



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 PM GMT

PDB ID : 4B3I  
Title : Crystal structure of Mycobacterium tuberculosis fatty acid beta- oxidation complex with CoenzymeA bound at the hydratase active sites  
Authors : Venkatesan, R.; Wierenga, R.K.  
Deposited on : 2012-07-24  
Resolution : 2.63 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

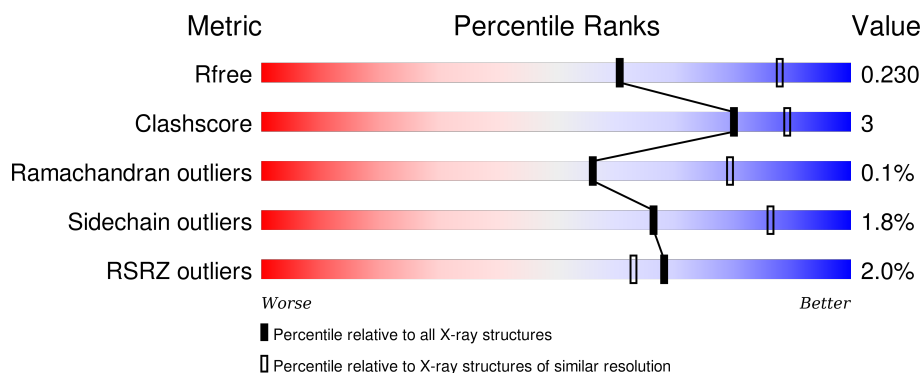
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	736	<div> <div>90%</div> <div>9%</div> </div>
1	B	736	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>
2	C	403	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
2	D	403	<div> <div>2%</div> <div>92%</div> <div>8%</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	SO4	B	1725	-	-	-	X
4	GOL	A	1729	-	-	-	X
4	GOL	B	1730	-	-	-	X
5	COA	A	1730	-	-	-	X
5	COA	B	1731	-	-	-	X
6	ADP	A	1731	-	-	-	X
6	ADP	C	1414	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17910 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 FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	731	Total	C	N	O	S	0	5	0
			5454	3453	940	1040	21			
1	B	728	Total	C	N	O	S	0	6	0
			5405	3423	925	1037	20			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP O53872
A	-14	GLY	-	EXPRESSION TAG	UNP O53872
A	-13	SER	-	EXPRESSION TAG	UNP O53872
A	-12	SER	-	EXPRESSION TAG	UNP O53872
A	-11	HIS	-	EXPRESSION TAG	UNP O53872
A	-10	HIS	-	EXPRESSION TAG	UNP O53872
A	-9	HIS	-	EXPRESSION TAG	UNP O53872
A	-8	HIS	-	EXPRESSION TAG	UNP O53872
A	-7	HIS	-	EXPRESSION TAG	UNP O53872
A	-6	HIS	-	EXPRESSION TAG	UNP O53872
A	-5	SER	-	EXPRESSION TAG	UNP O53872
A	-4	GLN	-	EXPRESSION TAG	UNP O53872
A	-3	ASP	-	EXPRESSION TAG	UNP O53872
A	-2	PRO	-	EXPRESSION TAG	UNP O53872
A	-1	ASN	-	EXPRESSION TAG	UNP O53872
A	0	SER	-	EXPRESSION TAG	UNP O53872
B	-15	MET	-	EXPRESSION TAG	UNP O53872
B	-14	GLY	-	EXPRESSION TAG	UNP O53872
B	-13	SER	-	EXPRESSION TAG	UNP O53872
B	-12	SER	-	EXPRESSION TAG	UNP O53872
B	-11	HIS	-	EXPRESSION TAG	UNP O53872
B	-10	HIS	-	EXPRESSION TAG	UNP O53872
B	-9	HIS	-	EXPRESSION TAG	UNP O53872
B	-8	HIS	-	EXPRESSION TAG	UNP O53872

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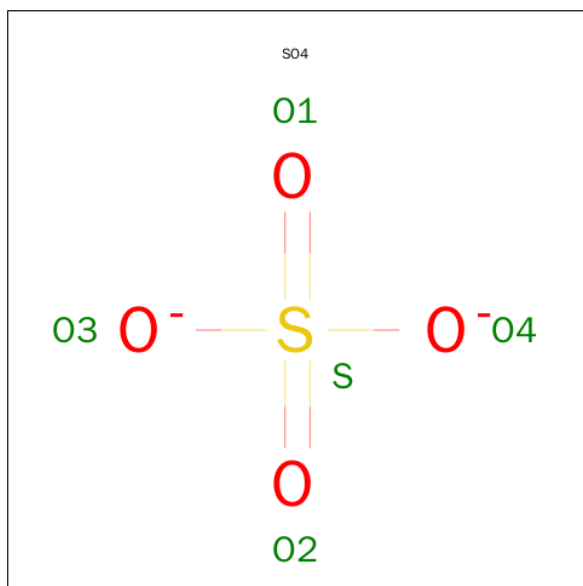
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	EXPRESSION TAG	UNP O53872
B	-6	HIS	-	EXPRESSION TAG	UNP O53872
B	-5	SER	-	EXPRESSION TAG	UNP O53872
B	-4	GLN	-	EXPRESSION TAG	UNP O53872
B	-3	ASP	-	EXPRESSION TAG	UNP O53872
B	-2	PRO	-	EXPRESSION TAG	UNP O53872
B	-1	ASN	-	EXPRESSION TAG	UNP O53872
B	0	SER	-	EXPRESSION TAG	UNP O53872

- Molecule 2 is a protein called FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	402	Total	C	N	O	S	0	3	0
			2976	1859	529	573	15			
2	D	403	Total	C	N	O	S	0	2	0
			2968	1854	525	574	15			

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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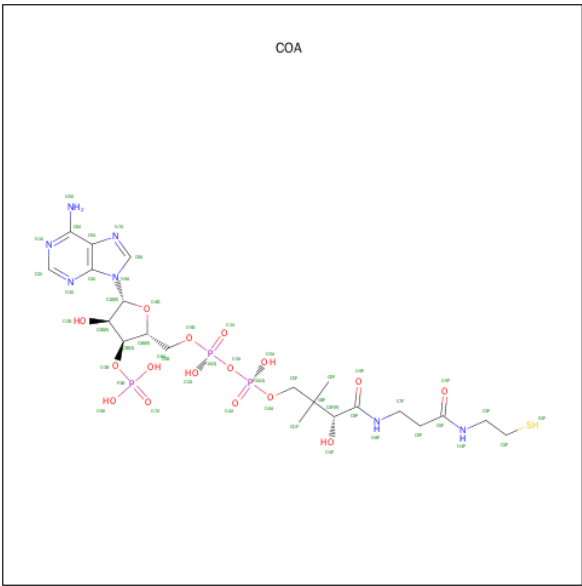
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



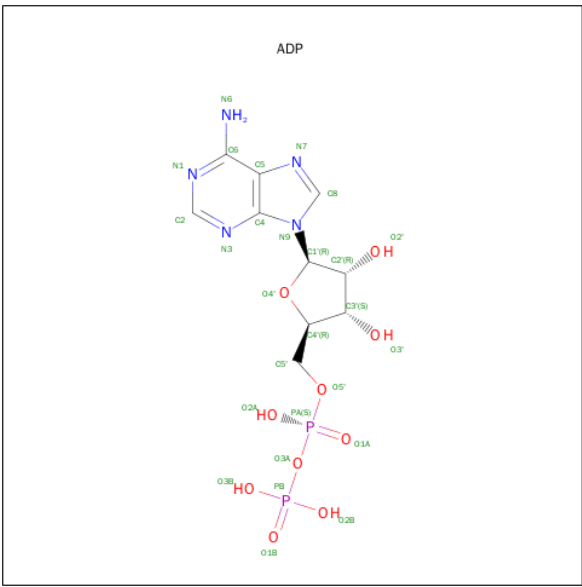
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

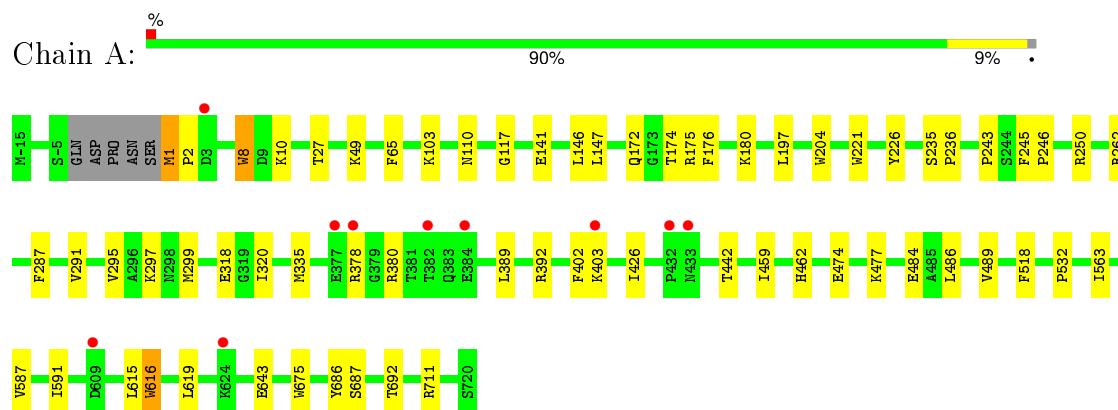
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	235	Total	O	0	0
			235	235		
7	B	254	Total	O	0	0
			254	254		
7	C	168	Total	O	0	0
			168	168		
7	D	122	Total	O	0	0
			122	122		

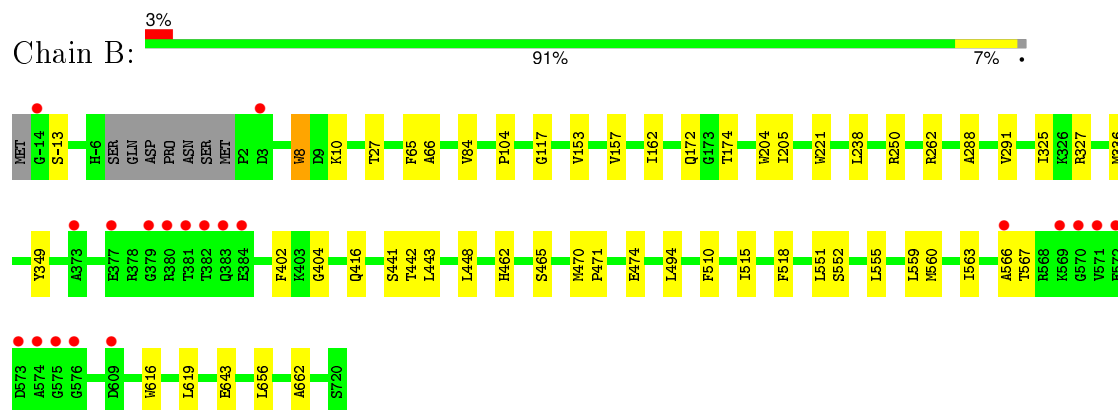
### 3 Residue-property plots

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.

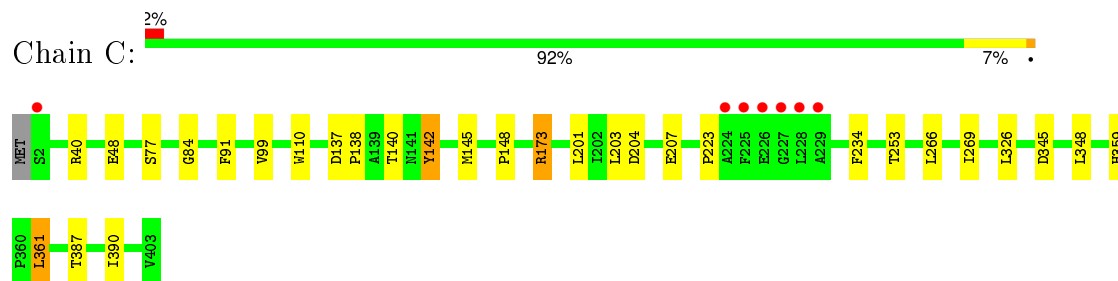
- Molecule 1: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB



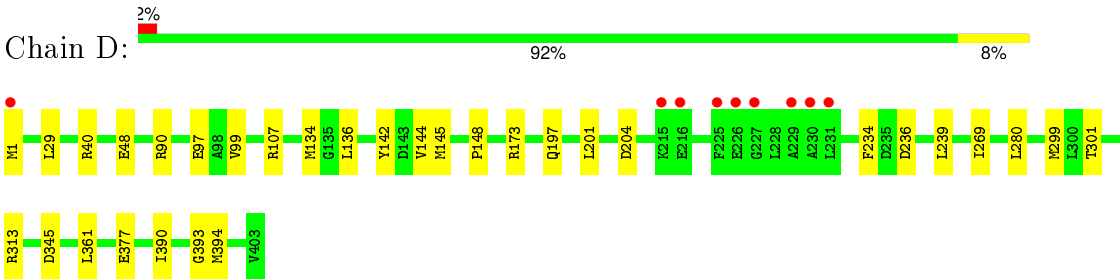
- Molecule 1: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB



- Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA



- Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	248.16Å 135.97Å 118.16Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.63 49.68 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.63) 100.0 (49.68-2.63)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.186 , 0.229 0.187 , 0.230	Depositor DCC
$R_{free}$ test set	5449 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 109047 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, GOL, SO4, ADP

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	0.40	3/5574 (0.1%)	0.51	0/7547
1	B	0.41	2/5527 (0.0%)	0.51	0/7490
2	C	0.40	0/3030	0.55	0/4103
2	D	0.40	0/3019	0.54	0/4092
All	All	0.40	5/17150 (0.0%)	0.52	0/23232

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	TRP	CD2-CE2	5.23	1.47	1.41
1	A	675	TRP	CD2-CE2	5.16	1.47	1.41
1	A	616	TRP	CD2-CE2	5.05	1.47	1.41
1	B	204	TRP	CD2-CE2	5.03	1.47	1.41
1	A	204	TRP	CD2-CE2	5.01	1.47	1.41

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	5454	0	5477	40	0
1	B	5405	0	5399	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2976	0	2996	25	0
2	D	2968	0	2975	25	0
3	A	35	0	0	0	0
3	B	45	0	0	0	0
3	C	50	0	0	0	0
3	D	30	0	0	0	0
4	A	12	0	16	2	0
4	B	6	0	8	0	0
5	A	48	0	32	0	0
5	B	48	0	32	0	0
6	A	27	0	12	0	0
6	C	27	0	12	0	0
7	A	235	0	0	3	0
7	B	254	0	0	3	0
7	C	168	0	0	0	0
7	D	122	0	0	1	0
All	All	17910	0	16959	116	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 3.

All (116) 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:262[A]:ARG:NE	2:C:142[A]:TYR:CE2	1.98	1.29
1:A:262[B]:ARG:HG3	1:A:262[B]:ARG:HH11	1.06	1.12
1:B:262[A]:ARG:HD3	2:C:142[A]:TYR:CD2	1.86	1.10
7:B:2147:HOH:O	2:D:197[A]:GLN:NE2	1.89	1.01
1:A:262[B]:ARG:CG	1:A:262[B]:ARG:HH11	1.73	0.99
1:B:262[A]:ARG:CD	2:C:142[A]:TYR:CD2	2.47	0.97
1:A:103:LYS:HE3	7:A:2018:HOH:O	1.66	0.93
1:A:262[B]:ARG:HG3	1:A:262[B]:ARG:NH1	1.80	0.90
1:B:262[A]:ARG:NE	2:C:142[A]:TYR:CD2	2.42	0.87
7:B:2147:HOH:O	2:D:197[A]:GLN:CD	2.15	0.80
2:D:90:ARG:HD3	2:D:394:MET:HE2	1.65	0.76
1:B:27:THR:HG21	1:B:66:ALA:HB3	1.67	0.75
1:B:84:VAL:HG11	1:B:291:VAL:HG11	1.68	0.74
7:B:2147:HOH:O	2:D:197[A]:GLN:OE1	2.05	0.72
2:C:84:GLY:HA2	2:D:394:MET:HE3	1.73	0.70
2:D:90:ARG:HH11	2:D:394:MET:HE1	1.57	0.70
2:D:40:ARG:HD2	2:D:48:GLU:OE2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HG3	1:B:448:LEU:HD23	1.77	0.67
1:B:563:ILE:HA	1:B:566:ALA:HB3	1.77	0.66
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.77	0.65
2:C:110:TRP:HD1	2:D:313:ARG:HD3	1.62	0.64
2:C:173:ARG:NH2	2:C:348:LEU:O	2.30	0.64
1:A:287:PHE:CE2	1:A:291:VAL:HG21	2.33	0.64
1:B:262[A]:ARG:HD3	2:C:142[A]:TYR:CG	2.33	0.63
1:B:559:LEU:O	1:B:563:ILE:HG23	1.99	0.63
1:A:711:ARG:HB3	4:A:1728:GOL:H2	1.80	0.63
1:A:262[B]:ARG:CG	1:A:262[B]:ARG:NH1	2.45	0.62
2:D:197[B]:GLN:OE1	7:D:2074:HOH:O	0.62	0.62
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.15	0.61
1:A:297:LYS:HE3	7:A:2132:HOH:O	2.02	0.59
1:B:27:THR:CG2	1:B:66:ALA:HB3	2.32	0.58
2:C:40:ARG:NH2	2:C:77:SER:O	2.32	0.58
1:B:262[A]:ARG:CD	2:C:142[A]:TYR:CE2	2.80	0.58
1:B:8[A]:TRP:CZ3	1:B:10:LYS:HB2	2.40	0.57
1:A:65:PHE:HB3	1:A:117:GLY:HA2	1.87	0.56
1:B:262[A]:ARG:CZ	2:C:142[A]:TYR:CE2	2.86	0.54
1:A:711:ARG:HH11	4:A:1728:GOL:H12	1.73	0.54
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.89	0.54
2:D:90:ARG:HH11	2:D:394:MET:CE	2.20	0.53
2:C:110:TRP:CH2	2:D:107:ARG:HD2	2.43	0.53
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.91	0.53
1:A:402:PHE:CD2	1:A:426:ILE:HG12	2.44	0.53
1:B:616:TRP:O	1:B:619:LEU:HB2	2.09	0.53
1:B:65:PHE:HB3	1:B:117:GLY:HA2	1.90	0.53
2:C:203:LEU:HD11	2:C:207:GLU:HG3	1.91	0.52
2:D:201:LEU:HD11	2:D:204:ASP:HB3	1.92	0.52
1:B:552:SER:O	1:B:555:LEU:O	2.28	0.51
1:A:141:GLU:HG3	1:A:147:LEU:C	2.31	0.51
2:C:201:LEU:HD11	2:C:204:ASP:HB3	1.93	0.51
1:B:515:ILE:HD11	1:B:551:LEU:HD21	1.94	0.50
2:D:134:MET:HB2	2:D:144:VAL:HG21	1.94	0.50
1:B:336:MET:SD	1:B:465:SER:HB3	2.52	0.50
1:A:243:PRO:HG3	2:D:136:LEU:HD23	1.94	0.49
1:A:686:TYR:O	1:A:692:THR:HA	2.12	0.49
1:A:8[A]:TRP:CZ3	1:A:10:LYS:HB2	2.47	0.49
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.94	0.49
1:B:84:VAL:HG11	1:B:291:VAL:CG1	2.39	0.49
1:B:262[A]:ARG:NE	2:C:142[A]:TYR:HE2	1.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8[A]:TRP:HZ3	1:A:10:LYS:HB2	1.78	0.48
1:A:65:PHE:HB3	1:A:117:GLY:CA	2.43	0.48
1:B:325:ILE:HB	1:B:349:TYR:CE1	2.49	0.47
1:B:327:ARG:HB3	1:B:404:GLY:O	2.15	0.47
2:D:148:PRO:HD3	2:D:234:PHE:CD1	2.50	0.47
2:C:140:THR:HG21	2:D:29:LEU:HD23	1.96	0.46
1:A:442:THR:HG21	1:A:563:ILE:HG12	1.98	0.46
1:B:8[A]:TRP:HZ3	1:B:10:LYS:HB2	1.79	0.46
1:A:245:PHE:HB2	1:A:246:PRO:HD3	1.98	0.46
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.31	0.46
1:A:221:TRP:HA	1:A:226:TYR:CD1	2.50	0.46
1:B:27:THR:HG21	1:B:66:ALA:CB	2.42	0.45
2:C:223:PRO:HA	2:C:253:THR:HG22	1.98	0.45
1:B:442:THR:HG21	1:B:563:ILE:CG2	2.46	0.45
1:A:518:PHE:HB2	1:A:643:GLU:CD	2.37	0.45
1:A:295:VAL:HG12	1:A:299:MET:HE3	1.98	0.45
2:D:390:ILE:HB	2:D:394:MET:HB2	1.97	0.45
1:B:656:LEU:HD13	1:B:662:ALA:HB2	1.98	0.45
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.99	0.44
1:A:587:VAL:O	1:A:591:ILE:HG12	2.17	0.44
7:A:2110:HOH:O	2:D:142[B]:TYR:CZ	2.68	0.44
1:A:378:ARG:HH21	1:A:380:ARG:NH2	2.15	0.44
2:C:40:ARG:HD3	2:C:48:GLU:OE2	2.18	0.44
2:D:299:MET:O	2:D:393:GLY:HA2	2.17	0.44
2:D:301:THR:HG22	2:D:301:THR:O	2.18	0.44
1:A:616:TRP:O	1:A:619:LEU:HB2	2.17	0.44
1:B:510:PHE:CD1	1:B:656:LEU:HD11	2.53	0.44
1:A:250:ARG:HD2	2:D:142[B]:TYR:CE2	2.53	0.44
2:C:91:PHE:HB2	2:C:390:ILE:HG23	2.00	0.44
2:D:1:MET:HA	2:D:107:ARG:HH21	1.82	0.43
1:A:378:ARG:HH21	1:A:380:ARG:HH22	1.65	0.43
1:B:560:MET:HA	1:B:563:ILE:HG12	1.99	0.43
1:B:65:PHE:HB3	1:B:117:GLY:CA	2.49	0.43
1:A:235:SER:HA	1:A:236:PRO:HD3	1.90	0.43
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.39	0.43
2:D:90:ARG:HH21	2:D:97:GLU:CD	2.21	0.43
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.99	0.43
1:A:287:PHE:O	1:A:291:VAL:HG23	2.19	0.43
1:A:616:TRP:HE3	1:A:619:LEU:HD13	1.83	0.43
1:B:470:MET:HA	1:B:471:PRO:HD3	1.79	0.43
2:C:326:LEU:HD13	2:C:387:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:VAL:HG13	2:C:269:ILE:HD11	2.01	0.42
2:C:359:HIS:CE1	2:C:361:LEU:HA	2.54	0.42
1:B:325:ILE:HB	1:B:349:TYR:HE1	1.83	0.42
1:A:532:PRO:HB2	1:A:615:LEU:HD13	2.02	0.42
2:D:1:MET:HA	2:D:107:ARG:NH2	2.34	0.42
1:A:1:MET:HA	1:A:2:PRO:HD3	1.94	0.42
2:C:148:PRO:HD3	2:C:234:PHE:CD1	2.55	0.41
1:A:320:ILE:HG21	1:A:484:GLU:HA	2.01	0.41
1:A:176:PHE:CD1	1:A:180:LYS:HD2	2.56	0.41
1:B:104:PRO:HG2	1:B:205:ILE:HG23	2.02	0.41
1:A:477:LYS:HB2	1:A:486:LEU:HD21	2.02	0.41
1:B:563:ILE:HA	1:B:566:ALA:CB	2.49	0.41
1:A:110:ASN:HA	1:A:197:LEU:HD11	2.03	0.41
1:B:153:VAL:O	1:B:157:VAL:HG23	2.21	0.40
2:C:137:ASP:HA	2:C:138:PRO:HD3	1.95	0.40
1:B:288:ALA:HA	1:B:291:VAL:HG12	2.04	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	732/736 (100%)	708 (97%)	23 (3%)	1 (0%)	56	79
1	B	730/736 (99%)	710 (97%)	20 (3%)	0	100	100
2	C	403/403 (100%)	390 (97%)	12 (3%)	1 (0%)	52	76
2	D	403/403 (100%)	391 (97%)	11 (3%)	1 (0%)	52	76
All	All	2268/2278 (100%)	2199 (97%)	66 (3%)	3 (0%)	56	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	361	LEU
1	A	318	GLU

### 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	560/566 (99%)	549 (98%)	11 (2%)	63	85
1	B	553/566 (98%)	543 (98%)	10 (2%)	66	86
2	C	309/310 (100%)	304 (98%)	5 (2%)	70	88
2	D	307/310 (99%)	300 (98%)	7 (2%)	58	81
All	All	1729/1752 (99%)	1696 (98%)	33 (2%)	66	85

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8[A]	TRP
1	A	8[B]	TRP
1	A	27	THR
1	A	49	LYS
1	A	172	GLN
1	A	174	THR
1	A	175	ARG
1	A	335	MET
1	A	403	LYS
1	A	687	SER
1	B	-13	SER
1	B	8[A]	TRP
1	B	8[B]	TRP
1	B	172	GLN
1	B	174	THR
1	B	402	PHE
1	B	441	SER
1	B	443	LEU

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Mol	Chain	Res	Type
1	B	494	LEU
1	B	567	THR
2	C	142[A]	TYR
2	C	142[B]	TYR
2	C	173	ARG
2	C	266	LEU
2	C	345	ASP
2	D	145	MET
2	D	173	ARG
2	D	236	ASP
2	D	239	LEU
2	D	280	LEU
2	D	345	ASP
2	D	377	GLU

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

### 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](#)

39 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	SO4	A	1721	-	4,4,4	0.36	0	6,6,6	0.16	0
3	SO4	A	1722	-	4,4,4	0.40	0	6,6,6	0.23	0
3	SO4	A	1723	-	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	A	1724	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	A	1725	-	4,4,4	0.38	0	6,6,6	0.17	0
3	SO4	A	1726	-	4,4,4	0.40	0	6,6,6	0.14	0
3	SO4	A	1727	-	4,4,4	0.33	0	6,6,6	0.15	0
4	GOL	A	1728	-	5,5,5	0.29	0	5,5,5	0.27	0
4	GOL	A	1729	-	5,5,5	0.30	0	5,5,5	0.29	0
5	COA	A	1730	-	40,50,50	0.86	2 (5%)	50,75,75	1.54	5 (10%)
6	ADP	A	1731	-	22,29,29	1.04	1 (4%)	27,45,45	2.10	5 (18%)
3	SO4	B	1721	-	4,4,4	0.37	0	6,6,6	0.12	0
3	SO4	B	1722	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	B	1723	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	B	1724	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	B	1725	-	4,4,4	0.32	0	6,6,6	0.17	0
3	SO4	B	1726	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	B	1727	-	4,4,4	0.39	0	6,6,6	0.07	0
3	SO4	B	1728	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	B	1729	-	4,4,4	0.37	0	6,6,6	0.17	0
4	GOL	B	1730	-	5,5,5	0.30	0	5,5,5	0.33	0
5	COA	B	1731	-	40,50,50	0.87	2 (5%)	50,75,75	1.63	7 (14%)
3	SO4	C	1404	-	4,4,4	0.27	0	6,6,6	0.19	0
3	SO4	C	1405	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	C	1406	-	4,4,4	0.37	0	6,6,6	0.16	0
3	SO4	C	1407	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	C	1408	-	4,4,4	0.35	0	6,6,6	0.14	0
3	SO4	C	1409	-	4,4,4	0.40	0	6,6,6	0.17	0
3	SO4	C	1410	-	4,4,4	0.34	0	6,6,6	0.15	0
3	SO4	C	1411	-	4,4,4	0.41	0	6,6,6	0.09	0
3	SO4	C	1412	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	C	1413	-	4,4,4	0.42	0	6,6,6	0.12	0
6	ADP	C	1414	-	22,29,29	1.15	2 (9%)	27,45,45	1.79	2 (7%)
3	SO4	D	1404	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	D	1405	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	D	1406	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	D	1407	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	D	1408	-	4,4,4	0.36	0	6,6,6	0.15	0
3	SO4	D	1409	-	4,4,4	0.38	0	6,6,6	0.08	0

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	SO4	A	1721	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1722	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1723	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1724	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1725	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1726	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1727	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1728	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1729	-	-	0/4/4/4	0/0/0/0
5	COA	A	1730	-	-	0/44/64/64	0/3/3/3
6	ADP	A	1731	-	-	0/12/32/32	0/3/3/3
3	SO4	B	1721	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1722	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1723	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1724	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1725	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1726	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1727	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1728	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1729	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1730	-	-	0/4/4/4	0/0/0/0
5	COA	B	1731	-	-	0/44/64/64	0/3/3/3
3	SO4	C	1404	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1405	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1406	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1407	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1408	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1409	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1410	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1411	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1412	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1413	-	-	0/0/0/0	0/0/0/0
6	ADP	C	1414	-	-	0/12/32/32	0/3/3/3
3	SO4	D	1404	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1405	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1406	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1407	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1408	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1409	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1731	COA	O4B-C1B	2.20	1.44	1.41
6	C	1414	ADP	O4'-C1'	2.31	1.44	1.41
5	A	1730	COA	O4B-C1B	2.35	1.44	1.41
6	A	1731	ADP	C5-C4	3.26	1.47	1.40
5	A	1730	COA	C5A-C4A	3.27	1.47	1.40
5	B	1731	COA	C5A-C4A	3.31	1.48	1.40
6	C	1414	ADP	C5-C4	3.52	1.48	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1731	COA	N3A-C2A-N1A	-7.94	122.82	128.89
6	A	1731	ADP	N3-C2-N1	-7.87	122.87	128.89
5	A	1730	COA	N3A-C2A-N1A	-7.57	123.10	128.89
6	C	1414	ADP	N3-C2-N1	-7.11	123.45	128.89
6	A	1731	ADP	C4'-O4'-C1'	-3.80	105.54	109.72
5	A	1730	COA	P2A-O3A-P1A	-3.62	122.56	132.73
6	A	1731	ADP	C4-C5-N7	-3.23	106.51	109.48
5	B	1731	COA	P2A-O3A-P1A	-3.09	124.04	132.73
5	B	1731	COA	C4A-C5A-N7A	-3.04	106.68	109.48
6	C	1414	ADP	C4-C5-N7	-3.02	106.70	109.48
5	B	1731	COA	C2B-C1B-N9A	-2.80	110.02	114.29
5	A	1730	COA	C4A-C5A-N7A	-2.80	106.91	109.48
6	A	1731	ADP	PA-O3A-PB	-2.78	123.34	132.67
5	A	1730	COA	C1B-N9A-C4A	-2.00	123.92	126.94
5	B	1731	COA	O9A-P3B-O8A	2.03	115.12	107.38
5	B	1731	COA	CEP-CBP-CAP	2.17	113.30	109.34
5	A	1730	COA	O4B-C1B-N9A	2.51	113.36	108.10
6	A	1731	ADP	O4'-C1'-N9	2.73	113.82	108.10
5	B	1731	COA	O4B-C1B-N9A	2.84	114.05	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1728	GOL	2	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	731/736 (99%)	-0.28	10 (1%) 78 74	22, 40, 63, 90	0
1	B	728/736 (98%)	-0.20	20 (2%) 58 52	23, 38, 71, 115	0
2	C	402/403 (99%)	-0.26	7 (1%) 73 68	21, 29, 47, 102	0
2	D	403/403 (100%)	-0.25	9 (2%) 65 59	21, 34, 51, 84	0
All	All	2264/2278 (99%)	-0.24	46 (2%) 68 63	21, 36, 64, 115	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	226	GLU	5.4
1	B	573	ASP	5.4
2	D	225	PHE	4.6
2	C	229	ALA	4.5
1	B	566	ALA	4.4
1	B	381	THR	4.1
1	B	576	GLY	4.0
2	C	227	GLY	3.8
1	B	575	GLY	3.7
1	B	-14	GLY	3.6
1	B	377	GLU	3.6
1	B	574	ALA	3.5
1	B	570	GLY	3.2
1	B	3	ASP	3.2
1	B	572	GLU	3.2
1	B	382	THR	3.2
2	C	225	PHE	3.1
1	A	433	ASN	3.1
2	D	227	GLY	3.1
1	A	3	ASP	3.1
1	A	382	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	379	GLY	3.0
1	B	571	VAL	3.0
2	C	228	LEU	2.9
2	D	1	MET	2.7
1	A	378	ARG	2.6
1	B	609	ASP	2.5
2	C	2	SER	2.4
2	C	224	ALA	2.4
1	A	432	PRO	2.4
1	B	569	LYS	2.4
1	B	383	GLN	2.3
1	A	609	ASP	2.3
1	B	380	ARG	2.3
1	A	403	LYS	2.3
2	D	230	ALA	2.2
1	B	384	GLU	2.2
1	B	373	ALA	2.2
2	D	216	GLU	2.2
1	A	384	GLU	2.2
1	A	624	LYS	2.2
2	D	226	GLU	2.2
2	D	231	LEU	2.1
2	D	215	LYS	2.1
2	D	229	ALA	2.0
1	A	377	GLU	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ADP	A	1731	27/27	0.73	0.36	14.48	92,105,119,121	0
6	ADP	C	1414	27/27	0.76	0.36	14.00	67,87,109,110	0
4	GOL	A	1729	6/6	0.91	0.23	10.94	48,50,50,51	0
3	SO4	B	1725	5/5	0.73	0.37	7.40	57,57,58,58	5
4	GOL	B	1730	6/6	0.87	0.22	3.98	53,54,54,54	0
5	COA	A	1730	48/48	0.94	0.22	2.83	49,59,65,67	0
5	COA	B	1731	48/48	0.90	0.21	2.08	66,76,82,83	0
3	SO4	C	1405	5/5	0.99	0.23	1.36	48,49,50,51	0
3	SO4	C	1412	5/5	0.89	0.20	1.27	47,48,49,49	5
3	SO4	C	1413	5/5	0.96	0.21	1.13	58,61,64,64	0
3	SO4	C	1408	5/5	0.96	0.25	1.00	51,52,53,53	5
3	SO4	D	1408	5/5	0.97	0.18	0.59	64,64,66,66	0
4	GOL	A	1728	6/6	0.94	0.14	-0.23	54,55,56,57	0
3	SO4	B	1722	5/5	0.98	0.12	-0.46	55,55,56,56	0
3	SO4	A	1722	5/5	0.98	0.11	-0.64	47,49,51,51	0
3	SO4	B	1721	5/5	0.97	0.12	-0.96	50,51,51,52	0
3	SO4	A	1721	5/5	0.98	0.11	-1.94	46,47,47,48	0
3	SO4	C	1406	5/5	0.95	0.23	-	65,67,68,69	0
3	SO4	D	1406	5/5	0.96	0.31	-	61,62,64,65	0
3	SO4	D	1409	5/5	0.78	0.25	-	93,94,96,97	5
3	SO4	A	1724	5/5	0.85	0.20	-	66,67,69,69	5
3	SO4	B	1729	5/5	0.90	0.19	-	85,86,87,88	0
3	SO4	C	1407	5/5	0.95	0.33	-	72,74,76,77	0
3	SO4	A	1725	5/5	0.83	0.23	-	39,40,40,41	5
3	SO4	D	1405	5/5	0.97	0.25	-	59,60,61,61	0
3	SO4	C	1404	5/5	0.99	0.11	-	37,40,41,41	0
3	SO4	A	1727	5/5	0.86	0.35	-	23,23,23,23	5
3	SO4	D	1404	5/5	0.96	0.10	-	70,72,73,73	0
3	SO4	B	1724	5/5	0.89	0.21	-	43,44,44,44	5
3	SO4	D	1407	5/5	0.99	0.23	-	59,60,60,60	0
3	SO4	A	1726	5/5	0.83	0.31	-	48,48,49,50	5
3	SO4	B	1728	5/5	0.95	0.28	-	62,63,63,64	0
3	SO4	B	1726	5/5	0.93	0.20	-	46,46,48,48	5
3	SO4	C	1409	5/5	0.94	0.27	-	49,49,51,53	5
3	SO4	C	1410	5/5	0.93	0.16	-	44,46,46,47	5
3	SO4	B	1727	5/5	0.90	0.17	-	30,30,31,31	5
3	SO4	C	1411	5/5	0.90	0.21	-	47,48,48,49	5
3	SO4	A	1723	5/5	0.96	0.19	-	67,68,69,69	0
3	SO4	B	1723	5/5	0.91	0.32	-	62,63,64,64	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.