



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:44 AM EDT

PDB ID : 1JLL
Title : Crystal Structure Analysis of the E197betaA Mutant of E. coli SCS
Authors : Fraser, M.E.
Deposited on : 2001-07-16
Resolution : 2.69 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 : 2.23.2
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) : 2.23.2

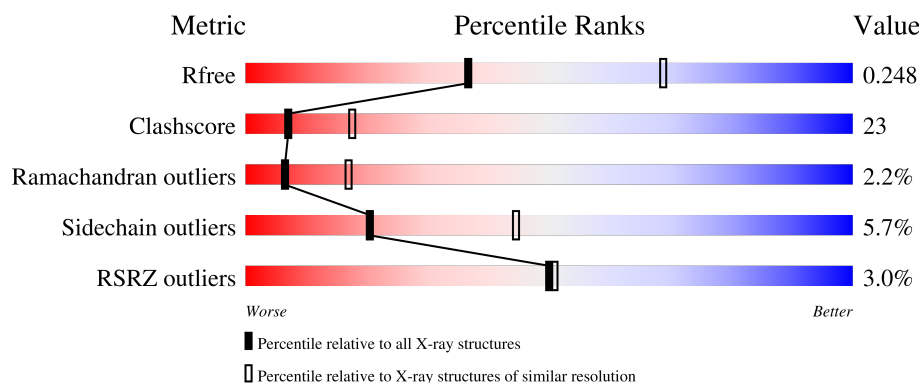
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>..</div> </div> </div>
1	D	288	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>40%</div> <div>.</div> </div> </div>
2	B	388	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>6%</div> </div> </div>
2	E	388	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>34%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	D	1601	-	-	X	-
4	COA	B	1903	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10255 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 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2069	1313	346	399	11			
1	D	287	Total	C	N	O	S	0	0	0
			2069	1313	346	399	11			

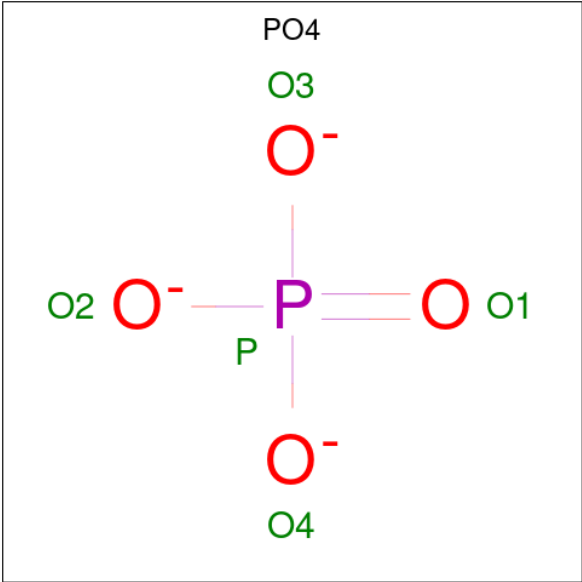
- Molecule 2 is a protein called succinyl-CoA synthetase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			2904	1834	509	548	13			
2	E	385	Total	C	N	O	S	0	0	0
			2881	1821	505	542	13			

There are 2 discrepancies between the modelled and reference sequences:

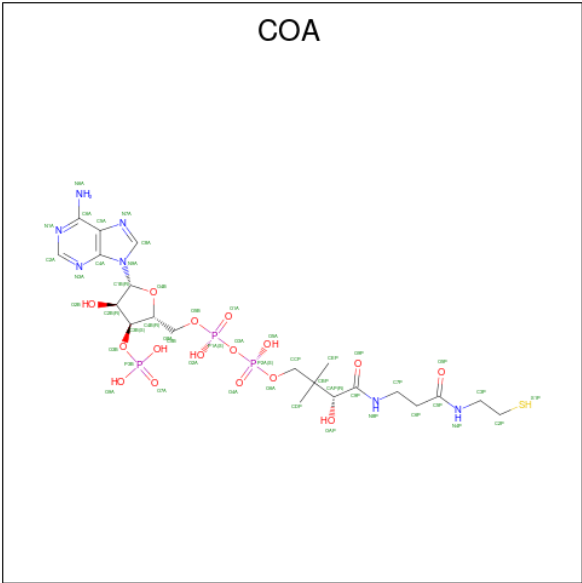
Chain	Residue	Modelled	Actual	Comment	Reference
B	197	ALA	GLU	engineered mutation	UNP P0A836
E	197	ALA	GLU	engineered mutation	UNP P0A836

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
4	B	1	Total	C	N	O	S	0	0
			17	11	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
4	E	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

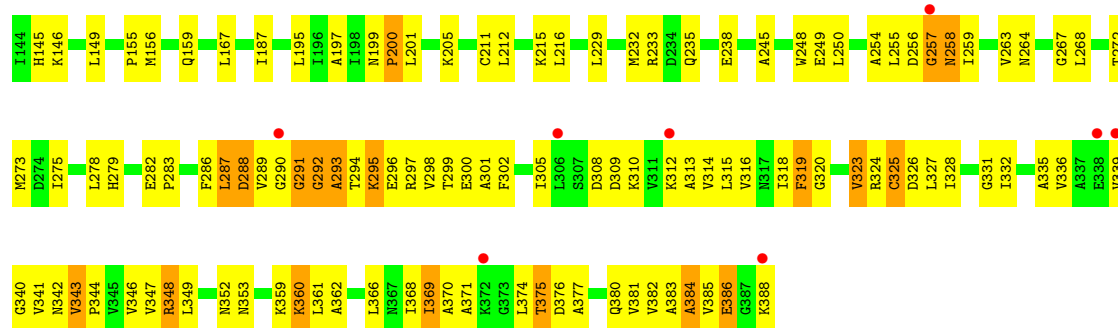
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total	O	0	0
			57	57		
6	B	46	Total	O	0	0
			46	46		
6	D	34	Total	O	0	0
			34	34		

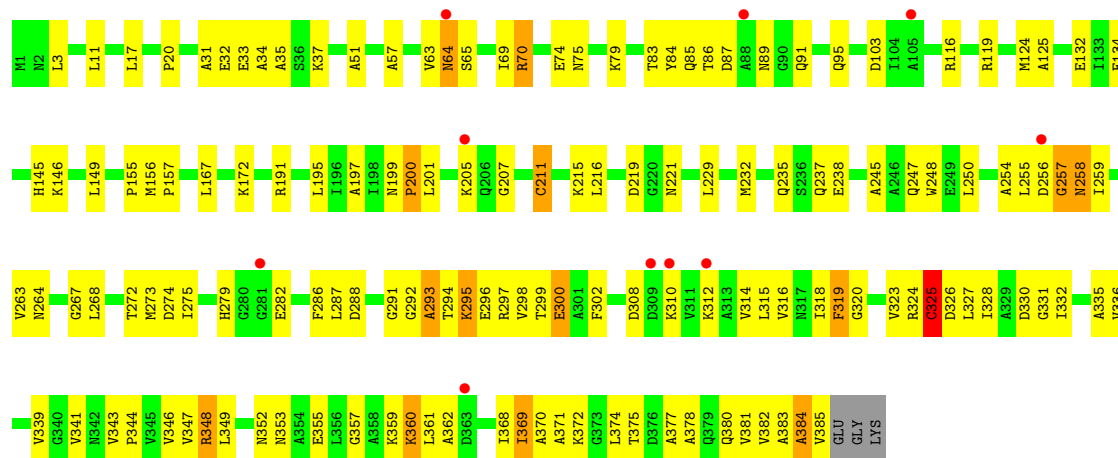
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	56	Total	O	0	0
			56	56		



• Molecule 2: succinyl-CoA synthetase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.06Å 97.06Å 389.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.38 – 2.69 34.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.5 (34.38-2.69) 91.5 (34.38-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.259 0.218 , 0.248	Depositor DCC
R_{free} test set	1000 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SO4, 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	0.82	1/2103 (0.0%)	0.88	1/2849 (0.0%)
1	D	0.75	1/2103 (0.0%)	0.87	1/2849 (0.0%)
2	B	0.76	0/2946	0.85	1/3984 (0.0%)
2	E	0.76	4/2923 (0.1%)	0.88	1/3956 (0.0%)
All	All	0.77	6/10075 (0.1%)	0.87	4/13638 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	CYS	CB-SG	-8.79	1.67	1.82
2	E	132	GLU	CG-CD	6.50	1.61	1.51
1	D	77	CYS	CB-SG	-6.21	1.71	1.82
2	E	132	GLU	CB-CG	5.54	1.62	1.52
2	E	211	CYS	CB-SG	5.35	1.91	1.82
2	E	300	GLU	CG-CD	5.05	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	GLY	N-CA-C	6.13	128.42	113.10
2	E	201	LEU	N-CA-C	-5.92	95.01	111.00
2	B	201	LEU	N-CA-C	-5.85	95.20	111.00
1	D	139	GLY	N-CA-C	5.85	127.72	113.10

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	2069	0	2129	114	0
1	D	2069	0	2129	120	0
2	B	2904	0	2961	134	0
2	E	2881	0	2939	122	0
3	A	5	0	0	1	0
3	D	5	0	0	2	0
4	A	42	0	24	2	0
4	B	17	0	18	2	0
4	D	42	0	24	1	0
4	E	8	0	7	2	0
5	B	10	0	0	1	0
5	E	10	0	0	0	0
6	A	57	0	0	3	0
6	B	46	0	0	3	0
6	D	34	0	0	2	0
6	E	56	0	0	5	0
All	All	10255	0	10231	465	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 23.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:369:ILE:HG22	2:E:370:ALA:H	1.23	1.04
2:B:369:ILE:HG22	2:B:370:ALA:H	1.25	0.98
2:E:295:LYS:HG2	2:E:331:GLY:HA2	1.46	0.97
2:B:295:LYS:HG2	2:B:331:GLY:HA2	1.46	0.94
1:A:145:GLY:HA3	1:A:170:GLY:HA3	1.51	0.89
1:D:145:GLY:HA3	1:D:170:GLY:HA3	1.54	0.88
2:B:291:GLY:O	2:B:293:ALA:N	2.08	0.85
2:E:369:ILE:HG22	2:E:370:ALA:N	1.92	0.84
2:B:369:ILE:HG22	2:B:370:ALA:N	1.92	0.84
2:E:238:GLU:HG3	6:E:1928:HOH:O	1.79	0.81
1:D:139:GLY:HA2	1:D:142:HIS:ND1	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:308:ASP:OD1	2:E:310:LYS:HG2	1.82	0.80
2:B:343:VAL:HG12	2:B:344:PRO:HD2	1.63	0.79
2:B:310:LYS:HE3	6:B:1936:HOH:O	1.82	0.79
2:E:325:CYS:HB2	2:E:352:ASN:O	1.81	0.79
2:E:343:VAL:HB	2:E:344:PRO:HD2	1.62	0.78
2:B:325:CYS:HB2	2:B:352:ASN:O	1.83	0.78
1:A:169:PHE:CE1	1:A:287:LEU:HD23	2.18	0.78
1:A:139:GLY:HA2	1:A:142:HIS:ND1	1.99	0.77
2:E:369:ILE:HG21	2:E:380:GLN:OE1	1.86	0.76
1:D:124:PRO:HB2	1:D:176:GLY:O	1.85	0.76
2:B:369:ILE:CG2	2:B:370:ALA:H	1.99	0.75
2:E:64:ASN:ND2	6:E:1924:HOH:O	2.19	0.75
2:B:308:ASP:OD1	2:B:310:LYS:HG2	1.86	0.75
1:D:223:GLU:HG2	1:D:224:HIS:CD2	2.22	0.75
1:A:124:PRO:HB2	1:A:176:GLY:O	1.86	0.74
2:E:75:ASN:O	2:E:79:LYS:HD2	1.87	0.73
2:B:36:SER:HB2	6:D:1630:HOH:O	1.87	0.72
1:A:223:GLU:HG2	1:A:224:HIS:CD2	2.24	0.72
1:A:129:PRO:HG2	1:A:171:GLN:HB2	1.70	0.71
1:D:129:PRO:HG2	1:D:171:GLN:HB2	1.72	0.71
2:E:369:ILE:CG2	2:E:370:ALA:H	2.00	0.71
1:D:273:VAL:CG2	1:D:278:ASP:HB2	2.20	0.71
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.73	0.71
1:A:186:ASN:HD22	1:A:187:PHE:H	1.39	0.70
2:B:229:LEU:HD23	2:B:232:MET:HE3	1.73	0.70
2:E:103:ASP:HB3	2:E:205:LYS:HG3	1.74	0.70
2:B:302:PHE:CE1	2:B:314:VAL:HG11	2.27	0.70
2:B:279:HIS:O	2:B:382:VAL:HG11	1.92	0.69
2:B:369:ILE:HG21	2:B:380:GLN:OE1	1.92	0.69
1:D:169:PHE:CE1	1:D:287:LEU:HD23	2.27	0.69
1:A:273:VAL:HG23	1:A:278:ASP:HB2	1.75	0.69
2:E:258:ASN:H	2:E:258:ASN:HD22	1.39	0.69
2:E:315:LEU:HB2	2:E:381:VAL:HG11	1.72	0.68
1:D:273:VAL:HG23	1:D:278:ASP:HB2	1.75	0.68
2:B:75:ASN:O	2:B:79:LYS:HD2	1.93	0.67
2:B:103:ASP:HB3	2:B:205:LYS:HG3	1.76	0.67
2:E:279:HIS:O	2:E:382:VAL:HG11	1.95	0.67
1:A:39:THR:HG21	1:A:42:LYS:HD2	1.76	0.67
1:A:23:HIS:CD2	1:A:136:ILE:HG22	2.31	0.66
2:B:348:ARG:C	2:B:348:ARG:HD2	2.16	0.66
1:D:159:GLU:OE2	2:E:319:PHE:CD2	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:HG21	2:B:264:ASN:O	1.95	0.66
1:A:273:VAL:CG2	1:A:278:ASP:HB2	2.25	0.66
1:D:23:HIS:CG	1:D:136:ILE:HG22	2.31	0.66
1:D:186:ASN:HD22	1:D:187:PHE:H	1.42	0.66
1:D:285:THR:HG22	1:D:286:VAL:N	2.10	0.66
1:A:273:VAL:HG13	1:A:273:VAL:O	1.95	0.65
2:B:294:THR:O	2:B:298:VAL:HG23	1.96	0.65
2:E:325:CYS:O	2:E:349:LEU:HD13	1.97	0.65
1:D:273:VAL:HG13	1:D:273:VAL:O	1.95	0.65
2:E:383:ALA:O	2:E:385:VAL:N	2.30	0.65
1:D:9:LYS:HD3	1:D:35:VAL:HG11	1.78	0.64
1:A:23:HIS:CG	1:A:136:ILE:HG22	2.31	0.64
2:E:294:THR:O	2:E:298:VAL:HG23	1.97	0.64
1:A:124:PRO:CB	1:A:176:GLY:O	2.45	0.64
2:B:325:CYS:O	2:B:349:LEU:HD13	1.97	0.64
1:D:197:ASP:O	1:D:227:LYS:NZ	2.31	0.64
1:A:150:VAL:CG1	1:A:190:ILE:HG21	2.29	0.63
2:B:371:ALA:CB	2:B:377:ALA:HB2	2.28	0.63
1:D:23:HIS:CD2	1:D:136:ILE:HG22	2.33	0.63
1:A:275:SER:HB2	2:B:278:LEU:HD21	1.80	0.63
2:B:70:ARG:O	2:B:74:GLU:HG3	1.99	0.63
2:E:302:PHE:CE1	2:E:314:VAL:HG11	2.33	0.63
1:D:81:ILE:O	1:D:85:ILE:HG13	1.99	0.62
2:B:292:GLY:O	2:B:294:THR:N	2.28	0.62
1:D:124:PRO:CB	1:D:176:GLY:O	2.48	0.62
1:A:222:LYS:HB2	1:A:268:ALA:HB1	1.81	0.62
2:B:258:ASN:HD22	2:B:258:ASN:H	1.44	0.62
1:D:222:LYS:HB2	1:D:268:ALA:HB1	1.82	0.62
2:B:383:ALA:O	2:B:385:VAL:N	2.32	0.62
2:E:124:MET:HA	2:E:145:HIS:O	2.00	0.61
1:D:237:THR:HG23	2:E:274:ASP:OD1	1.99	0.61
1:D:39:THR:HG21	1:D:42:LYS:HD2	1.82	0.61
1:D:42:LYS:NZ	4:D:1301:COA:O7A	2.31	0.61
2:E:70:ARG:O	2:E:74:GLU:HG3	2.00	0.61
1:D:93:ILE:HD12	1:D:126:VAL:HG23	1.82	0.61
1:A:138:PRO:O	1:A:141:ILE:HG12	2.00	0.61
1:A:285:THR:HG22	1:A:286:VAL:N	2.16	0.61
1:A:275:SER:HB2	2:B:278:LEU:CD2	2.31	0.60
1:A:276:LEU:H	1:A:276:LEU:HD23	1.66	0.60
1:A:281:GLU:O	1:A:284:LYS:HB3	2.02	0.60
1:A:164:THR:HG22	1:A:283:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:PRO:O	1:D:141:ILE:HG12	2.02	0.60
1:D:156:LEU:HD11	1:D:234:ALA:HB2	1.84	0.60
2:E:296:GLU:CD	2:E:296:GLU:H	2.05	0.59
2:E:371:ALA:CB	2:E:377:ALA:HB2	2.32	0.59
1:D:164:THR:HG22	1:D:283:LEU:HD12	1.83	0.59
2:E:348:ARG:HD2	2:E:348:ARG:C	2.22	0.59
1:D:159:GLU:OE2	2:E:319:PHE:HD2	1.84	0.59
1:D:240:LYS:HG2	1:D:251:ILE:HG21	1.86	0.58
2:B:348:ARG:NH1	2:B:348:ARG:HG3	2.18	0.58
1:D:248:GLY:O	2:E:116:ARG:NH2	2.36	0.58
1:A:156:LEU:HD11	1:A:234:ALA:HB2	1.85	0.58
1:D:281:GLU:O	1:D:284:LYS:HB3	2.03	0.58
2:E:87:ASP:C	2:E:87:ASP:OD1	2.42	0.58
1:D:12:CYS:HB2	1:D:34:MET:HE1	1.84	0.58
1:A:240:LYS:HG2	1:A:251:ILE:HG21	1.86	0.58
2:E:229:LEU:HD23	2:E:232:MET:HE3	1.85	0.58
1:D:169:PHE:HZ	1:D:284:LYS:HA	1.70	0.57
2:E:318:ILE:HG22	2:E:319:PHE:N	2.19	0.57
1:A:151:SER:HB2	1:A:206:ILE:HB	1.85	0.57
2:B:233:ARG:NH2	5:B:1500:SO4:O4	2.37	0.57
2:E:248:TRP:CD2	2:E:300:GLU:HG3	2.39	0.57
1:A:30:TYR:O	1:A:30:TYR:CD1	2.57	0.57
2:B:385:VAL:O	2:B:388:LYS:HG3	2.04	0.57
2:B:310:LYS:HG3	6:B:1936:HOH:O	2.05	0.57
1:A:81:ILE:O	1:A:85:ILE:HG13	2.04	0.57
2:E:17:LEU:N	2:E:17:LEU:HD23	2.19	0.57
1:A:197:ASP:O	1:A:227:LYS:NZ	2.38	0.56
2:E:35:ALA:HB2	2:E:69:ILE:CD1	2.35	0.56
2:B:248:TRP:CD2	2:B:300:GLU:HG3	2.40	0.56
1:D:192:GLU:HG3	1:D:220:TYR:OH	2.04	0.56
1:A:192:GLU:HG3	1:A:220:TYR:OH	2.05	0.56
1:A:199:GLN:O	1:A:199:GLN:HG3	2.04	0.56
1:D:6:LYS:N	1:D:131:GLU:HB3	2.21	0.56
2:E:361:LEU:HD22	2:E:368:ILE:HG21	1.86	0.56
1:D:4:ILE:HD12	1:D:132:CYS:HB3	1.88	0.56
1:D:150:VAL:CG1	1:D:190:ILE:HG21	2.36	0.56
2:B:296:GLU:CD	2:B:296:GLU:H	2.08	0.56
1:D:155:THR:HG21	2:E:264:ASN:O	2.06	0.56
1:A:123:CYS:SG	4:A:1300:COA:C6P	2.94	0.56
1:D:67:ALA:HA	1:D:91:LEU:O	2.06	0.56
1:D:93:ILE:HD12	1:D:126:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HB2	2:B:116:ARG:HD3	1.88	0.55
1:A:164:THR:HG22	1:A:283:LEU:CD1	2.35	0.55
2:B:249:GLU:OE1	2:E:70:ARG:NH2	2.39	0.55
2:B:348:ARG:HG3	2:B:348:ARG:HH11	1.71	0.55
2:E:258:ASN:H	2:E:258:ASN:ND2	2.03	0.55
1:D:32:THR:HG23	1:D:132:CYS:SG	2.47	0.55
1:D:95:ILE:HA	1:D:124:PRO:HD2	1.87	0.55
1:A:57:ARG:NH1	1:A:86:ASP:O	2.40	0.55
1:D:11:ILE:HA	1:D:36:GLY:O	2.07	0.55
2:E:348:ARG:HH12	2:E:374:LEU:HB2	1.71	0.55
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.89	0.55
1:A:156:LEU:HG	2:B:267:GLY:C	2.27	0.55
2:B:258:ASN:H	2:B:258:ASN:ND2	2.04	0.55
2:B:3:LEU:HD12	2:B:216:LEU:HB2	1.88	0.55
2:E:191:ARG:HB3	2:E:229:LEU:HD11	1.89	0.55
1:A:95:ILE:HA	1:A:124:PRO:HD2	1.89	0.55
1:A:203:ILE:HB	1:A:229:VAL:HG22	1.89	0.55
2:B:35:ALA:HB2	2:B:69:ILE:CD1	2.36	0.55
2:B:87:ASP:C	2:B:87:ASP:OD1	2.46	0.55
2:B:87:ASP:OD1	2:B:89:ASN:N	2.38	0.55
2:B:340:GLY:O	2:B:342:ASN:OD1	2.24	0.55
1:D:142:HIS:CD2	1:D:161:VAL:HG11	2.42	0.55
1:D:203:ILE:HB	1:D:229:VAL:HG22	1.88	0.55
1:A:109:VAL:O	1:A:113:GLU:HG2	2.06	0.55
2:B:369:ILE:HD12	2:B:369:ILE:N	2.22	0.54
1:A:6:LYS:N	1:A:131:GLU:HB3	2.22	0.54
1:A:154:GLY:O	1:A:157:THR:HB	2.07	0.54
2:E:125:ALA:HB1	2:E:167:LEU:HD11	1.88	0.54
1:A:9:LYS:HD3	1:A:35:VAL:HG11	1.89	0.54
1:A:169:PHE:HZ	1:A:284:LYS:HA	1.73	0.54
2:B:229:LEU:HD23	2:B:232:MET:CE	2.37	0.54
1:D:246:HIS:NE2	3:D:1601:PO4:O2	2.40	0.54
2:B:263:VAL:HG12	2:B:264:ASN:N	2.23	0.54
2:B:302:PHE:HE1	2:B:314:VAL:HG11	1.72	0.54
1:D:164:THR:HG22	1:D:283:LEU:CD1	2.37	0.54
1:A:186:ASN:ND2	1:A:187:PHE:H	2.06	0.54
1:A:166:ASP:C	1:A:168:GLY:H	2.11	0.54
2:B:318:ILE:HG22	2:B:319:PHE:N	2.23	0.54
2:B:125:ALA:HB1	2:B:167:LEU:HD11	1.89	0.53
2:E:229:LEU:HD23	2:E:232:MET:CE	2.39	0.53
1:A:42:LYS:NZ	4:A:1300:COA:O7A	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LYS:HG2	1:D:169:PHE:O	2.08	0.53
1:D:151:SER:HB3	1:D:157:THR:OG1	2.07	0.53
2:E:87:ASP:OD1	2:E:89:ASN:N	2.38	0.53
2:E:343:VAL:HB	2:E:344:PRO:CD	2.38	0.53
2:B:359:LYS:O	2:B:361:LEU:N	2.41	0.53
1:D:30:TYR:O	1:D:30:TYR:CD1	2.61	0.53
2:E:328:ILE:O	2:E:332:ILE:HG13	2.08	0.53
2:E:325:CYS:SG	2:E:349:LEU:HB3	2.48	0.53
1:A:137:GLN:HB2	1:A:138:PRO:HD2	1.90	0.53
1:A:145:GLY:HA3	1:A:170:GLY:CA	2.31	0.53
2:B:17:LEU:N	2:B:17:LEU:HD23	2.23	0.53
1:A:146:LYS:HG2	1:A:169:PHE:O	2.08	0.53
2:B:141:PRO:HG2	6:B:1948:HOH:O	2.08	0.53
1:D:276:LEU:HD23	1:D:276:LEU:H	1.72	0.53
1:A:93:ILE:HD12	1:A:126:VAL:HG23	1.91	0.52
1:D:186:ASN:ND2	1:D:187:PHE:H	2.07	0.52
1:D:199:GLN:O	1:D:199:GLN:HG3	2.09	0.52
2:E:348:ARG:HG3	2:E:348:ARG:NH1	2.24	0.52
1:A:248:GLY:O	2:B:116:ARG:NH2	2.42	0.52
2:B:149:LEU:HD22	2:B:155:PRO:HB3	1.90	0.52
1:D:137:GLN:HB2	1:D:138:PRO:HD2	1.90	0.52
2:E:248:TRP:CE2	2:E:300:GLU:HG3	2.44	0.52
1:A:186:ASN:HD22	1:A:187:PHE:N	2.08	0.52
1:D:236:VAL:HA	1:D:258:ALA:HB3	1.92	0.52
2:E:372:LYS:HG3	6:E:1930:HOH:O	2.10	0.52
1:A:4:ILE:HD12	1:A:132:CYS:HB3	1.90	0.52
1:A:150:VAL:HG11	1:A:190:ILE:HB	1.92	0.52
1:D:145:GLY:HA3	1:D:170:GLY:CA	2.33	0.52
2:B:348:ARG:HH11	2:B:348:ARG:CG	2.23	0.52
2:E:263:VAL:HG12	2:E:264:ASN:N	2.25	0.52
2:E:263:VAL:HG11	2:E:268:LEU:HG	1.92	0.52
2:E:359:LYS:O	2:E:361:LEU:N	2.42	0.52
2:B:263:VAL:HG11	2:B:268:LEU:HG	1.92	0.52
1:A:246:HIS:HB2	1:A:249:ALA:HB2	1.92	0.51
2:B:332:ILE:O	2:B:336:VAL:HG23	2.10	0.51
2:E:51:ALA:CB	2:E:86:THR:HG23	2.40	0.51
1:A:12:CYS:HB2	1:A:34:MET:HE1	1.93	0.51
1:D:150:VAL:HG11	1:D:190:ILE:HB	1.91	0.51
1:D:191:LEU:HD13	1:D:221:ILE:HG13	1.93	0.51
2:E:35:ALA:HB2	2:E:69:ILE:HD12	1.93	0.51
1:A:153:SER:OG	2:B:267:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LYS:HG2	2:B:331:GLY:CA	2.32	0.51
2:E:3:LEU:HD12	2:E:216:LEU:HB2	1.93	0.51
2:E:330:ASP:OD1	2:E:360:LYS:HD2	2.11	0.51
1:D:186:ASN:HD22	1:D:187:PHE:N	2.09	0.51
1:D:240:LYS:HG2	1:D:251:ILE:CG2	2.40	0.51
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.45	0.50
1:D:273:VAL:HG21	1:D:278:ASP:HB2	1.93	0.50
2:B:328:ILE:O	2:B:332:ILE:HG13	2.11	0.50
2:E:320:GLY:HA2	4:E:1904:COA:H32	1.94	0.50
1:D:146:LYS:HD2	1:D:287:LEU:HD21	1.94	0.50
2:E:258:ASN:ND2	2:E:259:ILE:HG13	2.26	0.50
1:A:150:VAL:CG1	1:A:190:ILE:CG2	2.90	0.50
1:A:236:VAL:HA	1:A:258:ALA:HB3	1.93	0.50
1:D:42:LYS:O	1:D:52:VAL:HG12	2.12	0.50
2:B:258:ASN:ND2	2:B:259:ILE:HG13	2.27	0.50
2:E:359:LYS:O	2:E:360:LYS:C	2.50	0.50
2:E:346:VAL:HB	2:E:381:VAL:CG1	2.42	0.49
1:D:154:GLY:O	1:D:157:THR:HB	2.11	0.49
2:B:348:ARG:HH12	2:B:374:LEU:HB2	1.78	0.49
2:B:51:ALA:CB	2:B:86:THR:HG23	2.42	0.49
2:B:64:ASN:H	2:B:64:ASN:ND2	2.10	0.49
2:B:346:VAL:HB	2:B:381:VAL:HG13	1.94	0.49
2:E:369:ILE:CG2	2:E:370:ALA:N	2.64	0.49
1:A:189:ASP:O	1:A:193:MET:HG3	2.12	0.49
2:E:369:ILE:HD12	2:E:369:ILE:N	2.27	0.49
2:E:332:ILE:O	2:E:336:VAL:HG23	2.13	0.49
1:D:123:CYS:O	1:D:124:PRO:O	2.29	0.49
1:A:151:SER:HB3	1:A:157:THR:OG1	2.12	0.49
1:A:246:HIS:NE2	3:A:1600:PO4:O2	2.46	0.49
1:A:169:PHE:CD1	1:A:287:LEU:HD23	2.47	0.49
2:B:272:THR:O	2:B:275:ILE:HG22	2.12	0.49
2:B:335:ALA:O	2:B:339:VAL:HB	2.13	0.49
2:E:91:GLN:NE2	2:E:237:GLN:O	2.40	0.48
1:A:273:VAL:O	1:A:273:VAL:CG1	2.62	0.48
1:D:189:ASP:O	1:D:193:MET:HG3	2.14	0.48
2:E:119:ARG:HG3	2:E:119:ARG:HH11	1.77	0.48
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.48	0.48
2:B:140:THR:HB	2:B:143:LEU:HD12	1.95	0.48
2:E:64:ASN:ND2	2:E:64:ASN:H	2.11	0.48
1:A:273:VAL:HG22	1:A:275:SER:O	2.14	0.48
2:B:346:VAL:HB	2:B:381:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:CG1	1:D:204:VAL:HG23	2.44	0.48
1:A:240:LYS:HG2	1:A:251:ILE:CG2	2.43	0.48
2:B:361:LEU:HD22	2:B:368:ILE:HG21	1.96	0.48
1:D:109:VAL:O	1:D:113:GLU:HG2	2.13	0.48
1:D:151:SER:HB2	1:D:206:ILE:HB	1.96	0.48
2:E:245:ALA:HB1	2:E:250:LEU:HB2	1.96	0.48
2:E:348:ARG:HG3	2:E:348:ARG:HH11	1.78	0.48
2:B:359:LYS:O	2:B:360:LYS:C	2.52	0.48
1:D:285:THR:O	1:D:287:LEU:N	2.47	0.48
1:D:156:LEU:CD2	1:D:276:LEU:HD13	2.43	0.47
1:D:166:ASP:C	1:D:168:GLY:H	2.17	0.47
1:D:201:GLU:O	1:D:228:PRO:HD2	2.13	0.47
1:D:253:GLY:HA2	2:E:134:GLU:OE1	2.13	0.47
1:A:67:ALA:HA	1:A:91:LEU:O	2.14	0.47
1:A:172:SER:HB3	1:A:199:GLN:HG2	1.96	0.47
2:E:256:ASP:O	2:E:257:GLY:O	2.32	0.47
2:B:315:LEU:HD12	2:B:316:VAL:N	2.29	0.47
2:E:378:ALA:O	2:E:382:VAL:HG23	2.15	0.47
1:D:223:GLU:HG2	1:D:224:HIS:NE2	2.29	0.47
1:A:152:ARG:NH2	6:A:1619:HOH:O	2.34	0.47
2:B:336:VAL:HG13	2:B:341:VAL:HB	1.97	0.47
1:A:93:ILE:HD12	1:A:126:VAL:CG2	2.45	0.47
1:A:243:ARG:NE	6:A:1629:HOH:O	2.38	0.47
2:B:35:ALA:HB2	2:B:69:ILE:HD12	1.96	0.47
1:D:6:LYS:O	1:D:33:LYS:HE3	2.14	0.47
2:E:84:TYR:CE1	2:E:85:GLN:HG3	2.49	0.47
2:E:197:ALA:HB3	2:E:215:LYS:HB3	1.95	0.47
2:E:324:ARG:O	2:E:326:ASP:N	2.48	0.47
2:E:346:VAL:HB	2:E:381:VAL:HG13	1.96	0.47
2:B:369:ILE:CG2	2:B:370:ALA:N	2.63	0.47
2:B:33:GLU:O	2:B:37:LYS:HG3	2.15	0.47
1:D:159:GLU:OE2	2:E:319:PHE:CE2	2.67	0.47
1:A:12:CYS:O	1:A:15:PHE:HB2	2.16	0.47
2:B:366:LEU:O	2:B:368:ILE:N	2.42	0.47
1:A:1:SER:H2	1:A:197:ASP:CG	2.19	0.46
1:D:223:GLU:CG	1:D:223:GLU:O	2.63	0.46
1:D:159:GLU:OE2	2:E:348:ARG:NH2	2.48	0.46
2:E:235:GLN:O	2:E:238:GLU:HG2	2.15	0.46
2:B:324:ARG:O	2:B:326:ASP:N	2.49	0.46
2:E:272:THR:O	2:E:275:ILE:HG22	2.15	0.46
2:E:316:VAL:HB	2:E:347:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:359:LYS:O	2:E:362:ALA:N	2.48	0.46
1:A:273:VAL:HG21	1:A:278:ASP:C	2.36	0.46
2:B:197:ALA:HB3	2:B:215:LYS:HB3	1.97	0.46
2:B:318:ILE:HG21	2:B:328:ILE:CD1	2.45	0.46
1:D:3:LEU:HD21	1:D:193:MET:SD	2.54	0.46
1:A:221:ILE:HG22	1:A:222:LYS:N	2.30	0.46
1:D:127:ILE:HG22	1:D:174:CYS:HB2	1.96	0.46
1:A:123:CYS:O	1:A:124:PRO:O	2.34	0.46
2:B:156:MET:O	2:B:159:GLN:HB2	2.16	0.46
1:D:273:VAL:O	1:D:273:VAL:CG1	2.62	0.46
1:D:273:VAL:HG21	1:D:278:ASP:C	2.35	0.46
2:E:119:ARG:HG3	2:E:119:ARG:NH1	2.31	0.46
1:A:181:PRO:CB	2:B:116:ARG:HD3	2.46	0.46
2:B:292:GLY:O	2:B:294:THR:HG23	2.16	0.46
2:E:315:LEU:HD12	2:E:316:VAL:N	2.31	0.46
1:D:151:SER:CB	1:D:206:ILE:HB	2.46	0.46
1:D:181:PRO:HB2	2:E:116:ARG:HD3	1.98	0.46
2:B:103:ASP:HB3	2:B:205:LYS:CG	2.44	0.45
2:B:124:MET:CE	2:B:146:LYS:HE2	2.46	0.45
2:E:383:ALA:C	2:E:385:VAL:H	2.19	0.45
1:A:142:HIS:CD2	1:A:161:VAL:HG11	2.51	0.45
1:A:277:ALA:CB	2:B:375:THR:HG23	2.46	0.45
2:B:383:ALA:C	2:B:385:VAL:H	2.19	0.45
2:B:133:ILE:O	2:B:133:ILE:HG13	2.17	0.45
2:E:32:GLU:O	6:E:1947:HOH:O	2.21	0.45
1:A:155:THR:OG1	2:B:268:LEU:HB2	2.16	0.45
2:B:140:THR:CB	2:B:143:LEU:HD12	2.47	0.45
2:E:348:ARG:HH11	2:E:348:ARG:CG	2.29	0.45
1:A:147:VAL:CG1	1:A:204:VAL:HG23	2.47	0.45
1:D:150:VAL:CG1	1:D:190:ILE:CG2	2.94	0.45
2:B:324:ARG:NH1	2:B:326:ASP:OD1	2.50	0.45
1:A:113:GLU:HG2	1:A:113:GLU:H	1.62	0.45
2:B:235:GLN:O	2:B:238:GLU:HG2	2.16	0.45
2:B:325:CYS:SG	2:B:349:LEU:HB3	2.56	0.45
2:E:199:ASN:HA	2:E:200:PRO:HA	1.76	0.45
2:B:359:LYS:O	2:B:362:ALA:N	2.50	0.44
2:E:254:ALA:C	2:E:255:LEU:HD12	2.37	0.44
2:B:263:VAL:O	2:B:289:VAL:HG23	2.18	0.44
1:D:121:PRO:HG2	1:D:180:ASP:OD2	2.17	0.44
2:B:323:VAL:O	4:B:1903:COA:H22	2.16	0.44
1:A:223:GLU:O	1:A:223:GLU:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ASP:O	2:B:257:GLY:O	2.35	0.44
2:B:320:GLY:O	4:B:1903:COA:H21	2.18	0.44
2:B:32:GLU:OE2	2:B:70:ARG:NH1	2.51	0.44
2:B:254:ALA:C	2:B:255:LEU:HD12	2.38	0.44
1:D:98:GLY:HA2	2:E:221:ASN:ND2	2.33	0.44
2:E:341:VAL:HG12	2:E:343:VAL:H	1.83	0.44
1:A:223:GLU:O	1:A:223:GLU:HG3	2.17	0.44
1:D:1:SER:H2	1:D:197:ASP:CG	2.21	0.44
1:A:151:SER:CB	1:A:206:ILE:HB	2.47	0.44
2:B:10:GLN:O	2:B:13:ALA:HB3	2.18	0.44
1:A:164:THR:O	1:A:169:PHE:HB2	2.18	0.43
2:B:245:ALA:HB1	2:B:250:LEU:HB2	2.00	0.43
2:B:348:ARG:NH1	2:B:348:ARG:CG	2.81	0.43
2:E:33:GLU:O	2:E:37:LYS:HG3	2.19	0.43
1:D:57:ARG:NH1	1:D:86:ASP:O	2.52	0.43
2:E:256:ASP:OD1	2:E:256:ASP:N	2.39	0.43
2:E:257:GLY:HA3	2:E:282:GLU:O	2.18	0.43
1:A:166:ASP:C	1:A:168:GLY:N	2.72	0.43
1:A:285:THR:O	1:A:287:LEU:N	2.51	0.43
2:E:291:GLY:O	2:E:293:ALA:N	2.38	0.43
2:E:324:ARG:NH1	2:E:326:ASP:OD1	2.51	0.43
1:A:6:LYS:O	1:A:33:LYS:HE3	2.18	0.43
2:B:301:ALA:O	2:B:305:ILE:HG13	2.18	0.43
1:D:196:LYS:O	1:D:196:LYS:HG2	2.19	0.43
1:D:221:ILE:HG22	1:D:222:LYS:N	2.34	0.43
1:D:229:VAL:HG12	1:D:270:VAL:HG13	2.01	0.43
2:E:299:THR:OG1	2:E:335:ALA:HB2	2.19	0.43
1:A:223:GLU:HG2	1:A:224:HIS:NE2	2.34	0.43
1:D:57:ARG:HG3	1:D:87:ALA:CB	2.49	0.43
1:D:156:LEU:HG	2:E:267:GLY:C	2.39	0.43
1:D:274:ARG:HA	1:D:274:ARG:HD3	1.78	0.43
1:A:133:LYS:NZ	1:A:137:GLN:O	2.45	0.43
1:D:246:HIS:HB2	1:D:249:ALA:HB2	2.01	0.43
2:E:258:ASN:HD22	2:E:258:ASN:N	2.03	0.43
1:A:15:PHE:CD2	1:A:37:GLY:HA3	2.53	0.43
1:A:155:THR:HB	2:B:268:LEU:HD22	1.99	0.43
1:A:158:TYR:CD1	1:A:158:TYR:N	2.87	0.43
2:B:313:ALA:HB2	2:B:385:VAL:HG13	2.00	0.43
2:E:219:ASP:OD1	2:E:221:ASN:HB2	2.18	0.43
1:A:156:LEU:CD2	1:A:276:LEU:HD13	2.49	0.43
1:A:191:LEU:HD13	1:A:221:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:PRO:HD3	2:B:211:CYS:O	2.18	0.43
2:B:312:LYS:O	2:B:385:VAL:HG12	2.19	0.43
1:D:99:ILE:HD12	1:D:121:PRO:CB	2.49	0.43
2:E:20:PRO:HD3	2:E:211:CYS:O	2.19	0.43
2:E:335:ALA:O	2:E:339:VAL:HB	2.19	0.43
1:D:246:HIS:NE2	3:D:1601:PO4:P	2.92	0.42
2:E:330:ASP:OD1	2:E:360:LYS:CD	2.67	0.42
1:D:227:LYS:HB3	1:D:228:PRO:HD2	2.00	0.42
2:E:149:LEU:HD22	2:E:155:PRO:HB3	2.00	0.42
2:E:172:LYS:HE3	2:E:207:GLY:O	2.19	0.42
1:A:273:VAL:HG22	1:A:275:SER:H	1.83	0.42
2:B:316:VAL:HB	2:B:347:VAL:HG22	2.00	0.42
1:D:57:ARG:HG3	1:D:87:ALA:HB2	2.02	0.42
1:D:200:THR:O	1:D:227:LYS:HD3	2.20	0.42
1:D:223:GLU:O	1:D:223:GLU:HG3	2.19	0.42
2:E:308:ASP:OD2	2:E:310:LYS:HG3	2.19	0.42
1:A:274:ARG:HD3	1:A:274:ARG:HA	1.79	0.42
2:B:15:TYR:CD1	2:B:187:ILE:HG12	2.54	0.42
2:B:282:GLU:HA	2:B:283:PRO:HD2	1.90	0.42
2:B:344:PRO:HG3	2:B:384:ALA:HB1	2.02	0.42
2:B:374:LEU:C	2:B:376:ASP:N	2.72	0.42
1:D:127:ILE:HG13	1:D:133:LYS:HB2	2.02	0.42
1:D:169:PHE:CD1	1:D:287:LEU:HD23	2.53	0.42
2:E:63:VAL:HB	6:E:1924:HOH:O	2.20	0.42
1:A:167:TYR:HB2	1:A:169:PHE:CD2	2.55	0.42
1:D:196:LYS:O	1:D:196:LYS:CG	2.68	0.42
2:E:235:GLN:HA	2:E:238:GLU:HG2	2.01	0.42
1:A:167:TYR:C	1:A:169:PHE:H	2.23	0.42
2:B:312:LYS:C	2:B:343:VAL:HG11	2.40	0.42
2:B:318:ILE:HG13	2:B:328:ILE:HD13	2.01	0.42
2:B:352:ASN:O	2:B:353:ASN:HB2	2.19	0.42
2:E:32:GLU:OE1	2:E:70:ARG:HD2	2.20	0.42
2:E:357:GLY:O	2:E:361:LEU:HG	2.20	0.42
1:D:221:ILE:HA	1:D:225:VAL:HG23	2.01	0.41
1:A:127:ILE:HG22	1:A:174:CYS:HB2	2.02	0.41
2:B:385:VAL:O	2:B:386:GLU:C	2.59	0.41
1:D:204:VAL:HA	1:D:230:VAL:O	2.19	0.41
2:E:273:MET:SD	2:E:286:PHE:HB2	2.60	0.41
1:D:285:THR:HG22	1:D:286:VAL:H	1.85	0.41
2:E:272:THR:O	2:E:273:MET:C	2.58	0.41
2:E:318:ILE:HG21	2:E:328:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:352:ASN:O	2:E:353:ASN:HB2	2.20	0.41
1:A:11:ILE:HG23	1:A:65:ALA:CB	2.50	0.41
1:A:94:THR:O	1:A:121:PRO:HA	2.20	0.41
1:A:200:THR:O	1:A:227:LYS:HD3	2.20	0.41
2:B:124:MET:HA	2:B:145:HIS:O	2.21	0.41
2:B:273:MET:SD	2:B:286:PHE:HB2	2.61	0.41
2:B:78:GLY:HA3	2:E:247:GLN:NE2	2.36	0.41
1:D:72:VAL:CG1	1:D:76:PHE:HB2	2.50	0.41
1:D:230:VAL:HG21	1:D:283:LEU:HD23	2.03	0.41
2:B:287:LEU:HD13	2:B:288:ASP:N	2.36	0.41
2:B:299:THR:OG1	2:B:335:ALA:HB2	2.20	0.41
1:D:94:THR:O	1:D:121:PRO:HA	2.20	0.41
1:D:136:ILE:HG12	6:D:1619:HOH:O	2.20	0.41
2:E:320:GLY:H	4:E:1904:COA:H21	1.85	0.41
1:A:199:GLN:O	1:A:199:GLN:CG	2.66	0.41
2:B:258:ASN:HD22	2:B:258:ASN:N	2.09	0.41
2:B:312:LYS:HG3	2:B:388:LYS:O	2.20	0.41
1:D:56:VAL:O	1:D:60:VAL:HG23	2.21	0.41
2:E:156:MET:HA	2:E:157:PRO:HD3	1.87	0.41
2:E:318:ILE:CG2	2:E:319:PHE:N	2.82	0.41
2:E:344:PRO:HG3	2:E:384:ALA:HB1	2.03	0.41
1:D:273:VAL:HG22	1:D:275:SER:H	1.86	0.41
1:D:2:ILE:O	1:D:4:ILE:N	2.46	0.40
1:D:158:TYR:CD1	1:D:158:TYR:N	2.87	0.40
1:A:146:LYS:HD2	1:A:287:LEU:HD21	2.01	0.40
1:A:159:GLU:OE2	2:B:348:ARG:NH2	2.54	0.40
1:D:11:ILE:HG23	1:D:65:ALA:CB	2.51	0.40
1:A:5:ASP:HB2	1:A:131:GLU:OE1	2.20	0.40
2:B:212:LEU:HD12	2:B:212:LEU:HA	1.93	0.40
2:B:290:GLY:O	2:B:291:GLY:C	2.59	0.40
1:D:42:LYS:O	1:D:52:VAL:CG1	2.69	0.40
2:E:57:ALA:CB	2:E:83:THR:HG22	2.51	0.40
2:E:312:LYS:O	2:E:385:VAL:HG12	2.21	0.40
1:A:3:LEU:HD21	1:A:193:MET:SD	2.62	0.40
1:A:124:PRO:O	6:A:1655:HOH:O	2.21	0.40
1:A:246:HIS:HB2	1:A:249:ALA:CB	2.51	0.40
2:B:199:ASN:HA	2:B:200:PRO:HA	1.76	0.40
2:B:312:LYS:HA	2:B:312:LYS:HD3	1.84	0.40
2:B:369:ILE:N	2:B:369:ILE:CD1	2.85	0.40
1:D:123:CYS:C	1:D:124:PRO:O	2.60	0.40
1:D:142:HIS:CD2	1:D:161:VAL:CG1	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:O	1:A:228:PRO:HD2	2.21	0.40
2:B:256:ASP:OD1	2:B:256:ASP:N	2.39	0.40
2:E:31:ALA:O	2:E:34:ALA:HB3	2.21	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	285/288 (99%)	258 (90%)	21 (7%)	6 (2%)	7	18
1	D	285/288 (99%)	252 (88%)	27 (10%)	6 (2%)	7	18
2	B	386/388 (100%)	348 (90%)	27 (7%)	11 (3%)	5	11
2	E	383/388 (99%)	351 (92%)	25 (6%)	7 (2%)	8	21
All	All	1339/1352 (99%)	1209 (90%)	100 (8%)	30 (2%)	6	17

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	THR
2	B	292	GLY
2	B	293	ALA
2	B	384	ALA
1	D	285	THR
1	D	286	VAL
2	E	384	ALA
1	A	139	GLY
1	A	286	VAL
2	B	257	GLY
2	B	325	CYS
2	B	360	LYS

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Mol	Chain	Res	Type
2	B	386	GLU
1	D	139	GLY
2	E	257	GLY
2	E	292	GLY
2	E	293	ALA
2	E	325	CYS
2	E	360	LYS
1	A	124	PRO
2	B	309	ASP
1	D	3	LEU
1	D	124	PRO
2	B	139	GLU
2	B	291	GLY
1	D	138	PRO
1	A	3	LEU
1	A	138	PRO
2	B	369	ILE
2	E	369	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/218 (100%)	209 (96%)	8 (4%)	34	63
1	D	217/218 (100%)	208 (96%)	9 (4%)	30	59
2	B	297/297 (100%)	276 (93%)	21 (7%)	14	34
2	E	295/297 (99%)	275 (93%)	20 (7%)	16	36
All	All	1026/1030 (100%)	968 (94%)	58 (6%)	20	44

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

Mol	Chain	Res	Type
1	A	57	ARG
1	A	77	CYS
1	A	113	GLU

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Mol	Chain	Res	Type
1	A	117	ARG
1	A	124	PRO
1	A	150	VAL
1	A	186	ASN
1	A	278	ASP
2	B	11	LEU
2	B	65	SER
2	B	70	ARG
2	B	95	GLN
2	B	116	ARG
2	B	124	MET
2	B	138	GLU
2	B	139	GLU
2	B	195	LEU
2	B	200	PRO
2	B	258	ASN
2	B	287	LEU
2	B	288	ASP
2	B	295	LYS
2	B	297	ARG
2	B	319	PHE
2	B	323	VAL
2	B	327	LEU
2	B	343	VAL
2	B	348	ARG
2	B	375	THR
1	D	57	ARG
1	D	77	CYS
1	D	100	PRO
1	D	113	GLU
1	D	117	ARG
1	D	150	VAL
1	D	186	ASN
1	D	262	PHE
1	D	278	ASP
2	E	11	LEU
2	E	64	ASN
2	E	65	SER
2	E	70	ARG
2	E	95	GLN
2	E	146	LYS
2	E	195	LEU

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Mol	Chain	Res	Type
2	E	200	PRO
2	E	258	ASN
2	E	287	LEU
2	E	288	ASP
2	E	295	LYS
2	E	297	ARG
2	E	319	PHE
2	E	323	VAL
2	E	325	CYS
2	E	327	LEU
2	E	348	ARG
2	E	355	GLU
2	E	375	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	186	ASN
1	A	224	HIS
2	B	64	ASN
2	B	94	ASN
2	B	95	GLN
2	B	247	GLN
2	B	258	ASN
2	B	342	ASN
2	B	353	ASN
1	D	186	ASN
1	D	224	HIS
2	E	64	ASN
2	E	94	ASN
2	E	95	GLN
2	E	247	GLN
2	E	258	ASN
2	E	353	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
5	SO4	B	1500	-	4,4,4	0.40	0	6,6,6	0.29	0
5	SO4	B	1400	-	4,4,4	0.29	0	6,6,6	0.63	0
5	SO4	E	1501	-	4,4,4	0.38	0	6,6,6	0.33	0
4	COA	B	1903	2	14,16,50	7.55	6 (42%)	19,21,75	4.49	13 (68%)
4	COA	E	1904	2	6,7,50	1.91	2 (33%)	6,7,75	5.54	4 (66%)
3	PO4	A	1600	-	4,4,4	1.75	1 (25%)	6,6,6	0.47	0
5	SO4	E	1401	-	4,4,4	0.26	0	6,6,6	0.35	0
3	PO4	D	1601	-	4,4,4	1.62	1 (25%)	6,6,6	0.38	0
4	COA	D	1301	-	36,44,50	0.96	1 (2%)	45,68,75	2.00	13 (28%)
4	COA	A	1300	-	36,44,50	0.88	0	45,68,75	1.94	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	E	1904	2	-	1/6/6/64	-
4	COA	D	1301	-	-	1/37/57/64	0/3/3/3
4	COA	A	1300	-	-	1/37/57/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	B	1903	2	-	5/20/20/64	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1903	COA	CBP-CAP	27.03	1.73	1.55
4	B	1903	COA	C2P-S1P	3.97	1.94	1.80
4	B	1903	COA	C6P-C5P	3.89	1.58	1.51
4	E	1904	COA	C6P-C5P	3.16	1.61	1.51
4	B	1903	COA	C7P-N8P	3.00	1.53	1.46
4	B	1903	COA	C3P-N4P	2.93	1.52	1.46
4	E	1904	COA	C2P-S1P	2.42	1.89	1.80
4	B	1903	COA	CCP-CBP	2.35	1.58	1.53
3	A	1600	PO4	P-O2	-2.31	1.47	1.54
3	D	1601	PO4	P-O2	-2.18	1.48	1.54
4	D	1301	COA	CDP-CBP	-2.14	1.49	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1904	COA	C6P-C5P-N4P	10.27	126.64	115.79
4	B	1903	COA	CEP-CBP-CCP	-8.11	93.05	108.80
4	E	1904	COA	C3P-N4P-C5P	7.22	136.24	122.84
4	B	1903	COA	C6P-C5P-N4P	7.11	128.39	116.42
4	B	1903	COA	CAP-C9P-N8P	6.88	130.27	116.58
4	B	1903	COA	O5P-C5P-C6P	-6.58	109.98	122.02
4	B	1903	COA	OAP-CAP-CBP	-5.86	98.83	109.45
4	A	1300	COA	CAP-C9P-N8P	5.81	128.14	116.58
4	D	1301	COA	CAP-C9P-N8P	5.74	128.00	116.58
4	B	1903	COA	C6P-C7P-N8P	5.35	122.69	111.90
4	A	1300	COA	CEP-CBP-CAP	5.27	117.95	108.82
4	B	1903	COA	CEP-CBP-CAP	4.82	120.69	109.59
4	D	1301	COA	CEP-CBP-CCP	-4.62	100.70	108.23
4	B	1903	COA	C3P-N4P-C5P	4.23	130.68	122.84
4	B	1903	COA	CDP-CBP-CAP	4.05	118.94	109.59
4	B	1903	COA	C7P-N8P-C9P	4.01	129.73	122.59
4	E	1904	COA	O5P-C5P-C6P	-3.99	110.94	122.08
4	D	1301	COA	CEP-CBP-CAP	3.92	115.61	108.82
4	B	1903	COA	O9P-C9P-N8P	-3.90	114.61	122.99
4	D	1301	COA	O9P-C9P-CAP	-3.83	109.37	121.06
4	D	1301	COA	CDP-CBP-CCP	3.82	114.45	108.23
4	A	1300	COA	CEP-CBP-CCP	-3.46	102.60	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1904	COA	C7P-C6P-C5P	3.26	123.67	113.30
4	A	1300	COA	O4B-C1B-C2B	-3.17	102.30	106.93
4	A	1300	COA	OAP-CAP-CBP	-3.16	102.80	110.25
4	D	1301	COA	P2A-O3A-P1A	-3.00	122.54	132.83
4	D	1301	COA	C6P-C7P-N8P	2.98	121.81	111.52
4	A	1300	COA	P2A-O3A-P1A	-2.95	122.69	132.83
4	D	1301	COA	O3B-P3B-O7A	-2.85	98.38	109.39
4	D	1301	COA	O4B-C1B-C2B	-2.82	102.81	106.93
4	D	1301	COA	OAP-CAP-CBP	-2.81	103.64	110.25
4	A	1300	COA	C6P-C7P-N8P	2.78	121.10	111.52
4	A	1300	COA	O9P-C9P-CAP	-2.69	112.86	121.06
4	A	1300	COA	CDP-CBP-CCP	2.68	112.61	108.23
4	D	1301	COA	C5A-C6A-N6A	2.52	124.18	120.35
4	D	1301	COA	O6A-CCP-CBP	2.47	114.52	110.55
4	B	1903	COA	CEP-CBP-CDP	-2.45	104.04	108.80
4	B	1903	COA	C2P-C3P-N4P	2.32	117.60	112.31
4	D	1301	COA	P2A-O6A-CCP	2.31	134.87	121.56
4	A	1300	COA	P2A-O6A-CCP	2.16	134.01	121.56
4	A	1300	COA	C5A-C6A-N6A	2.10	123.54	120.35
4	A	1300	COA	CDP-CBP-CAP	-2.06	105.25	108.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1903	COA	N8P-C9P-CAP-OAP
4	B	1903	COA	S1P-C2P-C3P-N4P
4	E	1904	COA	S1P-C2P-C3P-N4P
4	B	1903	COA	O9P-C9P-CAP-OAP
4	B	1903	COA	O9P-C9P-CAP-CBP
4	B	1903	COA	N8P-C9P-CAP-CBP
4	A	1300	COA	O4B-C4B-C5B-O5B
4	D	1301	COA	O4B-C4B-C5B-O5B

There are no ring outliers.

7 monomers are involved in 11 short contacts:

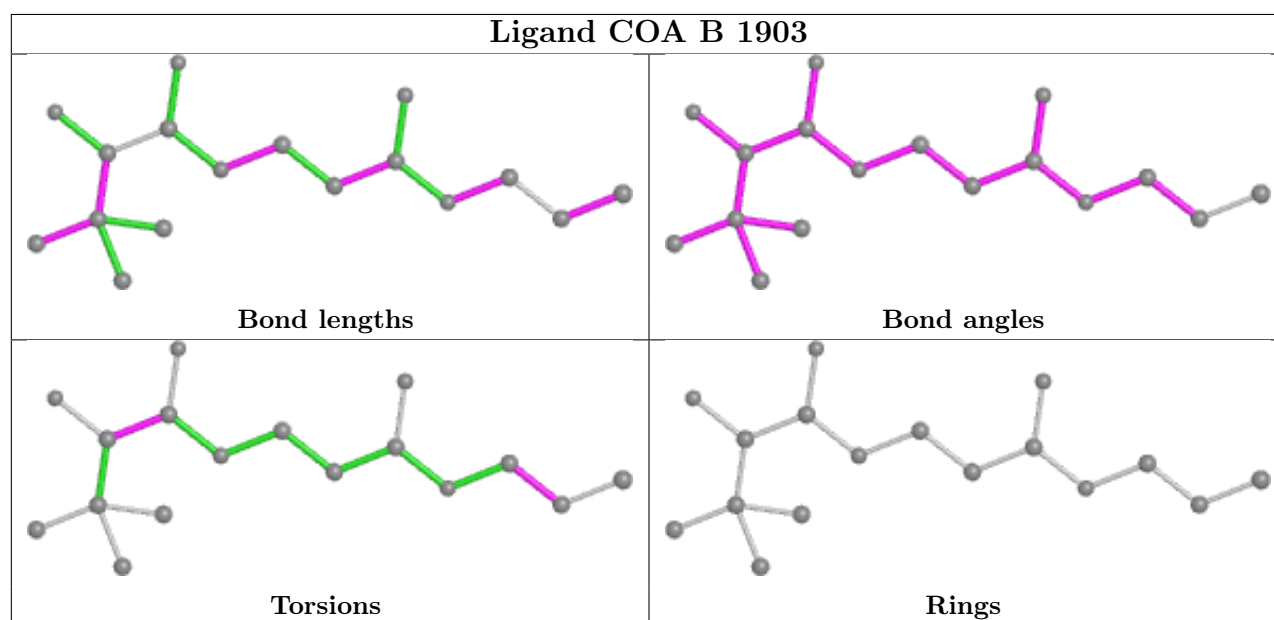
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1500	SO4	1	0
4	B	1903	COA	2	0
4	E	1904	COA	2	0

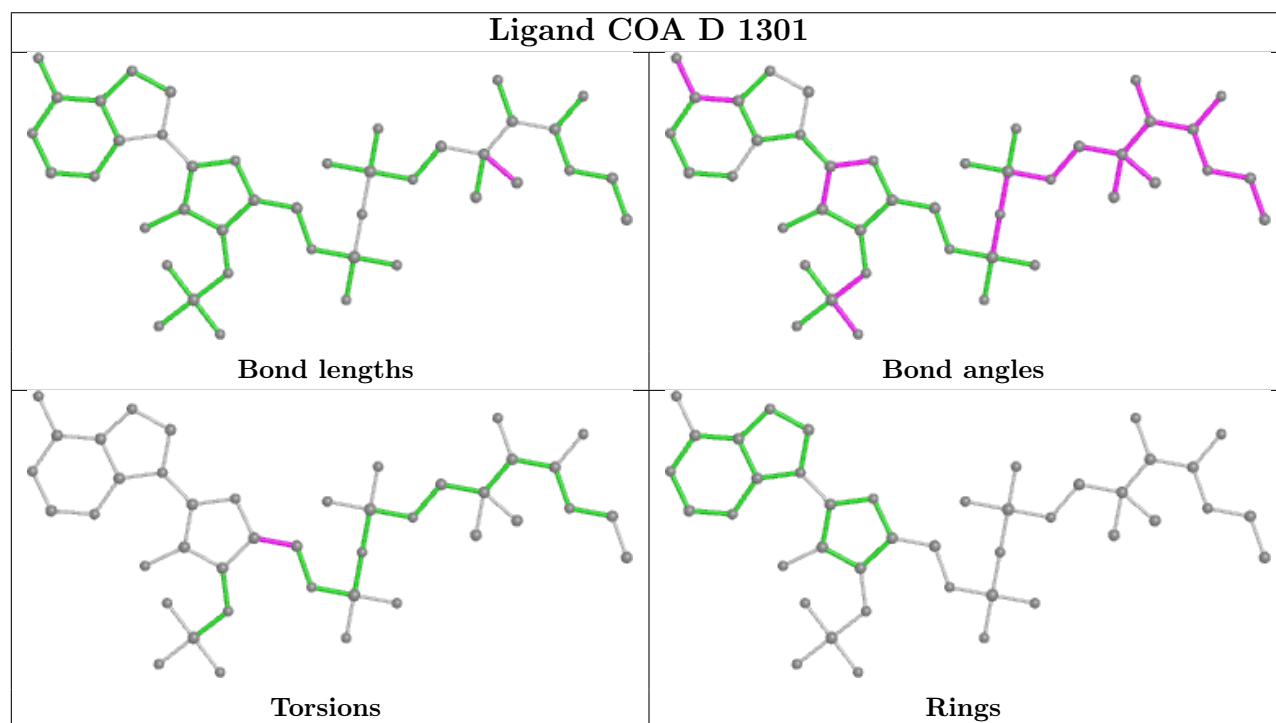
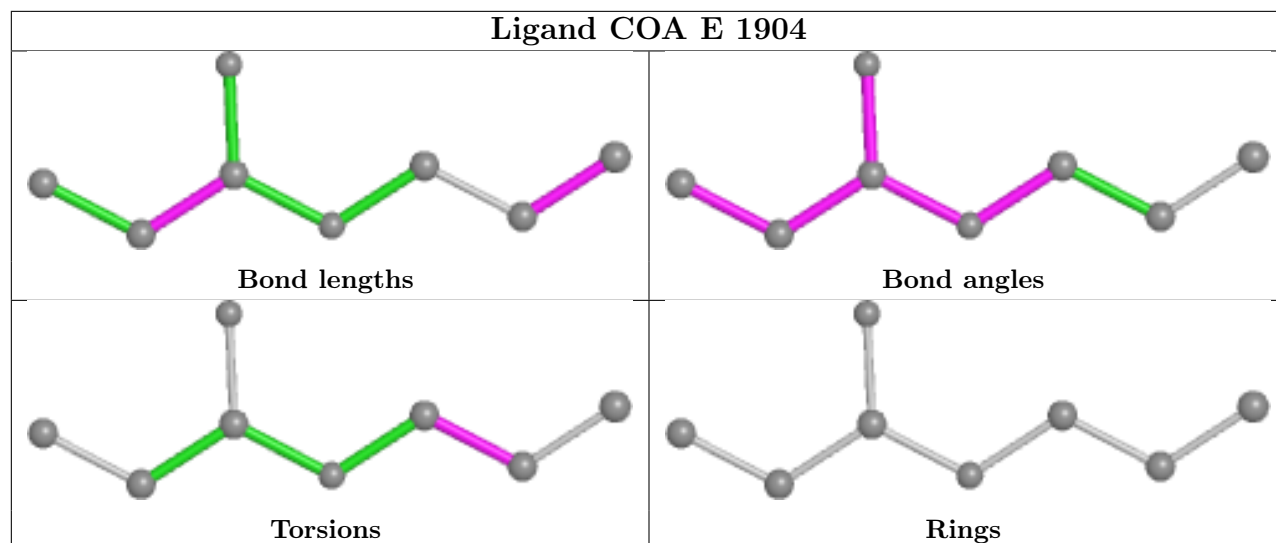
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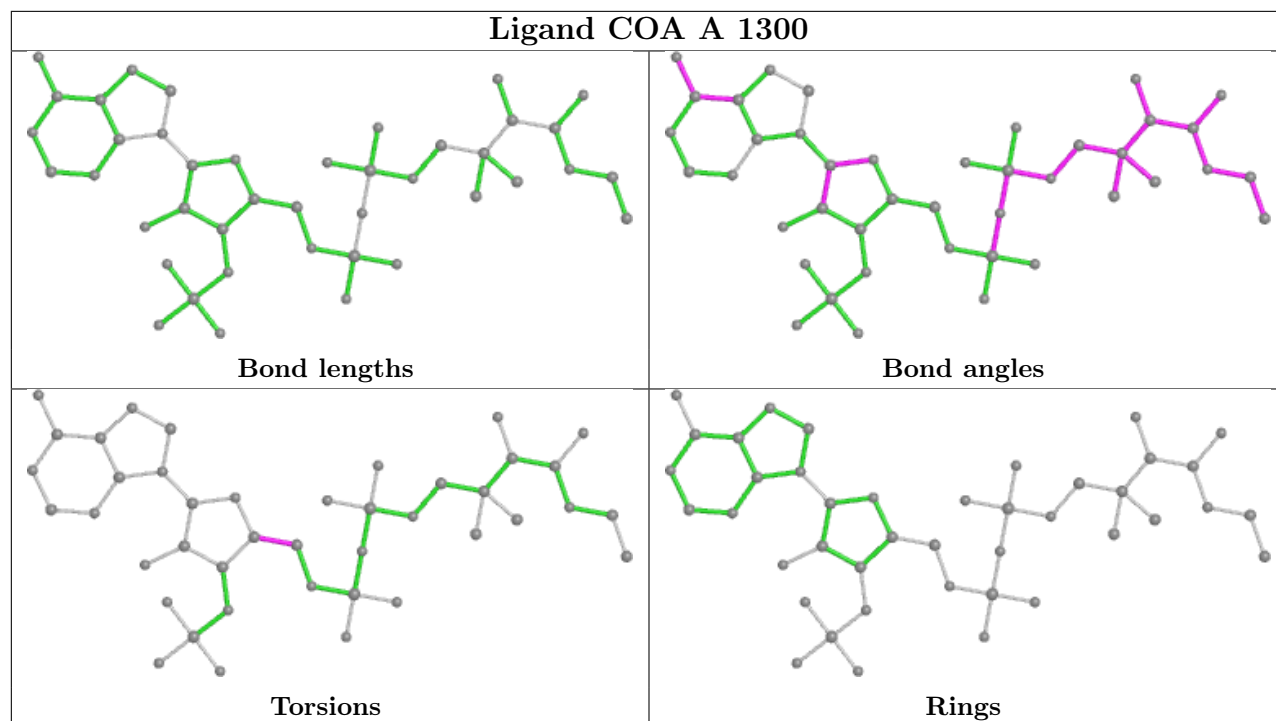
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1600	PO4	1	0
3	D	1601	PO4	2	0
4	D	1301	COA	1	0
4	A	1300	COA	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	287/288 (99%)	-0.07	6 (2%) 63 65	21, 42, 67, 82	0
1	D	287/288 (99%)	0.29	12 (4%) 36 35	29, 54, 78, 91	0
2	B	388/388 (100%)	0.08	12 (3%) 49 49	20, 48, 84, 96	0
2	E	385/388 (99%)	0.01	10 (2%) 56 57	25, 51, 79, 87	0
All	All	1347/1352 (99%)	0.07	40 (2%) 50 51	20, 49, 81, 96	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	88	ALA	5.3
1	A	254	GLY	4.2
1	D	7	ASN	4.0
2	B	312	LYS	4.0
2	B	339	VAL	3.8
2	B	140	THR	3.2
2	E	281	GLY	3.0
1	D	223	GLU	3.0
2	B	64	ASN	3.0
2	E	309	ASP	3.0
1	D	218	ALA	2.9
2	B	139	GLU	2.9
2	E	312	LYS	2.9
2	E	105	ALA	2.7
1	A	139	GLY	2.7
2	B	372	LYS	2.7
1	D	22	PHE	2.6
2	B	257	GLY	2.6
2	E	310	LYS	2.5
2	E	205	LYS	2.5
2	B	88	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	2.4
2	B	338	GLU	2.4
2	E	64	ASN	2.4
2	B	306	LEU	2.4
1	D	48	LEU	2.3
1	D	286	VAL	2.3
1	A	287	LEU	2.3
1	D	198	PRO	2.3
1	D	222	LYS	2.3
1	D	224	HIS	2.2
1	A	240	LYS	2.2
1	A	222	LYS	2.2
2	B	388	LYS	2.2
1	D	157	THR	2.2
2	E	363	ASP	2.2
2	E	256	ASP	2.1
2	B	290	GLY	2.1
1	D	168	GLY	2.0
1	D	42	LYS	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 monosaccharides 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.

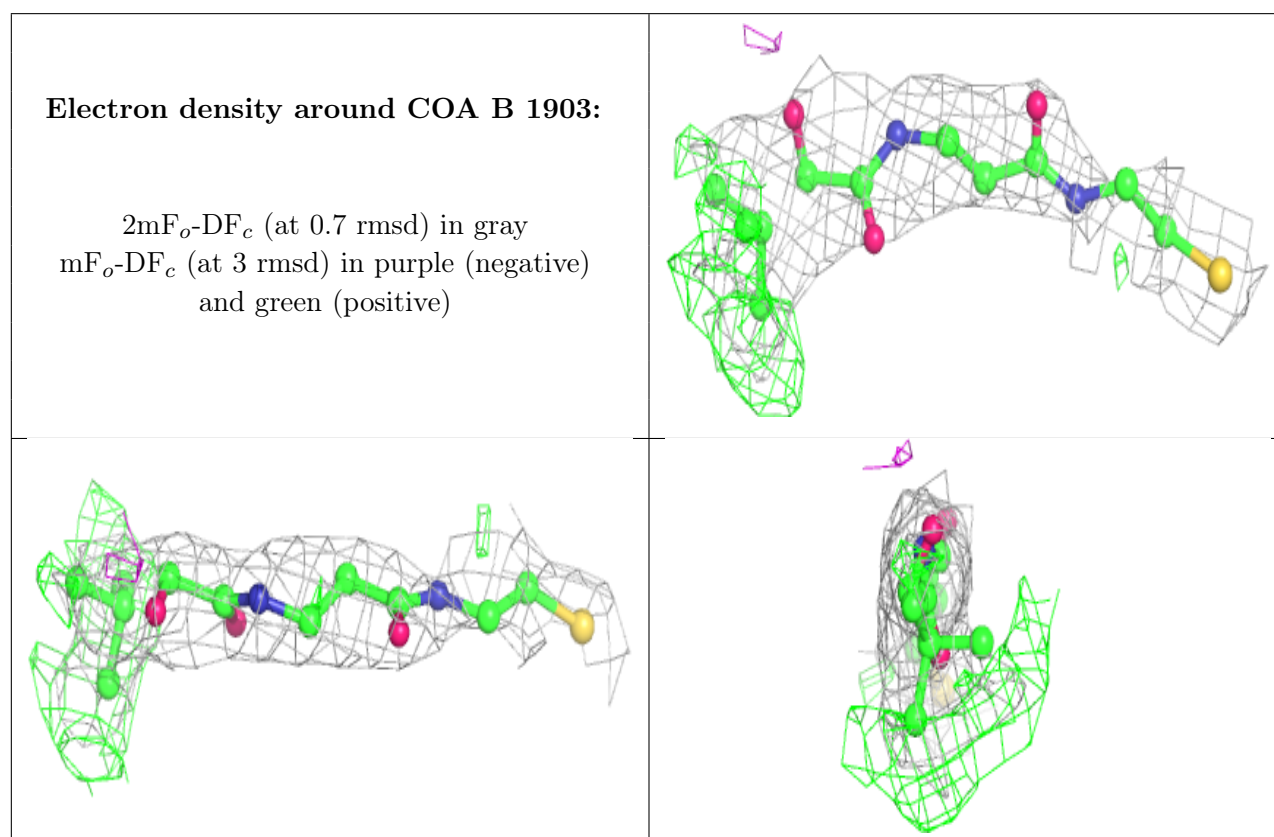
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	COA	B	1903	17/48	0.78	0.24	82,88,91,91	0
4	COA	E	1904	8/48	0.85	0.21	62,68,69,70	0
5	SO4	B	1500	5/5	0.92	0.36	34,34,36,37	5
4	COA	D	1301	42/48	0.93	0.17	50,61,67,68	0

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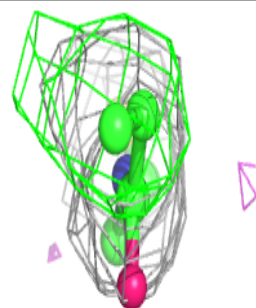
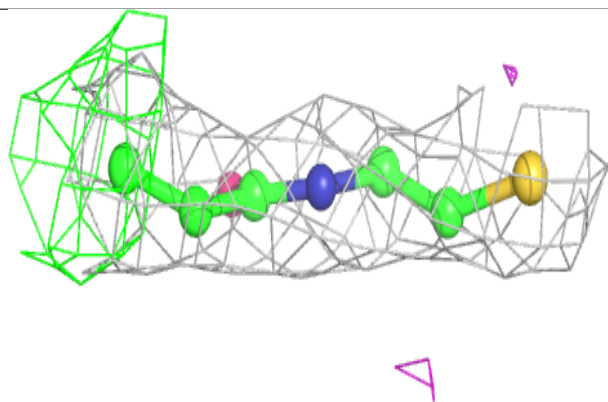
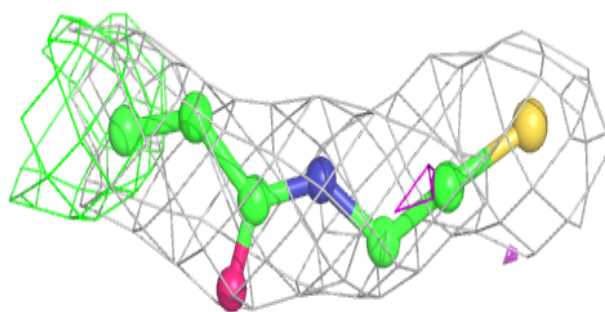
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	COA	A	1300	42/48	0.94	0.16	52,60,67,69	0
5	SO4	B	1400	5/5	0.96	0.12	59,60,61,63	0
3	PO4	A	1600	5/5	0.96	0.26	53,54,56,56	0
5	SO4	E	1401	5/5	0.96	0.19	70,70,72,72	0
5	SO4	E	1501	5/5	0.96	0.12	70,71,71,71	0
3	PO4	D	1601	5/5	0.98	0.22	54,57,57,58	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.

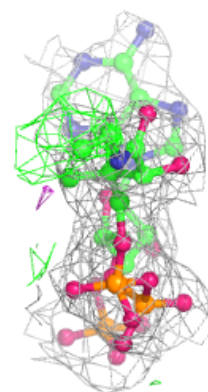
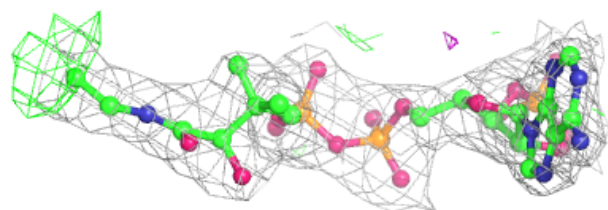
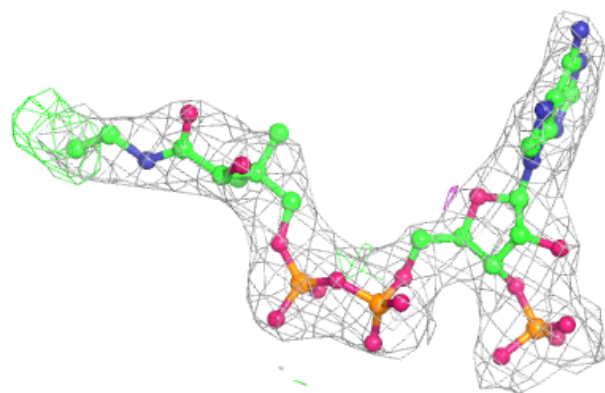


Electron density around COA E 1904:

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

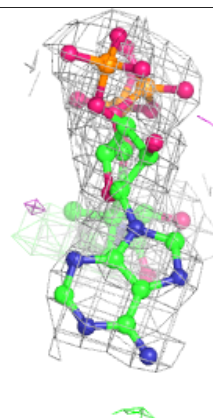
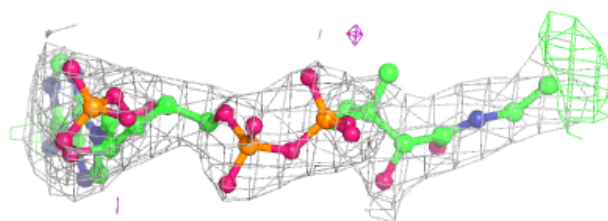
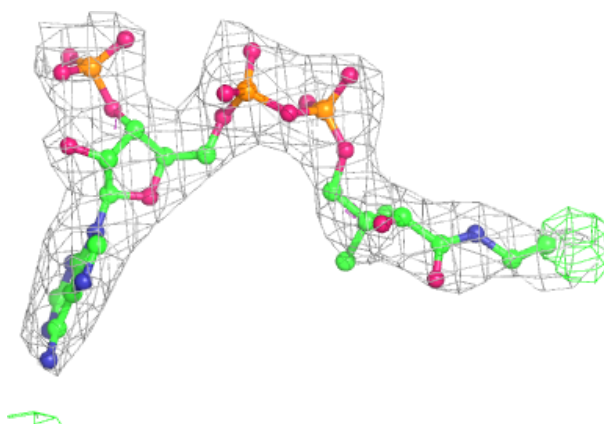
**Electron density around COA D 1301:**

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



Electron density around COA A 1300:

$2mF_o-DF_c$ (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.