



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2019 – 11:46 PM EDT

PDB ID : 6GFO
Title : cyanobacterial GAPDH with full-length CP12
Authors : McFarlane, C.R.; Murray, J.W.
Deposited on : 2018-05-01
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)
Xtrriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

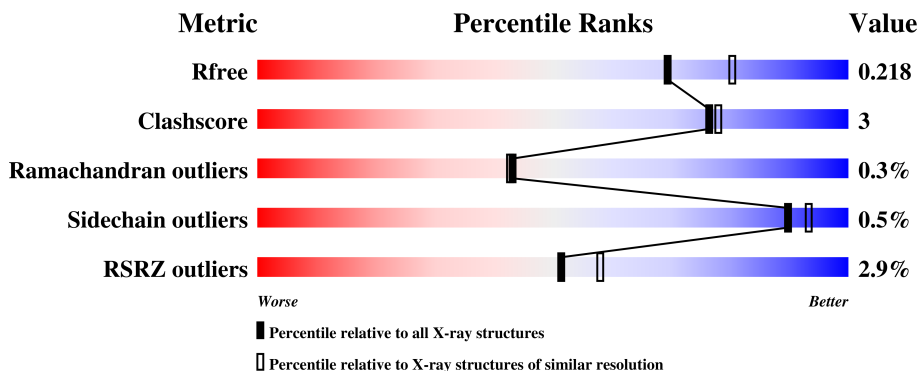
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



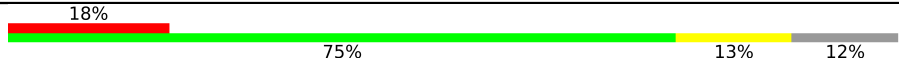
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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	339	
1	B	339	
1	C	339	
1	D	339	
2	E	77	

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Mol	Chain	Length	Quality of chain
2	F	77	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '18%', a large green segment labeled '75%', a yellow segment labeled '13%', and a grey segment on the far right labeled '12%'.</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11974 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2585	1618	460	492	15	0	1	0
1	B	338	2582	1617	459	491	15	0	1	0
1	C	338	2585	1618	460	492	15	0	1	0
1	D	338	2585	1618	460	492	15	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8DIW5
A	0	SER	-	expression tag	UNP Q8DIW5
B	-1	GLY	-	expression tag	UNP Q8DIW5
B	0	SER	-	expression tag	UNP Q8DIW5
C	-1	GLY	-	expression tag	UNP Q8DIW5
C	0	SER	-	expression tag	UNP Q8DIW5
D	-1	GLY	-	expression tag	UNP Q8DIW5
D	0	SER	-	expression tag	UNP Q8DIW5

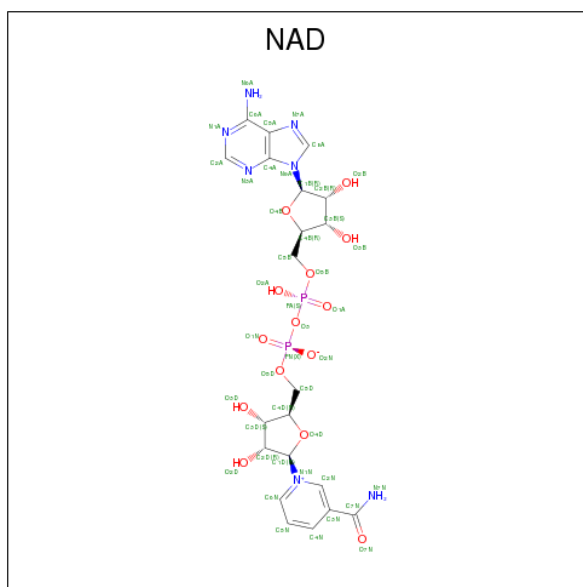
- Molecule 2 is a protein called CP12 polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	75	587	347	104	131	5	0	0	0
2	F	68	531	316	93	118	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

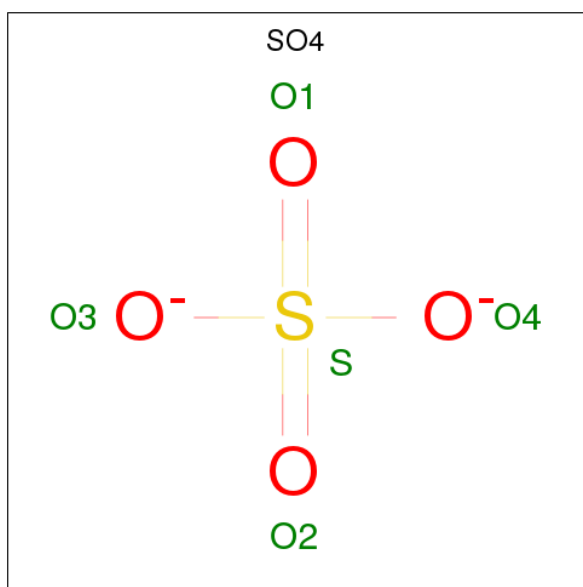
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q8DHX3
E	0	SER	-	expression tag	UNP Q8DHX3
F	-1	GLY	-	expression tag	UNP Q8DHX3
F	0	SER	-	expression tag	UNP Q8DHX3

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

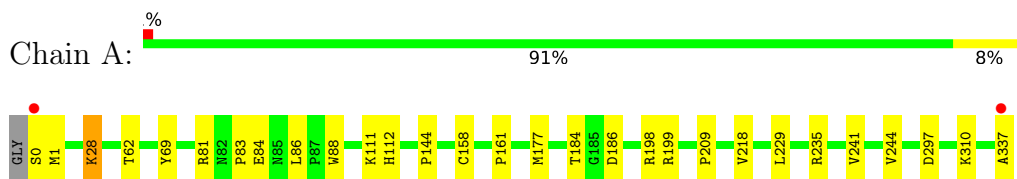
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	90	Total	O	0	0
			90	90		
5	C	92	Total	O	0	0
			92	92		
5	D	48	Total	O	0	0
			48	48		
5	E	3	Total	O	0	0
			3	3		
5	F	14	Total	O	0	0
			14	14		

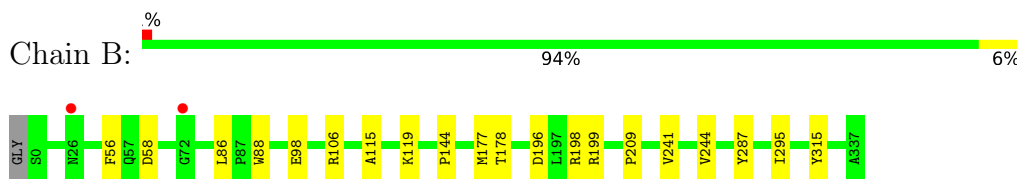
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

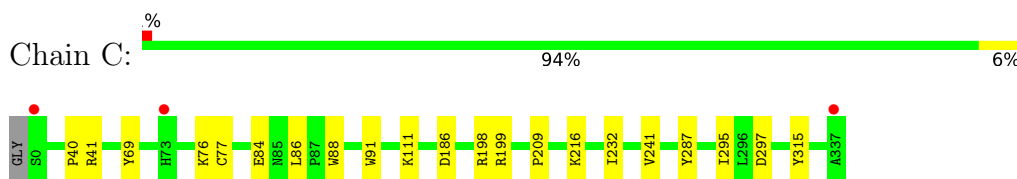
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



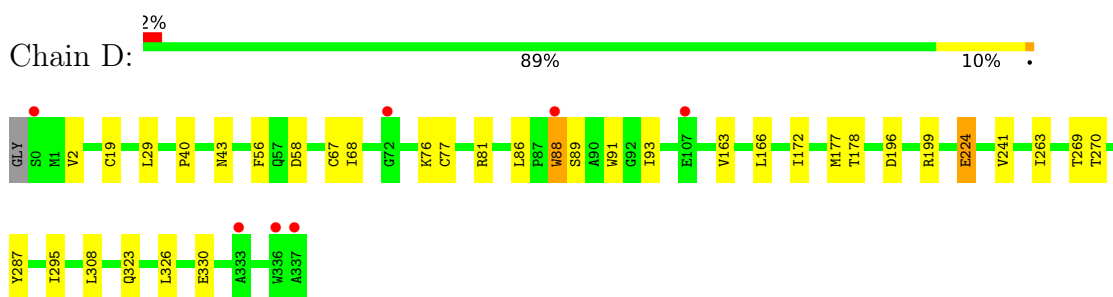
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



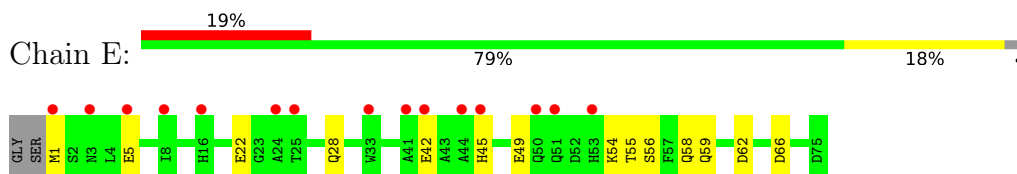
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



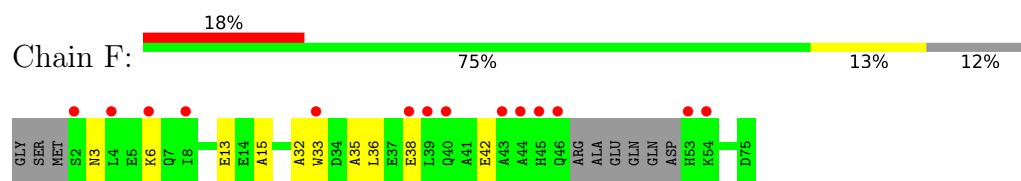
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 2: CP12 polypeptide



● Molecule 2: CP12 polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.45Å 141.05Å 81.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.63 – 2.10 70.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.63-2.10) 99.9 (70.63-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.171 , 0.218 0.171 , 0.218	Depositor DCC
R_{free} test set	4599 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtrriage
Anisotropy	0.936	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/2635	0.58	0/3580
1	B	0.40	0/2635	0.57	0/3580
1	C	0.38	0/2635	0.56	0/3580
1	D	0.34	0/2635	0.54	0/3580
2	E	0.30	0/595	0.41	0/802
2	F	0.30	0/538	0.45	0/724
All	All	0.37	0/11673	0.55	0/15846

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

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	2585	0	2569	17	0
1	B	2582	0	2570	13	0
1	C	2585	0	2569	17	0
1	D	2585	0	2569	20	1
2	E	587	0	510	8	0
2	F	531	0	462	6	0
3	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	C	5	0	0	0	0
5	A	91	0	0	1	0
5	B	90	0	0	1	0
5	C	92	0	0	1	0
5	D	48	0	0	0	0
5	E	3	0	0	0	0
5	F	14	0	0	0	0
All	All	11974	0	11353	76	1

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 3.

All (76) 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:C:86:LEU:HD13	1:C:88:TRP:CZ2	2.04	0.91
1:B:86:LEU:HD13	1:B:88:TRP:CZ2	2.07	0.88
1:A:86:LEU:HD13	1:A:88:TRP:CZ2	2.20	0.77
1:A:28:LYS:HD2	5:A:1101:HOH:O	1.92	0.70
1:A:297:ASP:OD2	1:C:198:ARG:NH2	2.24	0.69
2:E:54:LYS:NZ	2:E:62:ASP:OD2	2.32	0.62
1:B:196:ASP:OD2	1:B:199:ARG:NH1	2.32	0.62
2:E:56:SER:HA	2:E:59:GLN:HG3	1.85	0.58
1:C:86:LEU:HD13	1:C:88:TRP:HZ2	1.67	0.58
1:B:86:LEU:CD1	1:B:88:TRP:CZ2	2.85	0.57
1:A:198:ARG:NH2	1:C:297:ASP:OD2	2.38	0.57
1:B:244:VAL:HG23	1:B:315:TYR:CE2	2.41	0.55
2:F:35:ALA:O	2:F:38:GLU:HG2	2.07	0.54
1:D:43:ASN:HB3	1:D:68:ILE:HD11	1.92	0.51
2:F:42:GLU:N	2:F:42:GLU:OE2	2.44	0.51
1:D:40:PRO:HG3	1:D:77:CYS:HB2	1.93	0.51
1:B:244:VAL:HG23	1:B:315:TYR:HE2	1.75	0.51
2:E:22:GLU:HG2	2:E:28:GLN:NE2	2.27	0.50
1:C:186:ASP:OD2	1:C:199:ARG:NH1	2.42	0.50
1:C:41:ARG:HG2	1:C:41:ARG:NH1	2.27	0.50
1:C:41:ARG:HG2	1:C:41:ARG:HH11	1.76	0.50
1:C:40:PRO:HG3	1:C:77:CYS:HB2	1.94	0.49
1:B:86:LEU:HD13	1:B:88:TRP:HZ2	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:NZ	1:B:144:PRO:O	2.46	0.49
1:D:56:PHE:CZ	1:D:58:ASP:HB2	2.48	0.49
1:D:88:TRP:CE3	1:D:93:ILE:HG13	2.48	0.49
1:D:19:CYS:SG	1:D:323:GLN:NE2	2.86	0.48
1:C:76:LYS:HE3	1:C:91:TRP:CD1	2.49	0.48
1:D:269:THR:OG1	1:D:270:THR:N	2.46	0.48
2:E:49:GLU:O	2:E:54:LYS:HB2	2.14	0.48
1:A:144:PRO:HB2	1:A:337:ALA:HB3	1.96	0.47
1:A:86:LEU:HD13	1:A:88:TRP:HZ2	1.76	0.47
2:E:55:THR:N	2:E:58:GLN:OE1	2.44	0.47
1:A:177:MET:HG3	1:A:244:VAL:HG13	1.98	0.46
1:B:198:ARG:HD3	1:B:209:PRO:O	2.15	0.46
1:C:186:ASP:OD2	1:C:199:ARG:HD3	2.15	0.46
1:C:287:TYR:CE1	1:C:295:ILE:HG21	2.51	0.46
1:D:166:LEU:HD21	1:D:263:ILE:HD11	1.97	0.46
1:A:84:GLU:HG3	1:A:111:LYS:HD3	1.97	0.46
1:D:76:LYS:HE3	1:D:91:TRP:CZ2	2.50	0.46
1:A:218:VAL:HB	1:A:229:LEU:HD12	1.98	0.45
1:A:198:ARG:HD3	1:A:209:PRO:O	2.16	0.45
1:D:2:VAL:HB	1:D:29:LEU:HD23	1.98	0.45
1:A:0:SER:OG	1:A:1:MET:N	2.49	0.45
2:E:1:MET:SD	2:E:5:GLU:HB2	2.56	0.45
1:C:84:GLU:HG3	1:C:111:LYS:HB3	1.98	0.45
1:D:86:LEU:HD13	1:D:88:TRP:CZ2	2.51	0.45
1:D:177:MET:HG2	1:D:178:THR:N	2.33	0.44
1:C:198:ARG:HD3	1:C:209:PRO:O	2.18	0.44
1:A:184:THR:OG1	1:A:186:ASP:OD1	2.31	0.43
1:A:199:ARG:HH21	1:A:235:ARG:NH2	2.16	0.43
1:C:69:TYR:OH	2:F:13:GLU:HG2	2.18	0.43
1:A:310:LYS:HE2	1:C:232:ILE:HG12	2.00	0.43
1:B:56:PHE:CZ	1:B:58:ASP:HB2	2.54	0.42
1:D:196:ASP:OD2	1:D:199:ARG:NH1	2.47	0.42
1:B:106:ARG:NH2	5:B:1104:HOH:O	2.46	0.42
1:D:67:CYS:SG	1:D:76:LYS:HG2	2.59	0.42
2:F:15:ALA:HA	2:F:32:ALA:HB1	2.01	0.42
1:D:163:VAL:HG13	1:D:172:ILE:HD12	2.02	0.42
2:F:3:ASN:O	2:F:6:LYS:HB2	2.19	0.42
1:A:62:THR:HG22	1:A:69:TYR:HB2	2.00	0.42
1:D:43:ASN:CB	1:D:68:ILE:HD11	2.49	0.42
2:E:42:GLU:HA	2:E:45:HIS:HB2	2.01	0.42
1:D:224:GLU:CD	1:D:224:GLU:H	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HB2	5:C:1128:HOH:O	2.20	0.41
1:D:81:ARG:NH2	2:E:66:ASP:OD2	2.52	0.41
1:A:158:CYS:O	1:A:161:PRO:HD2	2.20	0.41
1:A:83:PRO:HB3	1:A:112:HIS:CE1	2.56	0.41
1:D:308:LEU:HD12	1:D:308:LEU:HA	1.92	0.41
1:C:76:LYS:HE3	1:C:91:TRP:CG	2.56	0.41
1:D:326:LEU:O	1:D:330:GLU:HG2	2.21	0.41
1:B:287:TYR:CE1	1:B:295:ILE:HG21	2.56	0.41
2:F:33:TRP:CZ3	2:F:36:LEU:HD23	2.55	0.41
1:B:177:MET:HG2	1:B:178:THR:N	2.35	0.41
1:D:287:TYR:CE1	1:D:295:ILE:HG21	2.56	0.40
1:B:88:TRP:CD1	1:B:115:ALA:HB3	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:SER:OG	1:D:89:SER:OG[2_665]	1.85	0.35

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	337/339 (99%)	324 (96%)	12 (4%)	1 (0%)	43	43
1	B	337/339 (99%)	321 (95%)	15 (4%)	1 (0%)	43	43
1	C	337/339 (99%)	322 (96%)	14 (4%)	1 (0%)	43	43
1	D	337/339 (99%)	324 (96%)	12 (4%)	1 (0%)	43	43
2	E	73/77 (95%)	73 (100%)	0	0	100	100
2	F	64/77 (83%)	64 (100%)	0	0	100	100
All	All	1485/1510 (98%)	1428 (96%)	53 (4%)	4 (0%)	43	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	VAL
1	B	241	VAL
1	C	241	VAL
1	D	241	VAL

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	278/277 (100%)	276 (99%)	2 (1%)	85 89
1	B	278/277 (100%)	277 (100%)	1 (0%)	92 95
1	C	278/277 (100%)	277 (100%)	1 (0%)	92 95
1	D	278/277 (100%)	276 (99%)	2 (1%)	85 89
2	E	59/61 (97%)	59 (100%)	0	100 100
2	F	54/61 (88%)	54 (100%)	0	100 100
All	All	1225/1230 (100%)	1219 (100%)	6 (0%)	90 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	81	ARG
1	B	98	GLU
1	C	315	TYR
1	D	88	TRP
1	D	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	D	129	ASN

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Mol	Chain	Res	Type
1	D	323	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](#)

5 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	NAD	A	1001	-	39,48,48	0.93	2 (5%)	44,73,73	1.32	6 (13%)
3	NAD	B	1001	-	39,48,48	0.82	1 (2%)	44,73,73	1.24	4 (9%)
3	NAD	C	1001	-	39,48,48	0.97	3 (7%)	44,73,73	1.14	2 (4%)
4	SO4	C	1002	-	4,4,4	0.40	0	6,6,6	0.13	0
3	NAD	D	1001	-	39,48,48	0.99	3 (7%)	44,73,73	1.19	5 (11%)

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	NAD	A	1001	-	-	0/22/62/62	0/5/5/5
3	NAD	B	1001	-	-	0/22/62/62	0/5/5/5
3	NAD	C	1001	-	-	0/22/62/62	0/5/5/5
4	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
3	NAD	D	1001	-	-	0/22/62/62	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	NAD	C2A-N3A	2.12	1.35	1.32
3	C	1001	NAD	O4D-C1D	2.15	1.44	1.41
3	C	1001	NAD	O4B-C1B	2.19	1.44	1.41
3	A	1001	NAD	O4D-C1D	2.38	1.44	1.41
3	B	1001	NAD	C5A-C4A	2.67	1.46	1.40
3	D	1001	NAD	C5A-C4A	2.86	1.47	1.40
3	D	1001	NAD	O4D-C1D	3.07	1.45	1.41
3	C	1001	NAD	C5A-C4A	3.16	1.47	1.40
3	A	1001	NAD	C5A-C4A	3.22	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1001	NAD	N3A-C2A-N1A	-3.44	123.14	128.68
3	A	1001	NAD	N3A-C2A-N1A	-3.40	123.20	128.68
3	C	1001	NAD	N3A-C2A-N1A	-3.39	123.21	128.68
3	B	1001	NAD	N3A-C2A-N1A	-3.36	123.27	128.68
3	C	1001	NAD	C4A-C5A-N7A	-3.05	106.22	109.40
3	B	1001	NAD	C4A-C5A-N7A	-2.71	106.58	109.40
3	D	1001	NAD	C4A-C5A-N7A	-2.55	106.75	109.40
3	A	1001	NAD	PN-O3-PA	-2.34	125.13	132.57
3	A	1001	NAD	C4A-C5A-N7A	-2.34	106.96	109.40
3	A	1001	NAD	O3D-C3D-C4D	-2.30	104.42	111.07
3	B	1001	NAD	C1B-N9A-C4A	-2.18	122.86	126.64
3	D	1001	NAD	O7N-C7N-N7N	-2.07	119.65	122.60
3	D	1001	NAD	C1B-N9A-C4A	-2.03	123.13	126.64
3	B	1001	NAD	C3N-C7N-N7N	2.28	120.35	117.75
3	A	1001	NAD	C2A-N1A-C6A	2.46	123.02	118.77
3	A	1001	NAD	C3N-C7N-N7N	2.77	120.90	117.75
3	D	1001	NAD	C3N-C7N-N7N	2.96	121.12	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	338/339 (99%)	-0.06	2 (0%) 89 91	18, 29, 52, 87	0
1	B	338/339 (99%)	-0.03	2 (0%) 89 91	20, 29, 52, 82	0
1	C	338/339 (99%)	0.05	3 (0%) 84 86	19, 31, 54, 95	0
1	D	338/339 (99%)	0.23	7 (2%) 63 68	21, 42, 74, 104	0
2	E	75/77 (97%)	1.41	15 (20%) 1 1	39, 77, 114, 136	0
2	F	68/77 (88%)	1.09	14 (20%) 1 1	31, 46, 110, 139	0
All	All	1495/1510 (99%)	0.16	43 (2%) 51 58	18, 33, 77, 139	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	ALA	7.8
2	E	25	THR	7.4
1	D	337	ALA	7.2
2	E	1	MET	7.1
2	F	4	LEU	6.6
2	E	33	TRP	6.3
1	A	337	ALA	5.7
1	D	72	GLY	5.2
2	F	53	HIS	5.0
2	F	2	SER	4.6
2	F	45	HIS	4.6
2	F	43	ALA	4.5
2	E	41	ALA	4.1
2	F	33	TRP	4.1
2	F	46	GLN	4.1
2	E	53	HIS	3.7
2	E	51	GLN	3.6
2	E	44	ALA	3.6
2	E	50	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	24	ALA	3.1
1	D	336	TRP	2.9
2	E	3	ASN	2.9
1	C	73	HIS	2.9
2	F	44	ALA	2.8
2	E	45	HIS	2.7
2	F	40	GLN	2.7
2	F	54	LYS	2.7
1	D	333	ALA	2.7
1	D	88	TRP	2.6
2	F	38	GLU	2.6
1	C	0	SER	2.5
2	F	8	ILE	2.5
1	A	0	SER	2.5
1	D	0	SER	2.4
1	B	72	GLY	2.4
2	E	42	GLU	2.4
2	E	8	ILE	2.3
1	B	26	ASN	2.3
1	D	107	GLU	2.2
2	F	39	LEU	2.1
2	F	6	LYS	2.1
2	E	5	GLU	2.0
2	E	16	HIS	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. 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	B-factors(\AA^2)	Q<0.9
4	SO4	C	1002	5/5	0.90	0.17	69,71,74,79	0
3	NAD	D	1001	44/44	0.96	0.11	24,30,41,43	0
3	NAD	B	1001	44/44	0.98	0.11	18,23,29,31	0
3	NAD	A	1001	44/44	0.98	0.10	19,26,31,33	0
3	NAD	C	1001	44/44	0.98	0.10	17,25,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.