	1.40
2	A	801	ACO	C3P-N4P	2.90	1.52	1.46
2	B	801	ACO	P2A-O6A	2.83	1.70	1.59
2	E	801	ACO	C5A-C4A	-2.81	1.33	1.40
2	E	801	ACO	O5P-C5P	-2.74	1.17	1.23
2	F	801	ACO	C5A-C4A	-2.73	1.33	1.40
2	F	801	ACO	C3P-N4P	2.72	1.52	1.46
2	C	801	ACO	C5A-C4A	-2.67	1.33	1.40
2	A	801	ACO	P2A-O6A	2.62	1.69	1.59
2	B	801	ACO	C5A-C4A	-2.59	1.34	1.40
2	A	801	ACO	O5P-C5P	-2.55	1.18	1.23
2	D	801	ACO	C5A-C4A	-2.50	1.34	1.40
2	C	801	ACO	O3B-C3B	-2.50	1.35	1.44
2	E	801	ACO	O3B-C3B	-2.48	1.35	1.44
2	D	801	ACO	C3P-N4P	2.46	1.51	1.46
2	E	801	ACO	C3P-N4P	2.45	1.51	1.46
2	D	801	ACO	O3B-C3B	-2.45	1.35	1.44
2	A	801	ACO	O3B-C3B	-2.41	1.35	1.44
2	B	801	ACO	O5P-C5P	-2.40	1.18	1.23
2	F	801	ACO	O3B-C3B	-2.31	1.35	1.44
2	B	801	ACO	O3B-C3B	-2.25	1.35	1.44
2	E	801	ACO	P3B-O8A	-2.20	1.46	1.54
2	B	801	ACO	C3P-N4P	2.16	1.51	1.46
2	C	801	ACO	C3P-N4P	2.11	1.51	1.46
2	B	801	ACO	O2B-C2B	2.07	1.47	1.43
2	F	801	ACO	O5P-C5P	-2.05	1.19	1.23
2	F	801	ACO	P3B-O8A	-2.02	1.47	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ACO	C5A-C6A-N6A	10.39	136.14	120.35
2	B	801	ACO	C5A-C6A-N6A	10.04	135.60	120.35
2	E	801	ACO	C5A-C6A-N6A	9.88	135.37	120.35
2	F	801	ACO	C5A-C6A-N6A	9.73	135.14	120.35
2	A	801	ACO	C5A-C6A-N6A	9.40	134.64	120.35
2	C	801	ACO	C5A-C6A-N6A	8.72	133.60	120.35
2	A	801	ACO	C7P-C6P-C5P	-7.41	100.02	112.36
2	E	801	ACO	C7P-C6P-C5P	-6.87	100.92	112.36
2	E	801	ACO	N6A-C6A-N1A	-6.53	105.02	118.57
2	D	801	ACO	N6A-C6A-N1A	-6.43	105.23	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ACO	N6A-C6A-N1A	-6.33	105.43	118.57
2	A	801	ACO	C7P-N8P-C9P	-6.26	111.43	122.59
2	B	801	ACO	N6A-C6A-N1A	-6.25	105.61	118.57
2	C	801	ACO	C7P-C6P-C5P	-5.89	102.54	112.36
2	F	801	ACO	N6A-C6A-N1A	-5.84	106.46	118.57
2	C	801	ACO	N3A-C2A-N1A	-5.82	119.58	128.68
2	E	801	ACO	C7P-N8P-C9P	-5.82	112.21	122.59
2	E	801	ACO	N3A-C2A-N1A	-5.59	119.95	128.68
2	C	801	ACO	N6A-C6A-N1A	-5.53	107.09	118.57
2	B	801	ACO	N3A-C2A-N1A	-5.34	120.33	128.68
2	A	801	ACO	N3A-C2A-N1A	-5.26	120.46	128.68
2	D	801	ACO	C7P-C6P-C5P	-5.15	103.78	112.36
2	D	801	ACO	N3A-C2A-N1A	-5.00	120.86	128.68
2	F	801	ACO	N3A-C2A-N1A	-4.84	121.11	128.68
2	C	801	ACO	C3P-N4P-C5P	-4.59	114.32	122.84
2	D	801	ACO	C7P-N8P-C9P	-4.41	114.72	122.59
2	C	801	ACO	P2A-O3A-P1A	-4.29	118.10	132.83
2	B	801	ACO	C7P-C6P-C5P	-4.28	105.23	112.36
2	C	801	ACO	C6P-C7P-N8P	-4.26	103.30	111.90
2	D	801	ACO	P2A-O3A-P1A	-4.10	118.74	132.83
2	E	801	ACO	C6P-C7P-N8P	-3.88	104.06	111.90
2	E	801	ACO	C3P-N4P-C5P	-3.78	115.83	122.84
2	C	801	ACO	C6P-C5P-N4P	3.69	122.63	116.42
2	B	801	ACO	CEP-CBP-CCP	3.61	114.13	108.23
2	B	801	ACO	C7P-N8P-C9P	-3.59	116.18	122.59
2	E	801	ACO	O6A-CCP-CBP	-3.57	104.81	110.55
2	F	801	ACO	P2A-O3A-P1A	-3.49	120.86	132.83
2	E	801	ACO	P2A-O3A-P1A	-3.45	120.98	132.83
2	A	801	ACO	C6P-C7P-N8P	-3.39	105.06	111.90
2	E	801	ACO	CDP-CBP-CAP	3.32	114.57	108.82
2	F	801	ACO	C7P-C6P-C5P	-3.23	106.97	112.36
2	E	801	ACO	C6P-C5P-N4P	3.12	121.67	116.42
2	E	801	ACO	C3B-C2B-C1B	3.05	106.64	99.89
2	B	801	ACO	P2A-O3A-P1A	-2.99	122.58	132.83
2	C	801	ACO	C7P-N8P-C9P	-2.93	117.37	122.59
2	B	801	ACO	O9P-C9P-N8P	-2.87	116.83	122.99
2	A	801	ACO	P2A-O3A-P1A	-2.85	123.05	132.83
2	D	801	ACO	C2P-C3P-N4P	-2.84	106.44	112.42
2	A	801	ACO	C3B-C2B-C1B	2.81	106.11	99.89
2	B	801	ACO	OAP-CAP-CBP	-2.77	103.72	110.25
2	A	801	ACO	O9P-C9P-N8P	-2.63	117.34	122.99
2	D	801	ACO	CEP-CBP-CCP	2.63	112.52	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ACO	C1B-N9A-C4A	-2.54	122.19	126.64
2	D	801	ACO	O9P-C9P-N8P	-2.51	117.61	122.99
2	C	801	ACO	C3B-C2B-C1B	2.49	105.42	99.89
2	F	801	ACO	O6A-CCP-CBP	-2.40	106.69	110.55
2	F	801	ACO	C2P-C3P-N4P	-2.37	107.44	112.42
2	C	801	ACO	O5P-C5P-C6P	-2.36	117.69	122.02
2	E	801	ACO	O9P-C9P-N8P	-2.36	117.92	122.99
2	D	801	ACO	C3B-C2B-C1B	2.32	105.02	99.89
2	D	801	ACO	O5B-C5B-C4B	-2.30	101.08	108.99
2	F	801	ACO	C7P-N8P-C9P	-2.22	118.63	122.59
2	D	801	ACO	CEP-CBP-CDP	-2.20	104.67	109.17
2	B	801	ACO	C3B-C2B-C1B	2.20	104.75	99.89
2	E	801	ACO	O5P-C5P-N4P	-2.19	118.88	123.01
2	B	801	ACO	C6P-C7P-N8P	-2.19	107.47	111.90
2	F	801	ACO	O9P-C9P-N8P	-2.18	118.32	122.99
2	D	801	ACO	C3P-N4P-C5P	-2.17	118.80	122.84
2	F	801	ACO	C3B-C2B-C1B	2.13	104.60	99.89
2	E	801	ACO	C5B-C4B-C3B	-2.06	107.56	114.40
2	D	801	ACO	CDP-CBP-CAP	2.06	112.39	108.82
2	A	801	ACO	OAP-CAP-CBP	-2.03	105.47	110.25
2	E	801	ACO	O5B-C5B-C4B	-2.02	102.05	108.99

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ACO	CCP-O6A-P2A-O3A
2	A	801	ACO	CCP-O6A-P2A-O4A
2	A	801	ACO	C3P-C2P-S1P-C
2	B	801	ACO	C5B-O5B-P1A-O3A
2	B	801	ACO	CCP-O6A-P2A-O5A
2	B	801	ACO	CBP-CCP-O6A-P2A
2	B	801	ACO	CDP-CBP-CCP-O6A
2	B	801	ACO	CEP-CBP-CCP-O6A
2	B	801	ACO	CAP-CBP-CCP-O6A
2	B	801	ACO	C3P-C2P-S1P-C
2	C	801	ACO	C5B-O5B-P1A-O1A
2	C	801	ACO	CDP-CBP-CCP-O6A
2	C	801	ACO	CEP-CBP-CCP-O6A
2	C	801	ACO	CAP-CBP-CCP-O6A
2	D	801	ACO	O4B-C4B-C5B-O5B
2	D	801	ACO	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	D	801	ACO	C5B-O5B-P1A-O2A
2	D	801	ACO	C5B-O5B-P1A-O3A
2	D	801	ACO	CDP-CBP-CCP-O6A
2	D	801	ACO	CAP-CBP-CCP-O6A
2	D	801	ACO	OAP-CAP-CBP-CCP
2	D	801	ACO	C9P-CAP-CBP-CCP
2	D	801	ACO	OAP-CAP-CBP-CDP
2	D	801	ACO	C9P-CAP-CBP-CDP
2	D	801	ACO	OAP-CAP-CBP-CEP
2	D	801	ACO	C9P-CAP-CBP-CEP
2	D	801	ACO	C3P-C2P-S1P-C
2	E	801	ACO	C5B-O5B-P1A-O3A
2	E	801	ACO	CCP-O6A-P2A-O3A
2	E	801	ACO	CCP-O6A-P2A-O4A
2	E	801	ACO	CCP-O6A-P2A-O5A
2	E	801	ACO	C9P-CAP-CBP-CCP
2	E	801	ACO	C9P-CAP-CBP-CDP
2	E	801	ACO	OAP-CAP-CBP-CEP
2	E	801	ACO	C9P-CAP-CBP-CEP
2	E	801	ACO	C3P-C2P-S1P-C
2	F	801	ACO	C5B-O5B-P1A-O1A
2	F	801	ACO	C5B-O5B-P1A-O3A
2	F	801	ACO	P1A-O3A-P2A-O6A
2	F	801	ACO	CEP-CBP-CCP-O6A
2	F	801	ACO	CAP-CBP-CCP-O6A
2	F	801	ACO	C3P-C2P-S1P-C
2	E	801	ACO	O4B-C4B-C5B-O5B
2	D	801	ACO	C3B-C4B-C5B-O5B
2	D	801	ACO	CEP-CBP-CCP-O6A
2	F	801	ACO	CDP-CBP-CCP-O6A
2	C	801	ACO	S1P-C2P-C3P-N4P
2	F	801	ACO	C3B-C4B-C5B-O5B
2	F	801	ACO	O4B-C4B-C5B-O5B
2	C	801	ACO	OAP-CAP-CBP-CDP
2	C	801	ACO	OAP-CAP-CBP-CEP
2	E	801	ACO	OAP-CAP-CBP-CDP
2	A	801	ACO	P1A-O3A-P2A-O4A
2	F	801	ACO	P2A-O3A-P1A-O1A
2	B	801	ACO	N8P-C9P-CAP-CBP
2	C	801	ACO	P1A-O3A-P2A-O6A
2	D	801	ACO	P1A-O3A-P2A-O6A
2	A	801	ACO	CEP-CBP-CCP-O6A

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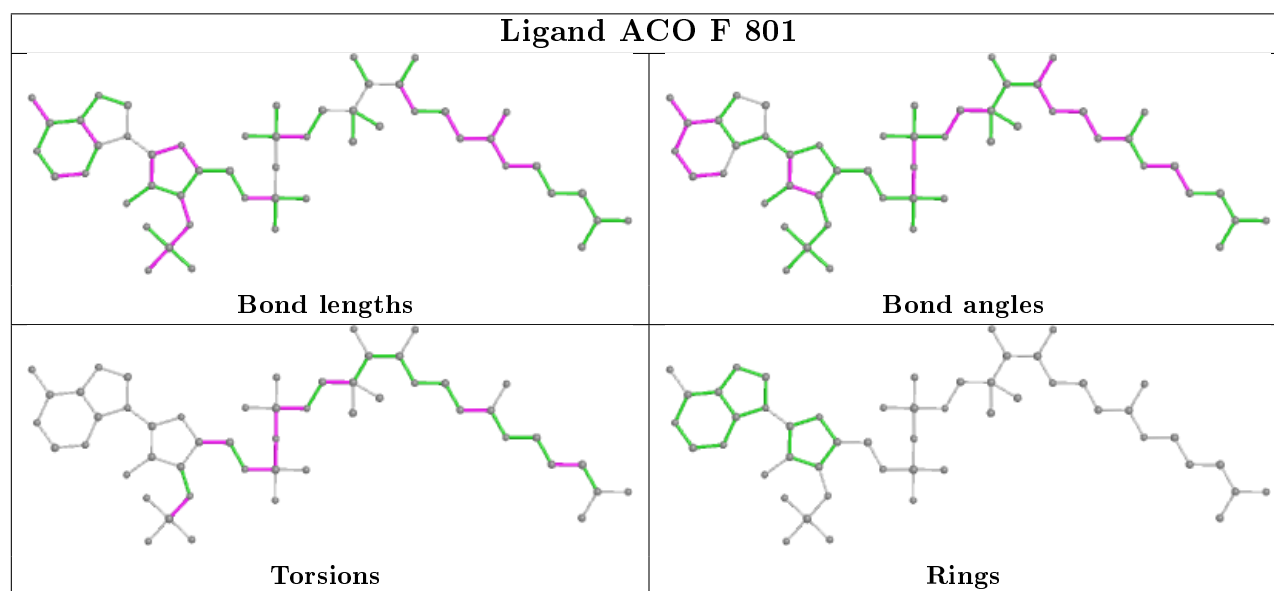
Mol	Chain	Res	Type	Atoms
2	B	801	ACO	CCP-O6A-P2A-O3A
2	C	801	ACO	C5B-O5B-P1A-O3A
2	F	801	ACO	C3B-O3B-P3B-O8A
2	B	801	ACO	P2A-O3A-P1A-O2A
2	A	801	ACO	CBP-CCP-O6A-P2A
2	D	801	ACO	CBP-CCP-O6A-P2A
2	B	801	ACO	C5B-O5B-P1A-O1A
2	B	801	ACO	C5B-O5B-P1A-O2A
2	B	801	ACO	CCP-O6A-P2A-O4A
2	C	801	ACO	C5B-O5B-P1A-O2A
2	E	801	ACO	C5B-O5B-P1A-O2A
2	F	801	ACO	CCP-O6A-P2A-O4A
2	A	801	ACO	CAP-CBP-CCP-O6A
2	C	801	ACO	OAP-CAP-CBP-CCP
2	E	801	ACO	CAP-CBP-CCP-O6A
2	E	801	ACO	OAP-CAP-CBP-CCP
2	E	801	ACO	C3B-C4B-C5B-O5B
2	A	801	ACO	CDP-CBP-CCP-O6A
2	E	801	ACO	CDP-CBP-CCP-O6A
2	E	801	ACO	CEP-CBP-CCP-O6A
2	C	801	ACO	C3P-C2P-S1P-C
2	A	801	ACO	P1A-O3A-P2A-O5A
2	D	801	ACO	P2A-O3A-P1A-O1A
2	C	801	ACO	C3B-O3B-P3B-O7A
2	B	801	ACO	C9P-CAP-CBP-CEP
2	F	801	ACO	O5P-C5P-C6P-C7P
2	A	801	ACO	C3B-O3B-P3B-O9A
2	A	801	ACO	OAP-CAP-CBP-CEP
2	B	801	ACO	OAP-CAP-CBP-CEP
2	E	801	ACO	C3B-O3B-P3B-O8A
2	F	801	ACO	CCP-O6A-P2A-O3A
2	B	801	ACO	O4B-C4B-C5B-O5B
2	D	801	ACO	P2A-O3A-P1A-O2A
2	E	801	ACO	P2A-O3A-P1A-O1A
2	C	801	ACO	CBP-CCP-O6A-P2A
2	A	801	ACO	CCP-O6A-P2A-O5A
2	E	801	ACO	C5B-O5B-P1A-O1A
2	A	801	ACO	O4B-C4B-C5B-O5B
2	C	801	ACO	O4B-C4B-C5B-O5B
2	B	801	ACO	O9P-C9P-CAP-CBP

There are no ring outliers.

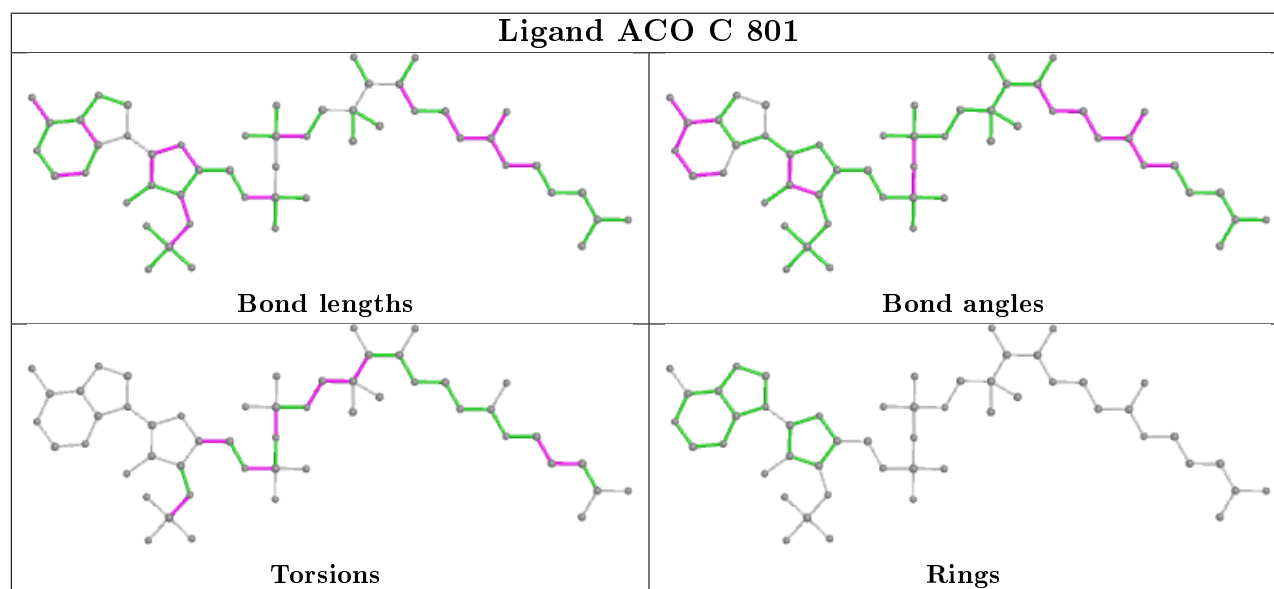
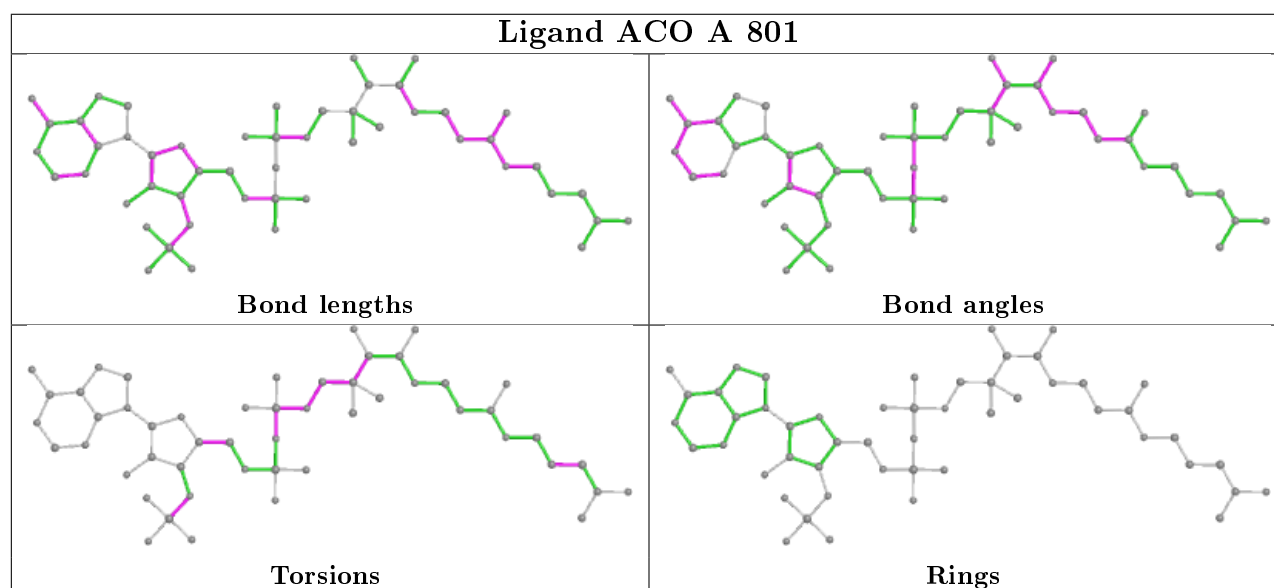
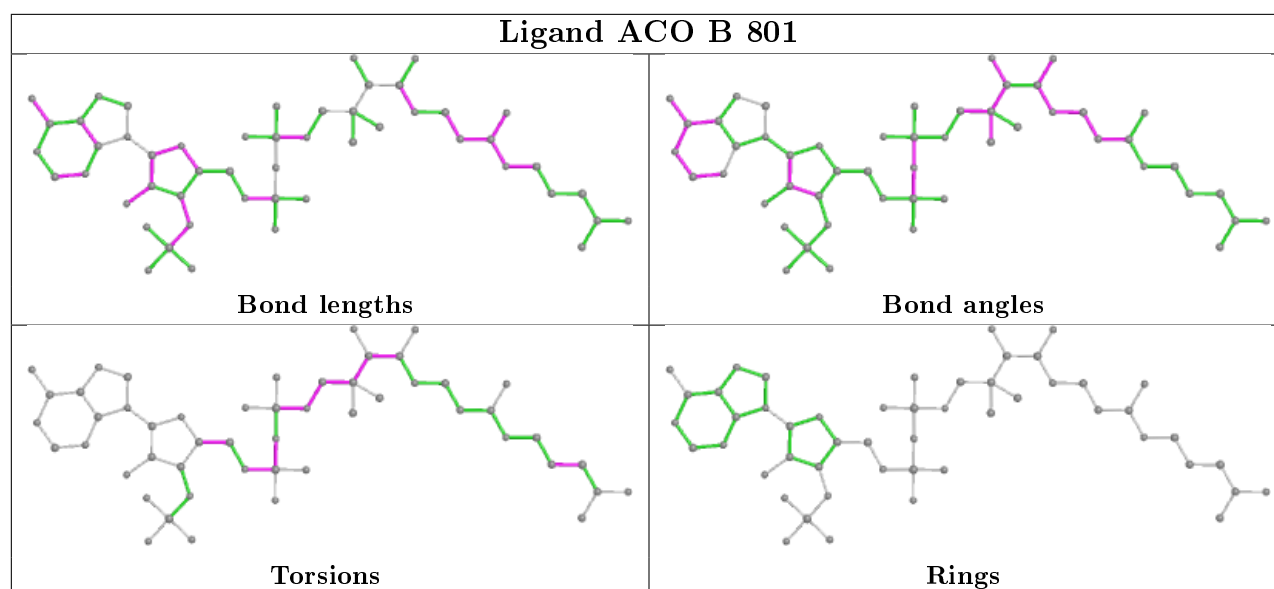
6 monomers are involved in 26 short contacts:

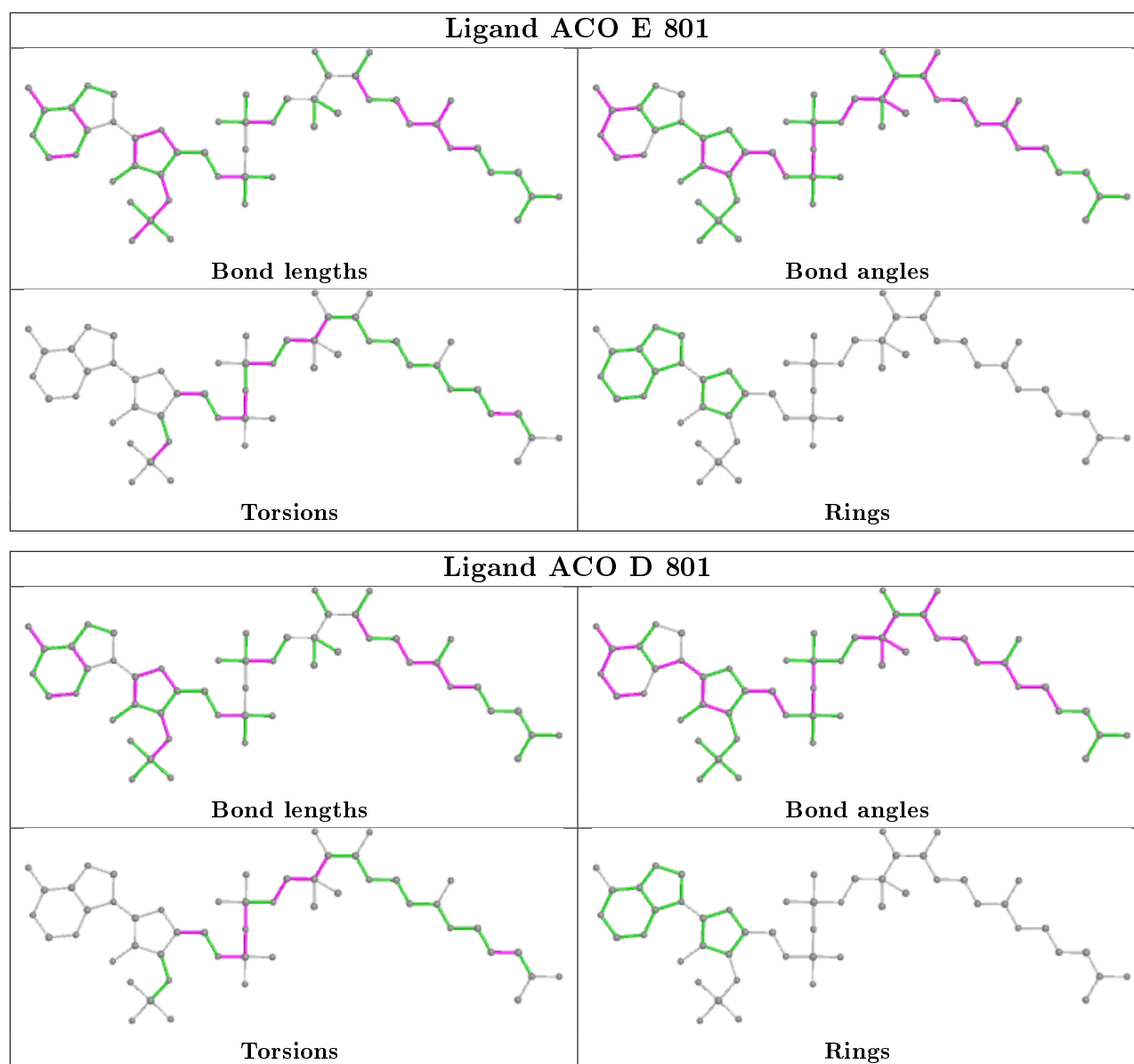
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	ACO	6	0
2	B	801	ACO	4	0
2	A	801	ACO	3	0
2	C	801	ACO	4	0
2	E	801	ACO	4	0
2	D	801	ACO	5	0

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	749/791 (94%)	1.74	232 (30%) 0 0	75, 154, 238, 253	0
1	B	748/791 (94%)	0.95	118 (15%) 2 1	70, 141, 189, 220	0
1	C	750/791 (94%)	0.44	16 (2%) 63 65	60, 81, 121, 139	0
1	D	750/791 (94%)	0.39	7 (0%) 84 85	57, 78, 103, 119	0
1	E	751/791 (94%)	0.42	20 (2%) 54 55	69, 94, 122, 143	0
1	F	753/791 (95%)	0.52	41 (5%) 25 25	63, 95, 128, 145	0
All	All	4501/4746 (94%)	0.74	434 (9%) 8 6	57, 95, 196, 253	0

All (434) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	LEU	15.7
1	A	206	ASN	12.6
1	A	295	ILE	12.3
1	A	330	VAL	11.5
1	A	357	LEU	11.1
1	A	146	ILE	10.7
1	A	331	ASN	10.3
1	A	321	THR	10.3
1	A	391	LEU	10.2
1	B	132	PHE	10.0
1	A	334	LEU	9.9
1	A	182	VAL	9.7
1	A	320	ALA	9.6
1	B	126	ALA	9.5
1	B	241	GLY	9.4
1	A	203	ILE	9.3
1	A	339	ILE	9.0
1	A	218	ILE	8.9
1	A	319	ILE	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	8.9
1	A	271	VAL	8.7
1	A	185	ALA	8.7
1	A	403	TRP	8.5
1	A	333	VAL	8.5
1	A	294	ILE	8.4
1	A	224	ALA	8.4
1	A	402	LEU	8.1
1	A	307	PRO	8.0
1	A	296	PHE	7.9
1	A	147	ASN	7.8
1	A	363	LEU	7.7
1	A	266	LEU	7.5
1	A	205	VAL	7.5
1	A	204	VAL	7.4
1	A	386	PHE	7.4
1	A	392	ILE	7.4
1	A	125	ALA	7.2
1	A	264	GLU	7.1
1	A	298	MET	7.0
1	A	366	LEU	6.9
1	A	318	ILE	6.9
1	A	219	PHE	6.8
1	A	272	PHE	6.7
1	A	282	THR	6.6
1	A	305	ILE	6.6
1	A	208	ALA	6.5
1	A	145	GLY	6.4
1	B	136	VAL	6.4
1	A	186	ALA	6.4
1	A	172	PHE	6.3
1	A	198	MET	6.3
1	A	332	ASN	6.3
1	A	124	VAL	6.2
1	A	229	ILE	6.2
1	A	396	PHE	6.1
1	A	351	ILE	6.1
1	A	193	ILE	6.0
1	A	122	ILE	6.0
1	A	283	PRO	6.0
1	A	169	ILE	5.9
1	A	393	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	5.9
1	A	103	VAL	5.8
1	A	132	PHE	5.7
1	A	275	LEU	5.7
1	A	181	ILE	5.7
1	A	34	ILE	5.7
1	B	90	LEU	5.6
1	A	297	ALA	5.6
1	B	139	LEU	5.6
1	A	189	ASN	5.5
1	A	126	ALA	5.5
1	A	273	VAL	5.5
1	A	183	SER	5.4
1	A	262	LEU	5.4
1	A	361	HIS	5.4
1	A	411	ALA	5.3
1	A	82	VAL	5.3
1	A	434	ALA	5.3
1	B	143	PHE	5.2
1	A	280	ALA	5.1
1	A	178	GLY	5.1
1	A	255	SER	5.1
1	B	172	PHE	5.0
1	A	115	ALA	4.9
1	B	169	ILE	4.9
1	B	278	ALA	4.9
1	B	238	ILE	4.9
1	A	395	PRO	4.9
1	A	362	ALA	4.9
1	B	224	ALA	4.8
1	A	399	ARG	4.8
1	A	190	ALA	4.8
1	B	88	ALA	4.8
1	B	124	VAL	4.7
1	B	245	GLY	4.7
1	A	348	SER	4.6
1	A	270	ASP	4.6
1	A	184	GLY	4.6
1	A	231	MET	4.6
1	A	180	ALA	4.6
1	B	125	ALA	4.5
1	A	401	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	338	SER	4.4
1	A	15	THR	4.4
1	A	207	GLY	4.4
1	A	144	GLY	4.4
1	A	222	LEU	4.4
1	A	111	PHE	4.4
1	B	135	ALA	4.4
1	A	139	LEU	4.4
1	A	497	ARG	4.4
1	A	278	ALA	4.3
1	A	405	ALA	4.3
1	B	218	ILE	4.3
1	A	209	GLY	4.3
1	A	216	ALA	4.3
1	A	114	PHE	4.2
1	A	211	SER	4.2
1	A	171	VAL	4.2
1	A	83	ILE	4.2
1	B	89	VAL	4.2
1	B	83	ILE	4.1
1	B	171	VAL	4.1
1	A	388	ARG	4.1
1	A	406	PRO	4.1
1	B	340	PHE	4.1
1	B	253	PHE	4.1
1	A	258	GLU	4.0
1	B	51	ALA	4.0
1	A	364	ALA	4.0
1	A	355	MET	4.0
1	B	275	LEU	4.0
1	A	136	VAL	4.0
1	A	223	GLY	4.0
1	A	337	PRO	4.0
1	B	231	MET	3.9
1	B	284	GLU	3.9
1	A	432	LEU	3.9
1	B	222	LEU	3.9
1	A	253	PHE	3.9
1	A	80	VAL	3.9
1	A	709	LEU	3.8
1	A	81	ALA	3.8
1	B	219	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	141	PRO	3.8
1	A	326	TYR	3.8
1	B	57	ALA	3.8
1	B	82	VAL	3.8
1	A	385	LYS	3.7
1	B	174	ASP	3.7
1	A	230	ILE	3.7
1	B	351	ILE	3.7
1	B	182	VAL	3.7
1	A	412	ALA	3.7
1	B	36	VAL	3.7
1	B	148	LEU	3.7
1	A	123	GLU	3.7
1	B	266	LEU	3.6
1	A	414	LYS	3.6
1	A	370	ASP	3.6
1	A	167	MET	3.6
1	A	340	PHE	3.6
1	A	344	LEU	3.6
1	B	286	LEU	3.6
1	A	70	VAL	3.6
1	F	359	ALA	3.6
1	B	95	ILE	3.6
1	A	120	PHE	3.5
1	A	176	GLN	3.5
1	A	421	ALA	3.5
1	A	210	ALA	3.5
1	A	90	LEU	3.5
1	B	396	PHE	3.5
1	B	247	ASN	3.5
1	B	510	LEU	3.5
1	A	284	GLU	3.4
1	A	265	ALA	3.4
1	A	269	ALA	3.4
1	B	147	ASN	3.4
1	A	110	LEU	3.4
1	B	79	LEU	3.4
1	A	435	LEU	3.4
1	A	491	LEU	3.4
1	B	279	GLY	3.4
1	E	747	LEU	3.4
1	A	174	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	261	THR	3.3
1	A	187	LEU	3.3
1	A	148	LEU	3.3
1	A	293	PRO	3.3
1	F	253	PHE	3.2
1	B	103	VAL	3.2
1	A	135	ALA	3.2
1	A	510	LEU	3.2
1	F	266	LEU	3.2
1	A	56	VAL	3.2
1	A	299	ALA	3.2
1	A	608	LEU	3.2
1	B	52	TYR	3.2
1	B	159	ILE	3.1
1	A	113	GLN	3.1
1	B	75	ALA	3.1
1	F	216	ALA	3.1
1	B	142	THR	3.1
1	B	205	VAL	3.1
1	A	276	SER	3.1
1	E	34	ILE	3.1
1	A	306	THR	3.1
1	B	111	PHE	3.1
1	A	27	GLN	3.1
1	A	309	LYS	3.1
1	B	281	LEU	3.1
1	B	467	PRO	3.0
1	A	138	VAL	3.0
1	B	110	LEU	3.0
1	F	363	LEU	3.0
1	A	142	THR	3.0
1	A	215	CYS	3.0
1	A	762	PHE	3.0
1	B	249	TYR	3.0
1	B	120	PHE	3.0
1	A	33	LYS	3.0
1	A	98	ALA	3.0
1	A	317	ALA	2.9
1	B	356	LYS	2.9
1	A	92	LEU	2.9
1	B	74	THR	2.9
1	B	363	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	507	ILE	2.9
1	A	335	GLY	2.9
1	A	36	VAL	2.9
1	A	408	VAL	2.9
1	A	75	ALA	2.9
1	A	274	GLY	2.9
1	B	243	THR	2.9
1	F	404	VAL	2.9
1	B	280	ALA	2.9
1	A	137	ARG	2.9
1	A	486	ILE	2.9
1	B	122	ILE	2.9
1	E	727	ILE	2.9
1	B	48	LEU	2.9
1	A	359	ALA	2.9
1	A	607	PHE	2.8
1	A	603	LEU	2.8
1	A	67	PRO	2.8
1	F	146	ILE	2.8
1	E	603	LEU	2.8
1	B	339	ILE	2.8
1	F	525	PHE	2.8
1	B	230	ILE	2.8
1	B	507	ILE	2.8
1	A	304	GLU	2.8
1	A	191	CYS	2.8
1	C	466	PHE	2.8
1	F	230	ILE	2.8
1	F	272	PHE	2.8
1	B	273	VAL	2.8
1	F	171	VAL	2.8
1	B	37	ILE	2.8
1	B	392	ILE	2.8
1	F	206	ASN	2.7
1	A	368	ARG	2.7
1	D	172	PHE	2.7
1	F	219	PHE	2.7
1	A	724	ILE	2.7
1	B	337	PRO	2.7
1	A	109	ILE	2.7
1	A	119	VAL	2.7
1	A	286	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	213	ASN	2.7
1	B	525	PHE	2.7
1	A	68	ALA	2.7
1	B	170	PRO	2.7
1	B	248	LYS	2.7
1	A	525	PHE	2.7
1	B	250	LYS	2.7
1	E	474	VAL	2.6
1	E	510	LEU	2.6
1	F	262	LEU	2.6
1	B	355	MET	2.6
1	F	304	GLU	2.6
1	A	350	GLN	2.6
1	A	212	ALA	2.6
1	B	301	PRO	2.6
1	A	354	GLU	2.6
1	A	720	ALA	2.6
1	B	115	ALA	2.6
1	A	394	LYS	2.6
1	B	167	MET	2.6
1	B	267	ARG	2.6
1	B	724	ILE	2.6
1	A	602	LEU	2.6
1	A	289	MET	2.6
1	B	198	MET	2.6
1	D	148	LEU	2.5
1	B	289	MET	2.5
1	A	310	ALA	2.5
1	A	313	ALA	2.5
1	A	367	ALA	2.5
1	A	422	ILE	2.5
1	A	52	TYR	2.5
1	B	400	VAL	2.5
1	F	204	VAL	2.5
1	B	240	LYS	2.5
1	A	369	GLU	2.5
1	F	43	ALA	2.5
1	B	84	SER	2.5
1	B	109	ILE	2.5
1	F	278	ALA	2.5
1	C	510	LEU	2.5
1	B	336	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	444	ARG	2.5
1	A	232	CYS	2.5
1	B	71	TYR	2.5
1	C	138	VAL	2.5
1	C	481	LEU	2.4
1	D	132	PHE	2.4
1	A	349	THR	2.4
1	B	481	LEU	2.4
1	B	138	VAL	2.4
1	E	205	VAL	2.4
1	A	101	LYS	2.4
1	A	194	THR	2.4
1	A	631	ALA	2.4
1	E	757	VAL	2.4
1	F	388	ARG	2.4
1	B	402	LEU	2.4
1	F	117	ILE	2.4
1	A	353	GLU	2.4
1	A	143	PHE	2.4
1	A	711	PHE	2.4
1	A	308	ASP	2.3
1	A	706	ALA	2.3
1	E	542	LEU	2.3
1	B	688	VAL	2.3
1	B	25	TYR	2.3
1	A	358	ALA	2.3
1	B	127	THR	2.3
1	F	496	GLU	2.3
1	B	370	ASP	2.3
1	B	53[A]	SER	2.3
1	E	584	LEU	2.3
1	C	569	VAL	2.3
1	F	182	VAL	2.3
1	F	638	PHE	2.3
1	B	246	MET	2.3
1	D	491	LEU	2.3
1	F	50	LEU	2.3
1	B	58	ALA	2.3
1	F	729	LYS	2.3
1	A	79	LEU	2.3
1	F	339	ILE	2.3
1	A	433	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	384	PHE	2.3
1	C	351	ILE	2.3
1	A	301	PRO	2.3
1	F	602	LEU	2.3
1	C	146	ILE	2.3
1	E	507	ILE	2.3
1	A	213	ASN	2.2
1	E	252	TYR	2.2
1	B	464	ILE	2.2
1	A	102	PRO	2.2
1	B	366	LEU	2.2
1	F	510	LEU	2.2
1	B	334	LEU	2.2
1	F	281	LEU	2.2
1	F	486	ILE	2.2
1	A	85	ASN	2.2
1	A	179	THR	2.2
1	B	272	PHE	2.2
1	A	692	ILE	2.2
1	B	333	VAL	2.2
1	F	205	VAL	2.2
1	A	721	TYR	2.2
1	B	73	TYR	2.2
1	A	225	ARG	2.2
1	C	486	ILE	2.2
1	E	481	LEU	2.2
1	A	104	MET	2.2
1	F	754	ASP	2.2
1	B	600	PHE	2.2
1	A	73	TYR	2.2
1	A	407	GLU	2.2
1	B	723	LEU	2.2
1	A	84	SER	2.1
1	C	760	VAL	2.1
1	E	122	ILE	2.1
1	A	121	ASP	2.1
1	C	15	THR	2.1
1	B	285	MET	2.1
1	A	188	LEU	2.1
1	B	262	LEU	2.1
1	B	107	LYS	2.1
1	D	222	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	334	LEU	2.1
1	F	37	ILE	2.1
1	C	477	ALA	2.1
1	D	126	ALA	2.1
1	A	404	VAL	2.1
1	E	83	ILE	2.1
1	F	509	LEU	2.1
1	C	489	PRO	2.1
1	A	287	LYS	2.1
1	E	47	ASP	2.1
1	C	136	VAL	2.1
1	C	366	LEU	2.1
1	E	723	LEU	2.1
1	E	132	PHE	2.1
1	B	144	GLY	2.1
1	B	478	LEU	2.1
1	F	391	LEU	2.1
1	B	34	ILE	2.1
1	B	393	PRO	2.1
1	F	235	GLN	2.1
1	A	285	MET	2.1
1	A	95	ILE	2.0
1	A	18	PHE	2.0
1	F	143	PHE	2.0
1	A	151	ILE	2.0
1	A	640	ILE	2.0
1	C	135	ALA	2.0
1	B	156	CYS	2.0
1	C	363	LEU	2.0
1	F	408	VAL	2.0
1	E	46	LYS	2.0
1	B	178	GLY	2.0
1	F	51	ALA	2.0
1	F	186	ALA	2.0
1	A	214	SER	2.0
1	F	42	CYS	2.0
1	D	333	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

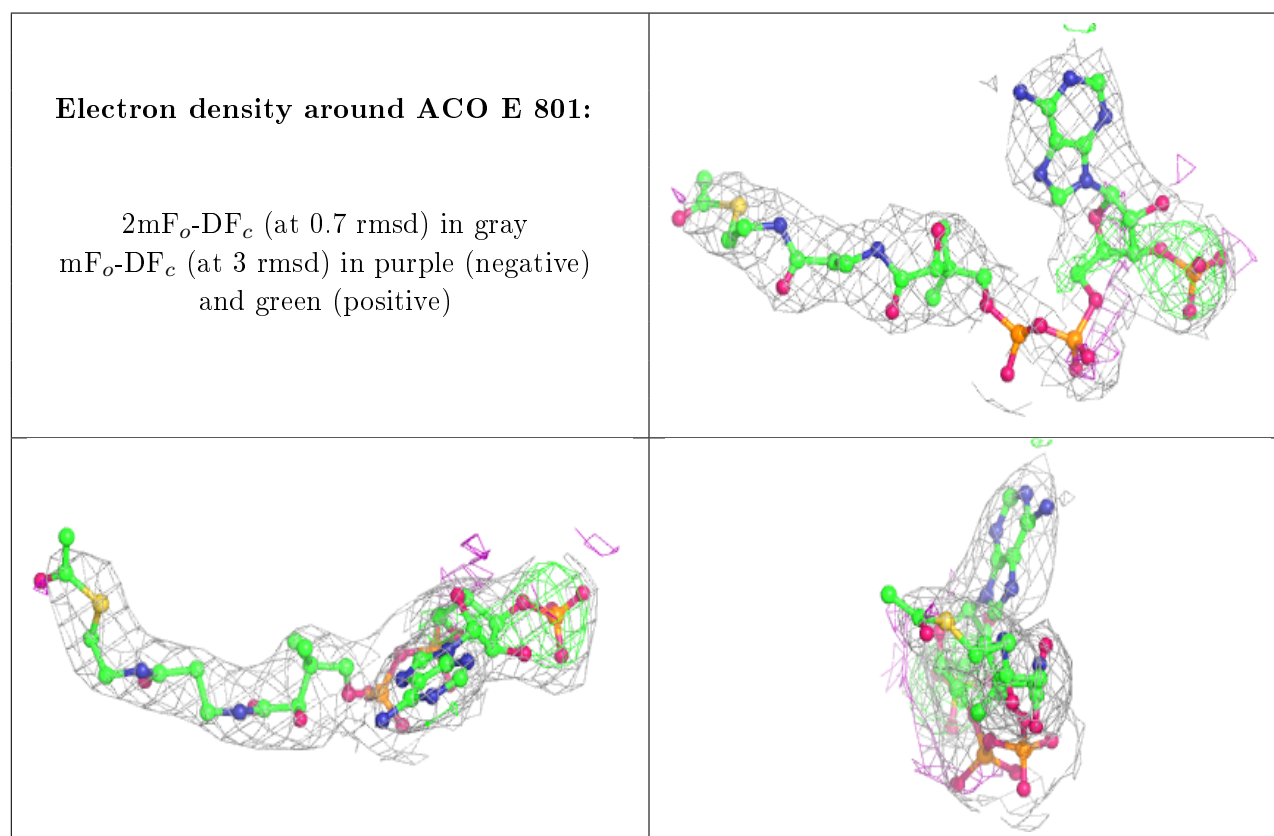
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

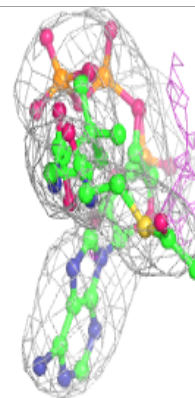
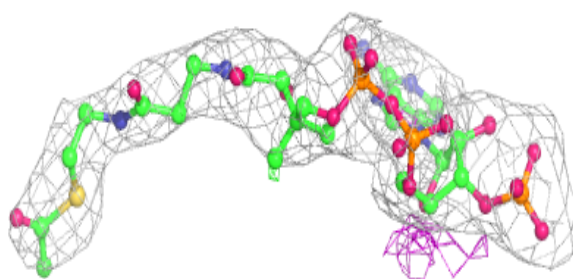
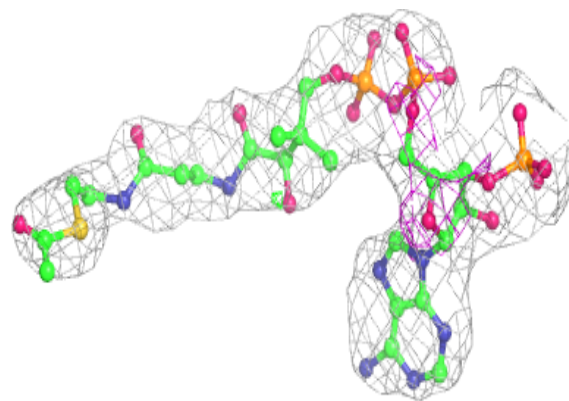
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACO	E	801	51/51	0.83	0.24	65,93,309,311	0
2	ACO	B	801	51/51	0.93	0.20	70,87,137,163	0
2	ACO	A	801	51/51	0.93	0.21	60,102,129,132	0
2	ACO	D	801	51/51	0.94	0.20	59,77,111,130	0
2	ACO	C	801	51/51	0.94	0.20	58,76,130,136	0
2	ACO	F	801	51/51	0.94	0.20	46,78,106,118	0

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

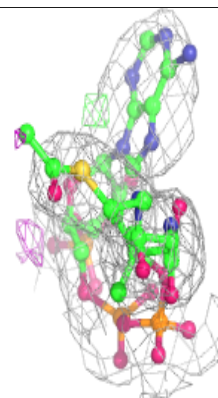
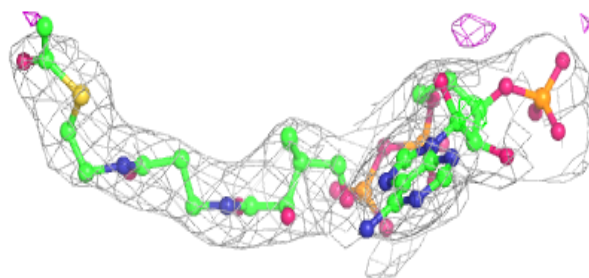
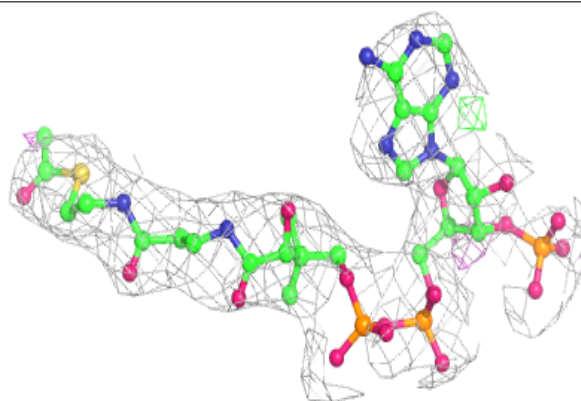


**Electron density around ACO B 801:**

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

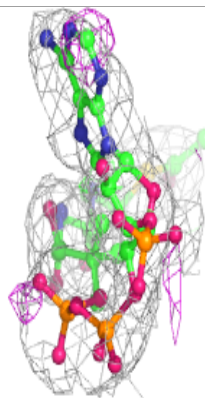
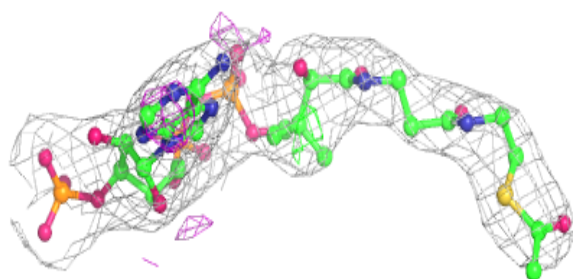
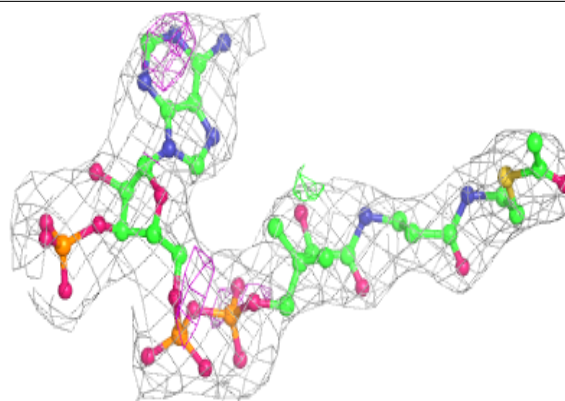
**Electron density around ACO A 801:**

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

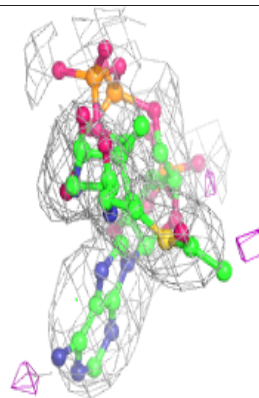
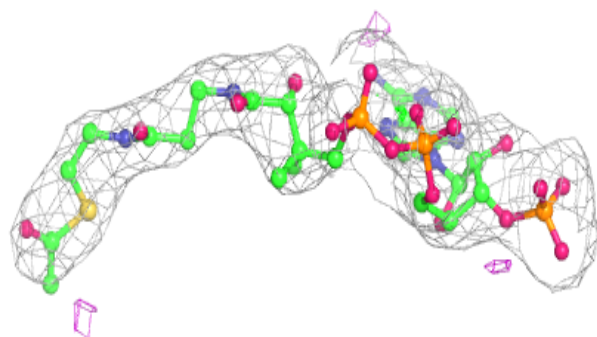
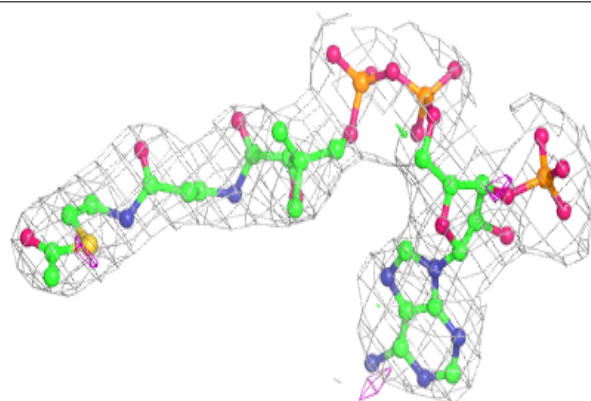


**Electron density around ACO D 801:**

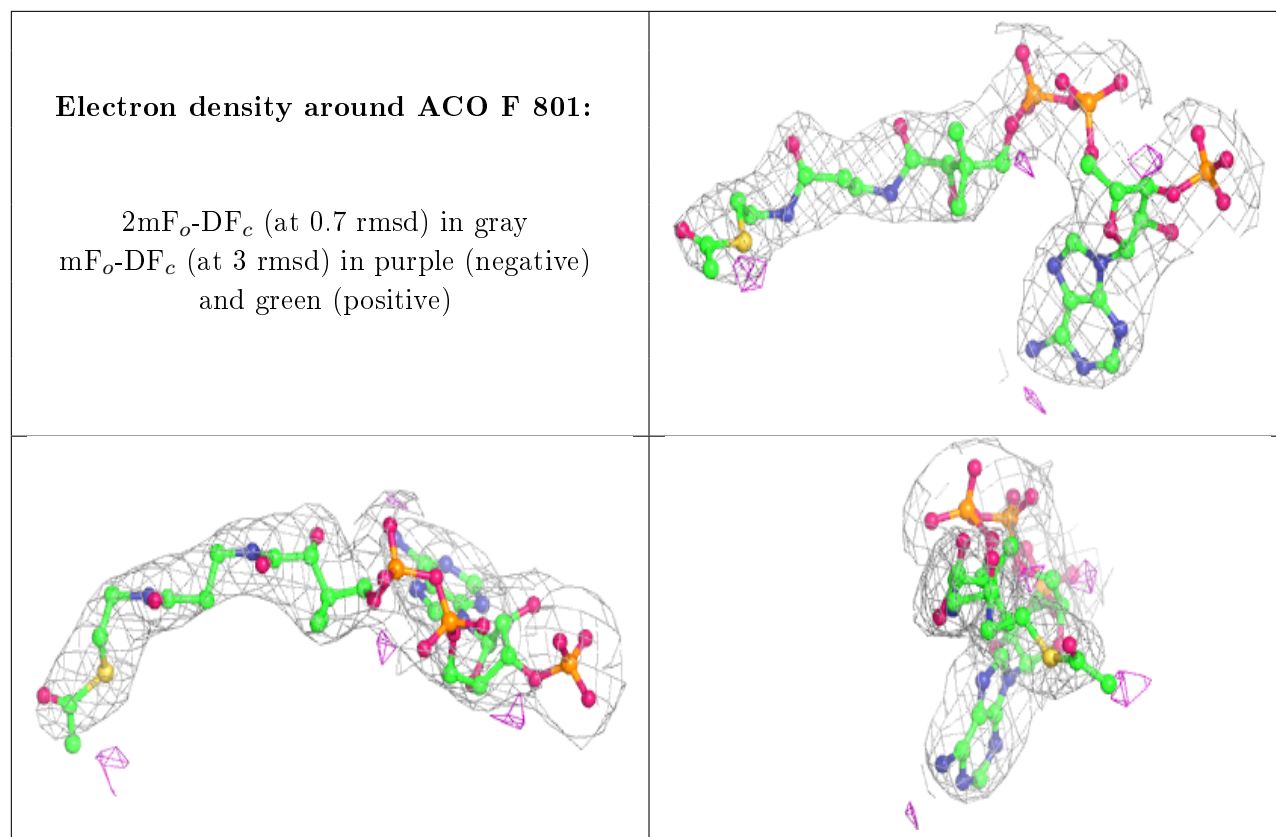
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ACO C 801:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.