



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 5K04 / pdb_00005k04
Title : The NatB Acetyltransferase Complex Bound To CoA and MES
Authors : Hong, H.; Cai, Y.; Zhang, S.; Han, A.
Deposited on : 2016-05-17
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

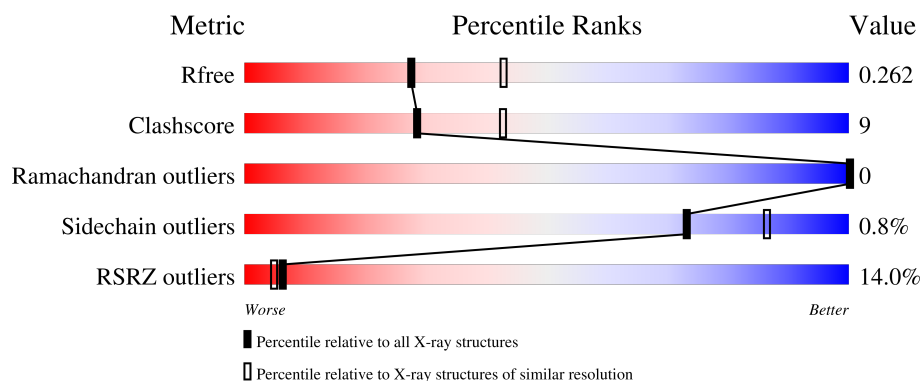
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	750	14% 81% 16% .
2	B	170	11% 71% 18% . 10%

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	MES	B	201	-	X	X	-
4	COA	B	202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7570 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5924	3831	954	1123	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP C4YFL7
A	-3	PRO	-	expression tag	UNP C4YFL7
A	-2	ALA	-	expression tag	UNP C4YFL7
A	-1	GLY	-	expression tag	UNP C4YFL7
A	0	SER	-	expression tag	UNP C4YFL7
A	269	LEU	SER	cloning artifact	UNP C4YFL7

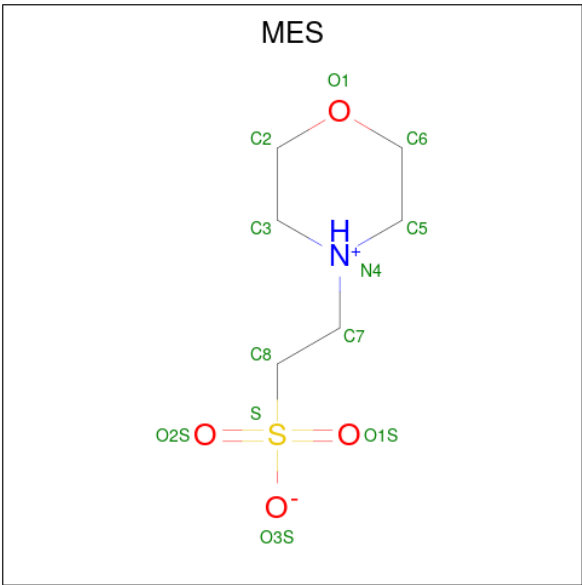
- Molecule 2 is a protein called N-terminal acetyltransferase B complex subunit NAT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1255	814	203	233	5			

There are 2 discrepancies between the modelled and reference sequences:

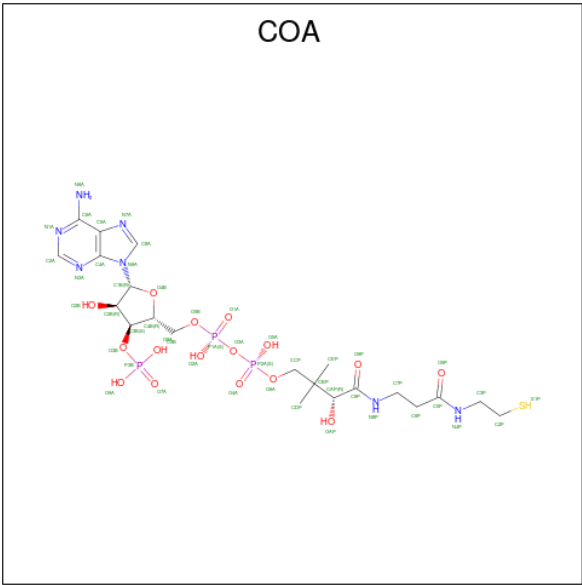
Chain	Residue	Modelled	Actual	Comment	Reference
B	81	LEU	SER	cloning artifact	UNP C4YDZ9
B	162	LEU	SER	cloning artifact	UNP C4YDZ9

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	B	1	48	21	7	16	3	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total 252	O 252	0	0
5	B	79	Total 79	O 79	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.45Å 108.45Å 223.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.82 – 2.40 24.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.82-2.40) 99.8 (24.82-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.199 , 0.239 0.227 , 0.262	Depositor DCC
R_{free} test set	1980 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7570	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: MES, 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	0.37	1/6037 (0.0%)	0.58	6/8164 (0.1%)
2	B	0.39	0/1281	0.72	3/1732 (0.2%)
All	All	0.37	1/7318 (0.0%)	0.60	9/9896 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PRO	N-CD	-7.13	1.37	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ASN	N-CA-C	14.72	133.69	113.37
2	B	49	THR	CB-CA-C	-13.54	87.48	109.41
2	B	49	THR	N-CA-C	10.88	123.36	109.65
1	A	482	GLY	N-CA-C	10.78	131.68	115.08
1	A	33	PRO	N-CA-CB	6.85	110.54	103.00
1	A	481	ASN	CA-C-N	-6.30	109.78	121.07
1	A	481	ASN	C-N-CA	-6.30	109.78	121.07
1	A	67	PRO	N-CA-C	6.08	125.00	112.47
2	B	51	ASN	N-CA-C	5.04	120.05	113.30

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	5924	0	5890	75	0
2	B	1255	0	1256	45	0
3	B	12	0	12	9	0
4	B	48	0	30	27	0
5	A	252	0	0	7	2
5	B	79	0	0	3	1
All	All	7570	0	7188	127	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (127) 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:B:79:THR:HG22	4:B:202:COA:C7P	1.55	1.35
2:B:79:THR:HG22	4:B:202:COA:H71	1.16	1.13
2:B:123:LEU:HD13	4:B:202:COA:H52A	1.29	1.08
3:B:201:MES:H82	4:B:202:COA:H31	1.37	1.03
2:B:79:THR:CG2	4:B:202:COA:H71	1.92	0.99
2:B:137:GLY:O	5:B:301:HOH:O	1.87	0.92
1:A:359:GLY:O	5:A:801:HOH:O	1.86	0.92
2:B:79:THR:CG2	4:B:202:COA:C7P	2.45	0.91
2:B:24:THR:HA	3:B:201:MES:H62	1.56	0.87
2:B:79:THR:HG22	4:B:202:COA:H72	1.54	0.87
2:B:79:THR:HA	4:B:202:COA:H72	1.56	0.86
1:A:340:LYS:NZ	5:A:804:HOH:O	2.14	0.81
1:A:384:GLN:NE2	1:A:714:ASP:O	2.14	0.80
2:B:78:VAL:H	3:B:201:MES:H72	1.48	0.78
1:A:44:GLU:HA	1:A:47:LEU:HD12	1.66	0.78
1:A:8:GLU:N	5:A:806:HOH:O	2.14	0.78
2:B:119:LEU:HD11	4:B:202:COA:C4A	2.13	0.77
2:B:77:ALA:HA	3:B:201:MES:H71	1.67	0.75
2:B:35:TYR:OH	2:B:76:THR:HG21	1.88	0.74
3:B:201:MES:C8	4:B:202:COA:H31	2.17	0.73
2:B:79:THR:HA	4:B:202:COA:C7P	2.18	0.73
1:A:437:HIS:O	1:A:441:ASN:HB2	1.90	0.72
2:B:79:THR:HG22	4:B:202:COA:C6P	2.20	0.72
1:A:44:GLU:CD	1:A:58:LYS:HB3	2.16	0.70
1:A:484:PHE:O	5:A:802:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LEU:O	5:B:302:HOH:O	2.12	0.68
1:A:351:TYR:HA	1:A:367:VAL:HG11	1.77	0.66
2:B:119:LEU:HD11	4:B:202:COA:N3A	2.10	0.66
1:A:178:GLU:OE2	5:A:803:HOH:O	2.13	0.64
2:B:164:PRO:O	5:B:303:HOH:O	2.14	0.64
2:B:73:THR:HG21	2:B:103:VAL:HG13	1.81	0.63
1:A:329:GLU:O	1:A:353:ARG:NH2	2.34	0.60
2:B:24:THR:HA	3:B:201:MES:C6	2.31	0.60
1:A:63:LEU:HD13	1:A:92:VAL:HG22	1.82	0.60
1:A:264:ASP:OD1	1:A:278:LYS:NZ	2.36	0.59
2:B:79:THR:CB	4:B:202:COA:H71	2.32	0.59
2:B:123:LEU:HD13	4:B:202:COA:C5B	2.20	0.59
2:B:123:LEU:CD1	4:B:202:COA:H52A	2.19	0.59
2:B:79:THR:CG2	4:B:202:COA:H72	2.25	0.58
2:B:2:THR:HG21	2:B:89:LEU:HD13	1.87	0.57
1:A:365:ASN:OD1	1:A:367:VAL:HG23	2.04	0.57
1:A:99:LYS:HD2	1:A:100:TYR:CZ	2.40	0.56
1:A:511:LEU:O	1:A:515:THR:HG23	2.06	0.56
1:A:709:ILE:O	1:A:713:MET:HG3	2.06	0.55
1:A:261:GLU:OE2	5:A:807:HOH:O	2.18	0.55
1:A:413:LEU:HD23	1:A:560:ILE:HD11	1.88	0.54
2:B:123:LEU:HB2	4:B:202:COA:O4B	2.07	0.54
1:A:354:PHE:HB2	1:A:367:VAL:HG21	1.89	0.53
2:B:72:HIS:HA	2:B:106:THR:HB	1.90	0.53
1:A:368:ASN:HA	1:A:371:THR:OG1	2.09	0.52
1:A:104:THR:HG21	1:A:134:ASN:HB2	1.91	0.52
1:A:457:TRP:CE2	1:A:509:LYS:HG2	2.44	0.52
1:A:69:ASP:OD2	1:A:72:THR:HG23	2.10	0.52
1:A:181:GLN:HE22	1:A:485:ASN:HB2	1.76	0.51
2:B:47:VAL:HG13	2:B:52:GLY:HA2	1.93	0.51
1:A:434:MET:HA	1:A:463:PHE:CD1	2.47	0.49
1:A:578:ILE:O	1:A:620:LYS:HE2	2.12	0.49
2:B:78:VAL:H	3:B:201:MES:C7	2.24	0.49
2:B:79:THR:HG22	4:B:202:COA:H62	1.93	0.49
1:A:215:MET:SD	1:A:231:THR:HG22	2.52	0.49
1:A:261:GLU:OE1	5:A:808:HOH:O	2.20	0.48
2:B:136:VAL:HG12	2:B:138:TYR:H	1.78	0.48
1:A:642:ASP:HA	1:A:645:LYS:HE2	1.94	0.48
4:B:202:COA:H61	4:B:202:COA:O9P	2.14	0.48
1:A:90:SER:OG	1:A:94:GLU:OE2	2.27	0.48
4:B:202:COA:H132	4:B:202:COA:H22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:CE2	1:A:247:LYS:HD2	2.49	0.48
2:B:73:THR:HG23	2:B:106:THR:OG1	2.14	0.47
1:A:363:ASP:OD2	4:B:202:COA:N6A	2.48	0.47
1:A:56:ILE:HD11	1:A:83:MET:HE2	1.95	0.47
2:B:24:THR:HG23	2:B:79:THR:HG21	1.95	0.47
1:A:288:ASN:OD1	1:A:290:GLU:HB2	2.15	0.47
4:B:202:COA:N8P	4:B:202:COA:H141	2.29	0.47
1:A:41:LEU:HD22	1:A:76:LEU:HG	1.96	0.47
1:A:47:LEU:O	1:A:51:GLN:N	2.34	0.46
1:A:641:THR:O	1:A:645:LYS:HG3	2.15	0.46
1:A:44:GLU:HG2	1:A:58:LYS:HD3	1.97	0.46
1:A:691:LYS:HD3	1:A:691:LYS:HA	1.82	0.46
1:A:112:PHE:O	1:A:116:ILE:HG13	2.16	0.45
1:A:387:ILE:HD12	1:A:713:MET:HE1	1.99	0.45
2:B:73:THR:OG1	2:B:109:ILE:HG23	2.15	0.45
1:A:361:GLU:HG3	1:A:362:TYR:CD2	2.52	0.45
4:B:202:COA:N8P	4:B:202:COA:CEP	2.80	0.45
2:B:77:ALA:HA	3:B:201:MES:C7	2.43	0.45
1:A:254:LYS:HD3	1:A:284:LEU:HG	1.98	0.45
2:B:49:THR:O	2:B:49:THR:OG1	2.23	0.45
3:B:201:MES:H51	4:B:202:COA:HN4	1.82	0.45
1:A:289:ILE:HG22	1:A:293:VAL:HG23	1.98	0.44
1:A:360:ALA:HB3	1:A:363:ASP:OD2	2.16	0.44
2:B:58:MET:HB2	2:B:58:MET:HE2	1.81	0.44
1:A:336:VAL:HA	1:A:370:LEU:HD11	1.98	0.44
1:A:613:PHE:CZ	1:A:617:LYS:HD2	2.53	0.44
1:A:392:LEU:O	1:A:396:LEU:HG	2.17	0.44
1:A:527:ILE:O	1:A:531:LYS:HG2	2.18	0.44
2:B:110:ASP:HA	2:B:159:MET:O	2.17	0.44
1:A:282:ASP:OD2	1:A:292:SER:OG	2.30	0.44
1:A:272:ARG:HH12	2:B:2:THR:HG22	1.82	0.44
1:A:727:LYS:O	1:A:731:LYS:HG3	2.19	0.43
1:A:523:LEU:O	1:A:527:ILE:HG12	2.18	0.43
1:A:136:LYS:HE3	1:A:136:LYS:HB3	1.81	0.43
1:A:149:HIS:O	1:A:153:GLN:HG2	2.18	0.43
1:A:668:ILE:HD11	1:A:693:PHE:HD2	1.83	0.43
2:B:2:THR:HG22	2:B:48:GLU:OE1	2.18	0.43
2:B:24:THR:CG2	2:B:79:THR:HG21	2.49	0.43
2:B:91:SER:HB3	2:B:127:LEU:HD21	2.01	0.43
1:A:88:GLU:O	1:A:92:VAL:HG23	2.19	0.43
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HG11	1:A:723:ILE:HD13	2.01	0.42
1:A:329:GLU:HG2	1:A:330:GLU:H	1.84	0.42
1:A:615:LEU:HD11	1:A:683:MET:HE1	2.02	0.42
2:B:79:THR:CA	4:B:202:COA:C7P	2.94	0.42
1:A:111:TRP:CD2	1:A:127:ILE:HG12	2.55	0.42
1:A:647:LEU:HB2	1:A:660:ASN:HB3	2.02	0.41
2:B:82:ASP:OD1	2:B:83:GLN:N	2.53	0.41
1:A:83:MET:O	1:A:85:MET:HG3	2.21	0.41
1:A:99:LYS:HB3	1:A:100:TYR:CD2	2.55	0.41
1:A:74:GLU:OE2	1:A:110:SER:OG	2.34	0.41
1:A:74:GLU:HG2	1:A:93:TYR:OH	2.21	0.41
1:A:133:LYS:HE2	1:A:133:LYS:HB2	1.92	0.41
1:A:332:LEU:HD11	1:A:367:VAL:HG22	2.03	0.41
1:A:551:TRP:CE3	1:A:556:LYS:HA	2.56	0.41
1:A:641:THR:HG22	1:A:697:PHE:CE1	2.56	0.41
1:A:119:TYR:CD1	1:A:495:LYS:HG2	2.56	0.41
4:B:202:COA:C6P	4:B:202:COA:O9P	2.69	0.40
1:A:85:MET:HB3	1:A:88:GLU:OE1	2.21	0.40
1:A:534:GLU:CD	1:A:588:LEU:HD21	2.46	0.40
2:B:80:VAL:HG13	2:B:89:LEU:HD23	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:815:HOH:O	5:B:367:HOH:O[8_554]	2.04	0.16
5:A:949:HOH:O	5:A:1017:HOH:O[5_454]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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	724/750 (96%)	704 (97%)	20 (3%)	0	100	100
2	B	147/170 (86%)	144 (98%)	3 (2%)	0	100	100
All	All	871/920 (95%)	848 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	658/706 (93%)	654 (99%)	4 (1%)	78	89
2	B	141/157 (90%)	139 (99%)	2 (1%)	59	79
All	All	799/863 (93%)	793 (99%)	6 (1%)	73	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	SER
1	A	463	PHE
1	A	483	VAL
1	A	617	LYS
2	B	2	THR
2	B	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	395	HIS
2	B	16	ASN
2	B	72	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	COA	B	202	-	47,50,50	5.84	27 (57%)	69,75,75	4.77	33 (47%)
3	MES	B	201	-	12,12,12	4.53	10 (83%)	15,16,16	3.14	9 (60%)

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	202	-	-	16/48/64/64	0/3/3/3
3	MES	B	201	-	-	4/6/14/14	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	COA	C8A-N9A	15.69	1.64	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	COA	C8A-N7A	13.49	1.57	1.31
4	B	202	COA	C5A-C4A	12.65	1.61	1.39
4	B	202	COA	C2A-N3A	10.50	1.52	1.33
4	B	202	COA	CCP-CBP	9.59	1.68	1.52
4	B	202	COA	C5A-N7A	9.17	1.55	1.39
4	B	202	COA	C2A-N1A	9.14	1.50	1.33
4	B	202	COA	C9P-N8P	8.11	1.52	1.33
4	B	202	COA	CEP-CBP	7.79	1.69	1.53
4	B	202	COA	C4A-N3A	7.44	1.48	1.34
3	B	201	MES	C7-N4	7.38	1.64	1.47
4	B	202	COA	CDP-CBP	7.24	1.68	1.53
3	B	201	MES	C8-S	6.90	1.87	1.77
4	B	202	COA	O9P-C9P	6.76	1.36	1.23
4	B	202	COA	C6P-C5P	6.61	1.64	1.51
3	B	201	MES	C5-N4	6.57	1.64	1.46
3	B	201	MES	C3-N4	6.51	1.64	1.46
4	B	202	COA	C4A-N9A	6.43	1.51	1.37
4	B	202	COA	C5A-C6A	6.26	1.58	1.41
4	B	202	COA	C5P-N4P	6.26	1.48	1.33
4	B	202	COA	C1B-N9A	6.03	1.63	1.46
4	B	202	COA	C6A-N1A	5.96	1.52	1.35
4	B	202	COA	O5P-C5P	5.55	1.34	1.23
4	B	202	COA	C7P-N8P	5.27	1.58	1.46
3	B	201	MES	O1-C6	3.86	1.57	1.42
3	B	201	MES	O1-C2	3.80	1.57	1.42
4	B	202	COA	C3B-C4B	3.78	1.62	1.52
4	B	202	COA	C6A-N6A	3.41	1.42	1.34
3	B	201	MES	O2S-S	2.74	1.52	1.45
3	B	201	MES	O1S-S	2.72	1.52	1.45
4	B	202	COA	O4B-C1B	2.48	1.47	1.42
4	B	202	COA	P3B-O3B	2.48	1.63	1.59
3	B	201	MES	C3-C2	2.45	1.59	1.50
3	B	201	MES	C5-C6	2.41	1.59	1.50
4	B	202	COA	P1A-O3A	-2.32	1.57	1.59
4	B	202	COA	C5B-C4B	2.17	1.58	1.51
4	B	202	COA	P2A-O5A	-2.15	1.45	1.55

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	COA	C3P-N4P-C5P	14.20	149.26	122.82
4	B	202	COA	C4A-N9A-C8A	14.17	120.61	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	COA	N3A-C2A-N1A	-12.75	109.29	128.58
4	B	202	COA	N9A-C8A-N7A	-11.81	97.18	113.94
4	B	202	COA	C2P-C3P-N4P	8.69	132.01	112.31
4	B	202	COA	C4B-O4B-C1B	-8.17	91.43	109.47
4	B	202	COA	C2A-N1A-C6A	7.76	131.48	118.73
4	B	202	COA	C7P-C6P-C5P	7.39	124.70	112.39
4	B	202	COA	O4B-C1B-C2B	7.37	122.38	106.62
4	B	202	COA	O2B-C2B-C3B	7.25	131.49	111.19
4	B	202	COA	N3A-C4A-N9A	7.19	139.39	127.17
4	B	202	COA	P3B-O3B-C3B	6.99	142.11	123.43
4	B	202	COA	C5A-C4A-N9A	-6.60	98.62	105.81
4	B	202	COA	C2A-N3A-C4A	6.35	127.33	111.83
4	B	202	COA	O3B-C3B-C2B	5.81	132.51	111.68
3	B	201	MES	C6-O1-C2	5.64	128.13	109.88
3	B	201	MES	C8-C7-N4	5.62	133.64	112.36
4	B	202	COA	C5A-N7A-C8A	5.44	112.00	103.45
3	B	201	MES	C5-N4-C3	5.33	120.31	108.84
4	B	202	COA	C1B-N9A-C8A	-5.04	115.91	127.09
4	B	202	COA	O2B-C2B-C1B	4.94	127.10	110.10
4	B	202	COA	O4B-C4B-C3B	4.61	114.65	104.92
4	B	202	COA	C5A-C4A-N3A	-4.27	120.83	126.72
4	B	202	COA	O5B-C5B-C4B	4.19	123.27	108.99
4	B	202	COA	O6A-CCP-CBP	4.18	117.26	110.55
4	B	202	COA	OAP-CAP-C9P	3.77	125.14	109.38
4	B	202	COA	P1A-O5B-C5B	3.75	142.83	121.35
4	B	202	COA	O4B-C4B-C5B	3.58	120.82	109.33
4	B	202	COA	P2A-O6A-CCP	3.51	140.26	121.12
3	B	201	MES	C6-C5-N4	3.35	115.21	110.12
3	B	201	MES	C2-C3-N4	3.32	115.17	110.12
4	B	202	COA	O9P-C9P-N8P	-3.28	116.03	122.98
3	B	201	MES	C7-N4-C3	3.25	119.89	111.24
3	B	201	MES	C7-N4-C5	3.21	119.79	111.24
4	B	202	COA	C3B-C2B-C1B	-3.16	92.95	99.89
4	B	202	COA	OAP-CAP-CBP	2.96	117.05	110.18
4	B	202	COA	O3B-C3B-C4B	2.76	119.75	110.03
4	B	202	COA	C6P-C7P-N8P	2.58	117.48	112.00
4	B	202	COA	C6A-C5A-C4A	-2.24	114.11	117.18
4	B	202	COA	O9A-P3B-O8A	2.14	115.84	107.80
3	B	201	MES	O1-C2-C3	2.14	116.37	111.77
3	B	201	MES	O1-C6-C5	2.11	116.31	111.77

There are no chirality outliers.

All (20) torsion outliers are listed below:

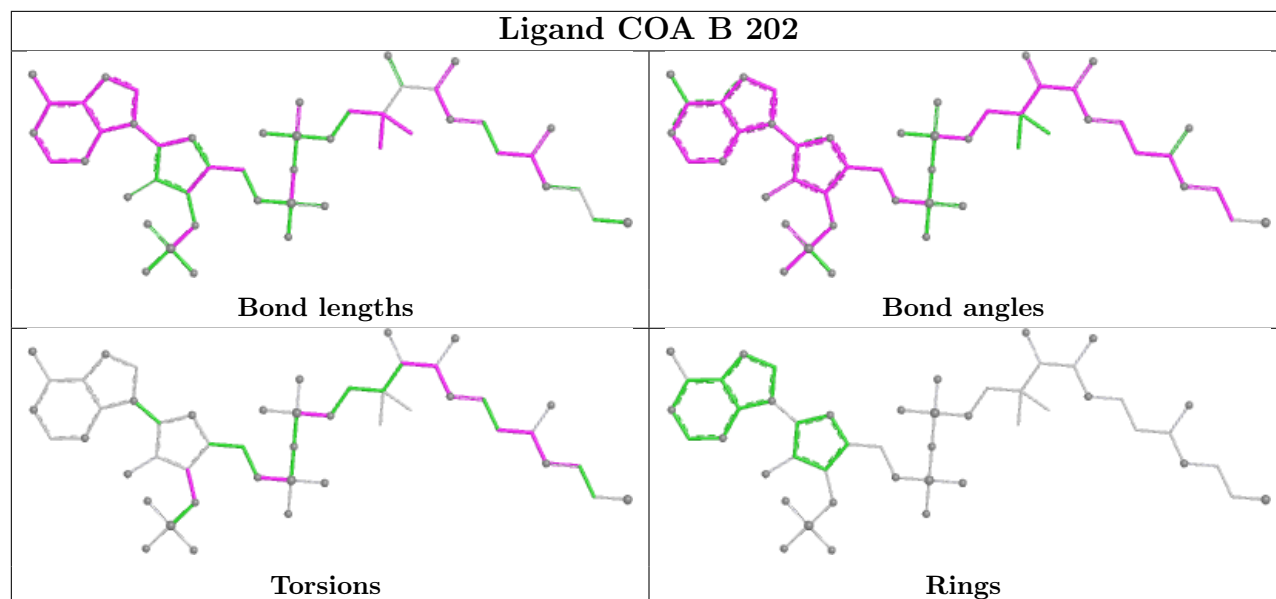
Mol	Chain	Res	Type	Atoms
3	B	201	MES	C7-C8-S-O1S
3	B	201	MES	C7-C8-S-O2S
3	B	201	MES	C7-C8-S-O3S
4	B	202	COA	C5B-O5B-P1A-O1A
4	B	202	COA	C5B-O5B-P1A-O3A
4	B	202	COA	CCP-O6A-P2A-O4A
4	B	202	COA	N8P-C9P-CAP-CBP
4	B	202	COA	CAP-C9P-N8P-C7P
4	B	202	COA	C6P-C5P-N4P-C3P
4	B	202	COA	O5P-C5P-N4P-C3P
4	B	202	COA	C2P-C3P-N4P-C5P
4	B	202	COA	C6P-C7P-N8P-C9P
4	B	202	COA	C2B-C3B-O3B-P3B
4	B	202	COA	O9P-C9P-CAP-OAP
4	B	202	COA	O5P-C5P-C6P-C7P
4	B	202	COA	N4P-C5P-C6P-C7P
4	B	202	COA	C5B-O5B-P1A-O2A
4	B	202	COA	CCP-O6A-P2A-O3A
3	B	201	MES	C8-C7-N4-C5
4	B	202	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

2 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	COA	27	0
3	B	201	MES	9	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	732/750 (97%)	0.96	105 (14%) 6 5	31, 49, 112, 149	0
2	B	153/170 (90%)	0.83	19 (12%) 8 6	32, 44, 86, 114	0
All	All	885/920 (96%)	0.93	124 (14%) 6 5	31, 48, 109, 149	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ASP	7.2
1	A	33	PRO	6.7
1	A	36	LEU	6.2
1	A	79	PHE	6.1
1	A	19	THR	6.1
2	B	138	TYR	5.9
1	A	20	TYR	5.8
1	A	38	TYR	5.6
1	A	9	ILE	5.5
1	A	13	ILE	4.9
1	A	119	TYR	4.9
1	A	41	LEU	4.9
1	A	42	GLN	4.7
2	B	65	GLN	4.6
1	A	10	ILE	4.6
1	A	12	PHE	4.5
2	B	69	LYS	4.5
1	A	50	GLY	4.4
1	A	17	ASN	4.4
1	A	15	GLN	4.3
1	A	118	LYS	4.3
1	A	67	PRO	4.1
1	A	51	GLN	4.0
1	A	325	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	32	SER	4.0
1	A	26	THR	4.0
1	A	86	GLU	4.0
2	B	68	LYS	3.9
2	B	66	LEU	3.8
1	A	54	LEU	3.7
1	A	441	ASN	3.6
2	B	136	VAL	3.6
1	A	135	GLY	3.6
1	A	21	ALA	3.5
1	A	75	LYS	3.5
1	A	421	ASP	3.5
1	A	43	ASN	3.4
1	A	37	PHE	3.4
1	A	39	HIS	3.4
1	A	599	ALA	3.4
1	A	289	ILE	3.3
1	A	14	ASP	3.3
1	A	68	ASN	3.2
2	B	148	ASN	3.2
1	A	317	THR	3.1
1	A	713	MET	3.1
1	A	323	LEU	3.0
1	A	49	SER	3.0
1	A	155	GLY	3.0
1	A	74	GLU	3.0
1	A	559	CYS	3.0
1	A	89	SER	3.0
1	A	521	GLY	3.0
1	A	76	LEU	2.9
1	A	87	LYS	2.9
1	A	518	GLY	2.9
2	B	59	MET	2.9
1	A	62	LEU	2.9
1	A	8	GLU	2.9
1	A	522	TYR	2.8
1	A	324	LYS	2.8
1	A	77	SER	2.8
1	A	80	PHE	2.8
1	A	24	LEU	2.8
1	A	85	MET	2.8
1	A	82	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	84	GLU	2.7
1	A	367	VAL	2.7
2	B	101	THR	2.7
1	A	158	ASP	2.6
1	A	25	ILE	2.6
1	A	29	LEU	2.6
1	A	358	GLU	2.6
2	B	70	GLU	2.6
1	A	23	SER	2.6
1	A	83	MET	2.6
1	A	153	GLN	2.6
1	A	30	ALA	2.6
1	A	98	LYS	2.6
1	A	121	PHE	2.5
1	A	650	GLU	2.5
1	A	346	ASP	2.5
1	A	57	LYS	2.5
1	A	103	SER	2.5
1	A	66	TYR	2.5
1	A	46	HIS	2.5
1	A	16	GLY	2.4
2	B	71	TRP	2.4
2	B	2	THR	2.4
1	A	520	ASP	2.4
1	A	71	LEU	2.4
1	A	52	ARG	2.4
1	A	129	MET	2.4
1	A	31	LYS	2.4
1	A	691	LYS	2.4
1	A	265	GLN	2.4
2	B	152	ASP	2.4
1	A	434	MET	2.4
1	A	45	ILE	2.3
2	B	49	THR	2.3
1	A	384	GLN	2.3
1	A	81	SER	2.3
1	A	630	SER	2.3
1	A	729	GLU	2.3
2	B	64	GLY	2.2
1	A	134	ASN	2.2
1	A	637	LYS	2.2
1	A	116	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	164	PRO	2.2
1	A	218	MET	2.2
1	A	91	LEU	2.2
1	A	469	GLN	2.2
1	A	65	ARG	2.2
1	A	72	THR	2.1
1	A	136	LYS	2.1
1	A	399	GLN	2.1
2	B	58	MET	2.1
1	A	485	ASN	2.1
1	A	329	GLU	2.1
1	A	322	SER	2.1
2	B	119	LEU	2.0
1	A	716	GLU	2.0
2	B	137	GLY	2.0
1	A	519	THR	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](#)

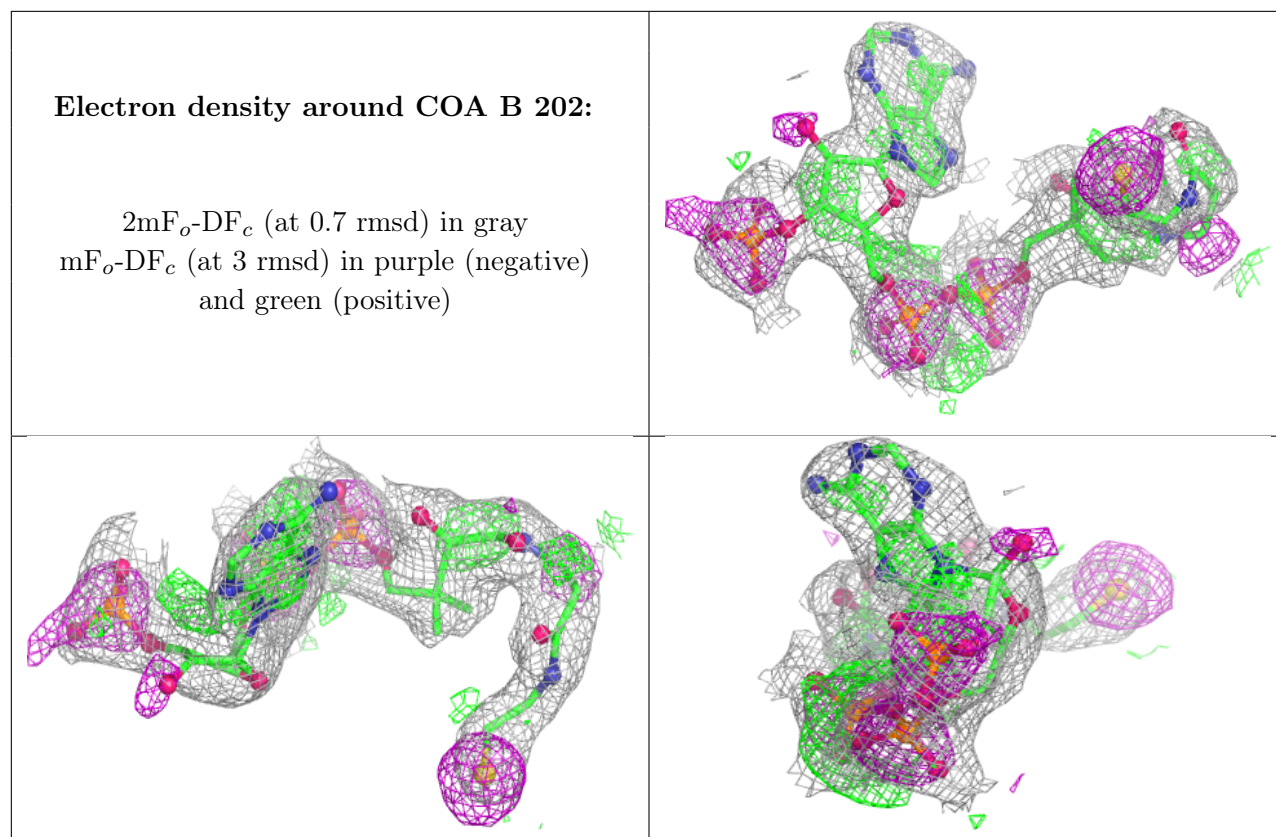
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	MES	B	201	12/12	0.74	0.32	46,78,100,101	0
4	COA	B	202	48/48	0.88	0.21	8,47,83,91	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.