



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 AM GMT

PDB ID : 2B4D  
Title : SSAT+COA+SP- SP disordered  
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Deposited on : 2005-09-23  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

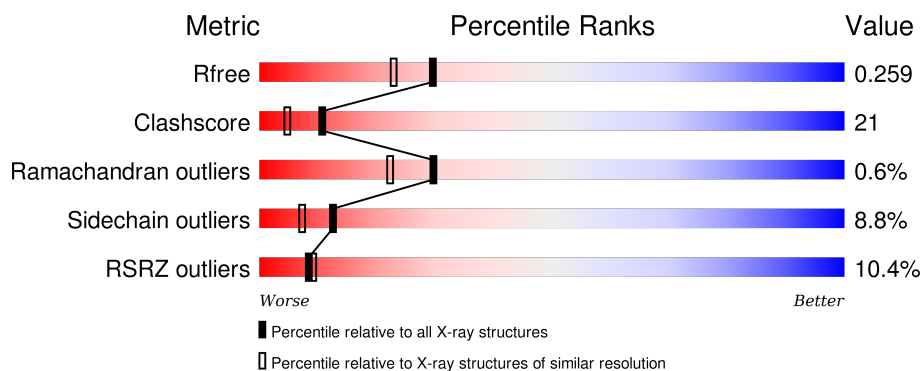
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	171	<div> <div>9%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
2	B	171	<div> <div>11%</div> <div>61%</div> <div>31%</div> <div>8%</div> <div>•</div> </div>

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	COA	A	201	X	-	-	-
3	COA	B	200	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2976 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.

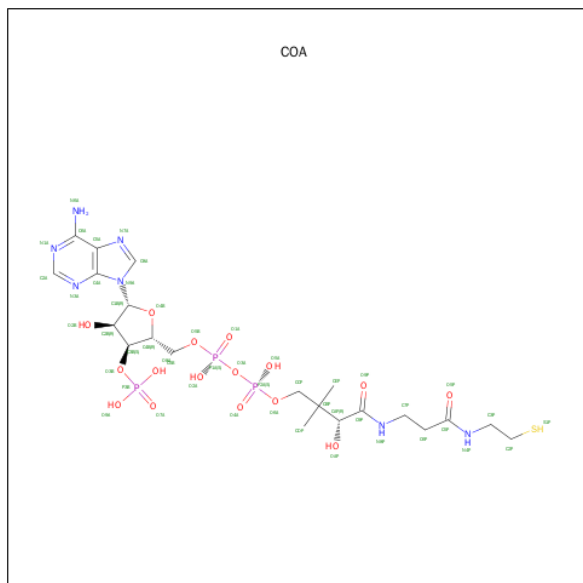
- Molecule 1 is a protein called Diamine acetyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	Se	0	0	0
			1401	910	224	257	4	6			

- Molecule 2 is a protein called Diamine acetyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	Se	3	0	0
			1404	912	224	258	4	6			

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	17	0
			48	21	7	16	3	1		
3	A	1	Total	C	N	O	P	S	27	0
			48	21	7	16	3	1		

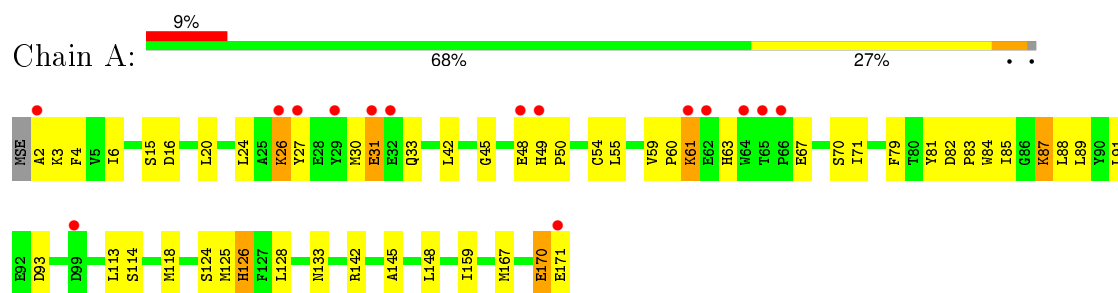
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total 41	O 41	0	0
4	B	34	Total 34	O 34	0	0

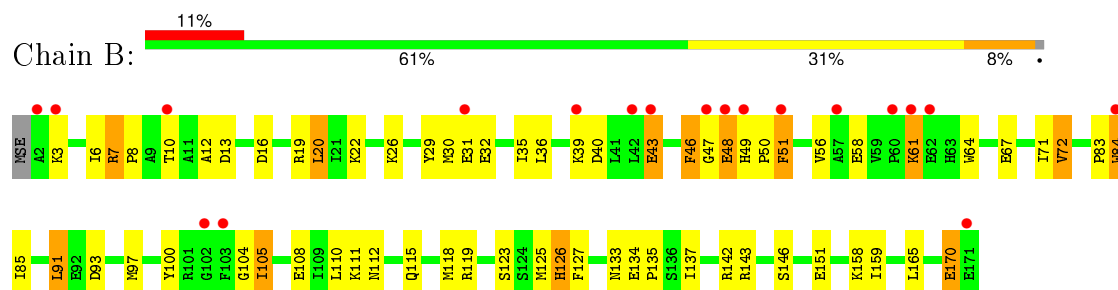
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Diamine acetyltransferase 1



#### • Molecule 2: Diamine acetyltransferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.00Å 74.00Å 64.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 19.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 96.3 (19.76-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.67 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , (Not available) 0.222 , 0.259	Depositor DCC
$R_{free}$ test set	1127 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.2	EDS
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 22575 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.65	1/1434 (0.1%)	0.76	0/1925
2	B	0.61	0/1424	0.78	0/1911
All	All	0.63	1/2858 (0.0%)	0.77	0/3836

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	CYS	CB-SG	-6.70	1.70	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	29	TYR	Sidechain

### 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	1401	0	1354	53	0
2	B	1404	0	1355	77	0
3	A	48	0	32	2	0
3	B	48	0	31	2	0
4	A	41	0	0	7	0
4	B	34	0	0	2	0
All	All	2976	0	2772	118	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 21.

All (118) 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:19:ARG:HH12	2:B:97:MSE:HE2	1.08	1.09
1:A:6:ILE:HG22	4:A:216:HOH:O	1.56	1.05
1:A:91:LEU:HB2	1:A:125:MSE:HE2	1.42	1.02
2:B:19:ARG:HH12	2:B:97:MSE:CE	1.71	1.01
1:A:55:LEU:HD22	4:A:216:HOH:O	1.63	0.98
2:B:72:VAL:HA	2:B:97:MSE:HE3	1.45	0.98
1:A:30:MSE:HG3	1:A:33:GLN:HG3	1.50	0.91
1:A:124:SER:OG	4:A:239:HOH:O	1.89	0.89
1:A:48:GLU:CD	1:A:48:GLU:H	1.73	0.89
1:A:113:LEU:HD13	1:A:125:MSE:HE1	1.56	0.88
1:A:170:GLU:HA	1:A:170:GLU:OE1	1.73	0.86
2:B:19:ARG:NH1	2:B:97:MSE:HE2	1.92	0.83
1:A:170:GLU:HG3	4:A:242:HOH:O	1.79	0.82
1:A:26:LYS:HB3	1:A:31:GLU:HG3	1.58	0.82
2:B:71:ILE:H	2:B:71:ILE:HD12	1.44	0.81
1:A:81:TYR:OH	2:B:36:LEU:HD13	1.85	0.77
2:B:71:ILE:O	2:B:97:MSE:HE3	1.88	0.73
2:B:118:MSE:HA	2:B:118:MSE:HE2	1.73	0.70
2:B:71:ILE:N	2:B:71:ILE:HD12	2.06	0.69
1:A:126:HIS:HD2	4:B:208:HOH:O	1.75	0.69
2:B:83:PRO:HG2	2:B:84:TRP:CE3	2.31	0.66
3:A:201:COA:O8A	3:A:201:COA:H4B	1.97	0.65
4:A:210:HOH:O	2:B:126:HIS:HD2	1.79	0.64
2:B:105:ILE:HD12	2:B:105:ILE:N	2.13	0.62
2:B:61:LYS:HE2	2:B:64:TRP:CZ2	2.34	0.62
4:A:239:HOH:O	2:B:159:ILE:N	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HE3	2:B:51:PHE:CE1	2.35	0.61
2:B:19:ARG:NH1	2:B:97:MSE:CE	2.55	0.61
1:A:26:LYS:HD3	1:A:26:LYS:O	2.01	0.60
2:B:170:GLU:OE1	2:B:170:GLU:HA	2.01	0.60
2:B:31:GLU:HG3	2:B:32:GLU:H	1.67	0.60
2:B:71:ILE:O	2:B:97:MSE:CE	2.50	0.59
1:A:59:VAL:HG22	1:A:70:SER:O	2.02	0.59
2:B:6:ILE:HG22	2:B:112:ASN:HD22	1.67	0.59
1:A:20:LEU:HD11	1:A:71:ILE:HG22	1.83	0.59
2:B:72:VAL:O	2:B:97:MSE:HG3	2.04	0.58
2:B:105:ILE:CD1	2:B:105:ILE:N	2.67	0.58
2:B:85:ILE:HD12	2:B:123:SER:OG	2.05	0.57
1:A:48:GLU:CD	1:A:48:GLU:N	2.53	0.56
1:A:87:LYS:HE3	2:B:51:PHE:CZ	2.42	0.55
1:A:170:GLU:HB2	2:B:111:LYS:NZ	2.22	0.55
2:B:142:ARG:NH1	3:B:200:COA:O8A	2.38	0.55
1:A:142:ARG:NH1	3:A:201:COA:O9A	2.40	0.54
2:B:71:ILE:H	2:B:71:ILE:CD1	2.17	0.54
2:B:133:ASN:O	2:B:137:ILE:HG13	2.07	0.54
2:B:146:SER:HB2	2:B:151:GLU:OE2	2.08	0.54
1:A:49:HIS:CE1	2:B:49:HIS:HD2	2.26	0.53
2:B:84:TRP:HE3	2:B:84:TRP:N	2.06	0.53
1:A:79:PHE:CD1	1:A:87:LYS:HE2	2.43	0.53
2:B:31:GLU:HG3	2:B:32:GLU:N	2.24	0.53
1:A:159:ILE:HD12	2:B:125:MSE:HE2	1.89	0.53
1:A:26:LYS:HB3	1:A:31:GLU:CG	2.36	0.52
2:B:36:LEU:HD12	2:B:40:ASP:HB2	1.90	0.52
1:A:79:PHE:HB3	1:A:87:LYS:CE	2.39	0.52
2:B:39:LYS:O	2:B:43:GLU:HG3	2.10	0.51
2:B:115:GLN:O	2:B:119:ARG:HD3	2.11	0.50
1:A:93:ASP:OD1	2:B:83:PRO:HG3	2.11	0.49
2:B:16:ASP:CG	2:B:71:ILE:HD13	2.33	0.49
1:A:113:LEU:HD13	1:A:125:MSE:CE	2.36	0.49
4:A:239:HOH:O	2:B:158:LYS:HB2	2.12	0.49
2:B:118:MSE:HE2	2:B:118:MSE:CA	2.42	0.49
2:B:47:GLY:O	2:B:48:GLU:HB2	2.12	0.49
2:B:39:LYS:NZ	2:B:39:LYS:HB3	2.28	0.49
2:B:46:PHE:CD1	2:B:46:PHE:N	2.80	0.49
1:A:2:ALA:N	1:A:63:HIS:CE1	2.82	0.48
1:A:82:ASP:HB3	1:A:85:ILE:HB	1.96	0.48
1:A:61:LYS:HE3	1:A:61:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:HG2	2:B:8:PRO:O	2.15	0.47
2:B:125:MSE:HE3	2:B:127:PHE:CE2	2.50	0.47
2:B:134:GLU:N	2:B:135:PRO:CD	2.78	0.47
2:B:20:LEU:HD11	2:B:97:MSE:HE2	1.98	0.46
1:A:84:TRP:CD1	2:B:30:MSE:HE2	2.50	0.46
1:A:59:VAL:HB	1:A:60:PRO:HD2	1.98	0.46
2:B:47:GLY:O	2:B:48:GLU:CB	2.63	0.46
1:A:88:LEU:HD22	1:A:124:SER:HB3	1.98	0.45
2:B:22:LYS:O	2:B:26:ALY:HG2	2.17	0.45
2:B:100:TYR:CD1	2:B:100:TYR:N	2.85	0.45
1:A:145:ALA:HA	2:B:158:LYS:O	2.16	0.45
1:A:170:GLU:CA	1:A:170:GLU:OE1	2.54	0.45
2:B:10:THR:HG23	2:B:12:ALA:H	1.81	0.45
1:A:167:MSE:O	2:B:111:LYS:HG3	2.17	0.44
1:A:3:LYS:HG2	1:A:4:PHE:N	2.32	0.44
2:B:105:ILE:CD1	2:B:105:ILE:H	2.29	0.44
2:B:61:LYS:HE2	2:B:64:TRP:CH2	2.52	0.44
1:A:83:PRO:HG3	2:B:93:ASP:OD2	2.17	0.44
2:B:84:TRP:CE3	2:B:84:TRP:N	2.86	0.44
2:B:16:ASP:OD2	2:B:19:ARG:NH2	2.41	0.43
1:A:167:MSE:HA	1:A:170:GLU:HG2	2.00	0.43
1:A:85:ILE:CG2	1:A:88:LEU:HD21	2.49	0.42
2:B:126:HIS:HE1	4:B:224:HOH:O	2.01	0.42
2:B:143:ARG:HH11	2:B:143:ARG:HG3	1.84	0.42
2:B:56:VAL:HB	2:B:71:ILE:HG23	2.01	0.42
1:A:2:ALA:N	1:A:63:HIS:NE2	2.67	0.42
1:A:83:PRO:O	2:B:35:ILE:CD1	2.68	0.42
2:B:143:ARG:NH1	2:B:143:ARG:HG3	2.34	0.42
2:B:6:ILE:HD13	2:B:108:GLU:HG2	2.02	0.42
2:B:7:ARG:HH21	2:B:58:GLU:CD	2.23	0.42
1:A:170:GLU:HB2	2:B:111:LYS:HZ2	1.84	0.42
1:A:61:LYS:N	1:A:61:LYS:HD3	2.34	0.42
2:B:10:THR:N	2:B:13:ASP:OD1	2.46	0.42
1:A:24:LEU:O	1:A:27:TYR:HB3	2.20	0.42
1:A:89:LEU:O	1:A:125:MSE:HA	2.20	0.41
1:A:89:LEU:HD22	1:A:125:MSE:HE3	2.01	0.41
1:A:79:PHE:HB3	1:A:87:LYS:HE2	2.02	0.41
2:B:170:GLU:CA	2:B:170:GLU:OE1	2.68	0.41
2:B:104:GLY:HA2	3:B:200:COA:O2A	2.20	0.41
1:A:114:SER:O	1:A:118:MSE:HG2	2.19	0.41
2:B:72:VAL:HG21	2:B:100:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:LEU:HB3	2:B:127:PHE:HB3	2.02	0.41
2:B:72:VAL:HG21	2:B:100:TYR:CE2	2.55	0.41
2:B:83:PRO:C	2:B:84:TRP:HE3	2.23	0.41
1:A:4:PHE:C	1:A:4:PHE:CD1	2.94	0.41
1:A:45:GLY:O	1:A:50:PRO:HB3	2.21	0.41
2:B:49:HIS:N	2:B:50:PRO:CD	2.84	0.41
2:B:165:LEU:HD23	2:B:165:LEU:HA	1.88	0.41
1:A:42:LEU:C	1:A:42:LEU:HD13	2.42	0.40
2:B:61:LYS:H	2:B:61:LYS:HD2	1.86	0.40
1:A:16:ASP:CB	1:A:71:ILE:HD12	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	168/171 (98%)	166 (99%)	2 (1%)	0	100	100
2	B	167/171 (98%)	160 (96%)	5 (3%)	2 (1%)	16	8
All	All	335/342 (98%)	326 (97%)	7 (2%)	2 (1%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	48	GLU
2	B	43	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/143 (104%)	137 (92%)	12 (8%)	15	9
2	B	148/142 (104%)	134 (90%)	14 (10%)	11	6
All	All	297/285 (104%)	271 (91%)	26 (9%)	12	7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	26	LYS
1	A	31	GLU
1	A	61	LYS
1	A	67	GLU
1	A	87	LYS
1	A	126	HIS
1	A	128	LEU
1	A	133	ASN
1	A	148	LEU
1	A	170	GLU
1	A	171	GLU
2	B	3	LYS
2	B	7	ARG
2	B	20	LEU
2	B	46	PHE
2	B	51	PHE
2	B	61	LYS
2	B	67	GLU
2	B	72	VAL
2	B	84	TRP
2	B	91	LEU
2	B	105	ILE
2	B	110	LEU
2	B	126	HIS
2	B	170	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS

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Mol	Chain	Res	Type
1	A	133	ASN
2	B	49	HIS
2	B	112	ASN
2	B	126	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ALY	B	26	2	10,11,12	1.94	3 (30%)	10,12,14	3.34	1 (10%)

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	ALY	B	26	2	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	ALY	CH-NZ	3.09	1.41	1.33
2	B	26	ALY	CE-NZ	3.20	1.53	1.46
2	B	26	ALY	OH-CH	3.45	1.31	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	ALY	CE-NZ-CH	10.29	139.19	122.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	26	ALY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	COA	A	201	-	40,50,50	1.63	6 (15%)	50,75,75	2.65	10 (20%)
3	COA	B	200	-	40,50,50	1.80	5 (12%)	50,75,75	2.19	10 (20%)

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	201	-	1/1/11/13	1/44/64/64	0/3/3/3
3	COA	B	200	-	1/1/11/13	0/44/64/64	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	COA	C7P-N8P	-5.89	1.32	1.46
3	A	201	COA	C7P-N8P	-4.95	1.34	1.46
3	B	200	COA	C7P-C6P	-3.73	1.39	1.51
3	A	201	COA	C7P-C6P	-3.44	1.40	1.51
3	B	200	COA	O4B-C4B	-3.39	1.37	1.45
3	A	201	COA	C2P-S1P	2.19	1.88	1.80
3	A	201	COA	P3B-O3B	2.24	1.66	1.60
3	B	200	COA	P3B-O7A	2.93	1.60	1.51
3	A	201	COA	P3B-O7A	3.01	1.61	1.51
3	A	201	COA	O4B-C1B	4.56	1.47	1.41
3	B	200	COA	O4B-C1B	5.94	1.48	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	COA	N3A-C2A-N1A	-10.83	120.60	128.89
3	B	200	COA	N3A-C2A-N1A	-10.81	120.62	128.89
3	A	201	COA	CDP-CBP-CCP	-7.59	98.66	108.50
3	A	201	COA	CEP-CBP-CCP	-5.79	100.99	108.50
3	B	200	COA	P2A-O3A-P1A	-3.69	122.37	132.73
3	B	200	COA	C4B-O4B-C1B	-3.30	106.10	109.72
3	B	200	COA	C2B-C1B-N9A	-3.17	109.45	114.29
3	A	201	COA	P2A-O3A-P1A	-3.09	124.06	132.73
3	B	200	COA	C2B-C3B-C4B	-2.81	98.01	103.29
3	B	200	COA	O4B-C1B-N9A	2.24	112.79	108.10
3	A	201	COA	CEP-CBP-CAP	2.27	113.50	109.34
3	A	201	COA	O4B-C1B-N9A	2.30	112.91	108.10
3	A	201	COA	O9A-P3B-O8A	2.78	117.95	107.38
3	B	200	COA	O9A-P3B-O8A	2.92	118.50	107.38
3	B	200	COA	C5B-C4B-C3B	3.10	125.48	114.31
3	B	200	COA	C6P-C7P-N8P	3.49	119.53	111.88
3	B	200	COA	O4B-C4B-C5B	3.56	122.05	109.32
3	A	201	COA	CEP-CBP-CDP	4.62	118.56	109.28
3	A	201	COA	CDP-CBP-CAP	5.25	118.94	109.34
3	A	201	COA	C6P-C7P-N8P	5.27	123.45	111.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	201	COA	CAP
3	B	200	COA	CAP

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	COA	P3B-O3B-C3B-C4B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	COA	2	0
3	B	200	COA	2	0

## 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, 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	164/171 (95%)	0.41	15 (9%) 11 12	9, 23, 43, 56	0
2	B	163/171 (95%)	0.74	19 (11%) 6 7	10, 23, 48, 58	0
All	All	327/342 (95%)	0.58	34 (10%) 8 9	9, 23, 48, 58	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ALA	12.3
2	B	49	HIS	5.9
2	B	47	GLY	5.6
1	A	29	TYR	5.5
2	B	48	GLU	5.5
1	A	171	GLU	4.3
2	B	51	PHE	3.9
1	A	66	PRO	3.8
1	A	32	GLU	3.7
1	A	49	HIS	3.7
1	A	27	TYR	3.2
2	B	171	GLU	3.2
1	A	64	TRP	3.0
2	B	62	GLU	3.0
2	B	84	TRP	3.0
1	A	31	GLU	2.9
1	A	65	THR	2.9
2	B	60	PRO	2.9
2	B	61	LYS	2.8
2	B	3	LYS	2.8
2	B	42	LEU	2.5
2	B	31	GLU	2.5
2	B	39	LYS	2.5
1	A	2	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	48	GLU	2.5
2	B	10	THR	2.5
2	B	43	GLU	2.4
2	B	102	GLY	2.4
1	A	26	LYS	2.3
1	A	62	GLU	2.2
1	A	61	LYS	2.1
2	B	103	PHE	2.1
1	A	99	ASP	2.1
2	B	57	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALY	B	26	12/13	0.87	0.17	-	18,28,40,40	3

## 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	COA	B	200	48/48	0.92	0.19	0.64	18,34,41,51	17
3	COA	A	201	48/48	0.90	0.18	0.52	34,44,53,55	27

## 6.5 Other polymers [i](#)

There are no such residues in this entry.