Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 07:36 pm BST

PDB ID	:	1CQJ
Title	:	CRYSTAL STRUCTURE OF DEPHOSPHORYLATED E. COLI SUCCINYL-COA SYNTHETASE
Authors	:	Joyce, M.A.; Fraser, M.E.; James, M.N.G.; Bridger, W.A.; Wolodko, W.T.
Deposited on	:	1999-08-06
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (i)) 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 ⓘ

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

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		17
Ramachandran outliers		0.4%
Sidechain outliers		5.2%
RSRZ outliers		0.1%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
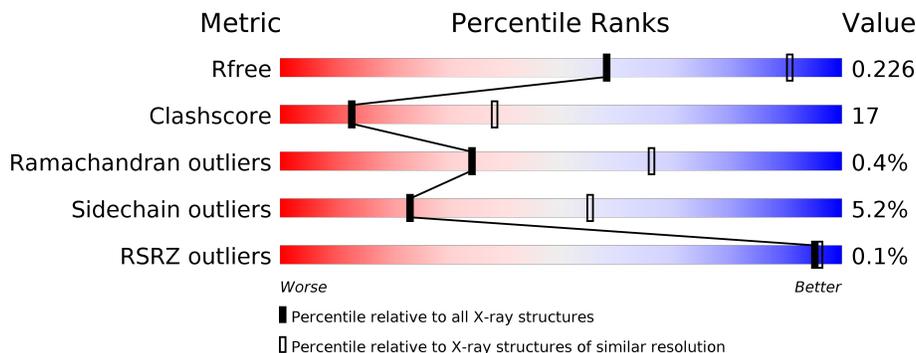
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	286	62%　　35%　•
1	D	286	59%　　38%　•
2	B	385	77%　　20%　•
2	E	385	78%　　21%　•

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10355 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 SUCCINYL-COA SYNTHETASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total 2061	C 1307	N 345	O 398	S 11	0	0	0
1	D	286	Total 2061	C 1307	N 345	O 398	S 11	0	0	0

- Molecule 2 is a protein called SUCCINYL-COA SYNTHETASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total 2885	C 1823	N 505	O 544	S 13	0	0	0
2	E	385	Total 2885	C 1823	N 505	O 544	S 13	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
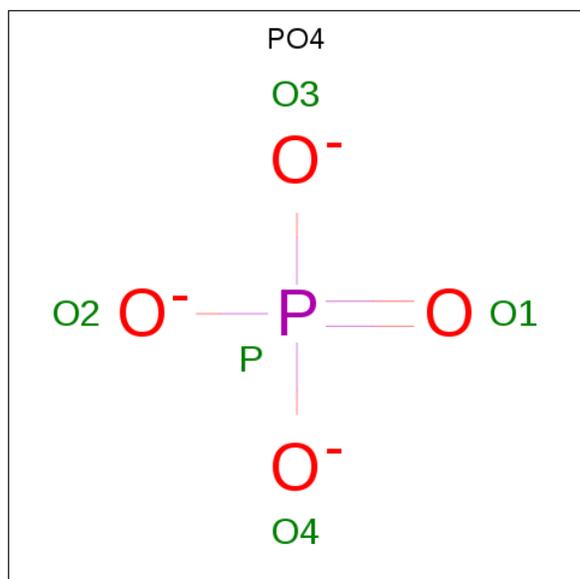
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total O P 5 4 1		0	0
3	B	1	Total O P 5 4 1		0	0
3	D	1	Total O P 5 4 1		0	0
3	E	1	Total O P 5 4 1		0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
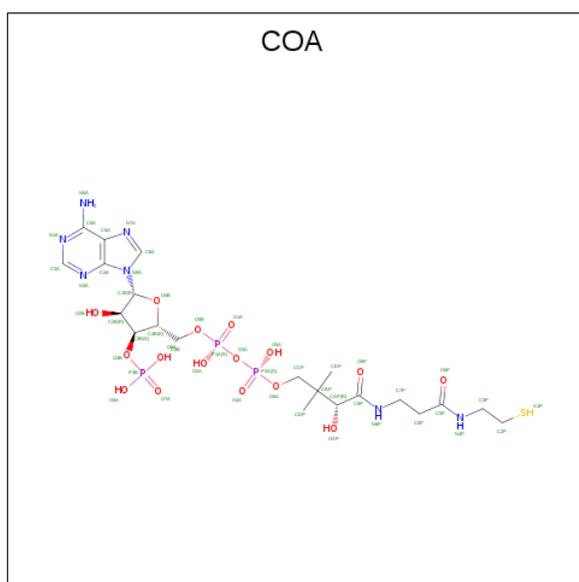
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C N O P S 48 21 7 16 3 1		0	0
4	B	1	Total C N O S 17 11 2 3 1		0	0
4	D	1	Total C N O P S 48 21 7 16 3 1		0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total O 65 65		0	0
5	B	112	Total O 112 112		0	0
5	D	64	Total O 64 64		0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	89	Total　　O 89　　　89		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: SUCCINYL-COA SYNTHETASE ALPHA CHAIN
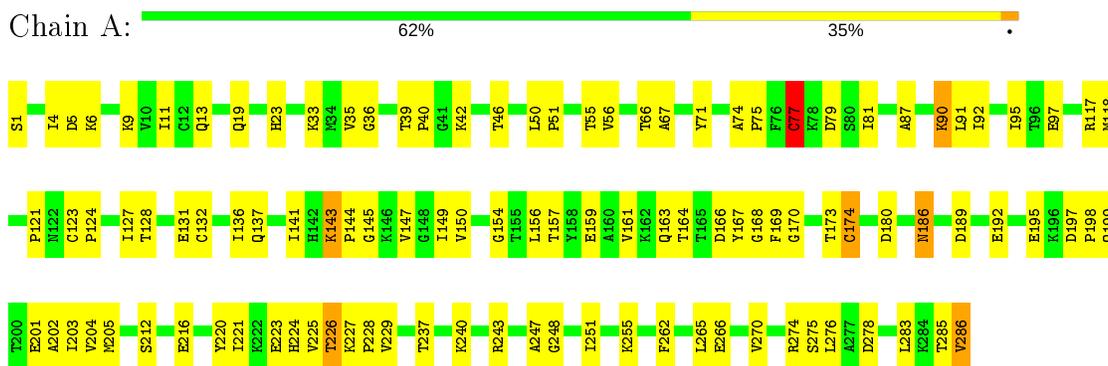
- Molecule 1: SUCCINYL-COA SYNTHETASE ALPHA CHAIN
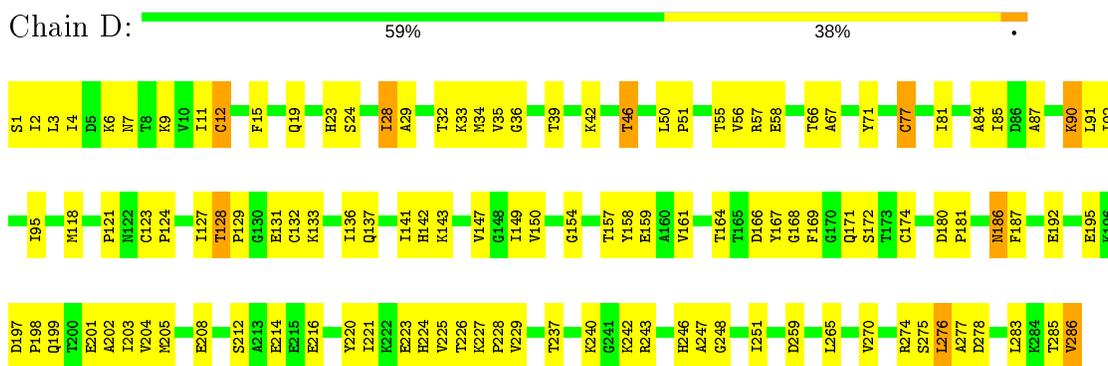
- Molecule 2: SUCCINYL-COA SYNTHETASE BETA CHAIN
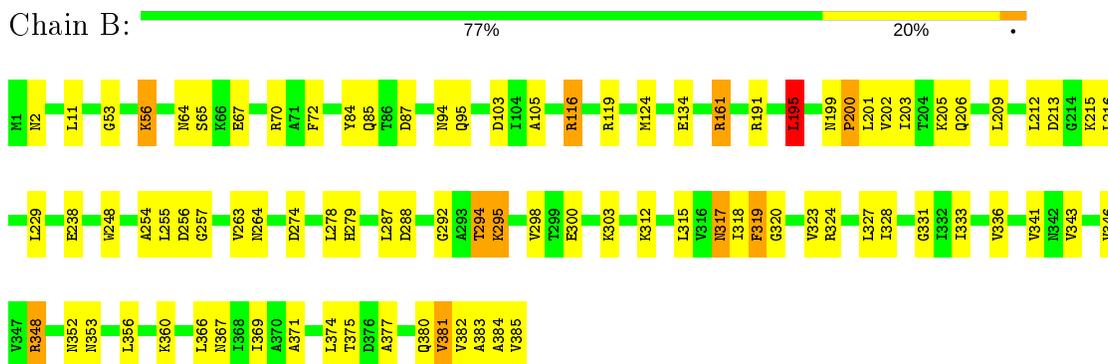
● Molecule 2: SUCCINYL-COA SYNTHETASE BETA CHAIN

Chain E:
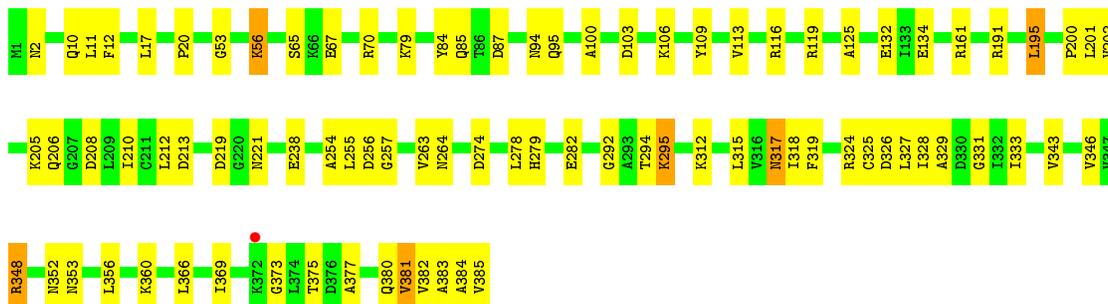
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.82Å 98.82Å 404.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.90) 98.7 (19.93-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.67 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.172 , 0.228 0.171 , 0.226	Depositor DCC
R_{free} test set	5121 reflections (11.38%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.3	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10355	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, PO4

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	0.74	2/2095 (0.1%)	0.89	1/2838 (0.0%)
1	D	0.75	2/2095 (0.1%)	0.89	0/2838
2	B	0.76	0/2927	0.87	5/3961 (0.1%)
2	E	0.76	0/2927	0.86	4/3961 (0.1%)
All	All	0.75	4/10044 (0.0%)	0.88	10/13598 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	CYS	CB-SG	-6.49	1.71	1.82
1	D	77	CYS	CB-SG	-5.78	1.72	1.81
1	D	12	CYS	CB-SG	-5.55	1.72	1.81
1	A	174	CYS	CB-SG	-5.29	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	161	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	B	201	LEU	N-CA-C	-6.18	94.32	111.00
2	E	195	LEU	CA-CB-CG	6.17	129.50	115.30
2	E	201	LEU	N-CA-C	-6.03	94.72	111.00
2	E	257	GLY	N-CA-C	-5.96	98.20	113.10
1	A	79	ASP	CB-CG-OD1	5.48	123.23	118.30
2	B	257	GLY	N-CA-C	-5.45	99.49	113.10
2	B	116	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	E	113	VAL	CB-CA-C	-5.35	101.23	111.40
2	B	195	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2061	0	2118	87	0
1	D	2061	0	2118	100	0
2	B	2885	0	2940	79	0
2	E	2885	0	2941	73	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	48	0	32	4	0
4	B	17	0	18	5	0
4	D	48	0	32	4	0
5	A	65	0	0	6	0
5	B	112	0	0	13	0
5	D	64	0	0	5	0
5	E	89	0	0	16	0
All	All	10355	0	10199	336	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 17.

All (336) 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)
4:B:903:COA:CBP	4:B:903:COA:CAP	1.78	1.56
2:E:56:LYS:H	2:E:56:LYS:HD2	0.98	1.08
2:B:56:LYS:H	2:B:56:LYS:HD2	0.91	1.04
2:B:56:LYS:HD2	2:B:56:LYS:N	1.75	0.99
2:E:56:LYS:N	2:E:56:LYS:HD2	1.82	0.93
1:D:221:ILE:HA	1:D:225:VAL:HG23	1.56	0.88
2:B:56:LYS:CD	2:B:56:LYS:H	1.81	0.86
4:B:903:COA:CDP	4:B:903:COA:CAP	2.55	0.84
1:A:33:LYS:HE2	5:A:916:HOH:O	1.79	0.83
2:E:20:PRO:HA	5:E:916:HOH:O	1.78	0.82
2:E:56:LYS:CD	2:E:56:LYS:H	1.88	0.82
2:E:213:ASP:HB3	5:E:966:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ILE:HG13	1:D:161:VAL:HG11	1.62	0.79
1:D:259:ASP:HB2	5:D:958:HOH:O	1.83	0.77
1:D:285:THR:O	1:D:286:VAL:HG13	1.85	0.77
1:A:221:ILE:HA	1:A:225:VAL:HG23	1.66	0.76
1:D:221:ILE:HA	1:D:225:VAL:CG2	2.16	0.76
1:A:285:THR:O	1:A:286:VAL:HG13	1.86	0.74
1:D:4:ILE:HD12	1:D:132:CYS:SG	2.28	0.73
1:D:197:ASP:O	1:D:227:LYS:NZ	2.22	0.72
2:E:295:LYS:HG2	2:E:331:GLY:HA2	1.71	0.72
1:A:141:ILE:HG13	1:A:161:VAL:HG11	1.71	0.71
1:A:163:GLN:HG3	5:A:949:HOH:O	1.91	0.71
1:A:9:LYS:HB3	1:A:35:VAL:HG11	1.74	0.70
1:D:123:CYS:HB2	1:D:124:PRO:HD2	1.72	0.69
1:A:197:ASP:O	1:A:227:LYS:NZ	2.25	0.69
1:D:229:VAL:HG12	1:D:270:VAL:HG13	1.75	0.68
2:B:295:LYS:HG2	2:B:331:GLY:HA2	1.75	0.68
1:D:192:GLU:HB2	1:D:220:TYR:OH	1.94	0.68
1:A:223:GLU:HG2	1:A:224:HIS:NE2	2.09	0.67
2:E:324:ARG:HG2	2:E:353:ASN:HD22	1.59	0.67
2:E:292:GLY:O	2:E:294:THR:HG23	1.94	0.67
1:A:221:ILE:HA	1:A:225:VAL:CG2	2.25	0.67
1:D:7:ASN:HA	1:D:33:LYS:NZ	2.11	0.66
2:E:279:HIS:HE1	2:E:375:THR:CG2	2.09	0.66
2:E:317:ASN:HD21	2:E:348:ARG:HH11	1.44	0.65
1:A:123:CYS:HB2	1:A:124:PRO:HD2	1.79	0.65
1:D:237:THR:HG23	2:E:274:ASP:OD1	1.96	0.65
2:E:324:ARG:CG	2:E:353:ASN:HD22	2.09	0.65
1:A:6:LYS:HE2	5:A:908:HOH:O	1.96	0.64
2:B:369:ILE:HD12	2:B:369:ILE:N	2.12	0.64
1:A:6:LYS:HG2	1:A:131:GLU:OE1	1.98	0.63
1:D:223:GLU:HG2	1:D:224:HIS:NE2	2.14	0.63
1:D:28:ILE:HG22	1:D:29:ALA:N	2.12	0.63
1:D:9:LYS:HB3	1:D:35:VAL:HG11	1.79	0.63
2:E:373:GLY:HA2	5:E:990:HOH:O	1.98	0.62
2:B:292:GLY:HA2	5:B:987:HOH:O	1.98	0.62
1:D:19:GLN:HG3	4:D:902:COA:H132	1.80	0.62
2:B:72:PHE:HA	5:B:930:HOH:O	1.98	0.62
1:D:285:THR:C	1:D:286:VAL:HG22	2.19	0.62
1:A:19:GLN:HG3	4:A:901:COA:H132	1.81	0.62
2:E:369:ILE:HD12	2:E:369:ILE:N	2.15	0.62
1:A:285:THR:O	1:A:286:VAL:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:GLY:O	2:B:294:THR:HG23	2.01	0.61
1:A:285:THR:C	1:A:286:VAL:HG22	2.21	0.61
1:D:248:GLY:O	2:E:116:ARG:NH2	2.34	0.61
1:D:46:THR:HG22	1:D:50:LEU:O	2.00	0.61
2:E:324:ARG:HB3	2:E:327:LEU:HD12	1.82	0.60
2:E:202:VAL:HG21	2:E:212:LEU:HD22	1.82	0.60
1:D:285:THR:O	1:D:286:VAL:HG22	2.01	0.60
2:E:324:ARG:HG2	2:E:326:ASP:OD1	2.02	0.59
1:D:6:LYS:HG2	1:D:131:GLU:OE1	2.02	0.59
2:E:208:ASP:HB2	5:E:967:HOH:O	2.01	0.59
2:B:279:HIS:HE1	2:B:375:THR:CG2	2.16	0.59
1:A:66:THR:HG22	5:A:933:HOH:O	2.01	0.59
1:A:154:GLY:O	1:A:157:THR:HB	2.03	0.58
1:D:39:THR:HG21	1:D:42:LYS:HD2	1.86	0.58
2:B:65:SER:HB2	2:B:67:GLU:OE1	2.02	0.58
1:A:127:ILE:HG22	1:A:174:CYS:HB2	1.85	0.58
2:B:320:GLY:HA2	4:B:903:COA:H32	1.86	0.57
1:D:127:ILE:HG22	1:D:174:CYS:HB2	1.86	0.57
1:D:187:PHE:HB2	5:D:950:HOH:O	2.02	0.57
2:E:79:LYS:HE2	5:E:931:HOH:O	2.03	0.57
1:D:202:ALA:CB	1:D:228:PRO:HG2	2.35	0.57
1:A:223:GLU:HG2	1:A:224:HIS:CD2	2.40	0.56
1:A:205:MET:HE3	1:A:265:LEU:HD21	1.87	0.56
2:E:106:LYS:HD3	5:E:939:HOH:O	2.05	0.56
1:D:201:GLU:O	1:D:228:PRO:HD2	2.06	0.56
1:A:229:VAL:HG12	1:A:270:VAL:HG13	1.88	0.56
1:D:6:LYS:O	1:D:33:LYS:HE3	2.06	0.56
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.41	0.56
1:D:202:ALA:HB2	1:D:228:PRO:HG2	1.88	0.56
1:D:223:GLU:HG2	1:D:224:HIS:CD2	2.41	0.56
2:B:202:VAL:HG21	2:B:212:LEU:HD22	1.87	0.56
2:E:103:ASP:HB3	2:E:205:LYS:HD2	1.88	0.55
2:E:53:GLY:HA2	2:E:56:LYS:HD3	1.89	0.55
1:D:12:CYS:O	1:D:15:PHE:HB2	2.06	0.55
1:D:186:ASN:H	1:D:186:ASN:HD22	1.55	0.55
1:D:198:PRO:HG2	1:D:199:GLN:H	1.72	0.55
1:D:164:THR:HG22	1:D:283:LEU:HD12	1.89	0.55
2:E:383:ALA:O	2:E:385:VAL:N	2.40	0.55
1:A:71:TYR:CE1	1:A:95:ILE:HG13	2.42	0.55
1:A:186:ASN:H	1:A:186:ASN:HD22	1.53	0.54
2:E:67:GLU:H	2:E:67:GLU:CD	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:SER:N	1:D:197:ASP:OD2	2.40	0.54
1:D:221:ILE:HG12	1:D:225:VAL:HG21	1.90	0.54
1:A:13:GLN:NE2	5:A:911:HOH:O	2.33	0.54
1:A:192:GLU:HB2	1:A:220:TYR:OH	2.07	0.54
2:E:84:TYR:CE1	2:E:85:GLN:HG3	2.42	0.54
2:E:65:SER:HB2	2:E:67:GLU:OE1	2.08	0.54
1:D:56:VAL:HG12	1:D:87:ALA:HB3	1.89	0.54
1:A:4:ILE:HD12	1:A:132:CYS:HB3	1.89	0.53
1:A:167:TYR:HB3	1:A:169:PHE:CE2	2.43	0.53
1:D:50:LEU:HB3	1:D:51:PRO:HD2	1.89	0.53
2:E:352:ASN:O	2:E:353:ASN:HB2	2.07	0.53
1:A:240:LYS:HG2	1:A:251:ILE:HG21	1.90	0.53
2:B:318:ILE:HG21	2:B:328:ILE:HD13	1.91	0.53
4:B:903:COA:CBP	4:B:903:COA:H10	2.18	0.53
1:D:167:TYR:HB3	1:D:169:PHE:CE2	2.43	0.53
2:B:103:ASP:HB3	2:B:205:LYS:HD2	1.91	0.53
2:B:248:TRP:HA	5:B:989:HOH:O	2.08	0.53
2:B:195:LEU:HD13	2:B:195:LEU:C	2.29	0.53
2:B:323:VAL:HA	5:B:994:HOH:O	2.08	0.53
2:B:383:ALA:O	2:B:385:VAL:N	2.42	0.53
1:A:212:SER:O	1:A:216:GLU:HG3	2.09	0.53
1:D:240:LYS:HG2	1:D:251:ILE:HG21	1.90	0.53
1:A:237:THR:HG23	2:B:274:ASP:OD1	2.09	0.53
1:A:275:SER:HB2	2:B:278:LEU:CD2	2.39	0.53
2:E:318:ILE:HG21	2:E:328:ILE:HD13	1.90	0.53
1:D:154:GLY:O	1:D:157:THR:HB	2.09	0.52
1:D:32:THR:HG23	1:D:132:CYS:SG	2.49	0.52
1:D:7:ASN:HA	1:D:33:LYS:HZ2	1.74	0.52
1:A:128:THR:O	1:A:128:THR:HG22	2.08	0.52
1:A:39:THR:HG21	1:A:42:LYS:HD2	1.92	0.52
1:D:141:ILE:HG13	1:D:161:VAL:CG1	2.35	0.52
1:D:166:ASP:C	1:D:168:GLY:H	2.13	0.52
1:A:166:ASP:C	1:A:168:GLY:H	2.11	0.52
1:D:71:TYR:CE1	1:D:95:ILE:HG13	2.45	0.52
2:E:161:ARG:NH1	5:E:954:HOH:O	2.41	0.52
1:A:66:THR:HB	1:A:90:LYS:HD3	1.92	0.52
1:D:180:ASP:HB3	1:D:181:PRO:CD	2.39	0.52
2:B:119:ARG:HG3	2:B:119:ARG:HH11	1.74	0.52
1:D:11:ILE:HA	1:D:36:GLY:O	2.10	0.52
1:A:201:GLU:O	1:A:228:PRO:HD2	2.10	0.51
2:B:67:GLU:CD	2:B:67:GLU:H	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:ASN:HB2	4:B:903:COA:O5P	2.11	0.51
2:B:352:ASN:O	2:B:353:ASN:HB2	2.11	0.51
1:A:243:ARG:HD2	1:A:247:ALA:HA	1.93	0.51
2:B:254:ALA:C	2:B:255:LEU:HD12	2.29	0.51
1:D:149:ILE:HG23	1:D:204:VAL:HB	1.92	0.51
2:B:206:GLN:HG2	5:B:967:HOH:O	2.09	0.51
1:A:1:SER:N	1:A:197:ASP:OD2	2.43	0.51
1:D:81:ILE:O	1:D:85:ILE:HG13	2.11	0.51
1:D:23:HIS:CE1	1:D:136:ILE:HG22	2.45	0.51
1:A:248:GLY:O	2:B:116:ARG:NH2	2.44	0.51
1:D:92:ILE:CG2	1:D:118:MET:HG3	2.41	0.50
2:E:119:ARG:HG3	2:E:119:ARG:HH11	1.77	0.50
2:E:2:ASN:ND2	5:E:911:HOH:O	2.44	0.50
1:D:129:PRO:HD2	1:D:172:SER:O	2.12	0.50
2:E:292:GLY:O	2:E:294:THR:N	2.44	0.50
2:B:213:ASP:HB3	5:B:964:HOH:O	2.11	0.50
1:D:285:THR:O	1:D:285:THR:HG22	2.12	0.49
2:E:317:ASN:ND2	2:E:348:ARG:HH11	2.10	0.49
2:B:263:VAL:HG22	2:B:317:ASN:HB3	1.93	0.49
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.94	0.49
1:D:56:VAL:HG11	1:D:84:ALA:HA	1.95	0.49
2:E:100:ALA:HB3	5:E:918:HOH:O	2.12	0.49
2:E:210:ILE:HB	5:E:968:HOH:O	2.11	0.49
2:E:254:ALA:C	2:E:255:LEU:HD12	2.33	0.49
2:E:263:VAL:HG22	2:E:317:ASN:HB3	1.94	0.49
2:E:106:LYS:CD	5:E:939:HOH:O	2.60	0.49
2:E:324:ARG:HD3	2:E:353:ASN:ND2	2.27	0.49
1:A:97:GLU:HB3	4:A:901:COA:H71	1.93	0.49
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.94	0.49
2:B:53:GLY:HA2	2:B:56:LYS:HD3	1.95	0.48
1:D:159:GLU:HG3	1:D:276:LEU:CD1	2.43	0.48
2:E:279:HIS:HE1	2:E:375:THR:HG22	1.78	0.48
2:E:356:LEU:O	2:E:356:LEU:HD12	2.13	0.48
1:A:9:LYS:HB3	1:A:35:VAL:CG1	2.43	0.48
1:A:67:ALA:HA	1:A:91:LEU:O	2.14	0.48
1:D:195:GLU:OE1	1:D:226:THR:N	2.42	0.48
1:A:195:GLU:OE1	1:A:226:THR:N	2.42	0.48
2:B:279:HIS:O	2:B:382:VAL:HG11	2.13	0.48
2:E:10:GLN:HG2	5:E:914:HOH:O	2.13	0.48
1:A:141:ILE:HG13	1:A:161:VAL:CG1	2.41	0.48
2:B:64:ASN:HA	5:B:926:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:LYS:O	1:D:33:LYS:CE	2.61	0.48
2:B:94:ASN:O	2:B:95:GLN:HG2	2.13	0.48
2:E:279:HIS:O	2:E:382:VAL:HG11	2.12	0.48
2:E:377:ALA:O	2:E:381:VAL:HG22	2.13	0.48
1:D:123:CYS:CB	1:D:124:PRO:HD2	2.41	0.48
4:D:902:COA:O2B	4:D:902:COA:O8A	2.31	0.48
2:B:369:ILE:N	2:B:369:ILE:CD1	2.77	0.48
2:E:132:GLU:HA	5:E:912:HOH:O	2.13	0.48
2:B:287:LEU:HD23	2:B:288:ASP:N	2.29	0.47
1:D:212:SER:O	1:D:216:GLU:HG3	2.14	0.47
1:A:149:ILE:HG23	1:A:204:VAL:HB	1.96	0.47
1:A:285:THR:HG22	1:A:285:THR:O	2.14	0.47
2:B:377:ALA:O	2:B:381:VAL:HG22	2.14	0.47
2:E:206:GLN:H	2:E:206:GLN:CD	2.18	0.47
1:D:66:THR:HB	1:D:90:LYS:HD3	1.95	0.47
1:D:7:ASN:HA	1:D:33:LYS:HZ1	1.80	0.47
1:D:19:GLN:CG	4:D:902:COA:H132	2.44	0.47
1:A:23:HIS:CE1	1:A:136:ILE:HG22	2.49	0.47
1:A:50:LEU:HB3	1:A:51:PRO:HD2	1.95	0.47
1:A:117:ARG:NH2	5:A:942:HOH:O	2.48	0.47
2:B:294:THR:O	2:B:298:VAL:HG23	2.15	0.47
2:B:356:LEU:O	2:B:356:LEU:HD12	2.15	0.47
1:D:208:GLU:OE2	1:D:246:HIS:ND1	2.39	0.47
1:D:275:SER:HB2	2:E:278:LEU:CD2	2.45	0.47
2:B:317:ASN:HD21	2:B:348:ARG:HH11	1.62	0.47
1:D:203:ILE:HB	1:D:229:VAL:HG22	1.96	0.46
1:A:262:PHE:O	1:A:266:GLU:HG3	2.16	0.46
2:B:279:HIS:HE1	2:B:375:THR:HG23	1.81	0.46
1:D:127:ILE:CD1	1:D:133:LYS:HG3	2.46	0.46
1:D:186:ASN:HD22	1:D:186:ASN:N	2.09	0.46
1:D:67:ALA:HA	1:D:91:LEU:O	2.16	0.46
1:A:221:ILE:HG12	1:A:225:VAL:HG21	1.96	0.46
2:E:279:HIS:HE1	2:E:375:THR:HG23	1.80	0.46
1:A:203:ILE:HB	1:A:229:VAL:HG22	1.97	0.46
1:D:142:HIS:HB3	1:D:171:GLN:OE1	2.15	0.46
2:E:333:ILE:HG23	2:E:366:LEU:HD12	1.97	0.46
1:A:195:GLU:OE1	1:A:225:VAL:HA	2.16	0.46
1:D:28:ILE:CG2	1:D:29:ALA:N	2.79	0.46
1:D:92:ILE:HG22	1:D:118:MET:HG3	1.97	0.46
1:D:127:ILE:HD12	1:D:133:LYS:HG3	1.97	0.46
1:A:202:ALA:CB	1:A:228:PRO:HG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ARG:HD2	1:D:247:ALA:HA	1.98	0.46
1:A:92:ILE:CG2	1:A:118:MET:HG3	2.46	0.45
2:B:191:ARG:HA	2:B:191:ARG:HD2	1.78	0.45
1:D:195:GLU:OE1	1:D:225:VAL:HA	2.16	0.45
2:B:105:ALA:HB3	2:B:203:ILE:O	2.16	0.45
1:D:180:ASP:HB3	1:D:181:PRO:HD2	1.98	0.45
2:E:325:CYS:HB2	2:E:352:ASN:O	2.16	0.45
1:A:186:ASN:N	1:A:186:ASN:HD22	2.12	0.45
1:A:159:GLU:HG3	1:A:276:LEU:CD1	2.47	0.45
1:A:77:CYS:O	1:A:81:ILE:HG13	2.16	0.45
1:D:147:VAL:CG1	1:D:204:VAL:HG23	2.47	0.45
2:B:119:ARG:NH1	2:B:119:ARG:HG3	2.31	0.45
2:B:333:ILE:HG23	2:B:366:LEU:HD12	1.99	0.45
2:E:282:GLU:N	5:E:981:HOH:O	2.50	0.45
1:A:164:THR:HG22	1:A:283:LEU:HD12	1.97	0.45
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.82	0.45
2:B:324:ARG:HH21	2:B:327:LEU:HD11	1.80	0.45
2:B:336:VAL:HG13	2:B:341:VAL:HB	1.99	0.45
2:B:84:TYR:CD1	2:B:85:GLN:HG3	2.51	0.45
1:A:275:SER:HB2	2:B:278:LEU:HD21	1.99	0.45
1:A:276:LEU:H	1:A:276:LEU:HD23	1.82	0.45
1:D:227:LYS:HB3	1:D:228:PRO:HD2	1.99	0.45
1:A:166:ASP:C	1:A:168:GLY:N	2.71	0.44
2:B:317:ASN:C	2:B:317:ASN:ND2	2.70	0.44
2:E:84:TYR:CD1	2:E:85:GLN:HG3	2.52	0.44
1:A:42:LYS:NZ	4:A:901:COA:O7A	2.43	0.44
2:B:254:ALA:O	2:B:255:LEU:HD12	2.17	0.44
2:E:12:PHE:HB3	2:E:17:LEU:HB2	1.99	0.44
2:E:279:HIS:CE1	2:E:375:THR:HG23	2.53	0.44
2:E:383:ALA:C	2:E:385:VAL:H	2.22	0.44
1:A:56:VAL:HG12	1:A:87:ALA:HB3	1.98	0.44
2:E:84:TYR:C	2:E:84:TYR:CD1	2.90	0.44
2:E:329:ALA:O	2:E:333:ILE:HG13	2.18	0.44
1:A:198:PRO:HG2	1:A:199:GLN:H	1.82	0.43
1:A:6:LYS:HE3	1:A:6:LYS:HB2	1.68	0.43
2:B:212:LEU:HD12	2:B:212:LEU:HA	1.81	0.43
1:A:143:LYS:HA	1:A:144:PRO:HD3	1.90	0.43
1:A:128:THR:HG1	1:A:173:THR:HG1	1.57	0.43
2:E:369:ILE:CD1	2:E:369:ILE:N	2.80	0.43
1:A:285:THR:O	1:A:286:VAL:CG1	2.64	0.43
1:D:229:VAL:O	1:D:270:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:LEU:HB2	2:E:381:VAL:HG11	2.00	0.43
2:B:317:ASN:HD22	2:B:317:ASN:C	2.20	0.43
2:E:317:ASN:HD21	2:E:348:ARG:NH1	2.13	0.43
1:D:192:GLU:O	1:D:192:GLU:HG3	2.18	0.43
1:A:202:ALA:HB2	1:A:228:PRO:HG2	2.00	0.43
2:B:383:ALA:C	2:B:385:VAL:H	2.22	0.43
2:B:263:VAL:HG12	2:B:264:ASN:N	2.34	0.43
2:B:300:GLU:OE2	2:B:303:LYS:NZ	2.52	0.43
2:B:371:ALA:CB	2:B:377:ALA:HB2	2.49	0.43
1:D:42:LYS:NZ	4:D:902:COA:O7A	2.48	0.43
2:E:360:LYS:HE2	2:E:360:LYS:HB3	1.86	0.43
1:A:4:ILE:HD12	1:A:132:CYS:SG	2.59	0.42
2:B:161:ARG:HD2	5:B:953:HOH:O	2.19	0.42
1:D:121:PRO:HG2	1:D:180:ASP:OD2	2.19	0.42
2:E:132:GLU:HG3	5:E:912:HOH:O	2.19	0.42
1:A:121:PRO:HG2	1:A:180:ASP:OD2	2.19	0.42
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.55	0.42
2:B:346:VAL:HB	2:B:381:VAL:HG13	2.02	0.42
1:D:166:ASP:C	1:D:168:GLY:N	2.72	0.42
1:D:57:ARG:O	1:D:58:GLU:C	2.54	0.42
2:E:191:ARG:HA	2:E:191:ARG:HD2	1.79	0.42
2:B:206:GLN:H	2:B:206:GLN:CD	2.23	0.42
2:B:380:GLN:O	2:B:383:ALA:HB3	2.20	0.42
1:D:24:SER:HA	5:D:911:HOH:O	2.19	0.42
2:E:109:TYR:O	2:E:125:ALA:HA	2.19	0.42
2:E:380:GLN:O	2:E:383:ALA:HB3	2.19	0.42
1:D:158:TYR:N	1:D:158:TYR:CD1	2.87	0.42
1:D:242:LYS:HE3	1:D:242:LYS:HB3	1.93	0.42
2:B:287:LEU:HD23	2:B:287:LEU:C	2.40	0.42
1:D:223:GLU:HG3	1:D:223:GLU:O	2.20	0.42
1:D:274:ARG:HD2	5:D:960:HOH:O	2.20	0.42
2:E:312:LYS:O	2:E:343:VAL:HB	2.20	0.42
1:D:92:ILE:O	1:D:118:MET:HA	2.20	0.41
1:A:147:VAL:CG1	1:A:204:VAL:HG23	2.51	0.41
1:D:128:THR:HG22	1:D:128:THR:O	2.20	0.41
1:D:187:PHE:HE2	1:D:214:GLU:OE2	2.04	0.41
2:E:119:ARG:HG3	2:E:119:ARG:NH1	2.35	0.41
2:E:219:ASP:OD1	2:E:221:ASN:HB2	2.20	0.41
1:A:145:GLY:HA3	1:A:170:GLY:HA3	2.01	0.41
1:A:255:LYS:HD2	1:A:255:LYS:HA	1.79	0.41
1:A:11:ILE:HA	1:A:36:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ARG:HB3	5:B:943:HOH:O	2.20	0.41
1:A:167:TYR:CB	1:A:169:PHE:CE2	3.03	0.41
2:B:229:LEU:HG	5:B:975:HOH:O	2.19	0.41
2:B:319:PHE:CD1	2:B:319:PHE:C	2.94	0.41
2:B:348:ARG:NH1	2:B:374:LEU:HD13	2.36	0.41
2:B:312:LYS:O	2:B:343:VAL:HB	2.21	0.41
1:D:246:HIS:HA	5:D:957:HOH:O	2.20	0.41
1:A:186:ASN:ND2	1:A:189:ASP:OD2	2.54	0.41
2:B:369:ILE:HG21	2:B:380:GLN:NE2	2.35	0.41
2:B:84:TYR:CD1	2:B:84:TYR:C	2.93	0.41
1:D:34:MET:O	1:D:50:LEU:CD1	2.69	0.41
2:B:215:LYS:O	2:B:216:LEU:HD23	2.20	0.41
1:A:92:ILE:HG22	1:A:118:MET:HG3	2.02	0.41
2:B:191:ARG:HD2	5:B:960:HOH:O	2.20	0.41
2:B:202:VAL:O	2:B:209:LEU:HA	2.21	0.41
1:A:13:GLN:NE2	1:A:56:VAL:HG21	2.36	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.76	0.41
2:B:116:ARG:HG3	5:B:941:HOH:O	2.20	0.41
1:D:6:LYS:HB2	1:D:6:LYS:HE3	1.69	0.41
1:D:192:GLU:O	1:D:192:GLU:CG	2.67	0.41
1:D:274:ARG:HG2	1:D:274:ARG:HH11	1.85	0.41
2:E:346:VAL:HB	2:E:381:VAL:HG13	2.02	0.41
2:E:79:LYS:CE	5:E:931:HOH:O	2.65	0.41
1:A:40:PRO:HD3	4:A:901:COA:C2A	2.51	0.40
2:B:360:LYS:HE2	2:B:360:LYS:HB3	1.83	0.40
2:B:292:GLY:O	2:B:294:THR:N	2.53	0.40
1:D:2:ILE:O	1:D:4:ILE:N	2.53	0.40
1:A:223:GLU:O	1:A:223:GLU:HG3	2.20	0.40
2:B:199:ASN:HA	2:B:200:PRO:HA	1.83	0.40
1:D:275:SER:C	1:D:277:ALA:H	2.24	0.40
2:E:263:VAL:HG12	2:E:264:ASN:N	2.37	0.40
2:E:94:ASN:O	2:E:95:GLN:HG2	2.22	0.40
1:A:5:ASP:C	1:A:5:ASP:OD1	2.60	0.40
1:D:197:ASP:OD1	1:D:198:PRO:HD2	2.21	0.40
1:D:205:MET:HE3	1:D:265:LEU:HD21	2.02	0.40
1:A:227:LYS:HB3	1:A:228:PRO:HD2	2.02	0.40
2:B:2:ASN:ND2	5:B:911:HOH:O	2.55	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	284/286 (99%)	261 (92%)	23 (8%)	0	100	100
1	D	284/286 (99%)	256 (90%)	27 (10%)	1 (0%)	34	66
2	B	383/385 (100%)	367 (96%)	14 (4%)	2 (0%)	29	61
2	E	383/385 (100%)	368 (96%)	13 (3%)	2 (0%)	29	61
All	All	1334/1342 (99%)	1252 (94%)	77 (6%)	5 (0%)	34	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	384	ALA
2	E	384	ALA
2	B	87	ASP
2	E	87	ASP
1	D	3	LEU

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	216/216 (100%)	205 (95%)	11 (5%)	24	56
1	D	216/216 (100%)	203 (94%)	13 (6%)	19	49
2	B	296/296 (100%)	280 (95%)	16 (5%)	22	54
2	E	296/296 (100%)	283 (96%)	13 (4%)	28	61
All	All	1024/1024 (100%)	971 (95%)	53 (5%)	23	55

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	55	THR
1	A	77	CYS
1	A	90	LYS
1	A	137	GLN
1	A	143	LYS
1	A	150	VAL
1	A	186	ASN
1	A	226	THR
1	A	278	ASP
1	A	286	VAL
2	B	11	LEU
2	B	56	LYS
2	B	70	ARG
2	B	124	MET
2	B	134	GLU
2	B	195	LEU
2	B	200	PRO
2	B	238	GLU
2	B	256	ASP
2	B	294	THR
2	B	295	LYS
2	B	317	ASN
2	B	319	PHE
2	B	348	ARG
2	B	367	ASN
2	B	381	VAL
1	D	28	ILE
1	D	46	THR
1	D	55	THR
1	D	77	CYS
1	D	90	LYS
1	D	128	THR
1	D	137	GLN
1	D	143	LYS
1	D	150	VAL
1	D	186	ASN
1	D	276	LEU
1	D	278	ASP
1	D	286	VAL
2	E	11	LEU
2	E	56	LYS

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Mol	Chain	Res	Type
2	E	70	ARG
2	E	134	GLU
2	E	195	LEU
2	E	200	PRO
2	E	238	GLU
2	E	256	ASP
2	E	295	LYS
2	E	317	ASN
2	E	319	PHE
2	E	348	ARG
2	E	381	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
2	B	2	ASN
2	B	50	HIS
2	B	221	ASN
2	B	279	HIS
2	B	317	ASN
2	B	342	ASN
2	B	380	GLN
1	D	186	ASN
2	E	2	ASN
2	E	50	HIS
2	E	235	GLN
2	E	279	HIS
2	E	317	ASN
2	E	353	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

7 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	#$|Z| > 2$
4	COA	D	902	-	41,50,50	0.94	1 (2%)	52,75,75	2.17	13 (25%)
4	COA	A	901	-	41,50,50	1.16	2 (4%)	52,75,75	2.33	14 (26%)
3	PO4	A	906	-	4,4,4	1.49	0	6,6,6	0.51	0
3	PO4	D	907	-	4,4,4	1.81	2 (50%)	6,6,6	0.46	0
3	PO4	E	905	-	4,4,4	1.76	2 (50%)	6,6,6	0.48	0
4	COA	B	903	2	14,16,50	9.31	5 (35%)	19,21,75	3.90	13 (68%)
3	PO4	B	904	-	4,4,4	1.59	1 (25%)	6,6,6	0.55	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
4	COA	B	903	2	-	3/20/20/64	-
4	COA	A	901	-	-	1/44/64/64	0/3/3/3
4	COA	D	902	-	-	1/44/64/64	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	COA	CBP-CAP	34.14	1.78	1.55
4	A	901	COA	C6P-C5P	4.78	1.60	1.51
4	B	903	COA	CCP-CBP	3.11	1.60	1.53
4	B	903	COA	C6P-C5P	3.09	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	COA	CEP-CBP	2.79	1.59	1.53
4	A	901	COA	CEP-CBP	-2.49	1.48	1.53
4	B	903	COA	C7P-N8P	2.49	1.51	1.46
3	D	907	PO4	P-O2	-2.42	1.47	1.54
4	D	902	COA	P2A-O6A	-2.40	1.49	1.59
3	E	905	PO4	P-O2	-2.16	1.48	1.54
3	D	907	PO4	P-O3	-2.09	1.48	1.54
3	B	904	PO4	P-O3	-2.04	1.48	1.54
3	E	905	PO4	P-O4	-2.00	1.48	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	903	COA	CEP-CBP-CCP	-8.64	92.03	108.80
4	A	901	COA	CEP-CBP-CCP	-8.03	95.14	108.23
4	D	902	COA	C3P-N4P-C5P	7.07	135.97	122.84
4	B	903	COA	CCP-CBP-CAP	6.97	125.65	109.59
4	D	902	COA	O5P-C5P-C6P	-6.87	109.45	122.02
4	A	901	COA	C6P-C5P-N4P	6.04	126.59	116.42
4	A	901	COA	O5P-C5P-C6P	-5.71	111.57	122.02
4	D	902	COA	CAP-C9P-N8P	-5.67	105.28	116.58
4	B	903	COA	CEP-CBP-CAP	5.48	122.21	109.59
4	A	901	COA	CEP-CBP-CAP	5.33	118.07	108.82
4	B	903	COA	C3P-N4P-C5P	4.62	131.42	122.84
4	B	903	COA	CDP-CBP-CAP	-4.61	98.96	109.59
4	A	901	COA	C7P-N8P-C9P	4.47	130.57	122.59
4	B	903	COA	C7P-C6P-C5P	4.10	119.19	112.36
4	B	903	COA	C6P-C5P-N4P	4.07	123.28	116.42
4	D	902	COA	CEP-CBP-CDP	4.05	117.42	109.17
4	D	902	COA	O5P-C5P-N4P	3.91	130.39	123.01
4	A	901	COA	C3P-N4P-C5P	3.76	129.83	122.84
4	A	901	COA	CDP-CBP-CCP	3.73	114.32	108.23
4	B	903	COA	CDP-CBP-CCP	-3.67	101.67	108.80
4	B	903	COA	CEP-CBP-CDP	3.62	115.83	108.80
4	D	902	COA	CEP-CBP-CCP	-3.06	103.24	108.23
4	B	903	COA	O5P-C5P-C6P	-2.97	116.58	122.02
4	A	901	COA	C7P-C6P-C5P	2.91	117.21	112.36
4	A	901	COA	P2A-O3A-P1A	-2.80	123.23	132.83
4	A	901	COA	CAP-C9P-N8P	2.77	122.09	116.58
4	D	902	COA	P2A-O3A-P1A	-2.76	123.35	132.83
4	A	901	COA	O4B-C1B-C2B	-2.72	102.95	106.93
4	D	902	COA	O4B-C1B-C2B	-2.71	102.96	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	902	COA	C5A-C6A-N6A	2.61	124.33	120.35
4	D	902	COA	C7P-C6P-C5P	-2.53	108.14	112.36
4	B	903	COA	C7P-N8P-C9P	2.46	126.97	122.59
4	B	903	COA	C6P-C7P-N8P	2.44	116.83	111.90
4	D	902	COA	CDP-CBP-CCP	-2.33	104.43	108.23
4	D	902	COA	O9P-C9P-N8P	2.32	127.98	122.99
4	D	902	COA	C6P-C5P-N4P	2.22	120.16	116.42
4	A	901	COA	O9P-C9P-CAP	-2.17	114.43	121.06
4	A	901	COA	C2P-C3P-N4P	-2.15	107.40	112.31
4	B	903	COA	CAP-C9P-N8P	2.02	120.61	116.58
4	A	901	COA	C6P-C7P-N8P	-2.00	107.85	111.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	903	COA	C5P-C6P-C7P-N8P
4	B	903	COA	N8P-C9P-CAP-CBP
4	B	903	COA	O9P-C9P-CAP-CBP
4	A	901	COA	O4B-C4B-C5B-O5B
4	D	902	COA	O4B-C4B-C5B-O5B

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	902	COA	4	0
4	A	901	COA	4	0
4	B	903	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 902

Bond lengths

Bond angles

Torsions

Rings

Ligand COA A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand COA B 903

Bond lengths

Bond angles

Torsions

Rings
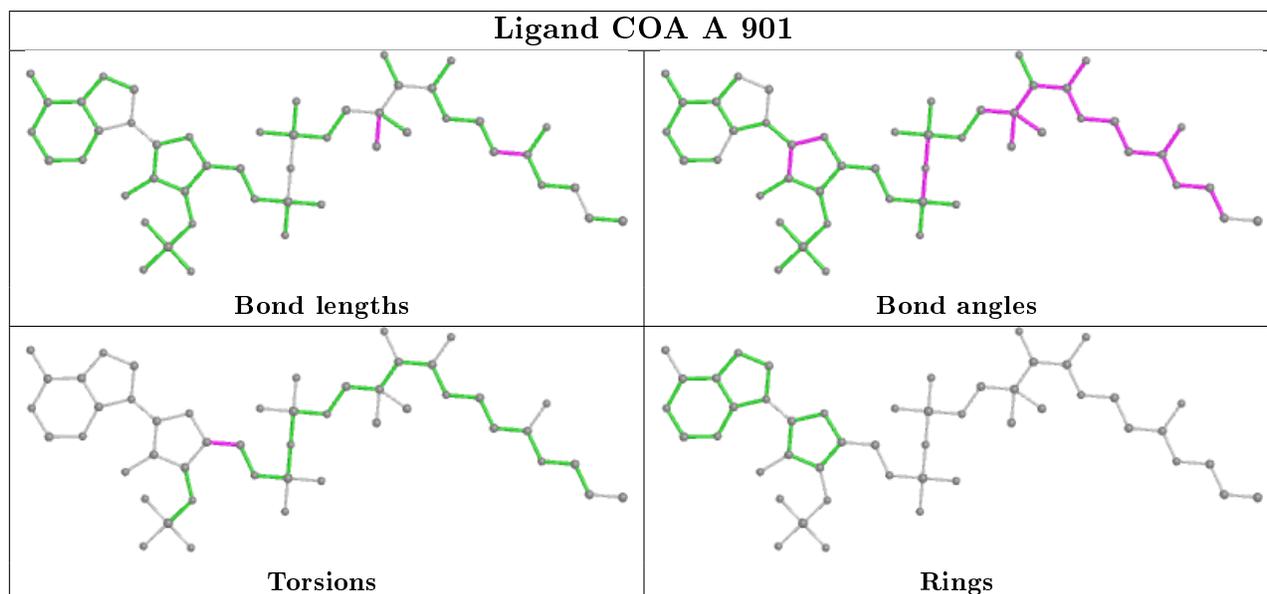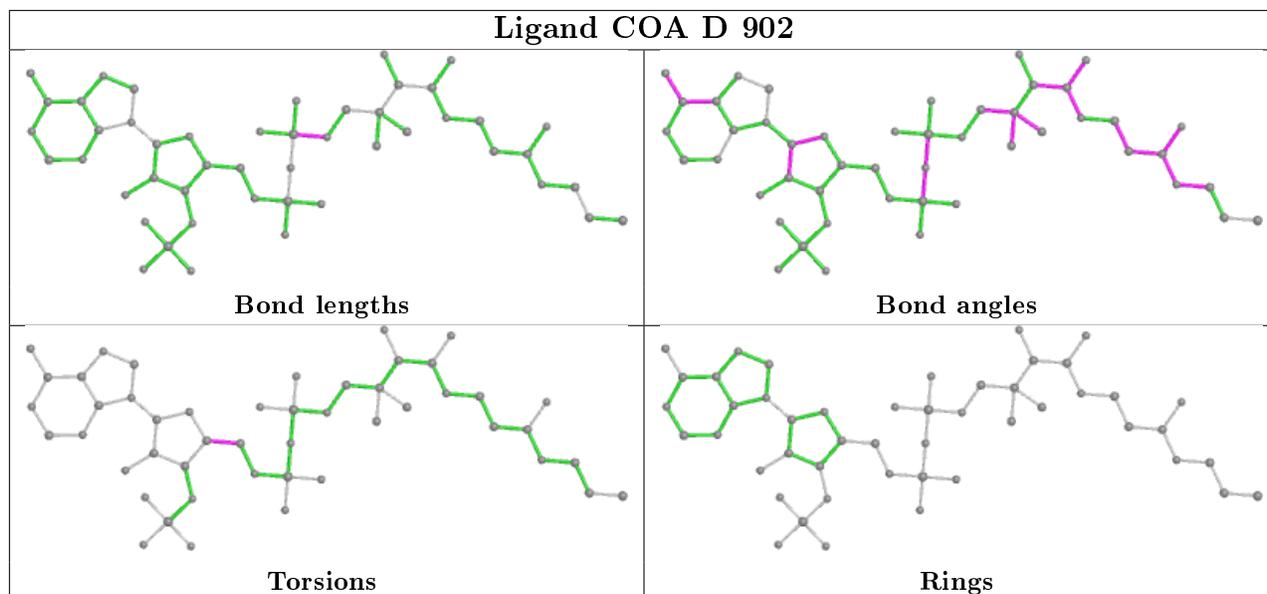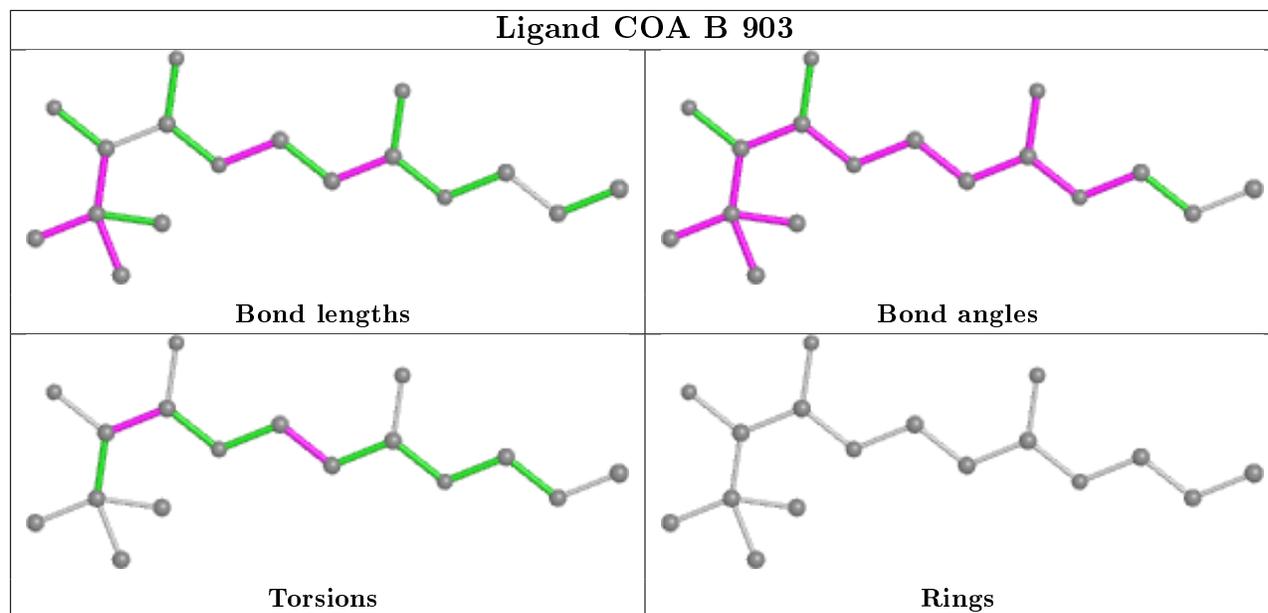
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6   Fit of model and data (i)

6.1   Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	286/286 (100%)	-0.85	0	100	100	12, 36, 56, 70	0
1	D	286/286 (100%)	-0.48	0	100	100	20, 49, 69, 82	0
2	B	385/385 (100%)	-0.80	0	100	100	13, 37, 59, 80	0
2	E	385/385 (100%)	-0.73	1 (0%)	94	94	15, 37, 68, 89	0
All	All	1342/1342 (100%)	-0.72	1 (0%)	95	96	12, 39, 65, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	372	LYS	2.4

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, 95th 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(Å²)	Q<0.9
4	COA	B	903	17/48	0.90	0.18	54,62,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COA	A	901	48/48	0.98	0.10	26,33,44,56	0
4	COA	D	902	48/48	0.98	0.12	25,34,47,53	0
3	PO4	B	904	5/5	0.98	0.09	69,70,70,71	0
3	PO4	D	907	5/5	0.99	0.09	38,38,39,40	0
3	PO4	E	905	5/5	0.99	0.07	54,54,55,55	0
3	PO4	A	906	5/5	1.00	0.06	38,40,41,42	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 B 903:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
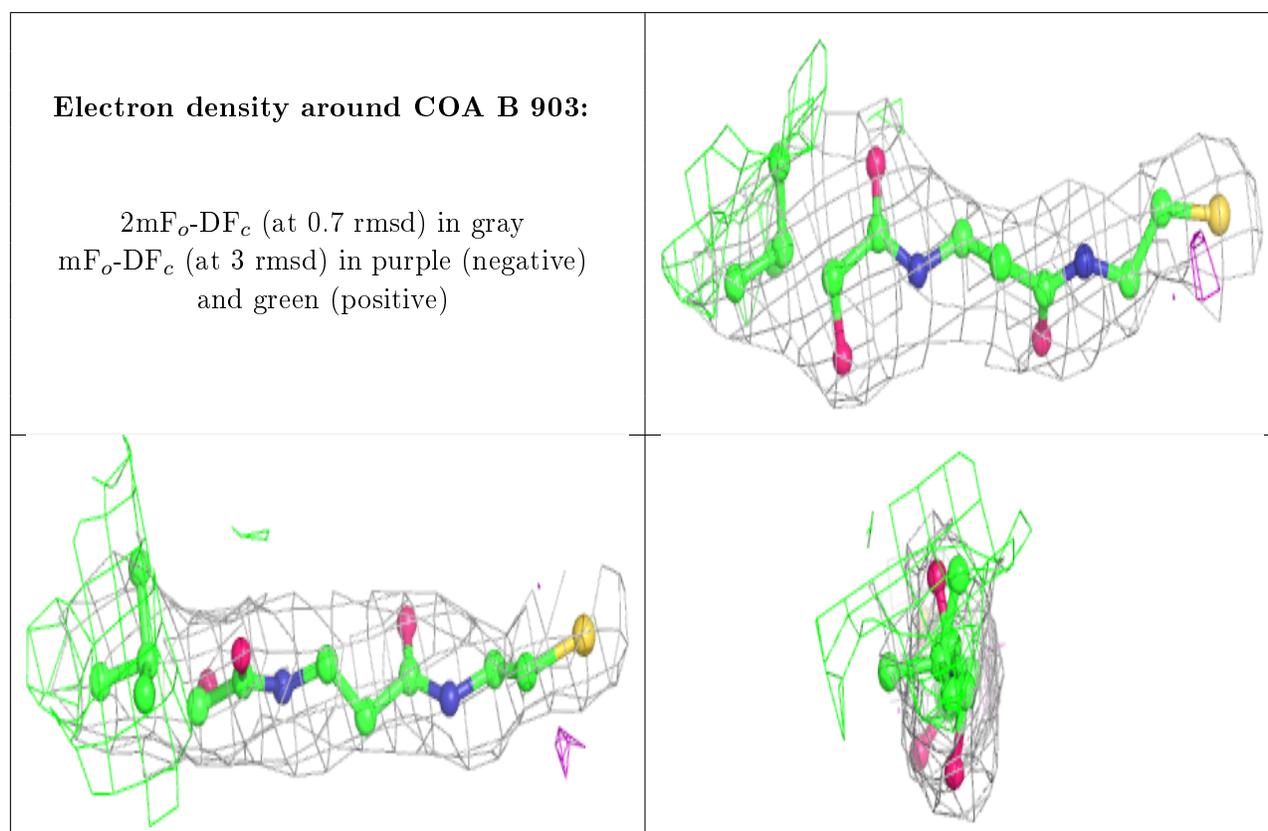
Electron density around COA A 901:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
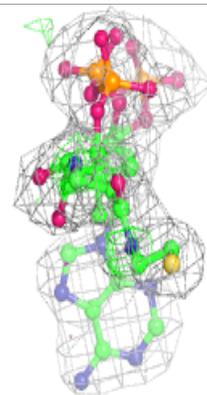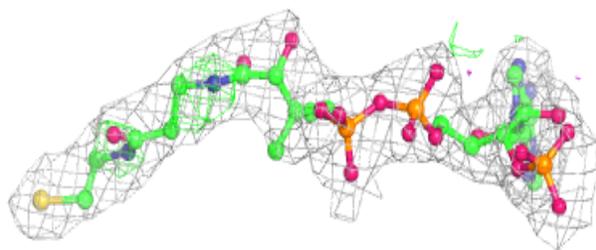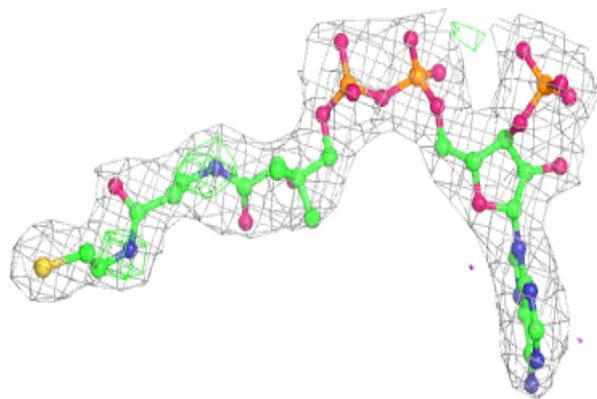
Electron density around COA D 902:

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

6.5 Other polymers (i)

There are no such residues in this entry.