



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YVK
Title : Crystal Structure of the Bacillus subtilis Acetyltransferase in complex with CoA, Northeast Structural Genomics Target SR237.
Authors : Forouhar, F.; Yong, W.; Xiao, R.; Ciano, M.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-02-15
Resolution : 3.01 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

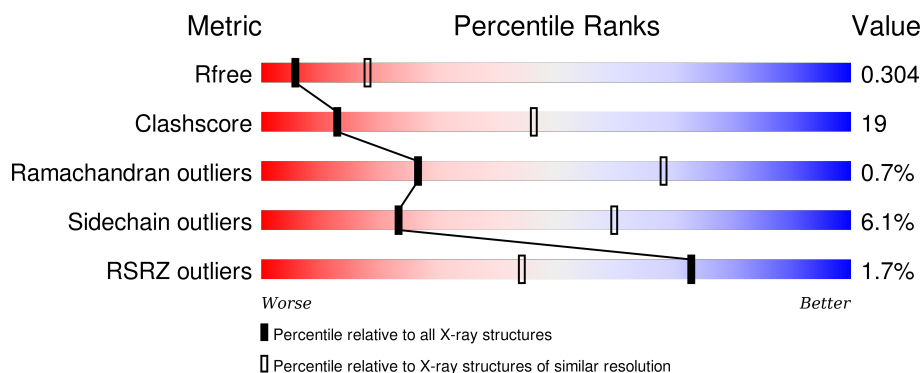
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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 ≥ 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	163	<div> <div> <div></div> <div>55%</div> <div>36%</div> <div>7%</div> </div> </div>
1	B	163	<div> <div>53%</div> <div>39%</div> <div>7%</div> </div>
1	C	163	<div> <div>4%</div> <div>53%</div> <div>38%</div> <div>7%</div> </div>
1	D	163	<div> <div>59%</div> <div>32%</div> <div>7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5076 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 hypothetical protein BSU33890.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	Se	0	0	0
			1221	778	202	237	3	1			
1	B	152	Total	C	N	O	S	Se	0	0	0
			1221	778	202	237	3	1			
1	C	152	Total	C	N	O	S	Se	0	0	0
			1221	778	202	237	3	1			
1	D	152	Total	C	N	O	S	Se	0	0	0
			1221	778	202	237	3	1			

There are 44 discrepancies between the modelled and reference sequences:

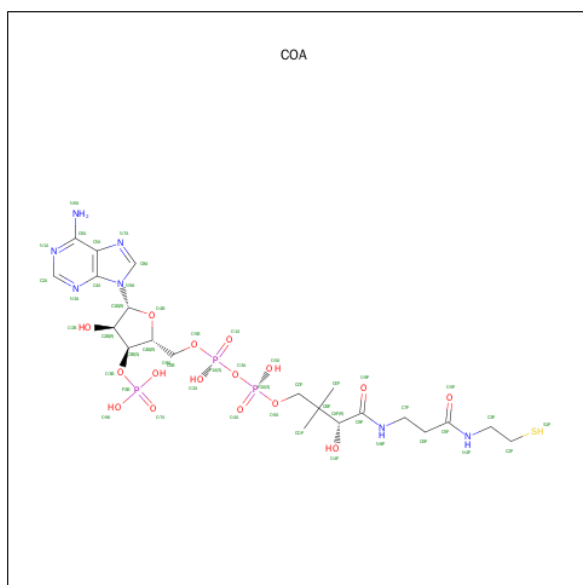
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O32248
A	3	MSE	MET	MODIFIED RESIDUE	UNP O32248
A	148	MSE	MET	MODIFIED RESIDUE	UNP O32248
A	156	LEU	-	EXPRESSION TAG	UNP O32248
A	157	GLU	-	EXPRESSION TAG	UNP O32248
A	158	HIS	-	EXPRESSION TAG	UNP O32248
A	159	HIS	-	EXPRESSION TAG	UNP O32248
A	160	HIS	-	EXPRESSION TAG	UNP O32248
A	161	HIS	-	EXPRESSION TAG	UNP O32248
A	162	HIS	-	EXPRESSION TAG	UNP O32248
A	163	HIS	-	EXPRESSION TAG	UNP O32248
B	1	MSE	MET	MODIFIED RESIDUE	UNP O32248
B	3	MSE	MET	MODIFIED RESIDUE	UNP O32248
B	148	MSE	MET	MODIFIED RESIDUE	UNP O32248
B	156	LEU	-	EXPRESSION TAG	UNP O32248
B	157	GLU	-	EXPRESSION TAG	UNP O32248
B	158	HIS	-	EXPRESSION TAG	UNP O32248
B	159	HIS	-	EXPRESSION TAG	UNP O32248
B	160	HIS	-	EXPRESSION TAG	UNP O32248
B	161	HIS	-	EXPRESSION TAG	UNP O32248
B	162	HIS	-	EXPRESSION TAG	UNP O32248

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Chain	Residue	Modelled	Actual	Comment	Reference
B	163	HIS	-	EXPRESSION TAG	UNP O32248
C	1	MSE	MET	MODIFIED RESIDUE	UNP O32248
C	3	MSE	MET	MODIFIED RESIDUE	UNP O32248
C	148	MSE	MET	MODIFIED RESIDUE	UNP O32248
C	156	LEU	-	EXPRESSION TAG	UNP O32248
C	157	GLU	-	EXPRESSION TAG	UNP O32248
C	158	HIS	-	EXPRESSION TAG	UNP O32248
C	159	HIS	-	EXPRESSION TAG	UNP O32248
C	160	HIS	-	EXPRESSION TAG	UNP O32248
C	161	HIS	-	EXPRESSION TAG	UNP O32248
C	162	HIS	-	EXPRESSION TAG	UNP O32248
C	163	HIS	-	EXPRESSION TAG	UNP O32248
D	1	MSE	MET	MODIFIED RESIDUE	UNP O32248
D	3	MSE	MET	MODIFIED RESIDUE	UNP O32248
D	148	MSE	MET	MODIFIED RESIDUE	UNP O32248
D	156	LEU	-	EXPRESSION TAG	UNP O32248
D	157	GLU	-	EXPRESSION TAG	UNP O32248
D	158	HIS	-	EXPRESSION TAG	UNP O32248
D	159	HIS	-	EXPRESSION TAG	UNP O32248
D	160	HIS	-	EXPRESSION TAG	UNP O32248
D	161	HIS	-	EXPRESSION TAG	UNP O32248
D	162	HIS	-	EXPRESSION TAG	UNP O32248
D	163	HIS	-	EXPRESSION TAG	UNP O32248

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

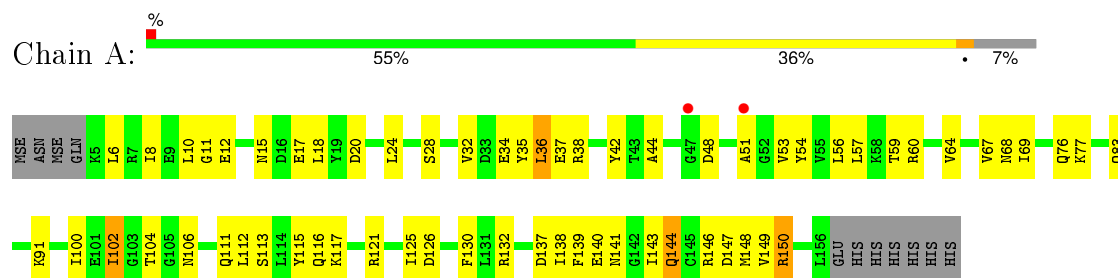


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

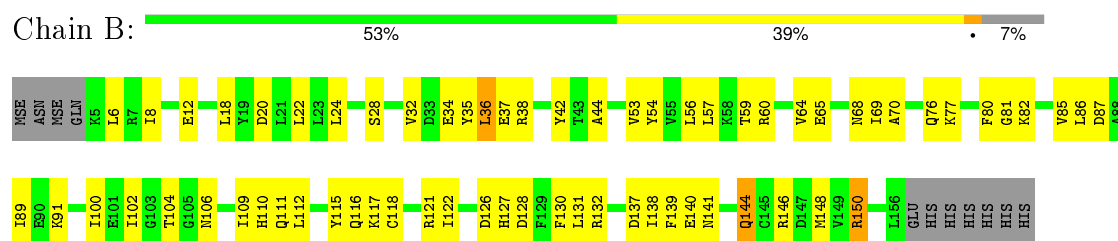
3 Residue-property plots [i](#)

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

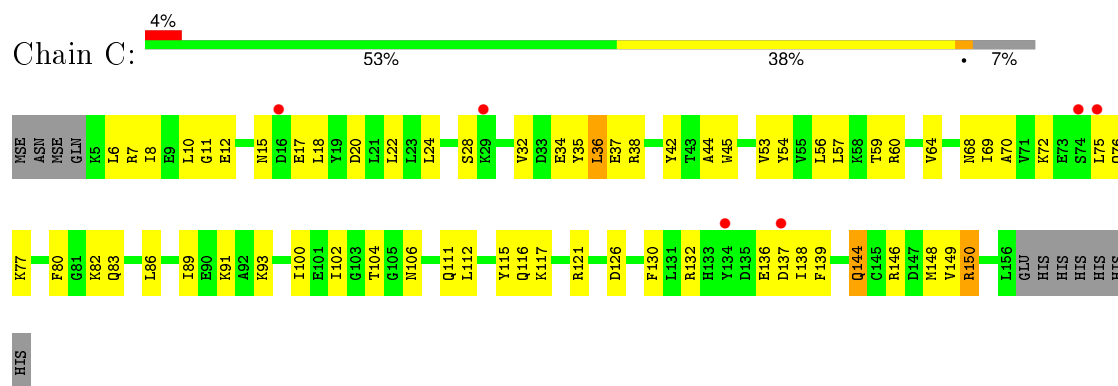
- Molecule 1: hypothetical protein BSU33890



- Molecule 1: hypothetical protein BSU33890

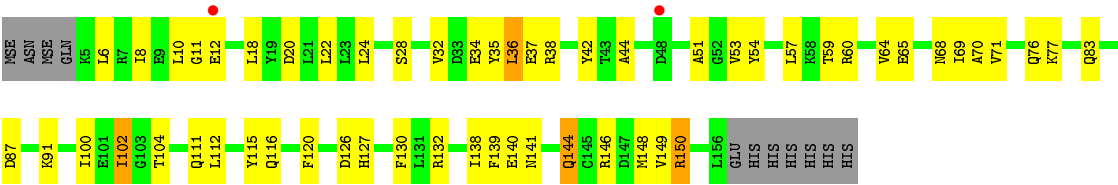


- Molecule 1: hypothetical protein BSU33890



- Molecule 1: hypothetical protein BSU33890





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.60Å 124.42Å 216.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.01 30.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	76.3 (30.00-3.01) 91.8 (30.00-3.01)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.284 0.262 , 0.304	Depositor DCC
R_{free} test set	1509 reflections (11.51%)	DCC
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	1.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 17.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 29303 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, 0.375 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

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	0.48	0/1238	0.58	0/1667
1	B	0.52	1/1238 (0.1%)	0.57	0/1667
1	C	0.49	0/1238	0.58	0/1667
1	D	0.48	0/1238	0.57	0/1667
All	All	0.49	1/4952 (0.0%)	0.57	0/6668

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	CYS	CB-SG	-5.13	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1221	0	1221	60	1
1	B	1221	0	1221	62	0
1	C	1221	0	1221	56	0
1	D	1221	0	1221	48	0
2	A	48	0	32	4	0
2	B	48	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	32	2	0
2	D	48	0	32	2	0
All	All	5076	0	5012	194	1

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 (194) 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:150:ARG:HH21	1:C:60:ARG:HD3	1.50	0.76
1:C:150:ARG:HG3	1:C:150:ARG:HH11	1.52	0.75
1:A:60:ARG:HD3	1:D:150:ARG:HH21	1.51	0.75
1:D:150:ARG:HH11	1:D:150:ARG:HG3	1.52	0.75
1:B:60:ARG:NH1	1:C:150:ARG:NH2	2.39	0.71
1:C:70:ALA:HA	2:C:203:COA:O9P	1.93	0.69
1:A:106:ASN:HB2	1:B:116:GLN:HE22	1.59	0.68
1:A:139:PHE:CE1	1:A:144:GLN:HG2	2.28	0.68
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.60	0.67
1:B:76:GLN:HB2	2:B:202:COA:O5A	1.95	0.67
1:D:139:PHE:CE1	1:D:144:GLN:HG2	2.30	0.67
1:B:65:GLU:OE2	1:C:60:ARG:NH1	2.30	0.65
1:D:138:ILE:N	1:D:138:ILE:HD12	2.12	0.64
1:B:150:ARG:HG3	1:B:150:ARG:HH11	1.63	0.63
1:B:139:PHE:CE1	1:B:144:GLN:HG2	2.33	0.63
1:B:104:THR:HG21	1:B:111:GLN:OE1	1.98	0.63
1:C:139:PHE:CE1	1:C:144:GLN:HG2	2.34	0.63
1:C:28:SER:O	1:C:32:VAL:HG23	1.98	0.63
1:C:121:ARG:NH2	1:D:146:ARG:HG3	2.14	0.62
1:B:8:ILE:HG12	1:B:44:ALA:HB2	1.80	0.62
1:A:121:ARG:HH21	1:B:146:ARG:HG3	1.65	0.62
1:A:28:SER:O	1:A:32:VAL:HG23	2.00	0.61
1:D:150:ARG:NH1	1:D:150:ARG:HG3	2.13	0.61
1:A:138:ILE:N	1:A:138:ILE:HD12	2.14	0.61
1:D:28:SER:O	1:D:32:VAL:HG23	2.01	0.61
1:D:60:ARG:HH11	1:D:60:ARG:HG2	1.66	0.61
1:A:150:ARG:NH2	1:D:60:ARG:NH1	2.48	0.61
1:C:121:ARG:HH21	1:D:146:ARG:HG3	1.66	0.61
1:A:121:ARG:NH2	1:B:146:ARG:HG3	2.15	0.60
1:B:60:ARG:HH11	1:B:60:ARG:HG2	1.65	0.60
1:C:150:ARG:NH1	1:C:150:ARG:HG3	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HE3	2:B:202:COA:O7A	2.02	0.60
1:B:28:SER:O	1:B:32:VAL:HG23	2.01	0.60
1:B:138:ILE:N	1:B:138:ILE:HD12	2.17	0.59
1:C:104:THR:HG21	1:C:111:GLN:OE1	2.02	0.59
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.66	0.59
1:C:60:ARG:HG2	1:C:60:ARG:HH11	1.68	0.58
1:D:8:ILE:HG12	1:D:44:ALA:HB2	1.84	0.58
1:A:104:THR:HG21	1:A:111:GLN:OE1	2.03	0.58
1:B:60:ARG:HD3	1:C:150:ARG:HH21	1.69	0.58
1:A:60:ARG:HD3	1:D:150:ARG:NH2	2.16	0.58
1:C:138:ILE:N	1:C:138:ILE:HD12	2.18	0.58
1:D:38:ARG:HD2	1:D:57:LEU:HD11	1.85	0.57
1:D:76:GLN:O	1:D:77:LYS:HB2	2.04	0.57
1:A:76:GLN:O	1:A:77:LYS:HB2	2.04	0.57
1:B:32:VAL:O	1:B:36:LEU:HB2	2.05	0.57
1:A:111:GLN:OE1	2:A:201:COA:H32	2.04	0.57
1:B:150:ARG:NH2	1:C:60:ARG:HD3	2.16	0.57
1:A:32:VAL:O	1:A:36:LEU:HB2	2.05	0.56
1:A:38:ARG:HD2	1:A:57:LEU:HD11	1.87	0.56
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.19	0.56
1:C:8:ILE:HG12	1:C:44:ALA:HB2	1.88	0.56
1:C:106:ASN:HB2	1:D:116:GLN:HE22	1.71	0.56
1:A:139:PHE:CZ	1:A:144:GLN:HG2	2.41	0.56
1:A:8:ILE:HG12	1:A:44:ALA:HB2	1.88	0.55
1:A:59:THR:C	1:D:59:THR:HG22	2.28	0.54
1:A:125:ILE:HG13	1:B:122:ILE:HG22	1.88	0.54
1:D:139:PHE:CZ	1:D:144:GLN:HG2	2.42	0.54
1:B:53:VAL:HG22	1:B:54:TYR:N	2.23	0.54
1:B:150:ARG:NH1	1:B:150:ARG:HG3	2.23	0.54
1:B:130:PHE:HB2	1:B:146:ARG:HA	1.90	0.54
1:A:130:PHE:HB2	1:A:146:ARG:HA	1.89	0.54
1:B:139:PHE:CZ	1:B:144:GLN:HG2	2.43	0.54
1:C:130:PHE:HB2	1:C:146:ARG:HA	1.90	0.54
1:D:130:PHE:HB2	1:D:146:ARG:HA	1.89	0.53
1:B:112:LEU:O	1:B:116:GLN:HG3	2.07	0.53
1:C:38:ARG:HD2	1:C:57:LEU:HD11	1.89	0.53
1:C:76:GLN:O	1:C:77:LYS:HB2	2.08	0.53
1:C:117:LYS:HE3	2:C:203:COA:O8A	2.08	0.53
1:D:104:THR:HG21	1:D:111:GLN:OE1	2.07	0.53
1:B:76:GLN:O	1:B:77:LYS:HB2	2.08	0.52
1:A:60:ARG:NH1	1:D:65:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HD2	1:B:57:LEU:HD11	1.91	0.52
1:D:32:VAL:O	1:D:36:LEU:HB2	2.09	0.51
1:A:150:ARG:HH21	1:D:60:ARG:HD3	1.76	0.51
1:B:70:ALA:HA	2:B:202:COA:O9P	2.10	0.51
1:C:139:PHE:CZ	1:C:144:GLN:HG2	2.45	0.51
1:B:111:GLN:HB3	1:B:115:TYR:CE2	2.46	0.51
1:A:42:TYR:O	1:A:53:VAL:HG23	2.10	0.51
1:A:112:LEU:O	1:A:116:GLN:HG3	2.10	0.51
1:A:116:GLN:HE22	1:B:106:ASN:HD22	1.59	0.50
1:B:81:GLY:N	2:B:202:COA:O4A	2.41	0.50
1:B:127:HIS:ND1	1:D:127:HIS:ND1	2.59	0.50
1:A:143:ILE:HG12	1:B:117:LYS:HG3	1.92	0.50
1:B:8:ILE:HG12	1:B:44:ALA:CB	2.42	0.50
1:B:36:LEU:HD13	1:B:36:LEU:O	2.12	0.50
1:C:42:TYR:O	1:C:53:VAL:HG23	2.11	0.50
1:C:112:LEU:O	1:C:116:GLN:HG3	2.12	0.50
1:A:53:VAL:HG22	1:A:54:TYR:N	2.28	0.49
1:A:113:SER:HB2	1:B:109:ILE:HD13	1.95	0.49
1:A:117:LYS:NZ	2:A:201:COA:O2B	2.45	0.49
1:A:59:THR:HA	1:D:59:THR:HA	1.94	0.49
1:B:126:ASP:HB3	1:B:148:MSE:HB3	1.95	0.49
1:A:126:ASP:HB3	1:A:148:MSE:HB3	1.95	0.48
1:B:6:LEU:HD13	1:B:80:PHE:CE1	2.48	0.48
1:B:6:LEU:HD13	1:B:80:PHE:CD1	2.48	0.48
1:C:32:VAL:O	1:C:36:LEU:HB2	2.12	0.48
1:C:126:ASP:HB3	1:C:148:MSE:HB3	1.94	0.48
1:D:126:ASP:HB3	1:D:148:MSE:HB3	1.95	0.48
1:D:112:LEU:O	1:D:116:GLN:HG3	2.14	0.48
1:B:42:TYR:O	1:B:53:VAL:HG23	2.14	0.48
1:D:42:TYR:O	1:D:53:VAL:HG23	2.14	0.48
1:D:53:VAL:HG22	1:D:54:TYR:N	2.29	0.48
1:C:20:ASP:O	1:C:24:LEU:HG	2.14	0.47
1:A:60:ARG:N	1:D:59:THR:HG22	2.29	0.47
1:C:53:VAL:HG22	1:C:54:TYR:N	2.30	0.47
1:D:8:ILE:HG12	1:D:44:ALA:CB	2.44	0.47
1:D:138:ILE:N	1:D:138:ILE:CD1	2.78	0.47
1:A:59:THR:HG22	1:D:59:THR:C	2.36	0.47
1:D:111:GLN:HB3	1:D:115:TYR:CE2	2.50	0.46
1:A:111:GLN:HB3	1:A:115:TYR:CE2	2.50	0.46
1:C:64:VAL:O	1:C:100:ILE:HA	2.15	0.46
1:D:64:VAL:O	1:D:100:ILE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:OH	1:A:91:LYS:HG3	2.16	0.46
1:C:32:VAL:HA	1:C:35:TYR:CE2	2.51	0.46
1:A:116:GLN:NE2	1:B:106:ASN:HD22	2.13	0.46
1:D:54:TYR:OH	1:D:91:LYS:HG3	2.16	0.46
1:A:64:VAL:O	1:A:100:ILE:HA	2.15	0.46
1:B:32:VAL:HA	1:B:35:TYR:CE2	2.51	0.45
1:B:54:TYR:OH	1:B:91:LYS:HG3	2.17	0.45
1:B:60:ARG:CZ	1:C:150:ARG:NH2	2.79	0.45
1:D:22:LEU:HA	1:D:68:ASN:HD21	1.82	0.45
1:C:137:ASP:HB3	1:C:139:PHE:CE2	2.52	0.45
1:B:64:VAL:O	1:B:100:ILE:HA	2.16	0.45
1:A:32:VAL:HA	1:A:35:TYR:CE2	2.52	0.45
1:B:82:LYS:HE2	1:B:86:LEU:HD11	1.98	0.45
1:C:54:TYR:OH	1:C:91:LYS:HG3	2.17	0.45
1:A:117:LYS:HE3	2:A:201:COA:O2B	2.17	0.44
1:A:6:LEU:HD11	1:A:51:ALA:CB	2.47	0.44
1:C:111:GLN:HB3	1:C:115:TYR:CE2	2.52	0.44
1:A:10:LEU:HG	1:A:11:GLY:N	2.33	0.44
1:B:20:ASP:O	1:B:24:LEU:HG	2.18	0.44
1:C:6:LEU:HD13	1:C:80:PHE:CD1	2.52	0.44
1:A:138:ILE:N	1:A:138:ILE:CD1	2.80	0.44
1:B:110:HIS:NE2	2:B:202:COA:H4B	2.33	0.43
1:C:72:LYS:HE3	1:C:75:LEU:HD12	2.00	0.43
1:C:82:LYS:HE2	1:C:86:LEU:HD11	2.01	0.43
1:A:56:LEU:HD22	1:A:64:VAL:CG2	2.49	0.43
1:A:20:ASP:O	1:A:24:LEU:HG	2.18	0.43
1:D:140:GLU:HG2	1:D:141:ASN:CG	2.39	0.43
1:C:22:LEU:HA	1:C:68:ASN:HD21	1.84	0.43
1:B:59:THR:HG22	1:C:59:THR:C	2.39	0.43
1:B:68:ASN:OD1	1:B:69:ILE:N	2.52	0.43
1:D:32:VAL:HA	1:D:35:TYR:CE2	2.54	0.43
1:A:117:LYS:CE	2:A:201:COA:O2B	2.67	0.43
1:D:6:LEU:HD11	1:D:51:ALA:CB	2.49	0.43
1:D:20:ASP:O	1:D:24:LEU:HG	2.19	0.43
1:D:70:ALA:HA	2:D:204:COA:O9P	2.19	0.43
1:B:22:LEU:HA	1:B:68:ASN:HD21	1.83	0.42
1:D:87:ASP:CG	1:D:91:LYS:HZ3	2.22	0.42
1:D:68:ASN:OD1	1:D:69:ILE:N	2.52	0.42
1:C:6:LEU:HB2	1:C:83:GLN:NE2	2.34	0.42
1:D:6:LEU:HB2	1:D:83:GLN:NE2	2.34	0.42
1:D:10:LEU:HG	1:D:11:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HB2	1:A:83:GLN:NE2	2.34	0.42
1:A:102:ILE:HG23	1:A:102:ILE:O	2.18	0.42
1:A:147:ASP:OD2	1:B:121:ARG:NH2	2.53	0.42
1:A:137:ASP:HB3	1:A:139:PHE:CE2	2.55	0.42
1:A:140:GLU:HG2	1:A:141:ASN:CG	2.40	0.42
1:D:112:LEU:HD11	1:D:149:VAL:HG11	2.02	0.41
1:A:56:LEU:HD22	1:A:64:VAL:HG22	2.02	0.41
1:C:68:ASN:OD1	1:C:69:ILE:N	2.53	0.41
1:C:144:GLN:NE2	1:C:146:ARG:HH11	2.18	0.41
1:C:89:ILE:O	1:C:93:LYS:HG3	2.20	0.41
1:C:10:LEU:HG	1:C:11:GLY:N	2.35	0.41
1:B:60:ARG:NH1	1:C:150:ARG:HH22	2.15	0.41
1:C:6:LEU:HD13	1:C:80:PHE:CE1	2.55	0.41
1:C:137:ASP:HB3	1:C:139:PHE:HE2	1.86	0.41
1:C:112:LEU:HD11	1:C:149:VAL:HG11	2.03	0.41
1:C:15:ASN:OD1	1:C:17:GLU:HB3	2.20	0.41
1:B:59:THR:HA	1:C:59:THR:HA	2.03	0.41
1:C:8:ILE:HG12	1:C:44:ALA:CB	2.49	0.41
1:A:112:LEU:HD11	1:A:149:VAL:HG11	2.03	0.41
1:B:130:PHE:N	1:B:130:PHE:CD1	2.89	0.41
1:D:102:ILE:HG22	1:D:120:PHE:CE2	2.56	0.41
1:B:85:VAL:O	1:B:89:ILE:HG13	2.21	0.41
1:C:7:ARG:NH2	1:C:45:TRP:CE3	2.84	0.41
1:C:7:ARG:HH22	1:C:45:TRP:HE3	1.62	0.41
1:A:68:ASN:OD1	1:A:69:ILE:N	2.54	0.41
1:C:136:GLU:OE1	1:C:136:GLU:HA	2.20	0.41
1:B:137:ASP:HB3	1:B:139:PHE:CE2	2.55	0.40
1:A:57:LEU:CD2	1:A:67:VAL:HG11	2.52	0.40
1:C:56:LEU:HD22	1:C:64:VAL:CG2	2.51	0.40
1:A:15:ASN:OD1	1:A:17:GLU:HB3	2.21	0.40
1:A:8:ILE:HG12	1:A:44:ALA:CB	2.50	0.40
1:B:140:GLU:HG2	1:B:141:ASN:CG	2.42	0.40
1:B:87:ASP:CG	1:B:91:LYS:HZ3	2.24	0.40
1:D:71:VAL:HG23	2:D:204:COA:H132	2.04	0.40
1:C:60:ARG:NH1	1:C:60:ARG:HG2	2.35	0.40
1:B:56:LEU:HD22	1:B:64:VAL:HG22	2.03	0.40
1:B:128:ASP:O	1:B:131:LEU:HB2	2.21	0.40
1:A:106:ASN:HD22	1:B:116:GLN:NE2	2.20	0.40
1:A:36:LEU:O	1:A:36:LEU:HD13	2.22	0.40
1:B:56:LEU:HD22	1:B:64:VAL:CG2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:OD2	1:A:48:ASP:OD2[3_656]	1.72	0.48

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	150/163 (92%)	129 (86%)	20 (13%)	1 (1%)	26	68
1	B	150/163 (92%)	130 (87%)	19 (13%)	1 (1%)	26	68
1	C	150/163 (92%)	131 (87%)	18 (12%)	1 (1%)	26	68
1	D	150/163 (92%)	131 (87%)	18 (12%)	1 (1%)	26	68
All	All	600/652 (92%)	521 (87%)	75 (12%)	4 (1%)	26	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ILE
1	A	102	ILE
1	D	102	ILE
1	C	102	ILE

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	132/140 (94%)	124 (94%)	8 (6%)	23	60
1	B	132/140 (94%)	124 (94%)	8 (6%)	23	60
1	C	132/140 (94%)	124 (94%)	8 (6%)	23	60
1	D	132/140 (94%)	124 (94%)	8 (6%)	23	60
All	All	528/560 (94%)	496 (94%)	32 (6%)	23	60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	18	LEU
1	A	34	GLU
1	A	36	LEU
1	A	37	GLU
1	A	132	ARG
1	A	144	GLN
1	A	150	ARG
1	B	12	GLU
1	B	18	LEU
1	B	34	GLU
1	B	36	LEU
1	B	37	GLU
1	B	132	ARG
1	B	144	GLN
1	B	150	ARG
1	C	12	GLU
1	C	18	LEU
1	C	34	GLU
1	C	36	LEU
1	C	37	GLU
1	C	132	ARG
1	C	144	GLN
1	C	150	ARG
1	D	12	GLU
1	D	18	LEU
1	D	34	GLU
1	D	36	LEU
1	D	37	GLU
1	D	132	ARG
1	D	144	GLN
1	D	150	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	83	GLN
1	A	116	GLN
1	A	123	GLN
1	A	144	GLN
1	B	76	GLN
1	B	83	GLN
1	B	116	GLN
1	B	133	HIS
1	B	144	GLN
1	C	76	GLN
1	C	83	GLN
1	C	116	GLN
1	C	123	GLN
1	C	144	GLN
1	D	76	GLN
1	D	83	GLN
1	D	116	GLN
1	D	144	GLN

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	A	201	-	40,50,50	2.86	12 (30%)	50,75,75	3.94	19 (38%)
2	COA	B	202	-	40,50,50	2.81	16 (40%)	50,75,75	4.13	18 (36%)
2	COA	C	203	-	40,50,50	2.88	16 (40%)	50,75,75	3.86	17 (34%)
2	COA	D	204	-	40,50,50	2.90	18 (45%)	50,75,75	3.92	17 (34%)

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	201	-	-	0/44/64/64	0/3/3/3
2	COA	B	202	-	-	0/44/64/64	0/3/3/3
2	COA	C	203	-	-	0/44/64/64	0/3/3/3
2	COA	D	204	-	-	0/44/64/64	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	204	COA	P2A-O6A	-3.01	1.45	1.59
2	A	201	COA	P2A-O6A	-2.99	1.45	1.59
2	C	203	COA	P2A-O6A	-2.78	1.46	1.59
2	B	202	COA	P2A-O6A	-2.71	1.46	1.59
2	B	202	COA	P2A-O5A	-2.53	1.44	1.54
2	C	203	COA	P2A-O5A	-2.43	1.44	1.54
2	A	201	COA	P2A-O5A	-2.37	1.44	1.54
2	B	202	COA	P3B-O3B	-2.30	1.53	1.60
2	D	204	COA	P2A-O5A	-2.26	1.45	1.54
2	A	201	COA	P3B-O9A	-2.20	1.46	1.54
2	B	202	COA	P1A-O1A	-2.10	1.43	1.51
2	C	203	COA	P3B-O9A	-2.03	1.47	1.54
2	D	204	COA	P3B-O9A	-2.02	1.47	1.54
2	D	204	COA	P1A-O1A	-2.01	1.43	1.51
2	D	204	COA	C3B-C4B	-2.00	1.47	1.52
2	B	202	COA	C6A-N1A	2.07	1.47	1.37
2	D	204	COA	C2P-C3P	2.08	1.59	1.51
2	C	203	COA	C6A-N1A	2.11	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	204	COA	OAP-CAP	2.14	1.46	1.42
2	D	204	COA	C6A-N1A	2.14	1.48	1.37
2	C	203	COA	OAP-CAP	2.14	1.46	1.42
2	C	203	COA	C5B-C4B	2.23	1.58	1.51
2	A	201	COA	C6A-N6A	2.25	1.41	1.34
2	D	204	COA	CEP-CBP	2.34	1.58	1.53
2	B	202	COA	C2P-C3P	2.34	1.60	1.51
2	B	202	COA	C5B-C4B	2.35	1.59	1.51
2	C	203	COA	CEP-CBP	2.41	1.58	1.53
2	A	201	COA	CEP-CBP	2.45	1.59	1.53
2	C	203	COA	C7P-C6P	2.49	1.59	1.51
2	B	202	COA	C6A-N6A	2.53	1.42	1.34
2	C	203	COA	C6A-N6A	2.72	1.43	1.34
2	D	204	COA	C7P-C6P	2.79	1.60	1.51
2	B	202	COA	C8A-N7A	2.79	1.40	1.34
2	B	202	COA	C7P-C6P	2.94	1.60	1.51
2	D	204	COA	C6A-N6A	3.02	1.44	1.34
2	D	204	COA	C8A-N7A	3.03	1.40	1.34
2	C	203	COA	C8A-N7A	3.22	1.40	1.34
2	A	201	COA	C8A-N7A	3.63	1.41	1.34
2	B	202	COA	C9P-N8P	3.78	1.41	1.33
2	D	204	COA	C9P-N8P	4.26	1.42	1.33
2	A	201	COA	C9P-N8P	4.34	1.42	1.33
2	B	202	COA	C5P-N4P	4.35	1.43	1.33
2	C	203	COA	C9P-N8P	4.55	1.43	1.33
2	A	201	COA	C5P-N4P	4.68	1.44	1.33
2	C	203	COA	C5P-N4P	4.75	1.44	1.33
2	D	204	COA	C5P-N4P	5.18	1.45	1.33
2	C	203	COA	O4B-C1B	5.43	1.48	1.41
2	A	201	COA	O4B-C1B	5.55	1.48	1.41
2	D	204	COA	O4B-C1B	5.57	1.48	1.41
2	B	202	COA	O4B-C1B	5.61	1.48	1.41
2	C	203	COA	C2A-N1A	6.30	1.45	1.33
2	D	204	COA	C2A-N1A	6.38	1.46	1.33
2	A	201	COA	C2A-N1A	6.40	1.46	1.33
2	B	202	COA	C2A-N1A	6.62	1.46	1.33
2	B	202	COA	C2A-N3A	7.31	1.45	1.32
2	A	201	COA	C4A-N3A	7.49	1.46	1.35
2	D	204	COA	C4A-N3A	7.60	1.46	1.35
2	C	203	COA	C4A-N3A	7.66	1.47	1.35
2	B	202	COA	C4A-N3A	7.93	1.47	1.35
2	D	204	COA	C2A-N3A	8.07	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	COA	C2A-N3A	8.28	1.46	1.32
2	C	203	COA	C2A-N3A	8.35	1.46	1.32

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	COA	N3A-C2A-N1A	-20.38	113.29	128.89
2	D	204	COA	N3A-C2A-N1A	-19.65	113.85	128.89
2	C	203	COA	N3A-C2A-N1A	-19.43	114.02	128.89
2	A	201	COA	N3A-C2A-N1A	-19.13	114.25	128.89
2	B	202	COA	CDP-CBP-CCP	-16.22	87.47	108.50
2	A	201	COA	CDP-CBP-CCP	-14.07	90.26	108.50
2	D	204	COA	CDP-CBP-CCP	-13.84	90.56	108.50
2	C	203	COA	CDP-CBP-CCP	-13.43	91.09	108.50
2	A	201	COA	C5B-C4B-C3B	-4.36	98.62	114.31
2	D	204	COA	C5B-C4B-C3B	-4.10	99.53	114.31
2	C	203	COA	C5B-C4B-C3B	-3.56	101.50	114.31
2	A	201	COA	P2A-O3A-P1A	-3.37	123.25	132.73
2	B	202	COA	C5B-C4B-C3B	-3.10	103.15	114.31
2	D	204	COA	O6A-CCP-CBP	-3.07	105.61	110.55
2	A	201	COA	O6A-CCP-CBP	-2.46	106.59	110.55
2	C	203	COA	P2A-O3A-P1A	-2.44	125.88	132.73
2	B	202	COA	O3A-P1A-O5B	-2.16	97.21	102.94
2	C	203	COA	CDP-CBP-CAP	2.06	113.11	109.34
2	A	201	COA	O4B-C1B-N9A	2.12	112.54	108.10
2	B	202	COA	C4A-C5A-N7A	2.18	111.48	109.48
2	A	201	COA	C2B-C3B-C4B	2.18	107.40	103.29
2	A	201	COA	C7P-C6P-C5P	2.21	115.95	112.31
2	D	204	COA	C6P-C7P-N8P	2.23	116.77	111.88
2	B	202	COA	C3B-C2B-C1B	2.24	105.35	99.98
2	D	204	COA	O4B-C1B-N9A	2.37	113.05	108.10
2	C	203	COA	C2B-C3B-C4B	2.37	107.75	103.29
2	B	202	COA	O4B-C4B-C5B	2.38	117.82	109.32
2	B	202	COA	C3P-N4P-C5P	2.40	127.52	122.79
2	B	202	COA	C6P-C7P-N8P	2.43	117.22	111.88
2	B	202	COA	O3B-P3B-O7A	2.44	113.21	107.11
2	C	203	COA	C3B-C2B-C1B	2.46	105.88	99.98
2	B	202	COA	C2B-C3B-C4B	2.46	107.92	103.29
2	D	204	COA	C3B-C2B-C1B	2.48	105.93	99.98
2	D	204	COA	C2B-C3B-C4B	2.55	108.08	103.29
2	C	203	COA	CEP-CBP-CCP	2.58	111.84	108.50
2	D	204	COA	CEP-CBP-CAP	2.59	114.07	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	203	COA	O4B-C4B-C5B	2.62	118.70	109.32
2	B	202	COA	C7P-N8P-C9P	2.67	127.81	122.53
2	C	203	COA	CEP-CBP-CAP	2.70	114.27	109.34
2	D	204	COA	O3B-P3B-O7A	2.79	114.08	107.11
2	A	201	COA	CEP-CBP-CAP	2.81	114.47	109.34
2	D	204	COA	C7P-N8P-C9P	2.82	128.11	122.53
2	A	201	COA	C2A-N1A-C6A	2.84	123.84	118.77
2	A	201	COA	O4B-C4B-C5B	2.87	119.58	109.32
2	A	201	COA	CEP-CBP-CCP	2.88	112.23	108.50
2	A	201	COA	C3B-C2B-C1B	2.91	106.95	99.98
2	C	203	COA	C2A-N1A-C6A	2.93	124.01	118.77
2	C	203	COA	C3P-N4P-C5P	2.94	128.57	122.79
2	C	203	COA	C6P-C7P-N8P	2.94	118.34	111.88
2	B	202	COA	C7P-C6P-C5P	2.97	117.20	112.31
2	D	204	COA	O4B-C4B-C5B	3.00	120.05	109.32
2	A	201	COA	C3P-N4P-C5P	3.01	128.72	122.79
2	C	203	COA	O3B-P3B-O7A	3.10	114.85	107.11
2	D	204	COA	C3P-N4P-C5P	3.14	128.97	122.79
2	A	201	COA	C6P-C7P-N8P	3.18	118.86	111.88
2	D	204	COA	C2A-N1A-C6A	3.20	124.48	118.77
2	B	202	COA	C2A-N1A-C6A	3.23	124.53	118.77
2	B	202	COA	CEP-CBP-CAP	3.25	115.27	109.34
2	B	202	COA	C2B-C1B-N9A	3.42	119.51	114.29
2	D	204	COA	CEP-CBP-CCP	3.51	113.06	108.50
2	A	201	COA	O3B-P3B-O7A	3.53	115.92	107.11
2	D	204	COA	C7P-C6P-C5P	3.54	118.14	112.31
2	C	203	COA	C7P-N8P-C9P	3.93	130.30	122.53
2	A	201	COA	C2B-C1B-N9A	3.93	120.29	114.29
2	B	202	COA	CEP-CBP-CCP	4.06	113.77	108.50
2	C	203	COA	C7P-C6P-C5P	4.17	119.18	112.31
2	A	201	COA	C7P-N8P-C9P	4.22	130.88	122.53
2	B	202	COA	O3A-P2A-O6A	4.86	115.84	102.94
2	A	201	COA	O3A-P2A-O6A	5.37	117.19	102.94
2	C	203	COA	O3A-P2A-O6A	5.50	117.53	102.94
2	D	204	COA	O3A-P2A-O6A	5.51	117.57	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	COA	4	0
2	B	202	COA	5	0
2	C	203	COA	2	0
2	D	204	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	151/163 (92%)	0.00	2 (1%) 79 52	36, 60, 83, 86	0
1	B	151/163 (92%)	-0.07	0 100 100	37, 61, 83, 86	0
1	C	151/163 (92%)	0.11	6 (3%) 42 17	38, 60, 84, 87	0
1	D	151/163 (92%)	0.09	2 (1%) 79 52	37, 60, 83, 86	0
All	All	604/652 (92%)	0.03	10 (1%) 73 44	36, 61, 84, 87	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	SER	2.6
1	C	137	ASP	2.5
1	D	48	ASP	2.4
1	C	16	ASP	2.4
1	C	75	LEU	2.3
1	A	51	ALA	2.2
1	C	29	LYS	2.1
1	C	134	TYR	2.1
1	D	12	GLU	2.1
1	A	47	GLY	2.1

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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	COA	C	203	48/48	0.86	0.26	0.52	72,81,109,111	0
2	COA	B	202	48/48	0.89	0.25	0.28	42,68,93,94	0
2	COA	D	204	48/48	0.93	0.21	-0.38	49,63,93,94	0
2	COA	A	201	48/48	0.92	0.20	-0.52	37,54,72,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.