



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:03 am BST

PDB ID : 4NSQ
Title : Crystal structure of PCAF
Authors : Lin, J.Y.; Cai, Y.F.
Deposited on : 2013-11-28
Resolution : 2.31 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

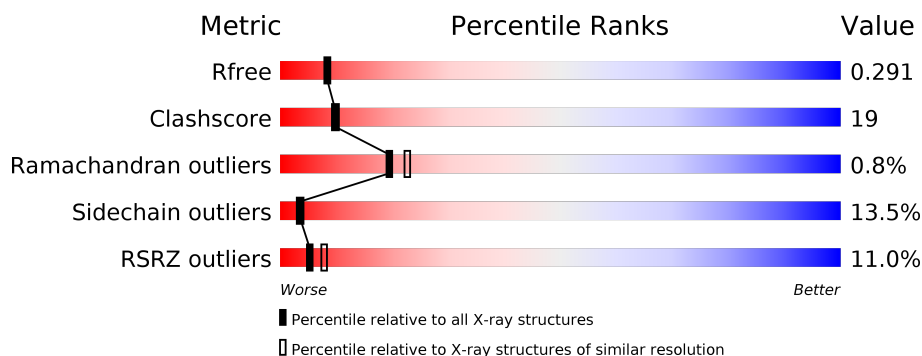
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	190	<div> <div>6%</div> <div> <div>54%</div> <div>24%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	190	<div> <div>5%</div> <div> <div>55%</div> <div>25%</div> <div>••</div> <div>17%</div> </div> </div>
1	C	190	<div> <div>12%</div> <div> <div>54%</div> <div>23%</div> <div>5%</div> <div>17%</div> </div> </div>
1	D	190	<div> <div>13%</div> <div> <div>48%</div> <div>27%</div> <div>7%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5296 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 KAT2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1276	836	213	219	8			
1	B	157	Total	C	N	O	S	0	0	0
			1276	836	213	219	8			
1	C	157	Total	C	N	O	S	0	0	0
			1276	836	213	219	8			
1	D	157	Total	C	N	O	S	0	0	0
			1276	836	213	219	8			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	MET	-	EXPRESSION TAG	UNP Q92831
A	470	GLY	-	EXPRESSION TAG	UNP Q92831
A	471	SER	-	EXPRESSION TAG	UNP Q92831
A	472	SER	-	EXPRESSION TAG	UNP Q92831
A	473	HIS	-	EXPRESSION TAG	UNP Q92831
A	474	HIS	-	EXPRESSION TAG	UNP Q92831
A	475	HIS	-	EXPRESSION TAG	UNP Q92831
A	476	HIS	-	EXPRESSION TAG	UNP Q92831
A	477	HIS	-	EXPRESSION TAG	UNP Q92831
A	478	HIS	-	EXPRESSION TAG	UNP Q92831
A	479	SER	-	EXPRESSION TAG	UNP Q92831
A	480	SER	-	EXPRESSION TAG	UNP Q92831
A	481	GLY	-	EXPRESSION TAG	UNP Q92831
A	482	LEU	-	EXPRESSION TAG	UNP Q92831
A	483	VAL	-	EXPRESSION TAG	UNP Q92831
A	484	PRO	-	EXPRESSION TAG	UNP Q92831
A	485	ARG	-	EXPRESSION TAG	UNP Q92831
A	486	GLY	-	EXPRESSION TAG	UNP Q92831
A	487	SER	-	EXPRESSION TAG	UNP Q92831
A	488	HIS	-	EXPRESSION TAG	UNP Q92831
A	489	MET	-	EXPRESSION TAG	UNP Q92831

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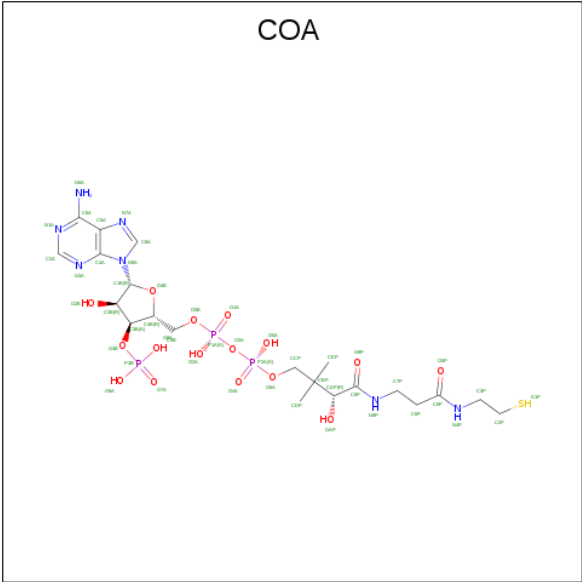
Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ALA	-	EXPRESSION TAG	UNP Q92831
A	491	SER	-	EXPRESSION TAG	UNP Q92831
A	492	LYS	-	EXPRESSION TAG	UNP Q92831
B	469	MET	-	EXPRESSION TAG	UNP Q92831
B	470	GLY	-	EXPRESSION TAG	UNP Q92831
B	471	SER	-	EXPRESSION TAG	UNP Q92831
B	472	SER	-	EXPRESSION TAG	UNP Q92831
B	473	HIS	-	EXPRESSION TAG	UNP Q92831
B	474	HIS	-	EXPRESSION TAG	UNP Q92831
B	475	HIS	-	EXPRESSION TAG	UNP Q92831
B	476	HIS	-	EXPRESSION TAG	UNP Q92831
B	477	HIS	-	EXPRESSION TAG	UNP Q92831
B	478	HIS	-	EXPRESSION TAG	UNP Q92831
B	479	SER	-	EXPRESSION TAG	UNP Q92831
B	480	SER	-	EXPRESSION TAG	UNP Q92831
B	481	GLY	-	EXPRESSION TAG	UNP Q92831
B	482	LEU	-	EXPRESSION TAG	UNP Q92831
B	483	VAL	-	EXPRESSION TAG	UNP Q92831
B	484	PRO	-	EXPRESSION TAG	UNP Q92831
B	485	ARG	-	EXPRESSION TAG	UNP Q92831
B	486	GLY	-	EXPRESSION TAG	UNP Q92831
B	487	SER	-	EXPRESSION TAG	UNP Q92831
B	488	HIS	-	EXPRESSION TAG	UNP Q92831
B	489	MET	-	EXPRESSION TAG	UNP Q92831
B	490	ALA	-	EXPRESSION TAG	UNP Q92831
B	491	SER	-	EXPRESSION TAG	UNP Q92831
B	492	LYS	-	EXPRESSION TAG	UNP Q92831
C	469	MET	-	EXPRESSION TAG	UNP Q92831
C	470	GLY	-	EXPRESSION TAG	UNP Q92831
C	471	SER	-	EXPRESSION TAG	UNP Q92831
C	472	SER	-	EXPRESSION TAG	UNP Q92831
C	473	HIS	-	EXPRESSION TAG	UNP Q92831
C	474	HIS	-	EXPRESSION TAG	UNP Q92831
C	475	HIS	-	EXPRESSION TAG	UNP Q92831
C	476	HIS	-	EXPRESSION TAG	UNP Q92831
C	477	HIS	-	EXPRESSION TAG	UNP Q92831
C	478	HIS	-	EXPRESSION TAG	UNP Q92831
C	479	SER	-	EXPRESSION TAG	UNP Q92831
C	480	SER	-	EXPRESSION TAG	UNP Q92831
C	481	GLY	-	EXPRESSION TAG	UNP Q92831
C	482	LEU	-	EXPRESSION TAG	UNP Q92831
C	483	VAL	-	EXPRESSION TAG	UNP Q92831

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Chain	Residue	Modelled	Actual	Comment	Reference
C	484	PRO	-	EXPRESSION TAG	UNP Q92831
C	485	ARG	-	EXPRESSION TAG	UNP Q92831
C	486	GLY	-	EXPRESSION TAG	UNP Q92831
C	487	SER	-	EXPRESSION TAG	UNP Q92831
C	488	HIS	-	EXPRESSION TAG	UNP Q92831
C	489	MET	-	EXPRESSION TAG	UNP Q92831
C	490	ALA	-	EXPRESSION TAG	UNP Q92831
C	491	SER	-	EXPRESSION TAG	UNP Q92831
C	492	LYS	-	EXPRESSION TAG	UNP Q92831
D	469	MET	-	EXPRESSION TAG	UNP Q92831
D	470	GLY	-	EXPRESSION TAG	UNP Q92831
D	471	SER	-	EXPRESSION TAG	UNP Q92831
D	472	SER	-	EXPRESSION TAG	UNP Q92831
D	473	HIS	-	EXPRESSION TAG	UNP Q92831
D	474	HIS	-	EXPRESSION TAG	UNP Q92831
D	475	HIS	-	EXPRESSION TAG	UNP Q92831
D	476	HIS	-	EXPRESSION TAG	UNP Q92831
D	477	HIS	-	EXPRESSION TAG	UNP Q92831
D	478	HIS	-	EXPRESSION TAG	UNP Q92831
D	479	SER	-	EXPRESSION TAG	UNP Q92831
D	480	SER	-	EXPRESSION TAG	UNP Q92831
D	481	GLY	-	EXPRESSION TAG	UNP Q92831
D	482	LEU	-	EXPRESSION TAG	UNP Q92831
D	483	VAL	-	EXPRESSION TAG	UNP Q92831
D	484	PRO	-	EXPRESSION TAG	UNP Q92831
D	485	ARG	-	EXPRESSION TAG	UNP Q92831
D	486	GLY	-	EXPRESSION TAG	UNP Q92831
D	487	SER	-	EXPRESSION TAG	UNP Q92831
D	488	HIS	-	EXPRESSION TAG	UNP Q92831
D	489	MET	-	EXPRESSION TAG	UNP Q92831
D	490	ALA	-	EXPRESSION TAG	UNP Q92831
D	491	SER	-	EXPRESSION TAG	UNP Q92831
D	492	LYS	-	EXPRESSION TAG	UNP Q92831

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

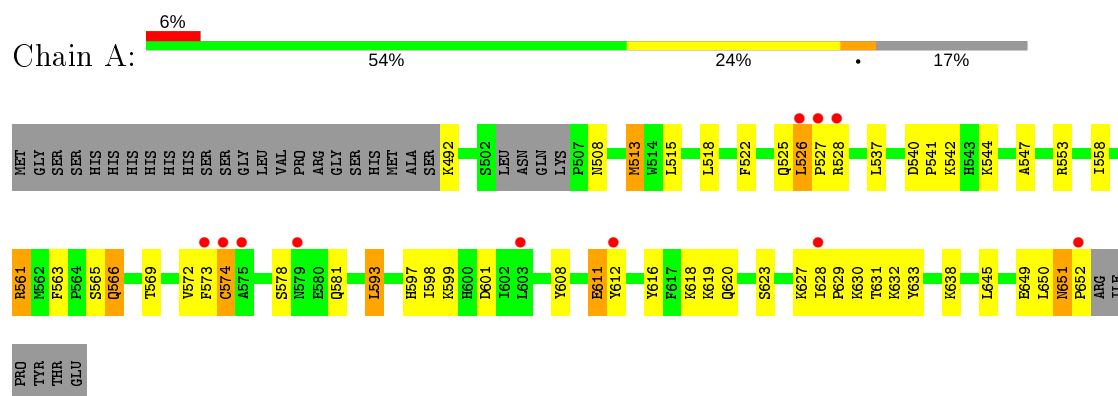


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

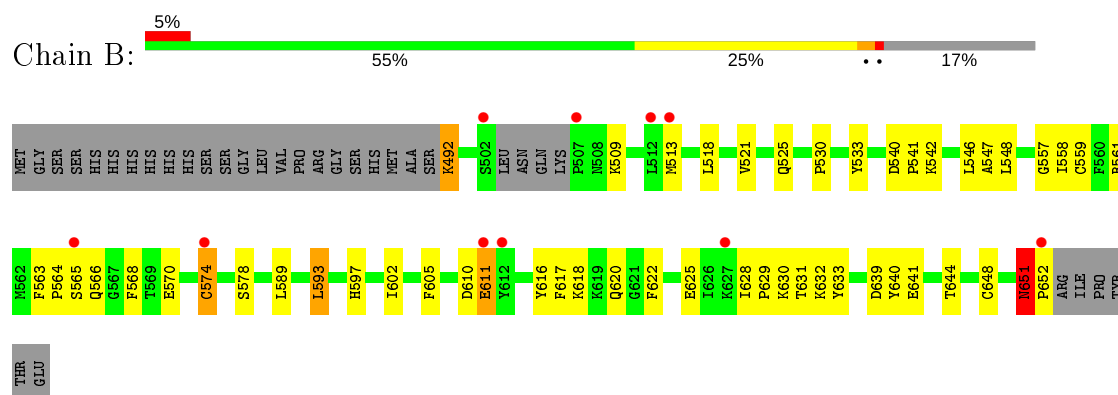
3 Residue-property plots [i](#)

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.

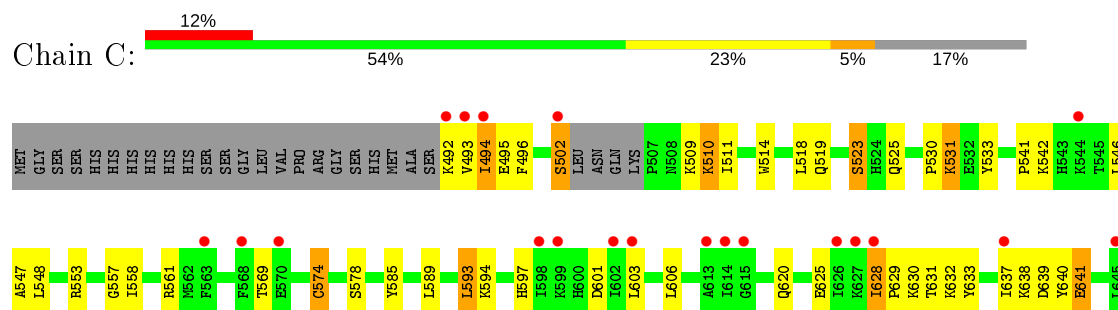
• Molecule 1: Histone acetyltransferase KAT2B

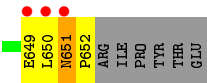


• Molecule 1: Histone acetyltransferase KAT2B

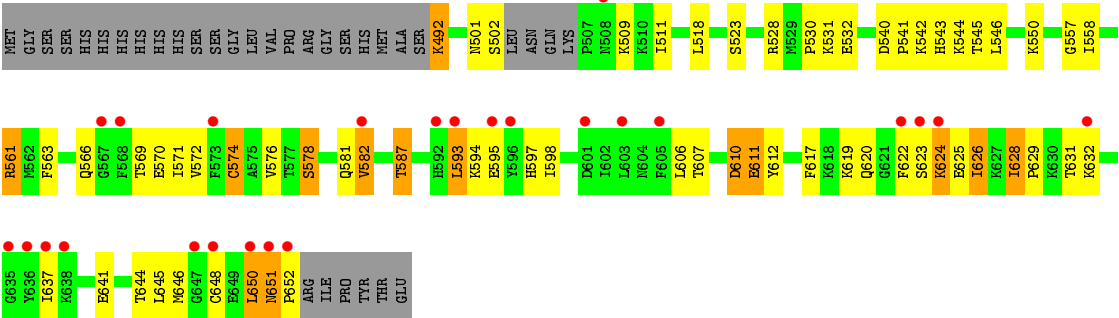


• Molecule 1: Histone acetyltransferase KAT2B





● Molecule 1: Histone acetyltransferase KAT2B



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	65.57Å 65.57Å 187.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.26 – 2.31 45.26 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.26-2.31) 88.1 (45.26-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.229 , 0.275 0.240 , 0.291	Depositor DCC
R_{free} test set	1988 reflections (6.06%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5296	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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

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	0.71	0/1309	0.61	0/1760
1	B	0.78	2/1309 (0.2%)	0.59	0/1760
1	C	0.68	0/1309	0.57	0/1760
1	D	0.58	0/1309	0.55	0/1760
All	All	0.69	2/5236 (0.0%)	0.58	0/7040

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	559	CYS	CB-SG	5.40	1.91	1.82
1	B	570	GLU	CG-CD	5.16	1.59	1.51

There are no bond angle outliers.

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	1276	0	1297	44	0
1	B	1276	0	1297	46	0
1	C	1276	0	1297	38	0
1	D	1276	0	1297	74	0
2	A	48	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	32	4	0
2	C	48	0	32	8	0
2	D	48	0	32	10	0
All	All	5296	0	5316	205	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 (205) 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:B:651:ASN:HB2	1:B:652:PRO:CD	1.42	1.49
1:A:651:ASN:HB2	1:A:652:PRO:CD	1.59	1.32
1:C:651:ASN:HB2	1:C:652:PRO:CD	1.62	1.29
1:A:525:GLN:O	1:A:527:PRO:HD3	1.28	1.25
1:B:651:ASN:CB	1:B:652:PRO:HD2	1.67	1.22
1:D:624:LYS:HD3	1:D:644:THR:HG21	1.17	1.11
1:A:651:ASN:HB2	1:A:652:PRO:HD3	1.21	1.10
1:C:651:ASN:CB	1:C:652:PRO:HD2	1.79	1.08
1:A:651:ASN:CB	1:A:652:PRO:CD	2.30	1.08
1:D:598:ILE:HD11	1:D:651:ASN:O	1.59	1.03
1:A:651:ASN:CB	1:A:652:PRO:HD2	1.90	1.02
1:A:537:LEU:HD12	1:A:573:PHE:CZ	1.98	0.99
1:D:651:ASN:HB2	1:D:652:PRO:HD2	1.42	0.97
1:D:624:LYS:HD3	1:D:644:THR:CG2	1.93	0.97
1:A:537:LEU:HD12	1:A:573:PHE:HZ	1.31	0.95
1:C:558:ILE:HG12	1:C:574:CYS:HB3	1.49	0.95
1:D:624:LYS:CD	1:D:644:THR:HG21	1.96	0.95
1:B:651:ASN:CB	1:B:652:PRO:CD	2.30	0.94
1:A:651:ASN:HB2	1:A:652:PRO:HD2	1.45	0.94
1:D:617:PHE:O	1:D:622:PHE:HB2	1.70	0.91
1:B:651:ASN:HB2	1:B:652:PRO:HD3	1.51	0.90
1:B:651:ASN:HB2	1:B:652:PRO:HD2	0.92	0.90
1:D:626:ILE:HD12	1:D:626:ILE:N	1.88	0.88
1:B:630:LYS:HA	1:B:633:TYR:CE2	2.08	0.88
1:A:651:ASN:CG	1:A:652:PRO:HD2	1.93	0.88
1:D:623:SER:O	1:D:646:MET:HG2	1.75	0.86
1:D:598:ILE:CD1	1:D:651:ASN:O	2.26	0.83
1:C:651:ASN:HB2	1:C:652:PRO:HD2	0.83	0.80
1:D:626:ILE:CD1	1:D:626:ILE:N	2.45	0.79
1:D:594:LYS:HG2	1:D:650:LEU:HD22	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:ASN:HB2	1:D:652:PRO:CD	2.12	0.77
1:A:525:GLN:O	1:A:527:PRO:CD	2.22	0.76
1:A:572:VAL:HG12	1:A:573:PHE:CD1	2.20	0.76
1:C:628:ILE:HG13	1:C:629:PRO:HD2	1.68	0.76
1:D:574:CYS:HG	2:D:700:COA:HS1	0.92	0.75
1:B:561:ARG:HD3	1:B:563:PHE:CZ	2.22	0.74
1:C:502:SER:HA	1:C:541:PRO:HB3	1.70	0.73
1:B:558:ILE:HG12	1:B:574:CYS:HB3	1.71	0.72
1:A:513:MET:HE1	1:D:532:GLU:HB3	1.71	0.71
1:C:493:VAL:C	1:C:494:ILE:HG12	2.11	0.71
1:A:628:ILE:HG13	1:A:629:PRO:HD2	1.73	0.70
1:D:622:PHE:HA	1:D:648:CYS:HB3	1.73	0.68
1:A:572:VAL:HG12	1:A:573:PHE:CE1	2.29	0.68
1:A:593:LEU:HD22	1:A:597:HIS:CE1	2.29	0.68
1:C:603:LEU:O	1:C:650:LEU:N	2.22	0.67
1:D:594:LYS:HG2	1:D:650:LEU:HD13	1.76	0.67
1:D:617:PHE:C	1:D:622:PHE:HB2	2.14	0.66
1:B:574:CYS:SG	2:B:700:COA:S1P	2.94	0.66
1:D:651:ASN:CB	1:D:652:PRO:HD2	2.24	0.66
1:D:594:LYS:CG	1:D:650:LEU:HD22	2.26	0.65
1:C:495:GLU:C	1:C:496:PHE:CD1	2.70	0.65
1:D:651:ASN:CB	1:D:652:PRO:CD	2.75	0.65
1:C:495:GLU:O	1:C:548:LEU:HD12	1.97	0.65
1:A:651:ASN:ND2	1:A:652:PRO:HD2	2.11	0.64
1:A:526:LEU:CD1	1:A:573:PHE:HB3	2.27	0.64
1:A:526:LEU:HD11	1:A:573:PHE:HB3	1.79	0.63
1:A:558:ILE:HG12	1:A:574:CYS:HB3	1.79	0.63
1:D:574:CYS:SG	2:D:700:COA:S1P	2.74	0.63
1:A:566:GLN:HG3	1:A:632:LYS:O	1.99	0.63
1:D:626:ILE:HG22	1:D:628:ILE:H	1.62	0.63
1:A:649:GLU:HG3	1:A:649:GLU:O	1.98	0.62
1:B:651:ASN:CG	1:B:652:PRO:HD2	2.18	0.62
1:B:548:LEU:HB2	1:B:589:LEU:HD21	1.80	0.61
1:B:563:PHE:HB2	1:B:568:PHE:O	2.01	0.61
1:D:620:GLN:HB2	1:D:622:PHE:CD2	2.36	0.61
1:B:563:PHE:N	1:B:564:PRO:HD3	2.15	0.61
1:A:528:ARG:NH2	1:A:611:GLU:OE2	2.33	0.61
1:C:603:LEU:HA	1:C:650:LEU:HB2	1.83	0.60
1:B:530:PRO:HG2	1:B:533:TYR:HB2	1.84	0.60
1:B:630:LYS:HG2	1:B:633:TYR:OH	2.02	0.59
1:D:501:ASN:O	1:D:502:SER:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ASN:O	1:A:652:PRO:C	2.41	0.59
1:D:582:VAL:O	1:D:582:VAL:HG12	2.02	0.59
1:C:630:LYS:HA	1:C:633:TYR:CE2	2.39	0.58
1:D:623:SER:O	1:D:646:MET:CG	2.50	0.57
1:D:593:LEU:HD22	1:D:597:HIS:CE1	2.40	0.57
1:D:620:GLN:HB2	1:D:622:PHE:HD2	1.69	0.57
1:B:525:GLN:HB3	2:B:700:COA:H72	1.88	0.56
1:C:639:ASP:OD1	1:C:640:TYR:N	2.39	0.56
1:D:594:LYS:CG	1:D:650:LEU:HD13	2.36	0.56
1:D:594:LYS:HE3	1:D:650:LEU:HD22	1.87	0.56
1:B:564:PRO:HG3	1:B:602:ILE:HD11	1.87	0.56
1:D:576:VAL:O	1:D:581:GLN:NE2	2.34	0.56
1:C:651:ASN:CB	1:C:652:PRO:CD	2.47	0.55
1:A:619:LYS:NZ	2:A:700:COA:O8A	2.36	0.55
1:B:561:ARG:HD3	1:B:563:PHE:CE2	2.42	0.55
1:D:594:LYS:HG2	1:D:650:LEU:CD2	2.34	0.55
1:A:561:ARG:HD2	1:A:563:PHE:CZ	2.42	0.54
1:D:563:PHE:HB3	1:D:566:GLN:HB2	1.89	0.54
1:D:558:ILE:HG12	1:D:574:CYS:HB3	1.88	0.54
1:B:563:PHE:N	1:B:564:PRO:CD	2.70	0.54
1:B:566:GLN:HG2	1:B:632:LYS:O	2.07	0.54
1:D:624:LYS:O	1:D:626:ILE:CD1	2.56	0.53
1:D:574:CYS:HG	2:D:700:COA:C2P	2.21	0.53
1:C:574:CYS:SG	2:C:700:COA:S1P	3.02	0.53
1:A:522:PHE:CE1	1:A:573:PHE:O	2.61	0.53
1:A:574:CYS:SG	2:A:700:COA:S1P	2.84	0.53
1:A:608:TYR:CE1	1:A:645:LEU:HB2	2.44	0.52
1:C:593:LEU:HD22	1:C:597:HIS:CD2	2.44	0.52
1:D:619:LYS:NZ	2:D:700:COA:O8A	2.43	0.52
1:B:628:ILE:HG13	1:B:629:PRO:HD2	1.90	0.51
1:D:509:LYS:O	1:D:509:LYS:HG3	2.10	0.51
1:D:626:ILE:H	1:D:626:ILE:CD1	2.20	0.51
1:C:574:CYS:HG	2:C:700:COA:HS1	1.51	0.51
1:D:578:SER:HA	1:D:581:GLN:HG3	1.91	0.51
1:D:587:THR:OG1	2:D:700:COA:O2A	2.27	0.51
1:B:509:LYS:O	1:B:513:MET:HG2	2.10	0.51
2:C:700:COA:N1A	2:C:700:COA:H133	2.25	0.51
1:B:563:PHE:O	1:B:566:GLN:N	2.33	0.51
1:A:572:VAL:HG12	1:A:573:PHE:CG	2.45	0.51
1:C:603:LEU:CA	1:C:650:LEU:HB2	2.41	0.51
1:D:532:GLU:H	1:D:532:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:PRO:HG2	1:B:533:TYR:CB	2.42	0.50
1:D:617:PHE:CE2	2:D:700:COA:H21	2.46	0.50
1:D:598:ILE:HD13	1:D:652:PRO:C	2.31	0.50
1:A:572:VAL:CG1	1:A:573:PHE:CE1	2.93	0.50
1:A:572:VAL:CG1	1:A:573:PHE:CZ	2.94	0.50
1:A:630:LYS:HA	1:A:633:TYR:CE2	2.47	0.49
1:A:593:LEU:CD2	1:A:597:HIS:HE1	2.26	0.49
1:A:518:LEU:HD11	1:A:547:ALA:HB2	1.94	0.49
1:D:528:ARG:NH1	1:D:611:GLU:OE2	2.41	0.48
1:C:546:LEU:O	1:C:557:GLY:HA2	2.13	0.48
1:D:594:LYS:HG2	1:D:650:LEU:CD1	2.43	0.48
1:C:625:GLU:O	1:C:625:GLU:HG3	2.13	0.48
1:D:617:PHE:HB3	1:D:622:PHE:CB	2.43	0.47
1:D:530:PRO:HB2	1:D:532:GLU:OE1	2.14	0.47
1:A:561:ARG:CD	1:A:563:PHE:CZ	2.97	0.47
1:B:639:ASP:OD1	1:B:640:TYR:N	2.47	0.47
1:D:606:LEU:HD22	1:D:645:LEU:HD11	1.96	0.47
1:C:525:GLN:HB3	2:C:700:COA:H72	1.95	0.47
1:C:649:GLU:O	1:C:649:GLU:HG3	2.14	0.47
1:D:542:LYS:O	1:D:561:ARG:HG2	2.15	0.47
1:B:616:TYR:O	1:B:620:GLN:HG2	2.15	0.46
1:D:546:LEU:O	1:D:557:GLY:HA2	2.14	0.46
1:D:571:ILE:HB	1:D:607:THR:HB	1.97	0.46
1:C:510:LYS:HD3	1:C:514:TRP:CZ2	2.51	0.46
1:D:574:CYS:CB	2:D:700:COA:HS1	2.27	0.46
1:B:564:PRO:C	1:B:566:GLN:N	2.69	0.46
1:B:593:LEU:HD13	1:B:605:PHE:CZ	2.51	0.46
1:D:594:LYS:CE	1:D:650:LEU:HD22	2.46	0.46
1:D:651:ASN:O	1:D:652:PRO:C	2.54	0.46
1:A:581:GLN:HB2	1:B:542:LYS:HE2	1.98	0.46
1:B:564:PRO:O	1:B:566:GLN:N	2.49	0.46
1:A:593:LEU:HD22	1:A:597:HIS:HE1	1.74	0.46
1:C:574:CYS:HG	2:C:700:COA:C2P	2.29	0.46
1:B:593:LEU:HD22	1:B:597:HIS:CE1	2.51	0.45
1:D:566:GLN:HG3	1:D:632:LYS:O	2.17	0.45
1:B:625:GLU:HG3	1:B:625:GLU:O	2.15	0.45
1:D:570:GLU:HG3	1:D:637:ILE:HG13	1.98	0.45
1:D:593:LEU:CD2	1:D:597:HIS:HE1	2.29	0.45
1:B:617:PHE:CE2	2:B:700:COA:H21	2.51	0.45
1:C:519:GLN:O	1:C:523:SER:OG	2.32	0.45
1:B:564:PRO:C	1:B:566:GLN:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:PRO:HG2	1:D:632:LYS:HG2	1.99	0.45
2:D:700:COA:N3A	2:D:700:COA:H2B	2.32	0.45
1:B:546:LEU:O	1:B:557:GLY:HA2	2.16	0.45
1:C:494:ILE:HD13	1:C:585:TYR:HE1	1.81	0.45
1:C:531:LYS:HG3	1:C:531:LYS:H	1.45	0.45
1:D:594:LYS:HG2	1:D:650:LEU:CG	2.47	0.45
1:C:641:GLU:H	1:C:641:GLU:HG2	1.51	0.45
1:B:518:LEU:HD11	1:B:547:ALA:HB2	1.99	0.45
1:D:625:GLU:C	1:D:626:ILE:HD12	2.35	0.45
1:D:628:ILE:HG13	1:D:629:PRO:HD2	1.99	0.44
1:A:616:TYR:O	1:A:620:GLN:HG2	2.17	0.44
2:C:700:COA:H2A	2:C:700:COA:H122	1.99	0.44
1:B:651:ASN:OD1	1:B:652:PRO:HD2	2.16	0.44
1:B:540:ASP:OD2	1:B:542:LYS:HB2	2.18	0.43
1:C:633:TYR:O	1:C:637:ILE:HG22	2.18	0.43
1:B:563:PHE:O	1:B:564:PRO:C	2.54	0.43
1:C:628:ILE:HG13	1:C:629:PRO:CD	2.45	0.43
1:B:566:GLN:CG	1:B:632:LYS:O	2.65	0.43
1:C:629:PRO:O	1:C:632:LYS:HB2	2.17	0.43
1:D:610:ASP:O	1:D:612:TYR:N	2.51	0.43
1:B:521:VAL:O	1:B:525:GLN:HG2	2.18	0.43
1:B:492:LYS:HA	1:B:492:LYS:HD2	1.65	0.43
1:B:542:LYS:HD2	1:B:561:ARG:HH21	1.84	0.43
1:D:625:GLU:O	1:D:625:GLU:HG3	2.18	0.43
1:C:496:PHE:N	1:C:496:PHE:CD1	2.87	0.43
1:A:542:LYS:HD2	1:A:561:ARG:NH2	2.33	0.42
1:B:622:PHE:CG	1:B:648:CYS:HB2	2.54	0.42
1:C:548:LEU:HB2	1:C:589:LEU:HD21	2.02	0.42
1:C:594:LYS:NZ	1:C:620:GLN:O	2.48	0.42
1:D:623:SER:O	1:D:646:MET:CB	2.66	0.42
1:A:565:SER:HB2	1:A:566:GLN:OE1	2.20	0.42
1:B:611:GLU:HG3	1:B:611:GLU:H	1.31	0.42
1:B:540:ASP:HA	1:B:541:PRO:HD3	1.79	0.42
1:D:582:VAL:N	2:D:700:COA:O5A	2.44	0.42
1:C:525:GLN:O	2:C:700:COA:H61	2.20	0.42
1:C:518:LEU:HD11	1:C:547:ALA:HB2	2.02	0.41
1:C:530:PRO:HG2	1:C:533:TYR:HB2	2.02	0.41
1:D:624:LYS:CE	1:D:644:THR:HG21	2.49	0.41
1:A:612:TYR:O	2:A:700:COA:N6A	2.53	0.41
1:D:593:LEU:CD2	1:D:597:HIS:CE1	3.04	0.41
1:A:593:LEU:HA	1:A:593:LEU:HD23	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:LYS:HB2	1:D:492:LYS:HE2	1.44	0.41
1:D:629:PRO:O	1:D:632:LYS:HB2	2.21	0.41
2:B:700:COA:H2B	2:B:700:COA:N3A	2.35	0.41
1:D:540:ASP:HA	1:D:541:PRO:HD3	1.79	0.41
1:D:543:HIS:CE1	1:D:572:VAL:HG21	2.55	0.41
1:D:518:LEU:HD13	1:D:545:THR:HG21	2.02	0.41
1:C:606:LEU:HA	1:C:606:LEU:HD23	1.80	0.40
1:D:619:LYS:NZ	2:D:700:COA:O3B	2.54	0.40
1:A:540:ASP:HA	1:A:541:PRO:HD3	1.84	0.40
2:C:700:COA:C2A	2:C:700:COA:H122	2.51	0.40
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.94	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	153/190 (80%)	146 (95%)	5 (3%)	2 (1%)	12	12
1	B	153/190 (80%)	145 (95%)	6 (4%)	2 (1%)	12	12
1	C	153/190 (80%)	147 (96%)	6 (4%)	0	100	100
1	D	153/190 (80%)	145 (95%)	7 (5%)	1 (1%)	22	26
All	All	612/760 (80%)	583 (95%)	24 (4%)	5 (1%)	19	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	651	ASN
1	A	526	LEU
1	B	565	SER
1	A	651	ASN

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Mol	Chain	Res	Type
1	D	582	VAL

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	139/168 (83%)	118 (85%)	21 (15%)	3	2
1	B	139/168 (83%)	128 (92%)	11 (8%)	12	15
1	C	139/168 (83%)	118 (85%)	21 (15%)	3	2
1	D	139/168 (83%)	117 (84%)	22 (16%)	2	2
All	All	556/672 (83%)	481 (86%)	75 (14%)	4	3

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	LYS
1	A	508	ASN
1	A	513	MET
1	A	544	LYS
1	A	553	ARG
1	A	561	ARG
1	A	566	GLN
1	A	569	THR
1	A	574	CYS
1	A	578	SER
1	A	593	LEU
1	A	598	ILE
1	A	599	LYS
1	A	601	ASP
1	A	611	GLU
1	A	618	LYS
1	A	623	SER
1	A	627	LYS
1	A	631	THR
1	A	638	LYS

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Mol	Chain	Res	Type
1	A	650	LEU
1	B	492	LYS
1	B	574	CYS
1	B	578	SER
1	B	593	LEU
1	B	610	ASP
1	B	611	GLU
1	B	618	LYS
1	B	631	THR
1	B	641	GLU
1	B	644	THR
1	B	651	ASN
1	C	492	LYS
1	C	494	ILE
1	C	502	SER
1	C	509	LYS
1	C	510	LYS
1	C	511	ILE
1	C	523	SER
1	C	531	LYS
1	C	542	LYS
1	C	553	ARG
1	C	561	ARG
1	C	569	THR
1	C	574	CYS
1	C	578	SER
1	C	593	LEU
1	C	601	ASP
1	C	628	ILE
1	C	631	THR
1	C	638	LYS
1	C	641	GLU
1	C	651	ASN
1	D	492	LYS
1	D	511	ILE
1	D	523	SER
1	D	531	LYS
1	D	544	LYS
1	D	550	LYS
1	D	561	ARG
1	D	569	THR
1	D	574	CYS

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Mol	Chain	Res	Type
1	D	578	SER
1	D	587	THR
1	D	593	LEU
1	D	595	GLU
1	D	610	ASP
1	D	611	GLU
1	D	624	LYS
1	D	626	ILE
1	D	628	ILE
1	D	631	THR
1	D	641	GLU
1	D	650	LEU
1	D	651	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	ASN
1	C	597	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	D	700	-	41,50,50	2.10	9 (21%)	52,75,75	1.53	11 (21%)
2	COA	B	700	-	41,50,50	2.11	8 (19%)	52,75,75	1.57	12 (23%)
2	COA	C	700	-	41,50,50	2.16	9 (21%)	52,75,75	1.56	10 (19%)
2	COA	A	700	-	41,50,50	2.18	8 (19%)	52,75,75	1.49	9 (17%)

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	D	700	-	-	13/44/64/64	0/3/3/3
2	COA	B	700	-	-	8/44/64/64	0/3/3/3
2	COA	C	700	-	-	6/44/64/64	0/3/3/3
2	COA	A	700	-	-	9/44/64/64	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	700	COA	C9P-N8P	7.47	1.49	1.33
2	D	700	COA	C9P-N8P	7.18	1.49	1.33
2	A	700	COA	C9P-N8P	7.16	1.49	1.33
2	B	700	COA	C9P-N8P	7.09	1.49	1.33
2	A	700	COA	C5P-N4P	6.43	1.48	1.33
2	C	700	COA	C5P-N4P	6.29	1.47	1.33
2	B	700	COA	C5P-N4P	6.04	1.47	1.33
2	D	700	COA	C5P-N4P	5.77	1.46	1.33
2	A	700	COA	C2B-C3B	-5.18	1.41	1.52
2	C	700	COA	C2B-C3B	-5.03	1.41	1.52
2	B	700	COA	C2B-C3B	-4.92	1.42	1.52
2	D	700	COA	C2B-C3B	-4.84	1.42	1.52
2	D	700	COA	C6A-N6A	3.89	1.48	1.34
2	C	700	COA	O5P-C5P	3.85	1.31	1.23
2	A	700	COA	C3B-C4B	-3.65	1.43	1.52
2	A	700	COA	O5P-C5P	3.59	1.30	1.23
2	C	700	COA	C6A-N6A	3.51	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	COA	C6A-N6A	3.45	1.46	1.34
2	A	700	COA	C6A-N6A	3.45	1.46	1.34
2	B	700	COA	C3B-C4B	-3.44	1.43	1.52
2	B	700	COA	O5P-C5P	3.40	1.30	1.23
2	D	700	COA	C3B-C4B	-3.34	1.43	1.52
2	D	700	COA	O5P-C5P	3.30	1.30	1.23
2	C	700	COA	C3B-C4B	-3.02	1.44	1.52
2	B	700	COA	C2A-N3A	2.59	1.36	1.32
2	D	700	COA	P3B-O8A	-2.46	1.45	1.54
2	C	700	COA	P3B-O8A	-2.34	1.45	1.54
2	B	700	COA	P3B-O8A	-2.25	1.46	1.54
2	A	700	COA	P3B-O8A	-2.22	1.46	1.54
2	D	700	COA	P2A-O4A	2.18	1.58	1.50
2	D	700	COA	C2A-N3A	2.17	1.35	1.32
2	A	700	COA	C2A-N3A	2.09	1.35	1.32
2	C	700	COA	O9P-C9P	2.07	1.27	1.23
2	C	700	COA	P2A-O4A	2.02	1.58	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	COA	N3A-C2A-N1A	-5.41	120.23	128.68
2	D	700	COA	N3A-C2A-N1A	-5.30	120.39	128.68
2	B	700	COA	N3A-C2A-N1A	-4.82	121.15	128.68
2	A	700	COA	N3A-C2A-N1A	-4.82	121.15	128.68
2	C	700	COA	P2A-O3A-P1A	-4.26	118.21	132.83
2	D	700	COA	P2A-O3A-P1A	-4.04	118.97	132.83
2	B	700	COA	P2A-O3A-P1A	-3.74	120.00	132.83
2	A	700	COA	P2A-O3A-P1A	-3.55	120.65	132.83
2	B	700	COA	C7P-C6P-C5P	3.24	117.76	112.36
2	C	700	COA	C6P-C7P-N8P	3.12	118.19	111.90
2	C	700	COA	C2B-C3B-C4B	2.85	108.28	103.22
2	A	700	COA	C6P-C5P-N4P	2.82	121.18	116.42
2	A	700	COA	C6P-C7P-N8P	2.81	117.57	111.90
2	D	700	COA	O5P-C5P-N4P	-2.80	117.73	123.01
2	C	700	COA	C3P-N4P-C5P	-2.70	117.83	122.84
2	D	700	COA	C2B-C3B-C4B	2.70	108.01	103.22
2	B	700	COA	C6P-C5P-N4P	2.68	120.94	116.42
2	C	700	COA	C6P-C5P-N4P	2.63	120.86	116.42
2	B	700	COA	O9P-C9P-N8P	-2.63	117.34	122.99
2	D	700	COA	O6A-CCP-CBP	2.62	114.75	110.55
2	D	700	COA	C6P-C5P-N4P	2.55	120.72	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	COA	O5B-C5B-C4B	2.55	117.76	108.99
2	A	700	COA	C7P-N8P-C9P	-2.52	118.10	122.59
2	C	700	COA	C1B-N9A-C4A	-2.52	122.22	126.64
2	B	700	COA	C2B-C3B-C4B	2.51	107.67	103.22
2	B	700	COA	C1B-N9A-C4A	-2.39	122.45	126.64
2	D	700	COA	C1B-N9A-C4A	-2.31	122.58	126.64
2	B	700	COA	O5P-C5P-N4P	-2.28	118.72	123.01
2	A	700	COA	C1B-N9A-C4A	-2.27	122.65	126.64
2	D	700	COA	C3P-N4P-C5P	-2.22	118.72	122.84
2	D	700	COA	C2A-N1A-C6A	2.21	122.54	118.75
2	B	700	COA	O6A-CCP-CBP	2.21	114.09	110.55
2	C	700	COA	C7P-N8P-C9P	-2.15	118.75	122.59
2	C	700	COA	C7P-C6P-C5P	2.15	115.94	112.36
2	A	700	COA	O4B-C1B-C2B	-2.13	103.81	106.93
2	A	700	COA	C7P-C6P-C5P	2.12	115.89	112.36
2	B	700	COA	C3P-N4P-C5P	-2.12	118.90	122.84
2	B	700	COA	C7P-N8P-C9P	-2.10	118.84	122.59
2	D	700	COA	O5B-C5B-C4B	2.07	116.12	108.99
2	C	700	COA	O5B-C5B-C4B	2.04	116.02	108.99
2	A	700	COA	CEP-CBP-CCP	2.04	111.56	108.23
2	D	700	COA	O9P-C9P-N8P	-2.03	118.63	122.99

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	700	COA	CCP-O6A-P2A-O3A
2	D	700	COA	CAP-CBP-CCP-O6A
2	D	700	COA	C5P-C6P-C7P-N8P
2	B	700	COA	CCP-O6A-P2A-O3A
2	B	700	COA	C5P-C6P-C7P-N8P
2	C	700	COA	CCP-O6A-P2A-O3A
2	C	700	COA	C5P-C6P-C7P-N8P
2	A	700	COA	N8P-C9P-CAP-OAP
2	A	700	COA	S1P-C2P-C3P-N4P
2	A	700	COA	C3B-C4B-C5B-O5B
2	D	700	COA	C3B-C4B-C5B-O5B
2	D	700	COA	O4B-C4B-C5B-O5B
2	B	700	COA	C3B-C4B-C5B-O5B
2	B	700	COA	O4B-C4B-C5B-O5B
2	C	700	COA	C3B-C4B-C5B-O5B
2	C	700	COA	O4B-C4B-C5B-O5B

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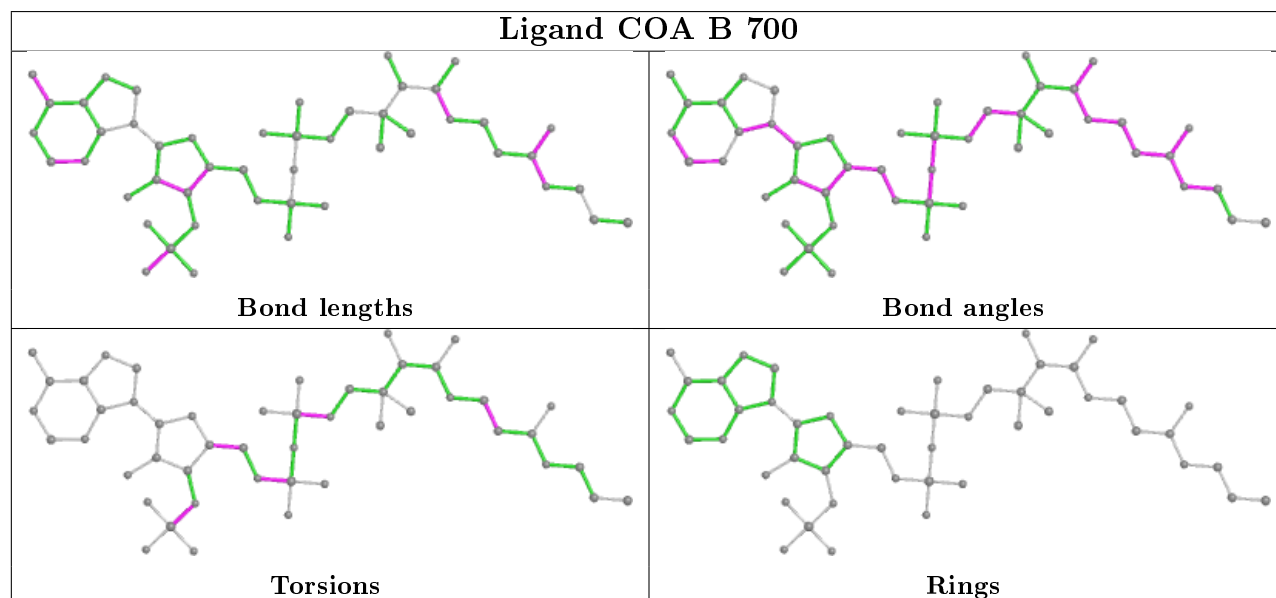
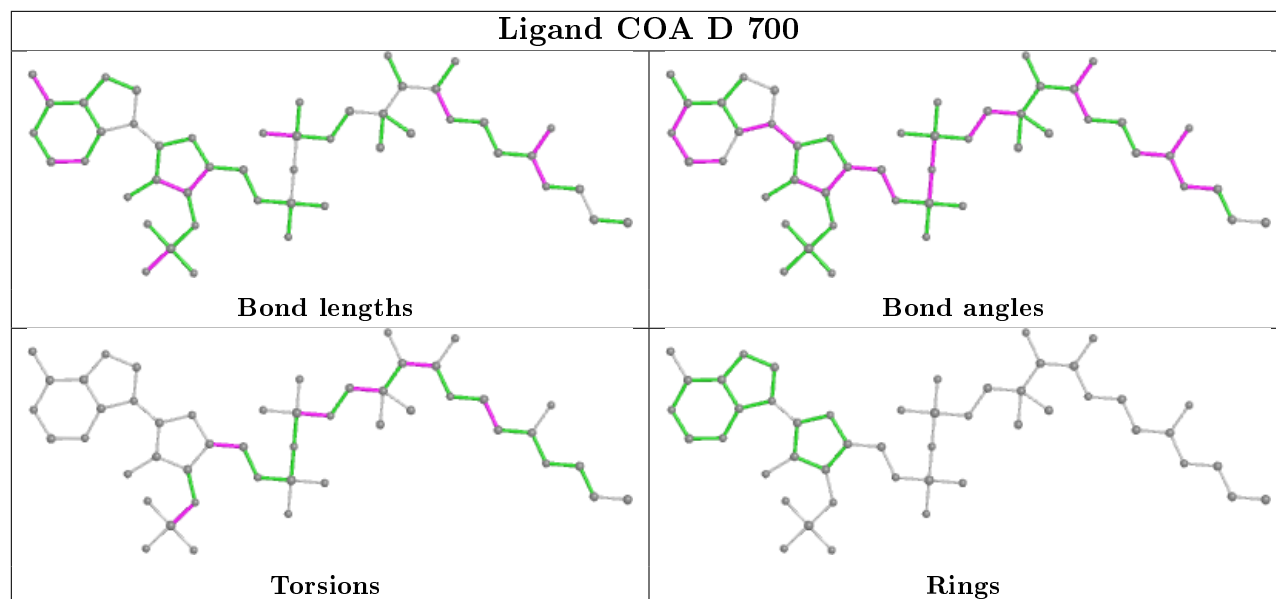
Mol	Chain	Res	Type	Atoms
2	A	700	COA	O4B-C4B-C5B-O5B
2	D	700	COA	CDP-CBP-CCP-O6A
2	D	700	COA	CEP-CBP-CCP-O6A
2	D	700	COA	O9P-C9P-CAP-OAP
2	A	700	COA	O9P-C9P-CAP-OAP
2	A	700	COA	C3B-O3B-P3B-O7A
2	D	700	COA	CCP-O6A-P2A-O5A
2	B	700	COA	CCP-O6A-P2A-O5A
2	C	700	COA	CCP-O6A-P2A-O5A
2	A	700	COA	C5P-C6P-C7P-N8P
2	D	700	COA	C3B-O3B-P3B-O7A
2	D	700	COA	N8P-C9P-CAP-OAP
2	D	700	COA	C3B-O3B-P3B-O8A
2	D	700	COA	C3B-O3B-P3B-O9A
2	B	700	COA	C3B-O3B-P3B-O8A
2	A	700	COA	CCP-O6A-P2A-O3A
2	A	700	COA	P1A-O3A-P2A-O4A
2	B	700	COA	C5B-O5B-P1A-O1A
2	B	700	COA	CCP-O6A-P2A-O4A
2	C	700	COA	C5B-O5B-P1A-O1A

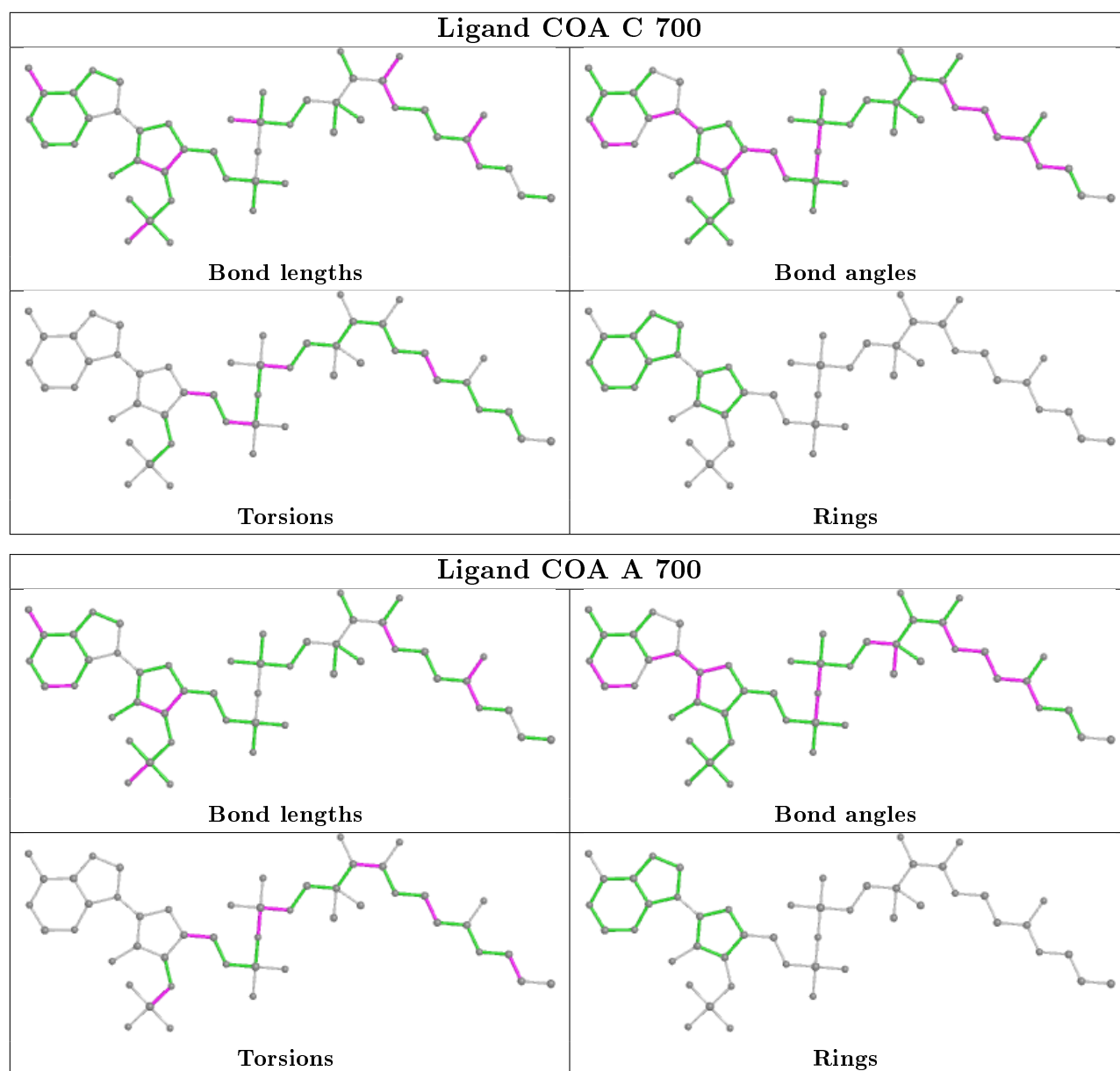
There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	700	COA	10	0
2	B	700	COA	4	0
2	C	700	COA	8	0
2	A	700	COA	3	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	157/190 (82%)	0.82	11 (7%) 16 22	53, 72, 104, 122	0
1	B	157/190 (82%)	0.86	10 (6%) 19 25	24, 69, 100, 134	0
1	C	157/190 (82%)	0.94	23 (14%) 2 3	53, 82, 114, 144	0
1	D	157/190 (82%)	1.30	25 (15%) 1 2	54, 87, 126, 158	0
All	All	628/760 (82%)	0.98	69 (10%) 5 8	24, 77, 115, 158	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	652	PRO	12.3
1	D	650	LEU	11.0
1	D	651	ASN	9.7
1	A	652	PRO	7.4
1	B	502	SER	7.0
1	D	593	LEU	6.8
1	D	622	PHE	6.5
1	C	493	VAL	5.7
1	C	650	LEU	5.3
1	D	605	PHE	4.9
1	C	494	ILE	4.8
1	C	492	LYS	4.7
1	D	601	ASP	4.7
1	B	507	PRO	4.6
1	C	628	ILE	4.5
1	D	582	VAL	4.2
1	C	602	ILE	4.1
1	D	568	PHE	4.0
1	C	651	ASN	4.0
1	D	648	CYS	3.9
1	C	598	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	636	TYR	3.7
1	D	596	TYR	3.7
1	D	603	LEU	3.6
1	B	652	PRO	3.6
1	D	567	GLY	3.5
1	C	603	LEU	3.4
1	B	612	TYR	3.2
1	D	647	GLY	3.2
1	A	628	ILE	3.2
1	A	573	PHE	3.1
1	C	626	ILE	2.9
1	D	635	GLY	2.9
1	B	627	LYS	2.9
1	A	579	ASN	2.8
1	D	637	ILE	2.8
1	D	623	SER	2.8
1	C	637	ILE	2.8
1	C	568	PHE	2.7
1	A	528	ARG	2.6
1	D	592	HIS	2.6
1	C	502	SER	2.6
1	B	565	SER	2.6
1	D	638	LYS	2.5
1	C	563	PHE	2.5
1	C	649	GLU	2.5
1	C	645	LEU	2.5
1	B	574	CYS	2.5
1	C	627	LYS	2.4
1	D	573	PHE	2.4
1	C	614	ILE	2.3
1	B	512	LEU	2.3
1	C	544	LYS	2.3
1	C	613	ALA	2.3
1	D	595	GLU	2.2
1	C	599	LYS	2.2
1	A	574	CYS	2.2
1	A	612	TYR	2.2
1	B	611	GLU	2.2
1	A	526	LEU	2.2
1	D	624	LYS	2.1
1	C	615	GLY	2.1
1	D	632	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	PRO	2.1
1	A	575	ALA	2.1
1	C	570	GLU	2.1
1	B	513	MET	2.0
1	D	508	ASN	2.0
1	A	603	LEU	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](#)

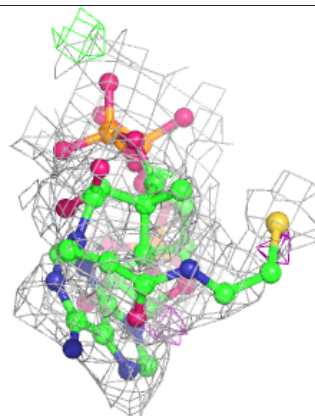
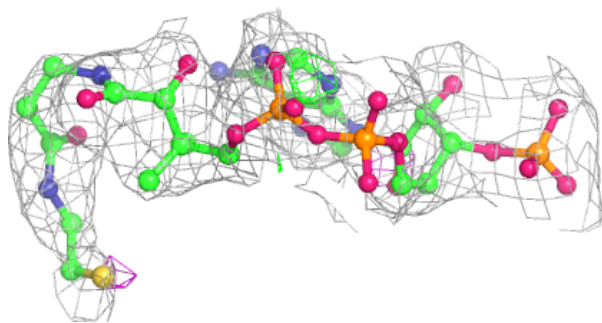
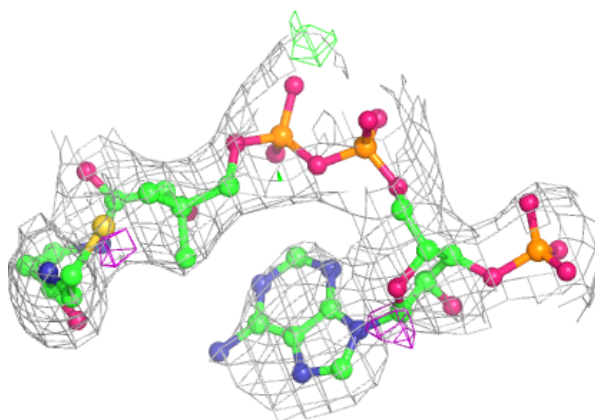
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	700	48/48	0.89	0.19	62,94,114,121	0
2	COA	B	700	48/48	0.89	0.19	59,78,99,112	0
2	COA	C	700	48/48	0.91	0.22	60,82,122,136	0
2	COA	A	700	48/48	0.92	0.19	64,77,98,103	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.

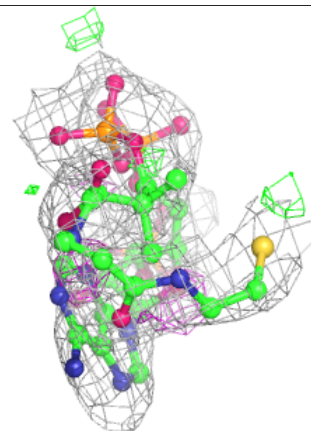
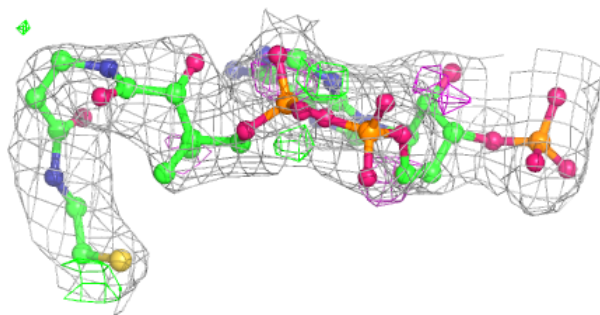
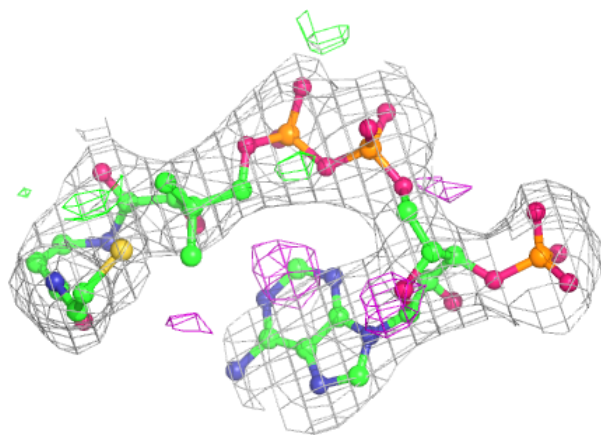
Electron density around COA D 700:

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



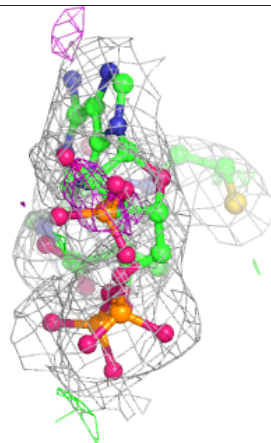
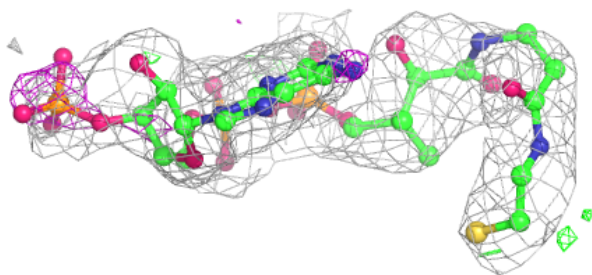
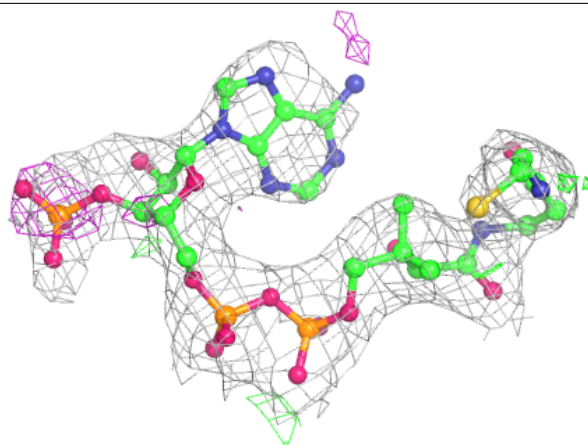
Electron density around COA B 700:

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



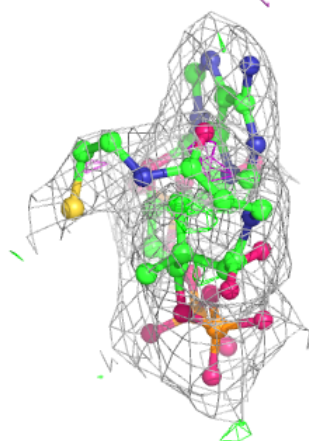
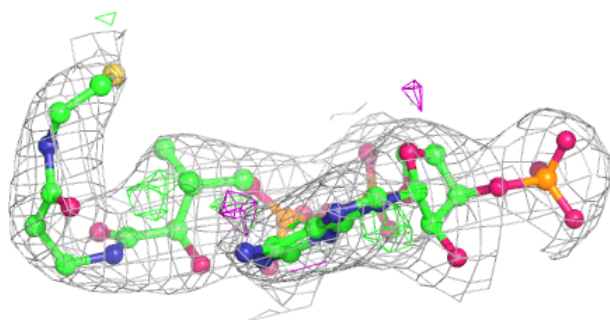
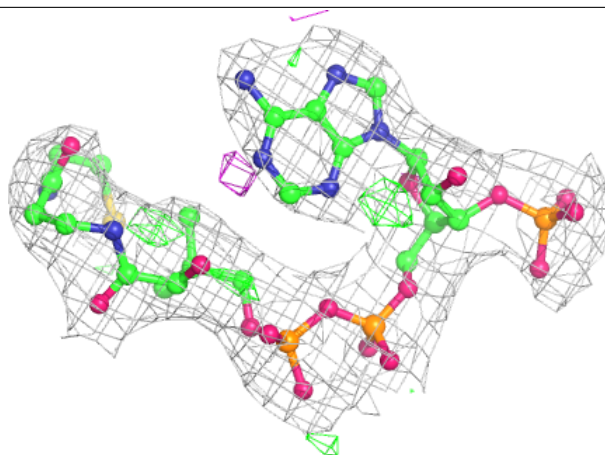
Electron density around COA C 700:

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



Electron density around COA A 700:

$2mF_o-DF_c$ (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.