



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:40 PM GMT

PDB ID : 5AE3  
Title : Ether Lipid-Generating Enzyme AGPS in complex with antimycin A  
Authors : Piano, V.; Benjamin, D.I.; Valente, S.; Nenci, S.; Marrocco, B.; Mai, A.; Aliverti, A.; Nomura, D.K.; Mattevi, A.  
Deposited on : 2015-08-25  
Resolution : 2.18 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

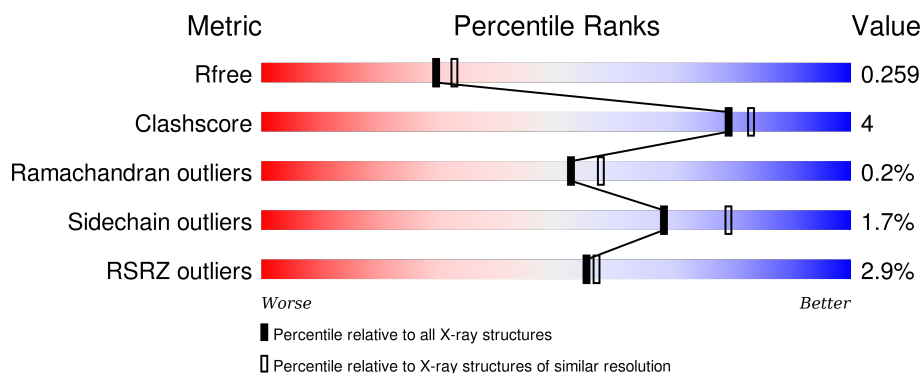
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	658	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>8%</div> <div>18%</div> </div> </div>
1	B	658	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>18%</div> </div> </div>
1	C	658	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>16%</div> </div> </div>
1	D	658	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>17%</div> </div> </div>

## 2 Entry composition [i](#)

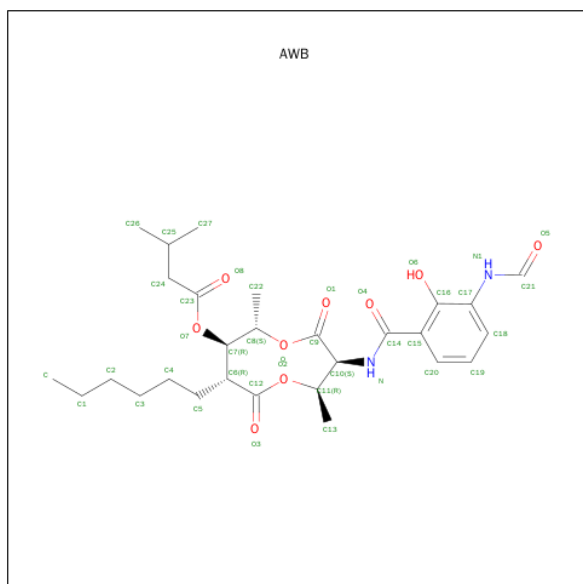
There are 5 unique types of molecules in this entry. The entry contains 18106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4252	2697	740	791	24			
1	B	539	Total	C	N	O	S	0	0	0
			4241	2696	734	787	24			
1	C	551	Total	C	N	O	S	0	2	0
			4333	2746	747	815	25			
1	D	547	Total	C	N	O	S	0	1	0
			4308	2729	752	803	24			

- Molecule 2 is [(2R,3S,6S,7R,8R)-3-[(3-FORMAMIDO-2-OXIDANYL-PHENYL)CARBONYLAMINO]-8-HEXYL-2,6-DIMETHYL-4,9-BIS(OXIDANYLIDENE)-1,5-DIOXONAN-7-YL] 3-METHYLBUTANOATE (three-letter code: AWB) (formula: C<sub>28</sub>H<sub>40</sub>N<sub>2</sub>O<sub>9</sub>).



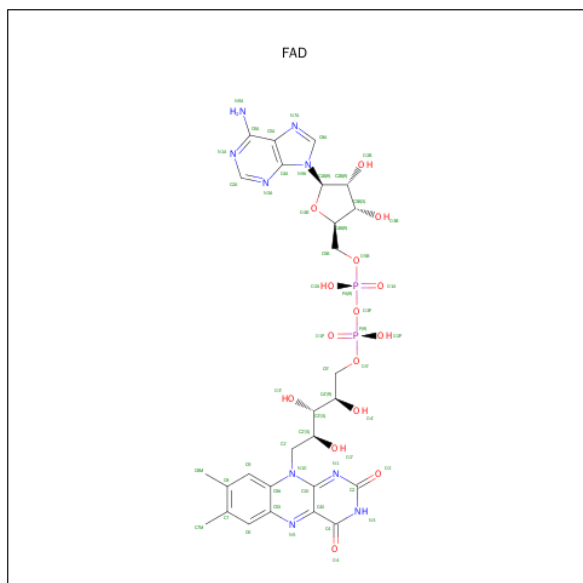
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	28	2	9		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			39	28	2	9		
2	C	1	Total	C	N	O	0	0
			39	28	2	9		
2	D	1	Total	C	N	O	0	0
			39	28	2	9		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).

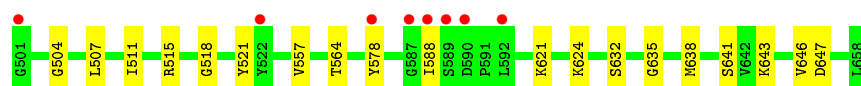


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

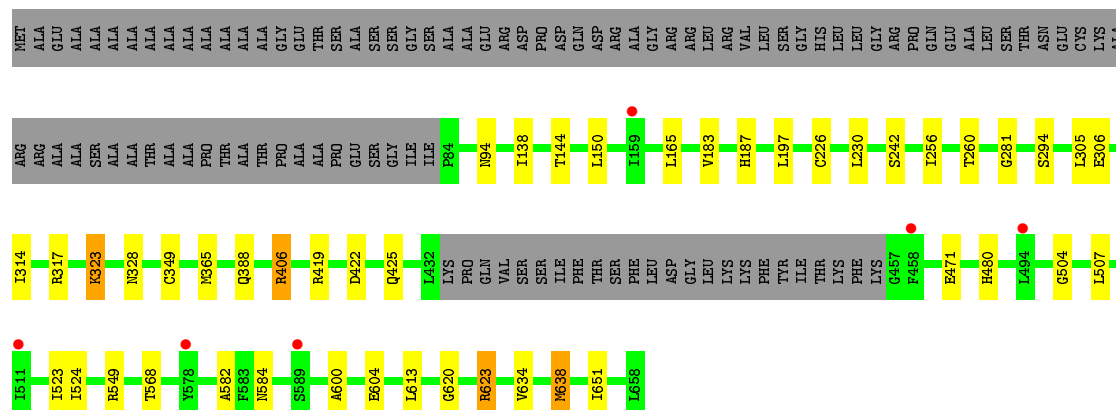
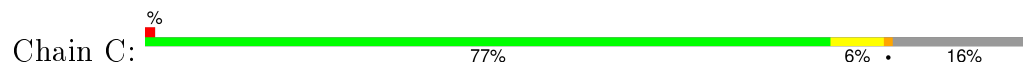
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total	O	0	0
			162	162		
5	B	119	Total	O	0	0
			119	119		
5	C	174	Total	O	0	0
			174	174		
5	D	134	Total	O	0	0
			134	134		

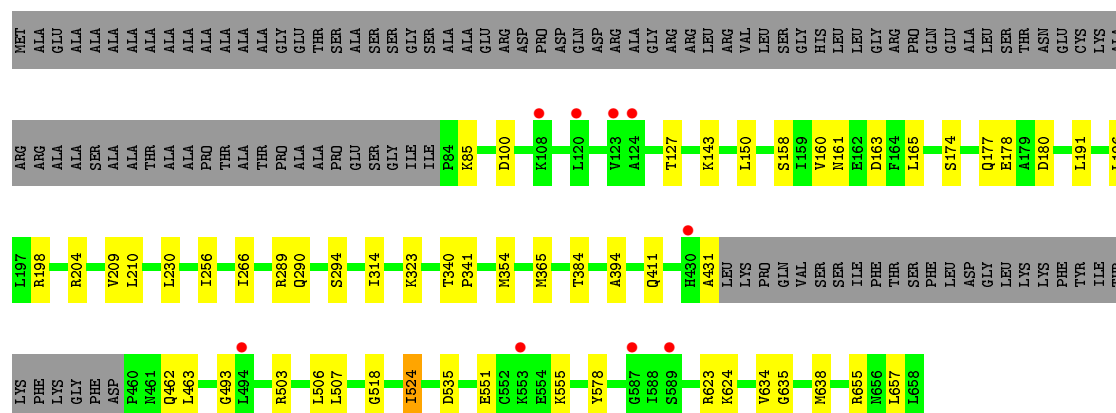
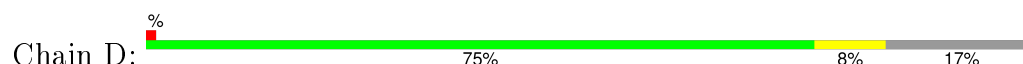




- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.16Å 98.85Å 107.72Å 90.80° 90.50° 94.79°	Depositor
Resolution (Å)	107.71 – 2.18 34.67 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.2 (107.71-2.18) 93.8 (34.67-2.18)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.191 , 0.259 0.197 , 0.259	Depositor DCC
$R_{free}$ test set	1333 reflections (1.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.7	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 123581 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD, AWB

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	0.80	0/4347	0.89	5/5876 (0.1%)
1	B	0.79	1/4337 (0.0%)	0.87	7/5867 (0.1%)
1	C	0.83	0/4436	0.91	8/6002 (0.1%)
1	D	0.80	0/4407	0.90	8/5959 (0.1%)
All	All	0.81	1/17527 (0.0%)	0.89	28/23704 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	641	SER	CB-OG	5.07	1.48	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	317	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	D	535	ASP	CB-CG-OD1	7.23	124.81	118.30
1	D	623	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	D	623	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	623	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	623	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	354	MET	CG-SD-CE	-6.52	89.76	100.20
1	D	100	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	463	LEU	CA-CB-CG	6.38	129.96	115.30
1	B	353	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	317	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	638	MET	CG-SD-CE	-5.74	91.02	100.20
1	A	623	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	515	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	406	ARG	CG-CD-NE	5.72	123.81	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	549	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	289	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	406	ARG	CA-CB-CG	5.59	125.70	113.40
1	D	198	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	140	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	353	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	353	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	87	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	342	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	406	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	406	ARG	NE-CZ-NH2	5.02	122.81	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	4252	0	4163	32	0
1	B	4241	0	4157	43	0
1	C	4333	0	4242	21	0
1	D	4308	0	4238	27	0
2	A	39	0	40	7	0
2	B	39	0	40	5	0
2	C	39	0	39	4	0
2	D	39	0	39	4	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	162	0	0	2	0
5	B	119	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	174	0	0	1	0
5	D	134	0	0	4	0
All	All	18106	0	17082	121	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 (121) 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:191:LEU:HD21	1:D:524:ILE:HG22	1.61	0.79
1:D:210:LEU:HD13	1:D:256:ILE:HG23	1.67	0.75
1:A:635:GLY:HA2	1:A:638:MET:HE3	1.69	0.73
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.23	0.70
1:A:140:LEU:O	1:A:142:HIS:N	2.26	0.69
1:D:518:GLY:HA3	2:D:800:AWB:H27	1.77	0.65
1:B:298:THR:HG21	1:B:379:ILE:HD12	1.80	0.63
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.80	0.63
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.85	0.59
1:B:230:LEU:HD13	1:B:256:ILE:HD11	1.83	0.59
1:A:635:GLY:HA2	1:A:638:MET:CE	2.34	0.58
1:D:551:GLU:O	1:D:555:LYS:HD3	2.04	0.58
1:B:421:MET:HG3	1:B:425:GLN:NE2	2.19	0.57
1:C:150:LEU:HD11	1:C:183:VAL:HB	1.87	0.57
1:C:425:GLN:O	2:C:800:AWB:H20	2.05	0.56
1:D:518:GLY:HA3	2:D:800:AWB:C27	2.34	0.56
1:D:507:LEU:HB2	2:D:800:AWB:C21	2.36	0.56
1:B:192:HIS:HB3	1:B:243:TYR:OH	2.05	0.56
1:B:635:GLY:HA2	1:B:638:MET:CE	2.35	0.55
1:B:421:MET:HG3	1:B:425:GLN:HE21	1.72	0.55
1:A:428:PHE:CZ	2:A:800:AWB:H22B	2.42	0.55
1:A:518:GLY:HA2	2:A:800:AWB:H27A	1.89	0.54
1:B:511:ILE:HG22	2:B:800:AWB:HA	1.89	0.54
1:B:133:GLN:NE2	1:B:139:ASN:O	2.32	0.54
1:A:365:MET:HE1	5:A:2087:HOH:O	2.07	0.54
1:D:411:GLN:CG	5:D:2098:HOH:O	2.56	0.54
1:B:425:GLN:O	2:B:800:AWB:H20	2.08	0.53
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.91	0.52
1:B:129:LYS:HG3	1:B:140:LEU:HD23	1.92	0.52
1:B:419:ARG:NH1	2:B:800:AWB:O5	2.42	0.52
1:D:127:THR:HG21	1:D:431:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:MET:SD	1:A:202:PHE:N	2.83	0.51
1:C:187:HIS:CE1	1:C:197:LEU:HD11	2.46	0.51
1:D:411:GLN:CD	5:D:2098:HOH:O	2.49	0.51
1:C:523:ILE:HG21	2:C:800:AWB:H26A	1.92	0.51
1:D:230:LEU:HD13	1:D:256:ILE:HD11	1.93	0.51
1:D:161:ASN:OD1	1:D:163:ASP:N	2.44	0.50
1:D:85:LYS:HZ1	1:D:174:SER:CB	2.24	0.50
1:D:624:LYS:HE3	1:D:655:ARG:O	2.12	0.50
1:A:475:GLU:O	1:A:479:GLN:HG3	2.11	0.49
1:A:518:GLY:CA	2:A:800:AWB:H27A	2.42	0.49
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.93	0.49
1:D:209:VAL:C	1:D:210:LEU:HD12	2.33	0.49
1:A:511:ILE:HD12	2:A:800:AWB:H13B	1.94	0.49
1:C:613:LEU:HD11	1:C:623:ARG:HB3	1.95	0.49
1:C:634:VAL:HG12	1:C:638:MET:HE2	1.95	0.49
1:B:557:VAL:HG22	1:B:588:ILE:HD11	1.95	0.48
1:B:140:LEU:CD1	1:B:521:TYR:CZ	2.97	0.48
1:A:342:ARG:HD2	1:A:645:TYR:CZ	2.49	0.48
1:A:314:ILE:HG23	1:A:365:MET:HG2	1.94	0.47
1:A:393:VAL:HG22	1:A:485:TYR:CE1	2.49	0.47
2:A:800:AWB:O	2:A:800:AWB:C12	2.62	0.47
1:B:139:ASN:O	1:B:140:LEU:CB	2.62	0.47
1:B:423:ASN:ND2	1:B:461:ASN:C	2.68	0.47
1:A:425:GLN:O	2:A:800:AWB:H20	2.14	0.47
1:B:340:THR:HB	1:B:646:VAL:HG13	1.96	0.47
1:C:226:CYS:HA	1:C:651:ILE:HD11	1.97	0.46
1:B:507:LEU:HB3	1:B:511:ILE:HD11	1.96	0.46
1:B:504:GLY:HA3	2:B:800:AWB:C21	2.46	0.46
1:B:187:HIS:CE1	1:B:197:LEU:HD11	2.51	0.46
2:D:800:AWB:O	2:D:800:AWB:C12	2.63	0.46
1:A:616:HIS:HA	1:B:355:SER:HB2	1.98	0.46
1:B:323:LYS:HG2	1:B:324:ASN:N	2.31	0.45
1:D:503:ARG:HA	1:D:506:LEU:HD12	1.98	0.45
1:A:588:ILE:HG21	1:A:591:PRO:HA	1.97	0.45
5:C:2093:HOH:O	1:D:634:VAL:HG23	2.15	0.45
1:A:424:GLN:NE2	1:A:562:LEU:HD12	2.32	0.45
1:D:191:LEU:C	1:D:191:LEU:HD13	2.36	0.45
1:D:158:SER:OG	1:D:177:GLN:HG2	2.16	0.45
1:B:474:ARG:O	1:B:478:LEU:HG	2.17	0.45
1:B:425:GLN:HG3	1:B:564:THR:OG1	2.16	0.45
1:A:419:ARG:O	1:A:466:ALA:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.98	0.45
1:A:426:PHE:CD2	1:A:463:LEU:HD12	2.51	0.45
1:C:260:THR:O	1:C:281:GLY:HA3	2.17	0.45
1:C:138:ILE:HG23	1:C:584:ASN:ND2	2.32	0.45
1:B:225:ALA:HA	1:B:230:LEU:HD12	2.00	0.44
2:C:800:AWB:C12	2:C:800:AWB:O	2.65	0.44
1:B:92:LYS:NZ	5:B:2007:HOH:O	2.51	0.44
1:D:635:GLY:HA2	1:D:638:MET:CE	2.48	0.44
1:B:518:GLY:CA	2:B:800:AWB:H27A	2.47	0.44
1:C:507:LEU:HB2	2:C:800:AWB:H21	2.01	0.43
1:D:127:THR:O	1:D:127:THR:HG22	2.18	0.43
1:A:230:LEU:HD13	1:A:256:ILE:HD11	2.00	0.43
1:A:585:TYR:HB2	1:A:591:PRO:HB3	2.01	0.43
1:A:160:VAL:HG11	1:A:165:LEU:HD13	2.01	0.43
1:B:422:ASP:C	1:B:422:ASP:OD1	2.56	0.43
1:A:346:GLU:O	1:B:632:SER:HB3	2.19	0.43
1:A:638:MET:HE1	1:B:345:ILE:HD13	2.01	0.43
1:A:286:GLU:OE2	1:A:289:ARG:NE	2.43	0.43
1:C:419:ARG:NH2	1:C:504:GLY:O	2.48	0.43
1:B:643:LYS:HD2	1:B:647:ASP:HB3	2.00	0.43
1:D:411:GLN:HG2	5:D:2098:HOH:O	2.19	0.42
1:B:621:LYS:HA	1:B:624:LYS:HD3	2.01	0.42
1:A:632:SER:HB3	1:B:346:GLU:O	2.19	0.42
1:B:267:LEU:HD12	1:B:277:HIS:CD2	2.54	0.42
1:B:286:GLU:OE2	1:B:289:ARG:NH2	2.50	0.42
1:C:422:ASP:OD1	1:C:422:ASP:C	2.58	0.42
1:B:112:GLU:OE1	5:B:2014:HOH:O	2.21	0.42
1:B:395:PHE:O	1:B:463:LEU:HD22	2.18	0.42
1:A:511:ILE:CD1	2:A:800:AWB:H13B	2.50	0.42
1:C:600:ALA:O	1:C:604:GLU:HG2	2.19	0.42
1:B:643:LYS:NZ	1:B:647:ASP:OD2	2.51	0.42
1:A:136:PHE:CD2	1:A:523:ILE:HD13	2.55	0.42
1:D:394:ALA:O	1:D:493:GLY:HA2	2.20	0.42
1:C:242:SER:O	1:C:620:GLY:HA3	2.19	0.42
1:A:535:ASP:HB3	1:B:272:ASN:HB3	2.02	0.41
1:A:129:LYS:HG3	1:A:140:LEU:HD22	2.02	0.41
1:C:524:ILE:O	1:C:582:ALA:HA	2.21	0.41
1:C:323:LYS:HG3	1:C:328:ASN:CG	2.40	0.41
1:C:305:LEU:HD12	1:C:306:GLU:N	2.35	0.41
1:A:426:PHE:CG	1:A:463:LEU:HD12	2.56	0.41
1:A:174:SER:HB3	5:A:2003:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:VAL:HG11	1:D:165:LEU:HD13	2.03	0.41
1:D:340:THR:HB	1:D:341:PRO:HD2	2.03	0.41
1:D:266:ILE:HD12	1:D:290:GLN:HB3	2.01	0.41
1:C:230:LEU:CD1	1:C:256:ILE:HD11	2.51	0.41
1:B:365:MET:HE2	5:B:2078:HOH:O	2.22	0.40
1:D:143:LYS:NZ	5:D:2014:HOH:O	2.52	0.40
1:C:94:ASN:HA	1:C:197:LEU:HD13	2.03	0.40
1:B:187:HIS:NE2	1:B:197:LEU:HD11	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/658 (81%)	512 (96%)	16 (3%)	3 (1%)	30	27
1	B	533/658 (81%)	515 (97%)	18 (3%)	0	100	100
1	C	549/658 (83%)	528 (96%)	21 (4%)	0	100	100
1	D	544/658 (83%)	530 (97%)	13 (2%)	1 (0%)	52	57
All	All	2157/2632 (82%)	2085 (97%)	68 (3%)	4 (0%)	52	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	142	HIS
1	D	657	LEU
1	A	156	PRO

### 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	456/545 (84%)	449 (98%)	7 (2%)	72	82
1	B	454/545 (83%)	448 (99%)	6 (1%)	76	85
1	C	467/545 (86%)	459 (98%)	8 (2%)	68	79
1	D	463/545 (85%)	452 (98%)	11 (2%)	57	67
All	All	1840/2180 (84%)	1808 (98%)	32 (2%)	68	79

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

Mol	Chain	Res	Type
1	A	88	GLN
1	A	90	LEU
1	A	142	HIS
1	A	526	GLU
1	A	555	LYS
1	A	559	PHE
1	A	578	TYR
1	B	90	LEU
1	B	130	ASP
1	B	140	LEU
1	B	174	SER
1	B	323	LYS
1	B	578	TYR
1	C	144	THR
1	C	165	LEU
1	C	294	SER
1	C	323	LYS
1	C	349	CYS
1	C	406	ARG
1	C	480	HIS
1	C	568	THR
1	D	150	LEU
1	D	178	GLU
1	D	180	ASP

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Mol	Chain	Res	Type
1	D	196	LEU
1	D	294	SER
1	D	323	LYS
1	D	384	THR
1	D	462	GLN
1	D	463	LEU
1	D	524	ILE
1	D	578	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	423	ASN
1	A	424	GLN
1	B	423	ASN
1	B	425	GLN
1	C	133	GLN
1	C	400	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](#)

11 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
4	SO4	A	1659	-	4,4,4	0.54	0	6,6,6	0.68	0
2	AWB	A	800	-	40,40,40	1.87	7 (17%)	31,54,54	1.74	8 (25%)
3	FAD	A	999	-	52,58,58	1.73	7 (13%)	52,89,89	2.48	13 (25%)
4	SO4	B	1659	-	4,4,4	0.77	0	6,6,6	0.74	0
2	AWB	B	800	-	40,40,40	1.74	7 (17%)	31,54,54	2.10	10 (32%)
3	FAD	B	999	-	52,58,58	1.52	9 (17%)	52,89,89	2.80	14 (26%)
2	AWB	C	800	-	40,40,40	1.79	7 (17%)	31,54,54	1.54	4 (12%)
3	FAD	C	999	-	52,58,58	1.36	8 (15%)	52,89,89	2.97	17 (32%)
4	SO4	D	1659	-	4,4,4	0.50	0	6,6,6	0.62	0
2	AWB	D	800	-	40,40,40	1.75	9 (22%)	31,54,54	2.09	10 (32%)
3	FAD	D	999	-	52,58,58	1.44	8 (15%)	52,89,89	2.69	13 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1659	-	-	0/0/0/0	0/0/0/0
2	AWB	A	800	-	-	0/37/53/53	0/1/2/2
3	FAD	A	999	-	-	0/30/50/50	0/6/6/6
4	SO4	B	1659	-	-	0/0/0/0	0/0/0/0
2	AWB	B	800	-	-	0/37/53/53	0/1/2/2
3	FAD	B	999	-	-	0/30/50/50	0/6/6/6
2	AWB	C	800	-	-	0/37/53/53	0/1/2/2
3	FAD	C	999	-	-	0/30/50/50	0/6/6/6
4	SO4	D	1659	-	-	0/0/0/0	0/0/0/0
2	AWB	D	800	-	-	0/37/53/53	0/1/2/2
3	FAD	D	999	-	-	0/30/50/50	0/6/6/6

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	AWB	O-C8	-4.69	1.38	1.46
2	B	800	AWB	C17-N1	-3.69	1.35	1.41
2	C	800	AWB	C17-N1	-3.39	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	FAD	C2-N1	-3.10	1.31	1.38
2	C	800	AWB	O-C8	-2.86	1.41	1.46
2	D	800	AWB	O-C8	-2.76	1.41	1.46
3	A	999	FAD	C6-C5X	-2.70	1.37	1.41
2	D	800	AWB	O7-C7	-2.61	1.40	1.44
2	D	800	AWB	C17-N1	-2.58	1.37	1.41
2	D	800	AWB	O2-C11	-2.57	1.42	1.46
3	B	999	FAD	C2-N1	-2.50	1.33	1.38
3	B	999	FAD	C2-N3	-2.44	1.33	1.38
2	A	800	AWB	O-C8	-2.40	1.42	1.46
3	C	999	FAD	O4B-C4B	-2.26	1.39	1.45
3	C	999	FAD	C1'-N10	-2.26	1.46	1.48
3	C	999	FAD	C2B-C1B	-2.25	1.50	1.53
3	C	999	FAD	O4B-C1B	2.24	1.44	1.41
3	B	999	FAD	C2A-N1A	2.29	1.38	1.33
2	A	800	AWB	C18-C17	2.30	1.43	1.39
3	D	999	FAD	C4-C4X	2.37	1.46	1.41
3	A	999	FAD	C5A-C4A	2.47	1.46	1.40
3	A	999	FAD	C10-N10	2.55	1.42	1.39
3	D	999	FAD	C4X-C10	2.62	1.45	1.40
3	D	999	FAD	C5A-C4A	2.70	1.46	1.40
3	C	999	FAD	C8-C7	2.72	1.48	1.41
2	B	800	AWB	C15-C16	2.90	1.46	1.41
3	C	999	FAD	C4-C4X	2.93	1.47	1.41
3	D	999	FAD	C8-C7	2.95	1.48	1.41
3	D	999	FAD	C10-N10	2.98	1.42	1.39
3	B	999	FAD	C8-C7	3.11	1.49	1.41
2	C	800	AWB	C17-C16	3.14	1.45	1.40
3	B	999	FAD	C5A-C4A	3.14	1.47	1.40
3	C	999	FAD	C4X-C10	3.18	1.46	1.40
3	B	999	FAD	O4B-C1B	3.19	1.45	1.41
3	C	999	FAD	C9A-C5X	3.25	1.49	1.42
2	D	800	AWB	O-C9	3.27	1.42	1.34
3	A	999	FAD	C1'-N10	3.48	1.52	1.48
2	D	800	AWB	C15-C16	3.50	1.47	1.41
3	B	999	FAD	C9A-C5X	3.58	1.50	1.42
3	D	999	FAD	C1'-N10	3.58	1.52	1.48
3	B	999	FAD	C4-C4X	3.58	1.48	1.41
3	B	999	FAD	C4X-C10	3.58	1.47	1.40
3	D	999	FAD	C9A-C5X	3.64	1.50	1.42
2	B	800	AWB	C17-C16	3.64	1.46	1.40
2	C	800	AWB	O7-C23	3.82	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	AWB	C15-C16	3.90	1.48	1.41
2	A	800	AWB	O7-C23	3.91	1.45	1.34
2	C	800	AWB	O-C9	3.94	1.43	1.34
2	B	800	AWB	O-C9	4.02	1.43	1.34
2	B	800	AWB	O7-C23	4.05	1.46	1.34
2	B	800	AWB	O2-C12	4.06	1.43	1.34
3	A	999	FAD	C8-C7	4.08	1.51	1.41
2	A	800	AWB	O-C9	4.15	1.44	1.34
2	D	800	AWB	C17-C16	4.17	1.47	1.40
2	D	800	AWB	O7-C23	4.23	1.46	1.34
2	A	800	AWB	O2-C12	4.31	1.44	1.34
2	D	800	AWB	O2-C12	4.63	1.45	1.34
2	A	800	AWB	C15-C16	5.09	1.50	1.41
2	A	800	AWB	C17-C16	5.28	1.49	1.40
3	A	999	FAD	C9A-C5X	5.42	1.54	1.42
2	C	800	AWB	O2-C12	5.89	1.48	1.34
3	A	999	FAD	C4X-C10	6.39	1.52	1.40

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	999	FAD	N3A-C2A-N1A	-9.49	121.41	128.87
3	B	999	FAD	N3A-C2A-N1A	-9.26	121.60	128.87
3	C	999	FAD	C4-C4X-C10	-8.04	114.80	119.94
3	A	999	FAD	N3A-C2A-N1A	-7.36	123.09	128.87
3	B	999	FAD	C4-C4X-C10	-5.50	116.42	119.94
3	D	999	FAD	C4X-C4-N3	-5.17	116.76	123.52
2	D	800	AWB	C7-O7-C23	-4.93	108.95	117.78
3	D	999	FAD	N3A-C2A-N1A	-4.93	125.00	128.87
3	D	999	FAD	C4-C4X-C10	-4.82	116.86	119.94
3	D	999	FAD	N3-C2-N1	-4.76	119.68	127.69
2	C	800	AWB	O5-C21-N1	-4.63	119.85	125.75
3	C	999	FAD	N3-C2-N1	-4.61	119.93	127.69
2	D	800	AWB	O5-C21-N1	-4.55	119.95	125.75
3	A	999	FAD	C4X-C4-N3	-4.47	117.68	123.52
3	B	999	FAD	C4X-C4-N3	-4.47	117.69	123.52
3	D	999	FAD	C1B-N9A-C4A	-4.42	121.88	126.81
3	B	999	FAD	N3-C2-N1	-4.30	120.45	127.69
3	A	999	FAD	C4-C4X-C10	-4.23	117.24	119.94
3	C	999	FAD	C1B-N9A-C4A	-4.11	122.22	126.81
2	B	800	AWB	C7-O7-C23	-4.04	110.55	117.78
3	A	999	FAD	O4B-C1B-N9A	-4.01	100.53	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	AWB	O5-C21-N1	-3.92	120.75	125.75
2	C	800	AWB	C18-C17-N1	-3.80	117.47	122.62
2	D	800	AWB	O8-C23-C24	-3.61	117.11	124.74
2	D	800	AWB	C18-C17-N1	-3.43	117.97	122.62
2	B	800	AWB	O2-C12-O3	-3.35	119.90	124.12
3	D	999	FAD	O4B-C1B-N9A	-3.33	101.81	108.11
2	A	800	AWB	C7-O7-C23	-3.26	111.94	117.78
3	A	999	FAD	N3-C2-N1	-3.20	122.30	127.69
2	D	800	AWB	C25-C24-C23	-3.05	101.30	114.97
2	B	800	AWB	O8-C23-C24	-2.98	118.43	124.74
2	A	800	AWB	O2-C12-O3	-2.94	120.42	124.12
3	C	999	FAD	O3B-C3B-C2B	-2.93	102.38	111.86
2	A	800	AWB	O8-C23-C24	-2.90	118.61	124.74
3	C	999	FAD	C4X-C4-N3	-2.87	119.77	123.52
3	C	999	FAD	O4B-C1B-N9A	-2.70	103.01	108.11
2	D	800	AWB	C27-C25-C24	-2.67	101.37	111.37
2	D	800	AWB	O-C9-O1	-2.58	120.87	124.12
2	B	800	AWB	O-C9-O1	-2.35	121.16	124.12
2	B	800	AWB	O4-C14-C15	-2.24	116.54	120.94
2	A	800	AWB	O-C9-O1	-2.16	121.39	124.12
3	B	999	FAD	C1B-N9A-C4A	-2.12	124.44	126.81
3	C	999	FAD	O2'-C2'-C3'	-2.01	103.78	108.96
2	B	800	AWB	C18-C17-N1	2.03	125.37	122.62
2	D	800	AWB	C27-C25-C26	2.07	120.62	110.52
3	C	999	FAD	C5X-C9A-N10	2.08	119.14	117.58
2	A	800	AWB	C19-C18-C17	2.09	122.96	118.57
2	A	800	AWB	C18-C17-N1	2.15	125.53	122.62
2	B	800	AWB	C10-N-C14	2.30	126.36	121.46
3	A	999	FAD	O2P-P-O1P	2.31	124.60	112.56
3	A	999	FAD	C2A-N1A-C6A	2.32	122.91	118.77
3	B	999	FAD	O2P-P-O1P	2.35	124.79	112.56
3	C	999	FAD	O2A-PA-O1A	2.43	125.19	112.56
3	A	999	FAD	O2A-PA-O1A	2.52	125.69	112.56
3	D	999	FAD	N6A-C6A-N1A	2.53	122.75	118.52
3	B	999	FAD	C2B-C1B-N9A	2.56	120.32	113.47
3	D	999	FAD	O2P-P-O1P	2.59	126.05	112.56
2	C	800	AWB	O-C9-C10	2.61	113.26	110.07
2	A	800	AWB	O-C9-C10	2.68	113.33	110.07
3	C	999	FAD	C2B-C3B-C4B	2.73	108.22	102.64
2	C	800	AWB	O7-C23-C24	2.78	116.98	111.60
3	A	999	FAD	C4X-N5-C5X	2.88	120.11	116.72
3	A	999	FAD	O3'-C3'-C4'	2.90	116.26	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FAD	C5X-C9A-N10	3.03	119.85	117.58
2	D	800	AWB	O7-C23-C24	3.13	117.67	111.60
3	B	999	FAD	C2A-N1A-C6A	3.14	124.38	118.77
3	A	999	FAD	C1'-N10-C9A	3.16	122.49	118.83
2	D	800	AWB	O-C9-C10	3.28	114.08	110.07
3	D	999	FAD	C4-C4X-N5	3.29	122.70	118.70
3	C	999	FAD	C1'-N10-C9A	3.38	122.75	118.83
3	B	999	FAD	C1'-N10-C9A	3.48	122.86	118.83
2	B	800	AWB	O-C9-C10	3.67	114.54	110.07
3	C	999	FAD	C4B-O4B-C1B	3.70	113.57	109.64
3	D	999	FAD	C5X-C9A-N10	3.73	120.37	117.58
3	C	999	FAD	C4X-N5-C5X	3.85	121.26	116.72
3	D	999	FAD	C4X-N5-C5X	3.87	121.28	116.72
3	C	999	FAD	O2'-C2'-C1'	3.88	119.52	109.93
3	C	999	FAD	C4-C4X-N5	4.01	123.58	118.70
3	D	999	FAD	C1'-N10-C9A	4.10	123.58	118.83
3	B	999	FAD	C4-C4X-N5	4.11	123.70	118.70
3	B	999	FAD	C4B-O4B-C1B	4.18	114.07	109.64
3	B	999	FAD	C4X-N5-C5X	4.44	121.95	116.72
3	A	999	FAD	C5X-C9A-N10	4.51	120.96	117.58
2	A	800	AWB	O7-C23-C24	5.13	121.54	111.60
2	B	800	AWB	O7-C23-C24	5.40	122.05	111.60
3	A	999	FAD	C4-N3-C2	10.08	123.57	115.16
3	C	999	FAD	C4-N3-C2	10.87	124.22	115.16
3	B	999	FAD	C4-N3-C2	11.13	124.44	115.16
3	D	999	FAD	C4-N3-C2	11.93	125.11	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	AWB	7	0
2	B	800	AWB	5	0
2	C	800	AWB	4	0
2	D	800	AWB	4	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	539/658 (81%)	0.03	15 (2%) 56 58	18, 35, 64, 81	0
1	B	539/658 (81%)	0.18	33 (6%) 25 26	18, 38, 66, 81	0
1	C	551/658 (83%)	-0.01	6 (1%) 82 83	17, 33, 60, 78	1 (0%)
1	D	547/658 (83%)	0.02	9 (1%) 74 75	18, 35, 61, 79	0
All	All	2176/2632 (82%)	0.06	63 (2%) 55 57	17, 35, 63, 81	1 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	589	SER	4.7
1	B	458	PHE	4.6
1	C	159	ILE	4.6
1	A	458	PHE	4.5
1	A	202	PHE	4.5
1	A	249	ALA	4.3
1	B	159	ILE	3.9
1	B	587	GLY	3.8
1	A	587	GLY	3.7
1	A	201	MET	3.6
1	B	589	SER	3.3
1	D	120	LEU	3.1
1	C	589	SER	3.0
1	A	195	PHE	3.0
1	D	123	VAL	2.9
1	A	159	ILE	2.9
1	B	233	ILE	2.8
1	D	494	LEU	2.8
1	A	86	LYS	2.8
1	B	459	ASP	2.8
1	D	589	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	155	THR	2.8
1	B	492	GLY	2.8
1	B	431	ALA	2.7
1	B	140	LEU	2.7
1	B	162	GLU	2.7
1	B	199	GLU	2.6
1	A	430	HIS	2.6
1	C	458	PHE	2.6
1	D	587	GLY	2.6
1	B	478	LEU	2.6
1	B	202	PHE	2.6
1	B	235	ILE	2.6
1	B	497	GLY	2.6
1	B	578	TYR	2.5
1	B	522	TYR	2.5
1	A	590	ASP	2.5
1	C	494	LEU	2.4
1	B	430	HIS	2.4
1	B	500	ASN	2.4
1	B	196	LEU	2.3
1	B	166	HIS	2.3
1	A	250	ASP	2.3
1	B	590	ASP	2.3
1	B	239	THR	2.3
1	C	578	TYR	2.3
1	B	592	LEU	2.3
1	A	200	GLY	2.3
1	B	501	GLY	2.2
1	D	124	ALA	2.2
1	B	163	ASP	2.2
1	C	511	ILE	2.2
1	B	496	ALA	2.2
1	B	460	PRO	2.2
1	D	430	HIS	2.2
1	B	493	GLY	2.2
1	D	553	LYS	2.2
1	A	166	HIS	2.1
1	D	108	LYS	2.1
1	B	89	GLU	2.1
1	B	462	GLN	2.1
1	B	588	ILE	2.0
1	B	201	MET	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( $\text{\AA}^2$ )	Q<0.9
2	AWB	A	800	39/39	0.86	0.18	1.51	32,44,63,67	0
4	SO4	D	1659	5/5	0.93	0.14	1.33	57,59,61,73	0
4	SO4	B	1659	5/5	0.93	0.14	1.33	49,60,66,69	0
2	AWB	B	800	39/39	0.90	0.17	0.90	39,46,71,74	0
4	SO4	A	1659	5/5	0.96	0.12	0.65	47,49,61,65	0
2	AWB	D	800	39/39	0.91	0.16	0.63	32,43,61,63	0
3	FAD	A	999	53/53	0.99	0.17	0.57	15,19,24,25	0
2	AWB	C	800	39/39	0.95	0.15	0.40	28,38,55,59	0
3	FAD	B	999	53/53	0.98	0.17	0.05	19,21,23,26	0
3	FAD	D	999	53/53	0.98	0.15	-0.09	15,19,23,24	0
3	FAD	C	999	53/53	0.99	0.14	-0.35	15,18,20,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.