



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:18 PM GMT

PDB ID : 4BCA  
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATESYN-  
THASE: Tyr578Phe mutant  
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Deposited on : 2012-10-01  
Resolution : 2.40 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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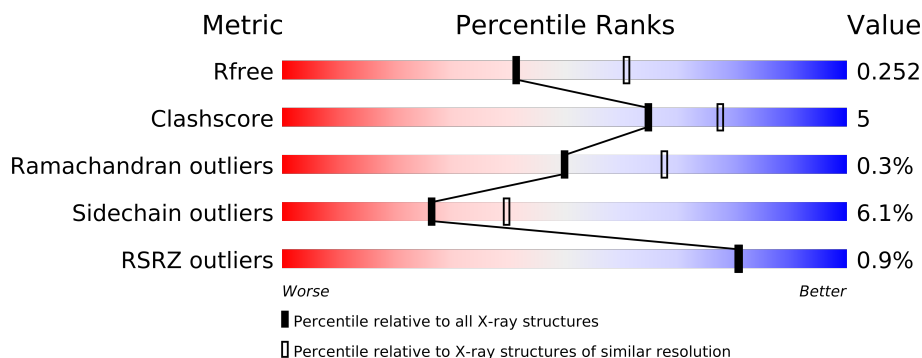
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	658	
1	B	658	
1	C	658	
1	D	658	

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	CL	A	1659	-	X
3	CL	B	1659	-	X
3	CL	C	1659	-	X
3	CL	D	1659	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	B	1661	-	X
4	SO4	D	1661	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18202 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 ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4393	2789	762	818	24			
1	B	543	Total	C	N	O	S	0	0	0
			4300	2732	747	797	24			
1	C	557	Total	C	N	O	S	0	2	0
			4412	2799	766	822	25			
1	D	550	Total	C	N	O	S	0	1	0
			4354	2761	757	811	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	PHE	TYR	ENGINEERED MUTATION	UNP P97275
B	578	PHE	TYR	ENGINEERED MUTATION	UNP P97275
C	578	PHE	TYR	ENGINEERED MUTATION	UNP P97275
D	578	PHE	TYR	ENGINEERED MUTATION	UNP P97275

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).

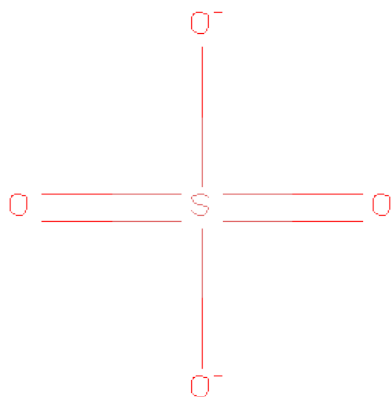


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



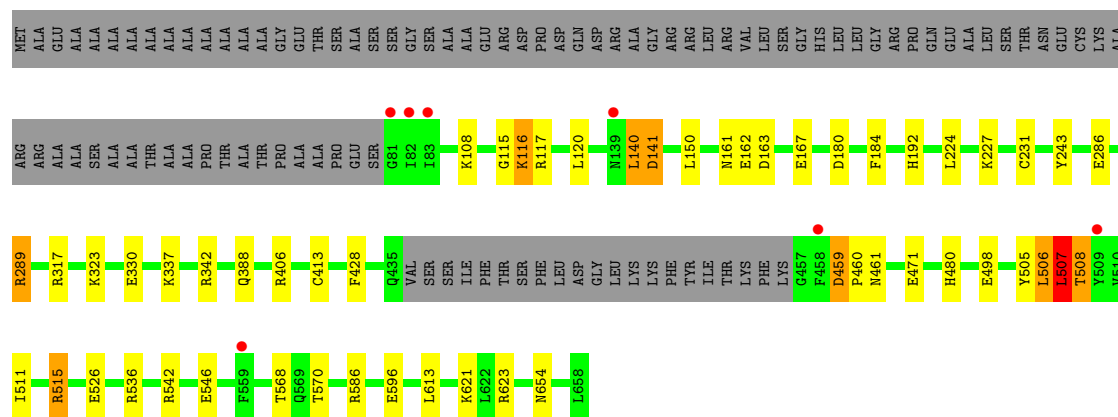
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	95	Total	O	0	0
			95	95		
5	C	143	Total	O	0	0
			143	143		
5	D	112	Total	O	0	0
			112	112		

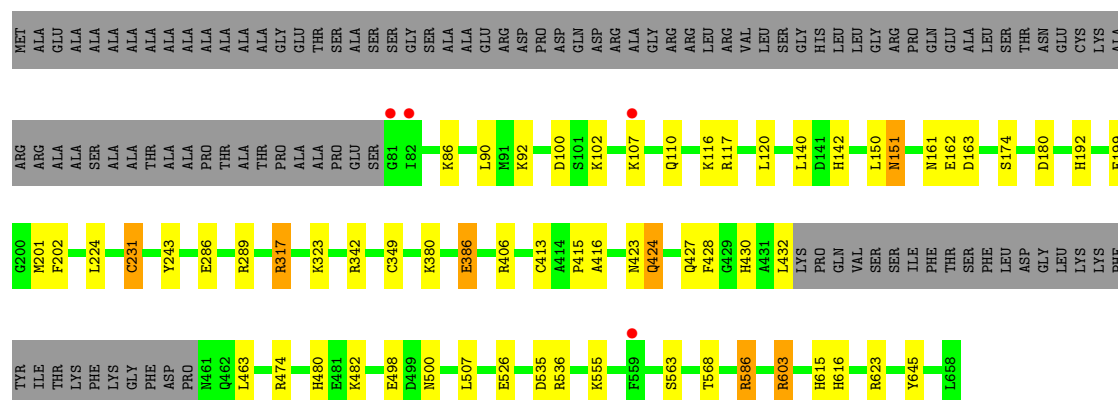


Chain C:



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE, PEROXISOMAL

## Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.68Å 99.32Å 107.98Å 90.43° 92.12° 95.20°	Depositor
Resolution (Å)	47.58 – 2.40 47.15 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.58-2.40) 98.7 (47.15-2.40)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.187 , 0.252 0.191 , 0.252	Depositor DCC
$R_{free}$ test set	1080 reflections (1.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 10.4	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 98366 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SO4, FAD, CL

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	0.93	2/4492 (0.0%)	0.90	6/6071 (0.1%)
1	B	0.89	0/4397	0.88	7/5942 (0.1%)
1	C	0.96	4/4518 (0.1%)	0.90	9/6107 (0.1%)
1	D	0.96	3/4454 (0.1%)	0.91	12/6020 (0.2%)
All	All	0.94	9/17861 (0.1%)	0.90	34/24140 (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	C	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	CYS	CB-SG	-6.42	1.71	1.82
1	C	546	GLU	CG-CD	5.95	1.60	1.51
1	D	386	GLU	CG-CD	5.93	1.60	1.51
1	C	330	GLU	CB-CG	5.86	1.63	1.52
1	D	231	CYS	CB-SG	-5.74	1.72	1.81
1	D	349	CYS	CB-SG	-5.74	1.72	1.81
1	A	399	GLU	CG-CD	5.71	1.60	1.51
1	A	386	GLU	CG-CD	5.70	1.60	1.51
1	C	330	GLU	CG-CD	5.30	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	603	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	C	317	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	D	603	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	D	536	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	B	603	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	623	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	D	603	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	C	623	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	515	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	463	LEU	CA-CB-CG	6.37	129.95	115.30
1	D	90	LEU	CA-CB-CG	6.13	129.41	115.30
1	D	380	LYS	CD-CE-NZ	-5.98	97.94	111.70
1	C	180	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	100	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	603	ARG	CD-NE-CZ	5.71	131.59	123.60
1	D	140	LEU	CA-CB-CG	5.69	128.38	115.30
1	B	140	LEU	CA-CB-CG	5.66	128.33	115.30
1	A	623	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	317	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	412	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	506	LEU	CA-CB-CG	5.53	128.01	115.30
1	C	515	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	174	SER	N-CA-CB	-5.42	102.37	110.50
1	D	623	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	623	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	542	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	463	LEU	CA-CB-CG	5.17	127.18	115.30
1	B	623	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	140	LEU	CA-CB-CG	5.13	127.10	115.30
1	D	536	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	638	MET	CG-SD-CE	5.11	108.37	100.20
1	D	317	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	515	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	289	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	460	PRO	Peptide
1	C	507	LEU	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	4393	0	0	29	0
1	B	4300	0	0	16	1
1	C	4412	0	0	24	1
1	D	4354	0	0	21	0
2	A	53	0	0	2	0
2	B	53	0	0	1	0
2	C	53	0	0	1	0
2	D	53	0	0	1	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
4	C	5	0	0	1	0
4	D	10	0	0	2	0
5	A	142	0	0	9	0
5	B	95	0	0	1	0
5	C	143	0	0	5	0
5	D	112	0	0	5	0
All	All	18202	0	0	94	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:MET:CG	5:A:2099:HOH:O	1.93	1.15
1:A:192:HIS:CB	1:A:243:TYR:OH	2.18	0.92
1:C:507:LEU:CD1	1:C:511:ILE:CG1	2.49	0.91
1:B:192:HIS:CB	1:B:243:TYR:OH	2.21	0.88
1:B:140:LEU:CB	5:B:2014:HOH:O	2.21	0.88
1:C:508:THR:CA	1:C:511:ILE:CD1	2.52	0.87
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.73	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:142:HIS:CE1	1:D:586:ARG:NH2	2.58	0.72
1:A:625:GLN:OE1	5:A:2132:HOH:O	2.07	0.71
1:D:192:HIS:CB	1:D:243:TYR:OH	2.37	0.71
1:C:161:ASN:OD1	1:C:163:ASP:N	2.25	0.70
1:A:569:GLN:NE2	5:A:2061:HOH:O	2.26	0.68
1:A:213:THR:O	5:A:2032:HOH:O	2.13	0.67
2:A:999:FAD:N5	3:A:1659:CL:CL	2.65	0.66
1:D:424:GLN:NE2	1:D:563:SER:O	2.30	0.65
1:B:503:ARG:O	1:B:505:TYR:N	2.30	0.65
1:C:480:HIS:ND1	4:C:1660:SO4:O3	2.29	0.64
2:D:999:FAD:N5	3:D:1659:CL:CL	2.68	0.64
1:D:386:GLU:CB	5:D:2084:HOH:O	2.45	0.64
1:C:515:ARG:NH2	5:C:2117:HOH:O	2.30	0.63
1:D:342:ARG:NE	1:D:645:TYR:O	2.33	0.61
1:C:461:ASN:CG	5:C:2112:HOH:O	2.39	0.61
1:B:195:PHE:O	1:B:196:LEU:C	2.40	0.60
1:C:507:LEU:CD1	1:C:511:ILE:CD1	2.80	0.59
1:B:139:ASN:O	1:B:140:LEU:CB	2.51	0.59
1:A:571:TYR:OH	1:A:615:HIS:CE1	2.56	0.58
1:A:286:GLU:OE2	1:A:289:ARG:NH2	2.36	0.58
2:C:999:FAD:N5	3:C:1659:CL:CL	2.73	0.58
1:C:508:THR:OG1	1:C:511:ILE:CD1	2.51	0.57
1:D:423:ASN:ND2	1:D:427:GLN:NE2	2.52	0.57
1:D:286:GLU:OE2	1:D:289:ARG:NH2	2.39	0.55
1:A:480:HIS:CE1	4:A:1661:SO4:O4	2.60	0.55
1:A:192:HIS:CG	1:A:243:TYR:OH	2.60	0.54
1:A:189:HIS:CE1	5:A:2027:HOH:O	2.59	0.54
1:A:192:HIS:CD2	1:A:243:TYR:OH	2.61	0.54
1:C:505:TYR:O	1:C:508:THR:N	2.41	0.54
1:C:141:ASP:OD1	1:C:141:ASP:N	2.41	0.53
1:D:161:ASN:OD1	1:D:163:ASP:N	2.42	0.52
1:D:92:LYS:NZ	5:D:2009:HOH:O	2.42	0.52
1:D:480:HIS:ND1	4:D:1660:SO4:O2	2.43	0.51
1:A:428:PHE:C	1:A:428:PHE:CD1	2.84	0.51
1:A:330:GLU:OE1	1:B:353:ARG:NH2	2.44	0.50
1:B:196:LEU:O	1:B:199:GLU:N	2.45	0.50
2:B:999:FAD:N5	3:B:1659:CL:CL	2.82	0.50
1:A:399:GLU:OE2	5:A:2094:HOH:O	2.19	0.50
1:B:423:ASN:ND2	1:B:427:GLN:NE2	2.60	0.49
1:D:413:CYS:O	1:D:480:HIS:NE2	2.46	0.49
1:A:349:CYS:SG	1:A:354:MET:CE	3.01	0.49
1:A:271:GLU:OE1	1:A:296:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:161:ASN:OD1	1:C:161:ASN:C	2.51	0.48
1:A:133:GLN:NE2	1:A:139:ASN:O	2.48	0.47
1:B:555:LYS:NZ	1:B:597:GLN:NE2	2.64	0.46
1:C:192:HIS:CB	1:C:243:TYR:OH	2.64	0.46
1:A:277:HIS:CE1	1:A:376:GLU:OE1	2.69	0.46
1:C:286:GLU:OE2	1:C:289:ARG:NH2	2.49	0.46
1:D:500:ASN:N	5:D:2095:HOH:O	2.49	0.46
1:D:415:PRO:O	1:D:416:ALA:C	2.55	0.45
1:C:570:THR:N	5:C:2069:HOH:O	2.49	0.45
1:A:388:GLN:NE2	5:A:2064:HOH:O	2.48	0.45
1:C:184:PHE:CD1	1:C:184:PHE:O	2.70	0.45
1:D:161:ASN:OD1	1:D:161:ASN:C	2.55	0.45
1:B:480:HIS:CE1	4:B:1660:SO4:O1	2.69	0.44
1:A:439:ILE:CG1	1:D:535:ASP:CB	2.96	0.44
5:C:2089:HOH:O	1:D:317:ARG:NH1	2.49	0.44
1:B:133:GLN:NE2	1:B:139:ASN:O	2.51	0.44
1:D:201:MET:SD	1:D:202:PHE:N	2.91	0.44
1:B:204:ARG:NH2	1:B:253:ARG:O	2.51	0.43
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.50	0.43
1:B:432:LEU:N	1:B:432:LEU:CD1	2.81	0.43
1:C:115:GLY:O	1:C:116:LYS:CD	2.67	0.43
1:A:167:GLU:OE2	1:A:227:LYS:NZ	2.51	0.43
1:C:459:ASP:CB	5:C:2111:HOH:O	2.67	0.43
1:C:507:LEU:C	1:C:507:LEU:CD1	2.87	0.43
1:D:151:ASN:C	1:D:151:ASN:ND2	2.71	0.43
1:A:480:HIS:CG	5:A:2110:HOH:O	2.72	0.42
1:C:508:THR:CB	1:C:511:ILE:CD1	2.97	0.42
1:C:167:GLU:OE2	1:C:227:LYS:NZ	2.52	0.42
1:C:413:CYS:O	1:C:480:HIS:NE2	2.52	0.42
1:A:201:MET:CG	1:A:202:PHE:N	2.82	0.42
2:A:999:FAD:C4X	3:A:1659:CL:CL	3.04	0.42
1:A:201:MET:SD	1:A:202:PHE:N	2.93	0.41
1:B:615:HIS:ND1	1:B:616:HIS:ND1	2.68	0.41
1:B:196:LEU:O	1:B:197:LEU:C	2.57	0.41
1:A:215:HIS:CD2	1:A:375:THR:OG1	2.73	0.41
1:A:118:TYR:OH	1:A:306:GLU:OE2	2.38	0.41
1:D:615:HIS:ND1	1:D:616:HIS:ND1	2.68	0.41
1:B:330:GLU:N	1:B:330:GLU:OE1	2.54	0.41
1:D:161:ASN:OD1	1:D:162:GLU:N	2.54	0.41
1:C:621:LYS:NZ	1:C:654:ASN:O	2.54	0.41
1:D:480:HIS:CE1	5:D:2088:HOH:O	2.74	0.40
1:C:505:TYR:C	1:C:507:LEU:N	2.75	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:505:TYR:O	1:A:508:THR:OG1	2.40	0.40
4:D:1661:SO4:O4	5:D:2067:HOH:O	2.20	0.40
1:A:189:HIS:CD2	5:A:2113:HOH:O	2.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:ASN:ND2	1:C:536:ARG:NH2[1_546]	2.14	0.06

## 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	549/658 (83%)	534 (97%)	15 (3%)	0	100	100
1	B	537/658 (82%)	514 (96%)	18 (3%)	5 (1%)	25	35
1	C	555/658 (84%)	528 (95%)	26 (5%)	1 (0%)	56	74
1	D	547/658 (83%)	525 (96%)	21 (4%)	1 (0%)	56	74
All	All	2188/2632 (83%)	2101 (96%)	80 (4%)	7 (0%)	50	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	504	GLY
1	B	195	PHE
1	B	196	LEU
1	C	506	LEU
1	B	503	ARG
1	D	430	HIS
1	B	477	VAL

### 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	476/545 (87%)	440 (92%)	36 (8%)	19	28
1	B	464/545 (85%)	436 (94%)	28 (6%)	27	41
1	C	479/545 (88%)	456 (95%)	23 (5%)	35	53
1	D	472/545 (87%)	444 (94%)	28 (6%)	28	42
All	All	1891/2180 (87%)	1776 (94%)	115 (6%)	26	40

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	105	LEU
1	A	107	LYS
1	A	108	LYS
1	A	116	LYS
1	A	120	LEU
1	A	162	GLU
1	A	165	LEU
1	A	174	SER
1	A	180	ASP
1	A	199	GLU
1	A	224	LEU
1	A	263	MET
1	A	323	LYS
1	A	342	ARG
1	A	354	MET
1	A	406	ARG
1	A	419	ARG
1	A	428	PHE
1	A	439	ILE
1	A	462	GLN
1	A	463	LEU
1	A	476	LYS
1	A	498	GLU
1	A	499	ASP
1	A	508	THR

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Mol	Chain	Res	Type
1	A	515	ARG
1	A	520	GLU
1	A	526	GLU
1	A	555	LYS
1	A	559	PHE
1	A	586	ARG
1	A	588	ILE
1	A	592	LEU
1	A	613	LEU
1	A	625	GLN
1	B	116	LYS
1	B	117	ARG
1	B	120	LEU
1	B	174	SER
1	B	180	ASP
1	B	195	PHE
1	B	199	GLU
1	B	298	THR
1	B	323	LYS
1	B	354	MET
1	B	384	THR
1	B	406	ARG
1	B	421	MET
1	B	428	PHE
1	B	432	LEU
1	B	476	LYS
1	B	478	LEU
1	B	498	GLU
1	B	507	LEU
1	B	515	ARG
1	B	516	ASP
1	B	520	GLU
1	B	526	GLU
1	B	555	LYS
1	B	568	THR
1	B	586	ARG
1	B	603	ARG
1	B	613	LEU
1	C	108	LYS
1	C	116	LYS
1	C	117	ARG
1	C	120	LEU

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Mol	Chain	Res	Type
1	C	140	LEU
1	C	141	ASP
1	C	150	LEU
1	C	162	GLU
1	C	224	LEU
1	C	323	LYS
1	C	337	LYS
1	C	342	ARG
1	C	406	ARG
1	C	428	PHE
1	C	459	ASP
1	C	498	GLU
1	C	507	LEU
1	C	508	THR
1	C	526	GLU
1	C	568	THR
1	C	586	ARG
1	C	596	GLU
1	C	613	LEU
1	D	86	LYS
1	D	102	LYS
1	D	107	LYS
1	D	110	GLN
1	D	116	LYS
1	D	117	ARG
1	D	120	LEU
1	D	150	LEU
1	D	151	ASN
1	D	174	SER
1	D	180	ASP
1	D	199	GLU
1	D	224	LEU
1	D	231	CYS
1	D	323	LYS
1	D	406	ARG
1	D	424	GLN
1	D	428	PHE
1	D	432	LEU
1	D	474	ARG
1	D	482	LYS
1	D	498	GLU
1	D	507	LEU

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Mol	Chain	Res	Type
1	D	526	GLU
1	D	555	LYS
1	D	568	THR
1	D	586	ARG
1	D	603	ARG

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z  > 2$
4	SO4	A	1660	-	4,4,4	0.26	0	6,6,6	1.09	1 (16%)
4	SO4	A	1661	-	4,4,4	0.56	0	6,6,6	0.46	0
2	FAD	A	999	-	58,58,58	1.27	7 (12%)	85,89,89	2.02	15 (17%)
4	SO4	B	1660	-	4,4,4	0.53	0	6,6,6	0.61	0
4	SO4	B	1661	-	4,4,4	0.36	0	6,6,6	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	B	999	-	58,58,58	1.35	8 (13%)	85,89,89	2.14	18 (21%)
4	SO4	C	1660	-	4,4,4	0.52	0	6,6,6	0.49	0
2	FAD	C	999	-	58,58,58	1.29	6 (10%)	85,89,89	2.18	18 (21%)
4	SO4	D	1660	-	4,4,4	0.34	0	6,6,6	0.63	0
4	SO4	D	1661	-	4,4,4	0.44	0	6,6,6	0.56	0
2	FAD	D	999	-	58,58,58	1.14	5 (8%)	85,89,89	2.03	19 (22%)

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
4	SO4	A	1660	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1661	-	-	0/0/0/0	0/0/0/0
2	FAD	A	999	-	-	0/34/50/50	0/1/6/6
4	SO4	B	1660	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1661	-	-	0/0/0/0	0/0/0/0
2	FAD	B	999	-	-	0/34/50/50	0/1/6/6
4	SO4	C	1660	-	-	0/0/0/0	0/0/0/0
2	FAD	C	999	-	-	0/34/50/50	0/1/6/6
4	SO4	D	1660	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1661	-	-	0/0/0/0	0/0/0/0
2	FAD	D	999	-	-	0/34/50/50	0/1/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	FAD	C1'-C2'	4.44	1.55	1.51
2	B	999	FAD	C1'-C2'	4.39	1.55	1.51
2	B	999	FAD	C4X-N5	3.74	1.44	1.36
2	C	999	FAD	C5X-N5	3.53	1.40	1.35
2	A	999	FAD	C1'-N10	3.42	1.52	1.48
2	C	999	FAD	C2A-N3A	3.08	1.38	1.32
2	D	999	FAD	C5X-N5	2.93	1.39	1.35
2	B	999	FAD	C2A-N3A	2.85	1.37	1.32
2	D	999	FAD	C6-C5X	-2.83	1.38	1.41
2	B	999	FAD	C5X-N5	2.80	1.39	1.35
2	C	999	FAD	C2B-C1B	-2.77	1.49	1.53
2	B	999	FAD	C1'-N10	2.72	1.51	1.48
2	C	999	FAD	C1'-N10	2.71	1.51	1.48
2	A	999	FAD	C4-N3	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	FAD	C1'-C2'	2.58	1.54	1.51
2	D	999	FAD	C2A-N3A	2.54	1.37	1.32
2	D	999	FAD	C9A-N10	2.47	1.42	1.38
2	A	999	FAD	C5X-N5	2.45	1.39	1.35
2	B	999	FAD	O4'-C4'	-2.45	1.37	1.43
2	A	999	FAD	C2A-N3A	2.41	1.37	1.32
2	A	999	FAD	C8A-N9A	2.38	1.40	1.36
2	B	999	FAD	C2A-N1A	2.37	1.38	1.33
2	C	999	FAD	C4A-N9A	2.36	1.41	1.37
2	B	999	FAD	C6-C5X	-2.31	1.39	1.41
2	A	999	FAD	C2A-N1A	2.13	1.38	1.33
2	D	999	FAD	PA-O3P	2.07	1.63	1.59

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	N3A-C2A-N1A	-10.86	119.63	128.71
2	C	999	FAD	N3A-C2A-N1A	-9.97	120.37	128.71
2	B	999	FAD	C2-N1-C10	8.92	123.96	114.98
2	B	999	FAD	N3A-C2A-N1A	-8.02	122.00	128.71
2	D	999	FAD	C2-N1-C10	7.99	123.03	114.98
2	D	999	FAD	N3A-C2A-N1A	-7.95	122.07	128.71
2	C	999	FAD	C4B-O4B-C1B	6.66	116.98	109.75
2	A	999	FAD	O4B-C1B-N9A	-6.42	102.47	108.44
2	A	999	FAD	C4X-N5-C5X	5.72	123.12	116.69
2	D	999	FAD	C4X-N5-C5X	5.31	122.65	116.69
2	B	999	FAD	O4'-C4'-C5'	-4.84	100.18	110.12
2	D	999	FAD	O4B-C1B-N9A	-4.61	104.16	108.44
2	C	999	FAD	C4X-N5-C5X	4.50	121.74	116.69
2	C	999	FAD	C2-N1-C10	4.46	119.47	114.98
2	D	999	FAD	C4X-C10-N1	-4.44	118.29	122.73
2	B	999	FAD	C4X-C10-N1	-4.33	118.40	122.73
2	C	999	FAD	N3A-C4A-N9A	4.21	133.03	125.43
2	B	999	FAD	C4A-C5A-N7A	-4.20	105.93	109.52
2	A	999	FAD	C2-N1-C10	4.13	119.14	114.98
2	C	999	FAD	O4'-C4'-C5'	-4.05	101.81	110.12
2	C	999	FAD	O4B-C1B-C2B	-4.03	100.60	106.77
2	C	999	FAD	O4B-C1B-N9A	-3.96	104.76	108.44
2	B	999	FAD	C5X-C9A-N10	3.78	120.53	116.80
2	B	999	FAD	C4X-N5-C5X	3.77	120.92	116.69
2	B	999	FAD	C4B-O4B-C1B	3.70	113.77	109.75
2	D	999	FAD	C1'-N10-C9A	3.69	122.46	118.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	999	FAD	C5A-C4A-N3A	-3.54	117.99	125.70
2	A	999	FAD	C1'-N10-C9A	3.47	122.24	118.87
2	C	999	FAD	C5'-C4'-C3'	3.43	118.53	112.06
2	D	999	FAD	O4'-C4'-C5'	-3.43	103.08	110.12
2	A	999	FAD	C5X-C9A-N10	3.40	120.15	116.80
2	C	999	FAD	C4A-C5A-N7A	-3.30	106.70	109.52
2	B	999	FAD	C8A-N9A-C4A	3.28	109.41	106.90
2	C	999	FAD	C4X-C10-N1	-3.26	119.47	122.73
2	A	999	FAD	C4-N3-C2	-3.23	118.76	125.39
2	C	999	FAD	C5X-C9A-N10	3.14	119.89	116.80
2	C	999	FAD	C2A-N3A-C4A	2.99	122.52	114.01
2	B	999	FAD	N3A-C4A-N9A	2.95	130.75	125.43
2	B	999	FAD	O4B-C1B-N9A	-2.90	105.75	108.44
2	C	999	FAD	C4-N3-C2	-2.86	119.52	125.39
2	C	999	FAD	C1'-N10-C9A	2.80	121.59	118.87
2	D	999	FAD	C4B-O4B-C1B	2.79	112.78	109.75
2	C	999	FAD	C9A-C5X-N5	-2.77	118.11	122.37
2	B	999	FAD	N7A-C8A-N9A	-2.76	106.55	114.36
2	D	999	FAD	C6-C5X-C9A	2.68	122.73	119.02
2	A	999	FAD	C9A-C5X-N5	-2.67	118.28	122.37
2	D	999	FAD	O3'-C3'-C4'	2.64	115.42	108.74
2	D	999	FAD	O4'-C4'-C3'	2.62	115.56	109.05
2	A	999	FAD	N3A-C4A-N9A	2.56	130.06	125.43
2	B	999	FAD	C10-C4X-N5	-2.56	117.35	120.45
2	D	999	FAD	N3A-C4A-N9A	2.53	130.01	125.43
2	A	999	FAD	C4X-C10-N1	-2.53	120.20	122.73
2	A	999	FAD	O2'-C2'-C1'	2.48	115.87	109.71
2	D	999	FAD	C2A-N1A-C6A	2.41	123.11	118.77
4	A	1660	SO4	O4-S-O3	2.39	119.16	109.08
2	B	999	FAD	C5'-C4'-C3'	2.37	116.54	112.06
2	C	999	FAD	C4-C4X-C10	2.35	120.74	116.95
2	D	999	FAD	C6A-C5A-C4A	2.34	121.54	117.25
2	D	999	FAD	C9A-C5X-N5	-2.34	118.79	122.37
2	B	999	FAD	P-O3P-PA	-2.31	124.90	131.68
2	B	999	FAD	C8A-N7A-C5A	2.28	110.64	103.58
2	A	999	FAD	O4'-C4'-C5'	-2.27	105.46	110.12
2	B	999	FAD	C1B-N9A-C4A	-2.26	122.74	126.64
2	B	999	FAD	C4-N3-C2	-2.24	120.80	125.39
2	D	999	FAD	C10-C4X-N5	-2.17	117.82	120.45
2	D	999	FAD	N7A-C8A-N9A	-2.13	108.32	114.36
2	D	999	FAD	C4-C4X-C10	2.08	120.30	116.95
2	D	999	FAD	C4A-C5A-N7A	-2.06	107.76	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C2A-N3A-C4A	2.06	119.87	114.01
2	A	999	FAD	C4-C4X-C10	2.05	120.26	116.95
2	A	999	FAD	O3'-C3'-C2'	-2.04	103.59	108.74

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	555/658 (84%)	-0.48	3 (0%) 88 88	10, 24, 49, 73	0
1	B	543/658 (82%)	-0.38	5 (0%) 81 81	13, 30, 60, 75	0
1	C	557/658 (84%)	-0.41	7 (1%) 74 73	9, 24, 51, 73	0
1	D	550/658 (83%)	-0.42	4 (0%) 84 84	9, 25, 53, 67	0
All	All	2205/2632 (83%)	-0.42	19 (0%) 81 81	9, 25, 54, 75	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ILE	4.9
1	C	82	ILE	4.3
1	D	559	PHE	3.4
1	A	83	ILE	2.9
1	C	83	ILE	2.8
1	A	156	PRO	2.7
1	C	81	GLY	2.6
1	D	81	GLY	2.5
1	D	82	ILE	2.5
1	C	509	TYR	2.5
1	D	107	LYS	2.4
1	B	162	GLU	2.3
1	B	199	GLU	2.3
1	C	139	ASN	2.3
1	B	202	PHE	2.3
1	C	458	PHE	2.2
1	B	197	LEU	2.2
1	C	559	PHE	2.2
1	B	81	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
3	CL	A	1659	1/1	0.23	21.39	36,36,36,36	0
3	CL	B	1659	1/1	0.20	16.24	56,56,56,56	0
3	CL	D	1659	1/1	0.26	4.76	44,44,44,44	0
4	SO4	B	1661	5/5	0.17	3.60	64,66,66,67	0
4	SO4	D	1661	5/5	0.18	2.43	41,44,53,53	0
3	CL	C	1659	1/1	0.20	2.13	39,39,39,39	0
4	SO4	A	1660	5/5	0.13	1.67	42,42,46,49	0
4	SO4	B	1660	5/5	0.15	1.03	47,49,51,51	0
4	SO4	C	1660	5/5	0.13	0.57	44,44,47,49	0
2	FAD	A	999	53/53	0.13	0.42	9,11,14,16	0
2	FAD	B	999	53/53	0.13	0.38	12,15,18,21	0
4	SO4	D	1660	5/5	0.12	0.08	36,38,39,43	0
4	SO4	A	1661	5/5	0.11	0.03	30,30,33,33	0
2	FAD	C	999	53/53	0.12	-0.03	7,9,12,15	0
2	FAD	D	999	53/53	0.11	-0.14	8,10,13,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.