Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:13 pm BST

PDB ID	:	5VJ1
Title	:	Crystal structure of a Pseudomonas malonate decarboxylase hetero-tetramer in complex with coenzyme A
Authors	:	Maderbocus, R.; Tong, L.
Deposited on	:	2017-04-18
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

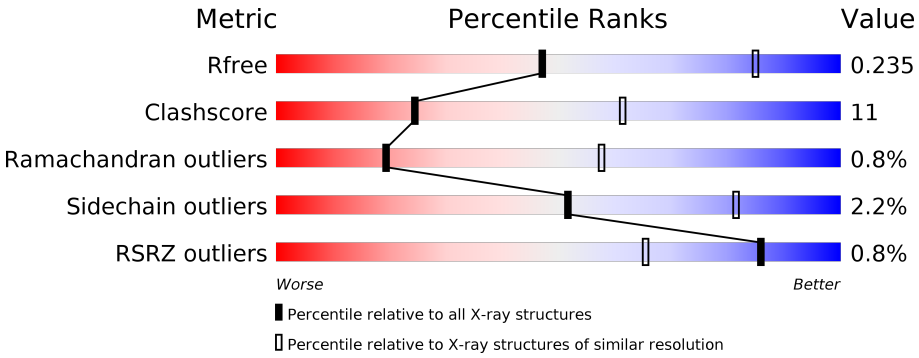
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	554	% 71% 26% ··
1	I	554	% 69% 28% ···
2	C	99	% 80% 18% ·
2	K	99	76% 22% ·
3	D	287	% 83% 14% ·
3	L	287	78% 18% ·

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Mol	Chain	Length	Quality of chain
4	E	284	
4	M	284	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18197 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 MdcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4284	2706	780	781	17			
1	I	548	Total	C	N	O	S	0	0	0
			4284	2706	780	781	17			

- Molecule 2 is a protein called MdcC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	97	Total	C	N	O	S	0	0	0
			735	465	129	139	2			
2	K	97	Total	C	N	O	S	0	0	0
			735	465	129	139	2			

- Molecule 3 is a protein called MdcD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	276	Total	C	N	O	S	0	0	0
			2063	1292	376	391	4			
3	L	276	Total	C	N	O	S	0	0	0
			2063	1292	376	391	4			

- Molecule 4 is a protein called MdcE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	263	Total	C	N	O	S	0	0	0
			1968	1239	368	356	5			
4	M	263	Total	C	N	O	S	0	0	0
			1968	1239	368	356	5			

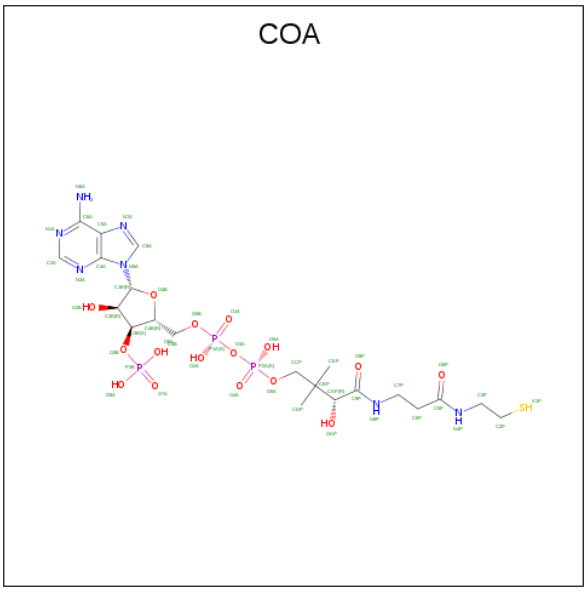
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	MET	-	initiating methionine	UNP A0A0C6EV56
E	-14	GLY	-	expression tag	UNP A0A0C6EV56
E	-13	SER	-	expression tag	UNP A0A0C6EV56
E	-12	SER	-	expression tag	UNP A0A0C6EV56
E	-11	HIS	-	expression tag	UNP A0A0C6EV56
E	-10	HIS	-	expression tag	UNP A0A0C6EV56
E	-9	HIS	-	expression tag	UNP A0A0C6EV56
E	-8	HIS	-	expression tag	UNP A0A0C6EV56
E	-7	HIS	-	expression tag	UNP A0A0C6EV56
E	-6	HIS	-	expression tag	UNP A0A0C6EV56
E	-5	SER	-	expression tag	UNP A0A0C6EV56
E	-4	GLN	-	expression tag	UNP A0A0C6EV56
E	-3	ASP	-	expression tag	UNP A0A0C6EV56
E	-2	PRO	-	expression tag	UNP A0A0C6EV56
E	-1	ASN	-	expression tag	UNP A0A0C6EV56
E	0	SER	-	expression tag	UNP A0A0C6EV56
M	-15	MET	-	initiating methionine	UNP A0A0C6EV56
M	-14	GLY	-	expression tag	UNP A0A0C6EV56
M	-13	SER	-	expression tag	UNP A0A0C6EV56
M	-12	SER	-	expression tag	UNP A0A0C6EV56
M	-11	HIS	-	expression tag	UNP A0A0C6EV56
M	-10	HIS	-	expression tag	UNP A0A0C6EV56
M	-9	HIS	-	expression tag	UNP A0A0C6EV56
M	-8	HIS	-	expression tag	UNP A0A0C6EV56
M	-7	HIS	-	expression tag	UNP A0A0C6EV56
M	-6	HIS	-	expression tag	UNP A0A0C6EV56
M	-5	SER	-	expression tag	UNP A0A0C6EV56
M	-4	GLN	-	expression tag	UNP A0A0C6EV56
M	-3	ASP	-	expression tag	UNP A0A0C6EV56
M	-2	PRO	-	expression tag	UNP A0A0C6EV56
M	-1	ASN	-	expression tag	UNP A0A0C6EV56
M	0	SER	-	expression tag	UNP A0A0C6EV56

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



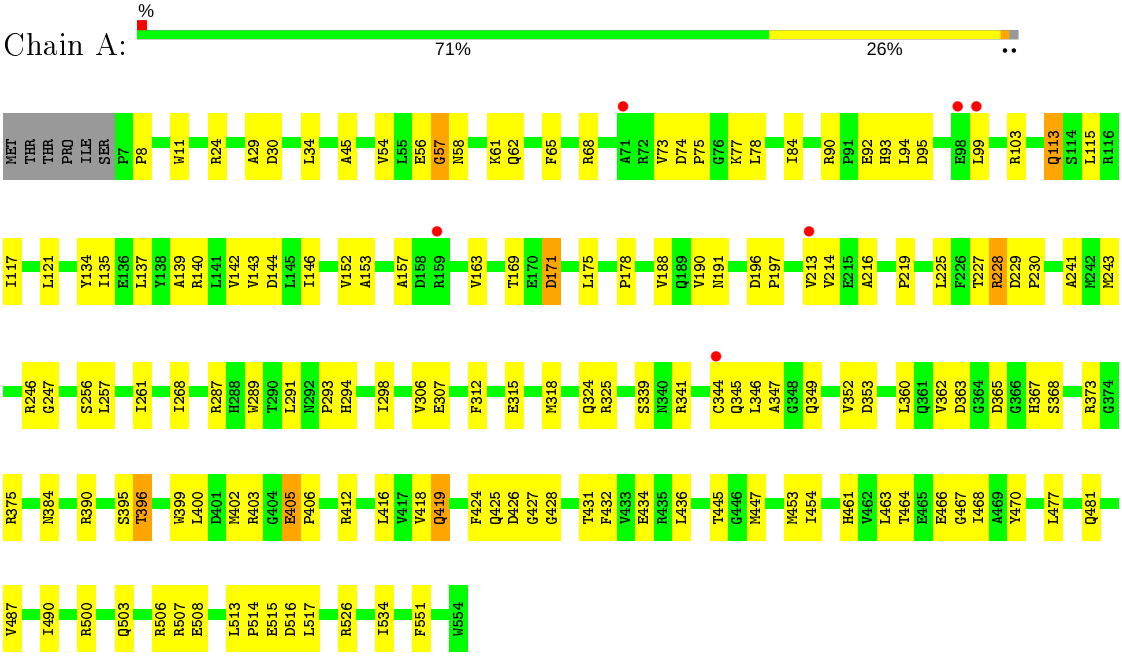
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
6	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

3 Residue-property plots (i)

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.

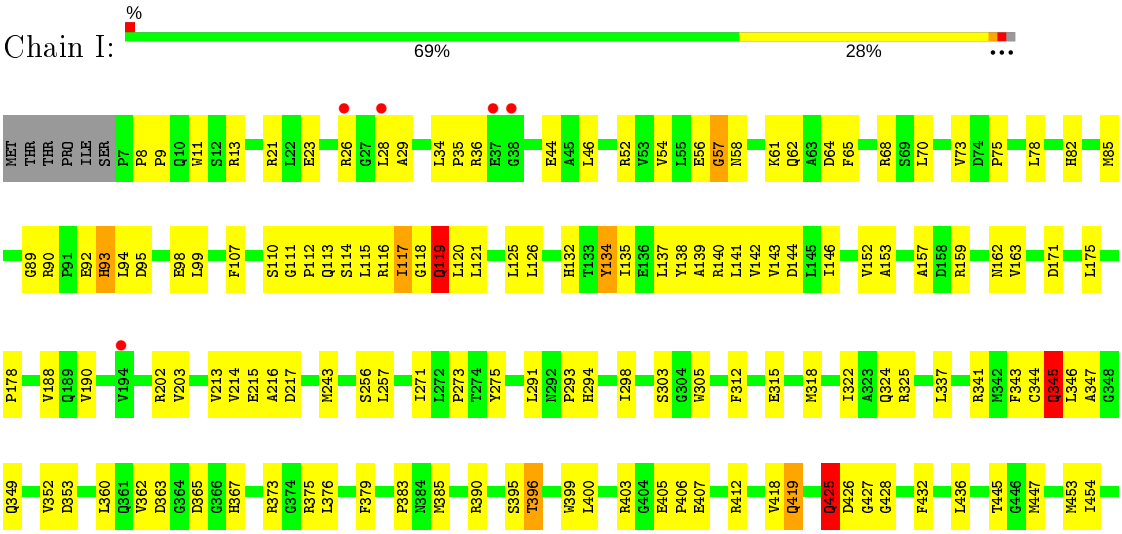
- Molecule 1: MdcA

Chain A:



- Molecule 1: MdcA

Chain I:

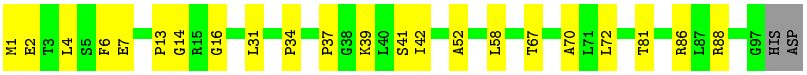


- Molecule 2: MdcC

Chain C:

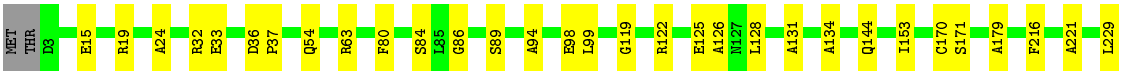
- Molecule 2: MdcC

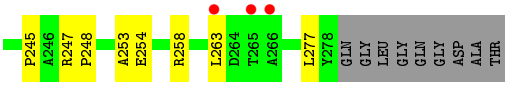
Chain K:



- Molecule 3: MdcD

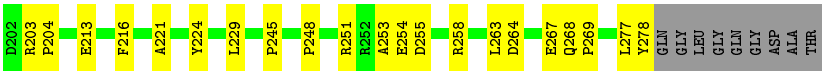
Chain D:





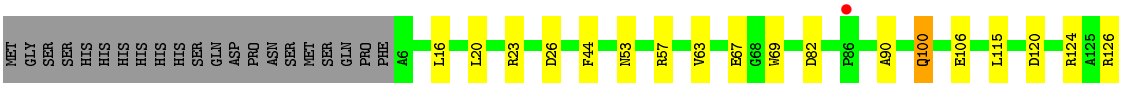
- Molecule 3: MdcD

Chain L:



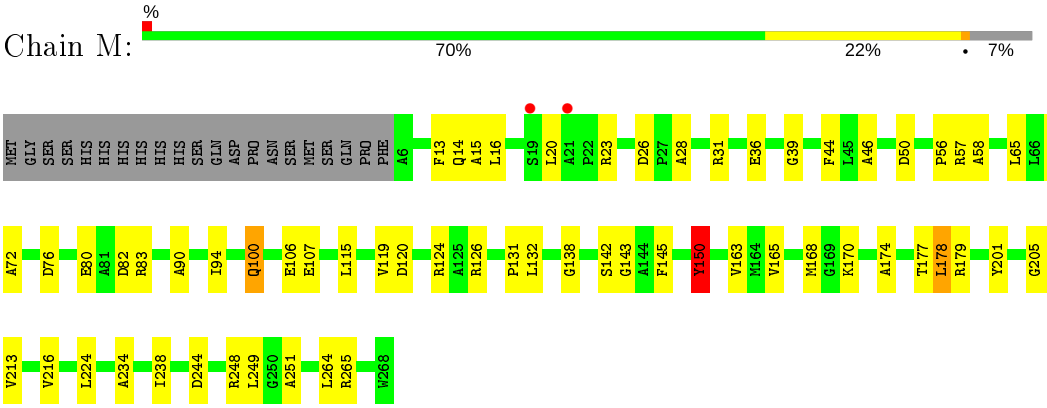
- Molecule 4: MdcE

Chain E:



• Molecule 4: MdcE

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.74Å 163.56Å 100.44Å 90.00° 94.01° 90.00°	Depositor
Resolution (Å)	47.90 – 3.00 47.90 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.90-3.00) 91.1 (47.90-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.173 , 0.233 0.176 , 0.235	Depositor DCC
R_{free} test set	3191 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18197	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, CL

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	0.47	0/4381	0.70	1/5944 (0.0%)
1	I	0.51	1/4381 (0.0%)	0.76	5/5944 (0.1%)
2	C	0.44	0/751	0.66	0/1017
2	K	0.45	0/751	0.68	0/1017
3	D	0.49	0/2093	0.67	0/2839
3	L	0.48	0/2093	0.68	0/2839
4	E	0.47	0/2007	0.70	0/2729
4	M	0.51	1/2007 (0.0%)	0.73	2/2729 (0.1%)
All	All	0.49	2/18464 (0.0%)	0.71	8/25058 (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	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	23	GLU	CB-CG	-6.52	1.39	1.52
4	M	150	TYR	CD1-CE1	-5.24	1.31	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	150	TYR	CB-CG-CD1	-8.20	116.08	121.00
1	I	345	GLN	CA-CB-CG	7.08	128.99	113.40
4	M	150	TYR	CB-CG-CD2	7.01	125.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	57	GLY	N-CA-C	-6.92	95.81	113.10
1	A	57	GLY	N-CA-C	-6.61	96.57	113.10
1	I	26	ARG	CG-CD-NE	5.62	123.61	111.80
1	I	425	GLN	CA-CB-CG	5.23	124.91	113.40
1	I	119	GLN	CB-CA-C	-5.19	100.02	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	119	GLN	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	4284	0	4281	105	1
1	I	4284	0	4281	143	1
2	C	735	0	724	10	0
2	K	735	0	724	15	0
3	D	2063	0	2071	28	1
3	L	2063	0	2071	31	1
4	E	1968	0	1994	49	0
4	M	1968	0	1994	44	0
5	A	1	0	0	0	0
6	D	48	0	32	6	0
6	L	48	0	32	5	0
All	All	18197	0	18204	395	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 (395) 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:I:119:GLN:HB2	1:I:120:LEU:HG	1.33	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:150:TYR:OH	4:M:201:TYR:OH	1.73	1.06
1:I:425:GLN:HA	1:I:425:GLN:HE21	1.22	1.00
1:A:464:THR:HG22	1:A:466:GLU:H	1.30	0.93
1:I:464:THR:HG22	1:I:466:GLU:H	1.33	0.92
1:I:360:LEU:HA	1:I:425:GLN:OE1	1.74	0.85
1:A:360:LEU:HA	1:A:425:GLN:NE2	1.92	0.85
3:L:24:ALA:HB1	3:L:229:LEU:HD21	1.59	0.84
1:A:73:VAL:HG11	1:A:78:LEU:HD12	1.65	0.78
1:I:426:ASP:O	1:I:428:GLY:N	2.15	0.77
1:I:418:VAL:HG22	1:I:461:HIS:HB2	1.66	0.77
1:A:360:LEU:HA	1:A:425:GLN:HE21	1.52	0.73
3:L:86:GLY:H	3:L:89:SER:HB3	1.52	0.73
1:A:68:ARG:HG2	1:A:92:GLU:HG2	1.71	0.71
1:I:73:VAL:HG11	1:I:78:LEU:HD12	1.72	0.71
1:I:119:GLN:CG	1:I:120:LEU:H	2.01	0.71
1:I:506:ARG:HD2	1:I:516:ASP:OD1	1.91	0.70
1:I:506:ARG:HD3	1:I:513:LEU:HG	1.74	0.70
3:D:86:GLY:H	3:D:89:SER:HB3	1.56	0.70
1:A:346:LEU:HD21	1:I:135:ILE:HG12	1.73	0.70
3:L:137:GLN:HE21	4:M:119:VAL:HG11	1.54	0.70
1:I:119:GLN:HG3	1:I:120:LEU:H	1.56	0.69
4:M:120:ASP:OD2	4:M:124:ARG:NH1	2.25	0.68
1:I:119:GLN:HB2	1:I:120:LEU:CG	2.18	0.68
4:M:205:GLY:HA3	4:M:251:ALA:HB2	1.76	0.68
1:I:157:ALA:HB2	1:I:190:VAL:HG11	1.75	0.68
1:A:135:ILE:HG12	1:I:346:LEU:HD21	1.73	0.68
6:D:301:COA:H31	4:E:168:MET:HE3	1.75	0.67
1:I:425:GLN:HA	1:I:425:GLN:NE2	2.04	0.67
6:D:301:COA:H31	4:E:168:MET:CE	2.24	0.67
1:A:246:ARG:HD3	1:A:517:LEU:O	1.95	0.67
1:A:349:GLN:HE22	1:I:349:GLN:HE22	1.42	0.67
3:L:33:GLU:HG2	3:L:36:ASP:HB3	1.76	0.67
3:D:24:ALA:HB1	3:D:229:LEU:HD21	1.77	0.67
1:A:506:ARG:HD3	1:A:513:LEU:HG	1.77	0.66
1:I:119:GLN:HE22	1:I:126:LEU:HD13	1.60	0.66
1:A:506:ARG:HD2	1:A:516:ASP:OD1	1.96	0.65
1:I:121:LEU:HD21	1:I:445:THR:HG23	1.77	0.65
1:A:418:VAL:HG22	1:A:461:HIS:HB2	1.78	0.65
1:I:419:GLN:NE2	1:I:454:ILE:HD12	2.13	0.64
1:I:34:LEU:HB2	1:I:214:VAL:HG22	1.79	0.64
1:A:445:THR:HB	1:A:447:MET:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:ARG:HG2	1:I:92:GLU:HG2	1.79	0.64
1:A:121:LEU:HD21	1:A:445:THR:HG23	1.79	0.63
1:I:116:ARG:O	1:I:119:GLN:N	2.31	0.62
1:A:298:ILE:HD11	1:A:318:MET:HE3	1.82	0.62
1:A:243:MET:HE1	1:A:467:GLY:HA2	1.80	0.62
6:L:301:COA:OAP	6:L:301:COA:H8A	1.99	0.62
1:A:347:ALA:HA	1:I:139:ALA:HB1	1.82	0.62
2:K:7:GLU:OE1	2:K:39:LYS:NZ	2.18	0.62
3:D:94:ALA:O	3:D:98:GLU:HG3	2.00	0.62
1:I:453:MET:HG2	1:I:454:ILE:HG13	1.80	0.61
1:A:188:VAL:HG13	1:A:213:VAL:HG12	1.81	0.61
2:K:41:SER:HB2	2:K:72:LEU:HD23	1.82	0.61
1:I:56:GLU:HG3	1:I:152:VAL:HG12	1.82	0.61
1:I:117:ILE:C	1:I:119:GLN:HG2	2.21	0.61
1:I:61:LYS:NZ	1:I:153:ALA:O	2.24	0.60
6:L:301:COA:H31	4:M:168:MET:HE3	1.83	0.60
1:A:56:GLU:HG3	1:A:152:VAL:HA	1.82	0.60
1:I:345:GLN:HE21	1:I:345:GLN:HA	1.67	0.60
1:I:419:GLN:HE22	1:I:454:ILE:HD12	1.67	0.60
3:L:94:ALA:O	3:L:98:GLU:HG3	2.02	0.60
1:I:120:LEU:HB3	1:I:125:LEU:HB2	1.83	0.60
3:D:134:ALA:HB2	4:E:150:TYR:HD2	1.67	0.59
1:I:117:ILE:CA	1:I:119:GLN:HG2	2.32	0.59
3:D:33:GLU:HG2	3:D:36:ASP:HB3	1.84	0.59
1:I:322:ILE:HG21	1:I:337:LEU:HB2	1.83	0.59
1:I:243:MET:HE1	1:I:514:PRO:HD3	1.83	0.59
1:I:73:VAL:O	1:I:75:PRO:HD3	2.02	0.59
2:K:88:ARG:HG2	2:K:88:ARG:HH11	1.67	0.59
3:D:131:ALA:HA	4:E:150:TYR:HE2	1.67	0.58
1:A:464:THR:HG22	1:A:466:GLU:N	2.12	0.58
1:I:171:ASP:OD1	1:I:341:ARG:HD2	2.03	0.58
1:A:426:ASP:O	1:A:428:GLY:N	2.34	0.58
1:I:464:THR:HG22	1:I:466:GLU:N	2.13	0.58
1:A:140:ARG:HE	1:A:144:ASP:HB2	1.66	0.58
1:A:243:MET:HE1	1:A:514:PRO:HD3	1.85	0.58
1:I:365:ASP:OD1	1:I:481:GLN:NE2	2.35	0.58
1:I:425:GLN:CA	1:I:425:GLN:HE21	2.05	0.58
1:A:425:GLN:OE1	1:A:425:GLN:HA	2.04	0.58
4:E:205:GLY:HA3	4:E:251:ALA:HB2	1.86	0.58
3:D:253:ALA:HA	4:E:69:TRP:CE3	2.39	0.57
1:I:508:GLU:HA	4:M:265:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:ARG:O	1:I:118:GLY:N	2.37	0.57
1:A:58:ASN:O	1:A:62:GLN:NE2	2.38	0.57
1:I:115:LEU:HD13	1:I:375:ARG:HG2	1.87	0.57
1:I:119:GLN:OE1	1:I:120:LEU:HD12	2.05	0.56
1:I:138:TYR:HA	1:I:141:LEU:HD12	1.86	0.56
3:L:119:GLY:O	6:L:301:COA:H62	2.05	0.56
1:I:58:ASN:O	1:I:62:GLN:NE2	2.39	0.56
1:I:243:MET:HE1	1:I:467:GLY:HA2	1.87	0.56
1:I:117:ILE:HA	1:I:119:GLN:HG2	1.88	0.56
1:I:188:VAL:HG13	1:I:213:VAL:HG12	1.87	0.56
1:I:57:GLY:HA2	1:I:62:GLN:OE1	2.06	0.56
4:M:213:VAL:HG23	4:M:216:VAL:HG22	1.86	0.56
3:D:36:ASP:HB2	3:D:37:PRO:HD2	1.87	0.56
1:I:119:GLN:NE2	1:I:126:LEU:HD13	2.21	0.56
1:I:116:ARG:O	1:I:119:GLN:HG2	2.07	0.55
4:E:126:ARG:HD3	4:E:151:GLN:O	2.07	0.55
1:I:163:VAL:HG21	1:I:188:VAL:HG11	1.88	0.55
1:A:257:LEU:HA	1:A:352:VAL:HG13	1.89	0.55
4:E:145:PHE:CE2	4:E:150:TYR:CE1	2.95	0.55
1:I:445:THR:HB	1:I:447:MET:HG3	1.89	0.55
1:A:171:ASP:OD1	1:A:341:ARG:HD2	2.06	0.54
3:L:36:ASP:HB2	3:L:37:PRO:HD2	1.87	0.54
1:I:396:THR:HG22	1:I:399:TRP:H	1.71	0.54
1:A:477:LEU:O	1:A:481:GLN:HG3	2.06	0.54
1:I:318:MET:HA	1:I:318:MET:HE2	1.90	0.54
1:A:94:LEU:HD11	1:A:113:GLN:HB3	1.90	0.54
1:I:9:PRO:O	1:I:13:ARG:NH1	2.41	0.54
1:A:243:MET:CE	1:A:467:GLY:HA2	2.37	0.54
3:L:177:ARG:NH2	3:L:213:GLU:OE2	2.38	0.54
3:L:216:PHE:HA	3:L:221:ALA:HB3	1.90	0.53
4:M:206:LEU:HD23	4:M:248:ARG:HB3	1.90	0.53
1:A:56:GLU:HG3	1:A:152:VAL:HG12	1.89	0.53
1:A:157:ALA:HB2	1:A:190:VAL:HG11	1.91	0.53
1:A:34:LEU:HB2	1:A:214:VAL:HG22	1.89	0.53
1:A:90:ARG:HB2	1:A:93:HIS:CE1	2.44	0.53
4:E:90:ALA:HA	4:E:131:PRO:HD2	1.91	0.53
1:A:453:MET:HG2	1:A:454:ILE:HG13	1.91	0.53
1:A:464:THR:HG21	1:A:487:VAL:O	2.08	0.53
1:A:54:VAL:HG11	1:A:175:LEU:HB3	1.91	0.53
1:A:115:LEU:HD22	1:A:375:ARG:HH11	1.74	0.52
1:I:61:LYS:HD3	1:I:153:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:345:GLN:HE22	1:I:385:MET:HE1	1.73	0.52
4:M:14:GLN:HG3	4:M:20:LEU:HD22	1.91	0.52
1:I:477:LEU:O	1:I:481:GLN:HG3	2.09	0.52
1:I:534:ILE:O	1:I:538:VAL:HG23	2.09	0.52
3:D:54:GLN:HB2	3:D:80:PHE:CE2	2.44	0.52
1:I:8:PRO:HG2	1:I:11:TRP:HB2	1.90	0.52
1:I:464:THR:HG21	1:I:487:VAL:O	2.09	0.52
4:E:206:LEU:HD23	4:E:248:ARG:HB3	1.91	0.52
4:M:65:LEU:HD11	4:M:106:GLU:HA	1.92	0.52
1:I:95:ASP:O	1:I:99:LEU:HG	2.10	0.52
3:D:153:ILE:HG22	3:D:179:ALA:HB1	1.92	0.51
3:L:88:VAL:O	3:L:92:LYS:HG3	2.10	0.51
4:E:150:TYR:HH	4:E:201:TYR:HH	1.58	0.51
1:I:117:ILE:HG22	1:I:376:LEU:HB2	1.92	0.51
3:L:248:PRO:HG2	3:L:251:ARG:HG3	1.93	0.51
4:M:234:ALA:O	4:M:238:ILE:HG13	2.09	0.51
1:A:57:GLY:HA2	1:A:62:GLN:OE1	2.11	0.51
1:I:112:PRO:HG2	1:I:113:GLN:HG2	1.93	0.51
4:M:100:GLN:HE21	4:M:143:GLY:H	1.58	0.51
4:E:120:ASP:OD2	4:E:124:ARG:NH1	2.45	0.50
1:A:503:GLN:HE21	4:E:249:LEU:HD12	1.77	0.50
1:A:163:VAL:HG21	1:A:188:VAL:HG11	1.93	0.50
1:A:73:VAL:O	1:A:75:PRO:HD3	2.12	0.50
1:I:117:ILE:HA	1:I:119:GLN:CD	2.32	0.50
3:D:84:SER:HB3	3:D:122:ARG:CA	2.42	0.50
4:E:16:LEU:HB3	4:E:44:PHE:CE2	2.46	0.50
1:A:508:GLU:HA	4:E:265:ARG:HD2	1.93	0.50
4:E:213:VAL:HG23	4:E:216:VAL:HG22	1.93	0.50
4:E:234:ALA:O	4:E:238:ILE:HG13	2.12	0.50
1:I:426:ASP:HA	2:K:81:THR:CG2	2.42	0.50
4:M:13:PHE:CE2	4:M:31:ARG:HB3	2.47	0.50
1:A:419:GLN:HE22	1:A:454:ILE:HD12	1.77	0.50
1:A:490:ILE:HD11	2:C:82:PRO:HB3	1.92	0.50
3:D:84:SER:HB3	3:D:122:ARG:HA	1.94	0.50
1:I:119:GLN:NE2	1:I:126:LEU:HD22	2.26	0.50
1:I:90:ARG:HB2	1:I:93:HIS:CE1	2.46	0.49
2:C:67:THR:OG1	4:E:209:ARG:HG3	2.11	0.49
2:K:67:THR:OG1	4:M:209:ARG:HA	2.12	0.49
3:D:32:ARG:NH2	4:E:267:GLN:O	2.42	0.49
1:I:363:ASP:HB3	1:I:436:LEU:HD13	1.94	0.49
1:A:95:ASP:O	1:A:99:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:NH2	1:I:457:ASP:OD2	2.45	0.49
3:D:119:GLY:O	6:D:301:COA:H62	2.11	0.49
4:E:67:GLU:H	4:E:67:GLU:CD	2.15	0.49
1:I:134:TYR:O	1:I:137:LEU:N	2.44	0.49
2:C:58:LEU:HD11	2:C:86:ARG:HB2	1.94	0.49
1:A:396:THR:HG22	1:A:399:TRP:CB	2.42	0.49
1:I:324:GLN:O	1:I:325:ARG:HD2	2.12	0.49
6:L:301:COA:H31	4:M:168:MET:CE	2.42	0.49
1:A:298:ILE:HD11	1:A:318:MET:CE	2.42	0.49
1:A:400:LEU:O	1:A:403:ARG:HG3	2.13	0.49
4:E:174:ALA:HB1	4:E:179:ARG:O	2.13	0.49
1:I:345:GLN:NE2	1:I:385:MET:CE	2.76	0.49
4:M:145:PHE:CZ	4:M:150:TYR:CE1	3.00	0.49
4:M:72:ALA:O	4:M:76:ASP:HB2	2.12	0.49
1:A:353:ASP:OD1	1:A:396:THR:HG21	2.13	0.48
2:K:13:PRO:HA	2:K:70:ALA:HB3	1.95	0.48
4:M:115:LEU:O	4:M:119:VAL:HG23	2.12	0.48
4:E:177:THR:HG21	4:E:179:ARG:HD2	1.94	0.48
1:I:118:GLY:C	1:I:119:GLN:HG3	2.32	0.48
1:A:139:ALA:HB1	1:I:347:ALA:HA	1.96	0.48
4:E:179:ARG:HB3	4:E:183:GLU:HG3	1.94	0.48
1:I:157:ALA:CB	1:I:190:VAL:HG11	2.44	0.48
1:A:30:ASP:O	1:A:30:ASP:OD1	2.32	0.48
1:I:132:HIS:NE2	1:I:140:ARG:NH1	2.62	0.48
1:A:225:LEU:O	1:A:261:ILE:HD11	2.14	0.48
1:A:396:THR:HG22	1:A:399:TRP:HB2	1.96	0.48
1:A:508:GLU:HG2	4:E:265:ARG:NE	2.29	0.48
1:A:74:ASP:HB3	1:A:77:LYS:HG3	1.96	0.48
1:I:115:LEU:HD22	1:I:375:ARG:HH11	1.79	0.48
3:L:73:LEU:HD12	3:L:113:LEU:HD23	1.95	0.48
4:E:188:ALA:O	4:E:195:ALA:HB2	2.14	0.47
1:I:303:SER:HB3	1:I:305:TRP:HD1	1.79	0.47
1:I:534:ILE:HG13	1:I:551:PHE:HB3	1.96	0.47
3:L:84:SER:HB3	3:L:122:ARG:HA	1.97	0.47
1:A:445:THR:O	1:A:445:THR:HG22	2.14	0.47
1:A:362:VAL:HA	1:A:367:HIS:O	2.14	0.47
3:L:127:ASN:ND2	4:M:165:VAL:O	2.37	0.47
4:E:100:GLN:H	4:E:100:GLN:HG3	1.16	0.47
4:E:53:ASN:ND2	4:E:67:GLU:OE2	2.47	0.47
1:I:271:ILE:HD12	1:I:275:TYR:HB3	1.95	0.47
1:I:257:LEU:HA	1:I:352:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:13:PRO:HD3	2:K:37:PRO:HB3	1.95	0.47
1:A:349:GLN:NE2	1:I:349:GLN:HE22	2.10	0.47
1:A:395:SER:OG	1:A:400:LEU:HD11	2.15	0.47
1:I:508:GLU:HG2	4:M:265:ARG:NE	2.30	0.47
4:M:44:PHE:HD2	4:M:94:ILE:HD11	1.79	0.47
4:E:63:VAL:HG12	4:E:115:LEU:HD11	1.96	0.47
1:I:550:ARG:HE	1:I:550:ARG:HB2	1.36	0.47
4:M:80:GLU:HA	4:M:83:ARG:HB2	1.95	0.47
3:D:128:LEU:HD21	4:E:254:ARG:HG2	1.97	0.47
1:I:56:GLU:HG3	1:I:152:VAL:HA	1.97	0.47
1:I:44:GLU:HG2	1:I:73:VAL:HG13	1.95	0.47
4:E:140:ALA:HB1	4:E:145:PHE:CD2	2.49	0.47
2:C:12:GLN:NE2	4:E:212:PRO:HB3	2.30	0.47
4:E:160:ASP:CG	4:E:216:VAL:HG21	2.35	0.47
1:A:94:LEU:HD21	1:A:117:ILE:HG12	1.97	0.46
2:C:1:MET:HG2	2:C:2:GLU:N	2.30	0.46
1:I:54:VAL:HG11	1:I:175:LEU:HB3	1.96	0.46
4:M:126:ARG:HB2	4:M:132:LEU:HD13	1.97	0.46
1:A:291:LEU:HD11	1:A:294:HIS:CE1	2.51	0.46
1:A:368:SER:CB	1:A:419:GLN:HE21	2.29	0.46
2:K:88:ARG:NH1	2:K:88:ARG:HG2	2.30	0.46
1:A:318:MET:HA	1:A:318:MET:HE2	1.98	0.46
4:E:198:ILE:HD11	4:E:207:LEU:HD11	1.98	0.46
1:I:400:LEU:O	1:I:403:ARG:HG3	2.15	0.46
1:A:229:ASP:HA	1:A:534:ILE:HD11	1.98	0.46
3:D:216:PHE:HA	3:D:221:ALA:HB3	1.97	0.46
4:E:57:ARG:HB2	4:E:106:GLU:OE1	2.14	0.46
3:L:251:ARG:HE	3:L:251:ARG:HB3	1.53	0.46
1:A:61:LYS:HD3	1:A:153:ALA:HB3	1.98	0.46
4:E:213:VAL:CG2	4:E:216:VAL:HG22	2.45	0.46
3:D:84:SER:HB3	3:D:122:ARG:CB	2.46	0.46
3:L:263:LEU:HD12	3:L:264:ASP:N	2.31	0.46
1:I:29:ALA:HB2	1:I:34:LEU:HD23	1.98	0.46
1:A:230:PRO:HD2	1:A:534:ILE:HD13	1.97	0.46
3:L:128:LEU:HD23	3:L:128:LEU:HA	1.71	0.46
1:A:293:PRO:HG2	1:A:315:GLU:H	1.81	0.45
1:A:405:GLU:HA	1:A:406:PRO:HD2	1.81	0.45
1:I:140:ARG:HE	1:I:144:ASP:HB2	1.82	0.45
3:L:84:SER:HB3	3:L:122:ARG:CA	2.46	0.45
3:L:216:PHE:CG	3:L:224:TYR:HB2	2.52	0.45
1:A:289:TRP:CD1	1:A:306:VAL:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:MET:HG2	2:K:2:GLU:N	2.30	0.45
1:A:140:ARG:HE	1:A:144:ASP:CB	2.29	0.45
1:A:349:GLN:HE22	1:I:349:GLN:NE2	2.12	0.45
1:A:362:VAL:O	1:A:432:PHE:HA	2.16	0.45
3:L:203:ARG:N	3:L:204:PRO:HD2	2.32	0.45
4:M:23:ARG:HB2	4:M:26:ASP:OD2	2.17	0.45
1:A:84:ILE:HG23	1:A:137:LEU:HD11	1.99	0.45
1:I:395:SER:OG	1:I:400:LEU:HD11	2.16	0.45
2:C:4:LEU:HD13	2:C:52:ALA:HA	1.97	0.45
1:I:64:ASP:OD2	1:I:68:ARG:NH1	2.50	0.45
2:C:86:ARG:O	2:C:90:GLU:HG3	2.17	0.45
1:I:21:ARG:HD3	1:I:46:LEU:O	2.17	0.45
1:I:345:GLN:NE2	1:I:385:MET:HE2	2.30	0.45
2:K:67:THR:OG1	4:M:209:ARG:HG3	2.16	0.45
1:A:312:PHE:CD1	1:A:344:CYS:HB3	2.51	0.45
2:K:4:LEU:HD13	2:K:52:ALA:HA	1.99	0.45
4:M:177:THR:O	4:M:178:LEU:HB2	2.16	0.45
1:A:534:ILE:HG13	1:A:551:PHE:HB3	1.98	0.45
1:I:312:PHE:CD1	1:I:344:CYS:HB3	2.52	0.45
1:A:65:PHE:CD2	1:A:216:ALA:HA	2.52	0.45
1:A:424:PHE:CE1	2:C:82:PRO:HG2	2.51	0.45
4:E:177:THR:O	4:E:178:LEU:HB2	2.17	0.44
1:I:28:LEU:HD12	1:I:28:LEU:O	2.17	0.44
1:A:324:GLN:O	1:A:325:ARG:HD2	2.17	0.44
4:M:145:PHE:CE2	4:M:150:TYR:CE1	3.05	0.44
4:M:46:ALA:HB2	4:M:94:ILE:HB	2.00	0.44
3:D:128:LEU:HA	3:D:128:LEU:HD23	1.73	0.44
1:I:119:GLN:HG3	1:I:120:LEU:N	2.30	0.44
1:I:119:GLN:HE22	1:I:126:LEU:HD22	1.82	0.44
1:I:162:ASN:HB3	1:I:203:VAL:HG13	1.98	0.44
2:K:16:GLY:O	2:K:34:PRO:HD3	2.18	0.44
1:A:8:PRO:HG2	1:A:11:TRP:HB2	2.00	0.44
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.82	0.44
1:A:463:LEU:HD13	1:A:468:ILE:HG12	1.98	0.44
1:A:507:ARG:HH12	4:E:265:ARG:HH21	1.66	0.44
1:I:362:VAL:HA	1:I:367:HIS:O	2.17	0.44
4:M:67:GLU:H	4:M:67:GLU:CD	2.20	0.44
1:A:196:ASP:HA	1:A:197:PRO:HD2	1.89	0.44
1:A:363:ASP:HB3	1:A:436:LEU:HD13	1.99	0.44
1:I:548:PRO:HG2	1:I:551:PHE:HD2	1.83	0.44
3:L:255:ASP:O	3:L:258:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:100:GLN:HG3	4:M:100:GLN:H	1.34	0.44
3:L:253:ALA:HA	4:M:69:TRP:CE3	2.53	0.44
1:A:24:ARG:HH21	1:A:45:ALA:HA	1.83	0.44
4:E:264:LEU:HA	4:E:264:LEU:HD23	1.88	0.44
1:A:390:ARG:NH1	1:A:412:ARG:HH22	2.15	0.43
1:A:142:VAL:HG12	1:A:178:PRO:HB3	1.98	0.43
1:I:121:LEU:HA	1:I:126:LEU:O	2.18	0.43
1:I:117:ILE:HA	1:I:119:GLN:CG	2.49	0.43
1:I:65:PHE:CD2	1:I:216:ALA:HA	2.53	0.43
4:M:90:ALA:HA	4:M:131:PRO:HD2	2.00	0.43
3:D:131:ALA:HA	4:E:150:TYR:CE2	2.49	0.43
1:I:85:MET:O	1:I:107:PHE:HA	2.18	0.43
1:I:119:GLN:CB	1:I:120:LEU:HG	2.24	0.43
1:A:247:GLY:O	1:A:470:TYR:OH	2.27	0.43
3:D:263:LEU:HD22	3:D:277:LEU:HD22	2.01	0.43
4:M:138:GLY:O	4:M:163:VAL:HA	2.19	0.43
4:E:145:PHE:CZ	4:E:150:TYR:CD1	3.07	0.43
1:I:405:GLU:HA	1:I:406:PRO:HD2	1.82	0.43
1:I:390:ARG:HD2	1:I:412:ARG:NH2	2.34	0.43
3:L:150:VAL:HG13	3:L:174:LEU:HD13	2.00	0.43
1:A:256:SER:O	1:A:353:ASP:HB2	2.18	0.43
4:E:23:ARG:HB2	4:E:26:ASP:OD2	2.19	0.43
3:L:44:PRO:HG2	3:L:45:TRP:CD1	2.54	0.43
4:M:174:ALA:HB1	4:M:179:ARG:O	2.19	0.43
1:A:227:THR:O	1:A:228:ARG:HD3	2.19	0.43
4:E:126:ARG:HG2	4:E:126:ARG:HH11	1.84	0.43
4:E:184:LEU:O	4:E:188:ALA:N	2.50	0.43
1:I:110:SER:OG	1:I:117:ILE:HD12	2.19	0.43
1:I:202:ARG:HG2	1:I:203:VAL:N	2.34	0.43
1:I:243:MET:CE	1:I:467:GLY:HA2	2.49	0.43
1:I:98:GLU:HA	1:I:125:LEU:HD13	2.00	0.43
3:L:268:GLN:HA	3:L:269:PRO:HD2	1.95	0.43
2:C:28:LEU:HD12	2:C:75:ILE:HG23	2.00	0.42
1:A:402:MET:HE2	1:A:416:LEU:HG	2.00	0.42
1:I:117:ILE:HG21	1:I:117:ILE:HD13	1.84	0.42
1:I:94:LEU:HD11	1:I:117:ILE:HG13	2.00	0.42
1:A:191:ASN:OD1	1:A:219:PRO:HA	2.18	0.42
1:A:312:PHE:HB3	1:A:341:ARG:NE	2.34	0.42
6:D:301:COA:H4B	6:D:301:COA:O9A	2.20	0.42
4:E:16:LEU:O	4:E:228:ARG:NH2	2.53	0.42
1:I:345:GLN:HE22	1:I:385:MET:CE	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:84:SER:HB3	3:D:122:ARG:HB2	2.00	0.42
1:I:112:PRO:C	1:I:114:SER:H	2.22	0.42
1:I:142:VAL:HG12	1:I:178:PRO:HB3	2.01	0.42
2:C:40:LEU:HD12	2:C:71:LEU:H	1.84	0.42
1:I:303:SER:HB3	1:I:305:TRP:CD1	2.55	0.42
1:I:379:PHE:HB3	1:I:383:PRO:CG	2.49	0.42
1:I:70:LEU:HD22	1:I:73:VAL:HG21	1.99	0.42
1:A:169:THR:HB	1:A:339:SER:O	2.20	0.42
1:A:345:GLN:NE2	1:A:384:ASN:HD22	2.17	0.42
1:I:36:ARG:HD3	1:I:215:GLU:O	2.19	0.42
1:A:29:ALA:HB2	1:A:34:LEU:HD23	2.01	0.42
3:D:247:ARG:HA	3:D:248:PRO:HD2	1.70	0.42
1:I:256:SER:O	1:I:353:ASP:HB2	2.19	0.42
1:I:362:VAL:O	1:I:432:PHE:HA	2.20	0.42
1:I:52:ARG:HA	1:I:82:HIS:HB3	2.02	0.42
1:I:34:LEU:HA	1:I:35:PRO:HD3	1.85	0.42
4:M:16:LEU:HB3	4:M:44:PHE:CE2	2.55	0.42
1:A:287:ARG:HD2	1:A:307:GLU:OE2	2.20	0.42
3:D:144:GLN:OE1	3:D:170:CYS:HA	2.20	0.42
6:D:301:COA:H31	4:E:168:MET:HE1	2.00	0.42
1:I:291:LEU:HD11	1:I:294:HIS:CE1	2.55	0.41
1:A:425:GLN:HG2	1:A:431:THR:OG1	2.20	0.41
1:I:273:PRO:HG2	1:I:530:ALA:HB2	2.02	0.41
1:I:64:ASP:O	1:I:68:ARG:HG3	2.20	0.41
1:I:89:GLY:O	1:I:113:GLN:HG3	2.19	0.41
4:M:56:PRO:C	4:M:58:ALA:H	2.23	0.41
1:A:61:LYS:NZ	1:A:153:ALA:O	2.48	0.41
1:A:365:ASP:OD1	1:A:481:GLN:NE2	2.50	0.41
3:L:263:LEU:HD22	3:L:277:LEU:HD22	2.01	0.41
1:I:120:LEU:O	1:I:125:LEU:N	2.40	0.41
1:I:379:PHE:HB3	1:I:383:PRO:HG2	2.02	0.41
4:E:126:ARG:HB2	4:E:132:LEU:HD13	2.03	0.41
1:I:98:GLU:HG3	1:I:120:LEU:CD2	2.50	0.41
4:M:36:GLU:OE1	4:M:39:GLY:HA2	2.19	0.41
1:I:68:ARG:NH2	1:I:217:ASP:OD1	2.54	0.41
1:I:534:ILE:HD13	1:I:534:ILE:HA	1.94	0.41
3:L:171:SER:HB3	3:L:245:PRO:HD3	2.02	0.41
3:D:171:SER:HB3	3:D:245:PRO:HD3	2.02	0.41
1:I:503:GLN:NE2	4:M:249:LEU:HD12	2.35	0.41
4:M:264:LEU:HA	4:M:264:LEU:HD23	1.75	0.41
3:L:127:ASN:OD1	4:M:165:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:99:LEU:HD23	3:D:99:LEU:HA	1.80	0.41
6:L:301:COA:H4B	6:L:301:COA:O9A	2.21	0.41
1:A:225:LEU:HA	1:A:225:LEU:HD12	1.84	0.41
1:A:396:THR:HG22	1:A:399:TRP:H	1.86	0.41
1:I:121:LEU:HD21	1:I:445:THR:CG2	2.46	0.41
1:I:298:ILE:HD11	1:I:318:MET:HE3	2.03	0.41
1:A:241:ALA:HA	1:A:268:ILE:HG12	2.02	0.41
3:D:258:ARG:HG3	3:D:258:ARG:HH11	1.86	0.41
1:I:293:PRO:HG2	1:I:315:GLU:H	1.86	0.41
3:L:153:ILE:HG22	3:L:179:ALA:HB1	2.03	0.41
3:L:277:LEU:O	3:L:278:TYR:HD2	2.04	0.41
4:M:28:ALA:HB3	4:M:50:ASP:CG	2.41	0.41
2:K:58:LEU:HD11	2:K:86:ARG:HB2	2.02	0.40
6:D:301:COA:OAP	6:D:301:COA:H8A	2.22	0.40
1:I:298:ILE:HD11	1:I:318:MET:CE	2.51	0.40
2:K:14:GLY:O	2:K:34:PRO:HB3	2.22	0.40
4:M:100:GLN:NE2	4:M:143:GLY:H	2.19	0.40
4:E:177:THR:CG2	4:E:179:ARG:HD2	2.50	0.40
2:K:6:PHE:HB2	2:K:42:ILE:HB	2.03	0.40
3:L:189:ILE:HD11	4:M:107:GLU:HG3	2.04	0.40
4:M:15:ALA:O	4:M:224:LEU:HD11	2.21	0.40
3:D:122:ARG:NH1	3:D:125:GLU:OE2	2.54	0.40
3:D:63:ARG:NH1	4:E:268:TRP:O	2.55	0.40
4:E:180:SER:OG	4:E:183:GLU:HG2	2.21	0.40
1:I:111:GLY:HA3	1:I:112:PRO:HD2	1.87	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)
1:A:526:ARG:NH1	3:L:15:GLU:OE2[2_556]	2.17	0.03
3:D:15:GLU:OE2	1:I:526:ARG:NH1[2_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	546/554 (99%)	507 (93%)	34 (6%)	5 (1%)	17 55
1	I	546/554 (99%)	503 (92%)	37 (7%)	6 (1%)	14 50
2	C	95/99 (96%)	92 (97%)	3 (3%)	0	100 100
2	K	95/99 (96%)	92 (97%)	3 (3%)	0	100 100
3	D	274/287 (96%)	260 (95%)	13 (5%)	1 (0%)	34 72
3	L	274/287 (96%)	260 (95%)	12 (4%)	2 (1%)	22 60
4	E	261/284 (92%)	234 (90%)	25 (10%)	2 (1%)	19 57
4	M	261/284 (92%)	234 (90%)	24 (9%)	3 (1%)	14 50
All	All	2352/2448 (96%)	2182 (93%)	151 (6%)	19 (1%)	19 57

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	117	ILE
1	I	373	ARG
1	I	427	GLY
1	A	113	GLN
1	A	373	ARG
1	A	427	GLY
3	D	126	ALA
3	L	126	ALA
4	M	178	LEU
4	E	142	SER
4	E	178	LEU
1	I	119	GLN
4	M	142	SER
1	A	134	TYR
1	A	143	VAL
1	I	134	TYR
4	M	57	ARG
1	I	143	VAL
3	L	156	PRO

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/457 (99%)	441 (98%)	10 (2%)	52	81
1	I	451/457 (99%)	442 (98%)	9 (2%)	55	83
2	C	78/80 (98%)	74 (95%)	4 (5%)	24	60
2	K	78/80 (98%)	77 (99%)	1 (1%)	69	89
3	D	202/209 (97%)	200 (99%)	2 (1%)	76	91
3	L	202/209 (97%)	198 (98%)	4 (2%)	55	83
4	E	189/209 (90%)	184 (97%)	5 (3%)	46	78
4	M	189/209 (90%)	184 (97%)	5 (3%)	46	78
All	All	1840/1910 (96%)	1800 (98%)	40 (2%)	52	81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	146	ILE
1	A	171	ASP
1	A	228	ARG
1	A	396	THR
1	A	405	GLU
1	A	419	GLN
1	A	434	GLU
1	A	500	ARG
1	A	515	GLU
2	C	15	ARG
2	C	31	LEU
2	C	43	GLN
2	C	66	GLN
3	D	19	ARG
3	D	254	GLU
4	E	20	LEU
4	E	82	ASP
4	E	100	GLN
4	E	150	TYR
4	E	244	ASP
1	I	93	HIS
1	I	146	ILE

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Mol	Chain	Res	Type
1	I	159	ARG
1	I	343	PHE
1	I	345	GLN
1	I	396	THR
1	I	407	GLU
1	I	419	GLN
1	I	425	GLN
2	K	31	LEU
3	L	174	LEU
3	L	201	ARG
3	L	254	GLU
3	L	267	GLU
4	M	82	ASP
4	M	100	GLN
4	M	150	TYR
4	M	170	LYS
4	M	244	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	345	GLN
1	A	387	HIS
1	A	419	GLN
2	C	91	GLN
3	D	184	ASN
1	I	93	HIS
1	I	345	GLN
1	I	349	GLN
1	I	387	HIS
1	I	419	GLN
1	I	425	GLN
3	L	106	ASN
3	L	137	GLN
3	L	184	ASN
4	M	100	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	COA	D	301	-	41,50,50	0.84	1 (2%)	52,75,75	1.07	3 (5%)
6	COA	L	301	-	41,50,50	0.84	1 (2%)	52,75,75	1.07	3 (5%)

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
6	COA	D	301	-	-	13/44/64/64	0/3/3/3
6	COA	L	301	-	-	9/44/64/64	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	COA	O4B-C1B	2.14	1.44	1.41
6	L	301	COA	O4B-C1B	2.11	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	301	COA	N3A-C2A-N1A	-4.42	121.77	128.68
6	D	301	COA	N3A-C2A-N1A	-4.40	121.80	128.68
6	D	301	COA	P2A-O3A-P1A	-3.31	121.48	132.83
6	L	301	COA	P2A-O3A-P1A	-3.30	121.50	132.83
6	D	301	COA	O4B-C1B-C2B	-2.95	102.62	106.93
6	L	301	COA	O4B-C1B-C2B	-2.60	103.13	106.93

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	COA	C5B-O5B-P1A-O2A
6	D	301	COA	CAP-CBP-CCP-O6A
6	D	301	COA	N8P-C9P-CAP-OAP
6	L	301	COA	C5B-O5B-P1A-O2A
6	L	301	COA	S1P-C2P-C3P-N4P
6	D	301	COA	C4B-C3B-O3B-P3B
6	L	301	COA	C2B-C3B-O3B-P3B
6	L	301	COA	C4B-C3B-O3B-P3B
6	D	301	COA	C2B-C3B-O3B-P3B
6	D	301	COA	O5P-C5P-N4P-C3P
6	D	301	COA	C6P-C5P-N4P-C3P
6	D	301	COA	O9P-C9P-CAP-OAP
6	D	301	COA	CDP-CBP-CCP-O6A
6	D	301	COA	CEP-CBP-CCP-O6A
6	D	301	COA	S1P-C2P-C3P-N4P
6	L	301	COA	P1A-O3A-P2A-O6A
6	D	301	COA	C5B-O5B-P1A-O3A
6	L	301	COA	C5B-O5B-P1A-O3A
6	D	301	COA	C5B-O5B-P1A-O1A
6	L	301	COA	C5B-O5B-P1A-O1A
6	L	301	COA	C2P-C3P-N4P-C5P
6	L	301	COA	P2A-O3A-P1A-O1A

There are no ring outliers.

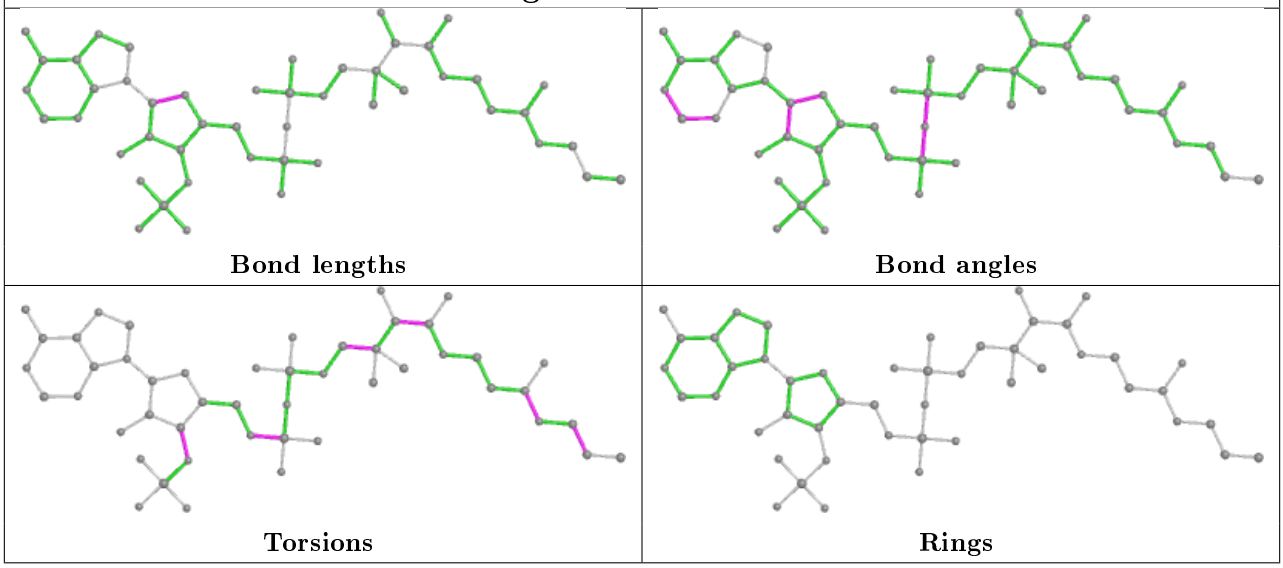
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	COA	6	0
6	L	301	COA	5	0

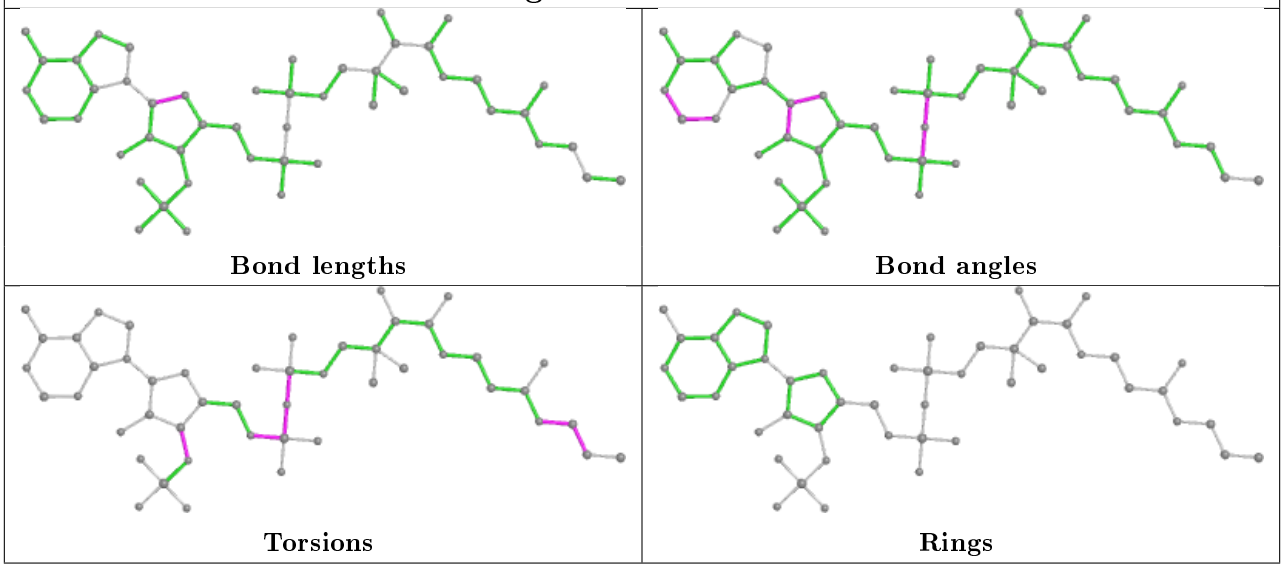
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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 D 301



Ligand COA L 301



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	548/554 (98%)	-0.03	6 (1%) 80 56	45, 60, 87, 104	0
1	I	548/554 (98%)	-0.02	5 (0%) 84 63	45, 61, 89, 103	0
2	C	97/99 (97%)	-0.17	1 (1%) 82 59	49, 60, 77, 103	0
2	K	97/99 (97%)	-0.15	0 100 100	45, 62, 75, 98	0
3	D	276/287 (96%)	-0.02	3 (1%) 80 56	47, 61, 83, 97	0
3	L	276/287 (96%)	-0.15	0 100 100	44, 60, 83, 96	0
4	E	263/284 (92%)	-0.19	1 (0%) 92 79	45, 67, 87, 103	0
4	M	263/284 (92%)	-0.11	2 (0%) 86 65	48, 66, 87, 107	0
All	All	2368/2448 (96%)	-0.08	18 (0%) 86 65	44, 62, 86, 107	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	19	SER	3.8
4	E	86	PRO	3.1
1	A	98	GLU	2.7
1	I	28	LEU	2.6
3	D	266	ALA	2.5
1	I	38	GLY	2.4
1	I	194	VAL	2.4
4	M	21	ALA	2.4
1	A	99	LEU	2.3
1	A	213	VAL	2.3
3	D	263	LEU	2.2
2	C	15	ARG	2.2
1	A	71	ALA	2.2
1	A	344	CYS	2.2
1	A	159	ARG	2.2
1	I	26	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	37	GLU	2.1
3	D	265	THR	2.1

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)

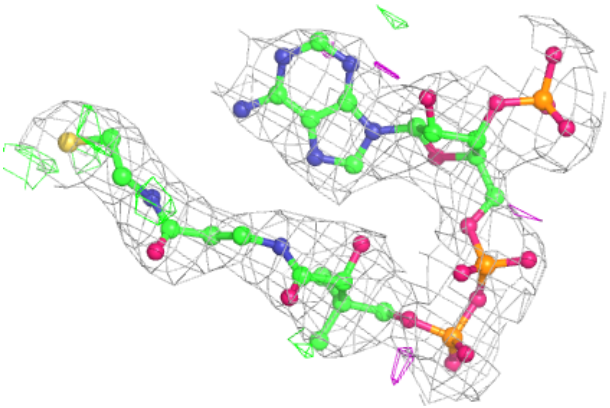
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

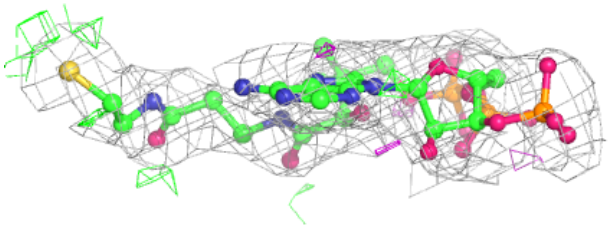
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	A	601	1/1	0.94	0.48	57,57,57,57	0
6	COA	D	301	48/48	0.94	0.22	53,64,80,82	0
6	COA	L	301	48/48	0.96	0.22	46,64,81,84	0

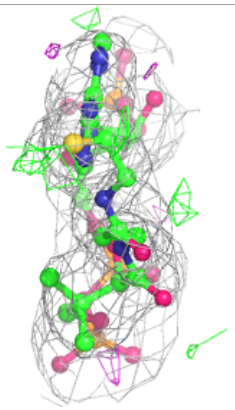
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 301:

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

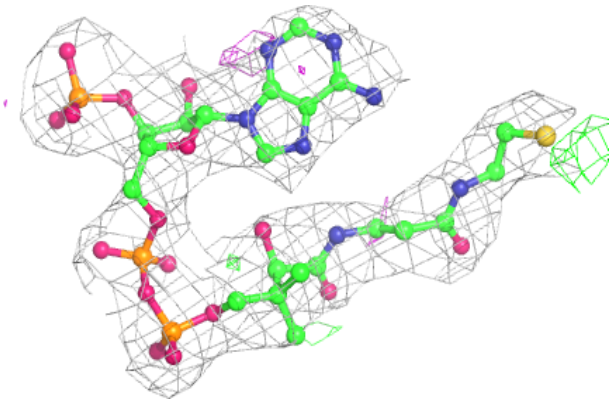


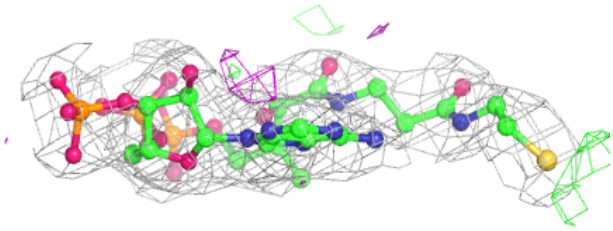


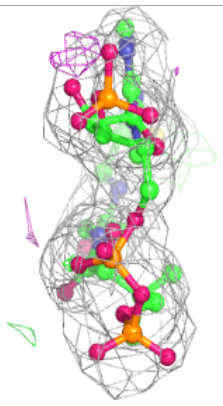


Electron density around COA L 301:

$2mF_o$-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.