



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:15 AM GMT

PDB ID : 2D52  
Title : Pentaketide chromone synthase (M207G mutant complexed with Coa)  
Authors : Kohno, T.; Morita, H.  
Deposited on : 2005-10-27  
Resolution : 1.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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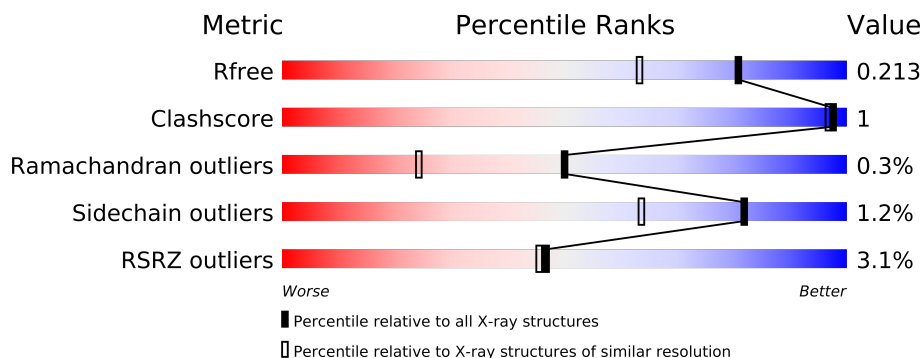
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6887 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

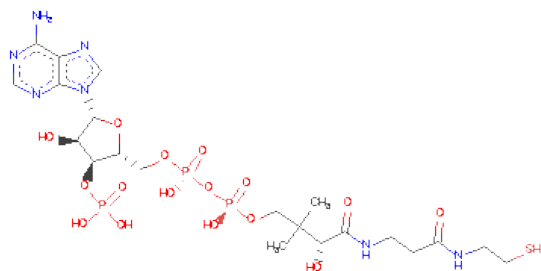
- Molecule 1 is a protein called pentaketide chromone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	6	0
			3167	2014	535	593	25			
1	B	395	Total	C	N	O	S	0	2	0
			3079	1964	520	571	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q58VP7
A	2	PRO	-	CLONING ARTIFACT	UNP Q58VP7
A	3	GLY	-	CLONING ARTIFACT	UNP Q58VP7
A	177	CSD	CYS	MODIFIED RESIDUE	UNP Q58VP7
A	210	GLY	MET	ENGINEERED	UNP Q58VP7
B	1	GLY	-	CLONING ARTIFACT	UNP Q58VP7
B	2	PRO	-	CLONING ARTIFACT	UNP Q58VP7
B	3	GLY	-	CLONING ARTIFACT	UNP Q58VP7
B	177	CSD	CYS	MODIFIED RESIDUE	UNP Q58VP7
B	210	GLY	MET	ENGINEERED	UNP Q58VP7

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



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

- Molecule 3 is water.

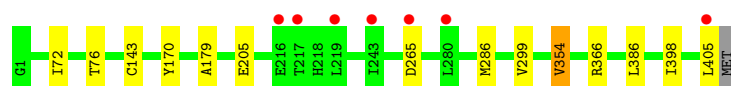
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	304	Total	O	0	0
			304	304		
3	B	241	Total	O	0	0
			241	241		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

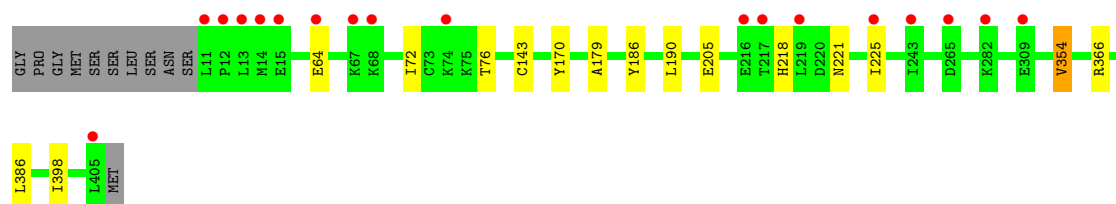
- Molecule 1: pentaketide chromone synthase

Chain A: 



- Molecule 1: pentaketide chromone synthase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.07Å 89.17Å 70.77Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 29.61 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.60) 100.0 (29.61-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.193 , 0.208 0.199 , 0.213	Depositor DCC
$R_{free}$ test set	6090 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 26.0	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 120439 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.59	0/3230	0.70	0/4379
1	B	0.59	0/3141	0.70	0/4259
All	All	0.59	0/6371	0.70	0/8638

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	TYR	Sidechain
1	B	170	TYR	Sidechain

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3167	0	3162	4	0
1	B	3079	0	3080	6	0
2	A	48	0	31	0	0
2	B	48	0	31	0	0
3	A	304	0	0	0	0
3	B	241	0	0	0	0
All	All	6887	0	6304	10	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (10) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:GLU:HG3	1:B:354:VAL:HB	1.85	0.57
1:B:143:CYS:SG	1:B:179:ALA:HB1	2.46	0.55
1:A:143:CYS:SG	1:A:179:ALA:HB1	2.49	0.53
1:A:205:GLU:HG3	1:A:354:VAL:HB	1.93	0.50
1:B:72:ILE:O	1:B:76:THR:HG23	2.18	0.43
1:A:386:LEU:HB3	1:A:398:ILE:HB	2.01	0.43
1:A:72:ILE:O	1:A:76:THR:HG23	2.18	0.43
1:B:386:LEU:HB3	1:B:398:ILE:HB	2.01	0.42
1:B:186:TYR:O	1:B:190:LEU:HG	2.18	0.42
1:B:221:ASN:O	1:B:225:ILE:HG12	2.20	0.42

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	408/406 (100%)	398 (98%)	9 (2%)	1 (0%)	56 29
1	B	394/406 (97%)	387 (98%)	6 (2%)	1 (0%)	50 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	802/812 (99%)	785 (98%)	15 (2%)	2 (0%)	50	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	VAL
1	B	354	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	343/338 (102%)	338 (98%)	5 (2%)	76	53
1	B	331/338 (98%)	328 (99%)	3 (1%)	87	74
All	All	674/676 (100%)	666 (99%)	8 (1%)	82	63

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	A	286	MET
1	A	299	VAL
1	A	366	ARG
1	A	405	LEU
1	B	64	GLU
1	B	218	HIS
1	B	366	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	221	ASN
1	B	328	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSD	A	177	1	7,7,8	8.83	3 (42%)	6,8,10	2.64	3 (50%)
1	CSD	B	177	1	7,7,8	8.90	3 (42%)	6,8,10	2.53	3 (50%)

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
1	CSD	A	177	1	-	1/3/6/8	0/0/0/0
1	CSD	B	177	1	-	1/3/6/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	CSD	O-C	18.04	1.23	1.11
1	A	177	CSD	O-C	17.79	1.23	1.11
1	B	177	CSD	OD1-SG	14.80	1.68	1.47
1	A	177	CSD	OD1-SG	14.79	1.68	1.47
1	A	177	CSD	CA-C	2.53	1.53	1.48
1	B	177	CSD	CA-C	2.43	1.52	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	CSD	C-CA-N	4.83	118.66	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	CSD	C-CA-N	4.22	118.04	113.83
1	B	177	CSD	OD2-SG-CB	3.14	110.04	97.42
1	A	177	CSD	OD2-SG-CB	3.00	109.48	97.42
1	B	177	CSD	CA-CB-SG	2.96	115.05	110.82
1	A	177	CSD	CA-CB-SG	2.72	114.70	110.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	177	CSD	CA-CB-SG-OD1
1	A	177	CSD	CA-CB-SG-OD1

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates 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	$\# Z  > 2$
2	COA	A	500	-	50,50,50	2.81	20 (40%)	75,75,75	2.90	31 (41%)
2	COA	B	501	-	50,50,50	2.79	20 (40%)	75,75,75	2.92	31 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	A	500	-	-	0/48/64/64	0/1/3/3
2	COA	B	501	-	-	0/48/64/64	0/1/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	COA	O5P-C5P	-9.22	1.02	1.23
2	B	501	COA	O5P-C5P	-9.21	1.03	1.23
2	A	500	COA	C2B-C1B	-5.80	1.45	1.53
2	A	500	COA	CCP-CBP	5.79	1.61	1.52
2	B	501	COA	CCP-CBP	5.65	1.61	1.52
2	B	501	COA	C2B-C1B	-5.58	1.45	1.53
2	A	500	COA	C4A-N3A	5.52	1.44	1.35
2	B	501	COA	C4A-N3A	5.37	1.43	1.35
2	A	500	COA	P1A-O5B	-5.13	1.36	1.59
2	B	501	COA	P1A-O5B	-5.11	1.36	1.59
2	B	501	COA	C1B-N9A	4.49	1.62	1.48
2	A	500	COA	C2A-N1A	4.41	1.42	1.33
2	A	500	COA	C1B-N9A	4.34	1.62	1.48
2	B	501	COA	C2A-N1A	4.31	1.42	1.33
2	B	501	COA	O4B-C1B	4.22	1.47	1.41
2	B	501	COA	C7P-N8P	4.13	1.56	1.46
2	A	500	COA	O4B-C1B	4.03	1.47	1.41
2	A	500	COA	CBP-CAP	4.00	1.59	1.55
2	A	500	COA	C7P-N8P	3.93	1.55	1.46
2	B	501	COA	CBP-CAP	3.75	1.59	1.55
2	A	500	COA	C3P-N4P	3.52	1.54	1.46
2	B	501	COA	O4B-C4B	3.22	1.52	1.45
2	A	500	COA	O4B-C4B	3.22	1.52	1.45
2	B	501	COA	C3P-N4P	2.95	1.53	1.46
2	B	501	COA	C2A-N3A	2.90	1.37	1.32
2	B	501	COA	P3B-O7A	2.88	1.60	1.51
2	A	500	COA	P3B-O7A	2.85	1.60	1.51
2	A	500	COA	C2A-N3A	2.82	1.37	1.32
2	B	501	COA	C5B-C4B	2.47	1.59	1.51
2	B	501	COA	O3B-C3B	2.40	1.51	1.44
2	A	500	COA	C5B-C4B	2.35	1.59	1.51
2	A	500	COA	O2B-C2B	-2.34	1.37	1.43
2	A	500	COA	O3B-C3B	2.33	1.51	1.44
2	B	501	COA	O2B-C2B	-2.32	1.37	1.43
2	B	501	COA	O9P-C9P	2.30	1.28	1.23
2	B	501	COA	C3B-C4B	2.22	1.59	1.52
2	A	500	COA	O9P-C9P	2.19	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	COA	C3B-C4B	2.16	1.59	1.52
2	B	501	COA	OAP-CAP	2.15	1.46	1.42
2	A	500	COA	OAP-CAP	2.12	1.46	1.42

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	COA	O4B-C1B-N9A	-9.69	99.43	108.44
2	A	500	COA	O4B-C1B-N9A	-9.26	99.83	108.44
2	A	500	COA	O5P-C5P-C6P	-7.84	106.32	121.92
2	A	500	COA	N3A-C2A-N1A	-7.76	122.22	128.71
2	B	501	COA	N3A-C2A-N1A	-7.67	122.30	128.71
2	B	501	COA	O5P-C5P-C6P	-7.62	106.77	121.92
2	B	501	COA	P3B-O3B-C3B	6.60	135.84	121.96
2	A	500	COA	P3B-O3B-C3B	6.20	135.01	121.96
2	B	501	COA	C2B-C3B-C4B	6.19	115.20	103.16
2	A	500	COA	C2B-C3B-C4B	6.19	115.20	103.16
2	A	500	COA	O2B-C2B-C3B	5.56	127.55	111.20
2	B	501	COA	O2B-C2B-C3B	5.52	127.45	111.20
2	B	501	COA	O5P-C5P-N4P	5.50	133.84	122.94
2	A	500	COA	O5P-C5P-N4P	5.24	133.32	122.94
2	B	501	COA	O4B-C1B-C2B	4.87	114.23	106.77
2	A	500	COA	O4B-C1B-C2B	4.81	114.15	106.77
2	A	500	COA	O2B-C2B-C1B	-4.45	97.75	111.23
2	B	501	COA	O2B-C2B-C1B	-4.37	98.00	111.23
2	B	501	COA	C2B-C1B-N9A	4.30	124.29	113.27
2	B	501	COA	CBP-CAP-C9P	4.15	116.76	112.73
2	A	500	COA	C2B-C1B-N9A	4.06	123.69	113.27
2	B	501	COA	C6P-C7P-N8P	-4.05	103.14	111.87
2	A	500	COA	CBP-CAP-C9P	3.79	116.41	112.73
2	A	500	COA	C6P-C7P-N8P	-3.72	103.84	111.87
2	B	501	COA	O4B-C4B-C3B	-3.59	96.72	104.88
2	A	500	COA	O4B-C4B-C3B	-3.55	96.80	104.88
2	A	500	COA	C4A-C5A-N7A	3.51	112.53	109.52
2	B	501	COA	C4A-C5A-N7A	3.44	112.47	109.52
2	B	501	COA	O9P-C9P-CAP	-3.40	114.27	120.48
2	A	500	COA	O9P-C9P-CAP	-3.39	114.29	120.48
2	A	500	COA	C2A-N1A-C6A	3.20	124.55	118.77
2	B	501	COA	C2A-N1A-C6A	3.17	124.49	118.77
2	A	500	COA	C3P-N4P-C5P	-3.15	116.43	122.84
2	A	500	COA	C7P-N8P-C9P	-3.13	116.14	122.57
2	A	500	COA	C3P-C2P-S1P	-3.06	105.47	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	COA	C3P-N4P-C5P	-3.02	116.69	122.84
2	B	501	COA	CDP-CBP-CAP	2.96	113.96	108.82
2	B	501	COA	C7P-N8P-C9P	-2.96	116.50	122.57
2	B	501	COA	C3P-C2P-S1P	-2.91	105.87	113.50
2	B	501	COA	O3B-P3B-O7A	-2.88	98.75	106.79
2	A	500	COA	CDP-CBP-CAP	2.83	113.73	108.82
2	B	501	COA	OAP-CAP-C9P	-2.82	103.50	110.76
2	A	500	COA	OAP-CAP-C9P	-2.80	103.54	110.76
2	B	501	COA	P1A-O5B-C5B	2.79	142.06	122.03
2	A	500	COA	P1A-O5B-C5B	2.72	141.59	122.03
2	A	500	COA	O3B-P3B-O7A	-2.72	99.20	106.79
2	A	500	COA	P2A-O3A-P1A	2.71	139.63	131.68
2	B	501	COA	P2A-O3A-P1A	2.59	139.28	131.68
2	A	500	COA	C2P-C3P-N4P	2.51	118.07	112.45
2	B	501	COA	O3A-P2A-O6A	2.28	113.59	103.41
2	A	500	COA	C8A-N9A-C1B	2.27	130.85	126.38
2	A	500	COA	O3A-P2A-O6A	2.25	113.48	103.41
2	B	501	COA	C8A-N9A-C1B	2.22	130.75	126.38
2	B	501	COA	O9A-P3B-O3B	2.13	113.23	107.09
2	A	500	COA	C6P-C5P-N4P	2.12	120.36	116.50
2	B	501	COA	O6A-CCP-CBP	-2.12	107.03	110.57
2	B	501	COA	C3B-C2B-C1B	-2.11	94.95	99.98
2	A	500	COA	C3B-C2B-C1B	-2.10	94.98	99.98
2	B	501	COA	O6A-P2A-O4A	-2.10	101.13	109.37
2	A	500	COA	O9A-P3B-O3B	2.10	113.12	107.09
2	A	500	COA	O6A-P2A-O4A	-2.09	101.20	109.37
2	B	501	COA	O9P-C9P-N8P	2.05	127.22	123.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/406 (99%)	-0.03	7 (1%) 67 67	7, 12, 24, 34	0
1	B	395/406 (97%)	-0.01	18 (4%) 31 30	6, 11, 27, 39	0
All	All	800/812 (98%)	-0.02	25 (3%) 47 45	6, 12, 26, 39	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	4.1
1	B	405	LEU	3.7
1	B	11	LEU	3.0
1	B	13	LEU	3.0
1	B	15	GLU	3.0
1	B	219	LEU	3.0
1	B	216	GLU	2.9
1	B	217	THR	2.8
1	B	14	MET	2.7
1	A	243	ILE	2.7
1	B	12	PRO	2.6
1	B	282	LYS	2.6
1	B	265	ASP	2.4
1	A	405	LEU	2.3
1	A	219	LEU	2.2
1	B	64	GLU	2.2
1	A	280	LEU	2.2
1	B	225	ILE	2.2
1	B	74	LYS	2.2
1	B	309	GLU	2.2
1	B	67	LYS	2.2
1	B	243	ILE	2.1
1	B	68	LYS	2.1
1	A	216	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	265	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	A	177	8/9	0.10	0.69	9,10,13,16	0
1	CSD	B	177	8/9	0.09	-0.03	9,10,12,16	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	COA	B	501	48/48	0.15	0.33	18,24,39,41	0
2	COA	A	500	48/48	0.13	0.20	17,22,34,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.