



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:44 AM GMT

PDB ID : 3PND
Title : FAD binding by ApbE protein from Salmonella enterica: a new class of FAD binding proteins
Authors : Boyd, J.M.; Endrizzi, J.A.; Hamilton, T.L.; Christopherson, M.R.; Mulder, D.W.; Downs, D.M.; Peters, J.W.
Deposited on : 2010-11-18
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

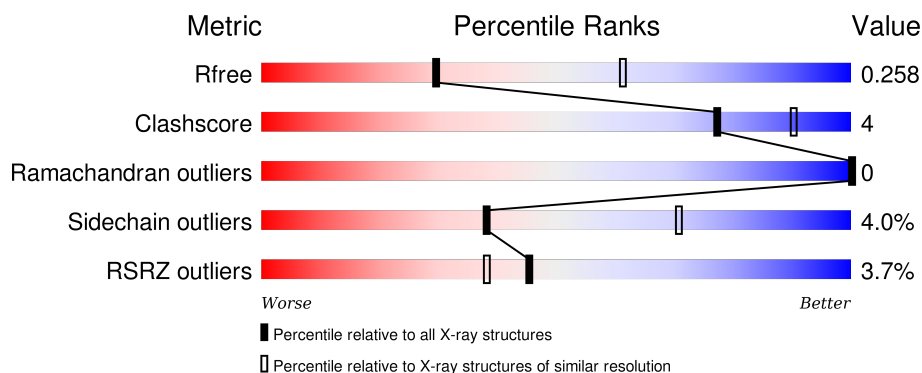
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>4%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	B	337	<div> <div>3%</div> <div>80%</div> <div>11%</div> <div>8%</div> </div>
1	C	337	<div> <div>4%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	D	337	<div> <div>4%</div> <div>80%</div> <div>11%</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
2	SO4	A	359	-	-	-	X
2	SO4	A	362	-	-	-	X
2	SO4	A	364	-	-	-	X
2	SO4	A	367	-	-	-	X
2	SO4	A	368	-	-	-	X
2	SO4	B	360	-	-	-	X
2	SO4	B	366	-	-	-	X
2	SO4	C	358	-	-	-	X
2	SO4	C	360	-	-	-	X
2	SO4	D	358	-	-	-	X
2	SO4	D	359	-	-	-	X
2	SO4	D	361	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10442 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 Thiamine biosynthesis lipoprotein ApbE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2437	1534	432	461	10			
1	B	309	Total	C	N	O	S	0	0	0
			2377	1500	420	447	10			
1	C	323	Total	C	N	O	S	0	0	0
			2476	1557	438	471	10			
1	D	310	Total	C	N	O	S	0	1	0
			2391	1509	423	449	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	INITIATING METHIONINE	UNP P41780
A	351	HIS	-	EXPRESSION TAG	UNP P41780
A	352	HIS	-	EXPRESSION TAG	UNP P41780
A	353	HIS	-	EXPRESSION TAG	UNP P41780
A	354	HIS	-	EXPRESSION TAG	UNP P41780
A	355	HIS	-	EXPRESSION TAG	UNP P41780
A	356	HIS	-	EXPRESSION TAG	UNP P41780
B	20	MET	-	INITIATING METHIONINE	UNP P41780
B	351	HIS	-	EXPRESSION TAG	UNP P41780
B	352	HIS	-	EXPRESSION TAG	UNP P41780
B	353	HIS	-	EXPRESSION TAG	UNP P41780
B	354	HIS	-	EXPRESSION TAG	UNP P41780
B	355	HIS	-	EXPRESSION TAG	UNP P41780
B	356	HIS	-	EXPRESSION TAG	UNP P41780
C	20	MET	-	INITIATING METHIONINE	UNP P41780
C	351	HIS	-	EXPRESSION TAG	UNP P41780
C	352	HIS	-	EXPRESSION TAG	UNP P41780
C	353	HIS	-	EXPRESSION TAG	UNP P41780
C	354	HIS	-	EXPRESSION TAG	UNP P41780
C	355	HIS	-	EXPRESSION TAG	UNP P41780
C	356	HIS	-	EXPRESSION TAG	UNP P41780

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	MET	-	INITIATING METHIONINE	UNP P41780
D	351	HIS	-	EXPRESSION TAG	UNP P41780
D	352	HIS	-	EXPRESSION TAG	UNP P41780
D	353	HIS	-	EXPRESSION TAG	UNP P41780
D	354	HIS	-	EXPRESSION TAG	UNP P41780
D	355	HIS	-	EXPRESSION TAG	UNP P41780
D	356	HIS	-	EXPRESSION TAG	UNP P41780

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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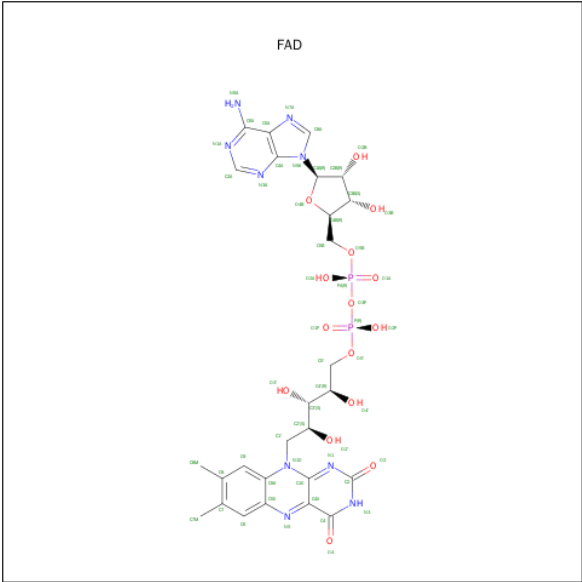
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

- 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		

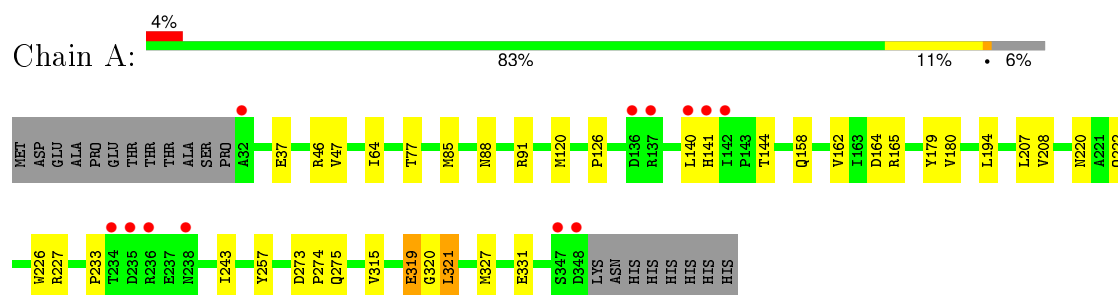
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	96	Total	O	0	0
			96	96		
4	C	91	Total	O	0	0
			91	91		
4	D	63	Total	O	0	0
			63	63		

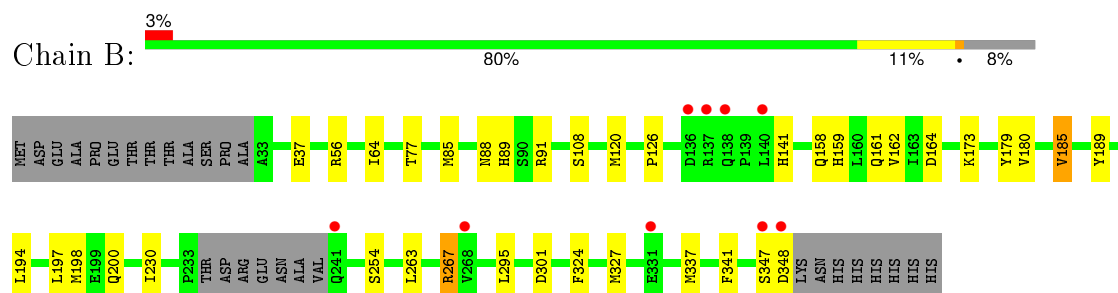
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

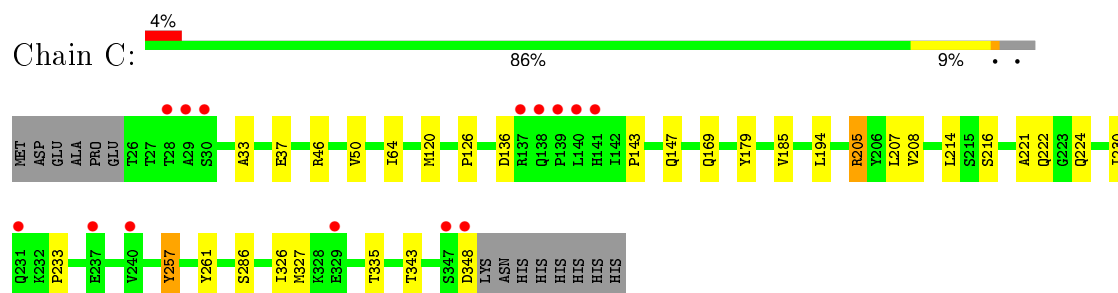
- Molecule 1: Thiamine biosynthesis lipoprotein ApbE



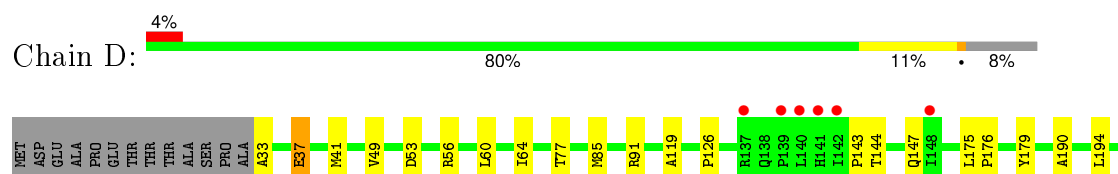
- Molecule 1: Thiamine biosynthesis lipoprotein ApbE



- Molecule 1: Thiamine biosynthesis lipoprotein ApbE



- Molecule 1: Thiamine biosynthesis lipoprotein ApbE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.10Å 120.85Å 212.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.60 – 2.75 32.60 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.60-2.75) 99.6 (32.60-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.254 0.205 , 0.258	Depositor DCC
R_{free} test set	2226 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 44205 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10442	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/2486	0.50	0/3376
1	B	0.29	0/2425	0.48	0/3291
1	C	0.30	0/2526	0.48	0/3433
1	D	0.30	0/2443	0.48	0/3316
All	All	0.30	0/9880	0.48	0/13416

There are no bond length outliers.

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	2437	0	2428	20	0
1	B	2377	0	2372	23	0
1	C	2476	0	2466	14	0
1	D	2391	0	2386	23	0
2	A	65	0	0	0	0
2	B	60	0	0	1	0
2	C	55	0	0	0	0
2	D	40	0	0	0	0
3	A	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	1	0
4	A	79	0	0	0	0
4	B	96	0	0	0	0
4	C	91	0	0	2	0
4	D	63	0	0	0	0
All	All	10442	0	9776	74	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 (74) 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:88:ASN:HD21	1:B:180:VAL:H	1.23	0.82
1:C:207:LEU:HD11	1:C:214:LEU:HD21	1.74	0.67
1:B:88:ASN:ND2	1:B:180:VAL:H	1.92	0.66
1:C:143:PRO:HA	1:C:147:GLN:HE21	1.61	0.64
1:A:88:ASN:HD21	1:A:180:VAL:H	1.47	0.63
1:A:126:PRO:HD3	1:A:179:TYR:HB3	1.82	0.61
1:C:33:ALA:HB2	1:C:221:ALA:HB2	1.83	0.60
1:C:194:LEU:HB3	1:C:208:VAL:HG11	1.84	0.60
1:D:64:ILE:HG23	1:D:194:LEU:HD11	1.83	0.59
1:A:64:ILE:HG23	1:A:194:LEU:HD11	1.85	0.58
1:C:64:ILE:HG23	1:C:194:LEU:HD11	1.86	0.58
1:B:77:THR:HA	1:B:85:MET:CE	2.34	0.57
1:D:126:PRO:HD3	1:D:179:TYR:HB3	1.84	0.57
1:B:254:SER:HB2	1:B:301:ASP:HB3	1.86	0.57
1:D:194:LEU:HB3	1:D:208:VAL:HG11	1.84	0.57
1:A:77:THR:HA	1:A:85:MET:CE	2.35	0.57
1:C:207:LEU:HD12	1:C:216:SER:HB3	1.86	0.56
1:A:165:ARG:HE	1:B:161:GLN:HE21	1.54	0.56
1:B:37:GLU:HB2	1:D:267:ARG:HD3	1.89	0.55
1:B:263:LEU:HD23	1:D:207:LEU:HD23	1.88	0.55
1:A:77:THR:HG22	1:A:85:MET:HE1	1.89	0.55
1:A:37:GLU:HG2	1:A:46:ARG:HG2	1.90	0.53
1:B:64:ILE:HG23	1:B:194:LEU:HD11	1.90	0.53
1:D:144:THR:H	1:D:147:GLN:HE21	1.56	0.53
1:B:126:PRO:HD3	1:B:179:TYR:HB3	1.89	0.53
1:B:77:THR:HA	1:B:85:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PRO:HB3	1:C:257:TYR:CE1	2.46	0.51
1:D:77:THR:HA	1:D:85:MET:HE3	1.92	0.51
1:B:91:ARG:NH1	2:B:362:SO4:O1	2.44	0.50
1:A:233:PRO:HA	1:A:257:TYR:CZ	2.47	0.50
1:A:77:THR:HA	1:A:85:MET:HE1	1.93	0.50
1:B:185:VAL:HG22	1:B:295:LEU:HG	1.93	0.50
1:D:205:ARG:HH11	1:D:219:MET:HB2	1.77	0.50
1:C:126:PRO:HD3	1:C:179:TYR:HB3	1.94	0.49
1:C:37:GLU:HG2	1:C:46:ARG:HG2	1.93	0.49
1:D:190:ALA:O	1:D:194:LEU:HB2	2.13	0.49
1:D:143:PRO:HA	1:D:147:GLN:HE21	1.78	0.48
1:A:207:LEU:HD12	1:A:226:TRP:HB3	1.95	0.48
1:C:169:GLN:HG3	4:C:408:HOH:O	2.12	0.48
1:B:189:TYR:HB2	1:B:295:LEU:HD12	1.94	0.48
1:A:47:VAL:HG22	1:A:208:VAL:HG12	1.96	0.47
1:A:88:ASN:ND2	1:A:180:VAL:H	2.11	0.47
1:D:49:VAL:HG11	1:D:198:MET:CE	2.45	0.46
1:A:227:ARG:HD2	1:A:243:ILE:HG21	1.96	0.46
1:C:194:LEU:HD23	1:C:208:VAL:HG13	1.97	0.46
1:D:194:LEU:HD23	1:D:208:VAL:HG13	1.98	0.46
1:D:326:ILE:HG12	1:D:335:THR:HG22	1.97	0.45
1:B:347:SER:O	1:B:348:ASP:HB3	2.16	0.45
1:C:224:GLN:HG2	4:C:480:HOH:O	2.17	0.45
1:D:41:MET:O	3:D:500:FAD:H2'	2.17	0.44
1:A:319:GLU:HB3	1:A:321:LEU:HD13	1.99	0.44
1:B:77:THR:HA	1:B:85:MET:HE3	2.00	0.43
1:D:119:ALA:HB1	1:D:306:VAL:HB	2.00	0.43
1:D:33:ALA:HB2	1:D:221:ALA:HB2	2.01	0.43
1:D:284:LEU:O	1:D:305:MET:HE1	2.19	0.43
1:B:197:LEU:HA	1:B:200:GLN:HE21	1.83	0.43
1:B:267:ARG:HD3	1:D:37:GLU:HG3	2.00	0.43
1:B:85:MET:HG3	1:B:89:HIS:CE1	2.54	0.43
1:D:144:THR:HG22	1:D:147:GLN:HG2	2.00	0.43
1:C:50:VAL:HB	1:C:205:ARG:HG3	2.00	0.42
1:B:230:ILE:HD13	1:B:341:PHE:HZ	1.84	0.42
1:A:220:ASN:HB3	1:A:222:GLN:H	1.84	0.42
1:A:162:VAL:HB	1:B:164:ASP:HB2	2.03	0.41
1:B:324:PHE:HD1	1:B:337:MET:HB3	1.85	0.41
1:D:175:LEU:HA	1:D:176:PRO:HD3	1.93	0.41
1:C:326:ILE:HG12	1:C:335:THR:HG22	2.03	0.41
1:D:330:GLY:C	1:D:332:GLY:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:O	1:A:319:GLU:HB2	2.20	0.41
1:D:77:THR:HA	1:D:85:MET:CE	2.50	0.41
1:A:319:GLU:N	1:A:320:GLY:HA2	2.36	0.41
1:B:159:HIS:O	1:B:173:LYS:HA	2.21	0.41
1:D:53:ASP:HB3	1:D:56:ARG:HG2	2.03	0.41
1:A:273:ASP:HA	1:A:274:PRO:HD3	1.95	0.40
1:A:164:ASP:HB2	1:B:162:VAL:HB	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	315/337 (94%)	307 (98%)	8 (2%)	0	100	100
1	B	305/337 (90%)	300 (98%)	5 (2%)	0	100	100
1	C	321/337 (95%)	314 (98%)	7 (2%)	0	100	100
1	D	307/337 (91%)	300 (98%)	7 (2%)	0	100	100
All	All	1248/1348 (93%)	1221 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/275 (94%)	246 (96%)	11 (4%)	35	68
1	B	251/275 (91%)	242 (96%)	9 (4%)	42	75
1	C	262/275 (95%)	250 (95%)	12 (5%)	33	65
1	D	253/275 (92%)	244 (96%)	9 (4%)	42	75
All	All	1023/1100 (93%)	982 (96%)	41 (4%)	38	71

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	120	MET
1	A	140	LEU
1	A	141	HIS
1	A	144	THR
1	A	158	GLN
1	A	275	GLN
1	A	319	GLU
1	A	321	LEU
1	A	327	MET
1	A	331	GLU
1	B	56	ARG
1	B	108	SER
1	B	120	MET
1	B	141	HIS
1	B	158	GLN
1	B	185	VAL
1	B	198	MET
1	B	267	ARG
1	B	327	MET
1	C	120	MET
1	C	136	ASP
1	C	185	VAL
1	C	205	ARG
1	C	222	GLN
1	C	230	ILE
1	C	257	TYR
1	C	261	TYR
1	C	286	SER
1	C	327	MET
1	C	343	THR
1	C	348	ASP
1	D	37	GLU

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Mol	Chain	Res	Type
1	D	60	LEU
1	D	91	ARG
1	D	199	GLU
1	D	224	GLN
1	D	258	ARG
1	D	305	MET
1	D	327	MET
1	D	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	168	HIS
1	A	169	GLN
1	A	200	GLN
1	A	313	GLN
1	A	340	GLN
1	B	88	ASN
1	B	89	HIS
1	B	161	GLN
1	B	200	GLN
1	C	147	GLN
1	D	147	GLN
1	D	283	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

48 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SO4	A	357	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	358	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	359	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	A	360	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	A	361	-	4,4,4	0.20	0	6,6,6	0.07	0
2	SO4	A	362	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	A	363	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	364	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	365	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	A	366	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	A	367	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	A	368	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	A	369	-	4,4,4	0.22	0	6,6,6	0.12	0
3	FAD	A	500	-	48,58,58	1.26	6 (12%)	54,89,89	2.08	7 (12%)
2	SO4	B	357	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	B	358	-	4,4,4	0.21	0	6,6,6	0.10	0
2	SO4	B	359	-	4,4,4	0.18	0	6,6,6	0.08	0
2	SO4	B	360	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	B	361	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	B	362	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	363	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	B	364	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	B	365	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	B	366	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	B	367	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	368	-	4,4,4	0.22	0	6,6,6	0.09	0
3	FAD	B	500	-	48,58,58	1.24	6 (12%)	54,89,89	2.11	9 (16%)
2	SO4	C	357	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	C	358	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	C	359	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	C	360	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	C	361	-	4,4,4	0.24	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	362	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	363	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	364	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	C	365	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	C	366	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	C	367	-	4,4,4	0.25	0	6,6,6	0.12	0
3	FAD	C	500	-	48,58,58	1.26	6 (12%)	54,89,89	2.08	7 (12%)
2	SO4	D	357	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	D	358	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	D	359	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	D	360	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	D	361	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	D	362	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	D	363	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	D	364	-	4,4,4	0.23	0	6,6,6	0.08	0
3	FAD	D	500	-	48,58,58	1.24	6 (12%)	54,89,89	2.05	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	357	-	-	0/0/0/0	0/0/0/0
2	SO4	A	358	-	-	0/0/0/0	0/0/0/0
2	SO4	A	359	-	-	0/0/0/0	0/0/0/0
2	SO4	A	360	-	-	0/0/0/0	0/0/0/0
2	SO4	A	361	-	-	0/0/0/0	0/0/0/0
2	SO4	A	362	-	-	0/0/0/0	0/0/0/0
2	SO4	A	363	-	-	0/0/0/0	0/0/0/0
2	SO4	A	364	-	-	0/0/0/0	0/0/0/0
2	SO4	A	365	-	-	0/0/0/0	0/0/0/0
2	SO4	A	366	-	-	0/0/0/0	0/0/0/0
2	SO4	A	367	-	-	0/0/0/0	0/0/0/0
2	SO4	A	368	-	-	0/0/0/0	0/0/0/0
2	SO4	A	369	-	-	0/0/0/0	0/0/0/0
3	FAD	A	500	-	-	0/30/50/50	0/6/6/6
2	SO4	B	357	-	-	0/0/0/0	0/0/0/0
2	SO4	B	358	-	-	0/0/0/0	0/0/0/0
2	SO4	B	359	-	-	0/0/0/0	0/0/0/0
2	SO4	B	360	-	-	0/0/0/0	0/0/0/0
2	SO4	B	361	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	362	-	-	0/0/0/0	0/0/0/0
2	SO4	B	363	-	-	0/0/0/0	0/0/0/0
2	SO4	B	364	-	-	0/0/0/0	0/0/0/0
2	SO4	B	365	-	-	0/0/0/0	0/0/0/0
2	SO4	B	366	-	-	0/0/0/0	0/0/0/0
2	SO4	B	367	-	-	0/0/0/0	0/0/0/0
2	SO4	B	368	-	-	0/0/0/0	0/0/0/0
3	FAD	B	500	-	-	0/30/50/50	0/6/6/6
2	SO4	C	357	-	-	0/0/0/0	0/0/0/0
2	SO4	C	358	-	-	0/0/0/0	0/0/0/0
2	SO4	C	359	-	-	0/0/0/0	0/0/0/0
2	SO4	C	360	-	-	0/0/0/0	0/0/0/0
2	SO4	C	361	-	-	0/0/0/0	0/0/0/0
2	SO4	C	362	-	-	0/0/0/0	0/0/0/0
2	SO4	C	363	-	-	0/0/0/0	0/0/0/0
2	SO4	C	364	-	-	0/0/0/0	0/0/0/0
2	SO4	C	365	-	-	0/0/0/0	0/0/0/0
2	SO4	C	366	-	-	0/0/0/0	0/0/0/0
2	SO4	C	367	-	-	0/0/0/0	0/0/0/0
3	FAD	C	500	-	-	0/30/50/50	0/6/6/6
2	SO4	D	357	-	-	0/0/0/0	0/0/0/0
2	SO4	D	358	-	-	0/0/0/0	0/0/0/0
2	SO4	D	359	-	-	0/0/0/0	0/0/0/0
2	SO4	D	360	-	-	0/0/0/0	0/0/0/0
2	SO4	D	361	-	-	0/0/0/0	0/0/0/0
2	SO4	D	362	-	-	0/0/0/0	0/0/0/0
2	SO4	D	363	-	-	0/0/0/0	0/0/0/0
2	SO4	D	364	-	-	0/0/0/0	0/0/0/0
3	FAD	D	500	-	-	0/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	FAD	C10-N1	2.04	1.39	1.35
3	B	500	FAD	C5X-N5	2.04	1.38	1.35
3	C	500	FAD	C10-N1	2.05	1.39	1.35
3	D	500	FAD	C5X-N5	2.05	1.38	1.35
3	A	500	FAD	C2A-N1A	2.42	1.38	1.33
3	B	500	FAD	C2A-N1A	2.45	1.38	1.33
3	D	500	FAD	C2A-N1A	2.49	1.38	1.33
3	C	500	FAD	C2A-N1A	2.49	1.38	1.33
3	A	500	FAD	C4-N3	2.65	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	FAD	C1'-N10	2.75	1.51	1.48
3	B	500	FAD	C1'-N10	2.78	1.51	1.48
3	C	500	FAD	C4-N3	2.96	1.38	1.33
3	B	500	FAD	C4-N3	3.00	1.38	1.33
3	D	500	FAD	C4-N3	3.06	1.38	1.33
3	C	500	FAD	C4X-N5	3.21	1.38	1.33
3	A	500	FAD	C4X-N5	3.24	1.38	1.33
3	B	500	FAD	C4X-N5	3.34	1.38	1.33
3	D	500	FAD	C4X-N5	3.38	1.38	1.33
3	C	500	FAD	C1'-N10	3.40	1.52	1.48
3	A	500	FAD	C1'-N10	3.44	1.52	1.48
3	C	500	FAD	C2A-N3A	3.45	1.38	1.32
3	A	500	FAD	C2A-N3A	3.65	1.38	1.32
3	B	500	FAD	C2A-N3A	3.70	1.38	1.32
3	D	500	FAD	C2A-N3A	3.75	1.38	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	FAD	N3A-C2A-N1A	-11.80	119.86	128.89
3	C	500	FAD	N3A-C2A-N1A	-11.53	120.07	128.89
3	A	500	FAD	N3A-C2A-N1A	-11.38	120.18	128.89
3	D	500	FAD	N3A-C2A-N1A	-11.30	120.24	128.89
3	A	500	FAD	P-O3P-PA	-3.70	122.33	132.73
3	B	500	FAD	P-O3P-PA	-3.63	122.53	132.73
3	D	500	FAD	P-O3P-PA	-3.36	123.30	132.73
3	C	500	FAD	P-O3P-PA	-3.15	123.89	132.73
3	D	500	FAD	C4X-C4-N3	-2.67	119.93	123.59
3	C	500	FAD	C4X-C4-N3	-2.66	119.95	123.59
3	B	500	FAD	C4X-C4-N3	-2.62	120.01	123.59
3	A	500	FAD	C4X-C4-N3	-2.60	120.03	123.59
3	D	500	FAD	C4A-C5A-N7A	-2.26	107.40	109.48
3	B	500	FAD	C2B-C1B-N9A	-2.06	111.14	114.29
3	D	500	FAD	C4B-O4B-C1B	2.01	111.92	109.72
3	B	500	FAD	C1'-C2'-C3'	2.04	115.67	109.82
3	B	500	FAD	C5X-C9A-N10	2.55	119.56	117.62
3	A	500	FAD	C1'-C2'-C3'	2.82	117.90	109.82
3	C	500	FAD	C4X-N5-C5X	2.88	120.07	116.76
3	D	500	FAD	C5X-C9A-N10	2.97	119.88	117.62
3	A	500	FAD	C4X-N5-C5X	2.99	120.21	116.76
3	B	500	FAD	C4X-N5-C5X	3.11	120.34	116.76
3	B	500	FAD	C1'-N10-C9A	3.11	122.35	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	500	FAD	C4X-N5-C5X	3.11	120.34	116.76
3	C	500	FAD	C1'-C2'-C3'	3.13	118.77	109.82
3	C	500	FAD	C5X-C9A-N10	3.17	120.03	117.62
3	A	500	FAD	C5X-C9A-N10	3.20	120.05	117.62
3	C	500	FAD	C4-N3-C2	5.35	119.87	115.25
3	B	500	FAD	C4-N3-C2	5.36	119.88	115.25
3	A	500	FAD	C4-N3-C2	5.41	119.92	115.25
3	D	500	FAD	C4-N3-C2	5.49	119.99	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	362	SO4	1	0
3	D	500	FAD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/337 (94%)	-0.09	12 (3%) 44 37	22, 35, 59, 99	0
1	B	309/337 (91%)	-0.12	9 (2%) 55 48	22, 35, 53, 111	0
1	C	323/337 (95%)	-0.05	14 (4%) 39 32	21, 34, 59, 85	0
1	D	310/337 (91%)	0.03	12 (3%) 43 36	24, 35, 58, 86	0
All	All	1259/1348 (93%)	-0.06	47 (3%) 45 38	21, 35, 57, 111	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	ASP	6.5
1	A	348	ASP	5.9
1	C	140	LEU	5.8
1	D	348	ASP	5.4
1	A	347	SER	5.3
1	B	348	ASP	5.2
1	B	137	ARG	4.8
1	A	137	ARG	4.7
1	A	140	LEU	4.7
1	C	137	ARG	4.1
1	B	140	LEU	3.9
1	D	139	PRO	3.7
1	C	28	THR	3.7
1	D	331	GLU	3.6
1	D	137	ARG	3.6
1	A	141	HIS	3.6
1	B	347	SER	3.5
1	D	347	SER	3.4
1	D	141	HIS	3.4
1	D	234	THR	3.4
1	C	139	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	136	ASP	3.1
1	D	142	ILE	3.0
1	C	237	GLU	3.0
1	A	238	ASN	2.8
1	B	136	ASP	2.7
1	A	235	ASP	2.7
1	C	141	HIS	2.7
1	C	30	SER	2.5
1	D	241	GLN	2.3
1	C	29	ALA	2.3
1	C	347	SER	2.3
1	D	148	ILE	2.3
1	C	231	GLN	2.3
1	D	330	GLY	2.2
1	D	140	LEU	2.2
1	B	241	GLN	2.2
1	C	138	GLN	2.2
1	C	240	VAL	2.2
1	A	142	ILE	2.1
1	B	268	VAL	2.1
1	B	138	GLN	2.1
1	A	236	ARG	2.1
1	B	331	GLU	2.0
1	A	32	ALA	2.0
1	C	329	GLU	2.0
1	A	234	THR	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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	358	5/5	0.81	0.41	12.94	112,115,116,118	0
2	SO4	B	360	5/5	0.85	0.30	8.81	97,98,100,101	0
2	SO4	A	362	5/5	0.86	0.25	4.83	77,82,83,89	0
2	SO4	C	360	5/5	0.88	0.21	3.60	96,97,98,99	0
2	SO4	A	364	5/5	0.86	0.21	3.20	101,104,106,107	0
2	SO4	A	367	5/5	0.72	0.30	2.86	117,120,121,122	0
2	SO4	D	359	5/5	0.92	0.18	2.76	84,85,86,87	0
2	SO4	D	358	5/5	0.90	0.24	2.59	84,85,87,90	0
2	SO4	D	361	5/5	0.77	0.29	2.34	109,111,112,112	0
2	SO4	A	368	5/5	0.87	0.25	2.26	95,97,99,101	0
2	SO4	B	366	5/5	0.94	0.24	2.21	94,96,97,97	0
2	SO4	A	359	5/5	0.78	0.28	2.18	96,100,103,107	0
2	SO4	C	364	5/5	0.90	0.28	1.86	93,93,94,97	0
2	SO4	C	362	5/5	0.89	0.18	1.66	81,85,87,88	0
2	SO4	C	357	5/5	0.95	0.21	1.59	47,50,53,62	0
2	SO4	A	361	5/5	0.93	0.21	0.95	73,75,76,76	0
2	SO4	B	364	5/5	0.95	0.15	0.91	42,44,54,58	0
2	SO4	C	365	5/5	0.82	0.30	0.81	113,115,117,119	0
2	SO4	B	365	5/5	0.85	0.21	0.66	104,106,107,109	0
3	FAD	D	500	53/53	0.93	0.15	-0.17	27,48,61,71	0
2	SO4	D	362	5/5	0.89	0.20	-0.39	92,94,96,97	0
2	SO4	A	366	5/5	0.93	0.14	-0.63	72,76,77,82	0
3	FAD	B	500	53/53	0.95	0.13	-0.65	17,36,51,66	0
3	FAD	A	500	53/53	0.96	0.12	-0.90	25,34,48,55	0
3	FAD	C	500	53/53	0.96	0.12	-0.99	15,26,40,50	0
2	SO4	B	362	5/5	0.97	0.13	-1.46	38,45,48,52	0
2	SO4	B	361	5/5	0.97	0.10	-1.49	54,62,63,64	0
2	SO4	D	360	5/5	0.98	0.08	-1.50	36,48,52,55	0
2	SO4	C	361	5/5	0.96	0.09	-1.68	40,41,43,46	0
2	SO4	C	363	5/5	0.97	0.08	-1.70	53,57,59,63	0
2	SO4	B	363	5/5	0.97	0.11	-2.40	42,47,52,55	0
2	SO4	A	360	5/5	0.96	0.13	-2.59	48,50,52,53	0
2	SO4	C	359	5/5	0.98	0.09	-3.32	58,62,64,66	0
2	SO4	B	357	5/5	0.94	0.14	-	81,82,84,84	0
2	SO4	A	369	5/5	0.92	0.15	-	72,72,76,76	0
2	SO4	A	363	5/5	0.85	0.20	-	107,108,108,110	0
2	SO4	D	357	5/5	0.95	0.15	-	45,52,54,57	0
2	SO4	A	358	5/5	0.84	0.28	-	104,108,109,113	0
2	SO4	B	358	5/5	0.91	0.20	-	76,77,78,80	0
2	SO4	D	364	5/5	0.82	0.35	-	105,106,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	C	366	5/5	0.80	0.32	-	105,106,107,108	0
2	SO4	B	368	5/5	0.82	0.34	-	103,105,106,107	0
2	SO4	A	365	5/5	0.92	0.17	-	72,80,80,82	0
2	SO4	B	367	5/5	0.89	0.25	-	85,92,95,95	0
2	SO4	D	363	5/5	0.79	0.33	-	95,100,102,102	0
2	SO4	A	357	5/5	0.97	0.14	-	44,47,55,59	0
2	SO4	C	367	5/5	0.84	0.35	-	122,123,126,127	0
2	SO4	B	359	5/5	0.96	0.13	-	62,62,66,68	0

6.5 Other polymers

There are no such residues in this entry.