



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:09 PM GMT

PDB ID : 3N0S  
Title : Crystal structure of BA2930 mutant (H183A) in complex with AcCoA  
Authors : Klimecka, M.M.; Chruszcz, M.; Porebski, P.J.; Cymborowski, M.; Anderson, W.F.; Minor, W.  
Deposited on : 2010-05-14  
Resolution : 2.15 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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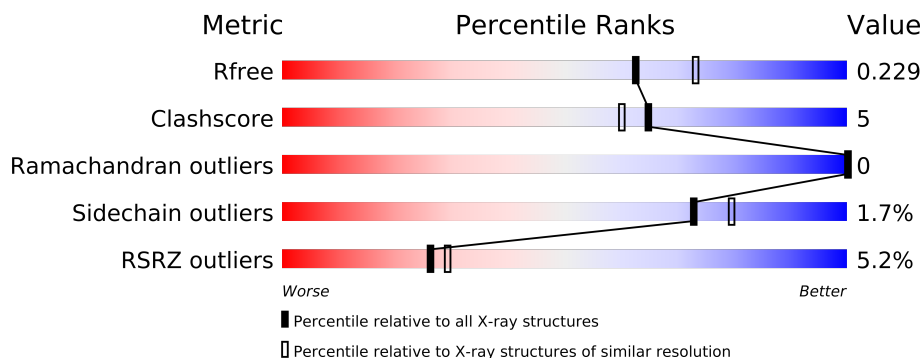
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.15 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	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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	268	
1	B	268	
1	C	268	
1	D	268	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	D	267	-	X
4	EPE	B	268	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8881 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.

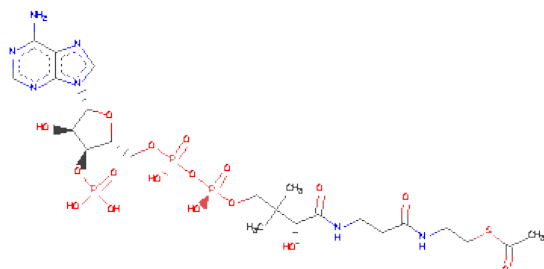
- Molecule 1 is a protein called Aminoglycoside N3-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	Se	0	0	0
			2063	1306	351	394	3	9			
1	D	265	Total	C	N	O	S	Se	0	0	0
			2070	1311	353	394	3	9			
1	C	264	Total	C	N	O	S	Se	0	1	0
			2063	1307	352	392	3	9			
1	B	266	Total	C	N	O	S	Se	0	2	0
			2090	1326	356	396	3	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81P86
A	-1	ASN	-	EXPRESSION TAG	UNP Q81P86
A	0	ALA	-	EXPRESSION TAG	UNP Q81P86
A	183	ALA	HIS	ENGINEERED MUTATION	UNP Q81P86
D	-2	SER	-	EXPRESSION TAG	UNP Q81P86
D	-1	ASN	-	EXPRESSION TAG	UNP Q81P86
D	0	ALA	-	EXPRESSION TAG	UNP Q81P86
D	183	ALA	HIS	ENGINEERED MUTATION	UNP Q81P86
C	-2	SER	-	EXPRESSION TAG	UNP Q81P86
C	-1	ASN	-	EXPRESSION TAG	UNP Q81P86
C	0	ALA	-	EXPRESSION TAG	UNP Q81P86
C	183	ALA	HIS	ENGINEERED MUTATION	UNP Q81P86
B	-2	SER	-	EXPRESSION TAG	UNP Q81P86
B	-1	ASN	-	EXPRESSION TAG	UNP Q81P86
B	0	ALA	-	EXPRESSION TAG	UNP Q81P86
B	183	ALA	HIS	ENGINEERED MUTATION	UNP Q81P86

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).

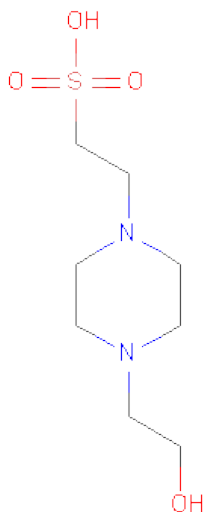


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

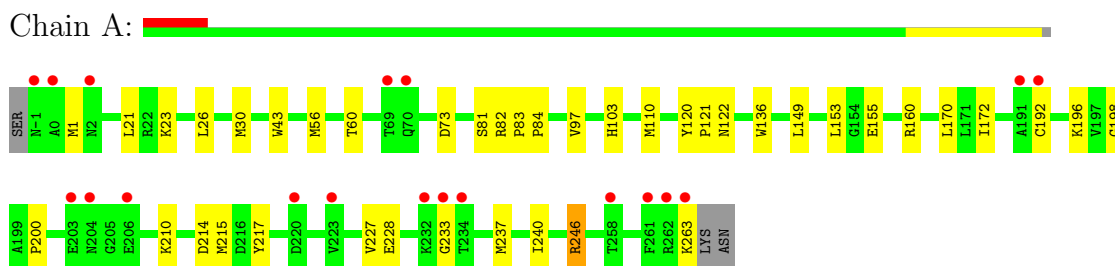
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	D	100	Total	O	0	0
			100	100		
5	C	81	Total	O	0	0
			81	81		
5	B	117	Total	O	0	0
			117	117		

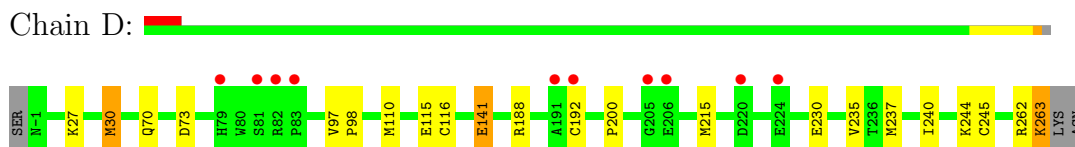
### 3 Residue-property plots

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.

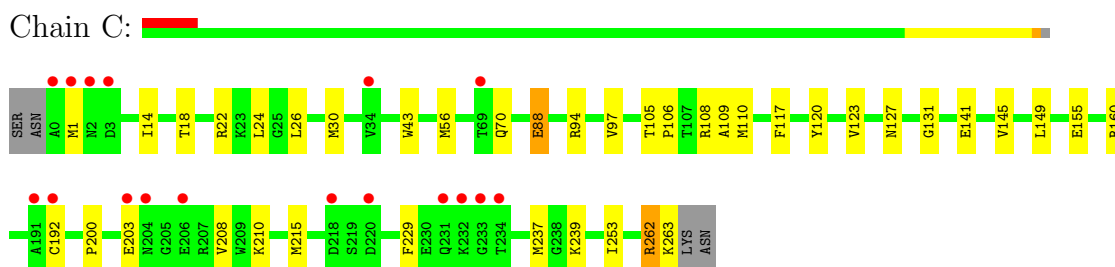
- Molecule 1: Aminoglycoside N3-acetyltransferase



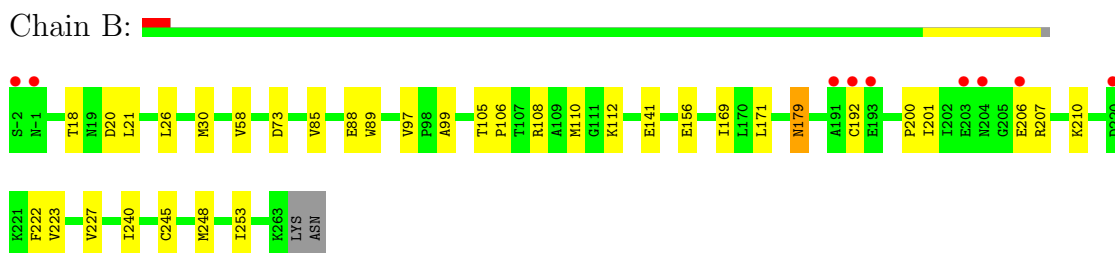
- Molecule 1: Aminoglycoside N3-acetyltransferase



- Molecule 1: Aminoglycoside N3-acetyltransferase



- Molecule 1: Aminoglycoside N3-acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.04Å 109.44Å 74.05Å 90.00° 111.86° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 30.24 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.15) 98.7 (30.24-2.14)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.173 , 0.228 0.178 , 0.229	Depositor DCC
$R_{free}$ test set	2931 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 19.4	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 57858 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.1708e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MG, EPE, ACO

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	0.87	0/2098	0.80	1/2833 (0.0%)
1	B	0.94	1/2126 (0.0%)	0.86	1/2869 (0.0%)
1	C	0.91	0/2098	0.84	4/2832 (0.1%)
1	D	0.97	4/2105 (0.2%)	0.84	1/2840 (0.0%)
All	All	0.92	5/8427 (0.1%)	0.84	7/11374 (0.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	CYS	CB-SG	8.53	1.96	1.82
1	D	116	CYS	CB-SG	-6.10	1.71	1.82
1	D	141	GLU	CG-CD	5.29	1.59	1.51
1	D	115	GLU	CG-CD	5.22	1.59	1.51
1	D	70	GLN	C-O	5.11	1.33	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	30	MSE	CG-SE-CE	-5.96	85.80	98.90
1	C	94	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	108	ARG	NE-CZ-NH2	5.33	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	MSE	CG-SE-CE	-5.17	87.53	98.90
1	C	24	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	24	LEU	CB-CG-CD2	-5.06	102.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	GLY	Peptide

## 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	2063	0	2046	28	0
1	B	2090	0	2083	23	0
1	C	2063	0	2052	26	0
1	D	2070	0	2066	12	0
2	A	51	0	34	1	0
2	B	51	0	34	1	0
2	C	51	0	34	1	0
2	D	51	0	34	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	15	0	17	1	0
5	A	76	0	0	0	0
5	B	117	0	0	1	0
5	C	81	0	0	1	0
5	D	100	0	0	1	0
All	All	8881	0	8400	89	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 5.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:248:MSE:HE3	1:B:253:ILE:HG21	1.35	1.07
1:A:110:MSE:HE1	2:A:266:ACO:H22	1.38	1.02
1:B:110:MSE:HE1	2:B:266:ACO:H22	1.45	0.99
1:D:110:MSE:HE1	2:D:266:ACO:H22	1.57	0.87
1:B:179:ASN:OD1	1:B:248:MSE:HE1	1.78	0.83
1:C:110:MSE:HE1	2:C:266:ACO:H22	1.60	0.83
1:A:56:MSE:HE3	1:A:136:TRP:CE2	2.18	0.78
1:C:97:VAL:HG13	1:C:200:PRO:HG3	1.66	0.78
1:A:192:CYS:HB2	1:A:215:MSE:SE	2.34	0.77
1:A:56:MSE:HE3	1:A:136:TRP:NE1	2.00	0.76
1:D:97:VAL:HG13	1:D:200:PRO:HG3	1.71	0.73
1:B:201:ILE:HD11	1:B:210:LYS:HD3	1.74	0.69
1:C:1:MSE:HE1	1:C:43:TRP:HD1	1.59	0.67
1:B:248:MSE:HE3	1:B:253:ILE:CG2	2.20	0.66
1:B:179:ASN:OD1	1:B:248:MSE:CE	2.44	0.65
1:C:155:GLU:OE1	1:C:160:ARG:NH1	2.28	0.65
1:C:26:LEU:HD12	1:C:30:MSE:SE	2.48	0.64
1:D:237:MSE:HE3	1:D:244:LYS:CE	2.30	0.62
1:A:56:MSE:CE	1:A:136:TRP:CE2	2.82	0.62
1:D:240:ILE:HG12	1:D:245:CYS:SG	2.40	0.61
1:D:262:ARG:HA	1:D:263:LYS:HB2	1.83	0.60
1:A:1:MSE:HE1	1:A:43:TRP:HD1	1.67	0.59
1:A:153:LEU:HD12	1:A:217:TYR:CD2	2.37	0.59
1:A:56:MSE:CE	1:A:136:TRP:NE1	2.66	0.57
1:C:192:CYS:O	1:C:215:MSE:HE2	2.07	0.55
1:A:97:VAL:HG13	1:A:200:PRO:HG3	1.89	0.55
1:C:117:PHE:O	1:C:123:VAL:HG21	2.07	0.55
1:C:239:LYS:NZ	5:C:370:HOH:O	2.40	0.54
1:B:21:LEU:HD22	1:B:26:LEU:HD22	1.90	0.54
1:A:26:LEU:HD12	1:A:30:MSE:HE1	1.90	0.53
1:A:215:MSE:HB3	1:A:217:TYR:CE1	2.43	0.53
1:B:88:GLU:HG2	1:B:88:GLU:O	2.09	0.53
1:A:149:LEU:HD21	1:A:210:LYS:HG2	1.91	0.53
1:A:21:LEU:HD23	1:A:240:ILE:HD11	1.91	0.52
1:C:127[B]:ASN:C	1:C:127[B]:ASN:OD1	2.49	0.51
1:B:73:ASP:OD1	1:B:108:ARG:HD2	2.10	0.51
4:B:268:EPE:N1	4:B:268:EPE:O1S	2.43	0.51
1:A:1:MSE:HE1	1:A:43:TRP:CD1	2.45	0.50
1:C:1:MSE:HE1	1:C:43:TRP:CD1	2.43	0.50
1:C:141:GLU:O	1:C:145:VAL:HG13	2.11	0.50
1:C:88:GLU:CD	1:C:88:GLU:H	2.14	0.50
1:B:248:MSE:CE	1:B:253:ILE:HG21	2.24	0.50
1:C:155:GLU:O	1:C:160:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:27:LYS:HB2	1:D:30:MSE:HE3	1.93	0.49
1:D:230:GLU:HG2	1:D:235:VAL:HG11	1.94	0.49
1:A:121:PRO:O	1:A:122:ASN:HB2	2.13	0.49
1:A:153:LEU:HD12	1:A:217:TYR:CE2	2.49	0.48
1:B:85:VAL:HB	1:B:89:TRP:CE3	2.50	0.47
1:B:88:GLU:CG	1:B:88:GLU:O	2.63	0.47
1:A:56:MSE:HE2	1:A:136:TRP:CZ2	2.50	0.46
1:B:156:GLU:OE1	1:B:156:GLU:HA	2.16	0.46
1:A:153:LEU:HB2	1:A:217:TYR:CZ	2.51	0.46
1:A:155:GLU:O	1:A:160:ARG:HG2	2.15	0.45
1:B:169:ILE:HD13	1:B:248:MSE:HE2	1.98	0.45
1:C:192:CYS:HB2	1:C:215:MSE:CG	2.47	0.45
1:D:188:ARG:NH2	5:D:320:HOH:O	2.48	0.45
1:C:18:THR:HG22	1:C:22:ARG:NH1	2.30	0.45
1:D:141:GLU:CD	1:D:141:GLU:H	2.20	0.45
1:C:56:MSE:HE1	1:C:120:TYR:CD2	2.52	0.45
1:D:192:CYS:HB2	1:D:215:MSE:SE	2.67	0.45
1:B:20:ASP:HB3	1:B:240:ILE:HD13	1.99	0.45
1:A:227:VAL:HG12	1:A:228:GLU:N	2.32	0.45
1:A:81:SER:O	1:A:84:PRO:HD3	2.16	0.45
1:B:222:PHE:CD1	1:B:222:PHE:N	2.85	0.44
1:B:18:THR:HG23	1:B:58:VAL:CG2	2.48	0.44
1:D:98:PRO:HG3	1:C:14:ILE:HD11	2.00	0.44
1:A:237:MSE:HE3	1:A:246:ARG:CG	2.47	0.44
1:A:82:ARG:HA	1:A:83:PRO:HA	1.81	0.43
1:B:105:THR:HA	1:B:106:PRO:HD3	1.90	0.43
1:A:170:LEU:HD21	1:A:172:ILE:HD11	2.01	0.43
1:B:223:VAL:O	1:B:227:VAL:HG23	2.18	0.43
1:C:109:ALA:O	1:C:110:MSE:HE2	2.18	0.43
1:B:97:VAL:HG13	1:B:200:PRO:HG3	2.00	0.43
1:B:112:LYS:HD2	5:B:314:HOH:O	2.18	0.42
1:A:56:MSE:HE1	1:A:120:TYR:CE2	2.54	0.42
1:C:18:THR:CG2	1:C:22:ARG:NH1	2.82	0.42
1:A:192:CYS:O	1:A:215:MSE:HE2	2.20	0.42
1:C:26:LEU:HD12	1:C:26:LEU:HA	1.95	0.42
1:B:171:LEU:O	1:B:245:CYS:HA	2.19	0.42
1:C:262:ARG:O	1:C:263:LYS:CB	2.67	0.42
1:D:262:ARG:HG3	1:D:262:ARG:O	2.19	0.42
1:C:149:LEU:HD21	1:C:210:LYS:HG2	2.02	0.41
1:A:56:MSE:HE3	1:A:136:TRP:CD1	2.55	0.41
1:A:198:GLY:HA2	1:A:210:LYS:O	2.21	0.41
1:C:237:MSE:HE3	1:C:237:MSE:HB3	1.98	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:70:GLN:HG2	1:C:131:GLY:HA2	2.02	0.41
1:B:99:ALA:HB2	1:B:207:ARG:HG3	2.02	0.41
1:C:229:PHE:CD2	1:C:253:ILE:HD13	2.56	0.41
1:C:105:THR:HA	1:C:106:PRO:HD3	1.91	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	263/268 (98%)	255 (97%)	8 (3%)	0	100	100
1	B	266/268 (99%)	258 (97%)	8 (3%)	0	100	100
1	C	263/268 (98%)	253 (96%)	10 (4%)	0	100	100
1	D	263/268 (98%)	255 (97%)	8 (3%)	0	100	100
All	All	1055/1072 (98%)	1021 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	228/224 (102%)	221 (97%)	7 (3%)	52	54
1	B	232/224 (104%)	229 (99%)	3 (1%)	80	87
1	C	228/224 (102%)	224 (98%)	4 (2%)	71	77
1	D	230/224 (103%)	228 (99%)	2 (1%)	87	92
All	All	918/896 (102%)	902 (98%)	16 (2%)	73	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	60	THR
1	A	73	ASP
1	A	103	HIS
1	A	196	LYS
1	A	214	ASP
1	A	263	LYS
1	D	73	ASP
1	D	263	LYS
1	C	88	GLU
1	C	203	GLU
1	C	208	VAL
1	C	262	ARG
1	B	141	GLU
1	B	179	ASN
1	B	206	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
2	ACO	A	266	-	53,53,53	1.29	7 (13%)	79,79,79	1.75	16 (20%)
2	ACO	B	266	-	53,53,53	1.44	6 (11%)	79,79,79	1.82	16 (20%)
4	EPE	B	268	-	15,15,15	1.38	1 (6%)	20,20,20	0.93	1 (5%)
2	ACO	C	266	-	53,53,53	1.37	7 (13%)	79,79,79	1.95	17 (21%)
2	ACO	D	266	-	53,53,53	1.55	7 (13%)	79,79,79	2.05	20 (25%)

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	ACO	A	266	-	-	0/51/67/67	0/1/3/3
2	ACO	B	266	-	-	0/51/67/67	0/1/3/3
4	EPE	B	268	-	-	0/9/19/19	0/1/1/1
2	ACO	C	266	-	-	0/51/67/67	0/1/3/3
2	ACO	D	266	-	-	0/51/67/67	0/1/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	266	ACO	P2A-O3A	-4.62	1.51	1.59
2	B	266	ACO	P1A-O3A	-4.37	1.52	1.59
4	B	268	EPE	C10-S	4.32	1.84	1.77
2	A	266	ACO	C4A-N9A	-4.12	1.31	1.37
2	D	266	ACO	C4A-N9A	-4.09	1.31	1.37
2	C	266	ACO	O4B-C1B	3.85	1.47	1.41
2	D	266	ACO	CCP-CBP	3.65	1.58	1.52
2	C	266	ACO	C4A-N9A	-3.65	1.32	1.37
2	A	266	ACO	P2A-O3A	-3.42	1.53	1.59
2	C	266	ACO	P3B-O7A	3.40	1.62	1.51
2	D	266	ACO	C4A-N3A	-3.31	1.30	1.35
2	B	266	ACO	C4A-N9A	-3.31	1.32	1.37
2	B	266	ACO	CCP-CBP	3.30	1.58	1.52
2	C	266	ACO	P2A-O3A	-3.19	1.54	1.59
2	B	266	ACO	O4B-C1B	3.00	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	266	ACO	C8A-N9A	-2.87	1.32	1.36
2	D	266	ACO	CBP-CAP	-2.68	1.52	1.55
2	C	266	ACO	CBP-CAP	-2.67	1.52	1.55
2	A	266	ACO	CCP-CBP	2.57	1.56	1.52
2	C	266	ACO	CCP-CBP	2.49	1.56	1.52
2	D	266	ACO	O4B-C1B	2.38	1.45	1.41
2	A	266	ACO	C5A-N7A	-2.28	1.31	1.40
2	D	266	ACO	C5P-N4P	-2.27	1.27	1.33
2	A	266	ACO	C2B-C1B	-2.25	1.50	1.53
2	A	266	ACO	C8A-N9A	-2.15	1.33	1.36
2	A	266	ACO	CBP-CAP	-2.07	1.53	1.55
2	B	266	ACO	C5B-C4B	2.06	1.58	1.51
2	C	266	ACO	P2A-O5A	-2.06	1.45	1.55

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	266	ACO	N3A-C2A-N1A	-10.45	119.97	128.71
2	C	266	ACO	N3A-C2A-N1A	-9.61	120.68	128.71
2	B	266	ACO	N3A-C2A-N1A	-8.98	121.20	128.71
2	A	266	ACO	N3A-C2A-N1A	-8.11	121.93	128.71
2	C	266	ACO	O4B-C1B-N9A	-4.69	104.08	108.44
2	D	266	ACO	C8A-N9A-C4A	4.25	110.14	106.90
2	C	266	ACO	C8A-N9A-C4A	4.21	110.11	106.90
2	C	266	ACO	C4B-O4B-C1B	-3.93	105.48	109.75
2	D	266	ACO	N3A-C4A-N9A	3.88	132.44	125.43
2	A	266	ACO	O5A-P2A-O3A	3.76	122.97	105.14
2	C	266	ACO	O5A-P2A-O3A	3.75	122.93	105.14
2	A	266	ACO	N3A-C4A-N9A	3.74	132.19	125.43
2	C	266	ACO	N3A-C4A-N9A	3.69	132.09	125.43
2	B	266	ACO	N3A-C4A-N9A	3.60	131.93	125.43
2	D	266	ACO	O5A-P2A-O3A	3.47	121.59	105.14
2	B	266	ACO	C4A-C5A-N7A	-3.46	106.56	109.52
2	A	266	ACO	CBP-CAP-C9P	-3.43	109.40	112.73
2	D	266	ACO	C7P-C6P-C5P	-3.31	106.61	112.25
2	D	266	ACO	O6A-P2A-O4A	-3.30	96.47	109.37
2	A	266	ACO	C4A-C5A-N7A	-3.12	106.85	109.52
2	D	266	ACO	C3P-N4P-C5P	-3.11	116.51	122.84
2	A	266	ACO	C7P-C6P-C5P	-3.11	106.96	112.25
2	B	266	ACO	O2B-C2B-C1B	-3.10	101.86	111.23
2	D	266	ACO	C4A-C5A-N7A	-3.09	106.87	109.52
2	B	266	ACO	C1B-N9A-C4A	-3.07	121.33	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	ACO	O9A-P3B-O3B	3.06	115.91	107.09
2	C	266	ACO	C2P-C3P-N4P	-3.05	105.60	112.50
2	C	266	ACO	P2A-O3A-P1A	-3.05	122.74	131.68
2	D	266	ACO	C1B-N9A-C4A	-3.04	121.39	126.64
2	D	266	ACO	O9A-P3B-O3B	3.00	115.74	107.09
2	D	266	ACO	O8A-P3B-O3B	-3.00	98.47	107.09
2	D	266	ACO	O2B-C2B-C1B	-2.94	102.34	111.23
2	D	266	ACO	CCP-CBP-CAP	2.83	112.83	108.70
2	B	266	ACO	C8A-N9A-C4A	2.82	109.05	106.90
2	B	266	ACO	O4B-C1B-N9A	-2.78	105.85	108.44
2	B	266	ACO	O5A-P2A-O3A	2.74	118.13	105.14
2	D	266	ACO	N7A-C8A-N9A	-2.66	106.83	114.36
2	A	266	ACO	C2P-C3P-N4P	-2.65	106.52	112.50
2	C	266	ACO	CEP-CBP-CDP	2.62	112.81	109.08
2	B	266	ACO	C2P-C3P-N4P	-2.60	106.62	112.50
2	D	266	ACO	C3P-C2P-S1P	-2.59	103.04	111.04
2	D	266	ACO	CBP-CAP-C9P	-2.58	110.23	112.73
2	A	266	ACO	P2A-O3A-P1A	-2.55	124.20	131.68
2	C	266	ACO	C4A-C5A-N7A	-2.54	107.35	109.52
2	D	266	ACO	C5A-C4A-N3A	-2.52	120.22	125.70
2	C	266	ACO	CBP-CAP-C9P	-2.47	110.34	112.73
2	A	266	ACO	C5A-C4A-N3A	-2.46	120.33	125.70
2	A	266	ACO	C2A-N1A-C6A	2.46	123.22	118.77
2	A	266	ACO	O4B-C1B-N9A	-2.46	106.15	108.44
2	A	266	ACO	C2B-C1B-N9A	-2.43	107.03	113.27
2	B	266	ACO	O8A-P3B-O3B	-2.33	100.39	107.09
2	C	266	ACO	N7A-C8A-N9A	-2.32	107.81	114.36
2	D	266	ACO	C2A-N3A-C4A	2.30	120.57	114.01
2	D	266	ACO	C2P-C3P-N4P	-2.29	107.33	112.50
2	B	266	ACO	C5A-C4A-N3A	-2.28	120.73	125.70
2	A	266	ACO	C4B-O4B-C1B	-2.23	107.33	109.75
2	C	266	ACO	CDP-CBP-CCP	-2.23	105.55	108.76
2	A	266	ACO	C2P-S1P-C	-2.20	92.45	101.38
2	D	266	ACO	P2A-O3A-P1A	-2.18	125.29	131.68
2	C	266	ACO	O2B-C2B-C1B	-2.18	104.64	111.23
2	B	266	ACO	N7A-C8A-N9A	-2.17	108.23	114.36
2	B	266	ACO	C7P-N8P-C9P	-2.16	118.13	122.57
2	C	266	ACO	C1B-N9A-C4A	-2.16	122.90	126.64
2	C	266	ACO	O2A-P1A-O3A	2.16	115.38	105.14
2	B	266	ACO	C3P-C2P-S1P	-2.08	104.62	111.04
4	B	268	EPE	C5-C6-N1	2.07	114.69	110.61
2	A	266	ACO	O9A-P3B-O8A	2.04	115.56	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	ACO	C2A-N1A-C6A	2.03	122.44	118.77
2	C	266	ACO	C5A-C4A-N3A	-2.02	121.30	125.70
2	A	266	ACO	O3B-C3B-C2B	-2.01	103.66	111.54

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	265/268 (98%)	0.29	19 (7%) 15 18	4, 12, 30, 47	7 (2%)
1	B	266/268 (99%)	0.16	9 (3%) 43 47	4, 13, 30, 46	8 (3%)
1	C	264/268 (98%)	0.26	17 (6%) 19 22	3, 12, 30, 35	4 (1%)
1	D	265/268 (98%)	0.16	10 (3%) 38 42	4, 12, 29, 37	4 (1%)
All	All	1060/1072 (98%)	0.22	55 (5%) 26 29	3, 12, 30, 47	23 (2%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	ALA	4.0
1	D	82	ARG	4.0
1	C	191	ALA	3.7
1	A	233	GLY	3.6
1	B	191	ALA	3.6
1	B	-2	SER	3.5
1	A	-1	ASN	3.5
1	C	204	ASN	3.5
1	B	192	CYS	3.5
1	C	2	ASN	3.4
1	A	232	LYS	3.4
1	D	192	CYS	3.3
1	C	234	THR	3.3
1	B	204	ASN	3.3
1	D	220	ASP	3.3
1	A	204	ASN	3.2
1	D	83	PRO	3.2
1	C	192	CYS	3.1
1	A	234	THR	3.0
1	A	262	ARG	3.0
1	B	203	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	220	ASP	3.0
1	D	205	GLY	2.8
1	C	232	LYS	2.7
1	B	206	GLU	2.7
1	A	203	GLU	2.7
1	A	263	LYS	2.7
1	C	34	VAL	2.7
1	C	203	GLU	2.6
1	A	0	ALA	2.6
1	A	191	ALA	2.6
1	A	192	CYS	2.5
1	A	261	PHE	2.5
1	B	193	GLU	2.5
1	C	218	ASP	2.4
1	A	206	GLU	2.4
1	B	220	ASP	2.4
1	C	69	THR	2.3
1	D	79	HIS	2.3
1	C	206	GLU	2.3
1	A	69	THR	2.3
1	C	231	GLN	2.2
1	A	258	THR	2.2
1	C	3	ASP	2.2
1	A	2	ASN	2.1
1	D	81	SER	2.1
1	D	206	GLU	2.1
1	B	-1	ASN	2.1
1	D	224	GLU	2.1
1	A	220	ASP	2.1
1	A	70	GLN	2.0
1	C	0	ALA	2.0
1	C	1	MSE	2.0
1	A	223	VAL	2.0
1	C	233	GLY	2.0

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

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

### 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
4	EPE	B	268	15/15	0.25	2.94	64,68,82,82	0
3	MG	D	267	1/1	0.14	2.32	45,45,45,45	0
2	ACO	D	266	51/51	0.16	0.90	14,27,48,50	0
2	ACO	B	266	51/51	0.16	0.55	15,27,44,47	0
2	ACO	C	266	51/51	0.15	0.49	17,28,48,49	0
2	ACO	A	266	51/51	0.15	0.19	20,31,51,52	0
3	MG	B	267	1/1	0.12	-0.41	37,37,37,37	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.