Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:47 am BST

PDB ID	:	5BZ4
Title	:	Crystal structure of a T1-like thiolase (CoA-complex) from Mycobacterium smegmatis
Authors	:	Janardan, N.; Harijan, R.K.; Kiema, T.R.; Wierenga, R.K.; Murthy, M.R.N.
Deposited on	:	2015-06-11
Resolution	:	2.43 Å(reported)

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

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

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

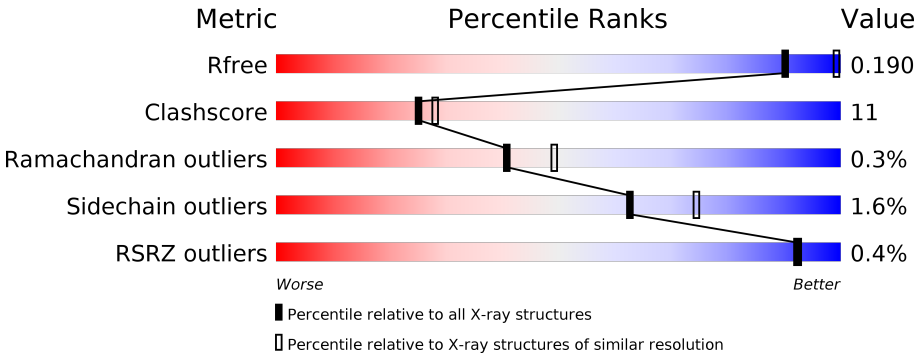
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	76% 22% •
1	B	407	77% 20% • •
1	C	407	% 77% 19% • •
1	D	407	76% 21% •
1	E	407	76% 20% • •
1	F	407	78% 20% •

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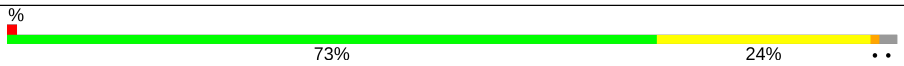
Mol	Chain	Length	Quality of chain
1	G	407	
1	H	407	
1	J	407	
1	K	407	
1	L	407	
1	M	407	

2 Entry composition

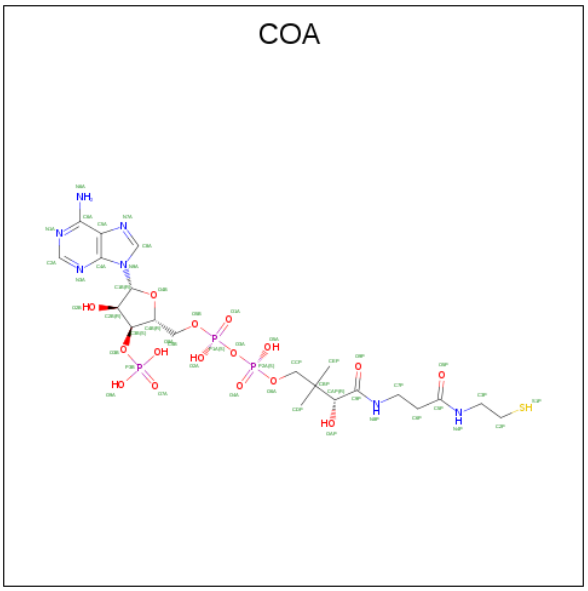
There are 3 unique types of molecules in this entry. The entry contains 36925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	1	0
			2912	1802	538	556	16			
1	B	398	Total	C	N	O	S	0	0	0
			2926	1813	537	560	16			
1	C	398	Total	C	N	O	S	0	0	0
			2903	1798	529	560	16			
1	D	397	Total	C	N	O	S	0	0	0
			2923	1811	536	560	16			
1	E	396	Total	C	N	O	S	0	0	0
			2918	1805	536	561	16			
1	F	399	Total	C	N	O	S	0	0	0
			2946	1824	541	565	16			
1	G	402	Total	C	N	O	S	0	0	0
			2956	1829	544	567	16			
1	H	397	Total	C	N	O	S	0	0	0
			2929	1813	539	561	16			
1	J	396	Total	C	N	O	S	0	0	0
			2905	1798	536	555	16			
1	K	400	Total	C	N	O	S	0	0	0
			2943	1821	540	566	16			
1	L	400	Total	C	N	O	S	0	0	0
			2929	1808	541	564	16			
1	M	397	Total	C	N	O	S	0	0	0
			2921	1808	536	561	16			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	167	Total	O	0	0
			167	167		
3	C	147	Total	O	0	0
			147	147		
3	D	145	Total	O	0	0
			145	145		
3	E	110	Total	O	0	0
			110	110		
3	F	114	Total	O	0	0
			114	114		
3	G	121	Total	O	0	0
			121	121		

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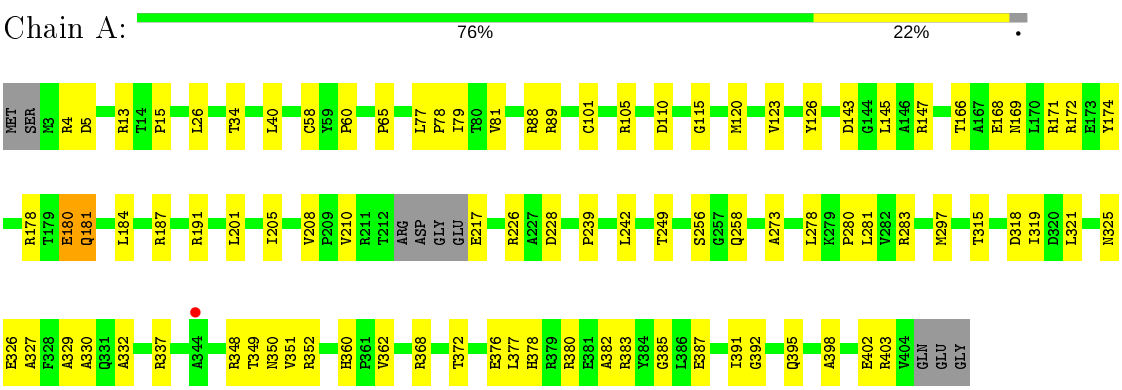
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	159	Total O 159 159	0	0
3	J	110	Total O 110 110	0	0
3	K	152	Total O 152 152	0	0
3	L	106	Total O 106 106	0	0
3	M	102	Total O 102 102	0	0

3 Residue-property plots

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

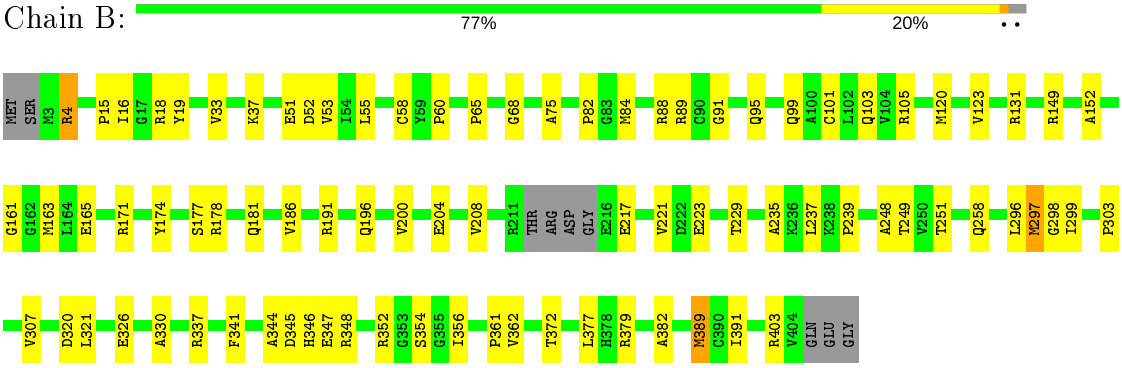
- Molecule 1: Beta-ketothiolase

Chain A:



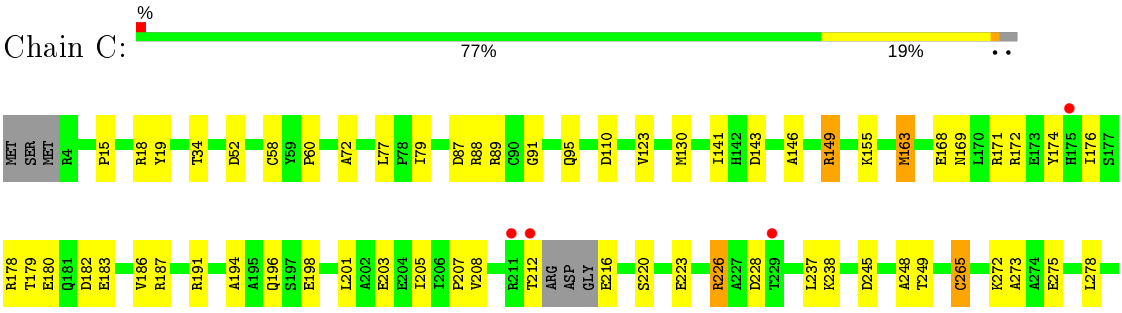
- Molecule 1: Beta-ketothiolase

Chain B:



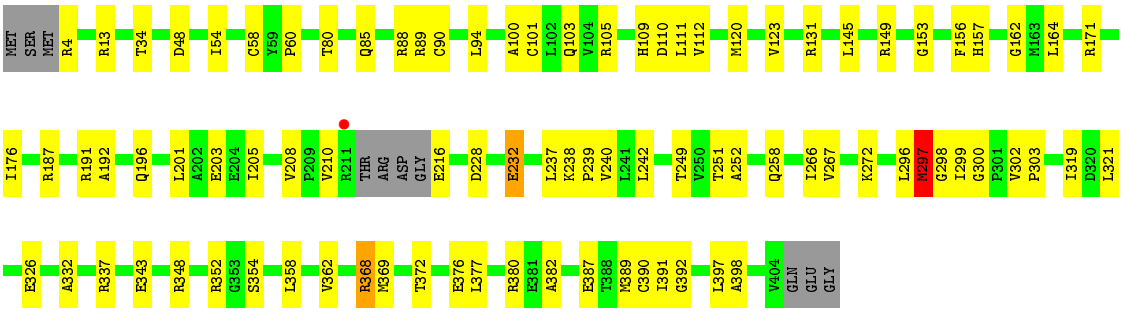
- Molecule 1: Beta-ketothiolase

Chain C:



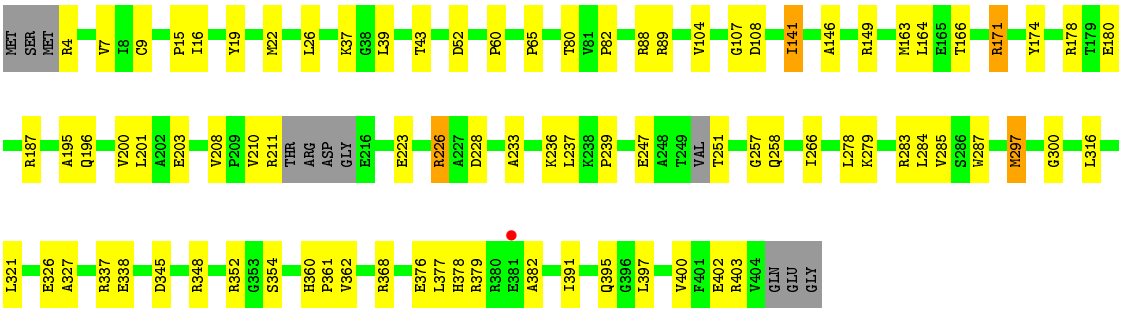
• Molecule 1: Beta-ketothiolase

Chain D:



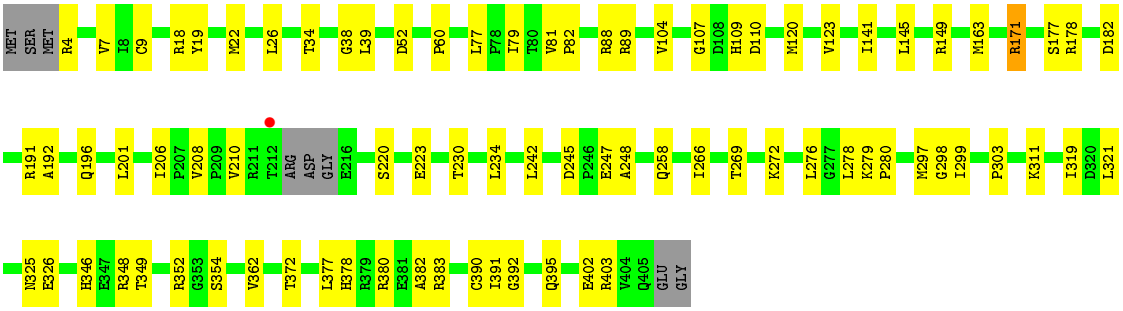
• Molecule 1: Beta-ketothiolase

Chain E:



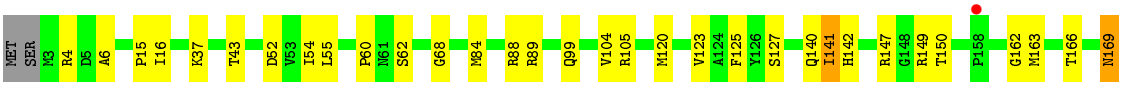
• Molecule 1: Beta-ketothiolase

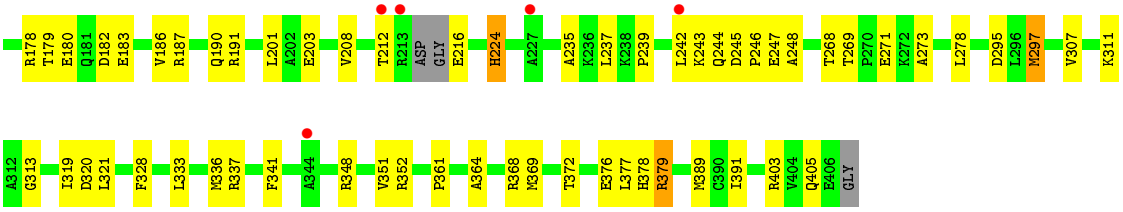
Chain F:



• Molecule 1: Beta-ketothiolase

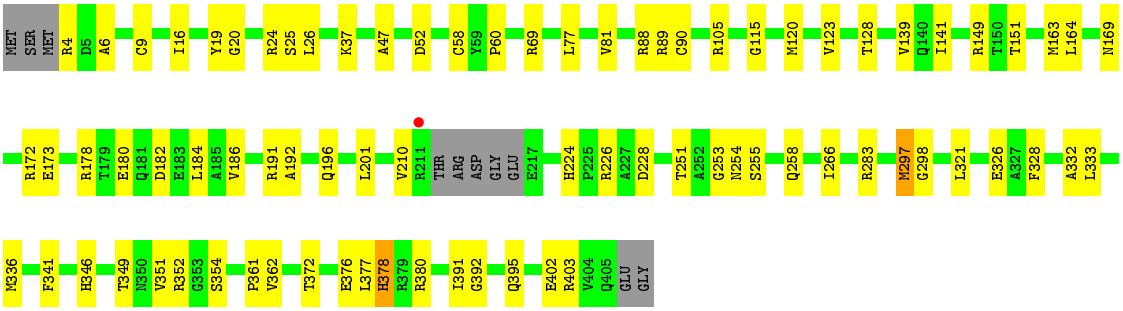
Chain G:





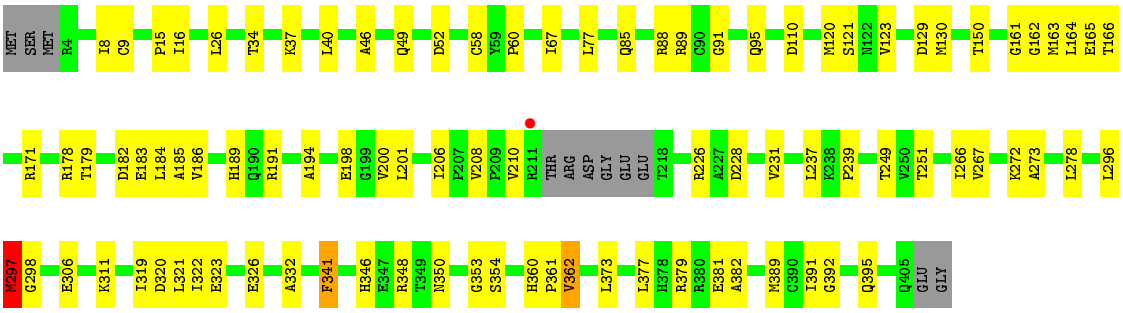
• Molecule 1: Beta-ketothiolase

Chain H:



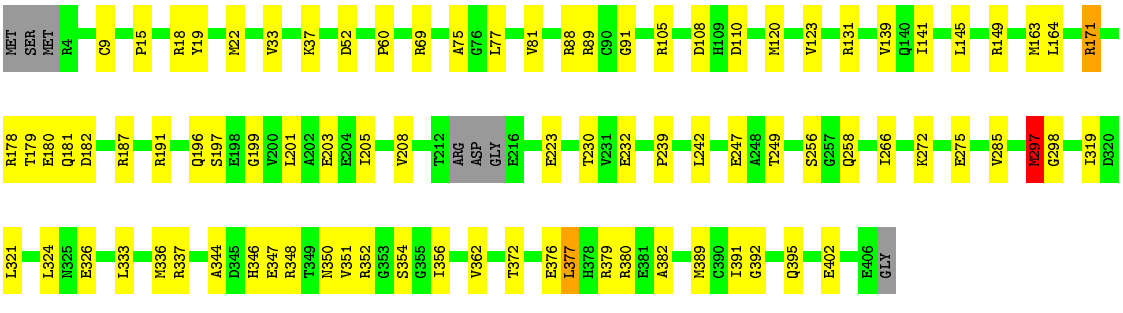
• Molecule 1: Beta-ketothiolase

Chain J:



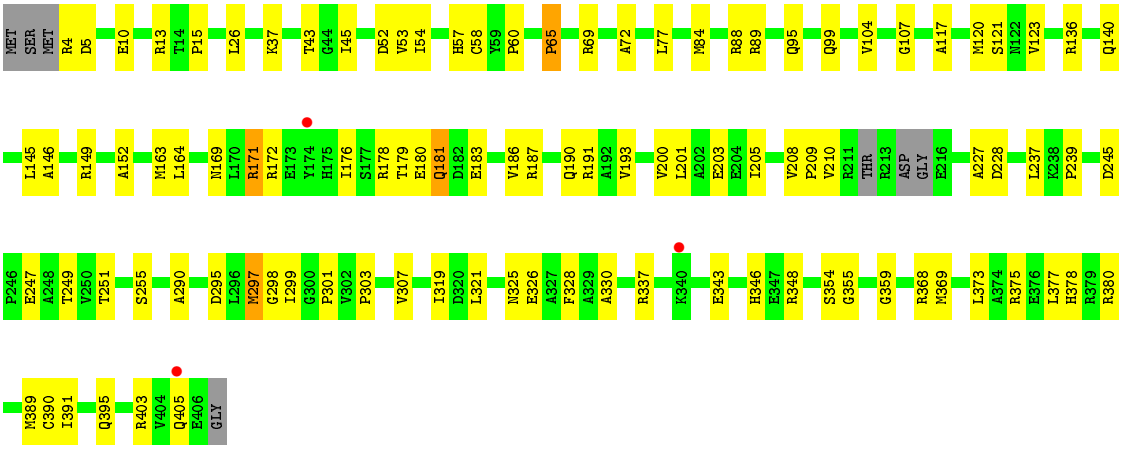
• Molecule 1: Beta-ketothiolase

Chain K:



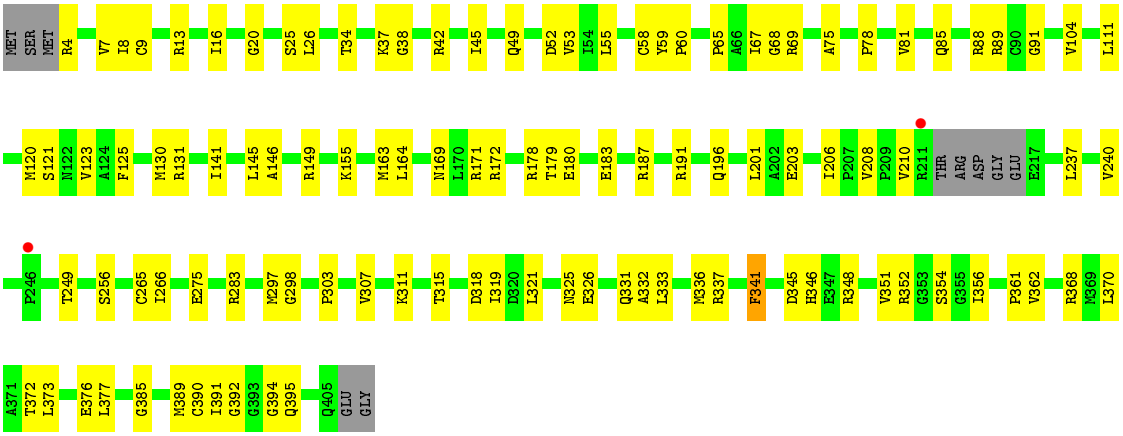
• Molecule 1: Beta-ketothiolase

Chain L:



- Molecule 1: Beta-ketothiolase

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	190.08Å 190.08Å 265.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 2.43 47.52 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.52-2.43) 98.9 (47.52-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.161 , 0.188 0.162 , 0.190	Depositor DCC
R_{free} test set	10163 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36925	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7670e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA

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	0/2956	0.61	0/4015
1	B	0.47	1/2970 (0.0%)	0.66	4/4029 (0.1%)
1	C	0.43	0/2946	0.63	2/4000 (0.1%)
1	D	0.43	0/2967	0.62	1/4025 (0.0%)
1	E	0.41	0/2961	0.60	0/4016
1	F	0.43	0/2990	0.60	0/4054
1	G	0.42	0/3000	0.63	0/4071
1	H	0.43	0/2973	0.61	1/4033 (0.0%)
1	J	0.41	0/2949	0.61	1/4003 (0.0%)
1	K	0.44	0/2987	0.61	1/4053 (0.0%)
1	L	0.39	0/2972	0.58	0/4030
1	M	0.40	0/2964	0.58	0/4021
All	All	0.42	1/35635 (0.0%)	0.61	10/48350 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	MET	CG-SD	-5.21	1.67	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	297	MET	CG-SD-CE	-8.85	86.05	100.20
1	B	297	MET	CG-SD-CE	-7.97	87.45	100.20
1	B	297	MET	CB-CG-SD	7.95	136.24	112.40
1	J	297	MET	CG-SD-CE	-7.78	87.76	100.20
1	H	297	MET	CG-SD-CE	-7.25	88.61	100.20
1	B	297	MET	CA-CB-CG	-6.26	102.66	113.30
1	K	297	MET	CG-SD-CE	-5.76	90.98	100.20
1	D	297	MET	CB-CG-SD	5.70	129.49	112.40
1	C	163	MET	CG-SD-CE	5.45	108.92	100.20
1	B	389	MET	CA-CB-CG	-5.13	104.58	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2912	0	2890	78	0
1	B	2926	0	2927	64	0
1	C	2903	0	2878	62	0
1	D	2923	0	2930	62	0
1	E	2918	0	2913	65	0
1	F	2946	0	2954	57	0
1	G	2956	0	2951	70	0
1	H	2929	0	2936	58	0
1	J	2905	0	2900	63	0
1	K	2943	0	2934	66	0
1	L	2929	0	2893	79	0
1	M	2921	0	2919	79	0
2	B	48	0	32	0	0
2	D	48	0	32	8	0
2	F	48	0	32	0	0
2	H	48	0	32	5	0
2	K	48	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	141	0	0	10	0
3	B	167	0	0	7	0
3	C	147	0	0	6	0
3	D	145	0	0	6	2
3	E	110	0	0	6	0
3	F	114	0	0	3	0
3	G	121	0	0	9	0
3	H	159	0	0	12	0
3	J	110	0	0	5	2
3	K	152	0	0	4	0
3	L	106	0	0	7	0
3	M	102	0	0	8	0
All	All	36925	0	35185	756	2

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 11.

All (756) 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:C:163:MET:HG2	1:C:297:MET:HE1	1.40	1.02
2:H:501:COA:H71	3:H:670:HOH:O	1.60	0.98
1:L:4:ARG:NH2	1:L:104:VAL:O	1.95	0.98
1:A:166:THR:HG21	1:A:297:MET:HB3	1.51	0.92
1:L:65:PRO:HB3	1:M:89:ARG:HH21	1.37	0.90
1:L:171:ARG:HA	1:L:176:ILE:HD12	1.55	0.88
1:J:297:MET:HG3	1:J:298:GLY:N	1.89	0.88
1:L:178:ARG:NH2	1:L:237:LEU:O	2.08	0.86
1:K:326:GLU:OE1	1:K:354:SER:OG	1.94	0.85
1:K:178:ARG:NH1	1:K:182:ASP:OD2	2.10	0.85
1:B:88:ARG:NH1	1:B:95:GLN:OE1	2.10	0.84
1:K:89:ARG:HB2	1:K:391:ILE:HG23	1.59	0.84
1:B:174:TYR:O	1:B:337:ARG:NH1	2.11	0.84
1:L:178:ARG:HH21	1:L:251:THR:HG21	1.42	0.84
1:K:297:MET:HG2	1:K:298:GLY:N	1.93	0.83
1:J:178:ARG:NH2	1:J:237:LEU:O	2.12	0.83
1:F:171:ARG:NH2	1:F:247:GLU:O	2.11	0.83
1:K:319:ILE:O	1:K:348:ARG:NH1	2.11	0.82
1:A:326:GLU:OE2	1:A:350:ASN:ND2	2.13	0.81
1:L:171:ARG:NH2	1:L:247:GLU:HB3	1.95	0.81
1:B:55:LEU:HD22	1:B:68:GLY:HA2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:OD1	1:C:172:ARG:NH2	2.16	0.79
1:A:89:ARG:NH2	3:A:502:HOH:O	2.16	0.79
1:G:88:ARG:NH2	1:H:52:ASP:OD1	2.17	0.78
1:L:181:GLN:NE2	1:L:330:ALA:HB2	2.00	0.77
1:G:52:ASP:OD1	1:H:88:ARG:NH2	2.16	0.77
1:C:88:ARG:NH1	1:C:95:GLN:OE1	2.19	0.76
1:F:352:ARG:HD2	1:F:372:THR:HG23	1.68	0.76
1:H:297:MET:HE1	1:H:392:GLY:HA2	1.67	0.76
1:C:352:ARG:NH2	3:C:502:HOH:O	2.13	0.75
1:H:326:GLU:OE1	1:H:354:SER:OG	2.04	0.75
1:A:319:ILE:O	1:A:348:ARG:NH1	2.20	0.75
1:E:89:ARG:HB2	1:E:391:ILE:HG23	1.66	0.75
1:A:376:GLU:HG3	1:A:380:ARG:HD2	1.68	0.75
1:G:37:LYS:NZ	3:G:502:HOH:O	2.20	0.75
1:A:174:TYR:O	1:A:337:ARG:NH1	2.20	0.74
1:K:145:LEU:HD13	1:K:258:GLN:NE2	2.02	0.74
1:L:10:GLU:OE2	1:L:375:ARG:NH2	2.20	0.74
1:F:196:GLN:HG2	1:F:201:LEU:HD12	1.70	0.73
1:G:224:HIS:O	1:G:224:HIS:ND1	2.20	0.73
2:H:501:COA:O4A	3:H:602:HOH:O	2.06	0.73
1:G:352:ARG:NH2	3:G:504:HOH:O	2.22	0.73
1:A:4:ARG:NH2	1:A:110:ASP:OD1	2.21	0.72
1:A:258:GLN:NE2	3:A:504:HOH:O	2.22	0.72
1:B:178:ARG:HH12	1:B:235:ALA:HA	1.53	0.72
1:C:297:MET:HG3	1:C:298:GLY:N	2.04	0.72
1:D:149:ARG:NH1	1:D:258:GLN:OE1	2.20	0.72
1:J:226:ARG:NH1	1:J:228:ASP:OD2	2.22	0.72
1:M:164:LEU:HD21	1:M:240:VAL:HB	1.72	0.72
1:C:187:ARG:HD2	1:C:191:ARG:HH21	1.54	0.72
1:C:155:LYS:NZ	3:C:506:HOH:O	2.22	0.72
1:H:297:MET:HG3	1:H:298:GLY:N	2.04	0.71
1:G:163:MET:HG2	1:G:297:MET:HE1	1.72	0.71
1:G:178:ARG:NH2	1:G:237:LEU:O	2.24	0.71
1:C:226:ARG:NH1	1:C:228:ASP:OD2	2.24	0.71
1:L:58:CYS:HB3	1:L:89:ARG:NH1	2.05	0.70
1:F:319:ILE:O	1:F:348:ARG:NH1	2.24	0.70
1:E:88:ARG:NH2	1:F:52:ASP:OD1	2.24	0.70
1:K:352:ARG:HD2	1:K:372:THR:HG23	1.74	0.70
1:G:321:LEU:HD12	1:G:377:LEU:HD23	1.74	0.69
1:M:58:CYS:HB3	1:M:89:ARG:NH1	2.07	0.69
1:D:203:GLU:OE1	3:D:601:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:TYR:O	3:C:501:HOH:O	2.10	0.69
1:E:178:ARG:NH2	1:E:237:LEU:O	2.26	0.69
1:A:143:ASP:OD1	1:B:131:ARG:NH2	2.19	0.69
1:A:181:GLN:OE1	1:A:330:ALA:HB2	1.93	0.69
1:E:166:THR:HG21	1:E:297:MET:HB3	1.75	0.69
1:A:325:ASN:O	3:A:501:HOH:O	2.11	0.68
1:L:180:GLU:OE1	1:L:337:ARG:NH2	2.26	0.68
1:A:88:ARG:NH2	1:B:52:ASP:OD1	2.27	0.68
1:L:325:ASN:O	3:L:501:HOH:O	2.10	0.68
1:M:155:LYS:NZ	3:M:510:HOH:O	2.25	0.68
1:B:89:ARG:HB2	1:B:391:ILE:HG23	1.76	0.68
1:G:179:THR:O	1:G:183:GLU:HG3	1.94	0.68
1:L:178:ARG:HG3	1:L:249:THR:HB	1.75	0.68
1:M:9:CYS:HB2	1:M:266:ILE:HB	1.76	0.67
1:G:55:LEU:HD22	1:G:68:GLY:HA2	1.76	0.67
1:J:306:GLU:OE2	3:J:501:HOH:O	2.13	0.67
1:M:297:MET:HG3	1:M:392:GLY:HA2	1.76	0.67
1:L:140:GLN:NE2	3:L:505:HOH:O	2.27	0.67
1:M:196:GLN:HG3	1:M:201:LEU:HD22	1.77	0.66
1:G:351:VAL:HG21	1:G:376:GLU:HG2	1.77	0.66
1:B:204:GLU:OE2	1:B:352:ARG:NH1	2.28	0.66
1:F:4:ARG:HH11	1:F:107:GLY:HA2	1.59	0.66
1:H:26:LEU:HD11	1:H:210:VAL:HG12	1.78	0.66
1:K:149:ARG:HG2	1:K:163:MET:HG2	1.76	0.66
1:H:89:ARG:HB2	1:H:391:ILE:HG23	1.76	0.66
1:K:191:ARG:NH2	1:K:346:HIS:O	2.27	0.66
1:K:37:LYS:NZ	3:K:603:HOH:O	2.21	0.66
1:M:163:MET:HG2	1:M:297:MET:HE2	1.78	0.66
1:L:52:ASP:OD1	1:M:88:ARG:NH2	2.29	0.66
1:G:88:ARG:HH22	1:H:52:ASP:CG	1.98	0.66
1:B:18:ARG:HG3	1:B:223:GLU:HG2	1.77	0.65
1:F:34:THR:HG21	1:F:208:VAL:HG22	1.77	0.65
1:M:37:LYS:HG3	1:M:75:ALA:HB1	1.78	0.65
1:D:34:THR:HG21	1:D:208:VAL:HG22	1.77	0.65
1:H:120:MET:HA	1:H:123:VAL:HG23	1.79	0.65
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.26	0.65
1:M:67:ILE:HG22	1:M:85:GLN:HB2	1.78	0.65
1:A:281:LEU:HA	1:A:378:HIS:CE1	2.32	0.65
1:D:156:PHE:O	1:D:157:HIS:ND1	2.29	0.65
1:E:345:ASP:OD1	1:E:348:ARG:NH1	2.30	0.65
1:F:325:ASN:O	3:F:602:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:ARG:HB2	1:G:391:ILE:HG23	1.79	0.65
1:F:326:GLU:OE1	1:F:354:SER:OG	2.12	0.64
1:J:34:THR:HG21	1:J:208:VAL:HG22	1.78	0.64
1:B:58:CYS:HB3	1:B:89:ARG:NH1	2.13	0.64
1:M:89:ARG:NH2	3:M:502:HOH:O	2.12	0.64
1:A:383:ARG:NH1	1:A:402:GLU:OE2	2.29	0.64
1:B:99:GLN:OE1	3:B:601:HOH:O	2.13	0.64
1:C:176:ILE:HG12	1:C:337:ARG:NH1	2.13	0.64
1:E:376:GLU:OE1	1:E:379:ARG:NH2	2.30	0.64
1:M:178:ARG:NH2	1:M:237:LEU:O	2.31	0.64
1:D:110:ASP:HB3	1:D:272:LYS:HD2	1.79	0.64
1:E:141:ILE:HD11	1:H:141:ILE:HD11	1.80	0.64
1:F:297:MET:HG3	1:F:392:GLY:HA2	1.79	0.64
1:G:4:ARG:NH2	1:G:104:VAL:O	2.31	0.64
1:D:58:CYS:O	1:D:89:ARG:NH2	2.29	0.63
1:J:88:ARG:NH1	1:J:95:GLN:OE1	2.29	0.63
1:F:89:ARG:NH2	3:F:605:HOH:O	2.32	0.63
1:C:319:ILE:O	1:C:348:ARG:NH1	2.31	0.63
1:D:4:ARG:NH2	1:D:109:HIS:O	2.32	0.63
1:F:4:ARG:NH1	1:F:107:GLY:HA2	2.14	0.63
1:G:245:ASP:O	1:G:247:GLU:N	2.31	0.63
1:G:149:ARG:NH2	3:G:506:HOH:O	2.24	0.63
1:H:164:LEU:HD12	3:H:653:HOH:O	1.98	0.63
1:L:319:ILE:O	1:L:348:ARG:NH1	2.31	0.63
1:M:120:MET:HA	1:M:123:VAL:HG23	1.80	0.63
1:E:19:TYR:HB2	1:E:258:GLN:HB3	1.81	0.63
1:L:171:ARG:HH22	1:L:247:GLU:HB3	1.62	0.63
1:D:258:GLN:HG3	2:D:501:COA:H71	1.81	0.62
1:G:52:ASP:CG	1:H:88:ARG:HH22	2.02	0.62
1:L:378:HIS:CD2	1:L:403:ARG:HG3	2.34	0.62
1:C:351:VAL:HG21	1:C:376:GLU:HG2	1.81	0.62
1:D:89:ARG:HB2	1:D:391:ILE:HG23	1.81	0.62
1:L:120:MET:HA	1:L:123:VAL:HG23	1.82	0.62
1:A:281:LEU:HA	1:A:378:HIS:HE1	1.63	0.62
1:C:163:MET:HG2	1:C:297:MET:CE	2.23	0.62
2:H:501:COA:H51A	2:H:501:COA:C8A	2.29	0.62
1:B:178:ARG:NH2	1:B:237:LEU:O	2.33	0.61
1:C:245:ASP:HB3	1:C:248:ALA:HB2	1.81	0.61
1:L:239:PRO:HA	1:L:251:THR:HG22	1.81	0.61
1:J:319:ILE:O	1:J:348:ARG:NH1	2.32	0.61
1:M:91:GLY:HA2	1:M:389:MET:SD	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLU:HB3	1:C:171:ARG:HH21	1.66	0.61
1:G:352:ARG:HD2	1:G:372:THR:HG23	1.82	0.61
1:J:163:MET:SD	1:J:297:MET:HE1	2.40	0.61
1:B:120:MET:HA	1:B:123:VAL:HG23	1.81	0.61
1:B:186:VAL:HG22	1:B:229:THR:HG22	1.82	0.61
1:L:89:ARG:NH2	3:L:508:HOH:O	2.30	0.61
1:C:297:MET:CE	1:C:392:GLY:HA2	2.31	0.61
1:E:15:PRO:HD2	1:E:208:VAL:HG23	1.83	0.61
1:F:321:LEU:HD11	1:F:380:ARG:HD2	1.83	0.61
1:K:247:GLU:OE1	3:K:601:HOH:O	2.16	0.61
1:E:200:VAL:O	1:E:203:GLU:HG2	2.00	0.60
1:H:69:ARG:NH1	1:H:81:VAL:O	2.34	0.60
1:L:88:ARG:NH1	1:L:95:GLN:OE1	2.34	0.60
1:M:303:PRO:O	1:M:307:VAL:HG23	2.01	0.60
1:G:120:MET:HA	1:G:123:VAL:HG23	1.84	0.60
1:K:203:GLU:OE1	1:K:379:ARG:NH2	2.34	0.60
1:E:391:ILE:HB	1:E:395:GLN:HB2	1.82	0.60
1:J:40:LEU:HD11	1:J:77:LEU:HD11	1.83	0.60
1:E:4:ARG:NH2	1:E:104:VAL:O	2.33	0.60
1:G:180:GLU:OE1	1:G:337:ARG:NH2	2.35	0.60
1:B:181:GLN:NE2	1:B:330:ALA:HB2	2.16	0.60
1:M:89:ARG:HB2	1:M:391:ILE:HG23	1.83	0.60
1:D:343:GLU:OE1	3:D:602:HOH:O	2.16	0.60
1:K:352:ARG:NH2	1:K:376:GLU:OE1	2.34	0.59
1:L:15:PRO:HD2	1:L:208:VAL:HG23	1.84	0.59
1:K:187:ARG:HD2	1:K:191:ARG:HH21	1.66	0.59
1:G:178:ARG:HH11	1:G:178:ARG:HG2	1.67	0.59
1:K:352:ARG:NH1	3:K:602:HOH:O	2.17	0.59
1:K:352:ARG:NH2	1:K:379:ARG:HH11	2.00	0.59
1:F:89:ARG:HB2	1:F:391:ILE:HG23	1.84	0.59
1:H:283:ARG:NH2	1:H:402:GLU:OE1	2.34	0.59
1:B:103:GLN:OE1	3:B:602:HOH:O	2.16	0.59
2:D:501:COA:O9P	2:D:501:COA:H131	2.03	0.59
1:J:52:ASP:OD1	1:K:88:ARG:NH2	2.32	0.59
1:L:321:LEU:HD11	1:L:380:ARG:HD2	1.84	0.59
1:L:65:PRO:HB3	1:M:89:ARG:NH2	2.14	0.59
1:B:297:MET:CG	1:B:298:GLY:N	2.65	0.58
1:E:377:LEU:HD12	1:E:382:ALA:HB3	1.84	0.58
1:M:275:GLU:OE2	3:M:503:HOH:O	2.16	0.58
1:D:48:ASP:OD2	3:D:603:HOH:O	2.17	0.58
1:A:65:PRO:HG2	1:B:152:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:HG1	1:C:216:GLU:N	2.01	0.58
1:C:353:GLY:O	3:C:504:HOH:O	2.16	0.58
1:C:58:CYS:O	1:C:89:ARG:NH2	2.35	0.58
1:G:16:ILE:O	3:G:501:HOH:O	2.17	0.58
1:B:37:LYS:NZ	3:B:610:HOH:O	2.35	0.58
1:H:47:ALA:HB1	1:H:77:LEU:HG	1.86	0.58
1:M:25:SER:OG	3:M:504:HOH:O	2.17	0.58
1:M:26:LEU:HD11	1:M:210:VAL:HG22	1.85	0.58
1:F:145:LEU:HD13	1:F:258:GLN:NE2	2.18	0.58
1:L:52:ASP:CG	1:M:88:ARG:HH22	2.08	0.58
1:A:391:ILE:HB	1:A:395:GLN:HB2	1.86	0.58
1:K:18:ARG:HG3	1:K:223:GLU:HG2	1.86	0.58
1:C:91:GLY:HA2	1:C:389:MET:SD	2.44	0.57
1:E:163:MET:HG2	1:E:297:MET:HE1	1.86	0.57
1:M:55:LEU:HD22	1:M:68:GLY:HA2	1.84	0.57
1:J:110:ASP:HB3	1:J:272:LYS:HD3	1.86	0.57
1:F:18:ARG:O	3:F:603:HOH:O	2.17	0.57
1:J:391:ILE:HB	1:J:395:GLN:HB2	1.85	0.57
1:L:186:VAL:HG12	1:L:190:GLN:HE21	1.70	0.57
1:M:169:ASN:OD1	1:M:172:ARG:NH2	2.38	0.57
1:E:9:CYS:HB2	1:E:266:ILE:HB	1.85	0.57
1:A:168:GLU:OE1	1:A:171:ARG:NH1	2.36	0.57
1:A:256:SER:OG	1:A:360:HIS:HB2	2.04	0.57
1:E:37:LYS:NZ	3:E:501:HOH:O	2.01	0.57
1:J:179:THR:O	1:J:183:GLU:HG3	2.05	0.57
1:J:297:MET:HE2	1:J:392:GLY:HA2	1.86	0.57
1:K:164:LEU:HD13	3:K:654:HOH:O	2.04	0.57
1:C:321:LEU:HD12	1:C:377:LEU:HD23	1.87	0.56
1:K:297:MET:HG2	1:K:298:GLY:CA	2.34	0.56
1:E:52:ASP:OD1	1:F:88:ARG:NH2	2.37	0.56
1:F:321:LEU:HD12	1:F:377:LEU:HD23	1.86	0.56
1:C:18:ARG:HG3	1:C:223:GLU:HG2	1.86	0.56
1:D:358:LEU:HD12	1:D:368:ARG:HH21	1.70	0.56
1:G:15:PRO:HD2	1:G:208:VAL:HG23	1.88	0.56
1:K:145:LEU:HD13	1:K:258:GLN:HE21	1.68	0.56
1:M:315:THR:O	1:M:318:ASP:HB2	2.05	0.56
1:A:273:ALA:HA	1:A:278:LEU:HD12	1.86	0.56
1:C:273:ALA:HB1	1:C:278:LEU:HB2	1.86	0.56
1:H:169:ASN:O	1:H:173:GLU:HG2	2.06	0.56
1:K:9:CYS:HB2	1:K:266:ILE:HB	1.87	0.56
1:K:180:GLU:OE1	1:K:337:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:THR:HG1	1:G:216:GLU:N	2.04	0.56
1:B:196:GLN:HE21	1:B:221:VAL:HG13	1.71	0.56
1:E:368:ARG:NH2	3:E:507:HOH:O	2.36	0.56
1:K:352:ARG:HH22	1:K:379:ARG:HH11	1.51	0.56
1:M:7:VAL:HG12	1:M:283:ARG:HB3	1.88	0.56
1:A:166:THR:HG22	3:A:566:HOH:O	2.05	0.56
1:G:405:GLN:NE2	3:G:507:HOH:O	2.26	0.56
1:M:111:LEU:HD21	1:M:266:ILE:HD12	1.88	0.56
1:D:376:GLU:HG3	1:D:380:ARG:HD2	1.88	0.55
1:L:405:GLN:CD	1:L:405:GLN:H	2.09	0.55
1:L:84:MET:SD	1:M:88:ARG:NH1	2.79	0.55
1:E:321:LEU:HD11	1:E:376:GLU:HG3	1.88	0.55
1:D:210:VAL:O	1:D:216:GLU:HA	2.07	0.55
1:E:26:LEU:HD11	1:E:210:VAL:HG12	1.88	0.55
1:J:89:ARG:HB2	1:J:391:ILE:HG23	1.89	0.55
1:A:89:ARG:HH21	1:B:65:PRO:HB3	1.71	0.55
1:E:226:ARG:NH1	1:E:228:ASP:OD2	2.39	0.55
1:A:34:THR:HG21	1:A:208:VAL:HG22	1.88	0.55
1:G:224:HIS:HD2	3:G:547:HOH:O	1.89	0.55
1:J:9:CYS:HB2	1:J:266:ILE:HB	1.88	0.55
1:J:322:ILE:HD12	1:J:341:PHE:HZ	1.72	0.55
1:C:178:ARG:NH2	1:C:237:LEU:O	2.35	0.54
1:E:52:ASP:CG	1:F:88:ARG:HH22	2.11	0.54
1:M:45:ILE:HD12	1:M:49:GLN:HB2	1.90	0.54
1:C:146:ALA:O	1:C:149:ARG:HG2	2.08	0.54
1:F:149:ARG:HD3	1:F:163:MET:HG2	1.90	0.54
1:M:16:ILE:HG23	1:M:361:PRO:HG3	1.90	0.54
1:M:351:VAL:HG21	1:M:376:GLU:HG2	1.90	0.54
1:F:9:CYS:HB2	1:F:266:ILE:HB	1.90	0.54
1:G:307:VAL:O	1:G:311:LYS:HG3	2.08	0.54
1:E:211:ARG:HG3	1:E:211:ARG:HH11	1.72	0.53
1:H:251:THR:N	1:H:254:ASN:OD1	2.37	0.53
1:L:121:SER:O	1:M:131:ARG:HD2	2.07	0.53
1:H:332:ALA:O	1:H:336:MET:HG3	2.06	0.53
1:D:352:ARG:HD2	1:D:372:THR:HG23	1.89	0.53
1:B:101:CYS:O	1:B:105:ARG:HG3	2.09	0.53
1:F:149:ARG:NH2	1:F:258:GLN:NE2	2.56	0.53
1:H:351:VAL:HG21	1:H:376:GLU:HG2	1.90	0.53
1:L:149:ARG:NH2	3:L:513:HOH:O	2.39	0.53
1:A:15:PRO:HD3	1:A:205:ILE:HG23	1.90	0.53
1:A:378:HIS:CD2	1:A:403:ARG:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:O	3:B:603:HOH:O	2.18	0.53
1:C:326:GLU:OE1	1:C:354:SER:OG	2.26	0.53
1:M:390:CYS:SG	3:M:568:HOH:O	2.59	0.53
1:C:332:ALA:O	1:C:336:MET:HG3	2.07	0.53
1:E:326:GLU:OE1	1:E:354:SER:OG	2.26	0.53
1:A:5:ASP:OD2	1:A:283:ARG:NE	2.38	0.53
1:L:391:ILE:HB	1:L:395:GLN:HB2	1.90	0.53
2:D:501:COA:H31	3:D:705:HOH:O	2.08	0.53
1:K:191:ARG:HH11	1:K:351:VAL:HA	1.74	0.53
1:E:163:MET:CG	1:E:297:MET:HE1	2.39	0.52
1:K:239:PRO:HB2	1:K:242:LEU:HB2	1.91	0.52
1:L:326:GLU:OE1	1:L:354:SER:OG	2.24	0.52
1:D:153:GLY:O	1:D:157:HIS:HB2	2.08	0.52
1:H:169:ASN:OD1	1:H:172:ARG:NH2	2.42	0.52
1:K:352:ARG:NE	1:K:376:GLU:OE1	2.40	0.52
1:G:333:LEU:HA	1:G:336:MET:HE2	1.92	0.52
1:L:171:ARG:HD2	1:L:249:THR:OG1	2.09	0.52
1:M:307:VAL:HG12	1:M:311:LYS:HE2	1.91	0.52
1:L:58:CYS:O	1:L:89:ARG:NH1	2.37	0.52
1:A:169:ASN:OD1	1:A:172:ARG:NH2	2.43	0.52
1:G:149:ARG:O	1:G:162:GLY:HA2	2.09	0.52
1:H:321:LEU:HD11	1:H:380:ARG:HD2	1.91	0.52
1:A:351:VAL:HG21	1:A:376:GLU:HG2	1.92	0.52
1:C:297:MET:HE2	1:C:392:GLY:HA2	1.91	0.52
1:D:100:ALA:HB1	1:D:112:VAL:HG21	1.90	0.52
1:K:196:GLN:O	1:K:199:GLY:N	2.42	0.52
1:L:193:VAL:HG11	1:L:227:ALA:HB2	1.92	0.52
1:A:178:ARG:HA	1:A:181:GLN:HE21	1.74	0.52
1:M:354:SER:HA	1:M:368:ARG:NH2	2.24	0.52
1:A:88:ARG:HH22	1:B:52:ASP:CG	2.13	0.52
1:E:352:ARG:HE	1:E:379:ARG:HH21	1.57	0.52
1:H:184:LEU:HD13	1:H:333:LEU:HG	1.92	0.52
1:M:146:ALA:HA	1:M:149:ARG:CZ	2.40	0.52
1:M:34:THR:HG21	1:M:208:VAL:HG22	1.92	0.52
1:M:354:SER:HA	1:M:368:ARG:HH21	1.74	0.52
1:A:171:ARG:NH2	1:A:172:ARG:HD3	2.25	0.51
1:G:307:VAL:HG12	1:G:311:LYS:HE3	1.92	0.51
1:D:326:GLU:HG2	1:D:332:ALA:HB2	1.92	0.51
1:J:373:LEU:O	1:J:377:LEU:HB2	2.11	0.51
1:K:297:MET:CE	1:K:392:GLY:HA2	2.39	0.51
1:K:352:ARG:HH22	1:K:379:ARG:NH1	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLU:HG2	1:A:332:ALA:HB2	1.91	0.51
1:F:382:ALA:O	1:F:403:ARG:NE	2.36	0.51
1:F:120:MET:HA	1:F:123:VAL:HG23	1.92	0.51
1:J:88:ARG:NH2	1:K:52:ASP:OD1	2.43	0.51
1:L:297:MET:HG2	1:L:298:GLY:N	2.25	0.51
1:L:378:HIS:HD2	1:L:403:ARG:HG3	1.74	0.51
1:M:125:PHE:HD2	1:M:141:ILE:HG22	1.75	0.51
1:L:4:ARG:NH2	1:L:107:GLY:H	2.08	0.51
1:C:273:ALA:HA	1:C:278:LEU:HD12	1.93	0.51
1:E:284:LEU:HD21	1:E:287:TRP:HD1	1.74	0.51
1:G:245:ASP:C	1:G:247:GLU:N	2.63	0.51
1:L:179:THR:O	1:L:183:GLU:HG3	2.10	0.51
1:A:378:HIS:HD2	1:A:403:ARG:HD2	1.76	0.51
1:J:171:ARG:HG3	1:J:249:THR:OG1	2.10	0.51
1:D:302:VAL:HB	1:D:303:PRO:HD3	1.93	0.51
1:G:6:ALA:HB2	1:G:105:ARG:HG2	1.93	0.50
1:H:378:HIS:CD2	1:H:403:ARG:HG3	2.46	0.50
1:A:326:GLU:HG2	1:A:332:ALA:CB	2.41	0.50
1:D:326:GLU:HG2	1:D:332:ALA:CB	2.41	0.50
1:M:179:THR:O	1:M:183:GLU:HG3	2.12	0.50
1:B:196:GLN:NE2	1:B:221:VAL:HG13	2.25	0.50
1:D:187:ARG:O	1:D:191:ARG:HG3	2.12	0.50
1:M:391:ILE:HB	1:M:395:GLN:HB2	1.93	0.50
1:A:226:ARG:HB3	1:A:228:ASP:OD1	2.11	0.50
1:K:171:ARG:NH2	1:K:247:GLU:HB2	2.26	0.50
1:L:58:CYS:HB3	1:L:89:ARG:HH11	1.74	0.50
1:H:6:ALA:HB2	1:H:105:ARG:HG3	1.93	0.50
1:H:163:MET:SD	1:H:297:MET:HE3	2.51	0.50
1:G:352:ARG:NE	1:G:376:GLU:OE1	2.43	0.50
1:B:58:CYS:HB3	1:B:89:ARG:HH11	1.75	0.50
1:C:176:ILE:HG12	1:C:337:ARG:HH12	1.77	0.50
1:D:297:MET:HE3	1:D:392:GLY:N	2.26	0.50
1:F:391:ILE:HB	1:F:395:GLN:HB2	1.93	0.50
1:H:352:ARG:HD2	1:H:372:THR:HG23	1.92	0.50
1:L:343:GLU:HA	1:L:346:HIS:ND1	2.25	0.50
1:E:257:GLY:N	3:E:515:HOH:O	2.45	0.50
1:H:90:CYS:HB3	3:H:618:HOH:O	2.11	0.50
1:K:75:ALA:HB3	1:K:77:LEU:HD13	1.93	0.50
1:L:187:ARG:O	1:L:191:ARG:HG3	2.12	0.50
1:L:88:ARG:NH2	1:M:52:ASP:OD2	2.43	0.50
1:D:171:ARG:HA	1:D:176:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:VAL:O	1:G:190:GLN:HG3	2.12	0.49
1:H:149:ARG:NH2	3:H:616:HOH:O	2.36	0.49
1:K:187:ARG:O	1:K:191:ARG:HG3	2.12	0.49
1:L:54:ILE:HD13	1:L:99:GLN:HE21	1.77	0.49
1:K:139:VAL:HG21	1:M:130:MET:HB3	1.94	0.49
1:A:13:ARG:HD3	1:A:368:ARG:HG2	1.93	0.49
1:C:333:LEU:HD23	1:C:336:MET:HE3	1.93	0.49
1:E:233:ALA:HA	1:E:236:LYS:HE3	1.94	0.49
1:J:121:SER:O	1:K:131:ARG:HD2	2.12	0.49
1:L:295:ASP:N	1:L:295:ASP:OD1	2.41	0.49
1:J:60:PRO:HG2	1:K:60:PRO:HG2	1.92	0.49
1:A:352:ARG:HD2	1:A:372:THR:HG23	1.94	0.49
1:A:321:LEU:HD12	1:A:377:LEU:HG	1.94	0.49
1:B:191:ARG:NH2	1:B:346:HIS:O	2.46	0.49
1:D:387:GLU:O	1:D:398:ALA:HA	2.13	0.49
1:E:166:THR:HG22	3:E:555:HOH:O	2.12	0.49
1:L:181:GLN:HE22	1:L:330:ALA:HB2	1.75	0.49
1:L:37:LYS:NZ	3:L:502:HOH:O	2.13	0.49
1:A:120:MET:HA	1:A:123:VAL:HG23	1.93	0.49
1:A:239:PRO:HD2	1:A:242:LEU:HD12	1.93	0.49
1:B:352:ARG:NH2	1:B:379:ARG:HH12	2.11	0.49
1:A:377:LEU:HD23	1:A:382:ALA:HB3	1.94	0.49
1:G:163:MET:HG2	1:G:297:MET:CE	2.41	0.49
1:G:245:ASP:C	1:G:247:GLU:H	2.15	0.49
1:H:226:ARG:NH1	1:H:228:ASP:OD2	2.46	0.49
1:J:297:MET:HG3	1:J:298:GLY:CA	2.41	0.49
1:A:315:THR:N	1:A:318:ASP:OD2	2.34	0.49
1:D:239:PRO:HD2	1:D:242:LEU:HD22	1.95	0.49
1:F:191:ARG:NH2	1:F:346:HIS:O	2.46	0.49
1:J:194:ALA:O	1:J:198:GLU:HG3	2.13	0.49
1:J:67:ILE:HG22	1:J:85:GLN:HB2	1.94	0.49
1:M:319:ILE:O	1:M:348:ARG:NH1	2.42	0.49
1:L:255:SER:HG	1:L:328:PHE:HD1	1.59	0.49
1:F:145:LEU:HD13	1:F:258:GLN:HE22	1.76	0.49
1:A:88:ARG:HH21	1:B:82:PRO:HB2	1.78	0.48
1:E:196:GLN:NE2	3:E:502:HOH:O	2.30	0.48
1:F:110:ASP:HB3	1:F:272:LYS:HD3	1.93	0.48
1:J:186:VAL:HG21	1:J:231:VAL:HG22	1.94	0.48
1:E:285:VAL:HB	1:E:400:VAL:HG12	1.95	0.48
1:F:18:ARG:HG3	1:F:223:GLU:HG2	1.94	0.48
1:G:169:ASN:N	1:G:169:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:ARG:HH22	1:K:52:ASP:CG	2.15	0.48
1:B:16:ILE:HG23	1:B:361:PRO:HG3	1.96	0.48
1:G:245:ASP:O	1:G:248:ALA:N	2.29	0.48
1:G:313:GLY:HA2	3:G:554:HOH:O	2.12	0.48
1:H:149:ARG:HD3	3:H:653:HOH:O	2.13	0.48
1:J:37:LYS:NZ	3:J:502:HOH:O	2.17	0.48
1:E:226:ARG:HD3	1:E:228:ASP:OD1	2.13	0.48
1:D:258:GLN:HG3	2:D:501:COA:C7P	2.44	0.48
1:M:373:LEU:O	1:M:377:LEU:HB2	2.13	0.48
1:H:255:SER:HG	1:H:328:PHE:HD2	1.59	0.48
1:M:180:GLU:OE1	1:M:337:ARG:NH2	2.47	0.48
1:M:89:ARG:HD3	1:M:89:ARG:HA	1.58	0.48
1:C:265:CYS:HB3	3:C:578:HOH:O	2.14	0.48
1:L:53:VAL:HG21	1:L:72:ALA:HB2	1.94	0.48
1:E:239:PRO:HA	1:E:251:THR:HG22	1.95	0.48
1:F:149:ARG:HH22	1:F:258:GLN:NE2	2.12	0.48
1:F:178:ARG:NE	1:F:182:ASP:OD2	2.45	0.48
1:K:120:MET:HA	1:K:123:VAL:HG23	1.96	0.48
1:K:19:TYR:HB2	1:K:258:GLN:O	2.14	0.48
1:M:183:GLU:OE1	3:M:505:HOH:O	2.19	0.48
1:B:163:MET:SD	1:B:297:MET:HE2	2.54	0.47
1:C:201:LEU:HB3	1:C:205:ILE:HD12	1.96	0.47
1:D:252:ALA:HA	2:D:501:COA:H132	1.96	0.47
1:G:245:ASP:HB3	1:G:248:ALA:HB2	1.94	0.47
1:A:88:ARG:NH1	1:B:84:MET:SD	2.88	0.47
1:F:19:TYR:HB2	1:F:258:GLN:O	2.14	0.47
1:D:101:CYS:O	1:D:105:ARG:HG3	2.14	0.47
1:H:191:ARG:NH1	1:H:349:THR:O	2.47	0.47
1:L:171:ARG:HG2	1:L:172:ARG:N	2.27	0.47
1:M:123:VAL:HG21	1:M:145:LEU:HD21	1.96	0.47
1:E:180:GLU:OE1	1:E:337:ARG:NH2	2.47	0.47
1:G:378:HIS:HA	1:G:403:ARG:HD2	1.96	0.47
1:K:196:GLN:HG2	1:K:201:LEU:HD12	1.97	0.47
1:L:146:ALA:O	1:L:149:ARG:HB2	2.14	0.47
1:L:163:MET:N	3:L:518:HOH:O	2.46	0.47
1:A:249:THR:HA	3:A:509:HOH:O	2.14	0.47
1:A:40:LEU:HD11	1:A:77:LEU:HD11	1.97	0.47
1:D:164:LEU:CD2	1:D:240:VAL:HB	2.45	0.47
1:F:278:LEU:O	1:F:280:PRO:HD3	2.13	0.47
1:F:39:LEU:HD11	1:F:266:ILE:HG12	1.96	0.47
1:J:120:MET:HA	1:J:123:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:391:ILE:HB	1:K:395:GLN:HB2	1.96	0.47
1:G:201:LEU:HA	1:G:201:LEU:HD23	1.75	0.47
1:D:377:LEU:HD12	1:D:382:ALA:HB3	1.96	0.47
1:J:163:MET:HG3	3:J:580:HOH:O	2.14	0.47
1:J:161:GLY:HA3	1:J:165:GLU:HB2	1.95	0.47
1:B:51:GLU:OE1	3:B:604:HOH:O	2.20	0.47
1:A:78:PRO:HG2	1:A:81:VAL:HG23	1.97	0.47
1:D:120:MET:HA	1:D:123:VAL:HG23	1.96	0.47
1:M:59:TYR:OH	3:M:501:HOH:O	2.10	0.47
1:A:210:VAL:O	1:A:217:GLU:N	2.48	0.47
1:C:52:ASP:OD1	1:D:88:ARG:NH2	2.47	0.47
1:E:60:PRO:HG2	1:F:60:PRO:HG2	1.97	0.47
1:G:239:PRO:HD2	1:G:242:LEU:HD12	1.97	0.47
1:A:256:SER:HB3	1:A:327:ALA:O	2.14	0.47
1:C:187:ARG:O	1:C:191:ARG:HG3	2.15	0.46
1:D:94:LEU:HD23	1:D:397:LEU:HG	1.97	0.46
1:F:7:VAL:HB	1:F:280:PRO:HB3	1.98	0.46
1:L:43:THR:HB	1:L:45:ILE:HG13	1.96	0.46
1:C:123:VAL:O	1:D:131:ARG:NH2	2.39	0.46
1:C:130:MET:HE1	1:C:141:ILE:HD11	1.97	0.46
1:C:383:ARG:HD3	1:C:384:TYR:CE2	2.50	0.46
1:D:300:GLY:O	1:D:303:PRO:HD2	2.15	0.46
1:E:7:VAL:HG12	1:E:283:ARG:HB3	1.97	0.46
1:G:297:MET:HG3	1:G:391:ILE:O	2.15	0.46
1:H:182:ASP:O	1:H:186:VAL:HG23	2.15	0.46
1:J:26:LEU:HD11	1:J:210:VAL:HG12	1.96	0.46
1:K:91:GLY:HA2	1:K:389:MET:SD	2.56	0.46
1:L:89:ARG:HE	1:M:65:PRO:HB2	1.79	0.46
1:J:191:ARG:NH1	1:J:346:HIS:O	2.45	0.46
1:G:84:MET:SD	1:H:88:ARG:NH1	2.88	0.46
1:J:326:GLU:HG2	1:J:332:ALA:CB	2.45	0.46
1:K:297:MET:HG2	1:K:298:GLY:HA2	1.96	0.46
1:B:297:MET:HG2	1:B:298:GLY:N	2.30	0.46
1:C:79:ILE:HG13	1:K:275:GLU:O	2.15	0.46
1:J:8:ILE:HD12	1:J:267:VAL:HG22	1.98	0.46
1:B:248:ALA:O	3:B:605:HOH:O	2.21	0.46
1:F:141:ILE:HG13	1:G:141:ILE:HD12	1.97	0.46
1:K:33:VAL:HG13	1:K:75:ALA:HA	1.98	0.46
1:C:180:GLU:OE1	1:C:337:ARG:NH2	2.41	0.46
1:C:89:ARG:HB2	1:C:391:ILE:HG23	1.98	0.46
1:F:299:ILE:O	1:F:303:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:ALA:HB1	1:G:278:LEU:HB2	1.96	0.46
1:J:239:PRO:HA	1:J:251:THR:HG22	1.98	0.46
1:A:178:ARG:HA	1:A:181:GLN:NE2	2.30	0.46
1:H:128:THR:O	3:H:604:HOH:O	2.20	0.46
1:L:54:ILE:HD13	1:L:99:GLN:NE2	2.31	0.46
1:B:4:ARG:H	1:B:4:ARG:HG2	1.53	0.46
1:C:34:THR:HG21	1:C:208:VAL:HG22	1.98	0.46
1:K:285:VAL:CG2	1:K:402:GLU:HB2	2.46	0.46
1:L:57:HIS:ND1	1:L:117:ALA:O	2.46	0.46
1:L:69:ARG:NH2	1:M:394:GLY:O	2.49	0.46
1:A:191:ARG:NH1	1:A:349:THR:O	2.49	0.45
1:B:344:ALA:O	1:B:347:GLU:HB2	2.15	0.45
1:D:319:ILE:O	1:D:348:ARG:NH1	2.49	0.45
1:F:22:MET:SD	1:F:223:GLU:HB2	2.56	0.45
1:F:242:LEU:HD12	1:F:245:ASP:O	2.16	0.45
1:M:325:ASN:O	1:M:326:GLU:HB2	2.17	0.45
1:D:297:MET:HE3	1:D:391:ILE:C	2.37	0.45
1:J:91:GLY:HA2	1:J:389:MET:SD	2.55	0.45
1:L:186:VAL:O	1:L:190:GLN:HG3	2.16	0.45
1:A:126:TYR:OH	1:A:147:ARG:HG2	2.16	0.45
1:C:337:ARG:HD3	3:C:501:HOH:O	2.16	0.45
1:F:38:GLY:HA3	1:F:206:ILE:HD12	1.98	0.45
1:E:108:ASP:HB3	1:F:311:LYS:NZ	2.30	0.45
1:G:187:ARG:O	1:G:191:ARG:HG3	2.16	0.45
1:G:203:GLU:OE1	1:G:379:ARG:NH1	2.50	0.45
1:A:65:PRO:HB2	1:B:89:ARG:HE	1.81	0.45
1:A:89:ARG:NH2	1:B:65:PRO:HB3	2.32	0.45
1:C:72:ALA:O	1:C:77:LEU:HB2	2.16	0.45
1:E:141:ILE:HD11	1:H:141:ILE:CD1	2.45	0.45
1:E:171:ARG:NH1	1:E:247:GLU:HB3	2.32	0.45
1:F:383:ARG:O	1:F:402:GLU:HA	2.16	0.45
1:J:200:VAL:HG11	1:J:379:ARG:NH1	2.31	0.45
1:B:163:MET:SD	1:B:297:MET:CE	3.05	0.45
1:B:177:SER:O	1:B:181:GLN:HG3	2.16	0.45
1:G:163:MET:CG	1:G:297:MET:HE1	2.44	0.45
1:A:321:LEU:HD11	1:A:376:GLU:HB3	1.97	0.45
1:B:161:GLY:HA3	1:B:165:GLU:HB2	1.98	0.45
1:B:352:ARG:NH1	3:B:603:HOH:O	2.48	0.45
1:E:4:ARG:CZ	1:E:107:GLY:HA2	2.47	0.45
1:C:171:ARG:HD3	1:C:249:THR:OG1	2.17	0.45
1:C:194:ALA:O	1:C:198:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD11	1:E:266:ILE:HG12	1.99	0.45
1:G:127:SER:HB2	1:G:140:GLN:O	2.17	0.45
1:D:111:LEU:HD21	1:D:266:ILE:HD12	1.99	0.45
1:J:297:MET:CE	1:J:392:GLY:HA2	2.45	0.45
1:L:26:LEU:HD11	1:L:210:VAL:HG12	1.98	0.45
1:L:373:LEU:O	1:L:377:LEU:HB2	2.16	0.45
1:E:16:ILE:HG23	1:E:361:PRO:HG3	1.99	0.45
1:L:169:ASN:OD1	1:L:172:ARG:NH2	2.49	0.45
1:M:42:ARG:NH1	1:M:203:GLU:O	2.39	0.45
1:A:181:GLN:HG2	1:A:329:ALA:HB3	1.98	0.44
1:B:303:PRO:O	1:B:307:VAL:HG23	2.17	0.44
1:E:211:ARG:HG3	1:E:211:ARG:NH1	2.32	0.44
1:M:256:SER:HA	1:M:356:ILE:HA	1.99	0.44
1:A:184:LEU:HD12	1:A:187:ARG:NH2	2.32	0.44
1:B:89:ARG:HA	1:B:89:ARG:HD3	1.57	0.44
1:F:192:ALA:O	1:F:196:GLN:HG3	2.17	0.44
1:J:350:ASN:HB3	1:J:353:GLY:O	2.17	0.44
1:D:232:GLU:OE2	3:D:604:HOH:O	2.20	0.44
1:E:163:MET:HG2	1:E:297:MET:CE	2.48	0.44
1:E:43:THR:HB	1:E:278:LEU:HD21	1.98	0.44
2:H:501:COA:N3A	2:H:501:COA:H2B	2.33	0.44
1:J:201:LEU:HA	1:J:201:LEU:HD23	1.79	0.44
1:A:60:PRO:HG2	1:B:60:PRO:HG2	1.99	0.44
1:H:58:CYS:O	1:H:89:ARG:NH2	2.50	0.44
1:A:5:ASP:OD1	3:A:503:HOH:O	2.21	0.44
1:D:123:VAL:HG21	1:D:145:LEU:HD21	1.99	0.44
1:E:283:ARG:NE	1:E:402:GLU:OE1	2.50	0.44
1:F:230:THR:O	1:F:234:LEU:HG	2.17	0.44
1:G:268:THR:OG1	1:G:269:THR:N	2.47	0.44
1:J:16:ILE:HG23	1:J:361:PRO:HG3	1.99	0.44
1:C:291:GLY:O	1:D:80:THR:HA	2.17	0.44
1:E:65:PRO:HB2	1:F:89:ARG:HD3	1.99	0.44
1:H:253:GLY:O	3:H:605:HOH:O	2.21	0.44
1:M:69:ARG:NH1	1:M:81:VAL:O	2.47	0.44
1:D:228:ASP:N	1:D:228:ASP:OD1	2.48	0.44
1:H:321:LEU:HD12	1:H:377:LEU:HD23	1.99	0.44
1:M:171:ARG:HD3	1:M:249:THR:OG1	2.17	0.44
1:F:191:ARG:NH1	1:F:349:THR:O	2.50	0.44
1:F:279:LYS:O	1:F:279:LYS:HG2	2.18	0.44
1:M:191:ARG:NH2	1:M:346:HIS:O	2.47	0.44
1:B:171:ARG:HG3	1:B:249:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASP:HB3	1:C:272:LYS:HD3	1.98	0.44
1:F:77:LEU:HD23	1:F:81:VAL:HG21	1.99	0.44
1:C:182:ASP:O	1:C:186:VAL:HG23	2.18	0.43
1:D:326:GLU:OE1	1:D:354:SER:OG	2.15	0.43
1:D:387:GLU:HG2	1:D:389:MET:HE1	2.00	0.43
1:G:182:ASP:OD1	3:G:503:HOH:O	2.21	0.43
1:G:319:ILE:O	1:G:348:ARG:NH1	2.49	0.43
1:G:368:ARG:NH2	1:G:369:MET:HG2	2.32	0.43
1:L:325:ASN:HB2	1:L:369:MET:SD	2.58	0.43
1:M:333:LEU:O	1:M:337:ARG:HG3	2.18	0.43
1:A:115:GLY:HA2	3:A:547:HOH:O	2.17	0.43
1:B:321:LEU:HD12	1:B:377:LEU:HD23	2.00	0.43
2:D:501:COA:C3P	3:D:705:HOH:O	2.65	0.43
1:F:26:LEU:HD11	1:F:210:VAL:HG12	1.99	0.43
1:F:298:GLY:HA2	1:F:390:CYS:CB	2.48	0.43
1:H:9:CYS:HB2	1:H:266:ILE:HB	2.00	0.43
1:G:224:HIS:C	1:G:224:HIS:ND1	2.71	0.43
1:J:171:ARG:HG3	1:J:249:THR:HG1	1.82	0.43
1:B:341:PHE:CD2	1:B:345:ASP:HB3	2.53	0.43
1:E:80:THR:O	1:E:82:PRO:HD3	2.19	0.43
1:G:163:MET:HB3	1:G:328:PHE:HE2	1.84	0.43
1:H:149:ARG:HB3	1:H:163:MET:HG2	2.01	0.43
1:M:20:GLY:N	1:M:121:SER:OG	2.30	0.43
1:M:336:MET:HG2	1:M:341:PHE:CD2	2.53	0.43
1:A:58:CYS:O	1:A:89:ARG:NH1	2.47	0.43
1:B:53:VAL:HG12	1:B:55:LEU:HD13	2.00	0.43
1:D:112:VAL:HG23	1:D:267:VAL:HB	2.00	0.43
1:H:19:TYR:HB2	1:H:258:GLN:O	2.19	0.43
1:L:208:VAL:HA	1:L:209:PRO:HD3	1.85	0.43
1:B:239:PRO:HA	1:B:251:THR:HG22	2.01	0.43
1:D:321:LEU:HD11	1:D:376:GLU:HG3	2.00	0.43
1:J:129:ASP:OD2	3:J:503:HOH:O	2.21	0.43
1:K:256:SER:HA	1:K:356:ILE:HA	2.01	0.43
1:G:178:ARG:HH12	1:G:235:ALA:HA	1.84	0.43
1:G:187:ARG:HD2	1:G:191:ARG:NH2	2.34	0.43
1:G:242:LEU:O	1:G:244:GLN:N	2.51	0.43
1:J:182:ASP:O	1:J:186:VAL:HG23	2.19	0.43
1:K:171:ARG:HD2	1:K:249:THR:OG1	2.18	0.43
1:K:230:THR:HB	1:K:232:GLU:OE1	2.17	0.43
1:L:172:ARG:NH1	1:L:245:ASP:OD2	2.51	0.43
1:C:297:MET:HE1	1:C:392:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ALA:O	1:E:149:ARG:HB2	2.18	0.43
1:J:162:GLY:O	1:J:166:THR:HG23	2.19	0.43
1:K:377:LEU:HD12	1:K:382:ALA:HB3	2.01	0.43
1:M:13:ARG:HD3	1:M:368:ARG:HB2	2.01	0.43
1:M:38:GLY:HA3	1:M:206:ILE:HG21	2.01	0.43
1:C:19:TYR:OH	1:D:131:ARG:HD3	2.18	0.43
1:E:195:ALA:HB1	1:E:201:LEU:HD13	2.01	0.43
1:H:20:GLY:HA2	1:H:24:ARG:HD3	2.00	0.43
2:K:501:COA:O1A	1:L:136:ARG:NH1	2.52	0.43
1:M:298:GLY:HA3	1:M:331:GLN:HG2	2.01	0.43
1:A:387:GLU:O	1:A:398:ALA:HA	2.19	0.43
2:D:501:COA:H62	2:D:501:COA:H31	1.70	0.43
1:E:279:LYS:HZ1	1:E:378:HIS:CD2	2.37	0.43
1:G:369:MET:SD	1:G:389:MET:HE2	2.59	0.43
1:H:16:ILE:HG23	1:H:361:PRO:HG3	2.01	0.43
2:H:501:COA:C5B	2:H:501:COA:C8A	2.96	0.43
1:J:184:LEU:HD21	1:J:326:GLU:CD	2.39	0.43
1:K:110:ASP:HB3	1:K:272:LYS:HD3	2.01	0.43
1:L:60:PRO:HG2	1:M:60:PRO:HG2	2.01	0.43
1:M:4:ARG:NH2	1:M:104:VAL:O	2.52	0.43
1:B:149:ARG:HG2	1:B:163:MET:HG2	2.01	0.42
1:B:91:GLY:HA2	1:B:389:MET:SD	2.59	0.42
1:C:187:ARG:HD2	1:C:191:ARG:NH2	2.28	0.42
1:D:297:MET:CG	1:D:298:GLY:N	2.78	0.42
1:C:60:PRO:HG2	1:D:60:PRO:HG2	2.00	0.42
1:L:200:VAL:O	1:L:203:GLU:HG2	2.19	0.42
1:L:5:ASP:OD1	3:L:503:HOH:O	2.22	0.42
1:D:239:PRO:HA	1:D:251:THR:HG22	2.00	0.42
1:E:378:HIS:HA	1:E:403:ARG:HD2	2.00	0.42
1:E:88:ARG:HH21	1:F:82:PRO:HB2	1.84	0.42
1:K:105:ARG:HE	1:K:105:ARG:HB3	1.61	0.42
1:L:13:ARG:O	1:L:205:ILE:HA	2.18	0.42
1:L:301:PRO:HD3	1:L:390:CYS:HA	2.01	0.42
1:A:89:ARG:HD3	1:A:89:ARG:HA	1.61	0.42
1:B:320:ASP:CB	1:B:382:ALA:HB1	2.48	0.42
1:H:196:GLN:HG2	1:H:201:LEU:HD22	2.01	0.42
1:J:360:HIS:CE1	1:J:362:VAL:HA	2.54	0.42
1:K:88:ARG:HG2	1:K:391:ILE:HD13	2.00	0.42
1:L:299:ILE:HA	1:L:299:ILE:HD12	1.85	0.42
1:M:326:GLU:HG2	1:M:332:ALA:CB	2.48	0.42
1:M:155:LYS:HB3	1:M:155:LYS:HE2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:352:ARG:HD2	1:M:372:THR:HG23	2.01	0.42
1:A:201:LEU:HD11	3:A:555:HOH:O	2.20	0.42
1:A:40:LEU:CD1	1:A:77:LEU:HD11	2.50	0.42
1:J:130:MET:SD	1:K:141:ILE:HD13	2.59	0.42
1:J:323:GLU:HG3	1:J:373:LEU:HB2	2.01	0.42
1:K:15:PRO:HD2	1:K:208:VAL:HG23	2.01	0.42
1:M:78:PRO:HG2	1:M:81:VAL:HG23	2.02	0.42
1:B:352:ARG:HD2	1:B:372:THR:HG23	2.01	0.42
1:D:237:LEU:HD21	2:D:501:COA:C4A	2.50	0.42
1:E:360:HIS:CE1	1:E:362:VAL:HA	2.54	0.42
1:H:178:ARG:HD3	3:H:728:HOH:O	2.18	0.42
1:A:65:PRO:HA	1:B:89:ARG:HH21	1.84	0.42
1:D:321:LEU:HD12	1:D:377:LEU:HD13	2.02	0.42
1:F:245:ASP:HB3	1:F:248:ALA:HB2	2.02	0.42
1:G:43:THR:HG22	3:G:529:HOH:O	2.19	0.42
1:L:239:PRO:CA	1:L:251:THR:HG22	2.46	0.42
1:A:123:VAL:HG21	1:A:145:LEU:HD21	2.02	0.42
1:A:15:PRO:HD2	1:A:208:VAL:HG23	2.01	0.42
1:D:90:CYS:HA	1:D:362:VAL:HG13	2.02	0.42
1:E:174:TYR:OH	1:E:338:GLU:OE2	2.24	0.42
1:H:115:GLY:HA2	3:H:727:HOH:O	2.20	0.42
1:E:141:ILE:HD11	1:H:141:ILE:CG1	2.50	0.42
1:J:273:ALA:HA	1:J:278:LEU:HD12	2.02	0.42
1:M:187:ARG:O	1:M:191:ARG:HG3	2.19	0.42
1:M:352:ARG:NH2	1:M:376:GLU:OE1	2.48	0.42
1:G:60:PRO:HG2	1:H:60:PRO:HG2	2.02	0.42
1:H:164:LEU:HG	1:H:328:PHE:CE2	2.55	0.42
1:H:192:ALA:O	1:H:196:GLN:HG3	2.20	0.42
1:K:333:LEU:HD23	1:K:336:MET:HE3	2.02	0.42
1:E:316:LEU:HD12	1:E:316:LEU:HA	1.88	0.41
1:J:163:MET:CG	1:J:297:MET:HE1	2.49	0.41
1:M:341:PHE:CE2	1:M:345:ASP:HB3	2.55	0.41
1:B:377:LEU:O	1:B:403:ARG:HD3	2.20	0.41
1:C:275:GLU:O	1:C:275:GLU:HG2	2.18	0.41
1:D:54:ILE:HD11	1:D:103:GLN:NE2	2.36	0.41
1:E:22:MET:SD	1:E:223:GLU:HB2	2.59	0.41
1:K:324:LEU:O	1:K:350:ASN:ND2	2.52	0.41
1:M:321:LEU:O	1:M:385:GLY:HA2	2.20	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.89	0.41
1:E:345:ASP:HA	1:E:348:ARG:HH11	1.85	0.41
1:G:166:THR:HG22	1:G:295:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:PRO:HD3	1:J:206:ILE:O	2.19	0.41
1:L:290:ALA:HA	3:M:572:HOH:O	2.20	0.41
1:A:180:GLU:OE1	3:A:505:HOH:O	2.22	0.41
1:A:352:ARG:NH1	3:A:510:HOH:O	2.45	0.41
1:B:19:TYR:HB2	1:B:258:GLN:O	2.19	0.41
1:C:143:ASP:HB3	1:C:146:ALA:HB3	2.02	0.41
1:C:196:GLN:HG2	1:C:201:LEU:HD22	2.03	0.41
1:C:87:ASP:HB3	1:D:85:GLN:HB3	2.02	0.41
1:J:150:THR:O	3:J:504:HOH:O	2.22	0.41
1:A:101:CYS:O	1:A:105:ARG:HG3	2.21	0.41
1:C:15:PRO:HD2	1:C:208:VAL:HG23	2.03	0.41
1:D:368:ARG:NH1	1:D:369:MET:HA	2.35	0.41
1:H:37:LYS:NZ	3:H:630:HOH:O	2.52	0.41
1:A:26:LEU:HD11	1:A:210:VAL:HG12	2.03	0.41
1:A:297:MET:HG3	1:A:392:GLY:HA2	2.02	0.41
1:D:192:ALA:O	1:D:196:GLN:HG3	2.20	0.41
1:E:327:ALA:HB2	3:E:579:HOH:O	2.20	0.41
1:E:352:ARG:HE	1:E:379:ARG:NH2	2.19	0.41
1:E:397:LEU:HA	1:E:397:LEU:HD12	1.96	0.41
1:G:147:ARG:O	1:G:150:THR:HB	2.21	0.41
1:J:171:ARG:C	1:J:171:ARG:HD2	2.41	0.41
1:J:46:ALA:HB3	1:J:49:GLN:HG2	2.02	0.41
1:J:311:LYS:NZ	1:K:108:ASP:O	2.46	0.41
1:K:22:MET:HE2	1:K:223:GLU:HB2	2.01	0.41
1:L:303:PRO:O	1:L:307:VAL:HG23	2.20	0.41
1:B:326:GLU:HB3	1:B:356:ILE:HG13	2.02	0.41
1:D:296:LEU:O	1:D:299:ILE:HG22	2.19	0.41
1:F:4:ARG:CZ	1:F:269:THR:HG21	2.51	0.41
1:G:62:SER:O	1:H:151:THR:OG1	2.35	0.41
1:J:326:GLU:HG2	1:J:332:ALA:HB2	2.02	0.41
1:M:8:ILE:HG13	1:M:370:LEU:HD21	2.01	0.41
1:C:179:THR:O	1:C:183:GLU:HG3	2.21	0.41
1:D:297:MET:HE1	1:D:390:CYS:SG	2.61	0.41
1:G:125:PHE:HA	1:G:142:HIS:O	2.20	0.41
1:J:321:LEU:HD23	1:J:321:LEU:HA	1.91	0.41
1:K:69:ARG:NH1	1:K:81:VAL:O	2.52	0.41
1:L:152:ALA:HA	1:M:65:PRO:HG2	2.01	0.41
1:M:321:LEU:HD23	1:M:321:LEU:HA	1.95	0.41
1:B:15:PRO:HD2	1:B:208:VAL:HG23	2.02	0.41
1:B:33:VAL:HG13	1:B:75:ALA:HA	2.02	0.41
1:D:149:ARG:O	1:D:162:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:VAL:HA	1:F:109:HIS:O	2.20	0.41
1:F:272:LYS:HE3	1:F:276:LEU:HD11	2.03	0.41
1:G:54:ILE:HD13	1:G:99:GLN:HE21	1.86	0.41
1:H:391:ILE:HB	1:H:395:GLN:HB2	2.03	0.41
1:L:368:ARG:NH2	1:L:369:MET:HG2	2.35	0.41
1:A:181:GLN:NE2	1:A:249:THR:HB	2.36	0.41
1:B:296:LEU:O	1:B:299:ILE:HG22	2.21	0.41
1:J:185:ALA:O	1:J:189:HIS:HD2	2.04	0.41
1:K:321:LEU:HD11	1:K:380:ARG:HD2	2.03	0.41
1:L:355:GLY:HA2	1:L:359:GLY:O	2.21	0.41
1:M:307:VAL:HG12	1:M:311:LYS:CE	2.51	0.41
1:C:212:THR:OG1	1:C:216:GLU:N	2.53	0.41
1:D:13:ARG:O	1:D:205:ILE:HA	2.21	0.41
1:H:297:MET:CG	1:H:298:GLY:N	2.80	0.41
1:K:297:MET:HE2	1:K:391:ILE:C	2.41	0.41
1:L:123:VAL:HG21	1:L:145:LEU:HD21	2.02	0.41
1:E:321:LEU:HD12	1:E:377:LEU:HD13	2.03	0.40
1:F:81:VAL:HA	1:F:82:PRO:HD3	1.84	0.40
1:B:58:CYS:SG	1:B:362:VAL:HG12	2.61	0.40
1:C:207:PRO:HB3	1:C:220:SER:HB3	2.03	0.40
1:D:171:ARG:HG3	1:D:249:THR:HG1	1.86	0.40
1:G:361:PRO:O	1:G:364:ALA:N	2.49	0.40
1:H:224:HIS:CG	3:H:669:HOH:O	2.75	0.40
1:G:320:ASP:O	1:G:348:ARG:HB2	2.22	0.40
1:A:278:LEU:O	1:A:280:PRO:HD3	2.21	0.40
1:A:377:LEU:HD11	1:A:385:GLY:HA3	2.04	0.40
1:H:191:ARG:NH2	1:H:346:HIS:O	2.47	0.40
1:J:296:LEU:O	1:J:298:GLY:N	2.55	0.40
1:J:320:ASP:CB	1:J:382:ALA:HB1	2.51	0.40
1:K:15:PRO:HD3	1:K:205:ILE:HG23	2.04	0.40
1:K:181:GLN:NE2	1:K:249:THR:OG1	2.54	0.40
1:K:344:ALA:O	1:K:347:GLU:HB2	2.21	0.40
1:L:72:ALA:O	1:L:77:LEU:HB2	2.22	0.40
1:M:53:VAL:HG12	1:M:55:LEU:HD13	2.03	0.40
1:A:105:ARG:HB3	1:A:105:ARG:HE	1.62	0.40
1:C:238:LYS:HG2	1:C:238:LYS:H	1.45	0.40
1:E:141:ILE:HD12	1:H:139:VAL:CG1	2.52	0.40
1:J:58:CYS:HB3	1:J:89:ARG:NH1	2.37	0.40

All (2) 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)
3:D:692:HOH:O	3:J:549:HOH:O[3_654]	1.99	0.21
3:D:603:HOH:O	3:J:502:HOH:O[3_654]	2.13	0.07

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	395/407 (97%)	384 (97%)	10 (2%)	1 (0%)	41	49
1	B	394/407 (97%)	379 (96%)	15 (4%)	0	100	100
1	C	394/407 (97%)	380 (96%)	13 (3%)	1 (0%)	41	49
1	D	393/407 (97%)	378 (96%)	14 (4%)	1 (0%)	41	49
1	E	390/407 (96%)	380 (97%)	9 (2%)	1 (0%)	41	49
1	F	395/407 (97%)	383 (97%)	10 (2%)	2 (0%)	29	34
1	G	398/407 (98%)	383 (96%)	13 (3%)	2 (0%)	29	34
1	H	393/407 (97%)	384 (98%)	8 (2%)	1 (0%)	41	49
1	J	392/407 (96%)	380 (97%)	10 (3%)	2 (0%)	29	34
1	K	396/407 (97%)	381 (96%)	14 (4%)	1 (0%)	41	49
1	L	395/407 (97%)	384 (97%)	11 (3%)	0	100	100
1	M	393/407 (97%)	382 (97%)	10 (2%)	1 (0%)	41	49
All	All	4728/4884 (97%)	4578 (97%)	137 (3%)	13 (0%)	41	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	VAL
1	F	362	VAL
1	J	297	MET
1	M	362	VAL
1	C	297	MET
1	D	297	MET

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Mol	Chain	Res	Type
1	J	362	VAL
1	E	300	GLY
1	G	246	PRO
1	G	243	LYS
1	F	79	ILE
1	K	362	VAL
1	H	362	VAL

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	293/309 (95%)	291 (99%)	2 (1%)	84	90
1	B	298/309 (96%)	295 (99%)	3 (1%)	76	84
1	C	293/309 (95%)	287 (98%)	6 (2%)	55	67
1	D	299/309 (97%)	294 (98%)	5 (2%)	60	73
1	E	298/309 (96%)	292 (98%)	6 (2%)	55	67
1	F	301/309 (97%)	297 (99%)	4 (1%)	69	80
1	G	301/309 (97%)	294 (98%)	7 (2%)	50	63
1	H	300/309 (97%)	295 (98%)	5 (2%)	60	73
1	J	295/309 (96%)	290 (98%)	5 (2%)	60	73
1	K	299/309 (97%)	294 (98%)	5 (2%)	60	73
1	L	294/309 (95%)	286 (97%)	8 (3%)	44	57
1	M	298/309 (96%)	296 (99%)	2 (1%)	84	90
All	All	3569/3708 (96%)	3511 (98%)	58 (2%)	62	74

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	181	GLN
1	B	4	ARG

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Mol	Chain	Res	Type
1	B	217	GLU
1	B	354	SER
1	C	149	ARG
1	C	203	GLU
1	C	226	ARG
1	C	265	CYS
1	C	337	ARG
1	C	341	PHE
1	D	201	LEU
1	D	232	GLU
1	D	238	LYS
1	D	337	ARG
1	D	368	ARG
1	E	141	ILE
1	E	164	LEU
1	E	171	ARG
1	E	187	ARG
1	E	226	ARG
1	E	297	MET
1	F	171	ARG
1	F	177	SER
1	F	220	SER
1	F	378	HIS
1	G	141	ILE
1	G	169	ASN
1	G	224	HIS
1	G	271	GLU
1	G	297	MET
1	G	341	PHE
1	G	379	ARG
1	H	4	ARG
1	H	25	SER
1	H	180	GLU
1	H	341	PHE
1	H	378	HIS
1	J	164	LEU
1	J	297	MET
1	J	341	PHE
1	J	354	SER
1	J	381	GLU
1	K	171	ARG
1	K	179	THR

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Mol	Chain	Res	Type
1	K	197	SER
1	K	297	MET
1	K	377	LEU
1	L	65	PRO
1	L	164	LEU
1	L	171	ARG
1	L	181	GLN
1	L	201	LEU
1	L	228	ASP
1	L	297	MET
1	L	389	MET
1	M	265	CYS
1	M	341	PHE

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

Mol	Chain	Res	Type
1	A	103	GLN
1	A	181	GLN
1	A	378	HIS
1	B	99	GLN
1	B	103	GLN
1	D	181	GLN
1	F	258	GLN
1	J	49	GLN
1	K	258	GLN
1	L	190	GLN
1	M	122	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	COA	F	501	-	41,50,50	3.90	10 (24%)	52,75,75	1.78	10 (19%)
2	COA	H	501	-	41,50,50	1.10	2 (4%)	52,75,75	1.65	14 (26%)
2	COA	B	501	-	41,50,50	3.83	11 (26%)	52,75,75	1.56	7 (13%)
2	COA	K	501	-	41,50,50	3.80	11 (26%)	52,75,75	2.07	15 (28%)
2	COA	D	501	-	41,50,50	1.16	2 (4%)	52,75,75	1.69	11 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	F	501	-	-	12/44/64/64	0/3/3/3
2	COA	H	501	-	-	19/44/64/64	0/3/3/3
2	COA	B	501	-	-	6/44/64/64	0/3/3/3
2	COA	K	501	-	-	17/44/64/64	0/3/3/3
2	COA	D	501	-	-	12/44/64/64	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	COA	C2B-C1B	-15.19	1.30	1.53
2	K	501	COA	C2B-C1B	-15.14	1.30	1.53
2	F	501	COA	O4B-C1B	14.96	1.62	1.41
2	B	501	COA	C2B-C1B	-14.91	1.31	1.53
2	B	501	COA	O4B-C1B	14.57	1.61	1.41
2	K	501	COA	O4B-C1B	14.49	1.61	1.41
2	F	501	COA	C3B-C4B	-6.08	1.36	1.52
2	K	501	COA	C3B-C4B	-5.85	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	COA	C3B-C4B	-5.66	1.37	1.52
2	F	501	COA	C2B-C3B	5.54	1.65	1.52
2	B	501	COA	C2B-C3B	5.45	1.65	1.52
2	K	501	COA	C2B-C3B	4.57	1.63	1.52
2	K	501	COA	C9P-N8P	4.17	1.42	1.33
2	B	501	COA	C9P-N8P	4.11	1.42	1.33
2	F	501	COA	C9P-N8P	3.94	1.42	1.33
2	F	501	COA	O4B-C4B	3.89	1.53	1.45
2	B	501	COA	C5P-N4P	3.86	1.42	1.33
2	B	501	COA	O4B-C4B	3.80	1.53	1.45
2	F	501	COA	C2A-N3A	3.69	1.38	1.32
2	B	501	COA	C2A-N3A	3.69	1.38	1.32
2	F	501	COA	C5P-N4P	3.55	1.41	1.33
2	K	501	COA	C5P-N4P	3.45	1.41	1.33
2	K	501	COA	O4B-C4B	3.32	1.52	1.45
2	K	501	COA	C2A-N3A	3.21	1.37	1.32
2	B	501	COA	C6A-N6A	3.08	1.45	1.34
2	F	501	COA	C6A-N6A	3.00	1.45	1.34
2	D	501	COA	C2B-C1B	-2.97	1.49	1.53
2	K	501	COA	C6A-N6A	2.94	1.44	1.34
2	K	501	COA	C2A-N1A	2.85	1.39	1.33
2	F	501	COA	C2A-N1A	2.66	1.38	1.33
2	B	501	COA	OAP-CAP	-2.51	1.37	1.42
2	B	501	COA	C2A-N1A	2.38	1.38	1.33
2	D	501	COA	P3B-O8A	-2.18	1.46	1.54
2	H	501	COA	C5A-C4A	2.12	1.46	1.40
2	H	501	COA	C5A-N7A	-2.11	1.32	1.39
2	K	501	COA	OAP-CAP	-2.05	1.38	1.42

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	501	COA	C7P-C6P-C5P	-7.69	99.55	112.36
2	D	501	COA	O6A-CCP-CBP	6.05	120.27	110.55
2	K	501	COA	N3A-C2A-N1A	-5.47	120.13	128.68
2	F	501	COA	N3A-C2A-N1A	-5.28	120.43	128.68
2	B	501	COA	C5A-C6A-N6A	5.18	128.23	120.35
2	B	501	COA	N3A-C2A-N1A	-5.04	120.80	128.68
2	F	501	COA	CEP-CBP-CCP	4.93	116.27	108.23
2	K	501	COA	C5A-C6A-N6A	4.88	127.77	120.35
2	H	501	COA	C4A-C5A-N7A	-4.31	104.91	109.40
2	F	501	COA	C5A-C6A-N6A	4.27	126.84	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	COA	N3A-C2A-N1A	-4.12	122.25	128.68
2	K	501	COA	C6P-C7P-N8P	3.92	119.81	111.90
2	K	501	COA	C7P-N8P-C9P	3.75	129.28	122.59
2	H	501	COA	O6A-CCP-CBP	3.74	116.56	110.55
2	F	501	COA	C7P-C6P-C5P	-3.64	106.30	112.36
2	D	501	COA	C1B-N9A-C4A	-3.52	120.46	126.64
2	B	501	COA	N6A-C6A-N1A	-3.48	111.36	118.57
2	D	501	COA	CEP-CBP-CCP	3.31	113.62	108.23
2	H	501	COA	C6P-C7P-N8P	3.19	118.33	111.90
2	K	501	COA	C3P-N4P-C5P	-3.17	116.96	122.84
2	H	501	COA	P2A-O3A-P1A	-3.12	122.14	132.83
2	F	501	COA	CDP-CBP-CAP	3.09	114.17	108.82
2	D	501	COA	C4A-C5A-N7A	-3.05	106.22	109.40
2	F	501	COA	C3P-N4P-C5P	-3.02	117.23	122.84
2	B	501	COA	C6P-C7P-N8P	-2.94	105.97	111.90
2	B	501	COA	C3B-C2B-C1B	2.87	106.26	99.89
2	H	501	COA	C5A-C6A-N6A	2.86	124.70	120.35
2	K	501	COA	O5P-C5P-N4P	-2.73	117.87	123.01
2	K	501	COA	C6P-C5P-N4P	2.72	121.00	116.42
2	B	501	COA	C1B-N9A-C4A	-2.71	121.88	126.64
2	F	501	COA	C6P-C7P-N8P	-2.70	106.45	111.90
2	H	501	COA	C6P-C5P-N4P	2.64	120.86	116.42
2	F	501	COA	O4B-C1B-C2B	-2.56	103.18	106.93
2	K	501	COA	N6A-C6A-N1A	-2.53	113.33	118.57
2	F	501	COA	C3B-C2B-C1B	2.51	105.45	99.89
2	H	501	COA	O4B-C1B-C2B	-2.49	103.29	106.93
2	F	501	COA	N6A-C6A-N1A	-2.46	113.47	118.57
2	H	501	COA	CEP-CBP-CAP	-2.40	104.67	108.82
2	D	501	COA	C6P-C7P-N8P	2.39	116.71	111.90
2	K	501	COA	O4B-C1B-C2B	-2.36	103.48	106.93
2	K	501	COA	CDP-CBP-CCP	2.34	112.05	108.23
2	H	501	COA	CDP-CBP-CAP	2.34	112.87	108.82
2	K	501	COA	CEP-CBP-CAP	-2.33	104.77	108.82
2	B	501	COA	C3P-N4P-C5P	-2.33	118.51	122.84
2	H	501	COA	C3B-C2B-C1B	2.30	104.98	99.89
2	H	501	COA	O5P-C5P-N4P	-2.26	118.74	123.01
2	H	501	COA	O9A-P3B-O8A	2.25	116.25	107.64
2	D	501	COA	CDP-CBP-CCP	-2.23	104.59	108.23
2	H	501	COA	O5A-P2A-O4A	2.22	123.20	112.24
2	D	501	COA	C7P-N8P-C9P	-2.12	118.81	122.59
2	D	501	COA	C2A-N1A-C6A	2.10	122.34	118.75
2	D	501	COA	C3B-C2B-C1B	-2.08	95.29	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	COA	O3B-P3B-O7A	-2.07	101.42	109.39
2	K	501	COA	O6A-CCP-CBP	-2.06	107.24	110.55
2	K	501	COA	C1B-N9A-C4A	-2.03	123.08	126.64
2	K	501	COA	P2A-O3A-P1A	-2.01	125.92	132.83
2	H	501	COA	O2A-P1A-O1A	2.01	122.18	112.24

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	COA	C5B-O5B-P1A-O1A
2	F	501	COA	C5B-O5B-P1A-O2A
2	F	501	COA	C5B-O5B-P1A-O3A
2	F	501	COA	CCP-O6A-P2A-O4A
2	F	501	COA	CCP-O6A-P2A-O5A
2	F	501	COA	CAP-CBP-CCP-O6A
2	H	501	COA	C4B-C5B-O5B-P1A
2	H	501	COA	CCP-O6A-P2A-O4A
2	H	501	COA	CDP-CBP-CCP-O6A
2	H	501	COA	CEP-CBP-CCP-O6A
2	H	501	COA	CAP-CBP-CCP-O6A
2	H	501	COA	OAP-CAP-CBP-CCP
2	H	501	COA	C9P-CAP-CBP-CCP
2	H	501	COA	OAP-CAP-CBP-CDP
2	H	501	COA	C9P-CAP-CBP-CDP
2	H	501	COA	OAP-CAP-CBP-CEP
2	H	501	COA	C9P-CAP-CBP-CEP
2	H	501	COA	N8P-C9P-CAP-OAP
2	H	501	COA	C2P-C3P-N4P-C5P
2	B	501	COA	CCP-O6A-P2A-O3A
2	B	501	COA	CCP-O6A-P2A-O4A
2	B	501	COA	CCP-O6A-P2A-O5A
2	B	501	COA	CAP-CBP-CCP-O6A
2	K	501	COA	O4B-C4B-C5B-O5B
2	K	501	COA	C5B-O5B-P1A-O1A
2	K	501	COA	C5B-O5B-P1A-O2A
2	K	501	COA	CDP-CBP-CCP-O6A
2	K	501	COA	CAP-CBP-CCP-O6A
2	K	501	COA	OAP-CAP-CBP-CCP
2	K	501	COA	C9P-CAP-CBP-CCP
2	K	501	COA	OAP-CAP-CBP-CDP
2	K	501	COA	C9P-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
2	K	501	COA	OAP-CAP-CBP-CEP
2	K	501	COA	C9P-CAP-CBP-CEP
2	K	501	COA	C5P-C6P-C7P-N8P
2	D	501	COA	C3B-O3B-P3B-O8A
2	D	501	COA	CCP-O6A-P2A-O3A
2	D	501	COA	O9P-C9P-CAP-CBP
2	D	501	COA	N8P-C9P-CAP-CBP
2	D	501	COA	O9P-C9P-CAP-OAP
2	D	501	COA	N8P-C9P-CAP-OAP
2	D	501	COA	CAP-C9P-N8P-C7P
2	D	501	COA	C6P-C5P-N4P-C3P
2	D	501	COA	O5P-C5P-N4P-C3P
2	K	501	COA	C6P-C7P-N8P-C9P
2	D	501	COA	O9P-C9P-N8P-C7P
2	F	501	COA	C3B-C4B-C5B-O5B
2	K	501	COA	C3B-C4B-C5B-O5B
2	F	501	COA	O4B-C4B-C5B-O5B
2	F	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	CEP-CBP-CCP-O6A
2	K	501	COA	CEP-CBP-CCP-O6A
2	H	501	COA	O5P-C5P-N4P-C3P
2	H	501	COA	C6P-C5P-N4P-C3P
2	H	501	COA	O9P-C9P-CAP-OAP
2	F	501	COA	CEP-CBP-CCP-O6A
2	K	501	COA	C5B-O5B-P1A-O3A
2	F	501	COA	P2A-O3A-P1A-O1A
2	H	501	COA	CBP-CCP-O6A-P2A
2	H	501	COA	CCP-O6A-P2A-O5A
2	D	501	COA	CCP-O6A-P2A-O4A
2	D	501	COA	CCP-O6A-P2A-O5A
2	F	501	COA	CCP-O6A-P2A-O3A
2	H	501	COA	CCP-O6A-P2A-O3A
2	K	501	COA	CCP-O6A-P2A-O4A

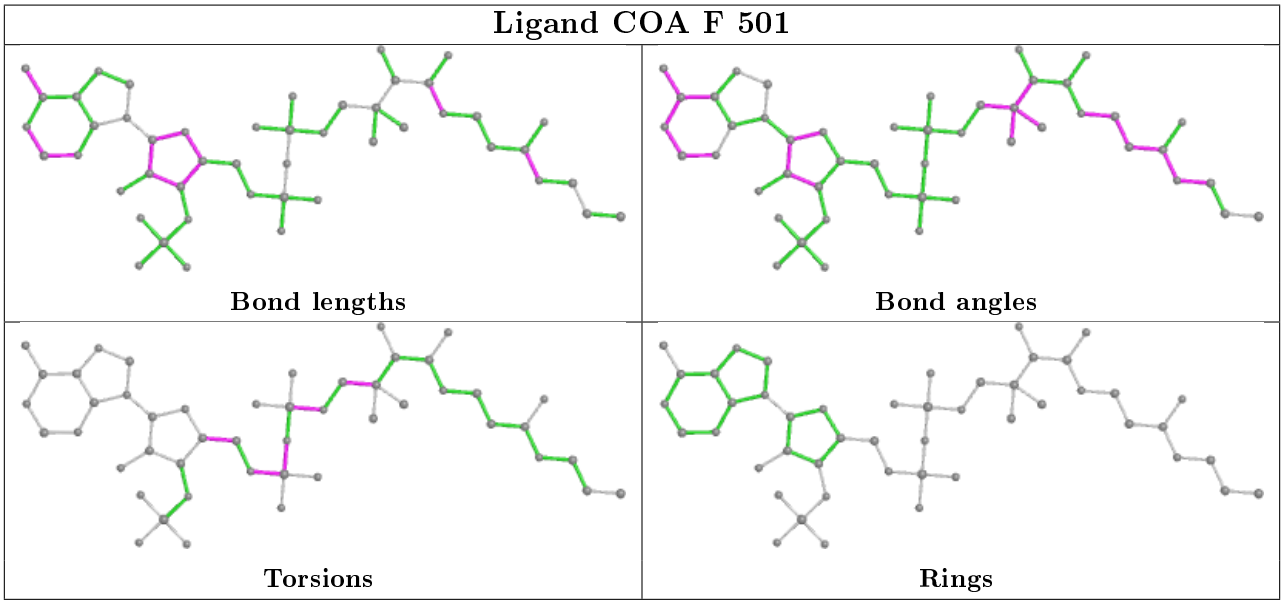
There are no ring outliers.

3 monomers are involved in 14 short contacts:

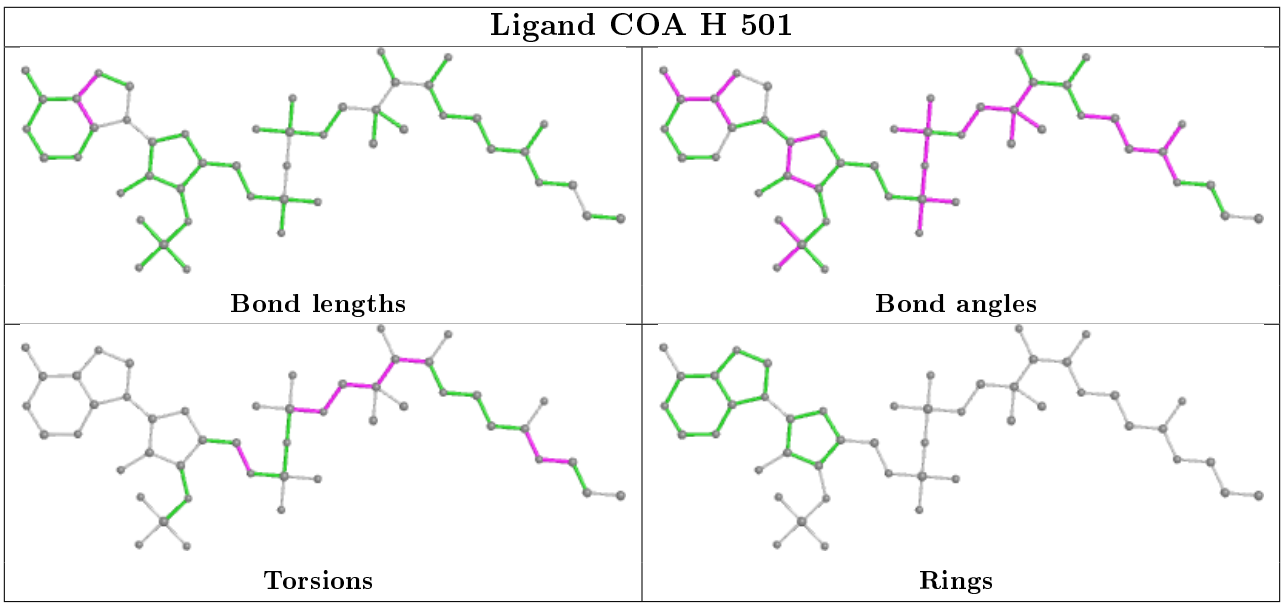
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	COA	5	0
2	K	501	COA	1	0
2	D	501	COA	8	0

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

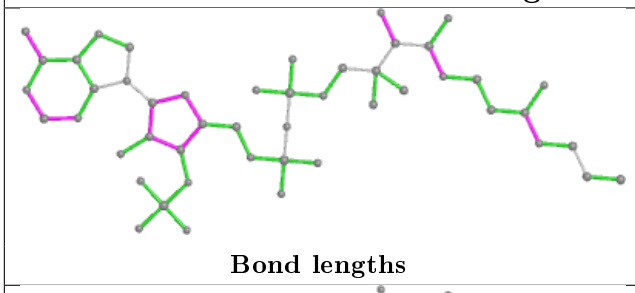
Ligand COA F 501



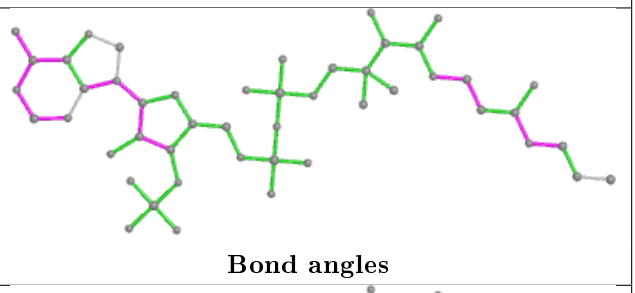
Ligand COA H 501



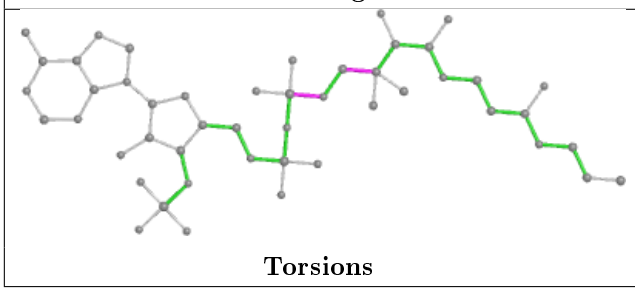
Ligand COA B 501



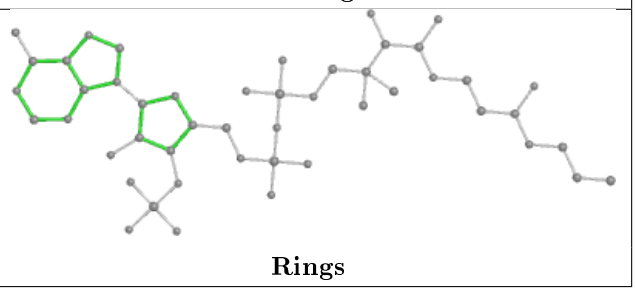
Bond lengths



Bond angles

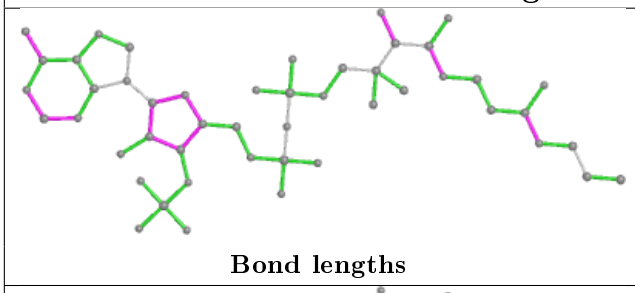


Torsions

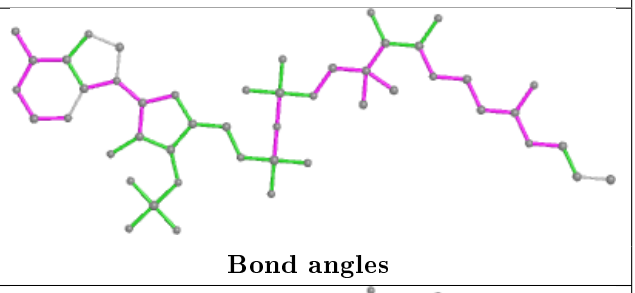


Rings

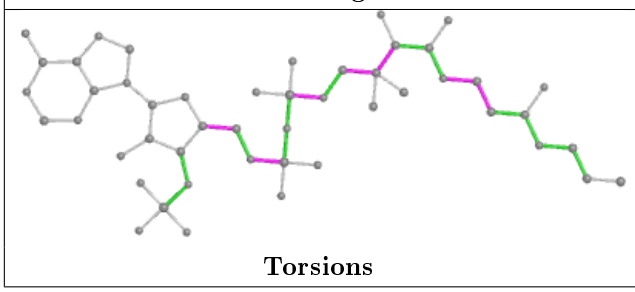
Ligand COA K 501



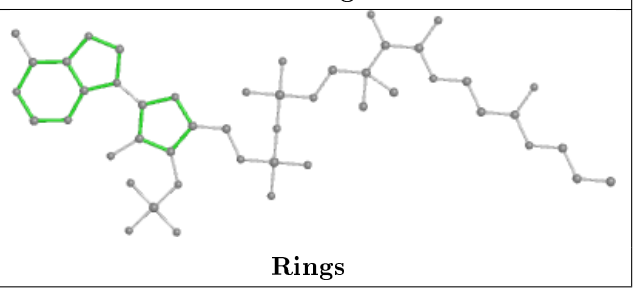
Bond lengths



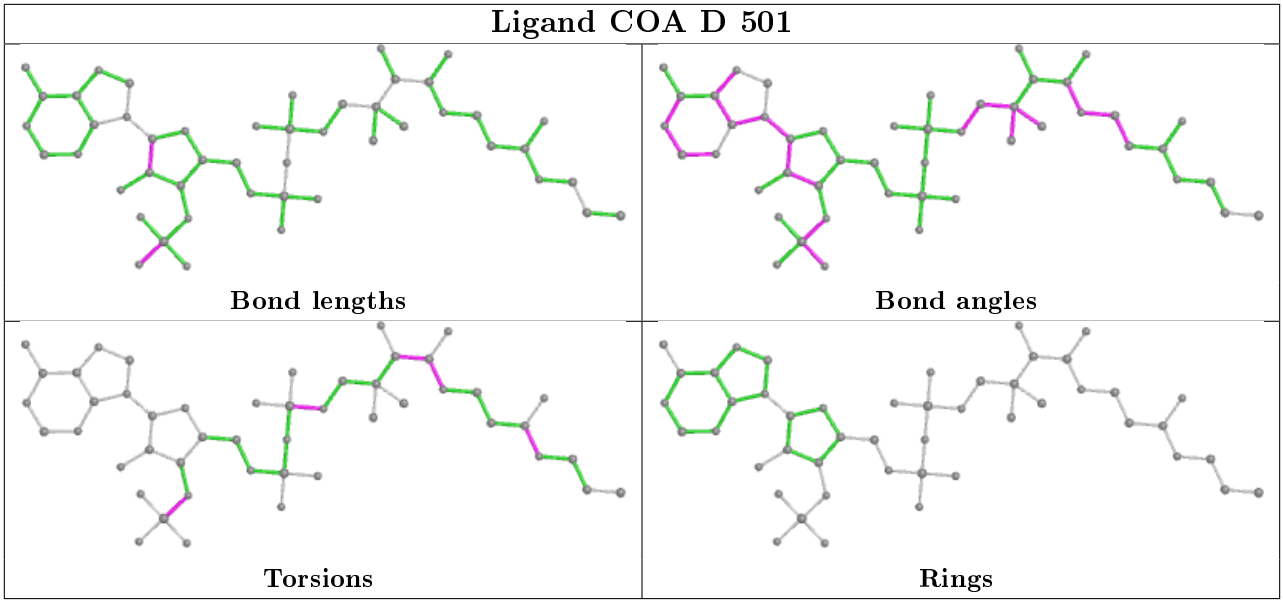
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	398/407 (97%)	-0.67	1 (0%) 94 94	22, 37, 57, 67	0
1	B	398/407 (97%)	-0.74	0 100 100	22, 32, 50, 63	0
1	C	398/407 (97%)	-0.56	4 (1%) 82 81	21, 37, 62, 74	0
1	D	397/407 (97%)	-0.72	1 (0%) 94 94	21, 32, 54, 73	0
1	E	396/407 (97%)	-0.50	1 (0%) 94 94	25, 43, 65, 75	0
1	F	399/407 (98%)	-0.64	1 (0%) 94 94	24, 36, 57, 81	0
1	G	402/407 (98%)	-0.55	6 (1%) 73 71	24, 37, 62, 86	0
1	H	397/407 (97%)	-0.70	1 (0%) 94 94	23, 33, 53, 72	0
1	J	396/407 (97%)	-0.63	1 (0%) 94 94	23, 38, 59, 74	0
1	K	400/407 (98%)	-0.68	0 100 100	21, 33, 58, 73	0
1	L	400/407 (98%)	-0.40	3 (0%) 86 85	24, 46, 75, 82	0
1	M	397/407 (97%)	-0.59	2 (0%) 91 91	27, 41, 61, 75	0
All	All	4778/4884 (97%)	-0.61	21 (0%) 92 92	21, 37, 61, 86	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	THR	4.3
1	L	174	TYR	3.3
1	F	212	THR	3.3
1	J	211	ARG	2.9
1	G	212	THR	2.8
1	G	213	ARG	2.8
1	C	211	ARG	2.8
1	M	246	PRO	2.7
1	G	242	LEU	2.6
1	G	344	ALA	2.5
1	M	211	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	175	HIS	2.4
1	L	405	GLN	2.4
1	D	211	ARG	2.3
1	G	158	PRO	2.2
1	C	229	THR	2.2
1	G	227	ALA	2.1
1	H	211	ARG	2.1
1	L	340	LYS	2.1
1	A	344	ALA	2.1
1	E	381	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

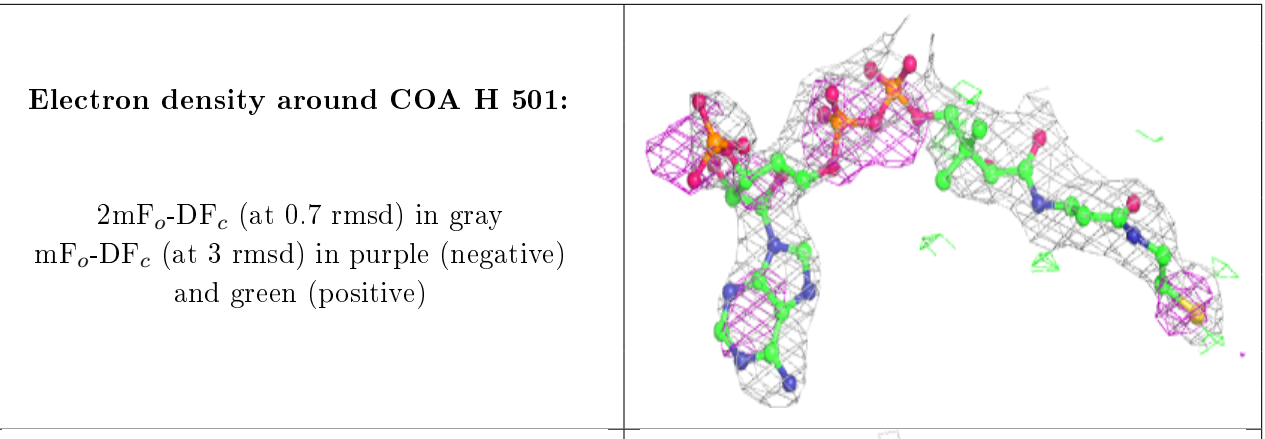
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	COA	H	501	48/48	0.77	0.28	38,57,78,98	0
2	COA	F	501	48/48	0.91	0.16	39,56,72,78	0
2	COA	B	501	48/48	0.92	0.16	29,50,73,91	0
2	COA	K	501	48/48	0.92	0.17	34,58,66,70	0
2	COA	D	501	48/48	0.94	0.31	20,20,20,20	0

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

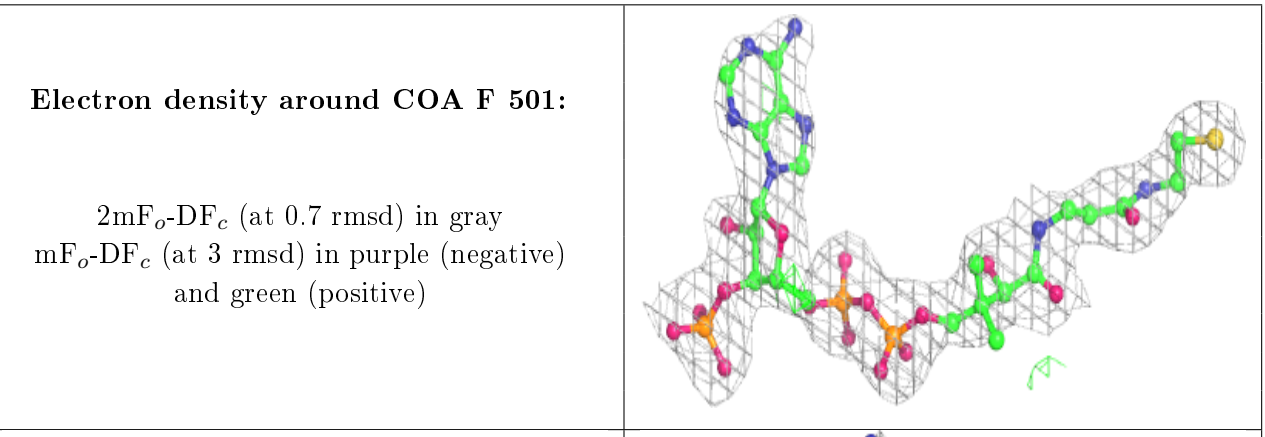
Electron density around COA H 501:

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



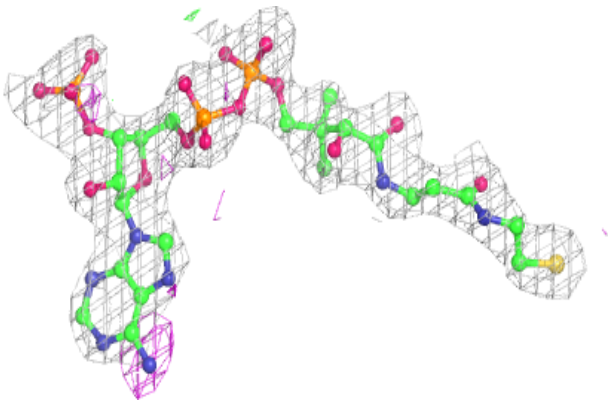
Electron density around COA F 501:

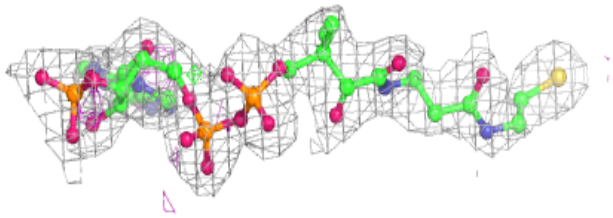
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

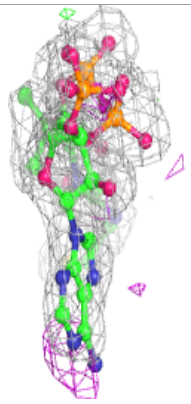


Electron density around COA B 501:

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

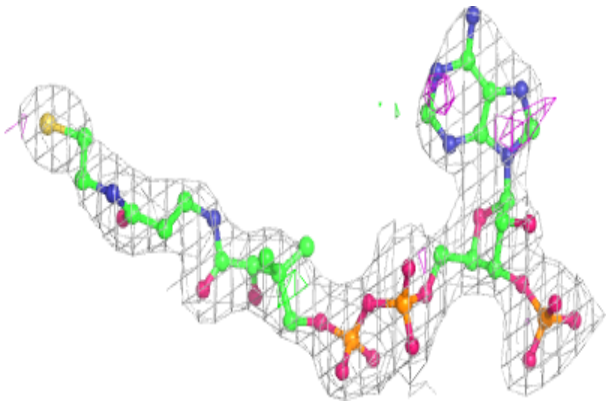


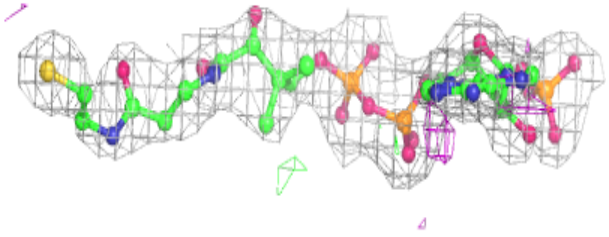


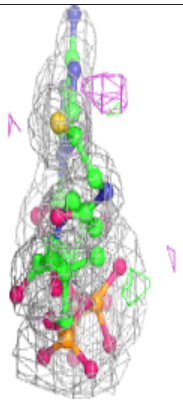


Electron density around COA K 501:

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

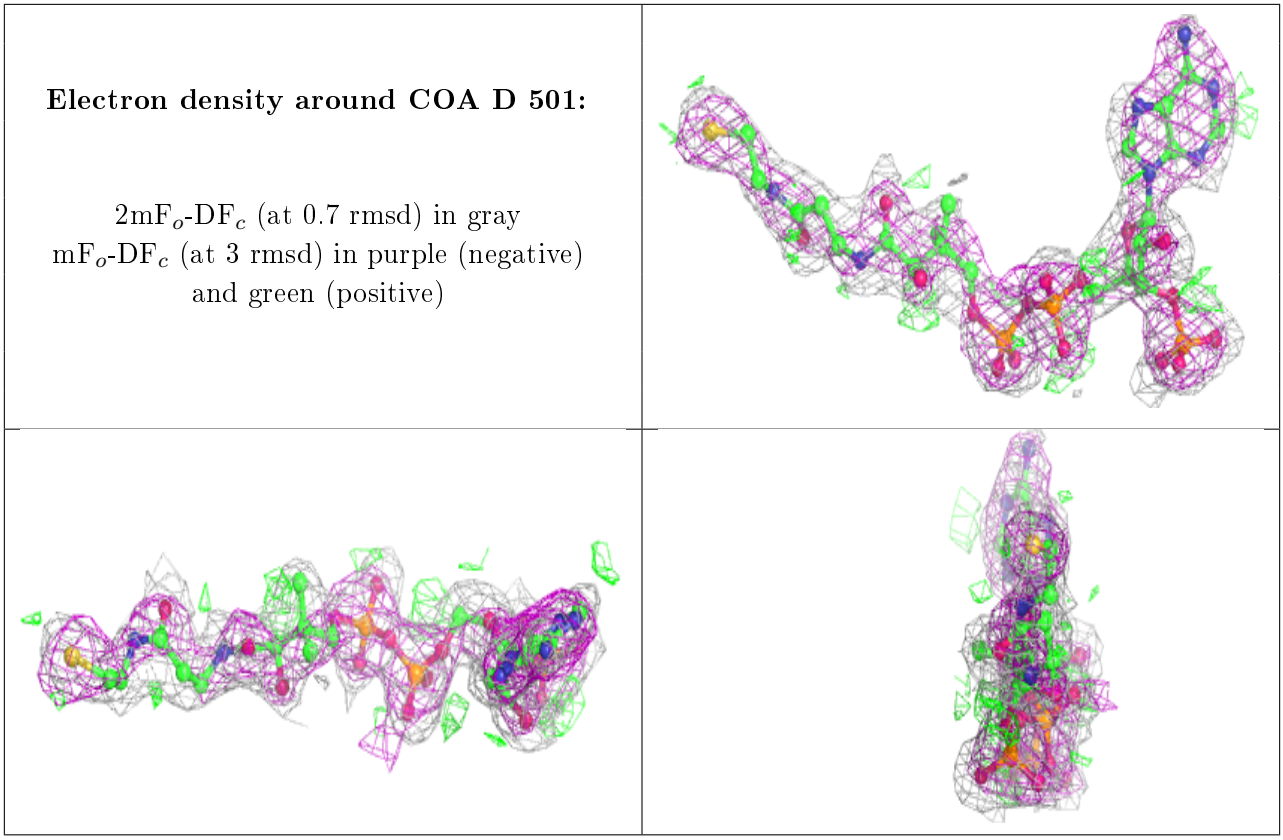






Electron density around COA D 501:

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



6.5 Other polymers

There are no such residues in this entry.