



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:24 am BST

PDB ID : 1P5R
Title : Formyl-CoA Transferase in complex with Coenzyme A
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Deposited on : 2003-04-28
Resolution : 2.50 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

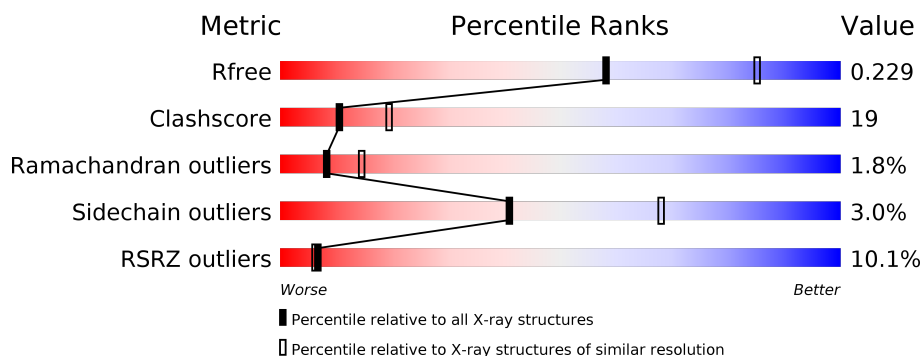
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	428	<div> <div>8%</div> <div>69%</div> <div>30%</div> </div>
1	B	428	<div> <div>12%</div> <div>64%</div> <div>33%</div> </div>

2 Entry composition [i](#)

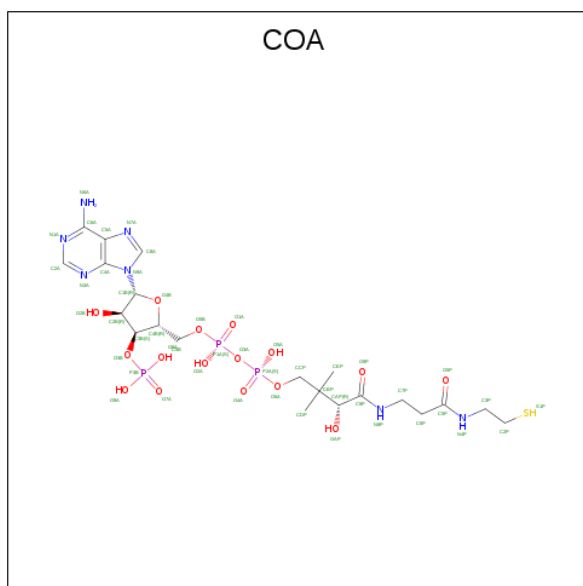
There are 3 unique types of molecules in this entry. The entry contains 6982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Formyl-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3312	2095	568	625	24			
1	B	427	Total	C	N	O	S	4	0	0
			3312	2095	568	625	24			

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

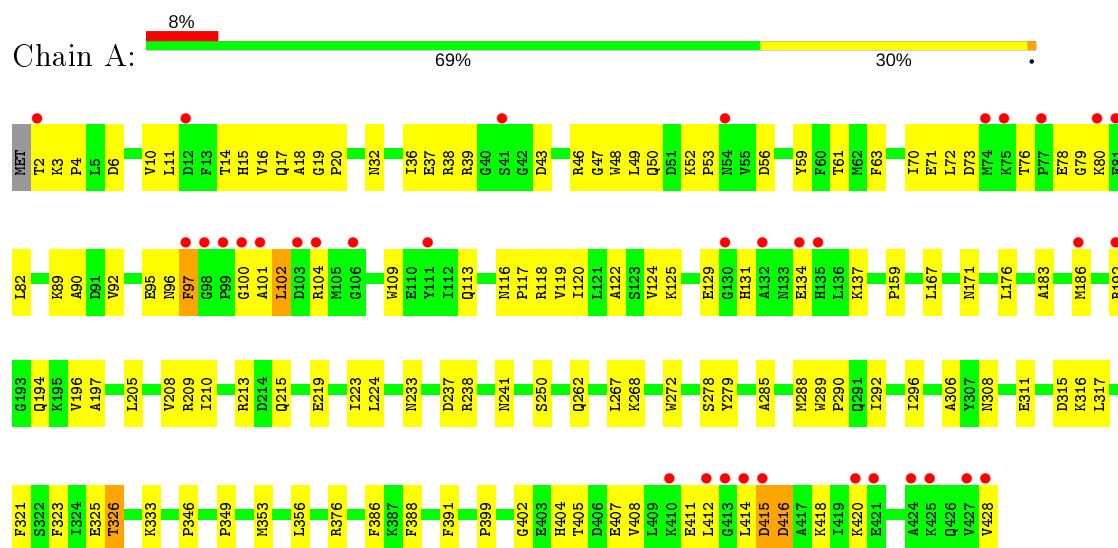
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total 150	O 150	0	0
3	B	112	Total 112	O 112	0	0

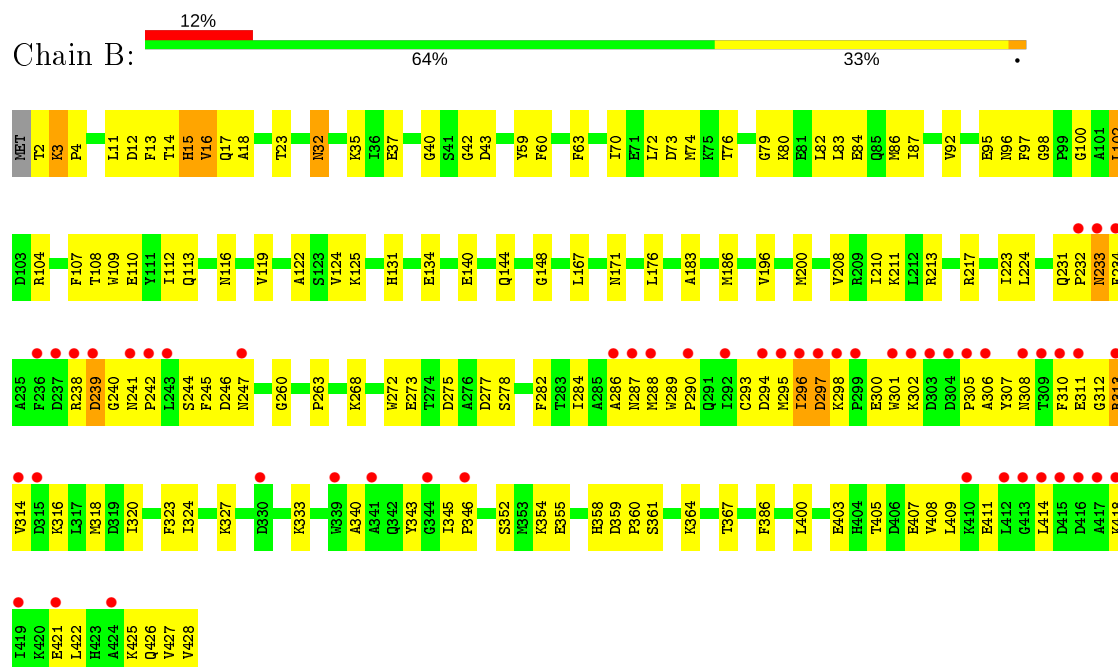
3 Residue-property plots [i](#)

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: Formyl-coenzyme A transferase



• Molecule 1: Formyl-coenzyme A transferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	151.40 Å 151.40 Å 99.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 2.50 29.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.88-2.50) 98.9 (29.79-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.236 0.186 , 0.229	Depositor DCC
R_{free} test set	1901 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6982	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/3386	0.60	0/4579
1	B	0.34	0/3386	0.59	0/4579
All	All	0.34	0/6772	0.59	0/9158

There are no bond length outliers.

There are no bond angle outliers.

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	3312	0	3250	119	0
1	B	3312	0	3250	141	0
2	A	48	0	32	8	0
2	B	48	0	32	4	0
3	A	150	0	0	5	0
3	B	112	0	0	3	0
All	All	6982	0	6564	246	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 (246) 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:405:THR:HG21	1:A:428:VAL:HG13	1.51	0.92
1:A:117:PRO:HB3	1:A:192:ARG:NH1	1.85	0.91
1:A:353:MET:HE1	1:B:148:GLY:HA3	1.55	0.87
1:A:11:LEU:HD23	1:A:90:ALA:HB2	1.58	0.85
1:A:418:LYS:H	1:A:418:LYS:HD2	1.43	0.83
1:B:76:THR:HG22	1:B:79:GLY:H	1.47	0.79
1:A:76:THR:HG22	1:A:79:GLY:H	1.49	0.78
1:A:122:ALA:HB1	1:A:176:LEU:HD11	1.68	0.75
1:A:95:GLU:HG2	1:A:102:LEU:HD12	1.67	0.75
1:A:78:GLU:O	1:A:82:LEU:HD23	1.87	0.74
1:B:405:THR:HG21	1:B:428:VAL:CG1	2.17	0.74
1:B:306:ALA:O	1:B:307:TYR:HD2	1.70	0.73
1:B:80:LYS:O	1:B:84:GLU:HG3	1.88	0.73
1:B:18:ALA:N	2:B:502:COA:S1P	2.58	0.73
1:A:219:GLU:OE2	1:B:358:HIS:HE1	1.72	0.73
1:A:124:VAL:HG23	1:A:176:LEU:HD22	1.69	0.72
1:A:43:ASP:O	1:A:46:ARG:HG3	1.90	0.71
1:A:414:LEU:HD12	1:A:414:LEU:H	1.56	0.71
1:A:238:ARG:HG3	3:A:534:HOH:O	1.91	0.70
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.75	0.69
1:A:129:GLU:HG3	1:A:134:GLU:OE2	1.92	0.69
1:A:405:THR:HG21	1:A:428:VAL:CG1	2.23	0.68
1:A:36:ILE:HG12	1:A:70:ILE:HD11	1.75	0.68
1:A:48:TRP:HD1	1:A:49:LEU:HG	1.59	0.68
1:B:70:ILE:HD11	1:B:408:VAL:HG11	1.77	0.67
1:B:76:THR:HG21	1:B:427:VAL:HG12	1.75	0.67
1:B:208:VAL:O	1:B:208:VAL:HG12	1.95	0.66
1:B:293:CYS:HB3	1:B:298:LYS:O	1.95	0.66
1:B:323:PHE:CE2	1:B:327:LYS:HE3	2.30	0.66
1:B:296:ILE:HG22	1:B:296:ILE:O	1.96	0.66
1:B:310:PHE:O	1:B:314:VAL:HG13	1.95	0.66
1:B:296:ILE:HD11	1:B:324:ILE:HG23	1.79	0.65
1:B:2:THR:O	1:B:3:LYS:HB2	1.96	0.65
1:A:18:ALA:N	2:A:501:COA:S1P	2.65	0.64
1:A:209:ARG:HD2	1:B:63:PHE:CE2	2.32	0.64
1:A:208:VAL:HG12	1:A:208:VAL:O	1.98	0.64
1:A:323:PHE:O	1:A:326:THR:HB	1.98	0.63
1:A:117:PRO:HB3	1:A:192:ARG:HH11	1.62	0.63
1:B:124:VAL:HG23	1:B:176:LEU:HD22	1.80	0.63
1:A:17:GLN:N	2:A:501:COA:S1P	2.72	0.63
1:A:10:VAL:HG22	1:A:92:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:PHE:HE2	1:B:327:LYS:HE3	1.65	0.62
1:A:289:TRP:HB3	1:A:290:PRO:HD3	1.80	0.62
1:B:405:THR:HG21	1:B:428:VAL:HG11	1.80	0.62
1:A:100:GLY:O	1:A:104:ARG:HG3	1.99	0.61
1:A:116:ASN:O	1:A:119:VAL:HG12	2.00	0.61
1:B:295:MET:C	1:B:297:ASP:H	2.01	0.61
1:A:89:LYS:NZ	1:A:412:LEU:HA	2.16	0.61
1:B:234:PHE:CD2	1:B:318:MET:HG3	2.36	0.61
1:B:116:ASN:O	1:B:119:VAL:HG12	2.02	0.60
1:A:418:LYS:CD	1:A:418:LYS:H	2.15	0.60
1:B:405:THR:HG21	1:B:428:VAL:HG13	1.83	0.59
1:A:17:GLN:HB3	2:A:501:COA:S1P	2.42	0.59
1:A:306:ALA:HB1	1:A:316:LYS:NZ	2.18	0.59
3:A:574:HOH:O	1:B:260:GLY:HA3	2.01	0.59
1:A:97:PHE:HB3	1:A:101:ALA:HB3	1.84	0.59
1:B:407:GLU:O	1:B:411:GLU:HG3	2.03	0.58
1:A:89:LYS:HZ2	1:A:412:LEU:HA	1.68	0.58
1:A:288:MET:CE	1:A:346:PRO:HD3	2.33	0.58
1:A:418:LYS:N	1:A:418:LYS:HD2	2.18	0.58
1:A:159:PRO:HB3	3:A:593:HOH:O	2.04	0.58
1:A:19:GLY:H	1:A:96:ASN:HD21	1.52	0.57
1:A:125:LYS:NZ	1:A:129:GLU:HB2	2.18	0.57
1:B:295:MET:HE3	1:B:345:ILE:HD12	1.85	0.57
1:A:288:MET:HE1	1:A:346:PRO:HD3	1.85	0.57
1:A:47:GLY:HA2	1:A:50:GLN:NE2	2.20	0.57
1:B:72:LEU:HD11	1:B:79:GLY:HA2	1.86	0.56
1:B:422:LEU:HD22	1:B:427:VAL:HG21	1.87	0.56
1:A:167:LEU:O	1:A:171:ASN:HB3	2.06	0.56
1:B:125:LYS:HD3	3:B:574:HOH:O	2.05	0.56
1:B:16:VAL:HG12	1:B:17:GLN:N	2.21	0.56
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.41	0.56
1:B:296:ILE:O	1:B:297:ASP:C	2.43	0.56
1:B:297:ASP:OD1	1:B:327:LYS:NZ	2.34	0.56
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.41	0.56
1:B:313:ARG:HD2	1:B:320:ILE:HD12	1.87	0.56
1:A:215:GLN:O	1:A:219:GLU:HG3	2.05	0.55
1:B:102:LEU:HD22	1:B:107:PHE:HB2	1.88	0.55
1:A:167:LEU:HD21	1:B:167:LEU:CD2	2.36	0.55
1:B:300:GLU:H	1:B:300:GLU:CD	2.09	0.55
1:B:427:VAL:HG23	1:B:428:VAL:HG23	1.89	0.55
1:B:343:TYR:HB2	1:B:345:ILE:HG13	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:PHE:CE2	1:B:318:MET:HG3	2.42	0.55
1:A:14:THR:HB	1:A:96:ASN:OD1	2.07	0.55
1:A:414:LEU:CD1	1:A:414:LEU:H	2.19	0.55
1:B:231:GLN:HG3	1:B:232:PRO:HD2	1.88	0.55
1:A:414:LEU:HD12	1:A:414:LEU:N	2.22	0.54
1:A:70:ILE:O	1:A:70:ILE:HG13	2.07	0.54
1:B:289:TRP:N	1:B:290:PRO:CD	2.70	0.54
1:A:311:GLU:H	1:A:311:GLU:CD	2.11	0.54
1:B:414:LEU:HD22	1:B:418:LYS:HD3	1.89	0.54
1:A:48:TRP:CD1	1:A:49:LEU:HG	2.41	0.54
1:A:407:GLU:O	1:A:411:GLU:HG3	2.08	0.53
1:B:70:ILE:HD11	1:B:408:VAL:HG21	1.90	0.53
1:B:100:GLY:O	1:B:104:ARG:HG3	2.08	0.53
1:B:70:ILE:HD11	1:B:408:VAL:CB	2.39	0.53
1:B:295:MET:CE	1:B:345:ILE:HD12	2.39	0.53
1:A:104:ARG:NH1	2:A:501:COA:O7A	2.42	0.52
1:A:70:ILE:HG22	1:A:405:THR:HA	1.91	0.52
1:A:353:MET:HE1	1:B:148:GLY:CA	2.35	0.52
1:B:17:GLN:N	2:B:502:COA:S1P	2.80	0.52
1:B:295:MET:HE2	1:B:340:ALA:HA	1.91	0.52
1:A:46:ARG:NH2	1:A:399:PRO:O	2.42	0.52
1:B:210:ILE:O	1:B:213:ARG:HB3	2.09	0.52
1:A:250:SER:HB2	1:B:354:LYS:HE3	1.92	0.51
1:B:131:HIS:O	1:B:134:GLU:HB2	2.10	0.51
1:B:208:VAL:HG12	1:B:211:LYS:HB2	1.92	0.51
1:B:320:ILE:O	1:B:323:PHE:HB3	2.10	0.51
1:B:104:ARG:NH1	2:B:502:COA:O7A	2.42	0.51
1:B:296:ILE:O	1:B:327:LYS:NZ	2.44	0.51
1:B:70:ILE:HD11	1:B:408:VAL:CG1	2.40	0.51
1:B:409:LEU:HD11	1:B:428:VAL:HG21	1.92	0.51
1:B:14:THR:HA	1:B:96:ASN:OD1	2.11	0.51
1:A:72:LEU:HD11	1:A:79:GLY:HA2	1.93	0.50
1:B:293:CYS:HB2	1:B:302:LYS:CE	2.40	0.50
1:A:11:LEU:HD12	1:A:36:ILE:HD11	1.93	0.50
1:B:110:GLU:H	1:B:110:GLU:CD	2.13	0.50
1:B:293:CYS:HB2	1:B:302:LYS:HE3	1.94	0.50
1:B:301:TRP:CD1	1:B:307:TYR:HD1	2.30	0.49
1:A:3:LYS:HG2	1:A:391:PHE:CE1	2.47	0.49
1:B:11:LEU:HG	1:B:13:PHE:CE1	2.46	0.49
1:B:224:LEU:HB2	1:B:245:PHE:CZ	2.48	0.49
1:B:298:LYS:HE3	1:B:323:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:O	1:B:76:THR:HB	2.13	0.49
1:A:186:MET:HG3	1:B:4:PRO:HA	1.94	0.49
1:B:301:TRP:CD1	1:B:307:TYR:CD1	3.00	0.49
1:B:268:LYS:HD3	1:B:272:TRP:CE2	2.48	0.48
1:A:267:LEU:HD22	1:A:325:GLU:HB2	1.94	0.48
1:A:292:ILE:O	1:A:296:ILE:HG12	2.13	0.48
1:B:305:PRO:HA	1:B:308:ASN:OD1	2.14	0.48
1:B:296:ILE:HA	1:B:327:LYS:HZ2	1.77	0.48
1:B:268:LYS:HD3	1:B:272:TRP:CD2	2.48	0.48
1:A:237:ASP:OD2	1:A:241:ASN:HB2	2.13	0.48
1:B:296:ILE:CA	1:B:327:LYS:HZ2	2.27	0.48
1:B:122:ALA:HA	1:B:196:VAL:O	2.14	0.48
1:A:11:LEU:CD1	1:A:36:ILE:HD11	2.44	0.48
1:A:268:LYS:HD3	1:A:272:TRP:CD2	2.49	0.48
1:A:3:LYS:HB2	1:A:6:ASP:OD2	2.14	0.48
1:A:120:ILE:HD13	1:A:183:ALA:CB	2.43	0.47
1:B:74:MET:SD	1:B:83:LEU:HD11	2.54	0.47
1:A:353:MET:CE	1:B:148:GLY:HA3	2.36	0.47
1:B:306:ALA:O	1:B:312:GLY:O	2.32	0.47
1:B:295:MET:C	1:B:297:ASP:N	2.68	0.47
1:B:421:GLU:HB3	1:B:425:LYS:HE3	1.94	0.47
1:A:131:HIS:O	1:A:134:GLU:HB2	2.14	0.47
1:B:83:LEU:O	1:B:87:ILE:HG13	2.14	0.47
1:A:109:TRP:O	1:A:113:GLN:HG3	2.14	0.47
1:A:56:ASP:HB2	1:A:376:ARG:HE	1.80	0.47
1:A:210:ILE:O	1:A:213:ARG:HB3	2.15	0.46
1:B:307:TYR:HE2	1:B:316:LYS:HE3	1.81	0.46
1:B:400:LEU:HB2	1:B:403:GLU:HB2	1.97	0.46
1:A:186:MET:SD	1:A:194:GLN:NE2	2.89	0.46
1:A:61:THR:HG21	3:A:634:HOH:O	2.15	0.45
1:B:311:GLU:CD	1:B:311:GLU:H	2.19	0.45
1:A:223:ILE:HG12	1:A:224:LEU:N	2.31	0.45
1:B:289:TRP:HB3	1:B:290:PRO:HD3	1.98	0.45
1:B:360:PRO:O	1:B:364:LYS:HG3	2.17	0.45
1:A:17:GLN:HB3	2:A:501:COA:HS1	1.81	0.45
1:B:200:MET:CE	2:B:502:COA:H32	2.46	0.45
1:A:315:ASP:OD1	1:A:316:LYS:HE3	2.17	0.45
1:A:71:GLU:HG3	1:A:402:GLY:HA3	1.99	0.45
1:B:301:TRP:CG	1:B:307:TYR:HD1	2.35	0.45
1:B:37:GLU:HB3	1:B:42:GLY:HA2	1.99	0.45
1:B:109:TRP:O	1:B:113:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LEU:O	1:B:171:ASN:HB3	2.17	0.45
1:A:415:ASP:H	1:A:418:LYS:HD3	1.82	0.44
1:B:16:VAL:HG12	1:B:17:GLN:H	1.81	0.44
1:A:95:GLU:HG2	1:A:102:LEU:CD1	2.41	0.44
1:A:39:ARG:HA	1:A:71:GLU:HB3	1.99	0.44
1:B:70:ILE:CD1	1:B:408:VAL:HG11	2.44	0.44
1:A:125:LYS:HE3	1:A:197:ALA:HB1	1.99	0.44
1:B:223:ILE:HG12	1:B:224:LEU:N	2.32	0.44
1:B:289:TRP:HH2	1:B:320:ILE:HD13	1.82	0.44
1:B:95:GLU:HG2	1:B:96:ASN:N	2.33	0.44
1:B:282:PHE:HE1	1:B:284:ILE:HG12	1.82	0.44
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.52	0.44
1:B:2:THR:O	1:B:3:LYS:CB	2.65	0.44
1:B:83:LEU:HD23	1:B:86:MET:HE3	1.99	0.44
1:B:306:ALA:O	1:B:316:LYS:HE2	2.18	0.44
1:B:296:ILE:HG22	1:B:298:LYS:HG3	1.99	0.43
1:A:38:ARG:HG2	2:A:501:COA:N6A	2.33	0.43
1:A:404:HIS:O	1:A:408:VAL:HG23	2.18	0.43
1:B:233:ASN:HB3	1:B:242:PRO:HB3	1.99	0.43
1:A:2:THR:HG22	1:A:3:LYS:HG3	2.01	0.43
1:B:359:ASP:OD2	1:B:361:SER:HB2	2.18	0.43
1:A:11:LEU:HD12	1:A:36:ILE:CD1	2.48	0.43
1:A:49:LEU:HD13	1:B:217:ARG:NH1	2.33	0.43
1:B:231:GLN:NE2	1:B:234:PHE:HB2	2.33	0.43
1:B:35:LYS:HE2	1:B:60:PHE:HE2	1.84	0.43
1:A:137:LYS:HD3	2:A:501:COA:H121	2.01	0.43
1:B:97:PHE:O	3:B:574:HOH:O	2.21	0.43
1:A:208:VAL:CG1	1:A:208:VAL:O	2.67	0.42
1:B:275:ASP:HB3	1:B:278:SER:HB2	2.01	0.42
1:A:205:LEU:HD23	1:B:367:THR:HG22	2.01	0.42
1:A:306:ALA:HB1	1:A:316:LYS:HZ2	1.85	0.42
1:B:244:SER:C	1:B:246:ASP:H	2.23	0.42
1:B:32:ASN:ND2	3:B:564:HOH:O	2.52	0.42
1:A:96:ASN:HB2	1:A:97:PHE:H	1.70	0.42
1:A:14:THR:HB	1:A:20:PRO:HD3	2.01	0.42
1:A:219:GLU:OE2	1:B:358:HIS:CE1	2.62	0.42
1:A:388:PHE:N	1:A:388:PHE:CD1	2.87	0.42
1:B:12:ASP:OD1	1:B:23:THR:HG21	2.20	0.42
1:B:307:TYR:CE2	1:B:316:LYS:HE3	2.54	0.42
1:A:76:THR:O	1:A:80:LYS:HG3	2.20	0.42
1:A:289:TRP:CD1	1:A:308:ASN:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLN:HG3	3:A:633:HOH:O	2.20	0.42
1:B:239:ASP:O	1:B:241:ASN:N	2.52	0.42
1:B:82:LEU:O	1:B:86:MET:HG3	2.20	0.42
1:A:317:LEU:HG	1:A:321:PHE:CE2	2.55	0.42
1:B:108:THR:O	1:B:112:ILE:HG13	2.20	0.42
1:B:76:THR:O	1:B:80:LYS:HG3	2.20	0.42
1:B:345:ILE:HA	1:B:346:PRO:HD3	1.87	0.42
1:B:122:ALA:HB1	1:B:176:LEU:HD11	2.01	0.41
1:B:15:HIS:HA	1:B:43:ASP:OD2	2.19	0.41
1:A:17:GLN:CA	2:A:501:COA:S1P	3.09	0.41
1:A:186:MET:CE	1:B:4:PRO:HG3	2.50	0.41
1:A:37:GLU:OE2	1:A:46:ARG:NH1	2.54	0.41
1:A:52:LYS:HA	1:A:53:PRO:HD2	1.88	0.41
1:B:241:ASN:HA	1:B:242:PRO:HD3	1.82	0.41
1:B:313:ARG:HD2	1:B:320:ILE:CD1	2.50	0.41
1:B:352:SER:OG	1:B:355:GLU:HG3	2.20	0.41
1:A:125:LYS:HZ3	1:A:129:GLU:HB2	1.82	0.41
1:A:278:SER:HA	1:A:333:LYS:HD2	2.03	0.41
1:A:288:MET:HE1	1:A:346:PRO:CD	2.50	0.41
1:A:285:ALA:HB3	1:A:288:MET:HE2	2.01	0.41
1:A:14:THR:CB	1:A:96:ASN:OD1	2.69	0.41
1:B:277:ASP:O	1:B:333:LYS:HD2	2.20	0.41
1:A:333:LYS:HB3	1:A:349:PRO:HB3	2.02	0.41
1:B:13:PHE:CE2	1:B:83:LEU:HD22	2.55	0.41
1:B:208:VAL:CG1	1:B:211:LYS:HB2	2.51	0.41
1:B:144:GLN:HG2	1:B:167:LEU:HB2	2.03	0.41
1:B:183:ALA:HA	1:B:186:MET:HE2	2.01	0.41
1:A:73:ASP:O	1:A:76:THR:HB	2.20	0.41
1:A:10:VAL:HG22	1:A:92:VAL:CG1	2.47	0.40
1:B:286:ALA:C	1:B:288:MET:H	2.25	0.40
1:A:120:ILE:HD13	1:A:183:ALA:HB3	2.03	0.40
1:B:278:SER:HA	1:B:333:LYS:HD2	2.04	0.40
1:B:295:MET:HB2	1:B:343:TYR:CE2	2.57	0.40
1:B:70:ILE:HG12	1:B:405:THR:HA	2.03	0.40
1:B:425:LYS:O	1:B:426:GLN:HB2	2.21	0.40
1:A:268:LYS:HG2	1:A:279:TYR:CE2	2.56	0.40
1:A:262:GLN:HE21	1:A:285:ALA:HA	1.86	0.40
1:A:416:ASP:O	1:A:420:LYS:HG3	2.22	0.40
1:A:3:LYS:HA	1:A:4:PRO:HD3	1.88	0.40
1:B:13:PHE:CZ	1:B:83:LEU:HD22	2.57	0.40
1:B:273:GLU:CD	1:B:273:GLU:H	2.22	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	425/428 (99%)	403 (95%)	20 (5%)	2 (0%)	29	48
1	B	425/428 (99%)	382 (90%)	30 (7%)	13 (3%)	4	5
All	All	850/856 (99%)	785 (92%)	50 (6%)	15 (2%)	8	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	97	PHE
1	B	3	LYS
1	B	238	ARG
1	B	16	VAL
1	B	263	PRO
1	B	296	ILE
1	B	98	GLY
1	B	140	GLU
1	B	233	ASN
1	B	287	ASN
1	B	297	ASP
1	B	240	GLY
1	B	313	ARG
1	B	40	GLY

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	350/351 (100%)	338 (97%)	12 (3%)	37	63
1	B	350/351 (100%)	341 (97%)	9 (3%)	46	72
All	All	700/702 (100%)	679 (97%)	21 (3%)	41	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	32	ASN
1	A	59	TYR
1	A	102	LEU
1	A	118	ARG
1	A	196	VAL
1	A	233	ASN
1	A	326	THR
1	A	356	LEU
1	A	386	PHE
1	A	415	ASP
1	A	416	ASP
1	B	15	HIS
1	B	32	ASN
1	B	59	TYR
1	B	92	VAL
1	B	102	LEU
1	B	239	ASP
1	B	247	ASN
1	B	294	ASP
1	B	386	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	262	GLN
1	A	363	GLN
1	B	9	ASN
1	B	32	ASN
1	B	188	HIS
1	B	206	ASN

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Mol	Chain	Res	Type
1	B	247	ASN
1	B	358	HIS
1	B	378	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](#)

2 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	501	-	41,50,50	1.51	3 (7%)	52,75,75	2.89	13 (25%)
2	COA	B	502	-	41,50,50	1.53	5 (12%)	52,75,75	2.80	15 (28%)

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	501	-	-	11/44/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	B	502	-	-	12/44/64/64	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	COA	O9P-C9P	5.69	1.34	1.23
2	B	502	COA	O9P-C9P	5.54	1.34	1.23
2	A	501	COA	C2A-N1A	3.25	1.40	1.33
2	B	502	COA	C2A-N1A	3.18	1.39	1.33
2	B	502	COA	P2A-O6A	-3.03	1.47	1.59
2	A	501	COA	P2A-O6A	-2.91	1.47	1.59
2	B	502	COA	C7P-N8P	2.19	1.51	1.46
2	B	502	COA	P3B-O8A	-2.02	1.47	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	COA	C6P-C7P-N8P	-11.31	89.07	111.90
2	B	502	COA	C6P-C7P-N8P	-10.68	90.33	111.90
2	B	502	COA	O6A-CCP-CBP	-9.43	95.38	110.55
2	A	501	COA	O6A-CCP-CBP	-9.13	95.87	110.55
2	A	501	COA	C7P-C6P-C5P	6.28	122.81	112.36
2	A	501	COA	C2P-C3P-N4P	-6.26	97.99	112.31
2	B	502	COA	C2P-C3P-N4P	-5.97	98.66	112.31
2	B	502	COA	C7P-C6P-C5P	5.85	122.09	112.36
2	A	501	COA	CAP-C9P-N8P	-4.74	107.15	116.58
2	B	502	COA	CAP-C9P-N8P	-4.34	107.93	116.58
2	A	501	COA	C6P-C5P-N4P	-4.34	109.12	116.42
2	A	501	COA	C7P-N8P-C9P	4.16	130.01	122.59
2	A	501	COA	CDP-CBP-CCP	4.16	115.02	108.23
2	B	502	COA	C6P-C5P-N4P	-4.13	109.48	116.42
2	A	501	COA	O9P-C9P-N8P	4.10	131.79	122.99
2	B	502	COA	O9P-C9P-N8P	4.01	131.60	122.99
2	B	502	COA	C7P-N8P-C9P	3.83	129.43	122.59
2	B	502	COA	CDP-CBP-CCP	3.80	114.43	108.23
2	B	502	COA	O4B-C1B-C2B	-2.58	103.15	106.93
2	A	501	COA	O4B-C1B-C2B	-2.51	103.26	106.93
2	B	502	COA	OAP-CAP-CBP	2.48	116.09	110.25
2	A	501	COA	O9A-P3B-O8A	2.40	116.81	107.64
2	A	501	COA	C5A-C6A-N6A	2.36	123.94	120.35
2	B	502	COA	O9A-P3B-O8A	2.32	116.50	107.64
2	B	502	COA	C5A-C6A-N6A	2.26	123.79	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	COA	O5P-C5P-N4P	2.20	127.17	123.01
2	B	502	COA	C3P-N4P-C5P	-2.13	118.89	122.84
2	B	502	COA	O5P-C5P-N4P	2.05	126.89	123.01

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	COA	CCP-O6A-P2A-O3A
2	A	501	COA	OAP-CAP-CBP-CCP
2	A	501	COA	C9P-CAP-CBP-CCP
2	A	501	COA	OAP-CAP-CBP-CDP
2	A	501	COA	C9P-CAP-CBP-CDP
2	A	501	COA	OAP-CAP-CBP-CEP
2	A	501	COA	C9P-CAP-CBP-CEP
2	A	501	COA	C5P-C6P-C7P-N8P
2	B	502	COA	CCP-O6A-P2A-O3A
2	B	502	COA	OAP-CAP-CBP-CCP
2	B	502	COA	C9P-CAP-CBP-CCP
2	B	502	COA	OAP-CAP-CBP-CDP
2	B	502	COA	C9P-CAP-CBP-CDP
2	B	502	COA	OAP-CAP-CBP-CEP
2	B	502	COA	C9P-CAP-CBP-CEP
2	B	502	COA	C5P-C6P-C7P-N8P
2	B	502	COA	S1P-C2P-C3P-N4P
2	A	501	COA	CCP-O6A-P2A-O5A
2	B	502	COA	CCP-O6A-P2A-O5A
2	A	501	COA	P2A-O3A-P1A-O1A
2	A	501	COA	P2A-O3A-P1A-O2A
2	B	502	COA	P2A-O3A-P1A-O1A
2	B	502	COA	P2A-O3A-P1A-O2A

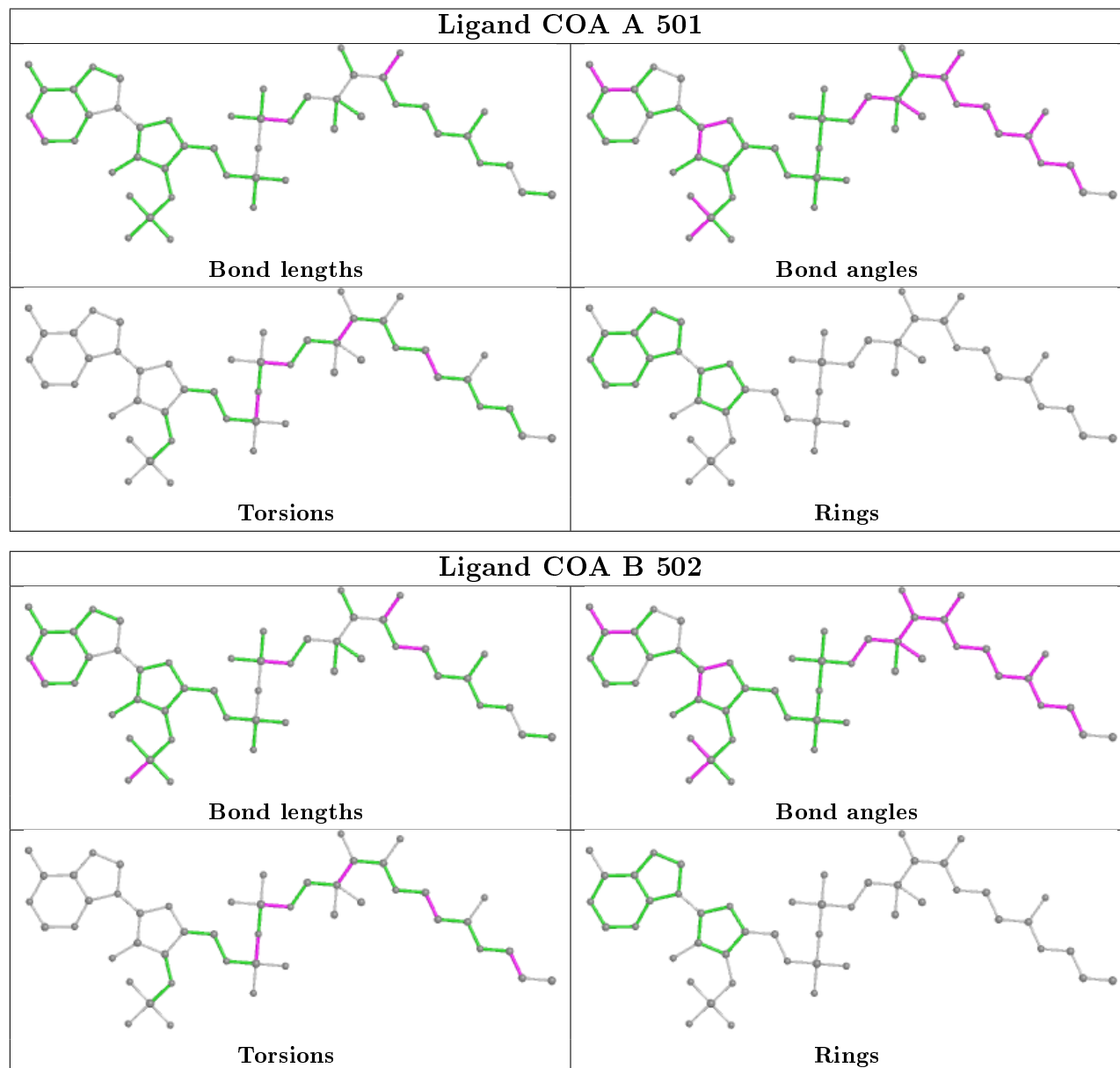
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	COA	8	0
2	B	502	COA	4	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 ⓘ

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, 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	427/428 (99%)	0.23	35 (8%) 11 11	17, 36, 97, 104	0
1	B	426/428 (99%)	0.46	51 (11%) 4 4	20, 42, 104, 117	0
All	All	853/856 (99%)	0.34	86 (10%) 7 6	17, 39, 98, 117	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	PRO	9.0
1	B	287	ASN	8.0
1	A	424	ALA	6.1
1	A	99	PRO	5.8
1	B	241	ASN	5.3
1	B	243	LEU	5.2
1	B	303	ASP	5.2
1	B	239	ASP	4.9
1	B	233	ASN	4.9
1	B	344	GLY	4.7
1	A	97	PHE	4.6
1	A	413	GLY	4.5
1	B	346	PRO	4.4
1	B	310	PHE	4.4
1	B	416	ASP	4.3
1	B	311	GLU	4.3
1	A	104	ARG	3.7
1	B	417	ALA	3.6
1	B	238	ARG	3.5
1	A	103	ASP	3.5
1	B	314	VAL	3.5
1	B	242	PRO	3.4
1	A	54	ASN	3.3
1	B	299	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	427	VAL	3.3
1	B	247	ASN	3.3
1	B	301	TRP	3.3
1	B	415	ASP	3.2
1	B	232	PRO	3.2
1	A	75	LYS	3.2
1	B	290	PRO	3.1
1	A	428	VAL	3.1
1	B	419	ILE	3.0
1	B	234	PHE	3.0
1	B	294	ASP	2.9
1	A	77	PRO	2.9
1	B	286	ALA	2.9
1	B	341	ALA	2.9
1	B	421	GLU	2.9
1	B	306	ALA	2.9
1	A	135	HIS	2.9
1	B	339	TRP	2.8
1	B	288	MET	2.8
1	B	237	ASP	2.7
1	B	298	LYS	2.7
1	A	134	GLU	2.7
1	A	425	LYS	2.7
1	B	304	ASP	2.7
1	B	308	ASN	2.6
1	B	309	THR	2.6
1	A	415	ASP	2.6
1	B	315	ASP	2.6
1	A	111	TYR	2.6
1	A	2	THR	2.5
1	A	80	LYS	2.5
1	B	418	LYS	2.5
1	A	414	LEU	2.5
1	B	297	ASP	2.5
1	A	421	GLU	2.4
1	A	101	ALA	2.4
1	B	236	PHE	2.4
1	A	106	GLY	2.4
1	B	414	LEU	2.4
1	A	81	GLU	2.3
1	A	412	LEU	2.3
1	B	410	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	186	MET	2.3
1	B	330	ASP	2.3
1	B	412	LEU	2.3
1	A	98	GLY	2.3
1	A	74	MET	2.2
1	A	420	LYS	2.2
1	A	100	GLY	2.2
1	B	413	GLY	2.2
1	A	192	ARG	2.2
1	B	424	ALA	2.1
1	A	130	GLY	2.1
1	B	302	LYS	2.1
1	B	295	MET	2.1
1	B	292	ILE	2.1
1	A	132	ALA	2.1
1	B	296	ILE	2.1
1	A	41	SER	2.1
1	B	313	ARG	2.0
1	A	12	ASP	2.0
1	A	410	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](#)

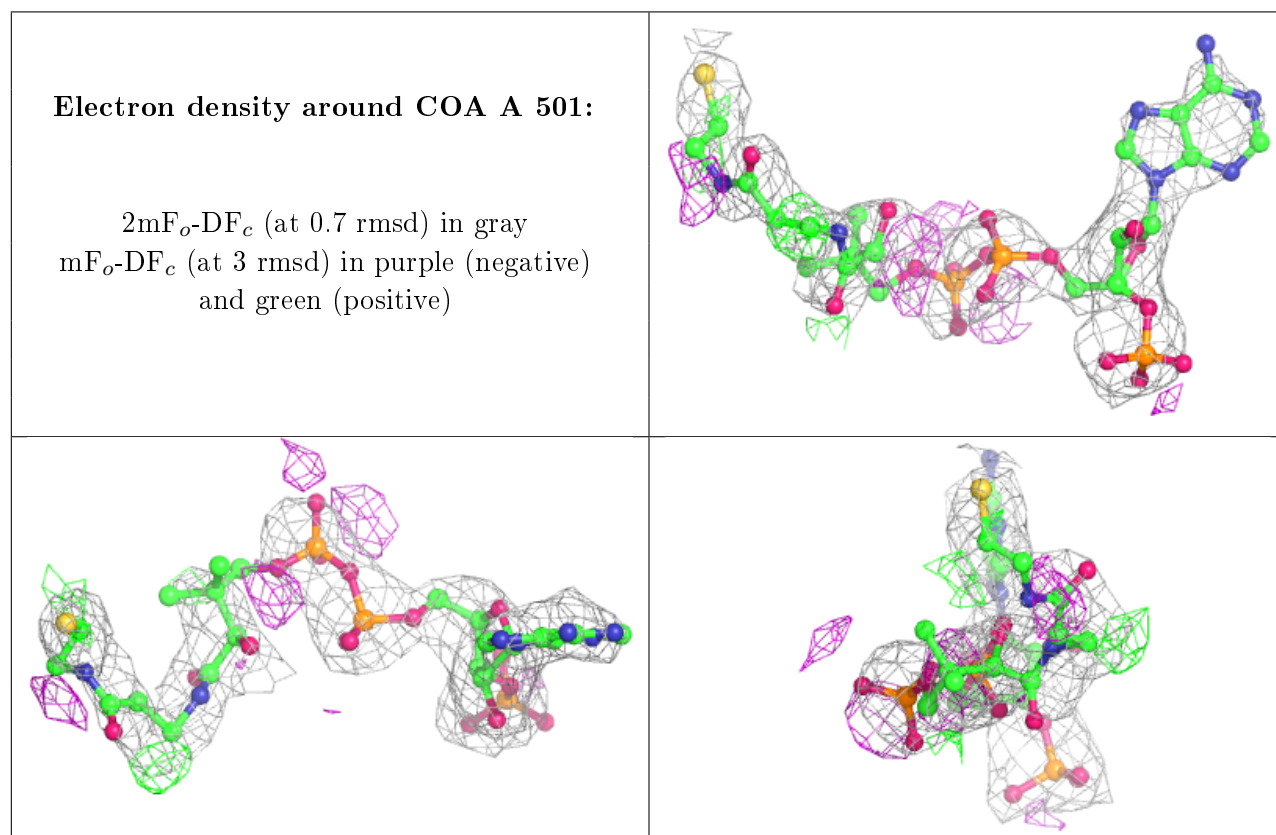
There are no carbohydrates in this entry.

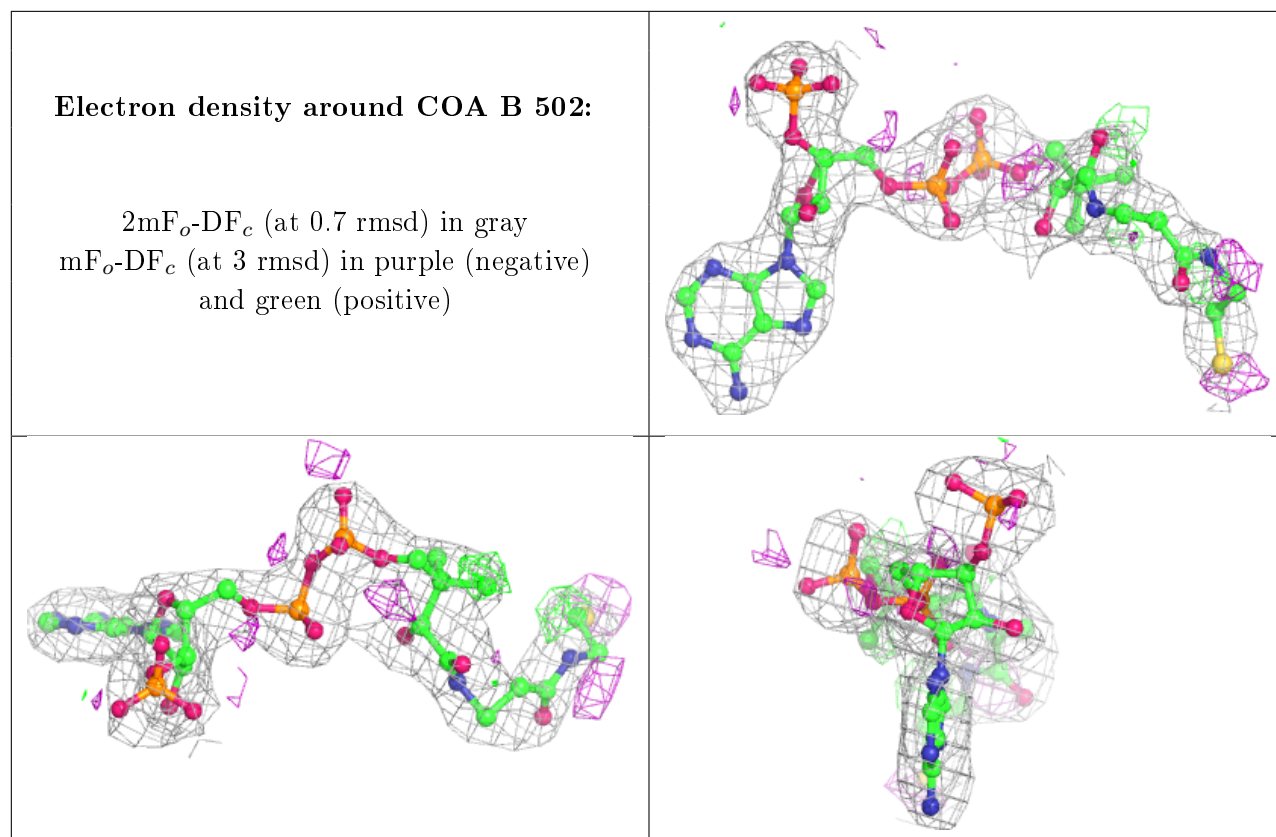
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	COA	A	501	48/48	0.80	0.30	82,101,104,105	0
2	COA	B	502	48/48	0.91	0.17	41,52,59,62	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.