



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:25 PM GMT

PDB ID : 3R7K  
Title : Crystal structure of a probable acyl CoA dehydrogenase from Mycobacterium abscessus ATCC 19977 / DSM 44196  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2011-03-22  
Resolution : 2.50 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



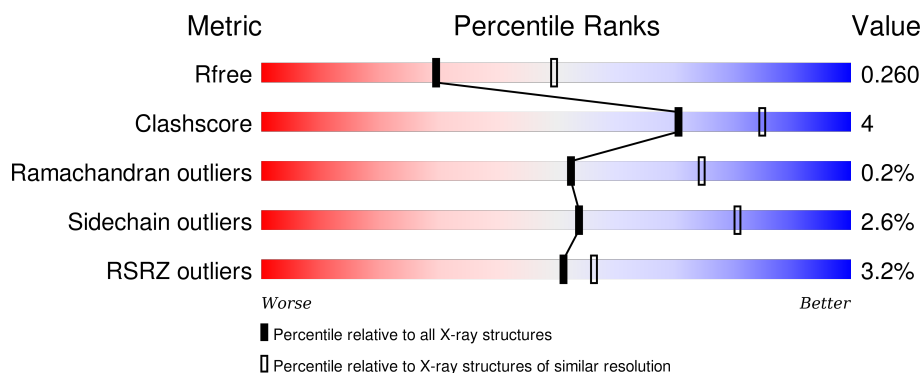
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	403	<div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	B	403	<div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	C	403	<div> <div>83%</div> <div>9%</div> <div>6%</div> </div>
1	D	403	<div> <div>85%</div> <div>8%</div> <div>7%</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	K	A	400	-	-	-	X



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11294 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 Probable acyl CoA dehydrogenase.

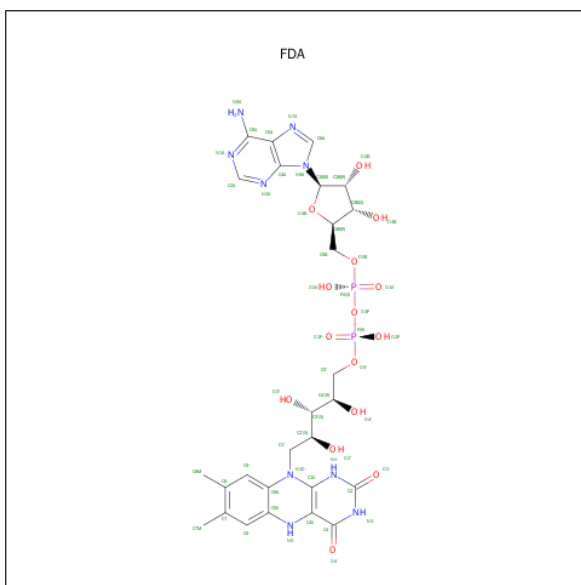
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2792	1741	508	528	15			
1	B	378	Total	C	N	O	S	0	0	0
			2736	1706	496	519	15			
1	C	377	Total	C	N	O	S	0	0	0
			2774	1731	506	523	14			
1	D	376	Total	C	N	O	S	0	0	0
			2722	1691	496	521	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP B1MPB5
A	-2	PRO	-	EXPRESSION TAG	UNP B1MPB5
A	-1	GLY	-	EXPRESSION TAG	UNP B1MPB5
A	0	SER	-	EXPRESSION TAG	UNP B1MPB5
B	-3	GLY	-	EXPRESSION TAG	UNP B1MPB5
B	-2	PRO	-	EXPRESSION TAG	UNP B1MPB5
B	-1	GLY	-	EXPRESSION TAG	UNP B1MPB5
B	0	SER	-	EXPRESSION TAG	UNP B1MPB5
C	-3	GLY	-	EXPRESSION TAG	UNP B1MPB5
C	-2	PRO	-	EXPRESSION TAG	UNP B1MPB5
C	-1	GLY	-	EXPRESSION TAG	UNP B1MPB5
C	0	SER	-	EXPRESSION TAG	UNP B1MPB5
D	-3	GLY	-	EXPRESSION TAG	UNP B1MPB5
D	-2	PRO	-	EXPRESSION TAG	UNP B1MPB5
D	-1	GLY	-	EXPRESSION TAG	UNP B1MPB5
D	0	SER	-	EXPRESSION TAG	UNP B1MPB5

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	2	Total	K	0	0
			2	2		
3	D	1	Total	K	0	0
			1	1		
3	C	2	Total	K	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		

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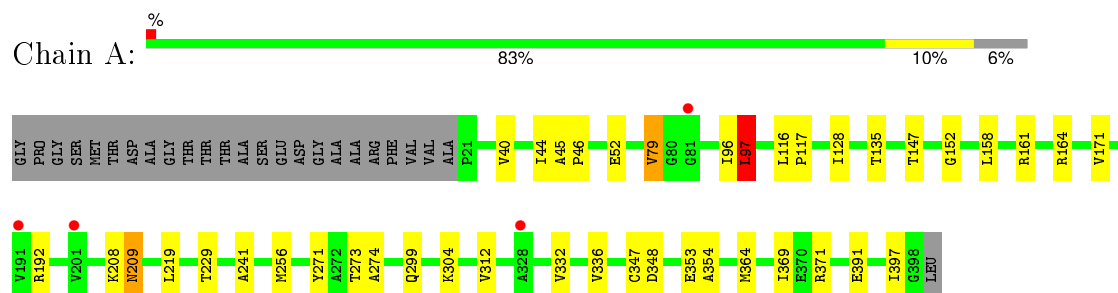
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	11	Total 11	O 11	0	0
4	C	13	Total 13	O 13	0	0
4	D	12	Total 12	O 12	0	0



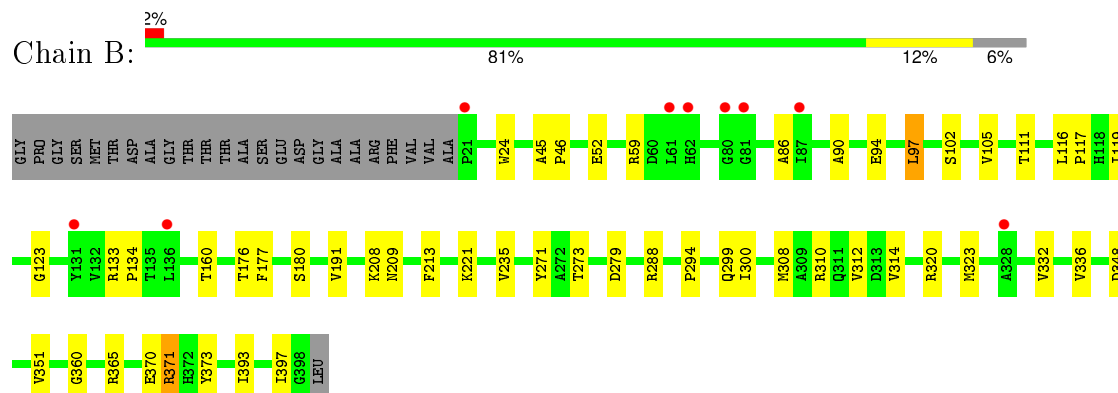
### 3 Residue-property plots [i](#)

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.

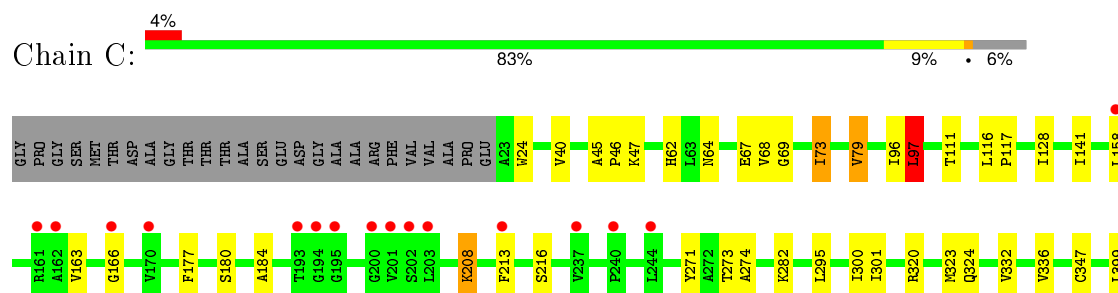
- Molecule 1: Probable acyl CoA dehydrogenase



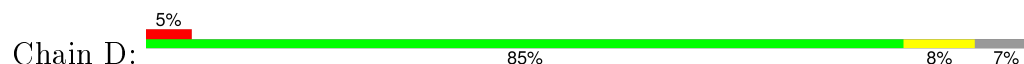
- Molecule 1: Probable acyl CoA dehydrogenase



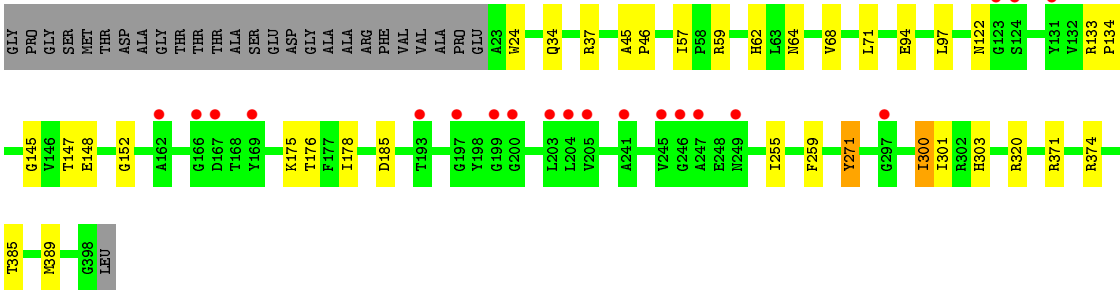
- Molecule 1: Probable acyl CoA dehydrogenase



- Molecule 1: Probable acyl CoA dehydrogenase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.25Å 121.12Å 172.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.50 49.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.52-2.50) 99.7 (49.52-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.208 , 0.259 0.214 , 0.260	Depositor DCC
$R_{free}$ test set	4843 reflections (8.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 62183 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: FDA, K

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	0.84	1/2838 (0.0%)	0.83	2/3848 (0.1%)
1	B	0.80	0/2782	0.82	5/3780 (0.1%)
1	C	0.83	3/2819 (0.1%)	0.82	1/3821 (0.0%)
1	D	0.70	0/2767	0.78	3/3758 (0.1%)
All	All	0.79	4/11206 (0.0%)	0.81	11/15207 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	CYS	CB-SG	-7.53	1.69	1.82
1	A	347	CYS	CB-SG	-6.70	1.70	1.82
1	C	274	ALA	CA-CB	5.37	1.63	1.52
1	C	67	GLU	CG-CD	5.15	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	LEU	CA-CB-CG	-6.78	99.71	115.30
1	C	97	LEU	CA-CB-CG	-6.67	99.95	115.30
1	B	279	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	374	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	374	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	59	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	348	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	348	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	97	LEU	CA-CB-CG	-5.19	103.36	115.30
1	B	97	LEU	CA-CB-CG	-5.08	103.61	115.30
1	B	371	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2733	30	0
1	B	2736	0	2620	31	0
1	C	2774	0	2712	24	0
1	D	2722	0	2585	19	0
2	A	53	0	33	1	0
2	B	53	0	33	2	0
2	C	53	0	33	1	0
2	D	53	0	33	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	0	0	0
4	B	11	0	0	0	0
4	C	13	0	0	0	0
4	D	12	0	0	0	0
All	All	11294	0	10782	96	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 4.

All (96) 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:D:34:GLN:OE1	1:D:37:ARG:NH1	2.24	0.70
1:B:86:ALA:HB1	1:B:323:MET:HE2	1.74	0.69
1:B:102:SER:HB3	1:B:105:VAL:HG23	1.75	0.68
1:A:97:LEU:HD22	1:A:273:THR:HA	1.77	0.67
1:B:86:ALA:HB1	1:B:323:MET:CE	2.24	0.67
1:B:299:GLN:HG2	1:C:300:ILE:HD13	1.77	0.66
1:B:97:LEU:HD22	1:B:273:THR:HA	1.78	0.65
1:A:79:VAL:HG22	1:A:128:ILE:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ALA:HB3	1:C:46:PRO:HD3	1.78	0.64
1:C:295:LEU:HB3	1:C:301:ILE:HD13	1.79	0.64
1:A:304:LYS:NZ	1:A:353:GLU:OE2	2.30	0.62
1:B:299:GLN:CG	1:C:300:ILE:HD13	2.30	0.62
1:D:62:HIS:O	1:D:71:LEU:HD22	2.01	0.61
1:C:320:ARG:O	1:C:324:GLN:HG3	2.01	0.61
1:A:79:VAL:HG13	1:A:79:VAL:O	2.01	0.61
1:A:158:LEU:C	1:A:158:LEU:HD12	2.22	0.60
1:A:332:VAL:O	1:A:336:VAL:HG23	2.03	0.59
1:C:332:VAL:HG23	1:C:336:VAL:HG23	1.84	0.59
1:A:304:LYS:HZ2	1:A:353:GLU:CD	2.06	0.58
1:B:308:MET:O	1:B:312:VAL:HG23	2.04	0.57
1:C:24:TRP:CH2	1:C:323:MET:CE	2.87	0.57
1:C:24:TRP:CZ2	1:C:323:MET:CE	2.88	0.56
1:A:79:VAL:HG22	1:A:128:ILE:HG21	1.87	0.56
1:D:59:ARG:NH2	1:D:185:ASP:OD2	2.36	0.56
1:A:299:GLN:HG2	1:D:300:ILE:CD1	2.35	0.56
1:A:208:LYS:O	1:A:209:ASN:CB	2.54	0.56
1:D:68:VAL:O	1:D:68:VAL:HG12	2.05	0.55
1:B:300:ILE:HA	1:C:300:ILE:HD11	1.89	0.55
1:C:24:TRP:CZ2	1:C:323:MET:HE2	2.42	0.54
1:C:158:LEU:HD12	1:C:158:LEU:C	2.27	0.54
1:A:147:THR:HG23	1:A:152:GLY:HA2	1.90	0.54
1:A:40:VAL:HG21	1:A:96:ILE:HA	1.90	0.53
1:B:97:LEU:CD2	1:B:273:THR:HA	2.39	0.53
1:A:299:GLN:HG2	1:D:300:ILE:HD12	1.91	0.52
1:B:365:ARG:HG2	1:B:370:GLU:OE1	2.10	0.52
1:C:97:LEU:HD22	1:C:273:THR:HA	1.91	0.52
2:A:420:FDA:H2A	1:B:300:ILE:HD11	1.92	0.51
1:A:299:GLN:CG	1:D:300:ILE:HD12	2.41	0.51
1:A:274:ALA:HB1	1:A:312:VAL:HG22	1.92	0.51
1:B:111:THR:HG21	1:B:180:SER:HB2	1.92	0.50
1:A:158:LEU:O	1:A:192:ARG:NH2	2.43	0.50
1:D:45:ALA:HB3	1:D:46:PRO:HD3	1.94	0.49
1:C:40:VAL:HG21	1:C:96:ILE:HA	1.93	0.49
1:B:52:GLU:OE1	1:B:371:ARG:HD3	2.12	0.49
1:B:208:LYS:O	1:B:209:ASN:CB	2.61	0.48
1:A:79:VAL:CG2	1:A:128:ILE:HG21	2.44	0.48
1:D:94:GLU:OE2	1:D:271:TYR:OH	2.17	0.48
1:C:24:TRP:CZ2	1:C:320:ARG:HG2	2.49	0.48
1:C:184:ALA:O	1:C:208:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:O	1:A:209:ASN:HB2	2.14	0.47
1:B:332:VAL:O	1:B:336:VAL:HG23	2.15	0.47
1:B:160:THR:CG2	1:B:191:VAL:HG12	2.45	0.47
1:C:62:HIS:CE1	1:C:141:ILE:CD1	2.98	0.47
1:B:119:ILE:O	1:B:123:GLY:N	2.48	0.47
1:B:24:TRP:CZ2	1:B:320:ARG:HG2	2.50	0.46
1:B:393:ILE:O	1:B:397:ILE:HG12	2.15	0.46
1:B:97:LEU:HD22	1:B:273:THR:CA	2.45	0.46
1:B:45:ALA:HB3	1:B:46:PRO:HD3	1.99	0.45
1:D:145:GLY:HA2	1:D:178:ILE:HD12	1.98	0.45
1:A:116:LEU:N	1:A:117:PRO:CD	2.79	0.45
1:D:64:ASN:O	1:D:68:VAL:HG23	2.17	0.45
1:A:52:GLU:OE1	1:A:371:ARG:HD3	2.17	0.45
1:A:79:VAL:O	1:A:79:VAL:CG1	2.63	0.45
1:A:116:LEU:HD21	1:A:135:THR:HB	1.99	0.45
1:B:351:VAL:HG11	1:B:373:TYR:HA	1.98	0.45
1:B:160:THR:HG22	1:B:191:VAL:HG12	1.99	0.44
1:C:24:TRP:CH2	1:C:323:MET:HE1	2.53	0.44
1:D:148:GLU:HG2	1:D:175:LYS:HD3	2.00	0.44
1:B:116:LEU:N	1:B:117:PRO:CD	2.81	0.44
1:A:364:MET:CE	1:B:221:LYS:HG2	2.48	0.43
1:B:90:ALA:O	1:B:94:GLU:HG3	2.19	0.43
1:A:164:ARG:HH12	1:A:241:ALA:HB1	1.84	0.43
1:B:177:PHE:HB3	2:B:420:FDA:C9	2.49	0.43
1:D:24:TRP:CZ2	1:D:320:ARG:HG2	2.54	0.43
1:A:45:ALA:HB3	1:A:46:PRO:HD3	2.00	0.42
1:B:177:PHE:O	2:B:420:FDA:C4X	2.66	0.42
1:C:332:VAL:O	1:C:332:VAL:HG23	2.19	0.42
1:A:397:ILE:HB	1:C:282:LYS:NZ	2.35	0.42
1:D:147:THR:HG23	1:D:152:GLY:HA2	2.02	0.42
1:C:69:GLY:O	1:C:73:ILE:HD13	2.20	0.42
1:C:116:LEU:N	1:C:117:PRO:CD	2.83	0.42
1:D:133:ARG:HB3	1:D:134:PRO:HD3	2.01	0.42
1:A:40:VAL:HG22	1:A:44:ILE:HD12	2.02	0.41
1:C:79:VAL:CG2	1:C:128:ILE:HG23	2.51	0.41
1:D:57:ILE:C	1:D:57:ILE:HD12	2.40	0.41
1:A:161:ARG:O	1:A:171:VAL:HA	2.20	0.41
1:A:219:LEU:HD12	1:A:229:THR:HG22	2.02	0.41
1:C:177:PHE:HB3	2:C:420:FDA:C9	2.51	0.41
1:C:111:THR:HG21	1:C:180:SER:HB2	2.03	0.41
1:B:288:ARG:O	1:B:294:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ILE:HG22	1:D:259:PHE:CZ	2.56	0.41
1:A:354:ALA:HB3	1:A:369:ILE:HD11	2.02	0.40
1:D:24:TRP:CE2	1:D:320:ARG:HD3	2.56	0.40
1:D:385:THR:O	1:D:389:MET:HG2	2.20	0.40
1:B:133:ARG:HB3	1:B:134:PRO:HD3	2.03	0.40
1:B:310:ARG:O	1:B:314:VAL:HG23	2.22	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	376/403 (93%)	365 (97%)	10 (3%)	1 (0%)	46	68
1	B	376/403 (93%)	365 (97%)	10 (3%)	1 (0%)	46	68
1	C	375/403 (93%)	363 (97%)	11 (3%)	1 (0%)	46	68
1	D	374/403 (93%)	358 (96%)	16 (4%)	0	100	100
All	All	1501/1612 (93%)	1451 (97%)	47 (3%)	3 (0%)	52	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	C	166	GLY
1	B	360	GLY

### 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	275/304 (90%)	270 (98%)	5 (2%)	66	88
1	B	259/304 (85%)	255 (98%)	4 (2%)	72	91
1	C	270/304 (89%)	258 (96%)	12 (4%)	35	60
1	D	256/304 (84%)	249 (97%)	7 (3%)	52	79
All	All	1060/1216 (87%)	1032 (97%)	28 (3%)	54	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	97	LEU
1	A	256	MET
1	A	271	TYR
1	A	391	GLU
1	B	176	THR
1	B	213	PHE
1	B	235	VAL
1	B	271	TYR
1	C	47	LYS
1	C	64	ASN
1	C	68	VAL
1	C	73	ILE
1	C	79	VAL
1	C	97	LEU
1	C	163	VAL
1	C	208	LYS
1	C	213	PHE
1	C	216	SER
1	C	271	TYR
1	C	399	LEU
1	D	122	ASN
1	D	176	THR
1	D	271	TYR
1	D	300	ILE
1	D	301	ILE
1	D	303	HIS
1	D	371	ARG

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



sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	C	260	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](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	FDA	A	420	-	48,58,58	0.99	2 (4%)	54,89,89	2.20	13 (24%)
2	FDA	B	420	-	48,58,58	0.99	4 (8%)	54,89,89	2.23	11 (20%)
2	FDA	C	420	-	48,58,58	1.09	6 (12%)	54,89,89	2.33	10 (18%)
2	FDA	D	420	-	48,58,58	1.11	3 (6%)	54,89,89	2.38	13 (24%)

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	FDA	A	420	-	-	0/30/50/50	0/6/6/6
2	FDA	B	420	-	-	0/30/50/50	0/6/6/6
2	FDA	C	420	-	-	0/30/50/50	0/6/6/6
2	FDA	D	420	-	-	0/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	420	FDA	C4A-N3A	2.01	1.38	1.35
2	C	420	FDA	C2A-N3A	2.02	1.35	1.32
2	C	420	FDA	C4-N3	2.04	1.36	1.33
2	B	420	FDA	C4X-N5	2.13	1.36	1.33
2	A	420	FDA	C9A-N10	2.13	1.41	1.38
2	B	420	FDA	O4B-C1B	2.20	1.44	1.41
2	D	420	FDA	O4B-C1B	2.23	1.44	1.41
2	C	420	FDA	C4X-N5	2.28	1.36	1.33
2	B	420	FDA	C4-N3	2.43	1.37	1.33
2	B	420	FDA	C10-N10	2.46	1.42	1.39
2	C	420	FDA	C9A-N10	2.57	1.42	1.38
2	D	420	FDA	C9A-N10	3.01	1.42	1.38
2	A	420	FDA	C10-N10	3.15	1.42	1.39
2	C	420	FDA	C10-N10	3.32	1.43	1.39
2	D	420	FDA	C10-N10	4.29	1.44	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	420	FDA	N3A-C2A-N1A	-11.16	120.35	128.89
2	C	420	FDA	N3A-C2A-N1A	-9.81	121.38	128.89
2	A	420	FDA	N3A-C2A-N1A	-9.14	121.89	128.89
2	B	420	FDA	N3A-C2A-N1A	-8.78	122.17	128.89
2	D	420	FDA	C1B-N9A-C4A	-4.69	119.86	126.94
2	B	420	FDA	O3P-PA-O5B	-4.30	91.52	102.94
2	C	420	FDA	C4X-C10-N10	-4.14	118.08	120.52
2	C	420	FDA	P-O3P-PA	-4.01	121.46	132.73
2	B	420	FDA	C4-C4X-C10	-3.85	117.48	119.94
2	B	420	FDA	C2B-C1B-N9A	-3.70	108.64	114.29
2	B	420	FDA	C4A-C5A-N7A	-3.64	106.13	109.48
2	D	420	FDA	C4X-C10-N10	-3.50	118.46	120.52
2	A	420	FDA	C2B-C1B-N9A	-3.47	108.99	114.29
2	D	420	FDA	P-O3P-PA	-3.46	123.01	132.73
2	C	420	FDA	C4-C4X-C10	-3.41	117.76	119.94
2	A	420	FDA	P-O3P-PA	-3.30	123.47	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	420	FDA	C4X-C10-N10	-3.27	118.59	120.52
2	C	420	FDA	C4X-C4-N3	-3.23	119.17	123.59
2	D	420	FDA	C4A-C5A-N7A	-3.15	106.58	109.48
2	D	420	FDA	C4-C4X-C10	-3.04	118.00	119.94
2	A	420	FDA	C4-C4X-C10	-2.99	118.03	119.94
2	A	420	FDA	C1B-N9A-C4A	-2.91	122.55	126.94
2	B	420	FDA	C4X-C4-N3	-2.88	119.65	123.59
2	D	420	FDA	O3P-PA-O5B	-2.67	95.87	102.94
2	B	420	FDA	C4X-C10-N10	-2.57	119.00	120.52
2	A	420	FDA	C4A-C5A-N7A	-2.49	107.19	109.48
2	C	420	FDA	C2B-C1B-N9A	-2.25	110.85	114.29
2	C	420	FDA	C4A-C5A-N7A	-2.13	107.52	109.48
2	A	420	FDA	C9A-C5X-N5	-2.11	119.23	122.36
2	D	420	FDA	C2B-C1B-N9A	-2.10	111.09	114.29
2	D	420	FDA	C4X-C4-N3	-2.09	120.73	123.59
2	B	420	FDA	O4B-C1B-N9A	2.02	112.32	108.10
2	B	420	FDA	O4'-C4'-C3'	2.04	114.14	109.02
2	A	420	FDA	O3P-P-O5'	2.17	108.68	102.94
2	C	420	FDA	O5'-P-O1P	2.23	118.27	109.62
2	A	420	FDA	O4B-C1B-N9A	2.41	113.15	108.10
2	A	420	FDA	C4-C4X-N5	2.56	121.83	118.72
2	D	420	FDA	O4B-C1B-N9A	2.63	113.61	108.10
2	D	420	FDA	C4X-N5-C5X	3.13	120.36	116.76
2	D	420	FDA	C4-C4X-N5	3.87	123.42	118.72
2	C	420	FDA	C4-C4X-N5	4.06	123.65	118.72
2	B	420	FDA	C4-C4X-N5	4.22	123.84	118.72
2	A	420	FDA	C4X-N5-C5X	4.52	121.96	116.76
2	D	420	FDA	C4-N3-C2	6.23	120.64	115.25
2	A	420	FDA	C4-N3-C2	6.72	121.06	115.25
2	B	420	FDA	C4-N3-C2	7.40	121.65	115.25
2	C	420	FDA	C4-N3-C2	7.77	121.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	420	FDA	1	0
2	B	420	FDA	2	0
2	C	420	FDA	1	0



## 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	378/403 (93%)	0.18	4 (1%) 82 84	36, 55, 77, 89	0
1	B	378/403 (93%)	0.17	9 (2%) 62 66	38, 58, 78, 92	0
1	C	377/403 (93%)	0.19	16 (4%) 40 45	36, 54, 83, 102	0
1	D	376/403 (93%)	0.32	20 (5%) 30 34	40, 66, 91, 107	0
All	All	1509/1612 (93%)	0.21	49 (3%) 51 56	36, 58, 84, 107	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	203	LEU	5.3
1	C	201	VAL	4.8
1	B	81	GLY	4.7
1	D	162	ALA	4.2
1	D	204	LEU	4.1
1	C	200	GLY	3.8
1	D	246	GLY	3.7
1	C	162	ALA	3.6
1	D	124	SER	3.5
1	D	245	VAL	3.5
1	D	169	TYR	3.4
1	D	193	THR	3.2
1	C	194	GLY	3.2
1	C	166	GLY	3.1
1	D	200	GLY	3.0
1	B	21	PRO	2.9
1	B	328	ALA	2.9
1	C	202	SER	2.8
1	D	249	ASN	2.8
1	D	166	GLY	2.8
1	A	328	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	2.6
1	A	81	GLY	2.6
1	D	131	TYR	2.6
1	D	247	ALA	2.6
1	A	201	VAL	2.5
1	C	158	LEU	2.5
1	D	199	GLY	2.5
1	B	61	LEU	2.5
1	D	167	ASP	2.4
1	C	161	ARG	2.4
1	C	244	LEU	2.4
1	C	195	GLY	2.3
1	C	193	THR	2.3
1	B	62	HIS	2.3
1	A	191	VAL	2.3
1	D	197	GLY	2.3
1	C	237	VAL	2.2
1	D	123	GLY	2.2
1	C	203	LEU	2.2
1	D	205	VAL	2.2
1	C	240	PRO	2.2
1	C	170	VAL	2.2
1	B	87	ILE	2.2
1	B	80	GLY	2.1
1	D	297	GLY	2.1
1	D	241	ALA	2.1
1	C	213	PHE	2.0
1	B	131	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	K	A	400	1/1	0.81	0.24	3.25	83,83,83,83	0
2	FDA	B	420	53/53	0.90	0.19	0.79	60,68,80,81	0
2	FDA	C	420	53/53	0.92	0.17	0.24	54,62,70,71	0
2	FDA	A	420	53/53	0.94	0.15	-0.03	46,55,60,61	0
3	K	C	400	1/1	0.86	0.10	-1.03	69,69,69,69	0
2	FDA	D	420	53/53	0.94	0.13	-1.12	56,61,66,67	0
3	K	D	400	1/1	0.86	0.10	-1.73	78,78,78,78	0
3	K	A	401	1/1	0.96	0.12	-	53,53,53,53	0
3	K	B	400	1/1	0.93	0.11	-	72,72,72,72	0
3	K	C	401	1/1	0.90	0.21	-	54,54,54,54	0

## 6.5 Other polymers

There are no such residues in this entry.