Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 07:55 am BST

PDB ID	:	2ZW4
Title	:	Crystal structure of bleomycin N-acetyltransferase complexed with coenzyme A in the orthorhombic crystal
Authors	:	Oda, K.; Matoba, Y.; Sugiyama, M.
Deposited on	:	2008-12-01
Resolution	:	2.70 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:

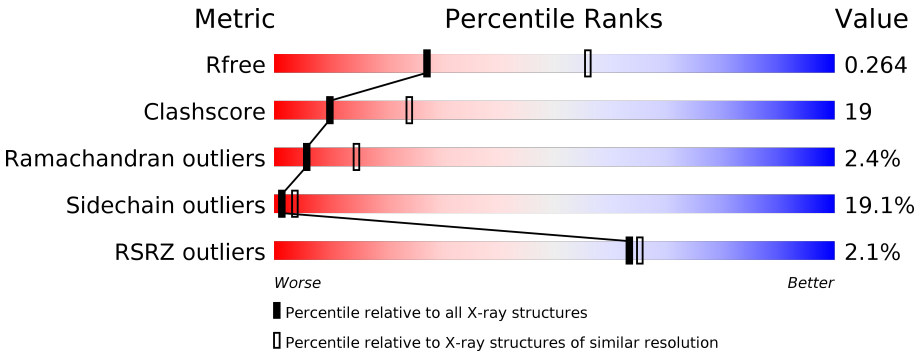
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	301	2% 60% 29% 8%
1	B	301	% 55% 34% 8%
1	C	301	2% 50% 41% 6%
1	D	301	2% 51% 39% 6%

2 Entry composition

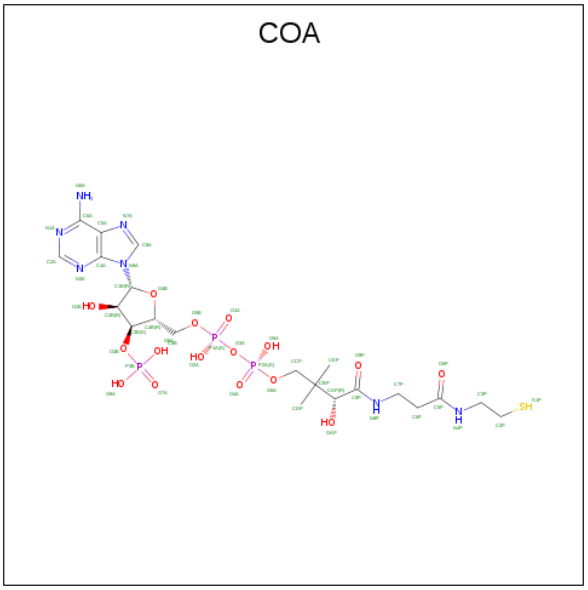
There are 4 unique types of molecules in this entry. The entry contains 9242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bleomycin acetyltransferase.

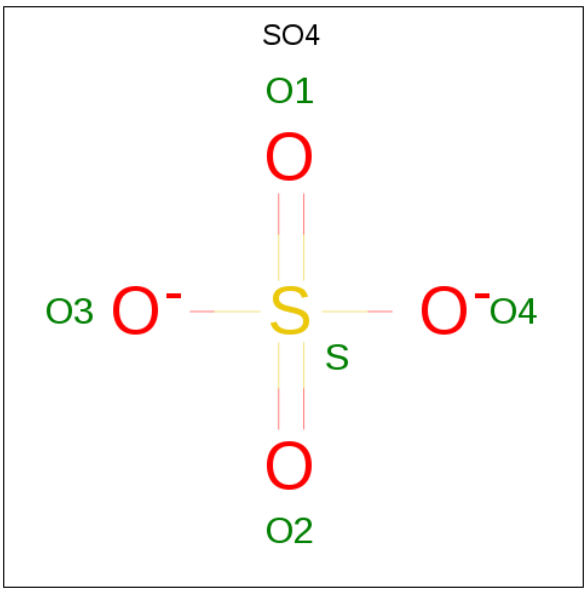
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	Se	0	0	0
			2219	1392	421	401	2	3			
1	B	294	Total	C	N	O	S	Se	0	0	0
			2219	1392	421	401	2	3			
1	C	293	Total	C	N	O	S	Se	0	0	0
			2209	1386	418	400	2	3			
1	D	293	Total	C	N	O	S	Se	0	0	0
			2209	1386	418	400	2	3			

- 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	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	61	Total O 61 61	0	0
4	B	40	Total O 40 40	0	0

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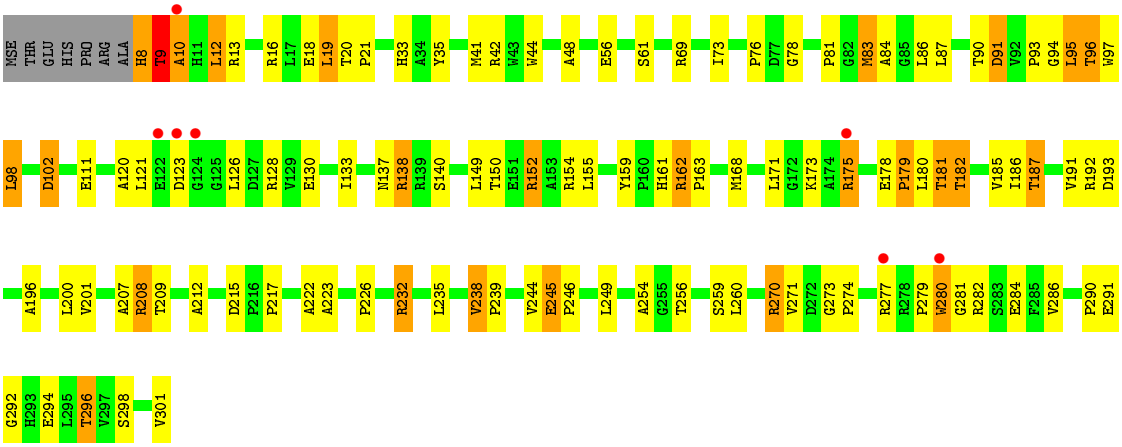
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	71	Total O 71 71	0	0
4	D	73	Total O 73 73	0	0

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.

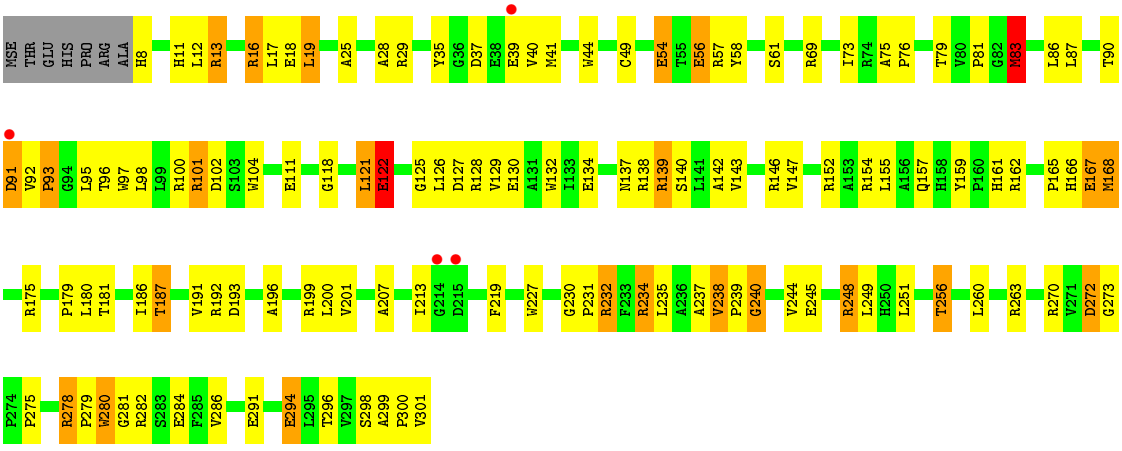
• Molecule 1: Bleomycin acetyltransferase

Chain A:



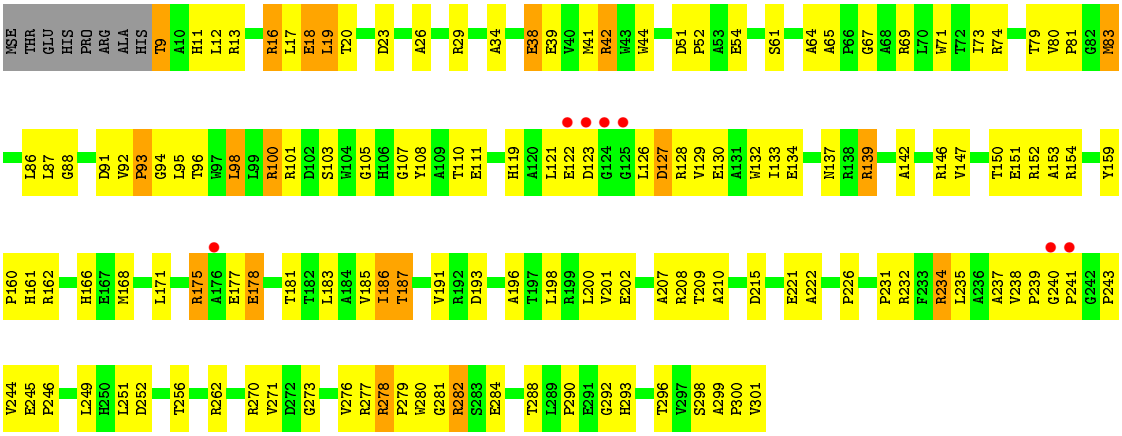
• Molecule 1: Bleomycin acetyltransferase

Chain B:



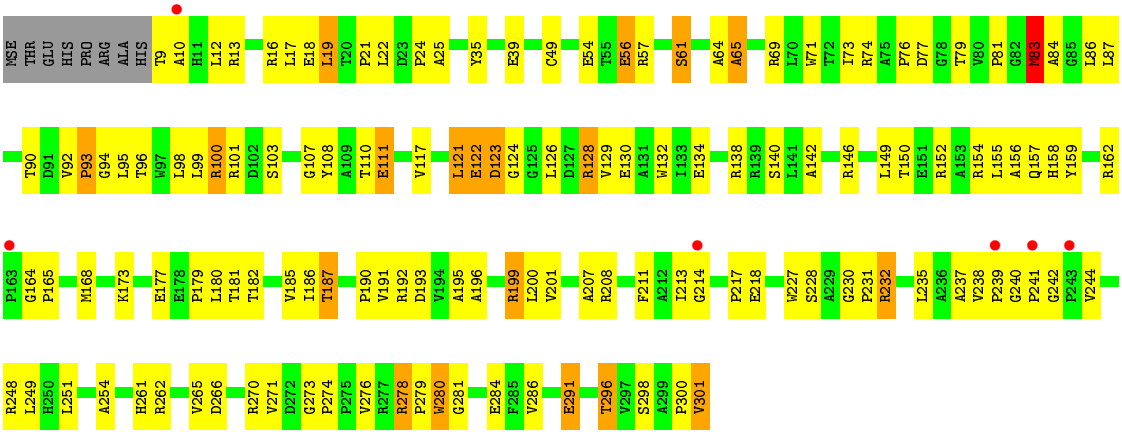
• Molecule 1: Bleomycin acetyltransferase

Chain C:



- Molecule 1: Bleomycin acetyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.22Å 96.33Å 181.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 41.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.70) 97.9 (41.17-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	5.56 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.191 , 0.257 0.198 , 0.264	Depositor DCC
R_{free} test set	1649 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9242	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.80% 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, SO4

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	0.34	0/2278	0.59	0/3116
1	B	0.33	0/2278	0.60	3/3116 (0.1%)
1	C	0.33	0/2267	0.61	0/3101
1	D	0.34	0/2267	0.59	1/3101 (0.0%)
All	All	0.33	0/9090	0.60	4/12434 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	273	GLY	N-CA-C	-5.99	98.12	113.10
1	D	83	MSE	CG-SE-CE	5.14	110.21	98.90
1	B	83	MSE	CG-SE-CE	5.14	110.20	98.90
1	B	168	MSE	CG-SE-CE	5.08	110.07	98.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2219	0	2185	79	0
1	B	2219	0	2185	100	0
1	C	2209	0	2178	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2209	0	2178	88	0
2	A	48	0	32	1	0
2	C	48	0	32	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	D	25	0	0	1	0
4	A	61	0	0	6	0
4	B	40	0	0	3	0
4	C	71	0	0	3	0
4	D	73	0	0	4	0
All	All	9242	0	8790	340	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (340) 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:A:162:ARG:HG3	1:A:163:PRO:HD2	1.49	0.94
1:D:132:TRP:HB3	1:D:168:MSE:HE2	1.49	0.92
1:D:49:CYS:HB3	1:D:54:GLU:HG2	1.55	0.88
1:B:79:THR:HG21	1:B:100:ARG:HH21	1.41	0.86
1:C:198:LEU:HD22	1:C:209:THR:HG22	1.58	0.85
1:B:284:GLU:HG2	1:B:298:SER:HB3	1.60	0.84
1:C:12:LEU:HB2	1:C:19:LEU:HB2	1.61	0.82
1:B:230:GLY:O	1:B:232:ARG:HD3	1.82	0.79
1:C:271:VAL:HG12	1:C:273:GLY:H	1.49	0.78
1:B:12:LEU:HB2	1:B:19:LEU:HB2	1.65	0.77
1:D:12:LEU:HB2	1:D:19:LEU:HB2	1.65	0.77
1:A:187:THR:HB	1:B:249:LEU:CD2	2.13	0.76
1:B:39:GLU:HG2	1:B:101:ARG:HE	1.51	0.75
1:B:201:VAL:HG12	1:B:207:ALA:HB3	1.67	0.74
1:A:201:VAL:HG12	1:A:207:ALA:HB3	1.68	0.74
1:D:230:GLY:O	1:D:232:ARG:HD2	1.88	0.73
1:C:210:ALA:HB3	1:C:221:GLU:HG2	1.71	0.73
1:A:83:MSE:HE2	1:A:98:LEU:HD23	1.71	0.73
1:B:272:ASP:HB2	1:B:286:VAL:H	1.53	0.72
1:D:95:LEU:HD21	1:D:117:VAL:CG2	2.19	0.72
1:A:249:LEU:CD2	1:B:187:THR:HB	2.19	0.71
1:D:201:VAL:HG12	1:D:207:ALA:HB3	1.72	0.71
1:B:79:THR:HG21	1:B:100:ARG:NH2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:HB3	4:A:555:HOH:O	1.91	0.70
1:C:249:LEU:CD2	1:D:187:THR:HB	2.21	0.70
1:C:201:VAL:HG12	1:C:207:ALA:HB3	1.73	0.70
1:B:238:VAL:HG22	1:B:239:PRO:HD2	1.74	0.70
1:A:187:THR:HB	1:B:249:LEU:HD23	1.73	0.70
1:B:118:GLY:O	1:B:122:GLU:HB2	1.91	0.69
1:A:191:VAL:O	1:A:238:VAL:HG12	1.92	0.69
1:B:90:THR:O	1:B:91:ASP:HB2	1.91	0.68
1:C:231:PRO:HG2	1:D:182:THR:O	1.94	0.68
1:B:93:PRO:HG3	1:B:126:LEU:HD22	1.74	0.68
1:C:83:MSE:HE2	1:C:98:LEU:HD23	1.76	0.67
1:C:150:THR:O	1:C:152:ARG:HD3	1.94	0.67
1:B:35:TYR:OH	1:B:83:MSE:HE2	1.94	0.67
1:B:286:VAL:HG11	1:B:294:GLU:HG2	1.76	0.66
1:D:71:TRP:O	1:D:83:MSE:HG2	1.95	0.66
1:B:132:TRP:HB3	1:B:168:MSE:HE2	1.78	0.66
1:D:95:LEU:HD21	1:D:117:VAL:HG22	1.76	0.66
1:A:245:GLU:HG3	1:B:245:GLU:HG3	1.76	0.66
1:C:100:ARG:HD3	1:C:103:SER:OG	1.96	0.65
1:A:280:TRP:HD1	1:A:282:ARG:HG3	1.60	0.65
1:C:151:GLU:HG2	4:D:584:HOH:O	1.96	0.65
1:B:180:LEU:N	1:B:180:LEU:HD23	2.12	0.65
1:A:83:MSE:HG2	1:A:84:ALA:N	2.11	0.65
1:A:149:LEU:HD23	1:A:173:LYS:HB2	1.79	0.64
1:D:49:CYS:CB	1:D:54:GLU:HG2	2.28	0.64
1:D:271:VAL:HG12	1:D:273:GLY:H	1.62	0.64
1:B:8:HIS:HB2	1:B:69:ARG:HD3	1.80	0.64
1:B:157:GLN:HG3	1:B:168:MSE:HG3	1.79	0.63
1:B:54:GLU:OE2	1:B:57:ARG:HD3	1.99	0.63
1:A:162:ARG:CG	1:A:163:PRO:HD2	2.26	0.63
1:D:261:HIS:O	1:D:265:VAL:HG23	1.99	0.63
1:A:179:PRO:O	1:A:181:THR:HG22	1.99	0.62
1:D:284:GLU:HG2	1:D:298:SER:HB2	1.80	0.62
1:B:213:ILE:HD12	1:B:219:PHE:HD2	1.65	0.62
1:D:16:ARG:HD3	1:D:111:GLU:OE1	2.00	0.62
1:C:175:ARG:HH11	1:C:175:ARG:HG3	1.65	0.62
1:C:87:LEU:HD12	1:C:95:LEU:N	2.14	0.62
1:A:90:THR:O	1:A:91:ASP:HB3	2.00	0.61
1:A:87:LEU:HD12	1:A:95:LEU:N	2.15	0.61
1:D:95:LEU:HB2	1:D:130:GLU:O	1.99	0.61
1:A:16:ARG:HD3	1:A:111:GLU:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:HIS:HB3	1:B:13:ARG:HH22	1.64	0.61
1:C:151:GLU:OE1	1:C:154:ARG:HD2	2.01	0.61
1:D:9:THR:HG22	1:D:21:PRO:HG3	1.83	0.60
1:A:286:VAL:HG22	1:A:296:THR:HB	1.83	0.60
1:C:187:THR:HB	1:D:249:LEU:CD2	2.31	0.60
1:C:202:GLU:OE1	1:C:209:THR:HG23	2.02	0.60
1:C:71:TRP:O	1:C:83:MSE:HG2	2.01	0.60
1:A:270:ARG:HH22	1:A:290:PRO:CG	2.15	0.60
1:D:35:TYR:OH	1:D:83:MSE:HE2	2.01	0.59
1:A:222:ALA:O	1:A:232:ARG:HB2	2.02	0.59
1:B:159:TYR:HB2	1:B:162:ARG:HG3	1.84	0.59
1:C:17:LEU:HD21	1:C:108:TYR:CD1	2.37	0.59
1:B:73:ILE:HG22	1:B:81:PRO:HG2	1.84	0.59
1:A:193:ASP:HB3	1:A:196:ALA:HB3	1.85	0.59
1:D:187:THR:HG21	1:D:249:LEU:HD21	1.83	0.59
1:B:25:ALA:HA	1:B:56:GLU:OE1	2.03	0.58
1:A:185:VAL:HG22	1:B:251:LEU:HD22	1.85	0.58
1:A:193:ASP:OD1	1:A:196:ALA:HB2	2.03	0.58
1:C:34:ALA:HB1	1:C:98:LEU:CD1	2.34	0.58
1:D:159:TYR:HB2	1:D:162:ARG:HG3	1.85	0.58
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.69	0.58
1:D:25:ALA:HA	1:D:56:GLU:OE1	2.03	0.58
1:D:9:THR:HG21	4:D:412:HOH:O	2.02	0.58
1:B:11:HIS:HB3	1:B:13:ARG:NH2	2.19	0.57
1:B:142:ALA:HB1	1:B:146:ARG:HH21	1.69	0.57
1:B:49:CYS:HB3	1:B:54:GLU:HB3	1.86	0.57
1:A:208:ARG:HE	1:A:226:PRO:HA	1.69	0.57
1:B:87:LEU:HD12	1:B:95:LEU:N	2.19	0.57
1:D:278:ARG:HD3	1:D:280:TRP:CZ2	2.40	0.57
1:C:147:VAL:O	1:C:147:VAL:HG12	2.05	0.57
1:D:284:GLU:HG2	1:D:298:SER:CB	2.34	0.57
1:C:93:PRO:HG2	1:C:128:ARG:O	2.04	0.57
1:C:119:HIS:ND1	1:C:123:ASP:HB2	2.20	0.56
1:C:198:LEU:O	1:C:202:GLU:HG3	2.04	0.56
1:D:193:ASP:HB3	1:D:196:ALA:HB3	1.86	0.56
1:A:8:HIS:CD2	1:A:9:THR:H	2.23	0.56
1:A:95:LEU:HB2	1:A:130:GLU:O	2.06	0.56
1:C:249:LEU:HD23	1:D:187:THR:HB	1.87	0.56
1:C:221:GLU:OE2	1:C:234:ARG:HD3	2.06	0.56
1:A:259:SER:HB3	1:B:180:LEU:HD11	1.87	0.56
1:B:187:THR:HG21	1:B:249:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:HB2	1:C:130:GLU:O	2.05	0.55
1:D:150:THR:O	1:D:152:ARG:HG2	2.06	0.55
1:B:238:VAL:HG22	1:B:239:PRO:CD	2.35	0.55
1:C:153:ALA:O	1:C:154:ARG:HG3	2.06	0.55
1:C:105:GLY:HA2	2:C:402:COA:H4B	1.87	0.55
1:B:132:TRP:CB	1:B:168:MSE:HE2	2.36	0.55
1:B:238:VAL:HG21	1:B:244:VAL:CG1	2.36	0.55
1:D:98:LEU:O	1:D:99:LEU:HD23	2.06	0.55
1:B:73:ILE:CG2	1:B:81:PRO:HG2	2.37	0.55
1:D:214:GLY:O	1:D:217:PRO:HA	2.07	0.55
1:A:201:VAL:HG12	1:A:207:ALA:CB	2.37	0.55
1:C:9:THR:N	4:C:583:HOH:O	2.41	0.54
1:A:150:THR:O	1:A:152:ARG:HD3	2.08	0.54
1:B:57:ARG:HG3	1:B:58:TYR:N	2.23	0.54
1:C:161:HIS:HD2	4:C:418:HOH:O	1.90	0.54
1:C:34:ALA:HB1	1:C:98:LEU:HD11	1.89	0.54
1:B:219:PHE:HZ	1:B:234:ARG:HD3	1.72	0.54
1:C:187:THR:HB	1:D:249:LEU:HD23	1.90	0.54
1:A:102:ASP:OD1	1:A:102:ASP:N	2.38	0.54
1:D:110:THR:OG1	1:D:146:ARG:NH1	2.40	0.54
1:A:150:THR:OG1	1:A:152:ARG:NH1	2.41	0.53
1:A:9:THR:O	1:A:21:PRO:HG3	2.08	0.53
1:A:8:HIS:N	1:A:8:HIS:CD2	2.76	0.53
1:A:86:LEU:HD23	1:A:94:GLY:O	2.09	0.53
1:B:281:GLY:C	1:B:282:ARG:HG2	2.29	0.53
1:D:179:PRO:HB2	1:D:180:LEU:HD22	1.90	0.53
1:D:54:GLU:HA	1:D:57:ARG:CZ	2.39	0.53
1:C:278:ARG:N	1:C:278:ARG:HD2	2.22	0.53
1:A:175:ARG:NH1	4:A:575:HOH:O	2.41	0.53
1:B:187:THR:HG21	1:B:249:LEU:CD2	2.39	0.53
1:A:18:GLU:HG3	4:A:652:HOH:O	2.09	0.52
1:A:271:VAL:HG12	1:A:273:GLY:H	1.74	0.52
1:B:121:LEU:O	1:B:175:ARG:CZ	2.58	0.52
1:C:191:VAL:O	1:C:237:ALA:HA	2.10	0.52
1:D:156:ALA:HB1	1:D:300:PRO:HG2	1.91	0.52
1:B:8:HIS:HB2	1:B:69:ARG:HH11	1.75	0.52
1:C:83:MSE:HE2	1:C:98:LEU:CD2	2.39	0.52
1:C:246:PRO:HB3	1:C:292:GLY:C	2.29	0.52
1:D:142:ALA:HB1	1:D:146:ARG:NH2	2.25	0.52
1:A:180:LEU:HB2	1:B:263:ARG:NH1	2.26	0.52
1:A:33:HIS:HD2	4:A:541:HOH:O	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ALA:HB1	1:B:300:PRO:HD2	1.92	0.51
1:C:139:ARG:NH1	1:C:139:ARG:HG3	2.25	0.51
1:A:223:ALA:HA	1:A:232:ARG:HB3	1.91	0.51
1:C:183:LEU:HD13	1:D:155:LEU:HA	1.92	0.51
1:D:100:ARG:HG3	1:D:103:SER:OG	2.10	0.51
1:D:165:PRO:HD3	1:D:301:VAL:HG21	1.92	0.51
1:C:132:TRP:HB3	1:C:168:MSE:HE3	1.93	0.51
1:B:17:LEU:HD12	1:B:111:GLU:HG2	1.91	0.51
1:A:133:ILE:HD12	1:A:171:LEU:HD13	1.92	0.51
1:A:254:ALA:HB3	1:B:181:THR:HG23	1.91	0.51
1:C:73:ILE:O	1:C:81:PRO:HD2	2.10	0.51
1:C:246:PRO:HA	1:C:293:HIS:ND1	2.26	0.50
1:C:23:ASP:OD1	1:C:26:ALA:HB3	2.10	0.50
1:B:95:LEU:HD23	1:B:97:TRP:HZ3	1.76	0.50
1:C:175:ARG:NH1	1:C:175:ARG:HG3	2.25	0.50
1:D:16:ARG:O	1:D:76:PRO:HG3	2.11	0.50
1:D:13:ARG:NH1	4:D:512:HOH:O	2.42	0.50
1:D:93:PRO:HB2	1:D:129:VAL:HA	1.93	0.50
1:C:73:ILE:CG2	1:C:81:PRO:HG2	2.41	0.50
1:B:69:ARG:NH2	4:B:610:HOH:O	2.44	0.50
1:D:208:ARG:NH2	1:D:227:TRP:O	2.45	0.50
1:C:271:VAL:HG12	1:C:273:GLY:N	2.24	0.49
1:A:249:LEU:HD23	1:B:187:THR:HB	1.94	0.49
1:A:120:ALA:O	1:A:126:LEU:HB2	2.12	0.49
1:A:35:TYR:CE1	1:A:98:LEU:HD21	2.47	0.49
1:B:159:TYR:HB3	1:B:161:HIS:CD2	2.47	0.49
1:B:219:PHE:CZ	1:B:234:ARG:HD3	2.47	0.49
1:C:281:GLY:O	1:C:282:ARG:HG2	2.12	0.49
1:A:178:GLU:H	1:A:178:GLU:CD	2.16	0.49
1:A:41:MSE:HG3	1:A:48:ALA:HA	1.95	0.49
1:A:83:MSE:HG2	1:A:84:ALA:H	1.78	0.49
1:C:110:THR:OG1	1:C:146:ARG:NH1	2.45	0.49
1:D:17:LEU:HD21	1:D:108:TYR:CD1	2.48	0.49
1:C:226:PRO:O	1:D:128:ARG:HD2	2.13	0.49
1:A:284:GLU:HG2	1:A:298:SER:HB3	1.95	0.49
1:D:191:VAL:O	1:D:237:ALA:HA	2.11	0.49
1:C:251:LEU:HD22	1:D:185:VAL:HG22	1.95	0.49
1:C:185:VAL:HG13	1:D:251:LEU:CD2	2.43	0.49
1:C:198:LEU:HD13	1:C:209:THR:CG2	2.43	0.49
1:B:278:ARG:HD3	1:B:280:TRP:CZ2	2.48	0.49
1:D:279:PRO:HG2	1:D:280:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ALA:HB1	1:C:300:PRO:HD2	1.95	0.48
1:A:246:PRO:HB3	1:A:292:GLY:C	2.34	0.48
1:B:284:GLU:HG2	1:B:298:SER:CB	2.36	0.48
1:D:81:PRO:O	1:D:100:ARG:HG2	2.13	0.48
1:B:278:ARG:HE	1:B:279:PRO:HD2	1.79	0.48
1:A:152:ARG:NH2	1:B:227:TRP:CZ2	2.82	0.48
1:B:279:PRO:C	1:B:281:GLY:H	2.17	0.47
1:C:222:ALA:O	1:C:232:ARG:HB2	2.14	0.47
1:B:193:ASP:OD2	1:B:196:ALA:HB2	2.14	0.47
1:C:284:GLU:OE1	1:C:298:SER:HB3	2.14	0.47
1:D:191:VAL:HG22	1:D:291:GLU:OE2	2.14	0.47
1:C:279:PRO:C	1:C:281:GLY:H	2.17	0.47
1:B:28:ALA:CB	1:B:56:GLU:HG3	2.45	0.47
1:C:210:ALA:CB	1:C:221:GLU:HG2	2.41	0.47
1:D:132:TRP:C	1:D:168:MSE:CE	2.83	0.47
1:A:182:THR:O	1:B:231:PRO:HG2	2.14	0.47
1:A:73:ILE:CG2	1:A:81:PRO:HG2	2.45	0.47
1:D:132:TRP:C	1:D:168:MSE:HE1	2.35	0.47
1:D:61:SER:O	1:D:64:ALA:HB3	2.14	0.47
1:D:73:ILE:CG2	1:D:81:PRO:HG2	2.45	0.47
1:B:132:TRP:N	1:B:132:TRP:CD1	2.83	0.47
1:B:134:GLU:HG3	1:B:166:HIS:CD2	2.49	0.47
1:C:208:ARG:HE	1:C:226:PRO:HA	1.79	0.47
1:A:155:LEU:CD1	1:A:168:MSE:HB2	2.46	0.46
1:A:12:LEU:HB2	1:A:19:LEU:HB2	1.96	0.46
1:A:16:ARG:O	1:A:76:PRO:HD3	2.16	0.46
1:B:191:VAL:O	1:B:237:ALA:HA	2.15	0.46
1:C:51:ASP:HB2	1:C:52:PRO:HD2	1.96	0.46
1:D:122:GLU:C	1:D:124:GLY:H	2.18	0.46
1:D:159:TYR:HB2	1:D:162:ARG:CG	2.45	0.46
1:B:191:VAL:HA	1:B:291:GLU:HG2	1.98	0.46
1:C:65:ALA:HB1	1:C:88:GLY:O	2.14	0.46
1:C:183:LEU:HD21	1:D:254:ALA:HB2	1.96	0.46
1:D:149:LEU:HD23	1:D:173:LYS:HB2	1.97	0.46
1:B:199:ARG:HD3	4:B:444:HOH:O	2.15	0.46
1:C:150:THR:O	1:C:152:ARG:CD	2.62	0.46
1:C:133:ILE:HD12	1:C:171:LEU:CD1	2.45	0.46
1:A:212:ALA:HB1	1:A:217:PRO:HB3	1.98	0.46
1:C:178:GLU:HG2	4:C:631:HOH:O	2.16	0.46
1:D:286:VAL:HG22	1:D:296:THR:HB	1.98	0.46
1:A:73:ILE:HG22	1:A:81:PRO:HG2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:PRO:HG3	1:D:126:LEU:HD22	1.97	0.45
1:A:270:ARG:HH22	1:A:290:PRO:CD	2.29	0.45
1:A:223:ALA:HA	1:A:232:ARG:CB	2.46	0.45
1:A:254:ALA:HB3	1:B:181:THR:CG2	2.47	0.45
1:C:16:ARG:HD3	1:C:111:GLU:OE1	2.17	0.45
1:C:198:LEU:CD2	1:C:209:THR:HG22	2.40	0.45
1:C:93:PRO:HB2	1:C:129:VAL:HG12	1.99	0.45
1:B:41:MSE:HE1	1:B:44:TRP:CD1	2.52	0.45
1:C:139:ARG:O	1:C:142:ALA:HB3	2.17	0.45
1:C:134:GLU:HG3	1:C:166:HIS:CD2	2.51	0.45
1:D:86:LEU:HD23	1:D:94:GLY:O	2.17	0.45
1:C:41:MSE:HE1	1:C:44:TRP:CD1	2.52	0.45
1:B:126:LEU:H	1:B:175:ARG:HH21	1.64	0.45
1:B:8:HIS:HB2	1:B:69:ARG:CD	2.46	0.44
1:D:158:HIS:HD2	1:D:164:GLY:C	2.21	0.44
1:D:77:ASP:OD1	1:D:79:THR:HG23	2.17	0.44
1:A:284:GLU:HG2	1:A:298:SER:CB	2.46	0.44
1:D:211:PHE:CD1	1:D:211:PHE:C	2.90	0.44
1:B:92:VAL:HG13	1:B:92:VAL:O	2.16	0.44
1:A:76:PRO:C	1:A:78:GLY:H	2.20	0.44
1:C:276:VAL:HB	1:C:278:ARG:NH1	2.32	0.44
1:B:134:GLU:HG3	1:B:166:HIS:HD2	1.83	0.44
1:B:16:ARG:O	1:B:76:PRO:HD3	2.18	0.44
1:A:138:ARG:HD2	4:A:479:HOH:O	2.17	0.44
1:B:143:VAL:O	1:B:147:VAL:HG23	2.17	0.44
1:B:278:ARG:HD3	1:B:280:TRP:CH2	2.53	0.44
1:D:142:ALA:HB1	1:D:146:ARG:HH21	1.82	0.43
1:B:75:ALA:HB1	1:B:76:PRO:HD2	2.00	0.43
1:B:104:TRP:HB2	1:C:11:HIS:CE1	2.52	0.43
1:D:107:GLY:HA2	3:D:404:SO4:O1	2.19	0.43
1:D:279:PRO:C	1:D:281:GLY:H	2.20	0.43
1:A:152:ARG:HG3	1:B:227:TRP:CD2	2.54	0.43
1:B:54:GLU:HG2	4:B:576:HOH:O	2.17	0.43
1:B:139:ARG:NH2	1:C:18:GLU:OE1	2.50	0.43
1:C:107:GLY:HA2	2:C:402:COA:H51A	2.01	0.43
1:B:238:VAL:HG21	1:B:244:VAL:HG11	2.00	0.43
1:B:279:PRO:HG2	1:B:280:TRP:CE3	2.53	0.43
1:D:180:LEU:N	1:D:180:LEU:HD22	2.33	0.43
1:C:159:TYR:HB2	1:C:162:ARG:HG3	1.99	0.43
1:D:195:ALA:HB2	1:D:217:PRO:HD2	1.99	0.43
1:C:278:ARG:HG3	1:C:280:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:HG2	1:C:42:ARG:H	1.69	0.43
1:D:54:GLU:HA	1:D:57:ARG:NH1	2.33	0.43
1:D:121:LEU:HD12	1:D:121:LEU:HA	1.86	0.43
1:B:126:LEU:O	1:B:175:ARG:NH2	2.52	0.43
1:C:147:VAL:O	1:C:147:VAL:CG1	2.67	0.43
1:A:86:LEU:HD23	1:A:95:LEU:HD12	2.00	0.43
1:B:213:ILE:HD12	1:B:219:PHE:CD2	2.50	0.43
1:C:86:LEU:HD23	1:C:94:GLY:O	2.19	0.42
1:D:199:ARG:HA	1:D:199:ARG:HD3	1.56	0.42
1:A:291:GLU:H	1:A:291:GLU:CD	2.21	0.42
1:C:64:ALA:O	1:C:65:ALA:C	2.58	0.42
1:D:9:THR:CG2	1:D:10:ALA:N	2.82	0.42
1:C:181:THR:HG22	1:D:254:ALA:HB3	2.00	0.42
1:B:256:THR:O	1:B:260:LEU:HG	2.19	0.42
1:B:54:GLU:O	1:B:57:ARG:HG2	2.19	0.42
1:C:193:ASP:OD1	1:C:196:ALA:HB2	2.18	0.42
1:C:20:THR:CG2	1:C:74:ARG:HE	2.32	0.42
1:C:67:GLY:HA2	1:C:69:ARG:NH2	2.33	0.42
1:A:208:ARG:NE	1:A:226:PRO:HA	2.33	0.42
1:B:37:ASP:HB3	1:B:40:VAL:HB	2.00	0.42
1:C:239:PRO:O	1:C:240:GLY:C	2.58	0.42
1:C:201:VAL:HG12	1:C:207:ALA:CB	2.46	0.42
1:A:260:LEU:HD23	1:B:180:LEU:HD13	2.02	0.42
1:C:81:PRO:O	1:C:100:ARG:HG3	2.19	0.42
1:B:154:ARG:NH2	1:B:167:GLU:OE1	2.53	0.42
1:C:277:ARG:C	1:C:278:ARG:HD2	2.41	0.42
1:C:38:GLU:HG3	1:C:42:ARG:NH2	2.35	0.42
1:D:190:PRO:HB3	1:D:238:VAL:HG11	2.02	0.42
1:A:138:ARG:HA	1:A:138:ARG:HD3	1.57	0.41
1:C:51:ASP:HB2	1:C:52:PRO:CD	2.50	0.41
1:C:186:ILE:HD12	1:C:232:ARG:CZ	2.50	0.41
1:D:157:GLN:NE2	1:D:168:MSE:HG3	2.34	0.41
1:D:22:LEU:HG	1:D:24:PRO:HD3	2.01	0.41
1:A:41:MSE:HE1	1:A:44:TRP:CD1	2.54	0.41
1:B:137:ASN:CG	1:B:140:SER:HB2	2.41	0.41
1:B:165:PRO:HB3	1:B:300:PRO:HG2	2.03	0.41
1:C:127:ASP:N	1:C:127:ASP:OD2	2.53	0.41
1:C:198:LEU:HD13	1:C:209:THR:HG21	2.02	0.41
1:C:92:VAL:HA	1:C:93:PRO:HD2	1.77	0.41
1:C:93:PRO:HG3	1:C:126:LEU:HD13	2.01	0.41
1:D:187:THR:HG21	1:D:249:LEU:CD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLY:O	1:B:126:LEU:HD23	2.20	0.41
1:D:154:ARG:HG3	4:D:584:HOH:O	2.18	0.41
1:D:64:ALA:O	1:D:65:ALA:C	2.58	0.41
1:B:95:LEU:HB2	1:B:130:GLU:O	2.20	0.41
1:C:73:ILE:O	1:C:80:VAL:HA	2.19	0.41
1:D:132:TRP:CB	1:D:168:MSE:HE2	2.36	0.41
1:C:185:VAL:HG23	1:D:231:PRO:HB3	2.02	0.41
1:C:42:ARG:HB3	1:C:42:ARG:HE	1.47	0.41
1:D:83:MSE:HG2	1:D:84:ALA:N	2.36	0.41
1:A:83:MSE:HE2	1:A:98:LEU:CD2	2.46	0.41
1:A:159:TYR:HD2	1:A:162:ARG:NH1	2.18	0.41
1:A:279:PRO:C	1:A:281:GLY:H	2.23	0.41
4:A:615:HOH:O	1:B:248:ARG:HD2	2.21	0.41
1:A:159:TYR:HB3	1:A:161:HIS:CD2	2.55	0.41
1:B:239:PRO:O	1:B:240:GLY:C	2.59	0.41
1:A:96:THR:O	1:A:97:TRP:HB3	2.21	0.41
1:B:231:PRO:O	1:B:232:ARG:HB3	2.20	0.41
1:C:133:ILE:HD12	1:C:171:LEU:HD13	2.02	0.41
1:A:140:SER:OG	2:A:401:COA:H31	2.20	0.41
1:D:262:ARG:HD2	1:D:266:ASP:OD2	2.20	0.41
1:B:139:ARG:O	1:B:143:VAL:HG23	2.21	0.40
1:D:134:GLU:CD	1:D:162:ARG:HH22	2.24	0.40
1:D:191:VAL:HG22	1:D:291:GLU:HG3	2.03	0.40
1:A:9:THR:HB	1:A:10:ALA:H	1.56	0.40
1:B:275:PRO:HA	1:B:284:GLU:O	2.22	0.40
1:B:92:VAL:HA	1:B:93:PRO:HD2	1.71	0.40
1:C:252:ASP:CG	1:C:282:ARG:HH22	2.24	0.40
1:A:20:THR:O	1:A:21:PRO:C	2.60	0.40
1:C:240:GLY:HA2	1:C:241:PRO:HD3	1.87	0.40
1:D:87:LEU:HD12	1:D:95:LEU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	292/301 (97%)	261 (89%)	23 (8%)	8 (3%)	5 12
1	B	292/301 (97%)	262 (90%)	25 (9%)	5 (2%)	9 23
1	C	291/301 (97%)	270 (93%)	16 (6%)	5 (2%)	9 23
1	D	291/301 (97%)	267 (92%)	14 (5%)	10 (3%)	3 8
All	All	1166/1204 (97%)	1060 (91%)	78 (7%)	28 (2%)	6 15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	10	ALA
1	A	239	PRO
1	B	122	GLU
1	B	240	GLY
1	D	123	ASP
1	A	137	ASN
1	B	93	PRO
1	B	280	TRP
1	C	243	PRO
1	D	93	PRO
1	D	228	SER
1	D	274	PRO
1	D	280	TRP
1	A	280	TRP
1	C	177	GLU
1	D	241	PRO
1	A	93	PRO
1	B	179	PRO
1	C	137	ASN
1	D	242	GLY
1	A	179	PRO
1	C	93	PRO
1	C	160	PRO
1	A	274	PRO
1	D	239	PRO
1	D	240	GLY
1	D	65	ALA

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	216/218 (99%)	173 (80%)	43 (20%)	1 3
1	B	216/218 (99%)	175 (81%)	41 (19%)	1 4
1	C	215/218 (99%)	173 (80%)	42 (20%)	1 3
1	D	215/218 (99%)	176 (82%)	39 (18%)	1 4
All	All	862/872 (99%)	697 (81%)	165 (19%)	1 4

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	9	THR
1	A	12	LEU
1	A	13	ARG
1	A	19	LEU
1	A	42	ARG
1	A	56	GLU
1	A	61	SER
1	A	69	ARG
1	A	83	MSE
1	A	91	ASP
1	A	95	LEU
1	A	96	THR
1	A	98	LEU
1	A	102	ASP
1	A	121	LEU
1	A	123	ASP
1	A	128	ARG
1	A	138	ARG
1	A	152	ARG
1	A	154	ARG
1	A	162	ARG
1	A	175	ARG
1	A	181	THR

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Mol	Chain	Res	Type
1	A	182	THR
1	A	186	ILE
1	A	187	THR
1	A	192	ARG
1	A	200	LEU
1	A	208	ARG
1	A	209	THR
1	A	215	ASP
1	A	232	ARG
1	A	235	LEU
1	A	238	VAL
1	A	244	VAL
1	A	245	GLU
1	A	256	THR
1	A	270	ARG
1	A	277	ARG
1	A	294	GLU
1	A	296	THR
1	A	301	VAL
1	B	13	ARG
1	B	16	ARG
1	B	18	GLU
1	B	19	LEU
1	B	29	ARG
1	B	54	GLU
1	B	56	GLU
1	B	61	SER
1	B	83	MSE
1	B	86	LEU
1	B	91	ASP
1	B	96	THR
1	B	98	LEU
1	B	101	ARG
1	B	102	ASP
1	B	121	LEU
1	B	122	GLU
1	B	127	ASP
1	B	128	ARG
1	B	129	VAL
1	B	138	ARG
1	B	139	ARG
1	B	152	ARG

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Mol	Chain	Res	Type
1	B	155	LEU
1	B	167	GLU
1	B	186	ILE
1	B	187	THR
1	B	192	ARG
1	B	200	LEU
1	B	232	ARG
1	B	234	ARG
1	B	235	LEU
1	B	238	VAL
1	B	248	ARG
1	B	256	THR
1	B	270	ARG
1	B	272	ASP
1	B	278	ARG
1	B	294	GLU
1	B	296	THR
1	B	301	VAL
1	C	9	THR
1	C	13	ARG
1	C	16	ARG
1	C	18	GLU
1	C	19	LEU
1	C	29	ARG
1	C	38	GLU
1	C	39	GLU
1	C	42	ARG
1	C	54	GLU
1	C	61	SER
1	C	79	THR
1	C	83	MSE
1	C	91	ASP
1	C	96	THR
1	C	98	LEU
1	C	100	ARG
1	C	101	ARG
1	C	121	LEU
1	C	122	GLU
1	C	127	ASP
1	C	139	ARG
1	C	175	ARG
1	C	178	GLU

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Mol	Chain	Res	Type
1	C	186	ILE
1	C	187	THR
1	C	200	LEU
1	C	215	ASP
1	C	234	ARG
1	C	235	LEU
1	C	238	VAL
1	C	244	VAL
1	C	245	GLU
1	C	256	THR
1	C	262	ARG
1	C	270	ARG
1	C	278	ARG
1	C	282	ARG
1	C	288	THR
1	C	290	PRO
1	C	296	THR
1	C	301	VAL
1	D	18	GLU
1	D	19	LEU
1	D	39	GLU
1	D	56	GLU
1	D	61	SER
1	D	69	ARG
1	D	74	ARG
1	D	83	MSE
1	D	90	THR
1	D	92	VAL
1	D	96	THR
1	D	100	ARG
1	D	101	ARG
1	D	111	GLU
1	D	121	LEU
1	D	122	GLU
1	D	123	ASP
1	D	128	ARG
1	D	138	ARG
1	D	140	SER
1	D	177	GLU
1	D	181	THR
1	D	186	ILE
1	D	187	THR

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Mol	Chain	Res	Type
1	D	192	ARG
1	D	199	ARG
1	D	200	LEU
1	D	213	ILE
1	D	218	GLU
1	D	232	ARG
1	D	235	LEU
1	D	244	VAL
1	D	248	ARG
1	D	270	ARG
1	D	276	VAL
1	D	278	ARG
1	D	291	GLU
1	D	296	THR
1	D	301	VAL

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

Mol	Chain	Res	Type
1	A	8	HIS
1	A	33	HIS
1	A	161	HIS
1	B	157	GLN
1	B	158	HIS
1	C	161	HIS
1	D	106	HIS
1	D	157	GLN
1	D	158	HIS

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)

11 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	A	401	-	41,50,50	1.21	4 (9%)	52,75,75	3.19	13 (25%)
3	SO4	B	403	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	D	410	-	4,4,4	0.25	0	6,6,6	0.14	0
2	COA	C	402	-	41,50,50	1.25	3 (7%)	52,75,75	1.54	5 (9%)
3	SO4	D	409	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	A	406	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	B	407	-	4,4,4	0.30	0	6,6,6	0.06	0
3	SO4	D	404	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	D	408	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	A	405	-	4,4,4	0.28	0	6,6,6	0.06	0
3	SO4	D	411	-	4,4,4	0.26	0	6,6,6	0.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	A	401	-	-	8/44/64/64	0/3/3/3
2	COA	C	402	-	-	9/44/64/64	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	COA	O4B-C1B	3.86	1.46	1.41
2	A	401	COA	O4B-C1B	3.43	1.45	1.41
2	C	402	COA	C2B-C1B	2.71	1.57	1.53
2	A	401	COA	C2B-C1B	2.57	1.57	1.53
2	A	401	COA	C8A-N7A	-2.21	1.30	1.34
2	A	401	COA	P3B-O9A	2.10	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	COA	P3B-O3B	2.09	1.63	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	COA	CEP-CBP-CAP	-12.01	88.00	108.82
2	A	401	COA	CDP-CBP-CAP	-10.74	90.21	108.82
2	A	401	COA	CEP-CBP-CCP	8.02	121.31	108.23
2	A	401	COA	CDP-CBP-CCP	7.20	119.98	108.23
2	C	402	COA	P2A-O3A-P1A	-6.79	109.52	132.83
2	A	401	COA	P2A-O3A-P1A	-6.57	110.29	132.83
2	C	402	COA	N3A-C2A-N1A	-4.96	120.92	128.68
2	A	401	COA	N3A-C2A-N1A	-4.68	121.36	128.68
2	A	401	COA	CEP-CBP-CDP	4.25	117.83	109.17
2	A	401	COA	O2A-P1A-O5B	2.60	119.82	107.75
2	C	402	COA	O2A-P1A-O5B	2.55	119.59	107.75
2	A	401	COA	P2A-O6A-CCP	-2.46	107.40	121.56
2	C	402	COA	P2A-O6A-CCP	-2.44	107.48	121.56
2	C	402	COA	P1A-O5B-C5B	-2.27	108.38	121.68
2	A	401	COA	P1A-O5B-C5B	-2.20	108.78	121.68
2	A	401	COA	CAP-C9P-N8P	2.18	120.93	116.58
2	A	401	COA	C6P-C5P-N4P	2.10	119.96	116.42
2	A	401	COA	O4B-C1B-C2B	-2.09	103.86	106.93

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	COA	C5B-O5B-P1A-O2A
2	A	401	COA	CEP-CBP-CCP-O6A
2	A	401	COA	N8P-C9P-CAP-OAP
2	A	401	COA	S1P-C2P-C3P-N4P
2	C	402	COA	C3B-O3B-P3B-O7A
2	C	402	COA	C3B-C4B-C5B-O5B
2	C	402	COA	O4B-C4B-C5B-O5B
2	C	402	COA	C5B-O5B-P1A-O1A
2	C	402	COA	P2A-O3A-P1A-O5B
2	A	401	COA	O9P-C9P-CAP-OAP
2	A	401	COA	O9P-C9P-CAP-CBP
2	A	401	COA	P2A-O3A-P1A-O5B
2	C	402	COA	C3B-O3B-P3B-O8A
2	C	402	COA	CCP-O6A-P2A-O3A

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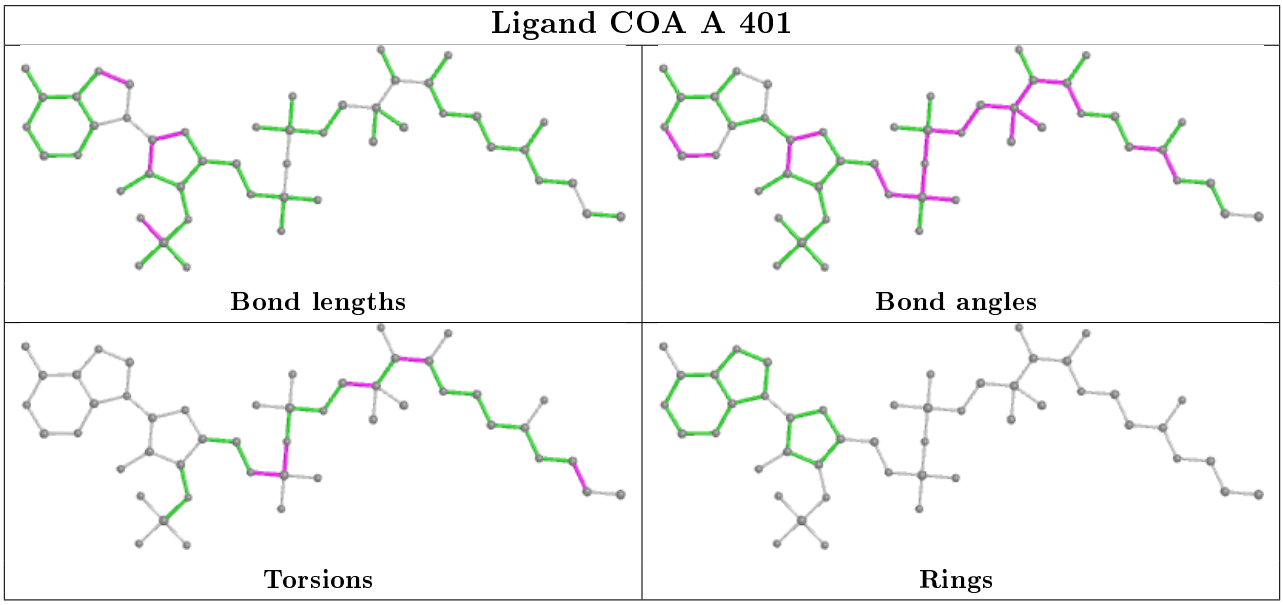
Mol	Chain	Res	Type	Atoms
2	C	402	COA	CEP-CBP-CCP-O6A
2	A	401	COA	C5B-O5B-P1A-O3A
2	C	402	COA	CCP-O6A-P2A-O5A

There are no ring outliers.

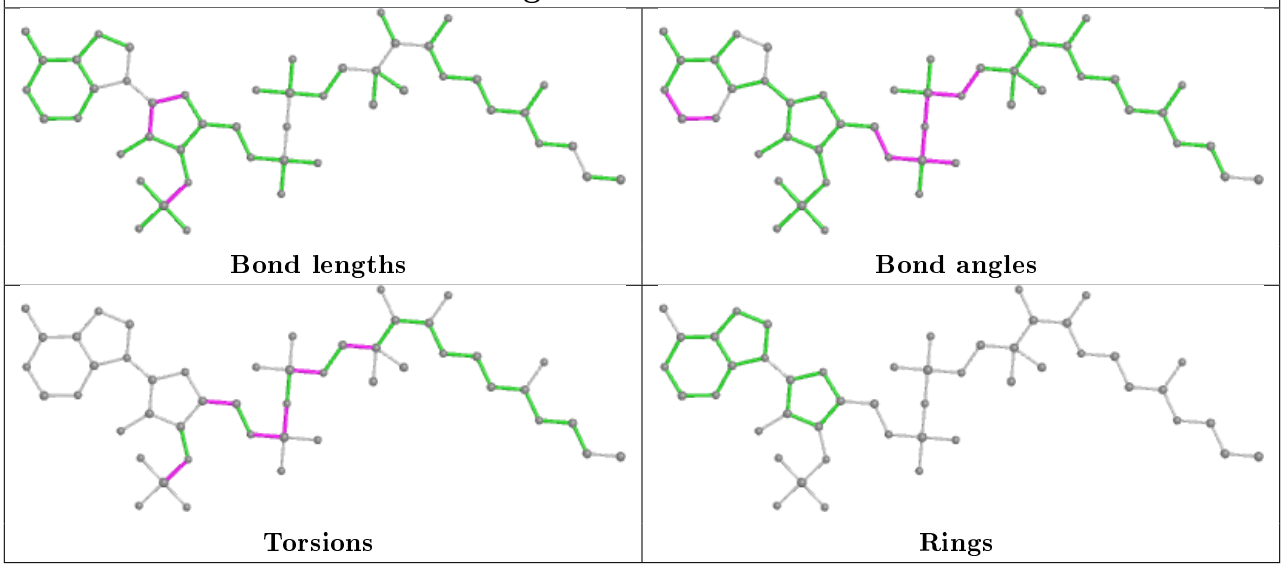
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	COA	1	0
2	C	402	COA	2	0
3	D	404	SO4	1	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 C 402



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	291/301 (96%)	-0.29	7 (2%)	59	60	7, 29, 68, 86	0
1	B	291/301 (96%)	-0.06	4 (1%)	75	77	13, 37, 63, 82	0
1	C	290/301 (96%)	-0.19	7 (2%)	59	60	10, 28, 64, 92	0
1	D	290/301 (96%)	-0.25	6 (2%)	63	65	8, 29, 62, 95	0
All	All	1162/1204 (96%)	-0.19	24 (2%)	63	65	7, 31, 64, 95	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	GLY	4.7
1	D	241	PRO	3.7
1	D	214	GLY	3.2
1	C	125	GLY	3.2
1	C	240	GLY	3.1
1	D	239	PRO	3.1
1	D	243	PRO	3.1
1	D	163	PRO	3.0
1	C	123	ASP	2.9
1	A	175	ARG	2.8
1	A	124	GLY	2.7
1	B	215	ASP	2.6
1	A	10	ALA	2.5
1	D	10	ALA	2.5
1	C	122	GLU	2.5
1	C	176	ALA	2.3
1	A	122	GLU	2.3
1	A	280	TRP	2.2
1	B	91	ASP	2.2
1	B	214	GLY	2.2
1	A	123	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	241	PRO	2.1
1	B	39	GLU	2.1
1	A	277	ARG	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)

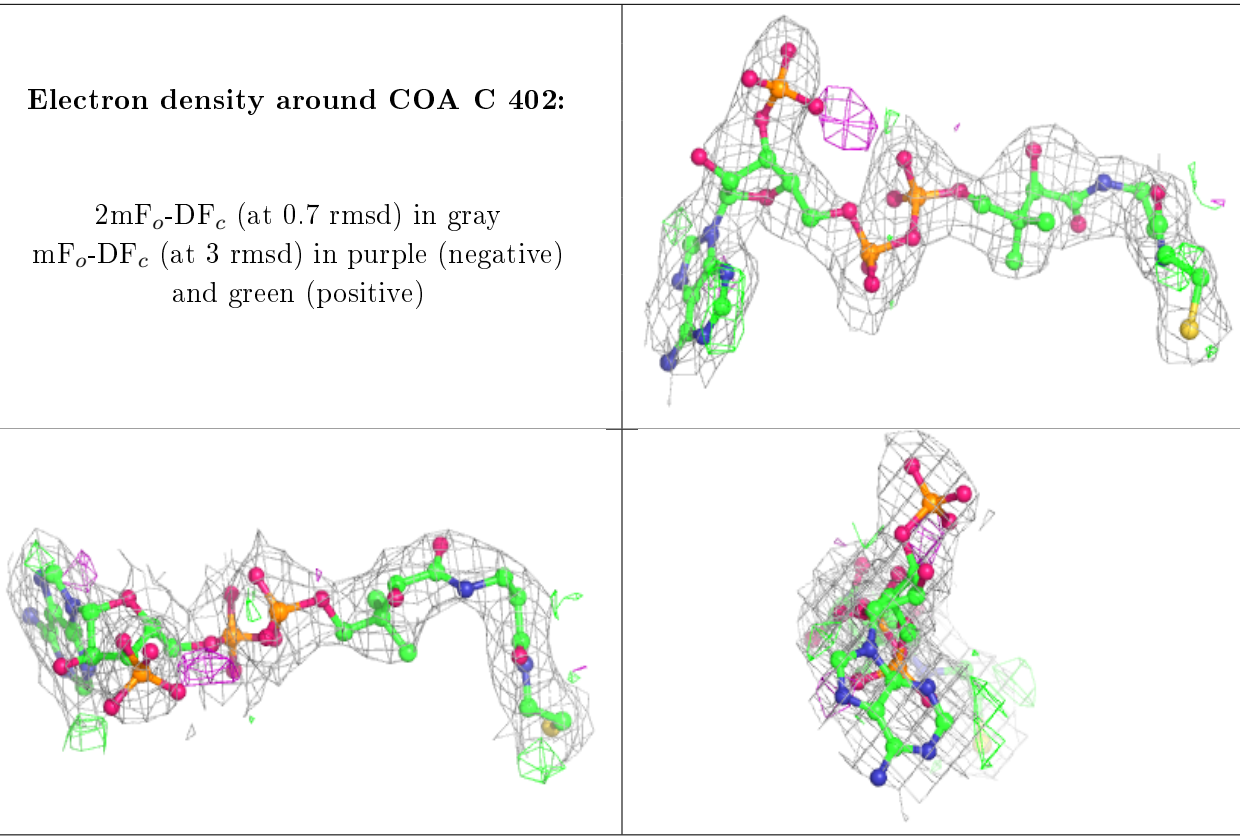
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	SO4	D	410	5/5	0.88	0.25	69,69,75,77	0
3	SO4	B	407	5/5	0.92	0.20	60,62,68,68	0
3	SO4	A	406	5/5	0.93	0.19	83,83,84,85	0
3	SO4	D	409	5/5	0.93	0.20	64,72,74,75	0
2	COA	C	402	48/48	0.94	0.16	4,30,60,75	0
3	SO4	D	411	5/5	0.94	0.19	46,65,69,70	0
2	COA	A	401	48/48	0.95	0.15	2,27,45,47	0
3	SO4	A	405	5/5	0.96	0.14	59,65,68,73	0
3	SO4	D	408	5/5	0.97	0.14	37,43,49,54	0
3	SO4	D	404	5/5	0.98	0.14	19,25,31,32	0
3	SO4	B	403	5/5	0.98	0.13	40,42,50,55	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.

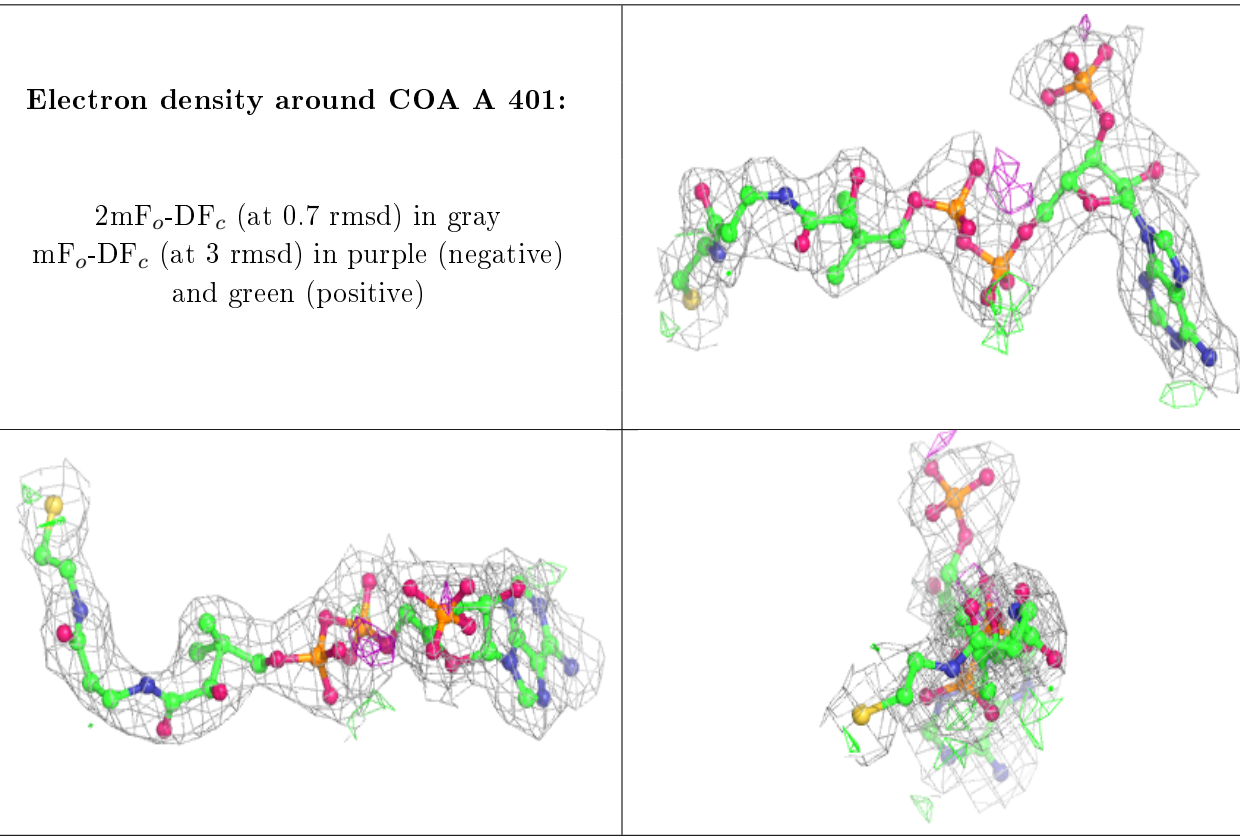
Electron density around COA C 402:

$2mF_o$-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 A 401:

$2mF_o$-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.