



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2026 – 05:50 pm BST

PDB ID : 9TZ6 / pdb_00009tz6
Title : Crystal structure of CREBBP-R1446H histone acetyltransferase domain in complex with CoA
Authors : Mechaly, A.E.; Zhang, W.; Haouz, A.; Green, M.; Rodrigues-Lima, F.
Deposited on : 2026-01-22
Resolution : 2.54 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 Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

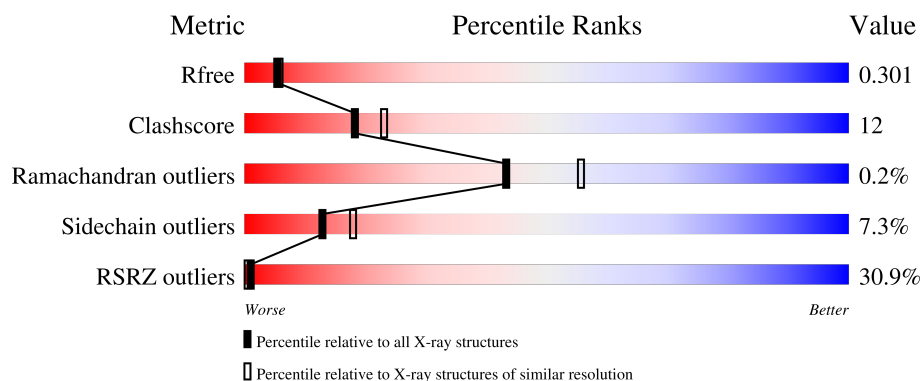
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	640	26% 62% 17% • 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4479 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 histone acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	1	0
			4413	2827	758	794	34			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1054	HIS	-	expression tag	UNP F8VPR5
A	1055	HIS	-	expression tag	UNP F8VPR5
A	1056	HIS	-	expression tag	UNP F8VPR5
A	1057	HIS	-	expression tag	UNP F8VPR5
A	1058	HIS	-	expression tag	UNP F8VPR5
A	1059	HIS	-	expression tag	UNP F8VPR5
A	1060	ASP	-	expression tag	UNP F8VPR5
A	1061	TYR	-	expression tag	UNP F8VPR5
A	1062	ASP	-	expression tag	UNP F8VPR5
A	1063	ILE	-	expression tag	UNP F8VPR5
A	1064	PRO	-	expression tag	UNP F8VPR5
A	1065	THR	-	expression tag	UNP F8VPR5
A	1066	THR	-	expression tag	UNP F8VPR5
A	1067	GLU	-	expression tag	UNP F8VPR5
A	1068	ASN	-	expression tag	UNP F8VPR5
A	1069	LEU	-	expression tag	UNP F8VPR5
A	1070	TYR	-	expression tag	UNP F8VPR5
A	1071	PHE	-	expression tag	UNP F8VPR5
A	1072	GLN	-	expression tag	UNP F8VPR5
A	1073	GLY	-	expression tag	UNP F8VPR5
A	1074	ALA	-	expression tag	UNP F8VPR5
A	1075	MET	-	expression tag	UNP F8VPR5
A	1076	GLY	-	expression tag	UNP F8VPR5
A	1077	SER	-	expression tag	UNP F8VPR5
A	1446	HIS	ARG	engineered mutation	UNP F8VPR5
A	1503	PHE	TYR	conflict	UNP F8VPR5
A	1613	SER	-	linker	UNP F8VPR5

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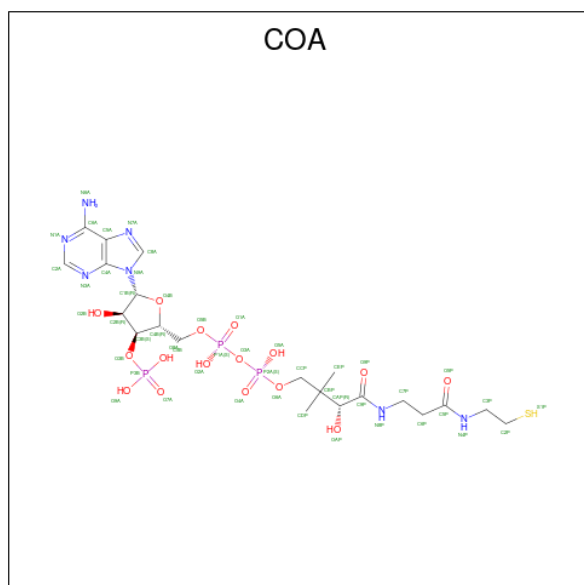
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1614	GLY	-	linker	UNP F8VPR5
A	1615	GLY	-	linker	UNP F8VPR5
A	1616	SER	-	linker	UNP F8VPR5
A	1617	GLY	-	linker	UNP F8VPR5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

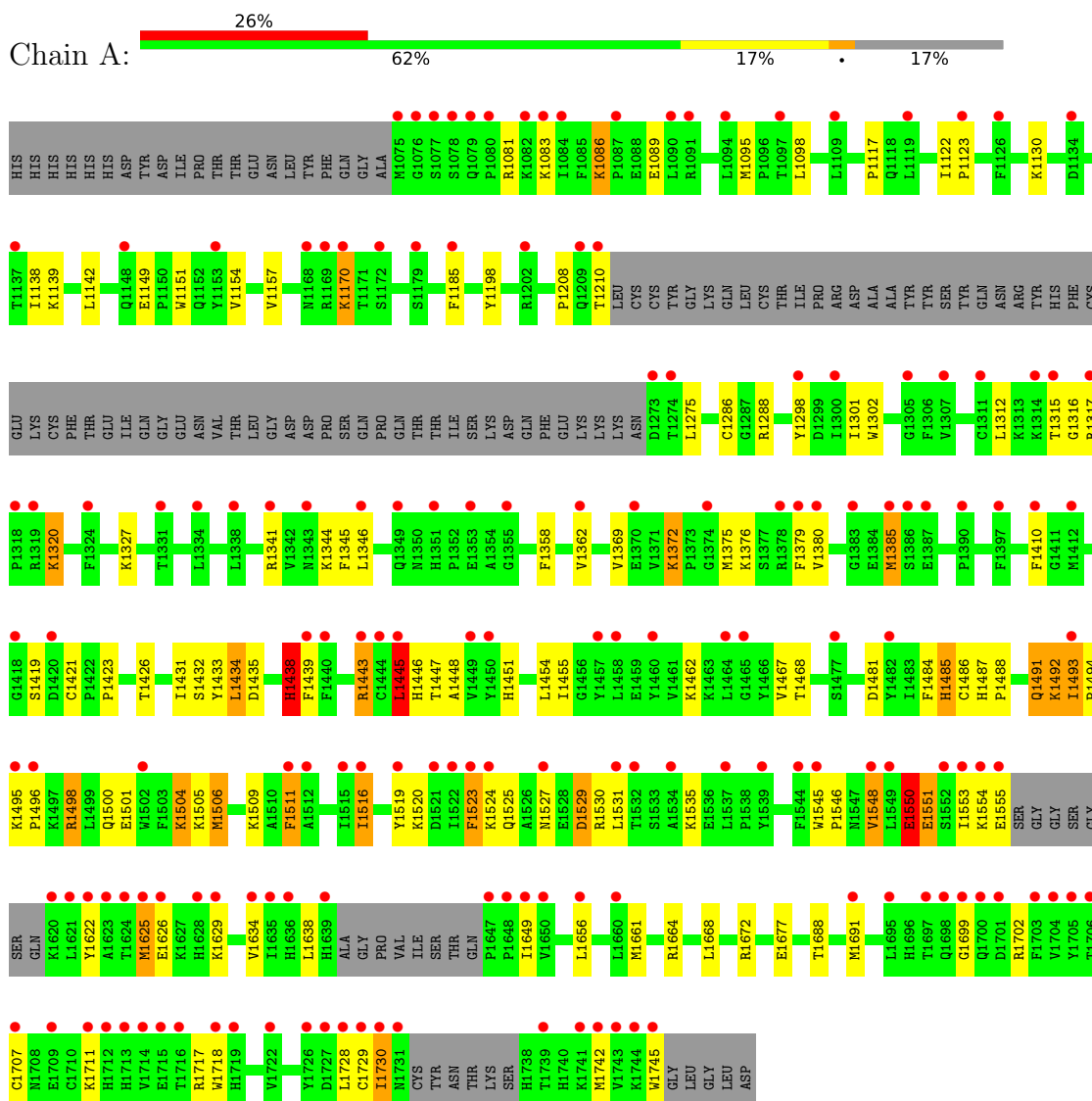
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: histone acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.88Å 146.84Å 154.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.34 – 2.54 77.34 – 2.54	Depositor EDS
% Data completeness (in resolution range)	41.7 (77.34-2.54) 41.7 (77.34-2.54)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.248 , 0.276 0.267 , 0.301	Depositor DCC
R_{free} test set	682 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4479	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: ZN, 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	0.78	8/4540 (0.2%)	1.13	20/6136 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1491	GLN	CA-C	-10.14	1.40	1.52
1	A	1491	GLN	CB-CG	-9.13	1.25	1.52
1	A	1491	GLN	CA-CB	-8.31	1.41	1.53
1	A	1491	GLN	CD-OE1	-8.30	1.07	1.23
1	A	1491	GLN	CG-CD	-7.81	1.32	1.52
1	A	1372	LYS	CA-C	5.74	1.60	1.52
1	A	1423	PRO	CA-C	5.38	1.54	1.51
1	A	1551	GLU	CA-C	5.05	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1491	GLN	CA-CB-CG	-12.99	88.12	114.10
1	A	1445	LEU	N-CA-CB	-8.07	98.55	110.49
1	A	1123	PRO	CA-C-N	7.34	130.44	120.38
1	A	1123	PRO	C-N-CA	7.34	130.44	120.38
1	A	1523	PHE	CA-CB-CG	-7.19	106.61	113.80
1	A	1438	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	1511	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	1550	GLU	CA-CB-CG	-6.10	101.90	114.10
1	A	1491	GLN	CB-CG-CD	-5.82	102.71	112.60
1	A	1529	ASP	CA-C-N	5.74	131.12	122.68
1	A	1529	ASP	C-N-CA	5.74	131.12	122.68
1	A	1491	GLN	CG-CD-OE1	-5.52	109.77	120.80
1	A	1491	GLN	CG-CD-NE2	5.50	124.65	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1446	HIS	CA-CB-CG	5.39	119.19	113.80
1	A	1484	PHE	CA-C-N	5.32	127.72	120.54
1	A	1484	PHE	C-N-CA	5.32	127.72	120.54
1	A	1485	HIS	N-CA-C	5.23	117.39	111.11
1	A	1699	GLY	N-CA-C	-5.07	105.27	112.37
1	A	1316	GLY	CA-C-N	5.03	127.40	120.67
1	A	1316	GLY	C-N-CA	5.03	127.40	120.67

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	4413	0	4278	103	0
2	A	4	0	0	0	0
3	A	48	0	32	6	0
4	A	14	0	0	0	0
All	All	4479	0	4310	106	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 12.

All (106) 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:1372:LYS:HB2	1:A:1550:GLU:OE2	1.72	0.89
1:A:1438:HIS:CE1	1:A:1443:ARG:HH21	1.90	0.89
1:A:1438:HIS:ND1	1:A:1443:ARG:NH2	2.21	0.89
1:A:1095:MET:HE3	1:A:1142:LEU:HD23	1.53	0.88
1:A:1728:LEU:HD12	1:A:1742:MET:HE2	1.54	0.88
1:A:1462:LYS:HB2	1:A:1638:LEU:HD23	1.56	0.88
1:A:1438:HIS:CE1	1:A:1443:ARG:NH2	2.43	0.87
1:A:1438:HIS:CG	1:A:1491:GLN:OE1	2.29	0.85
1:A:1438:HIS:CD2	1:A:1491:GLN:OE1	2.33	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:TYR:HB3	1:A:1301:ILE:HD12	1.62	0.81
1:A:1315:THR:HG22	1:A:1317:ARG:HB3	1.64	0.80
1:A:1410:PHE:CE2	1:A:1434:LEU:HD21	2.19	0.77
3:A:1805:COA:H4B	3:A:1805:COA:O9A	1.85	0.77
1:A:1435:ASP:HA	3:A:1805:COA:H72	1.66	0.76
1:A:1438:HIS:CE1	1:A:1491:GLN:OE1	2.39	0.76
1:A:1372:LYS:HB2	1:A:1550:GLU:CD	2.11	0.75
1:A:1372:LYS:CB	1:A:1550:GLU:OE2	2.35	0.75
1:A:1286:CYS:HB3	1:A:1288:ARG:HG2	1.70	0.74
1:A:1438:HIS:NE2	1:A:1439:PHE:CE1	2.57	0.72
1:A:1372:LYS:C	1:A:1550:GLU:OE1	2.36	0.69
1:A:1467:VAL:HG13	1:A:1468:THR:HG23	1.75	0.67
1:A:1455:ILE:HG12	1:A:1506:MET:CE	2.25	0.66
1:A:1481:ASP:OD1	1:A:1487:HIS:ND1	2.30	0.65
1:A:1523:PHE:CE2	1:A:1629:LYS:HB3	2.33	0.63
1:A:1138:ILE:HD13	1:A:1157:VAL:HG12	1.80	0.63
1:A:1372:LYS:O	1:A:1550:GLU:OE1	2.17	0.62
1:A:1545:TRP:HH2	1:A:1625:MET:HA	1.65	0.61
1:A:1688:THR:HA	1:A:1691:MET:HE3	1.82	0.61
1:A:1341:ARG:HH12	1:A:1455:ILE:HB	1.63	0.61
1:A:1095:MET:HE2	1:A:1098:LEU:HD23	1.83	0.61
1:A:1622:TYR:O	1:A:1626:GLU:HG2	2.00	0.60
1:A:1523:PHE:CE2	1:A:1626:GLU:HA	2.37	0.60
1:A:1718:TRP:CD1	1:A:1730:ILE:HG13	2.36	0.60
1:A:1527:ASN:O	1:A:1530:ARG:HG3	2.02	0.59
1:A:1455:ILE:HG12	1:A:1506:MET:HE2	1.85	0.58
1:A:1376:LYS:HG2	1:A:1380:VAL:CG1	2.34	0.57
1:A:1525:GLN:NE2	1:A:1529:ASP:OD2	2.37	0.57
1:A:1707:CYS:SG	1:A:1729:CYS:N	2.77	0.57
1:A:1302:TRP:HD1	1:A:1320:LYS:HE2	1.69	0.56
1:A:1486:CYS:HB3	1:A:1677:GLU:HB3	1.87	0.56
1:A:1451:HIS:O	1:A:1455:ILE:HG13	2.05	0.56
1:A:1286:CYS:CB	1:A:1288:ARG:HG2	2.37	0.55
1:A:1496:PRO:O	1:A:1500:GLN:HG3	2.07	0.54
1:A:1375:MET:H	1:A:1550:GLU:HG2	1.72	0.53
1:A:1545:TRP:CH2	1:A:1625:MET:HA	2.42	0.53
1:A:1717:ARG:HH21	1:A:1745:TRP:HE3	1.57	0.53
1:A:1520:LYS:HD2	1:A:1524:LYS:HD2	1.90	0.53
1:A:1523:PHE:CD2	1:A:1629:LYS:HB3	2.43	0.53
1:A:1433:TYR:CZ	1:A:1664:ARG:HD2	2.44	0.52
1:A:1345:PHE:HZ	1:A:1448:ALA:HB1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:HIS:ND1	1:A:1491:GLN:OE1	2.44	0.51
1:A:1385:MET:HE3	1:A:1535:LYS:HB2	1.92	0.51
1:A:1208:PRO:HG3	1:A:1275:LEU:HD21	1.92	0.50
1:A:1376:LYS:HG2	1:A:1380:VAL:HG12	1.94	0.50
1:A:1315:THR:CG2	1:A:1317:ARG:HB3	2.39	0.49
1:A:1504:LYS:NZ	1:A:1519:TYR:OH	2.46	0.49
1:A:1198:TYR:CE1	1:A:1288:ARG:HB2	2.47	0.49
1:A:1157:VAL:HG21	1:A:1185:PHE:CZ	2.48	0.49
1:A:1525:GLN:HG2	1:A:1634:VAL:HG11	1.95	0.48
1:A:1717:ARG:NH2	1:A:1745:TRP:HE3	2.11	0.48
1:A:1730:ILE:N	1:A:1730:ILE:HD12	2.29	0.48
1:A:1312:LEU:HA	1:A:1315:THR:HB	1.96	0.47
1:A:1419:SER:OG	1:A:1649:ILE:HG13	2.15	0.47
1:A:1434:LEU:HD11	1:A:1454:LEU:HD21	1.97	0.47
1:A:1493:ILE:O	3:A:1805:COA:N6A	2.49	0.46
1:A:1372:LYS:O	1:A:1376:LYS:HB2	2.16	0.46
1:A:1376:LYS:O	1:A:1380:VAL:HG12	2.16	0.46
1:A:1485:HIS:CE1	1:A:1672:ARG:HG2	2.50	0.46
1:A:1455:ILE:CG1	1:A:1506:MET:HE3	2.46	0.46
1:A:1523:PHE:CZ	1:A:1625:MET:C	2.94	0.46
1:A:1523:PHE:HZ	1:A:1625:MET:O	1.99	0.46
3:A:1805:COA:H131	3:A:1805:COA:O9P	2.14	0.46
1:A:1649:ILE:HD12	1:A:1649:ILE:O	2.16	0.46
1:A:1492:LYS:HE2	1:A:1492:LYS:HB2	1.68	0.45
1:A:1346:LEU:CD2	1:A:1445:LEU:CD2	2.95	0.45
1:A:1170:LYS:CD	1:A:1170:LYS:H	2.30	0.44
1:A:1516:ILE:HD13	1:A:1516:ILE:HA	1.89	0.44
1:A:1302:TRP:CD1	1:A:1320:LYS:HG2	2.53	0.44
1:A:1086:LYS:HG2	1:A:1089:GLU:CD	2.42	0.44
1:A:1149:GLU:HG2	1:A:1151:TRP:H	1.82	0.44
1:A:1083:LYS:HG2	1:A:1288:ARG:HH21	1.83	0.43
1:A:1435:ASP:OD1	1:A:1487:HIS:NE2	2.46	0.43
1:A:1545:TRP:HA	1:A:1548:VAL:HG12	2.00	0.43
1:A:1346:LEU:HD23	1:A:1445:LEU:HD21	2.01	0.43
1:A:1438:HIS:CD2	1:A:1488:PRO:HG2	2.54	0.43
1:A:1117:PRO:HB3	1:A:1122:ILE:O	2.19	0.42
3:A:1805:COA:O5P	3:A:1805:COA:N8P	2.53	0.42
1:A:1380:VAL:HG23	1:A:1385:MET:O	2.19	0.42
1:A:1668:LEU:O	1:A:1672:ARG:HG3	2.19	0.42
1:A:1362:VAL:CG2	1:A:1661:MET:HG3	2.49	0.42
1:A:1379:PHE:CD2	1:A:1535:LYS:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:PHE:CZ	1:A:1625:MET:O	2.73	0.42
1:A:1095:MET:HE1	1:A:1139:LYS:HG3	2.02	0.42
1:A:1494:PRO:HA	3:A:1805:COA:H62A	1.84	0.42
1:A:1327:LYS:HB2	1:A:1358:PHE:CE1	2.55	0.41
1:A:1345:PHE:CZ	1:A:1448:ALA:HB1	2.53	0.41
1:A:1494:PRO:HB3	1:A:1498:ARG:HG2	2.02	0.41
1:A:1485:HIS:ND1	1:A:1672:ARG:HG2	2.36	0.41
1:A:1546:PRO:O	1:A:1550:GLU:HB2	2.20	0.41
1:A:1419:SER:H	1:A:1649:ILE:CG1	2.33	0.41
1:A:1455:ILE:HD13	1:A:1509:LYS:HD2	2.03	0.41
1:A:1421:CYS:O	1:A:1426:THR:OG1	2.35	0.41
1:A:1511:PHE:HA	1:A:1516:ILE:O	2.21	0.41
1:A:1438:HIS:NE2	1:A:1439:PHE:CD1	2.89	0.40
1:A:1702:ARG:HA	1:A:1702:ARG:HE	1.86	0.40
1:A:1523:PHE:HE1	1:A:1625:MET:HG2	1.87	0.40

There are no symmetry-related clashes.

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	522/640 (82%)	501 (96%)	20 (4%)	1 (0%)	43 56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1438	HIS

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	491/586 (84%)	455 (93%)	36 (7%)	13	18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1081	ARG
1	A	1086	LYS
1	A	1130	LYS
1	A	1154	VAL
1	A	1170	LYS
1	A	1210	THR
1	A	1320	LYS
1	A	1344	LYS
1	A	1369	VAL
1	A	1385	MET
1	A	1431	ILE
1	A	1432	SER
1	A	1434	LEU
1	A	1443	ARG
1	A	1445	LEU
1	A	1447	THR
1	A	1492	LYS
1	A	1493	ILE
1	A	1495	LYS
1	A	1498	ARG
1	A	1501	GLU
1	A	1504	LYS
1	A	1505	LYS
1	A	1506	MET
1	A	1516	ILE
1	A	1531	LEU
1	A	1548	VAL
1	A	1550	GLU
1	A	1551	GLU
1	A	1553	ILE

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Mol	Chain	Res	Type
1	A	1554	LYS
1	A	1555	GLU
1	A	1625	MET
1	A	1656	LEU
1	A	1711	LYS
1	A	1730	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1146	GLN
1	A	1330	GLN
1	A	1517	ASN
1	A	1527	ASN
1	A	1675	HIS
1	A	1713	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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
3	COA	A	1805	-	44,50,50	1.12	4 (9%)	65,75,75	1.65	11 (16%)

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
3	COA	A	1805	-	-	15/48/64/64	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1805	COA	C5A-C4A	4.59	1.47	1.39
3	A	1805	COA	C5A-C6A	2.74	1.48	1.41
3	A	1805	COA	C8A-N7A	2.45	1.36	1.31
3	A	1805	COA	C5A-N7A	-2.15	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1805	COA	C5A-C4A-N3A	-6.15	118.73	126.75
3	A	1805	COA	N3A-C4A-N9A	4.81	135.01	127.08
3	A	1805	COA	C2A-N3A-C4A	3.86	120.87	111.75
3	A	1805	COA	P2A-O3A-P1A	-3.53	120.71	132.83
3	A	1805	COA	C4A-C5A-N7A	-3.28	106.62	110.62
3	A	1805	COA	N3A-C2A-N1A	-3.15	123.67	128.60
3	A	1805	COA	C3B-C2B-C1B	2.82	106.14	99.89
3	A	1805	COA	C5A-N7A-C8A	2.78	107.45	103.51
3	A	1805	COA	C4A-N9A-C8A	2.55	108.49	105.73
3	A	1805	COA	C6A-C5A-N7A	2.22	136.16	132.02
3	A	1805	COA	N9A-C8A-N7A	-2.01	111.17	113.91

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1805	COA	C4B-C3B-O3B-P3B
3	A	1805	COA	C5B-O5B-P1A-O2A
3	A	1805	COA	C5B-O5B-P1A-O3A
3	A	1805	COA	CCP-O6A-P2A-O4A

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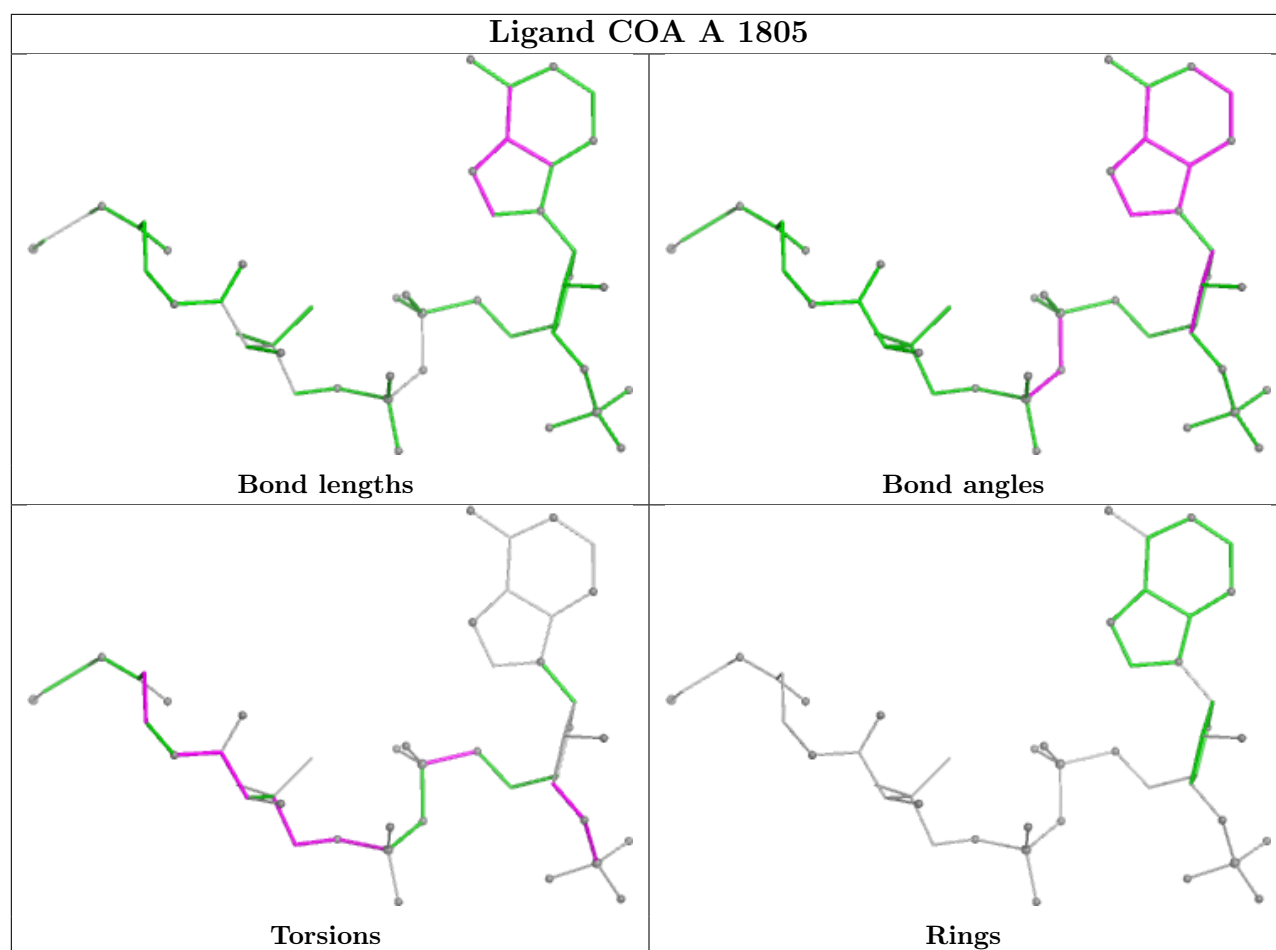
Mol	Chain	Res	Type	Atoms
3	A	1805	COA	CAP-CBP-CCP-O6A
3	A	1805	COA	CAP-C9P-N8P-C7P
3	A	1805	COA	CDP-CBP-CCP-O6A
3	A	1805	COA	CEP-CBP-CCP-O6A
3	A	1805	COA	O9P-C9P-N8P-C7P
3	A	1805	COA	C5P-C6P-C7P-N8P
3	A	1805	COA	O9P-C9P-CAP-OAP
3	A	1805	COA	CCP-O6A-P2A-O3A
3	A	1805	COA	C5B-O5B-P1A-O1A
3	A	1805	COA	C3B-O3B-P3B-O9A
3	A	1805	COA	CBP-CCP-O6A-P2A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1805	COA	6	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	531/640 (82%)	1.55	164 (30%) 1 0	39, 76, 145, 153	1 (0%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1714	VAL	7.0
1	A	1731	ASN	6.2
1	A	1076	GLY	5.8
1	A	1743	VAL	5.8
1	A	1703	PHE	5.7
1	A	1705	TYR	5.5
1	A	1534	ALA	5.5
1	A	1353	GLU	5.1
1	A	1537	LEU	5.0
1	A	1728	LEU	5.0
1	A	1522	ILE	4.9
1	A	1553	ILE	4.8
1	A	1716	THR	4.6
1	A	1704	VAL	4.5
1	A	1713	HIS	4.4
1	A	1080	PRO	4.4
1	A	1077	SER	4.3
1	A	1552	SER	4.3
1	A	1730	ILE	4.3
1	A	1555	GLU	4.3
1	A	1739	THR	4.2
1	A	1084	ILE	4.2
1	A	1706	THR	4.1
1	A	1718	TRP	4.1
1	A	1620	LYS	4.1
1	A	1711	LYS	4.1
1	A	1701	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1516	ILE	4.0
1	A	1549	LEU	4.0
1	A	1741	LYS	3.9
1	A	1745	TRP	3.9
1	A	1464	LEU	3.9
1	A	1545	TRP	3.8
1	A	1079	GLN	3.8
1	A	1170	LYS	3.8
1	A	1123	PRO	3.8
1	A	1346	LEU	3.8
1	A	1317	ARG	3.8
1	A	1512	ALA	3.6
1	A	1083	LYS	3.6
1	A	1449	VAL	3.6
1	A	1458	LEU	3.6
1	A	1210	THR	3.5
1	A	1649	ILE	3.5
1	A	1075	MET	3.5
1	A	1443	ARG	3.4
1	A	1650	VAL	3.4
1	A	1700	GLN	3.4
1	A	1444[A]	CYS	3.4
1	A	1082	LYS	3.4
1	A	1629	LYS	3.4
1	A	1341	ARG	3.4
1	A	1625	MET	3.3
1	A	1324	PHE	3.3
1	A	1622	TYR	3.3
1	A	1378	ARG	3.3
1	A	1712	HIS	3.3
1	A	1554	LYS	3.3
1	A	1698	GLN	3.2
1	A	1707	CYS	3.2
1	A	1729	CYS	3.2
1	A	1697	THR	3.2
1	A	1450	TYR	3.1
1	A	1532	THR	3.1
1	A	1362	VAL	3.0
1	A	1515	ILE	3.0
1	A	1457	TYR	3.0
1	A	1319	ARG	3.0
1	A	1338	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1390	PRO	2.9
1	A	1445	LEU	2.9
1	A	1621	LEU	2.9
1	A	1726	TYR	2.9
1	A	1691	MET	2.9
1	A	1097	THR	2.9
1	A	1440	PHE	2.9
1	A	1727	ASP	2.9
1	A	1647	PRO	2.9
1	A	1298	TYR	2.9
1	A	1078	SER	2.8
1	A	1656	LEU	2.8
1	A	1169	ARG	2.8
1	A	1305	GLY	2.8
1	A	1699	GLY	2.8
1	A	1385	MET	2.8
1	A	1519	TYR	2.8
1	A	1531	LEU	2.8
1	A	1387	GLU	2.8
1	A	1624	THR	2.8
1	A	1420	ASP	2.7
1	A	1439	PHE	2.7
1	A	1087	PRO	2.7
1	A	1318	PRO	2.7
1	A	1380	VAL	2.7
1	A	1477	SER	2.7
1	A	1482	TYR	2.7
1	A	1639	HIS	2.7
1	A	1660	LEU	2.6
1	A	1539	TYR	2.6
1	A	1273	ASP	2.6
1	A	1091	ARG	2.6
1	A	1314	LYS	2.6
1	A	1744	LYS	2.6
1	A	1094	LEU	2.6
1	A	1722	VAL	2.6
1	A	1172	SER	2.6
1	A	1153	TYR	2.5
1	A	1502	TRP	2.5
1	A	1397	PHE	2.5
1	A	1386	SER	2.5
1	A	1523	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1695	LEU	2.5
1	A	1351	HIS	2.5
1	A	1383	GLY	2.5
1	A	1715	GLU	2.5
1	A	1119	LEU	2.5
1	A	1527	ASN	2.5
1	A	1370	GLU	2.4
1	A	1355	GLY	2.4
1	A	1521	ASP	2.4
1	A	1418	GLY	2.3
1	A	1634	VAL	2.3
1	A	1623	ALA	2.3
1	A	1709	GLU	2.3
1	A	1636	HIS	2.3
1	A	1742	MET	2.3
1	A	1126	PHE	2.3
1	A	1410	PHE	2.3
1	A	1349	GLN	2.3
1	A	1493	ILE	2.3
1	A	1524	LYS	2.3
1	A	1460	TYR	2.3
1	A	1148	GLN	2.3
1	A	1628	HIS	2.3
1	A	1300	ILE	2.3
1	A	1185	PHE	2.3
1	A	1334	LEU	2.2
1	A	1635	ILE	2.2
1	A	1548	VAL	2.2
1	A	1168	ASN	2.2
1	A	1412	MET	2.2
1	A	1379	PHE	2.2
1	A	1648	PRO	2.2
1	A	1626	GLU	2.2
1	A	1109	LEU	2.2
1	A	1311	CYS	2.2
1	A	1511	PHE	2.2
1	A	1134	ASP	2.1
1	A	1179	SER	2.1
1	A	1544	PHE	2.1
1	A	1090	LEU	2.1
1	A	1274	THR	2.1
1	A	1331	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1202	ARG	2.1
1	A	1137	THR	2.1
1	A	1374	GLY	2.1
1	A	1495	LYS	2.1
1	A	1209	GLN	2.1
1	A	1307	VAL	2.1
1	A	1343	ASN	2.1
1	A	1465	GLY	2.0
1	A	1315	THR	2.0
1	A	1496	PRO	2.0
1	A	1719	HIS	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](#)

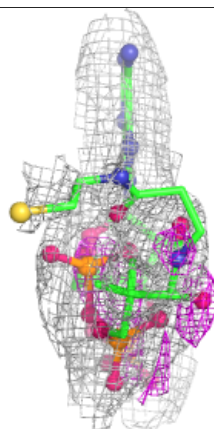
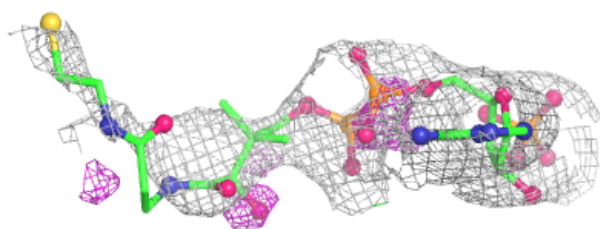
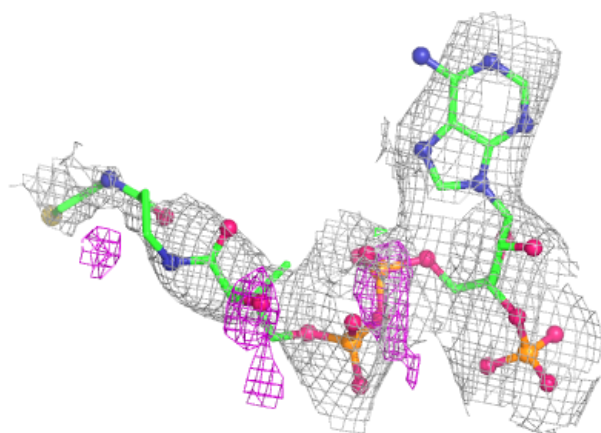
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
2	ZN	A	1803	1/1	0.65	0.17	236,236,236,236	0
3	COA	A	1805	48/48	0.79	0.18	120,125,128,128	0
2	ZN	A	1804	1/1	0.87	0.14	268,268,268,268	0
2	ZN	A	1802	1/1	0.99	0.04	81,81,81,81	0
2	ZN	A	1801	1/1	1.00	0.06	58,58,58,58	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 A 1805:

$2mF_o-DF_c$ (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.