



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 05:28 PM GMT

PDB ID : 1E6E  
Title : ADRENODOXIN REDUCTASE/ADRENODOXINCOMPLEX OF MITO-  
CHONDRIAL P450 SYSTEMS  
Authors : Mueller, J.J.; Lapko, A.; Bourenkov, G.; Ruckpaul, K.; Heinemann, U.  
Deposited on : 2000-08-15  
Resolution : 2.30 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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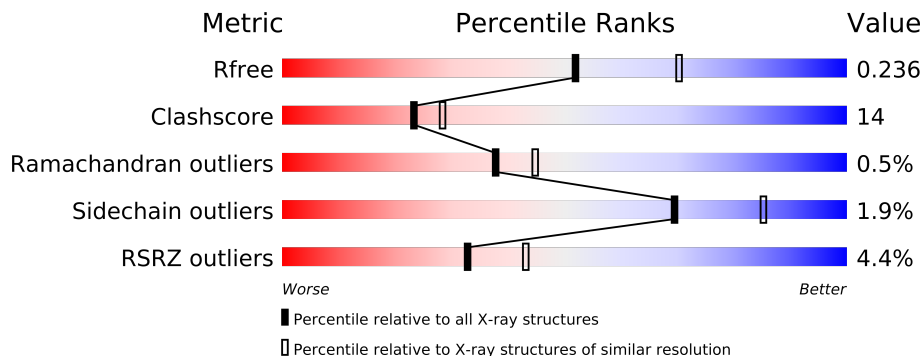
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	460	
1	C	460	
2	B	128	
2	D	128	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	C	3003	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9112 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 NADPH\ADRENODOXINOXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3518	2222	637	648	11			
1	C	456	Total	C	N	O	S	0	0	0
			3514	2220	636	647	11			

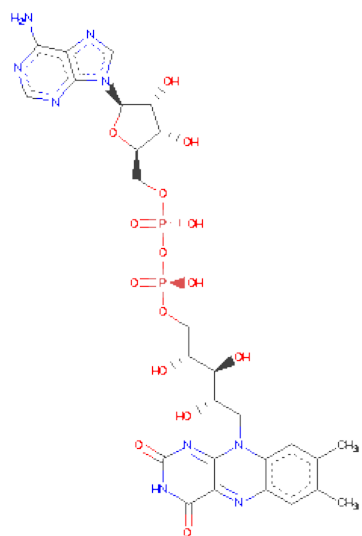
- Molecule 2 is a protein called ADRENODOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			858	529	147	174	8			
2	D	106	Total	C	N	O	S	0	0	0
			809	501	137	163	8			

There are 2 discrepancies between the modelled and reference sequences:

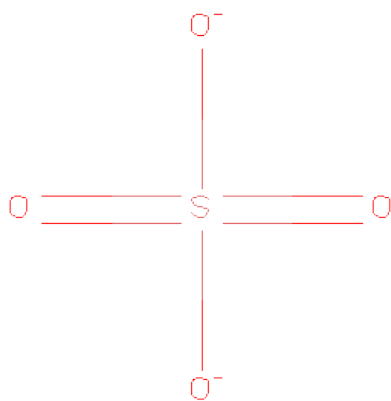
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	SER	ENGINEERED MUTATION	UNP P00257
D	1	GLY	SER	ENGINEERED MUTATION	UNP P00257

- Molecule 3 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
3	A	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		

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



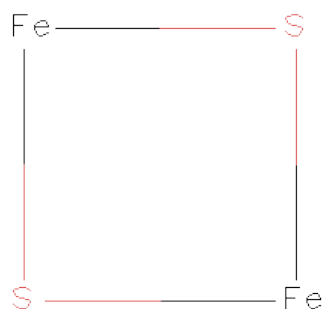
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is water.

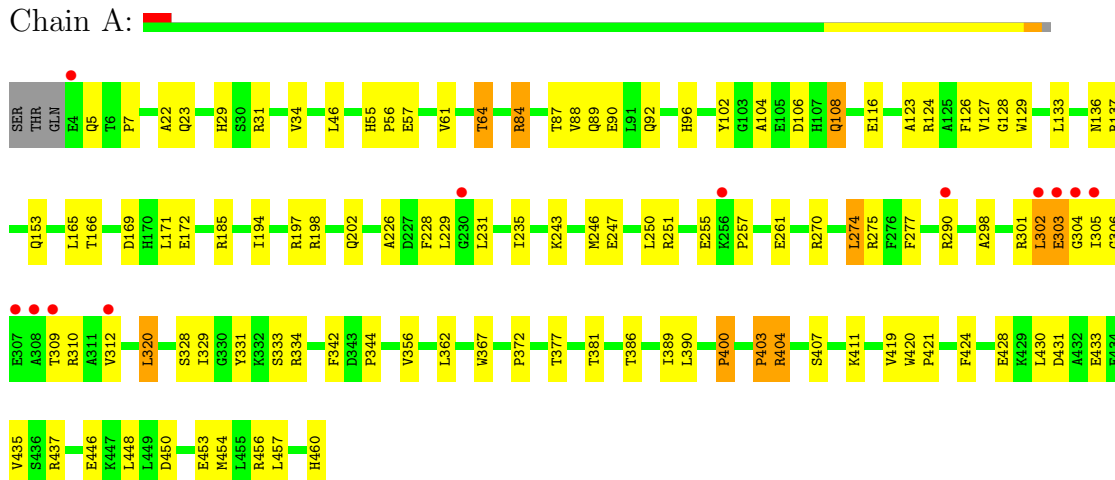
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	12	Total	O	0	0
			12	12		
6	C	123	Total	O	0	0
			123	123		
6	D	11	Total	O	0	0
			11	11		

### 3 Residue-property plots

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

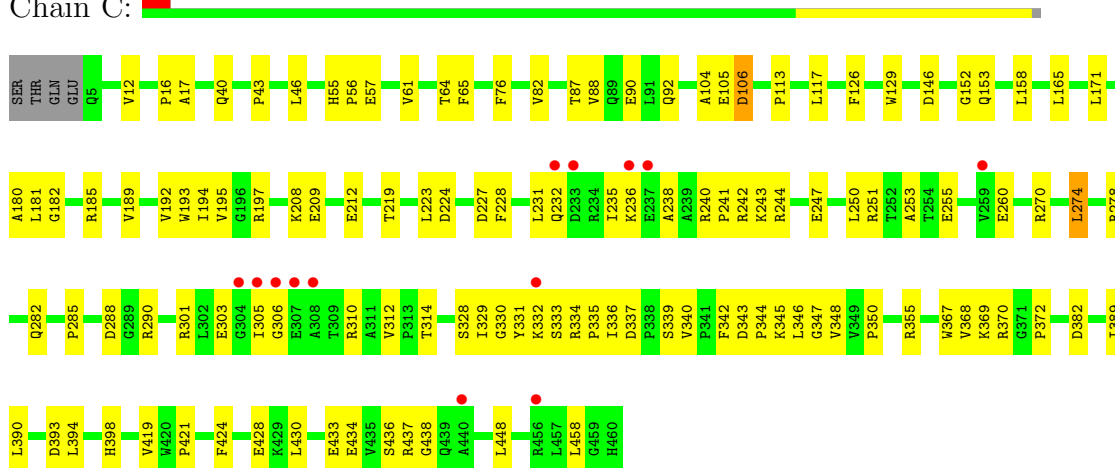
#### • Molecule 1: NADPH\ADRENODOXINOXIDOREDUCTASE

Chain A:



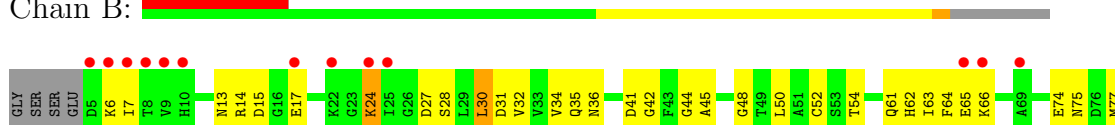
#### • Molecule 1: NADPH\ADRENODOXINOXIDOREDUCTASE

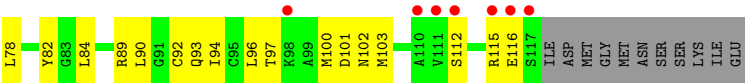
Chain C:



#### • Molecule 2: ADRENODOXIN

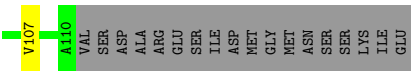
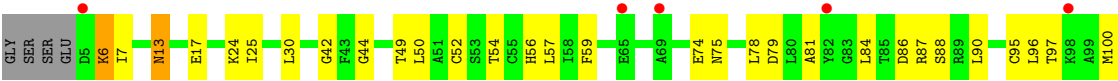
Chain B:





● Molecule 2: ADRENODOXIN

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.21Å 92.21Å 607.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.30 39.93 – 2.21	Depositor EDS
% Data completeness (in resolution range)	79.1 (19.97-2.30) 73.0 (39.93-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.22 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.222 , 0.268 0.224 , 0.236	Depositor DCC
$R_{free}$ test set	2907 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 24.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57539 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: FES, FAD, SO4

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	0/3597	0.59	0/4888
1	C	0.29	0/3593	0.57	0/4883
2	B	0.34	0/866	0.55	0/1168
2	D	0.38	1/817 (0.1%)	0.57	0/1102
All	All	0.31	1/8873 (0.0%)	0.57	0/12041

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	52	CYS	CB-SG	6.72	1.93	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3518	0	3542	105	0
1	C	3514	0	3541	96	0
2	B	858	0	836	39	0
2	D	809	0	791	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	3	0
3	C	53	0	31	2	0
4	A	15	0	0	0	0
4	C	10	0	0	0	0
5	B	4	0	0	1	0
5	D	4	0	0	1	0
6	A	128	0	0	5	0
6	B	12	0	0	1	0
6	C	123	0	0	3	0
6	D	11	0	0	0	0
All	All	9112	0	8772	255	0

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 14.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:113:PRO:HG2	1:C:282:GLN:HG3	1.44	0.95
2:D:81:ALA:HB3	2:D:84:LEU:HD13	1.53	0.90
1:A:302:LEU:H	1:A:302:LEU:HD23	1.37	0.90
1:A:235:ILE:HD12	1:A:246:MET:HB3	1.54	0.86
1:A:453:GLU:HG3	1:A:456:ARG:HH12	1.41	0.86
1:C:61:VAL:O	1:C:64:THR:HG22	1.77	0.85
1:A:400:PRO:HB3	1:A:404:ARG:NH2	1.94	0.83
2:D:7:ILE:HD11	2:D:96:LEU:HD22	1.60	0.82
1:C:434:GLU:HG2	1:C:448:LEU:HD23	1.63	0.81
1:C:240:ARG:HD3	2:D:84:LEU:HD23	1.61	0.81
2:D:6:LYS:HG2	2:D:24:LYS:HA	1.65	0.78
1:A:290:ARG:HB3	1:A:290:ARG:NH1	2.02	0.75
1:C:345:LYS:HG3	1:C:346:LEU:HD12	1.69	0.74
1:A:400:PRO:HB3	1:A:404:ARG:HH21	1.53	0.73
1:A:87:THR:OG1	1:A:90:GLU:HG3	1.89	0.72
2:D:6:LYS:HG3	2:D:25:ILE:HD13	1.70	0.72
2:B:7:ILE:HD11	2:B:96:LEU:HB3	1.71	0.71
2:B:34:VAL:HG13	2:B:35:GLN:H	1.55	0.71
1:C:104:ALA:HB1	1:C:331:TYR:O	1.90	0.71
1:A:172:GLU:HG2	1:A:185:ARG:HH22	1.55	0.70
1:A:302:LEU:H	1:A:302:LEU:CD2	2.04	0.70
2:B:112:SER:O	2:B:115:ARG:HG2	1.91	0.70
1:C:243:LYS:O	1:C:247:GLU:HG3	1.92	0.70
1:C:197:ARG:HE	1:C:310:ARG:HH22	1.40	0.69
1:A:84:ARG:HD2	1:C:193:TRP:CH2	2.27	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:106:ASP:OD2	1:C:334:ARG:HB3	1.93	0.69
1:A:302:LEU:N	1:A:302:LEU:HD23	2.08	0.67
1:A:84:ARG:HD2	1:C:193:TRP:HH2	1.61	0.66
1:A:169:ASP:HA	1:A:172:GLU:HG3	1.76	0.66
1:C:197:ARG:HH21	1:C:310:ARG:NH2	1.94	0.66
1:A:198:ARG:HH22	1:A:309:THR:HG22	1.61	0.65
1:A:108:GLN:HE21	1:A:108:GLN:HA	1.61	0.65
1:A:305:ILE:HG22	1:A:306:GLY:H	1.62	0.65
2:D:97:THR:N	2:D:100:MET:HE3	2.11	0.64
1:A:108:GLN:HB2	1:A:329:ILE:HG13	1.78	0.64
1:C:332:LYS:HD3	1:C:347:GLY:HA3	1.79	0.63
1:C:88:VAL:O	1:C:92:GLN:HG3	1.97	0.63
2:B:30:LEU:O	2:B:34:VAL:HG12	1.98	0.63
1:A:356:VAL:HG21	1:A:362:LEU:HG	1.80	0.63
1:A:106:ASP:O	1:A:331:TYR:HB3	1.97	0.63
1:A:231:LEU:O	1:A:235:ILE:HG12	1.99	0.63
1:C:337:ASP:HB3	1:C:340:VAL:HG23	1.80	0.63
1:C:430:LEU:HG	1:C:458:LEU:HD21	1.81	0.62
1:A:290:ARG:HH11	1:A:290:ARG:HB3	1.63	0.62
1:C:260:GLU:CD	1:C:260:GLU:H	2.01	0.62
1:A:88:VAL:O	1:A:92:GLN:HG3	1.99	0.62
1:C:355:ARG:CZ	1:C:389:ILE:HD11	2.30	0.62
1:A:305:ILE:HG22	1:A:306:GLY:N	2.14	0.62
1:C:372:PRO:HD3	6:C:2100:HOH:O	2.00	0.61
2:B:66:LYS:N	2:B:66:LYS:HD2	2.14	0.61
2:B:97:THR:N	2:B:100:MET:HE3	2.15	0.61
2:D:97:THR:H	2:D:100:MET:HE3	1.65	0.61
2:B:34:VAL:HG13	2:B:35:GLN:N	2.14	0.60
2:B:62:HIS:CE1	2:B:63:ILE:HG13	2.37	0.60
1:A:153:GLN:HG2	1:A:194:ILE:HG22	1.83	0.60
1:A:198:ARG:HD3	1:A:202:GLN:HG2	1.84	0.60
1:A:106:ASP:OD1	1:A:334:ARG:HD2	2.02	0.60
1:A:124:ARG:HD3	1:A:331:TYR:CE1	2.37	0.60
1:A:377:THR:O	1:A:381:THR:HG23	2.02	0.60
2:B:74:GLU:HG3	2:B:90:LEU:HD12	1.83	0.59
1:C:219:THR:HA	1:C:270:ARG:O	2.02	0.59
1:C:240:ARG:HD3	2:D:84:LEU:CD2	2.29	0.59
2:B:44:GLY:HA2	5:B:129:FES:S2	2.43	0.59
1:C:433:GLU:O	1:C:437:ARG:HG3	2.03	0.58
2:D:6:LYS:HG3	2:D:25:ILE:CD1	2.33	0.58
1:C:106:ASP:CG	1:C:334:ARG:HB3	2.23	0.58
1:A:29:HIS:HD2	1:A:31:ARG:H	1.49	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:244:ARG:CZ	2:D:75:ASN:HB3	2.34	0.58
1:C:343:ASP:OD1	1:C:345:LYS:HB3	2.04	0.58
1:C:305:ILE:HG22	1:C:306:GLY:H	1.69	0.58
2:B:65:GLU:HB2	2:B:66:LYS:HD2	1.86	0.58
1:A:328:SER:HA	6:A:2092:HOH:O	2.04	0.58
1:A:235:ILE:HD12	1:A:246:MET:CB	2.28	0.58
1:A:128:GLY:HA3	1:A:136:ASN:HD22	1.67	0.58
2:D:74:GLU:HG3	2:D:90:LEU:HD12	1.85	0.57
1:C:197:ARG:NE	1:C:310:ARG:HH22	2.02	0.57
2:B:28:SER:HA	2:B:94:ILE:O	2.04	0.57
1:C:335:PRO:HG3	1:C:342:PHE:CG	2.39	0.57
1:C:153:GLN:HG2	1:C:194:ILE:HG22	1.86	0.57
1:A:430:LEU:HG	1:A:448:LEU:HD12	1.87	0.57
1:A:342:PHE:O	1:A:344:PRO:HD3	2.04	0.56
1:C:419:VAL:O	1:C:421:PRO:HD3	2.05	0.56
1:A:420:TRP:CZ3	1:A:460:HIS:HA	2.41	0.56
2:D:13:ASN:HB3	2:D:17:GLU:HB2	1.86	0.56
1:C:301:ARG:HG3	1:C:314:THR:CG2	2.36	0.56
1:C:236:LYS:HE2	1:C:236:LYS:HA	1.87	0.55
2:D:95:CYS:O	2:D:100:MET:HE1	2.07	0.55
1:A:127:VAL:HG11	3:A:461:FAD:HM72	1.88	0.55
1:C:146:ASP:HA	1:C:189:VAL:HA	1.88	0.55
2:B:34:VAL:HG13	2:B:35:GLN:HG3	1.88	0.55
2:B:115:ARG:HG3	2:B:116:GLU:OE2	2.07	0.55
1:A:61:VAL:O	1:A:64:THR:HG23	2.07	0.54
1:C:303:GLU:HG3	1:C:312:VAL:HG11	1.88	0.54
1:C:328:SER:O	1:C:329:ILE:HG23	2.07	0.54
2:B:32:VAL:O	2:B:36:ASN:HB2	2.08	0.54
1:C:82:VAL:HB	1:C:336:ILE:HD11	1.88	0.54
1:C:194:ILE:HB	1:C:274:LEU:HD12	1.90	0.54
1:A:407:SER:HB2	1:A:411:LYS:HE3	1.90	0.54
1:A:231:LEU:O	1:A:231:LEU:HD23	2.08	0.54
1:C:232:GLN:O	1:C:236:LYS:HG2	2.08	0.53
1:C:126:PHE:O	1:C:129:TRP:HB3	2.08	0.53
1:C:342:PHE:HA	1:C:350:PRO:HD3	1.89	0.53
1:A:126:PHE:O	1:A:129:TRP:HB3	2.08	0.53
1:A:420:TRP:CH2	1:A:460:HIS:HA	2.44	0.52
2:B:42:GLY:O	2:B:54:THR:HB	2.10	0.52
1:C:57:GLU:CD	1:C:57:GLU:H	2.13	0.52
1:A:437:ARG:HB2	1:A:446:GLU:HB3	1.92	0.52
2:B:82:TYR:CD2	2:B:115:ARG:HD2	2.45	0.52
1:C:208:LYS:O	1:C:212:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:424:PHE:O	1:C:428:GLU:HG2	2.10	0.52
1:C:46:LEU:HB2	3:C:461:FAD:O4'	2.10	0.52
1:A:275:ARG:HH12	1:A:320:LEU:HD11	1.74	0.52
1:A:172:GLU:HG2	1:A:185:ARG:NH2	2.25	0.51
1:A:108:GLN:HG3	1:A:329:ILE:O	2.10	0.51
1:A:290:ARG:HH11	1:A:290:ARG:CB	2.24	0.51
2:B:6:LYS:NZ	2:B:6:LYS:HB2	2.26	0.51
1:A:46:LEU:HB2	3:A:461:FAD:O4'	2.11	0.51
1:A:61:VAL:HG12	2:B:45:ALA:HB1	1.92	0.51
1:A:251:ARG:HG3	1:A:255:GLU:OE2	2.11	0.50
2:B:48:GLY:HA2	2:B:92:CYS:SG	2.51	0.50
2:B:61:GLN:O	2:B:65:GLU:HG3	2.12	0.50
1:C:394:LEU:HD23	1:C:394:LEU:C	2.31	0.50
1:A:89:GLN:HG3	6:A:2094:HOH:O	2.10	0.50
1:A:104:ALA:HA	1:A:333:SER:HA	1.94	0.50
1:A:367:TRP:CD2	1:A:372:PRO:HA	2.46	0.50
2:B:100:MET:HB3	2:B:103:MET:HE2	1.93	0.50
1:C:334:ARG:HG2	1:C:334:ARG:HH11	1.76	0.50
1:A:194:ILE:HB	1:A:274:LEU:HD12	1.94	0.49
1:A:243:LYS:O	1:A:247:GLU:HG3	2.12	0.49
1:C:301:ARG:HG3	1:C:314:THR:HG22	1.94	0.49
1:C:57:GLU:HB2	2:D:49:THR:OG1	2.12	0.49
1:A:198:ARG:HH22	1:A:309:THR:CG2	2.25	0.49
1:A:84:ARG:HD3	6:A:2024:HOH:O	2.13	0.49
1:C:305:ILE:HG22	1:C:306:GLY:N	2.27	0.49
1:C:333:SER:O	1:C:342:PHE:CE1	2.66	0.48
1:A:116:GLU:HB2	1:C:303:GLU:OE2	2.13	0.48
2:D:42:GLY:O	2:D:54:THR:HB	2.14	0.48
2:B:27:ASP:HB3	2:B:31:ASP:HB2	1.94	0.48
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.79	0.48
1:C:228:PHE:HB3	1:C:250:LEU:HD23	1.95	0.48
1:C:335:PRO:HG3	1:C:342:PHE:CD2	2.48	0.48
1:C:238:ALA:HB1	1:C:242:ARG:HB3	1.95	0.48
1:C:105:GLU:HB2	6:C:2022:HOH:O	2.14	0.48
1:C:117:LEU:HD11	1:C:285:PRO:HB3	1.96	0.48
1:A:431:ASP:O	1:A:435:VAL:HG23	2.14	0.48
1:A:166:THR:HG21	1:A:171:LEU:HD13	1.96	0.48
2:B:15:ASP:OD1	2:B:17:GLU:HB2	2.14	0.48
1:A:390:LEU:HD23	1:A:390:LEU:C	2.34	0.47
2:D:56:HIS:NE2	2:D:88:SER:HB3	2.29	0.47
1:C:367:TRP:CD2	1:C:372:PRO:HA	2.49	0.47
1:C:348:VAL:HG22	1:C:368:VAL:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:PHE:HA	1:A:231:LEU:HD13	1.97	0.47
1:A:61:VAL:O	1:A:64:THR:CG2	2.62	0.47
1:C:152:GLY:HA3	1:C:329:ILE:HG23	1.96	0.47
1:A:133:LEU:HD23	1:A:136:ASN:ND2	2.30	0.47
2:B:82:TYR:HD2	2:B:115:ARG:HD2	1.79	0.47
1:A:165:LEU:HD22	1:A:270:ARG:HB3	1.97	0.47
1:A:231:LEU:HD21	1:A:235:ILE:HD11	1.97	0.46
1:A:390:LEU:HD23	1:A:390:LEU:O	2.16	0.46
1:A:116:GLU:HG3	1:C:303:GLU:HG2	1.98	0.46
1:A:55:HIS:N	1:A:56:PRO:CD	2.78	0.46
1:A:381:THR:HG22	6:B:2007:HOH:O	2.15	0.46
1:A:96:HIS:CD2	1:A:404:ARG:HG3	2.51	0.46
2:B:61:GLN:HE21	2:B:65:GLU:CG	2.29	0.46
1:C:390:LEU:C	1:C:390:LEU:HD23	2.36	0.46
1:A:453:GLU:O	1:A:457:LEU:HD23	2.16	0.46
2:B:7:ILE:HD11	2:B:96:LEU:HD13	1.97	0.46
1:A:275:ARG:NH1	1:A:320:LEU:HD11	2.31	0.46
1:A:453:GLU:HG3	1:A:456:ARG:NH1	2.20	0.46
1:C:240:ARG:HB3	1:C:241:PRO:HD3	1.97	0.45
2:D:59:PHE:O	2:D:87:ARG:NH1	2.49	0.45
1:C:12:VAL:HG13	1:C:82:VAL:HG21	1.98	0.45
1:A:102:TYR:HB2	3:A:461:FAD:C8A	2.47	0.45
2:B:52:CYS:O	2:B:77:MET:HE2	2.16	0.45
1:A:231:LEU:CD2	1:A:235:ILE:HD11	2.47	0.45
1:A:231:LEU:HD23	1:A:235:ILE:HG12	1.97	0.45
1:C:55:HIS:N	1:C:56:PRO:CD	2.80	0.45
1:C:224:ASP:HB3	1:C:227:ASP:OD2	2.17	0.45
2:D:30:LEU:HD11	2:D:44:GLY:HA3	1.97	0.45
1:A:29:HIS:CD2	1:A:31:ARG:H	2.31	0.45
1:A:57:GLU:H	1:A:57:GLU:CD	2.20	0.45
1:C:240:ARG:HG2	1:C:240:ARG:HH11	1.82	0.45
2:D:57:LEU:HD23	2:D:107:VAL:HG12	2.00	0.44
1:C:251:ARG:O	1:C:255:GLU:HB2	2.17	0.44
1:C:158:LEU:HD12	1:C:209:GLU:HB3	1.98	0.44
1:C:197:ARG:NH2	1:C:310:ARG:NH2	2.64	0.44
1:A:304:GLY:O	1:A:309:THR:HA	2.17	0.44
1:C:236:LYS:HE2	1:C:236:LYS:CA	2.47	0.44
1:C:181:LEU:O	1:C:185:ARG:CG	2.65	0.44
1:A:298:ALA:HB1	6:A:2089:HOH:O	2.18	0.44
1:A:5:GLN:O	1:A:7:PRO:HD3	2.18	0.44
1:A:407:SER:O	1:A:411:LYS:HG3	2.17	0.44
1:A:424:PHE:O	1:A:428:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:GLN:HB2	6:A:2003:HOH:O	2.18	0.44
1:C:342:PHE:O	1:C:344:PRO:HD3	2.18	0.43
1:A:433:GLU:O	1:A:437:ARG:HG3	2.18	0.43
1:C:61:VAL:O	1:C:64:THR:CG2	2.60	0.43
1:C:129:TRP:CZ2	1:C:180:ALA:HA	2.54	0.43
1:C:370:ARG:HD3	1:C:370:ARG:HA	1.81	0.43
1:A:456:ARG:HB3	1:A:456:ARG:NH1	2.34	0.43
1:C:113:PRO:HG2	1:C:282:GLN:CG	2.33	0.43
2:B:32:VAL:HG21	2:B:96:LEU:HD11	2.01	0.43
1:A:419:VAL:O	1:A:421:PRO:HD3	2.19	0.43
1:A:7:PRO:HG2	1:A:29:HIS:CE1	2.54	0.43
1:C:333:SER:O	1:C:342:PHE:CZ	2.71	0.43
1:C:250:LEU:HD13	1:C:250:LEU:C	2.39	0.43
2:B:101:ASP:O	2:B:102:ASN:HB2	2.19	0.43
1:C:43:PRO:HB3	1:C:76:PHE:CE1	2.54	0.43
1:C:223:LEU:HD13	1:C:253:ALA:HB2	2.01	0.43
1:C:240:ARG:NH1	2:D:79:ASP:OD1	2.52	0.42
2:B:24:LYS:HE2	2:B:27:ASP:OD2	2.19	0.42
1:C:337:ASP:OD1	1:C:339:SER:HB3	2.19	0.42
2:B:50:LEU:HD21	2:B:93:GLN:CD	2.39	0.42
1:C:231:LEU:O	1:C:235:ILE:HG13	2.18	0.42
2:D:7:ILE:HD11	2:D:96:LEU:CD2	2.42	0.42
1:A:305:ILE:CG2	1:A:306:GLY:N	2.82	0.42
2:D:50:LEU:HD22	2:D:74:GLU:HA	2.01	0.42
2:B:78:LEU:HG	2:B:84:LEU:HD11	2.01	0.42
1:A:123:ALA:CB	1:A:328:SER:HB3	2.50	0.42
1:C:16:PRO:HA	1:C:65:PHE:CZ	2.55	0.42
2:B:82:TYR:HD2	2:B:115:ARG:HH11	1.63	0.42
1:C:165:LEU:HD21	1:C:192:VAL:HG23	2.01	0.42
1:C:310:ARG:HD2	1:C:310:ARG:HA	1.91	0.42
1:A:407:SER:CB	1:A:411:LYS:HE3	2.49	0.42
2:D:44:GLY:HA2	5:D:129:FES:S2	2.60	0.42
1:C:40:GLN:NE2	6:C:2007:HOH:O	2.53	0.42
2:B:31:ASP:HA	2:B:34:VAL:HG12	2.01	0.42
1:A:124:ARG:HD3	1:A:331:TYR:CZ	2.54	0.42
2:B:97:THR:HG23	2:B:100:MET:HE3	2.01	0.42
1:A:226:ALA:HA	1:A:229:LEU:HG	2.00	0.42
2:B:64:PHE:HE1	2:B:89:ARG:HG2	1.85	0.42
1:A:22:ALA:CB	1:A:34:VAL:HG11	2.50	0.42
1:A:123:ALA:O	1:A:127:VAL:HG23	2.19	0.41
1:C:181:LEU:O	1:C:185:ARG:HG2	2.20	0.41
1:A:450:ASP:O	1:A:454:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:367:TRP:CG	1:A:372:PRO:HA	2.55	0.41
1:C:87:THR:OG1	1:C:90:GLU:HG3	2.21	0.41
1:C:369:LYS:HD3	1:C:382:ASP:OD2	2.20	0.41
1:A:303:GLU:HB3	1:A:312:VAL:HG22	2.03	0.41
2:B:100:MET:HB3	2:B:103:MET:CE	2.51	0.41
1:A:257:PRO:HB2	1:A:261:GLU:HB3	2.03	0.41
2:D:7:ILE:CD1	2:D:96:LEU:HD22	2.42	0.41
1:C:195:VAL:CG1	1:C:278:ARG:HB2	2.51	0.41
2:D:78:LEU:HG	2:D:84:LEU:HD11	2.01	0.41
1:C:182:GLY:HA2	1:C:185:ARG:HG3	2.03	0.41
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.86	0.41
1:C:393:ASP:HB3	1:C:398:HIS:HB2	2.03	0.41
2:B:13:ASN:OD1	2:B:14:ARG:N	2.52	0.41
1:A:247:GLU:O	1:A:251:ARG:HB2	2.21	0.40
1:C:288:ASP:OD1	1:C:290:ARG:HB2	2.21	0.40
1:A:305:ILE:CG2	1:A:306:GLY:H	2.31	0.40
1:C:17:ALA:HB3	3:C:461:FAD:O1P	2.21	0.40
1:A:386:THR:O	1:A:389:ILE:HG22	2.21	0.40
1:A:197:ARG:O	1:A:277:PHE:HA	2.21	0.40
1:C:436:SER:C	1:C:438:GLY:H	2.24	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	455/460 (99%)	425 (93%)	27 (6%)	3 (1%)	30	34
1	C	454/460 (99%)	429 (94%)	24 (5%)	1 (0%)	56	68
2	B	111/128 (87%)	100 (90%)	10 (9%)	1 (1%)	25	26
2	D	104/128 (81%)	93 (89%)	10 (10%)	1 (1%)	22	23
All	All	1124/1176 (96%)	1047 (93%)	71 (6%)	6 (0%)	38	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	GLU
1	A	403	PRO
1	C	330	GLY
2	D	13	ASN
1	A	404	ARG
2	B	41	ASP

### 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	375/379 (99%)	365 (97%)	10 (3%)	57	74
1	C	375/379 (99%)	372 (99%)	3 (1%)	89	96
2	B	95/111 (86%)	92 (97%)	3 (3%)	51	67
2	D	90/111 (81%)	88 (98%)	2 (2%)	64	81
All	All	935/980 (95%)	917 (98%)	18 (2%)	69	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	84	ARG
1	A	108	GLN
1	A	250	LEU
1	A	274	LEU
1	A	302	LEU
1	A	310	ARG
1	A	320	LEU
1	A	400	PRO
1	A	403	PRO
2	B	24	LYS
2	B	30	LEU
2	B	75	ASN
1	C	106	ASP
1	C	171	LEU
1	C	274	LEU
2	D	6	LYS

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Mol	Chain	Res	Type
2	D	86	ASP

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	23	GLN
1	A	28	HIS
1	A	29	HIS
1	A	108	GLN
1	A	136	ASN
1	A	452	GLN
2	B	61	GLN
2	B	75	ASN
1	C	24	HIS
1	C	28	HIS
1	C	107	HIS
1	C	232	GLN
1	C	392	GLN
1	C	452	GLN

### 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 ⓘ

9 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	3001	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	3004	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	A	3005	-	4,4,4	0.25	0	6,6,6	0.10	0
3	FAD	A	461	-	58,58,58	2.08	13 (22%)	85,89,89	1.62	17 (20%)
5	FES	B	129	2	0,4,4	0.00	-	0,4,4	0.00	-
4	SO4	C	3002	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	C	3003	-	4,4,4	0.26	0	6,6,6	0.05	0
3	FAD	C	461	-	58,58,58	2.21	15 (25%)	85,89,89	1.57	15 (17%)
5	FES	D	129	2	0,4,4	0.00	-	0,4,4	0.00	-

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	3001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	3004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	3005	-	-	0/0/0/0	0/0/0/0
3	FAD	A	461	-	-	0/34/50/50	0/1/6/6
5	FES	B	129	2	-	0/0/4/4	0/0/1/1
4	SO4	C	3002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	3003	-	-	0/0/0/0	0/0/0/0
3	FAD	C	461	-	-	0/34/50/50	0/1/6/6
5	FES	D	129	2	-	0/0/4/4	0/0/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	461	FAD	P-O3P	-6.71	1.47	1.59
3	C	461	FAD	C1'-C2'	6.58	1.57	1.51
3	C	461	FAD	P-O3P	-6.51	1.48	1.59
3	C	461	FAD	C9A-N10	5.21	1.46	1.38
3	A	461	FAD	C9A-N10	5.05	1.46	1.38
3	A	461	FAD	C1'-C2'	4.76	1.56	1.51
3	C	461	FAD	PA-O2A	-4.41	1.35	1.55
3	A	461	FAD	C4X-C10	4.41	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	461	FAD	C4X-C10	4.33	1.48	1.40
3	A	461	FAD	PA-O2A	-4.30	1.35	1.55
3	C	461	FAD	O4B-C1B	3.91	1.47	1.41
3	A	461	FAD	O4B-C1B	3.88	1.47	1.41
3	A	461	FAD	P-O2P	-3.70	1.38	1.55
3	C	461	FAD	P-O2P	-3.63	1.38	1.55
3	C	461	FAD	C2-N3	3.56	1.44	1.37
3	C	461	FAD	O5'-C5'	3.47	1.59	1.44
3	A	461	FAD	O5'-C5'	3.44	1.59	1.44
3	A	461	FAD	C2-N3	3.40	1.43	1.37
3	A	461	FAD	C4-C4X	2.71	1.45	1.41
3	C	461	FAD	C4-C4X	2.62	1.45	1.41
3	C	461	FAD	C8-C7	2.39	1.47	1.40
3	C	461	FAD	C4A-N3A	2.33	1.39	1.35
3	C	461	FAD	C2B-C1B	-2.33	1.50	1.53
3	C	461	FAD	C5X-N5	2.26	1.38	1.35
3	A	461	FAD	C8-C7	2.24	1.47	1.40
3	A	461	FAD	C2B-C1B	-2.18	1.50	1.53
3	A	461	FAD	C5X-N5	2.06	1.38	1.35
3	C	461	FAD	C4A-N9A	2.05	1.40	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	461	FAD	O4B-C1B-N9A	-5.84	103.00	108.44
3	C	461	FAD	O4B-C1B-N9A	-5.34	103.47	108.44
3	A	461	FAD	C2-N1-C10	5.21	120.23	114.98
3	C	461	FAD	C2-N1-C10	5.11	120.13	114.98
3	A	461	FAD	C4B-O4B-C1B	-3.67	105.77	109.75
3	A	461	FAD	C4X-C10-N10	-3.63	118.70	120.51
3	C	461	FAD	C4B-O4B-C1B	-3.59	105.85	109.75
3	C	461	FAD	C4X-C10-N10	-3.36	118.83	120.51
3	A	461	FAD	N3A-C2A-N1A	-3.12	126.10	128.71
3	A	461	FAD	O4B-C1B-C2B	-3.03	102.13	106.77
3	C	461	FAD	O4B-C1B-C2B	-3.02	102.14	106.77
3	C	461	FAD	N3A-C2A-N1A	-2.98	126.21	128.71
3	C	461	FAD	O5B-PA-O1A	-2.87	98.13	109.37
3	C	461	FAD	C5'-C4'-C3'	-2.84	106.71	112.06
3	C	461	FAD	P-O3P-PA	2.68	139.54	131.68
3	A	461	FAD	O5B-PA-O1A	-2.57	99.31	109.37
3	A	461	FAD	C1'-N10-C10	2.57	122.81	119.17
3	A	461	FAD	P-O3P-PA	2.53	139.09	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	461	FAD	C1'-N10-C9A	-2.47	116.47	118.87
3	C	461	FAD	N3A-C4A-N9A	2.46	129.87	125.43
3	A	461	FAD	C5'-C4'-C3'	-2.44	107.45	112.06
3	A	461	FAD	N3A-C4A-N9A	2.40	129.76	125.43
3	C	461	FAD	C2A-N1A-C6A	2.31	122.94	118.77
3	A	461	FAD	O5'-P-O1P	-2.26	100.53	109.37
3	C	461	FAD	O5'-P-O1P	-2.25	100.55	109.37
3	C	461	FAD	C5A-C4A-N9A	-2.21	103.97	107.16
3	A	461	FAD	O2A-PA-O3P	2.20	115.60	105.14
3	C	461	FAD	O2A-PA-O3P	2.19	115.52	105.14
3	A	461	FAD	C2A-N1A-C6A	2.17	122.69	118.77
3	A	461	FAD	C5A-C4A-N9A	-2.16	104.05	107.16
3	A	461	FAD	O3P-P-O5'	2.08	112.69	103.41
3	C	461	FAD	O3P-P-O5'	2.05	112.57	103.41

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	457/460 (99%)	-0.19	12 (2%) 53 63	9, 22, 47, 84	0
1	C	456/460 (99%)	-0.20	13 (2%) 49 59	11, 21, 50, 82	0
2	B	113/128 (88%)	0.76	20 (17%) 2 4	27, 53, 80, 84	0
2	D	106/128 (82%)	0.00	5 (4%) 30 40	22, 37, 55, 67	0
All	All	1132/1176 (96%)	-0.08	50 (4%) 33 43	9, 24, 61, 84	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	GLY	7.4
2	B	5	ASP	7.3
1	C	305	ILE	5.6
1	A	302	LEU	5.6
1	C	308	ALA	5.4
2	B	112	SER	4.8
1	A	308	ALA	4.5
1	A	304	GLY	4.5
2	B	115	ARG	3.8
2	D	5	ASP	3.7
2	B	7	ILE	3.6
1	C	304	GLY	3.6
2	B	117	SER	3.4
1	A	307	GLU	3.3
1	C	307	GLU	3.2
2	B	25	ILE	3.2
1	A	305	ILE	3.0
2	B	9	VAL	3.0
2	B	10	HIS	3.0
2	B	8	THR	3.0
1	A	309	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	237	GLU	2.9
1	A	230	GLY	2.8
2	D	65	GLU	2.8
2	B	98	LYS	2.8
2	B	22	LYS	2.7
2	B	66	LYS	2.7
1	A	303	GLU	2.6
1	C	236	LYS	2.6
2	D	82	TYR	2.6
2	B	17	GLU	2.6
2	B	6	LYS	2.5
2	B	24	LYS	2.5
2	B	69	ALA	2.4
2	D	69	ALA	2.3
1	C	232	GLN	2.3
2	B	110	ALA	2.3
1	A	4	GLU	2.2
1	C	233	ASP	2.2
1	C	259	VAL	2.2
1	A	290	ARG	2.2
1	A	312	VAL	2.2
2	D	98	LYS	2.2
1	C	456	ARG	2.1
2	B	65	GLU	2.1
2	B	116	GLU	2.1
1	C	332	LYS	2.1
1	A	256	LYS	2.1
1	C	440	ALA	2.1
2	B	111	VAL	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
4	SO4	C	3003	5/5	0.15	3.68	91,91,91,92	0
4	SO4	A	3004	5/5	0.12	0.99	68,68,69,69	0
3	FAD	A	461	53/53	0.14	0.32	12,18,28,30	0
4	SO4	C	3002	5/5	0.09	0.17	23,24,26,27	0
3	FAD	C	461	53/53	0.11	-0.21	9,14,18,22	0
4	SO4	A	3001	5/5	0.08	-0.38	19,19,20,21	0
4	SO4	A	3005	5/5	0.12	-0.64	43,44,45,46	0
5	FES	D	129	4/4	0.06	-1.26	20,20,22,22	0
5	FES	B	129	4/4	0.07	-1.62	25,26,27,29	0

## 6.5 Other polymers

There are no such residues in this entry.