



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:18 PM GMT

PDB ID : 1JNR
Title : Structure of adenylylsulfate reductase from the hyperthermophilic Archaeoglobus fulgidus at 1.6 resolution
Authors : Fritz, G.; Roth, A.; Schiffer, A.; Buechert, T.; Bourenkov, G.; Bartunik, H.D.; Huber, H.; Stetter, K.O.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2001-07-25
Resolution : 1.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

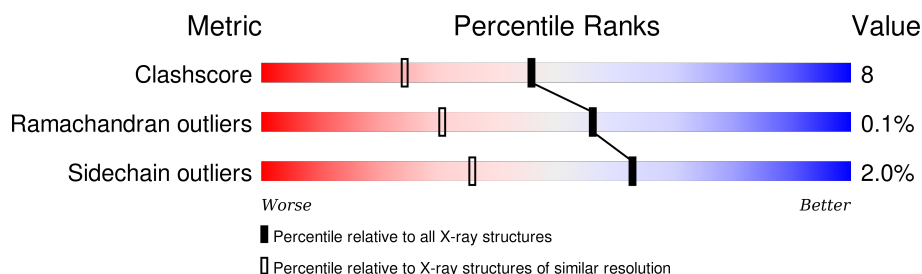
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	643	
1	C	643	
2	B	150	
2	D	150	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14542 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 adenylylsulfate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	8	0
			5199	3364	855	950	30			
1	C	642	Total	C	N	O	S	0	11	0
			5205	3369	853	953	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	ASN	LYS	CONFLICT	UNP O28603
C	183	ASN	LYS	CONFLICT	UNP O28603

- Molecule 2 is a protein called adenylylsulfate reductase.

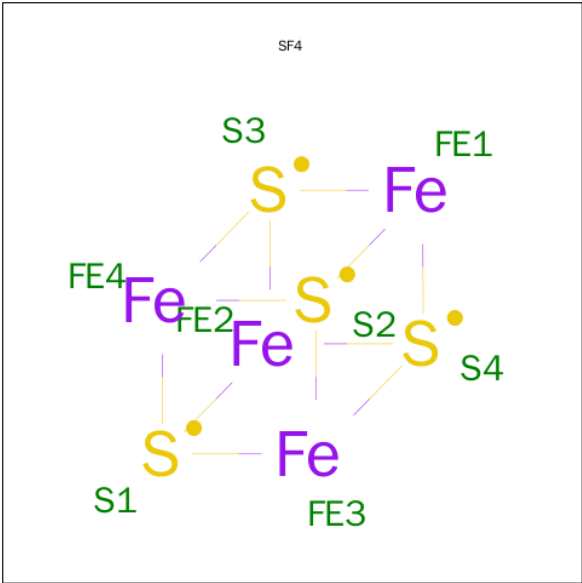
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	1	0
			1176	747	193	220	16			
2	D	149	Total	C	N	O	S	0	1	0
			1176	747	193	220	16			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	584	Total	O	0	3
			587	587		
6	B	170	Total	O	0	1
			171	171		
6	C	649	Total	O	0	10
			659	659		

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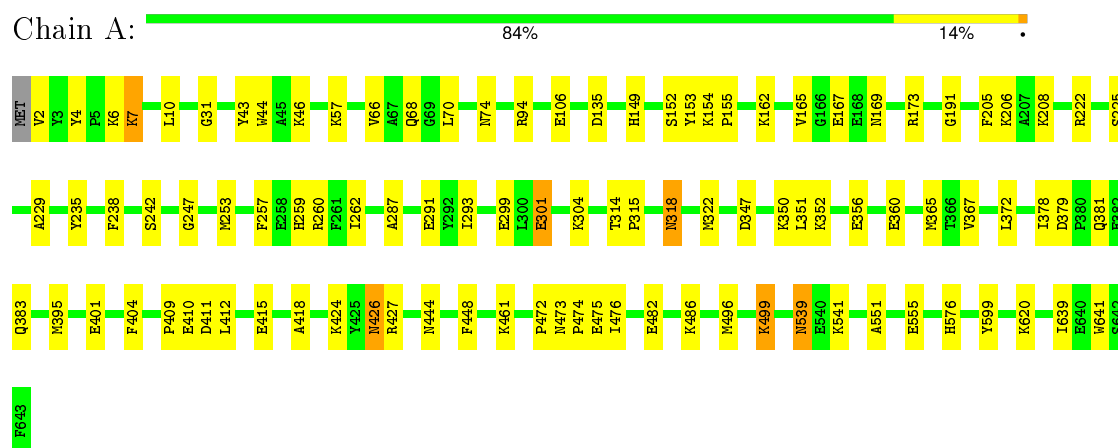
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	205	Total 207	O 207	0	2

3 Residue-property plots

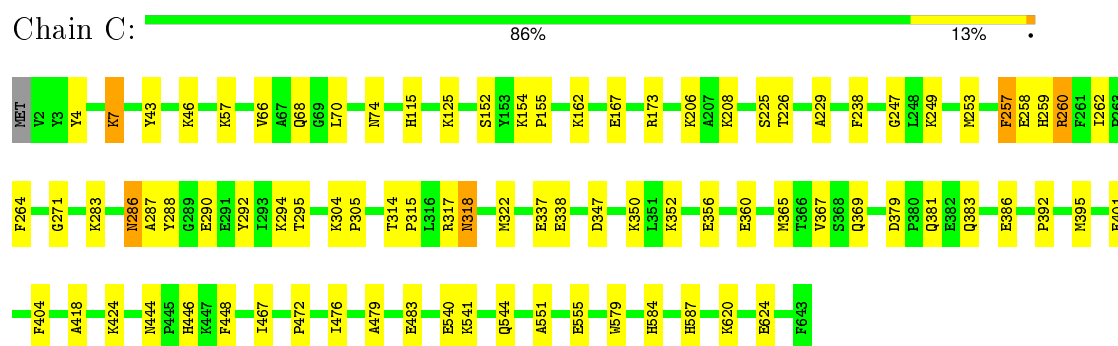
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

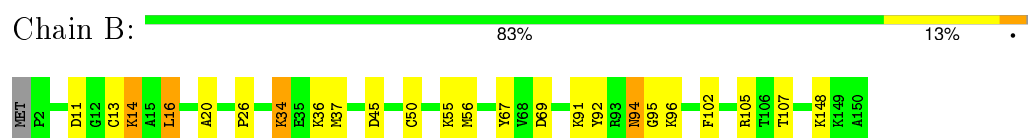
- Molecule 1: adenylylsulfate reductase



- Molecule 1: adenylylsulfate reductase



- Molecule 2: adenylylsulfate reductase



- Molecule 2: adenylylsulfate reductase

Chain D:

88%

11%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.60 Å 113.50 Å 193.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.59 – 1.60	Depositor
% Data completeness (in resolution range)	90.5 (27.59-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.180 , 0.202	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14542	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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: GOL, SF4, 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	0/5372	0.58	0/7269
1	C	0.31	0/5393	0.60	0/7300
2	B	0.30	0/1210	0.65	0/1632
2	D	0.32	0/1210	0.66	0/1632
All	All	0.30	0/13185	0.60	0/17833

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	5199	0	5094	92	0
1	C	5205	0	5100	84	0
2	B	1176	0	1151	26	0
2	D	1176	0	1151	16	0
3	A	53	0	29	2	0
3	C	53	0	29	0	0
4	B	16	0	0	1	0
4	D	16	0	0	1	0
5	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	18	0	24	4	0
6	A	587	0	0	6	0
6	B	171	0	0	3	0
6	C	659	0	0	6	0
6	D	207	0	0	3	0
All	All	14542	0	12586	194	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 8.

All (194) 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)
2:B:13:CYS:HB3	2:B:16:LEU:HD21	1.23	1.17
1:A:4:TYR:CE2	1:C:4:TYR:CD1	2.47	1.02
1:A:4:TYR:CE1	1:C:4:TYR:CE1	2.64	0.85
1:A:4:TYR:CE2	1:C:4:TYR:HD1	1.93	0.85
1:A:106:GLU:HB3	1:A:639[B]:ILE:HD13	1.58	0.85
1:A:106:GLU:HB3	1:A:639[A]:ILE:HD13	1.58	0.85
1:C:541:LYS:HE2	1:C:541:LYS:HA	1.58	0.85
1:A:4:TYR:CZ	1:C:4:TYR:CD1	2.65	0.84
1:C:379:ASP:H	1:C:383[B]:GLN:HE21	1.22	0.83
1:C:379:ASP:H	1:C:383[A]:GLN:HE21	1.22	0.83
2:B:16:LEU:H	2:B:16:LEU:HD13	1.44	0.82
1:A:259:HIS:HD2	1:A:401:GLU:H	1.26	0.81
1:C:259:HIS:HD2	1:C:401:GLU:H	1.28	0.81
1:C:379:ASP:H	1:C:383[B]:GLN:NE2	1.79	0.78
1:A:4:TYR:CE1	1:C:4:TYR:HE1	2.04	0.75
1:C:43:TYR:O	1:C:46:LYS:HE2	1.87	0.74
1:A:426:ASN:HD21	1:A:427:ARG:HH11	1.35	0.74
1:A:4:TYR:CD1	1:C:4:TYR:CE1	2.76	0.73
2:B:11:ASP:OD1	2:B:14:LYS:HG2	1.88	0.73
1:A:4:TYR:CD2	1:C:4:TYR:CD1	2.78	0.71
1:C:225:SER:HB3	1:C:229:ALA:HB3	1.72	0.70
1:A:225:SER:HB3	1:A:229:ALA:HB3	1.74	0.69
1:C:264:PHE:CE2	5:C:6504:GOL:H32	2.29	0.68
1:C:379:ASP:H	1:C:383[A]:GLN:NE2	1.79	0.68
1:C:115:HIS:HD2	2:D:134:GLU:OE2	1.77	0.68
1:A:4:TYR:CZ	1:C:4:TYR:HD1	2.07	0.67
1:C:125:LYS:HE2	6:D:7230:HOH:O	1.93	0.67
1:C:379:ASP:OD2	1:C:381:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ILE:HG12	1:A:383:GLN:HE21	1.58	0.67
1:C:352:LYS:O	1:C:356:GLU:HG3	1.94	0.66
2:B:94:ASN:C	2:B:94:ASN:HD22	2.01	0.64
2:D:96:LYS:HE2	2:D:98:LEU:HD21	1.78	0.64
1:C:264:PHE:CD2	5:C:6504:GOL:H32	2.32	0.64
1:A:378:ILE:HG12	1:A:383:GLN:NE2	2.12	0.64
1:A:539:ASN:C	1:A:539:ASN:HD22	2.01	0.64
1:C:317:ARG:HB3	5:C:6504:GOL:H11	1.80	0.63
1:C:68:GLN:HE22	1:C:367:VAL:H	1.46	0.63
1:A:379:ASP:OD2	1:A:381:GLN:HG2	1.97	0.63
1:A:4:TYR:CZ	1:C:4:TYR:CE1	2.87	0.63
1:A:253:MET:HG2	1:A:620:LYS:HB2	1.81	0.62
1:A:259:HIS:CD2	1:A:401:GLU:H	2.14	0.62
1:C:286:ASN:C	1:C:286:ASN:HD22	2.04	0.61
1:C:379:ASP:N	1:C:383[A]:GLN:HE21	1.96	0.61
1:C:379:ASP:N	1:C:383[B]:GLN:HE21	1.96	0.61
1:A:499:LYS:NZ	1:A:499:LYS:HB2	2.15	0.61
1:C:259:HIS:CD2	1:C:401:GLU:H	2.15	0.61
1:A:7:LYS:HE3	6:B:7116:HOH:O	2.01	0.60
1:A:411:ASP:O	2:B:148:LYS:NZ	2.32	0.60
2:B:94:ASN:ND2	2:B:96:LYS:H	1.99	0.60
1:A:301:GLU:HG2	1:A:304:LYS:HZ3	1.67	0.60
1:C:257:PHE:O	1:C:584:HIS:HD2	1.84	0.59
1:C:74:ASN:ND2	6:C:7082:HOH:O	2.27	0.59
1:A:352:LYS:O	1:A:356:GLU:HG3	2.03	0.59
1:C:260:ARG:HH21	1:C:584:HIS:HE1	1.49	0.59
1:A:6:LYS:HB3	1:A:7:LYS:HD3	1.84	0.58
2:B:34:LYS:HE3	6:B:7564:HOH:O	2.03	0.58
1:C:66:VAL:O	1:C:66:VAL:HG12	2.03	0.58
1:A:66:VAL:O	1:A:66:VAL:HG12	2.04	0.58
2:D:18:ARG:HD2	6:D:5259:HOH:O	2.04	0.58
1:A:68:GLN:HE22	1:A:367:VAL:H	1.51	0.57
1:A:222:ARG:HD3	6:C:7590[B]:HOH:O	2.04	0.57
1:A:94[A]:ARG:HG3	1:A:641:TRP:CE3	2.39	0.57
1:A:94[B]:ARG:HG3	1:A:641:TRP:CE3	2.39	0.57
1:A:378:ILE:HA	1:A:383:GLN:NE2	2.19	0.57
1:A:162:LYS:HE3	1:A:167:GLU:HB2	1.86	0.56
1:A:149:HIS:HD2	1:A:360:GLU:OE2	1.88	0.56
1:C:162:LYS:NZ	6:C:7351:HOH:O	2.38	0.56
1:A:301:GLU:O	1:A:304:LYS:HG3	2.07	0.55
1:A:409:PRO:HG2	1:A:412:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HE2	1:A:476:ILE:CD1	2.38	0.53
2:B:55:LYS:HB3	2:B:56:MET:HE1	1.90	0.53
1:A:411:ASP:O	2:B:148:LYS:CE	2.57	0.53
1:A:57:LYS:O	1:A:173:ARG:HA	2.09	0.53
1:C:162:LYS:NZ	1:C:167:GLU:HB3	2.24	0.53
1:A:154:LYS:HB3	1:A:155:PRO:HD3	1.90	0.53
1:A:482:GLU:HG3	1:A:486:LYS:HZ3	1.75	0.52
2:B:34:LYS:HD2	2:B:34:LYS:H	1.74	0.52
1:A:551:ALA:O	1:A:555:GLU:HG3	2.09	0.52
2:B:92:TYR:HB2	2:B:96:LYS:HB3	1.92	0.52
1:A:418:ALA:O	1:A:424:LYS:HE3	2.09	0.52
1:A:287:ALA:HB1	1:C:541:LYS:HG3	1.91	0.51
1:C:68:GLN:NE2	1:C:367:VAL:H	2.09	0.51
1:C:294:LYS:HD3	6:C:7500:HOH:O	2.11	0.51
1:A:541:LYS:HG3	1:C:287:ALA:HB1	1.93	0.51
1:C:115:HIS:HE1	6:D:5004:HOH:O	1.94	0.51
1:C:286:ASN:ND2	1:C:288:TYR:H	2.09	0.50
1:A:360:GLU:HB2	2:B:102:PHE:CE2	2.46	0.50
1:C:260:ARG:HH21	1:C:584:HIS:CE1	2.27	0.50
1:A:473:ASN:N	1:A:474:PRO:HD3	2.26	0.50
1:A:259:HIS:HD2	1:A:401:GLU:N	2.03	0.50
2:D:14:LYS:HD3	2:D:37:MET:CE	2.42	0.49
1:C:57:LYS:O	1:C:173:ARG:HA	2.13	0.49
1:C:262:ILE:HD11	1:C:392:PRO:HG3	1.95	0.49
1:C:206:LYS:HE2	1:C:476:ILE:HD11	1.93	0.49
1:C:286:ASN:ND2	1:C:290:GLU:H	2.11	0.49
1:A:68:GLN:HG2	2:B:50:CYS:HB2	1.94	0.49
1:C:283:LYS:HD2	6:C:7053:HOH:O	2.13	0.49
2:B:94:ASN:HD22	2:B:96:LYS:H	1.60	0.49
1:A:426:ASN:ND2	1:A:427:ARG:HH11	2.08	0.49
1:A:418:ALA:HB1	1:A:424:LYS:CE	2.43	0.49
1:C:152:SER:C	1:C:155:PRO:HD2	2.34	0.48
1:A:418:ALA:HB1	1:A:424:LYS:HE3	1.94	0.48
1:C:292:TYR:HA	1:C:295:THR:OG1	2.13	0.48
2:D:20:ALA:HB3	4:D:3110:SF4:S1	2.54	0.48
1:C:337:GLU:HG2	1:C:338:GLU:N	2.28	0.48
1:C:206:LYS:HE2	1:C:476:ILE:CD1	2.43	0.48
1:A:10:LEU:HD13	1:A:496:MET:CG	2.44	0.48
1:A:235:TYR:HA	3:A:1000:FAD:HM83	1.96	0.48
2:B:55:LYS:CB	2:B:56:MET:HE1	2.44	0.48
1:A:238:PHE:CE2	2:B:26:PRO:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASP:HB3	1:A:350:LYS:HB3	1.96	0.47
2:B:13:CYS:C	2:B:16:LEU:HD11	2.34	0.47
1:C:208:LYS:HB3	1:C:472:PRO:HG2	1.96	0.47
1:C:229:ALA:HA	2:D:67:TYR:CD2	2.50	0.47
1:C:70:LEU:HA	1:C:365[A]:MET:HB3	1.97	0.47
1:C:70:LEU:HA	1:C:365[B]:MET:HB3	1.97	0.47
1:A:475:GLU:HG3	6:A:7463:HOH:O	2.15	0.47
1:A:10:LEU:HD13	1:A:496:MET:HG2	1.97	0.47
1:A:68:GLN:NE2	1:A:367:VAL:H	2.13	0.46
6:A:6087:HOH:O	2:B:56:MET:HE3	2.16	0.46
1:C:418:ALA:O	1:C:424:LYS:HE3	2.16	0.46
1:A:314:THR:N	1:A:315:PRO:HD2	2.30	0.46
2:B:20:ALA:HB3	4:B:1110:SF4:S1	2.55	0.46
1:A:262:ILE:HD13	1:A:599:TYR:HA	1.97	0.46
1:C:238:PHE:CE2	2:D:26:PRO:HB2	2.51	0.46
2:D:134:GLU:HB3	2:D:135:PRO:HA	1.97	0.46
1:A:247:GLY:HA3	1:A:404:PHE:CZ	2.51	0.46
1:A:70:LEU:HA	1:A:365[B]:MET:HB3	1.98	0.46
1:A:70:LEU:HA	1:A:365[A]:MET:HB3	1.98	0.45
1:A:43:TYR:O	1:A:46:LYS:HE2	2.15	0.45
1:C:7:LYS:NZ	2:D:34:LYS:NZ	2.64	0.45
1:C:479:ALA:O	1:C:483:GLU:HG3	2.15	0.45
1:A:262:ILE:HD12	1:A:262:ILE:N	2.31	0.45
1:A:44:TRP:CZ2	1:A:461:LYS:HE3	2.52	0.45
1:A:259:HIS:CD2	1:A:401:GLU:HG2	2.51	0.45
1:C:7:LYS:CE	2:D:34:LYS:NZ	2.80	0.45
2:B:36:LYS:O	2:B:37:MET:HB2	2.17	0.45
2:B:91:LYS:HD3	6:B:7149:HOH:O	2.16	0.45
1:C:386:GLU:OE2	5:C:6505:GOL:H11	2.17	0.45
1:A:242:SER:OG	1:A:576:HIS:HD2	1.99	0.45
1:C:467:ILE:HA	1:C:472:PRO:HD2	1.99	0.44
1:C:253:MET:HG2	1:C:620:LYS:HB2	2.00	0.44
1:C:318:ASN:O	1:C:322:MET:HG2	2.17	0.44
1:C:154:LYS:HB3	1:C:155:PRO:HD3	2.00	0.44
1:A:541:LYS:HE2	6:A:7185:HOH:O	2.16	0.44
1:C:551:ALA:O	1:C:555:GLU:HG3	2.18	0.44
1:A:291:GLU:HG2	1:A:293:ILE:HG12	2.00	0.44
1:A:410:GLU:HG2	6:A:5772:HOH:O	2.17	0.44
1:A:208:LYS:HB3	1:A:472:PRO:HG2	2.00	0.44
1:C:360:GLU:HB2	2:D:102:PHE:CE2	2.53	0.44
1:C:347:ASP:HB3	1:C:350:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:7034:HOH:O	1:C:226:THR:HB	2.18	0.43
1:C:541:LYS:HE2	1:C:541:LYS:CA	2.37	0.43
1:C:259:HIS:HD2	1:C:401:GLU:N	2.05	0.43
1:C:304:LYS:HA	1:C:305:PRO:HA	1.83	0.43
1:C:540:GLU:O	1:C:544:GLN:HG3	2.17	0.43
1:A:499:LYS:HZ3	1:A:499:LYS:HB2	1.81	0.43
1:A:2:VAL:N	2:B:45:ASP:OD1	2.52	0.43
1:C:249:LYS:HE2	1:C:579:TRP:CH2	2.54	0.43
1:C:74:ASN:HB2	1:C:448:PHE:CG	2.53	0.42
1:C:259:HIS:CD2	1:C:401:GLU:HG2	2.54	0.42
1:C:446:HIS:HA	1:C:448:PHE:CE1	2.55	0.42
2:B:94:ASN:C	2:B:94:ASN:ND2	2.69	0.42
2:D:14:LYS:HA	2:D:14:LYS:HD2	1.88	0.42
2:B:94:ASN:HD22	2:B:95:GLY:N	2.18	0.42
1:C:260:ARG:NH2	1:C:584:HIS:HE1	2.13	0.42
1:A:152:SER:C	1:A:155:PRO:HD2	2.40	0.42
2:B:105:ARG:HG2	2:B:107:THR:H	1.85	0.42
1:A:351:LEU:HD22	6:A:5645:HOH:O	2.19	0.42
1:A:378:ILE:HA	1:A:383:GLN:HE21	1.82	0.42
2:D:25:CYS:HA	2:D:26:PRO:HD3	1.89	0.42
2:D:16:LEU:HD12	2:D:16:LEU:N	2.35	0.42
1:C:271:GLY:H	1:C:369:GLN:HE21	1.67	0.41
1:A:372:LEU:C	1:A:372:LEU:HD23	2.41	0.41
1:A:165:VAL:HG22	1:A:169:ASN:HB2	2.02	0.41
1:A:74:ASN:HB2	1:A:448:PHE:CG	2.55	0.41
1:A:301:GLU:HG2	1:A:304:LYS:NZ	2.34	0.41
1:C:286:ASN:C	1:C:286:ASN:ND2	2.72	0.41
1:C:258:GLU:HB3	1:C:587:HIS:HB3	2.03	0.41
1:A:31:GLY:HA3	3:A:1000:FAD:O5B	2.20	0.41
1:C:314:THR:N	1:C:315:PRO:HD2	2.36	0.41
1:A:191:GLY:HA3	1:A:205:PHE:O	2.20	0.41
1:A:539:ASN:ND2	1:A:539:ASN:C	2.73	0.41
1:A:318:ASN:O	1:A:322:MET:HG2	2.21	0.41
1:A:426:ASN:HD22	1:A:427:ARG:N	2.19	0.40
1:C:247:GLY:HA3	1:C:404:PHE:CZ	2.55	0.40
1:A:229:ALA:HA	2:B:67:TYR:CD2	2.57	0.40
1:C:162:LYS:HE2	6:C:6091:HOH:O	2.22	0.40
2:D:36:LYS:O	2:D:37:MET:HB2	2.21	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	648/643 (101%)	627 (97%)	21 (3%)	0	100	100
1	C	650/643 (101%)	631 (97%)	19 (3%)	0	100	100
2	B	148/150 (99%)	142 (96%)	4 (3%)	2 (1%)	14	2
2	D	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
All	All	1594/1586 (100%)	1546 (97%)	46 (3%)	2 (0%)	56	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	14	LYS
2	B	34	LYS

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	533/526 (101%)	518 (97%)	15 (3%)	51	22
1	C	536/526 (102%)	527 (98%)	9 (2%)	68	44
2	B	130/130 (100%)	127 (98%)	3 (2%)	58	29
2	D	130/130 (100%)	129 (99%)	1 (1%)	86	75
All	All	1329/1312 (101%)	1301 (98%)	28 (2%)	63	33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	135	ASP
1	A	153	TYR
1	A	257	PHE
1	A	260	ARG
1	A	299	GLU
1	A	301	GLU
1	A	318	ASN
1	A	395[A]	MET
1	A	395[B]	MET
1	A	415	GLU
1	A	426	ASN
1	A	444	ASN
1	A	499	LYS
1	A	539	ASN
2	B	16	LEU
2	B	69	ASP
2	B	94	ASN
1	C	7	LYS
1	C	257	PHE
1	C	260	ARG
1	C	286	ASN
1	C	318	ASN
1	C	395[A]	MET
1	C	395[B]	MET
1	C	444	ASN
1	C	624	GLU
2	D	69	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	149	HIS
1	A	259	HIS
1	A	310	GLN
1	A	318	ASN
1	A	381	GLN
1	A	383	GLN
1	A	426	ASN
1	A	497	GLN
1	A	539	ASN
1	A	576	HIS

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Mol	Chain	Res	Type
2	B	94	ASN
2	B	145	GLN
1	C	68	GLN
1	C	115	HIS
1	C	259	HIS
1	C	286	ASN
1	C	310	GLN
1	C	318	ASN
1	C	330	GLN
1	C	369	GLN
1	C	381	GLN
1	C	497	GLN
1	C	584	HIS
2	D	145	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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	1000	-	48,58,58	5.35	32 (66%)	54,89,89	2.98	21 (38%)
5	GOL	A	6503	-	5,5,5	0.81	0	5,5,5	0.89	0
4	SF4	B	1100	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1110	2	0,12,12	0.00	-	0,24,24	0.00	-
3	FAD	C	3000	-	48,58,58	5.11	30 (62%)	54,89,89	3.13	21 (38%)
5	GOL	C	6501	-	5,5,5	1.06	0	5,5,5	0.66	0
5	GOL	C	6504	-	5,5,5	0.74	0	5,5,5	0.67	0
5	GOL	C	6505	-	5,5,5	0.76	0	5,5,5	1.07	1 (20%)
4	SF4	D	3100	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	3110	2	0,12,12	0.00	-	0,24,24	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
3	FAD	A	1000	-	-	0/30/50/50	0/6/6/6
5	GOL	A	6503	-	-	0/4/4/4	0/0/0/0
4	SF4	B	1100	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1110	2	-	0/0/48/48	0/6/5/5
3	FAD	C	3000	-	-	0/30/50/50	0/6/6/6
5	GOL	C	6501	-	-	0/4/4/4	0/0/0/0
5	GOL	C	6504	-	-	0/4/4/4	0/0/0/0
5	GOL	C	6505	-	-	0/4/4/4	0/0/0/0
4	SF4	D	3100	2	-	0/0/48/48	0/6/5/5
4	SF4	D	3110	2	-	0/0/48/48	0/6/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C1'-N10	-23.09	1.24	1.48
3	C	3000	FAD	C1'-N10	-21.06	1.26	1.48
3	C	3000	FAD	C4'-C3'	-4.97	1.43	1.53
3	A	1000	FAD	PA-O1A	-4.67	1.34	1.51
3	C	3000	FAD	O2'-C2'	-4.59	1.33	1.43
3	A	1000	FAD	C4'-C3'	-3.90	1.45	1.53
3	C	3000	FAD	PA-O1A	-3.86	1.37	1.51
3	A	1000	FAD	O2'-C2'	-3.17	1.36	1.43
3	C	3000	FAD	O3'-C3'	-3.09	1.35	1.43
3	C	3000	FAD	O4-C4	-2.94	1.17	1.24
3	A	1000	FAD	O3'-C3'	-2.74	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C8A-N7A	-2.68	1.29	1.34
3	C	3000	FAD	C8A-N7A	-2.68	1.29	1.34
3	A	1000	FAD	PA-O2A	-2.37	1.44	1.54
3	A	1000	FAD	P-O1P	-2.16	1.43	1.51
3	A	1000	FAD	O4B-C4B	-2.16	1.40	1.45
3	A	1000	FAD	C6-C5X	2.12	1.45	1.41
3	A	1000	FAD	C9-C8	2.30	1.44	1.37
3	A	1000	FAD	C4-C4X	2.30	1.45	1.41
3	C	3000	FAD	C4-C4X	2.31	1.45	1.41
3	C	3000	FAD	PA-O5B	2.39	1.70	1.59
3	C	3000	FAD	C3B-C4B	2.68	1.60	1.53
3	C	3000	FAD	P-O1P	2.73	1.61	1.51
3	A	1000	FAD	C10-N1	3.05	1.40	1.35
3	C	3000	FAD	C4X-N5	3.38	1.38	1.33
3	C	3000	FAD	C5A-C4A	3.42	1.48	1.40
3	A	1000	FAD	C3B-C4B	3.55	1.62	1.53
3	A	1000	FAD	C5A-C4A	3.59	1.48	1.40
3	A	1000	FAD	C6-C7	3.64	1.47	1.37
3	C	3000	FAD	C10-N1	3.86	1.42	1.35
3	A	1000	FAD	C5X-N5	3.95	1.41	1.35
3	A	1000	FAD	C4X-N5	4.04	1.39	1.33
3	C	3000	FAD	C5X-N5	4.16	1.42	1.35
3	C	3000	FAD	C6-C7	4.27	1.49	1.37
3	C	3000	FAD	C2A-N1A	4.34	1.42	1.33
3	A	1000	FAD	C2A-N1A	4.48	1.42	1.33
3	C	3000	FAD	C2'-C3'	4.57	1.62	1.53
3	A	1000	FAD	O4B-C1B	4.58	1.47	1.41
3	A	1000	FAD	C2'-C3'	4.59	1.62	1.53
3	C	3000	FAD	C9-C9A	4.90	1.51	1.40
3	A	1000	FAD	C9-C9A	4.92	1.51	1.40
3	C	3000	FAD	C2A-N3A	5.10	1.41	1.32
3	C	3000	FAD	O2B-C2B	5.11	1.55	1.43
3	A	1000	FAD	O2B-C2B	5.42	1.55	1.43
3	A	1000	FAD	C2A-N3A	5.51	1.41	1.32
3	C	3000	FAD	C4A-N3A	5.56	1.43	1.35
3	C	3000	FAD	C4-N3	5.88	1.44	1.33
3	C	3000	FAD	O4B-C1B	6.19	1.49	1.41
3	C	3000	FAD	C10-N10	6.25	1.46	1.39
3	A	1000	FAD	C4-N3	6.85	1.45	1.33
3	A	1000	FAD	C9A-C5X	6.90	1.56	1.42
3	A	1000	FAD	C4A-N3A	7.06	1.46	1.35
3	C	3000	FAD	C9A-C5X	7.41	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C8-C7	7.50	1.61	1.41
3	C	3000	FAD	C8-C7	7.85	1.62	1.41
3	C	3000	FAD	C5'-C4'	8.04	1.64	1.51
3	A	1000	FAD	C10-N10	8.09	1.48	1.39
3	A	1000	FAD	C5'-C4'	8.58	1.64	1.51
3	C	3000	FAD	C4X-C10	8.60	1.57	1.41
3	A	1000	FAD	C9A-N10	8.76	1.50	1.38
3	C	3000	FAD	C9A-N10	9.18	1.51	1.38
3	A	1000	FAD	C4X-C10	9.19	1.58	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3000	FAD	N3A-C2A-N1A	-7.52	123.14	128.89
3	C	3000	FAD	C4-C4X-C10	-6.64	115.69	119.94
3	A	1000	FAD	N3A-C2A-N1A	-6.30	124.07	128.89
3	A	1000	FAD	C4-C4X-C10	-6.22	115.96	119.94
3	A	1000	FAD	C2B-C3B-C4B	-5.14	92.04	102.61
3	A	1000	FAD	C4X-C4-N3	-5.11	116.60	123.59
3	C	3000	FAD	P-O3P-PA	-4.99	118.71	132.73
3	C	3000	FAD	C2B-C3B-C4B	-4.77	92.80	102.61
3	C	3000	FAD	C4X-C4-N3	-4.68	117.20	123.59
3	A	1000	FAD	C6-C5X-N5	-4.03	113.78	118.96
3	C	3000	FAD	C4B-O4B-C1B	-4.00	105.32	109.72
3	C	3000	FAD	O3P-PA-O5B	-3.40	93.91	102.94
3	C	3000	FAD	C6-C5X-N5	-3.40	114.59	118.96
3	A	1000	FAD	P-O3P-PA	-3.38	123.23	132.73
3	A	1000	FAD	O5'-P-O1P	-2.72	99.07	109.62
3	C	3000	FAD	C5B-C4B-C3B	-2.64	104.75	115.21
3	A	1000	FAD	C5B-C4B-C3B	-2.39	105.72	115.21
3	C	3000	FAD	C9-C9A-C5X	-2.30	115.53	119.62
3	A	1000	FAD	C9-C9A-C5X	-2.30	115.54	119.62
5	C	6505	GOL	O2-C2-C1	-2.15	98.79	108.65
3	C	3000	FAD	C4X-C10-N10	-2.15	119.25	120.52
3	A	1000	FAD	O4'-C4'-C5'	-2.13	105.56	110.19
3	C	3000	FAD	O4'-C4'-C5'	-2.09	105.63	110.19
3	A	1000	FAD	C4B-O4B-C1B	-2.06	107.46	109.72
3	A	1000	FAD	C4X-N5-C5X	2.01	119.07	116.76
3	A	1000	FAD	N6A-C6A-N1A	2.14	123.79	119.20
3	A	1000	FAD	C8M-C8-C7	2.39	125.97	120.73
3	C	3000	FAD	C8M-C8-C7	2.44	126.08	120.73
3	C	3000	FAD	O3'-C3'-C4'	2.59	115.28	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	FAD	O3'-C3'-C4'	2.71	115.57	108.75
3	A	1000	FAD	O2'-C2'-C3'	2.74	115.92	109.02
3	A	1000	FAD	C6-C5X-C9A	2.95	122.86	118.98
3	C	3000	FAD	O2'-C2'-C3'	3.05	116.67	109.02
3	C	3000	FAD	O4'-C4'-C3'	3.28	117.26	109.02
3	C	3000	FAD	C4X-N5-C5X	3.45	120.73	116.76
3	C	3000	FAD	C6-C5X-C9A	3.84	124.03	118.98
3	A	1000	FAD	O4'-C4'-C3'	4.39	120.06	109.02
3	C	3000	FAD	O4B-C4B-C3B	6.13	117.50	105.15
3	A	1000	FAD	O4B-C4B-C3B	6.22	117.67	105.15
3	C	3000	FAD	C2B-C1B-N9A	6.36	124.00	114.29
3	A	1000	FAD	C2B-C1B-N9A	7.44	125.66	114.29
3	A	1000	FAD	C4-N3-C2	10.74	124.53	115.25
3	C	3000	FAD	C4-N3-C2	11.60	125.27	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	FAD	2	0
4	B	1110	SF4	1	0
5	C	6504	GOL	3	0
5	C	6505	GOL	1	0
4	D	3110	SF4	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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.