



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:40 am GMT

PDB ID : 3B1K
Title : Crystal structure of Glyceraldehyde-3-Phosphate Dehydrogenase complexed with CP12 in the absence of copper from *Synechococcus elongatus*
Authors : Matsumura, H.; Kai, A.; Inoue, T.
Deposited on : 2011-07-04
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

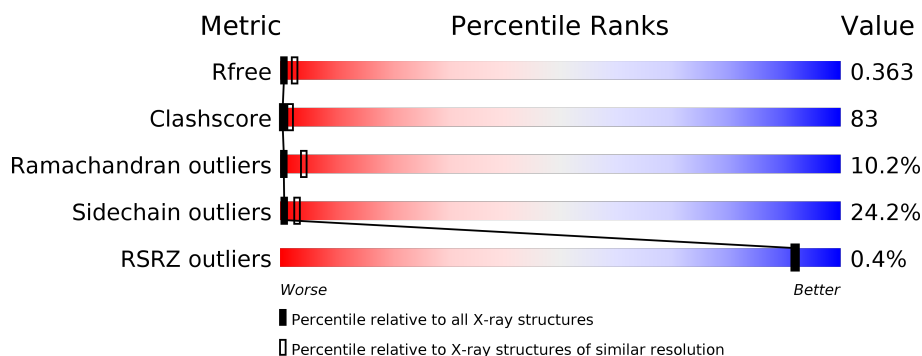
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



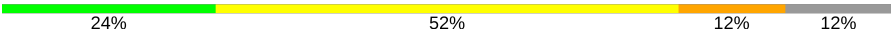
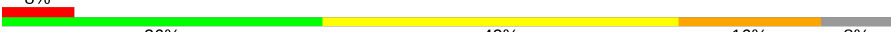
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	<div> <div>16%</div> <div>60%</div> <div>23%</div> <div>.</div> </div>
1	B	339	<div> <div>18%</div> <div>58%</div> <div>22%</div> <div>.</div> </div>
1	G	339	<div> <div>13%</div> <div>58%</div> <div>26%</div> <div>.</div> </div>
1	H	339	<div> <div>14%</div> <div>65%</div> <div>17%</div> <div>.</div> </div>
2	C	25	<div> <div>4%</div> <div>28%</div> <div>48%</div> <div>12%</div> <div>12%</div> </div>
2	D	25	<div> <div>4%</div> <div>32%</div> <div>44%</div> <div>8%</div> <div>8%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	25	
2	J	25	

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
3	NAD	G	340	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11278 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 (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	B	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	G	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	H	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			

- Molecule 2 is a protein called CP12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	S	0	0	0
			175	110	23	40	2			
2	D	23	Total	C	N	O	S	0	0	0
			182	114	24	42	2			
2	I	22	Total	C	N	O	S	0	0	0
			175	110	23	40	2			
2	J	23	Total	C	N	O	S	0	0	0
			182	114	24	42	2			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

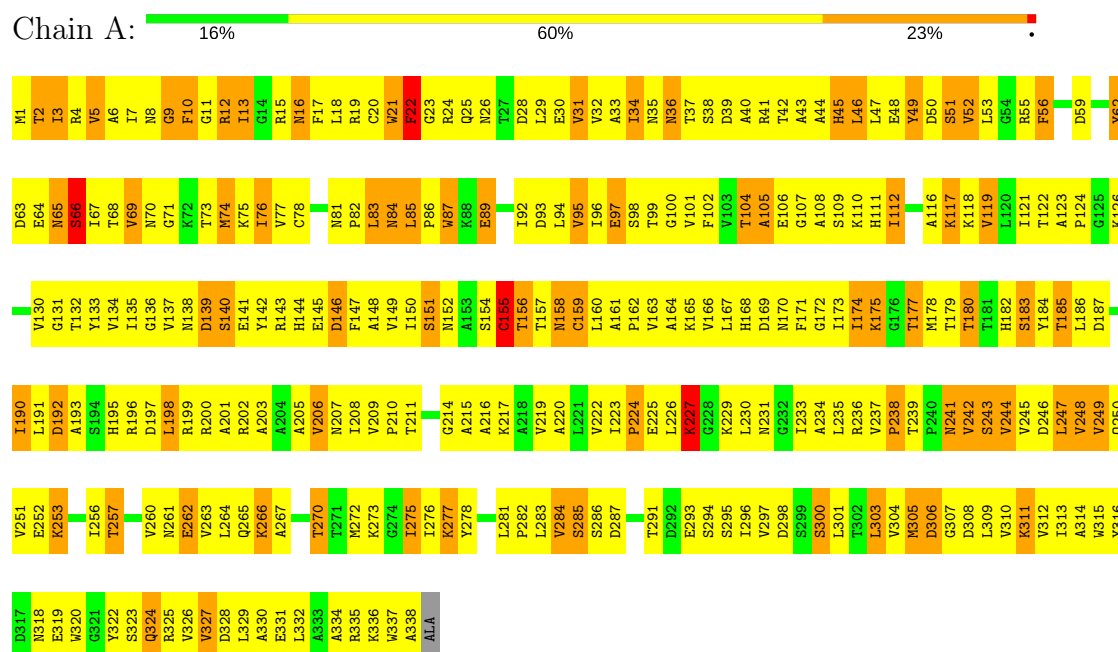
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total	O	0	0
			4	4		

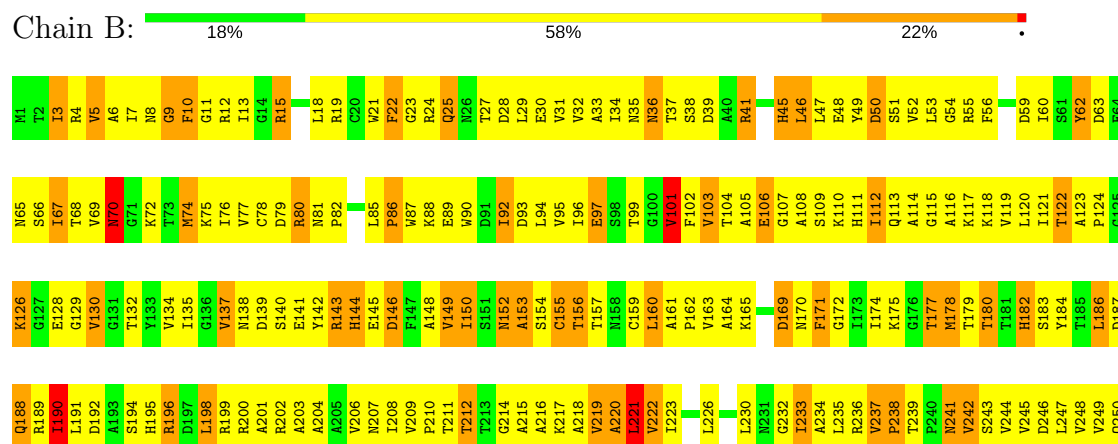
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 (NADP+)



- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)



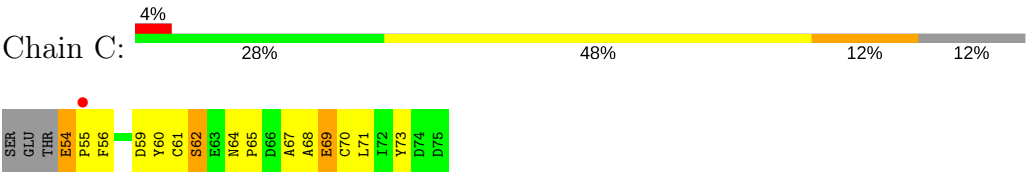


D308	L247	T185	A123	D63	M1
L309	V249	L186		E64	T2
V310	V248	D187	K126	R65	
K311	Q250	R188	G127	S66	V5
V312	V251	Q189	E128	I67	A6
I313	E252	L190	G129	T68	I7
A314	K253	L191	V130	V69	N8
W315	T254	D192	G131	N70	G9
Y316	T255	L193	T132	F10	F10
K317	T256	S194	Y133	K72	G11
N318	T257	H195	V134	T73	
E319	E258	R196	I135	M74	I13
W320	Q259	D197	G136	K75	G14
G321	V260	L198	V137	I76	R15
Y322	N261	R199	N138	V77	N16
K323	E262	R200	D139	C78	F17
Q324	V263	A201	S140	D79	L18
D328	L264	R202	E141	R80	R19
R325	Q265	K203	Y142	N81	C20
V326	T266	A204	R143	P82	W21
D328	A267	A205	H144	L83	F22
L329	Q268	V206	E145	N84	G23
	Q269	N207	D146	L85	R24
L332	T270	T208	F147	P86	
A333	T271	V209	A148	W87	T27
A334	M272		V149	K88	D28
R335	K273	T213	I150	E89	L29
K336	G274	G214	S151	W90	E30
W337	T275	A215	N152	D91	V31
	T276	A216	A153	I92	V32
A338	K277	K217	S154	D93	A33
ALA	T278	A218	C155	L94	I34
	T279	V219	T156	W95	N35
	D280	A220	T157	I96	N36
	L281	L221	N158	E97	T37
	P282	V222	C159	S98	S38
	L283	T223	L160	T99	D39
	V284	E224	A161	G100	A40
S285	S286	P225	P162	V101	R41
	D287	L226	V163	F102	T42
F288	D287	K227	A164	V103	A43
		G228	K165	T104	A44
	T291	K229	V166	A105	H45
D292	D292	L230	L167	E106	L46
E293	E293	N231	H168	G107	L47
S294	S294	G232	D169	A108	E48
S295	S295	T233	N170	S109	Y49
L296		K234	F171	K110	D50
V297	V297	L235	G172	H111	S51
D298	D298	R236	T173	I112	V52
S299	S299	V237	H174	Q113	L53
S300	S300	T238	K175	A114	G54
L301	L301	P239	G176	G115	R55
F302	F302	P240	T177	A116	F56
L303	L303	N241	M178	K117	N57
V304	V304	S243	T179	K118	A58
M305		V244	T180	V119	D59
D306				L120	I60
C307			S183	I121	S61
			Y184	T122	V62

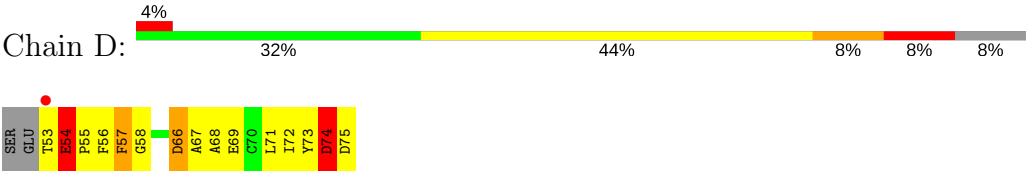
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)

G307	V245	S183	A123	Y62	M1
G308	D246	L184	P124	D63	I2
L309	L247	L185	G125	E64	T3
V310	V248	L186	K126	N65	R4
K311	V249		G127	S66	V5
V312	Q250	L190	E128	L67	A6
L313	V251	L191	G129	T68	I7
A314	E252	D192	V130	V69	N8
W315	K253	A193	G131	N70	G9
V316	P254	S194	T132	G71	F10
L317	T255	H195	Y133	K72	G11
K318	T256	R196	W134	T73	R12
E319	T257	D197	L135	M74	L13
W320	E258	L198	G136	K75	G14
G321	Q259	R199	V137	L76	R15
Y322	V260	R200	N138	V77	N16
S323	N261	A201	D139	C78	F17
Q324	E262	F202	S140	D79	L18
R325	V263	A203	E141	R80	R19
V326	L264	A204	Y142	N81	L20
V327	Q265	A205	R143	P82	C20
D328	K266	V206	H144	L83	W21
L329	A267	N207	E145	N84	F22
A330	S268	T208	D146	L85	G23
E331	Q269	V209	F147	P86	K24
L332	T270	P210	A148	N87	
A333	K271	T211	V149	R88	T27
R334	N272	T212	L150	E89	D28
S335	K273	G214	N152	I92	L29
K336	L275	A215	A153	D93	V31
W337	T276	A216	S154	L94	V32
A338	K277	K217	C155	V95	A33
ALA	V278	A218	T156	N96	I34
	S279	V219	T157	E97	N35
	D280	A220	N158	S98	N36
	L281	L221	C159	I99	T37
	T282	V222	L160	G100	S38
	L283	I223	A161	V101	D39
	V284	P224	P162	F102	A40
	S285	E225	V163	I103	R41
	S286	L226	A164	T104	T42
	T287	K227	C165	A105	A43
	F288	G228	V166	E106	A44
	R289	L230	L167	G107	H45
		K231	H168	A108	L46
	E293	N231	D169	S109	L47
	S294	G232	N170	K110	E48
	S295	I233	F171	H111	Y49
	L296	A234	G172	I112	D50
	V297	L235	I173	Q113	S51
	D298	R236	T174	A114	V52
	S299	V237	K175	G115	L53
	S300	P238	G176	A116	G54
	L301	T239	T177	K117	R55
	L302	P240	M178	L118	F56
	L303	K241	T179	V119	N57
	V304	T242	T180	L120	A58
	K305	S243	H181	I121	D59
	L306	V244	E182	T122	I60

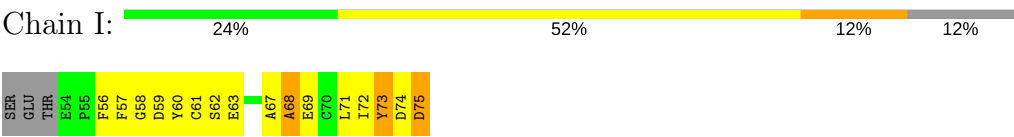
- Molecule 2: CP12



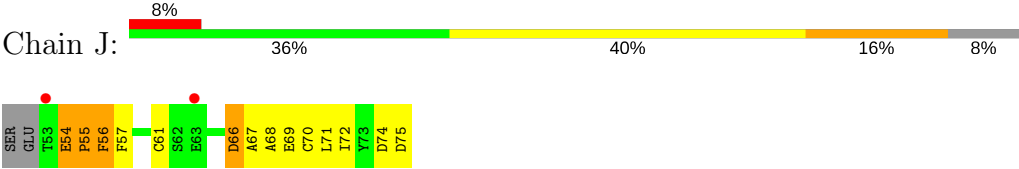
● Molecule 2: CP12



● Molecule 2: CP12



● Molecule 2: CP12



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.04Å 146.89Å 161.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.06 – 3.30 26.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	88.9 (26.06-3.30) 88.7 (26.06-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.252 , 0.363 0.247 , 0.363	Depositor DCC
R_{free} test set	1163 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11278	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.49 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.5976e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/2639	0.75	0/3590
1	B	0.51	0/2639	0.75	2/3590 (0.1%)
1	G	0.51	0/2639	0.74	1/3590 (0.0%)
1	H	0.49	0/2639	0.73	0/3590
2	C	0.50	0/180	0.63	0/245
2	D	0.46	0/187	0.60	0/255
2	I	0.72	0/180	0.67	0/245
2	J	0.41	0/187	0.64	0/255
All	All	0.51	0/11290	0.74	3/15360 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ILE	CB-CA-C	-6.11	99.38	111.60
1	B	264	LEU	CA-CB-CG	-5.98	101.54	115.30
1	G	206	VAL	CB-CA-C	-5.71	100.55	111.40

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	2596	0	2620	503	0
1	B	2596	0	2620	427	0
1	G	2596	0	2620	488	0
1	H	2596	0	2620	485	0
2	C	175	0	137	19	0
2	D	182	0	144	30	0
2	I	175	0	137	23	0
2	J	182	0	144	25	0
3	A	44	0	26	18	0
3	B	44	0	26	20	0
3	G	44	0	26	30	0
3	H	44	0	26	17	0
4	H	4	0	0	0	0
All	All	11278	0	11146	1854	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 83.

The worst 5 of 1854 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:G:247:LEU:HD12	1:G:248:VAL:H	1.10	1.16
1:B:305:MET:HB3	1:H:175:LYS:HD2	1.22	1.15
1:G:144:HIS:CD2	1:G:337:TRP:HA	1.84	1.12
1:A:31:VAL:HG12	1:A:74:MET:HG2	1.23	1.11
1:A:305:MET:HE2	1:G:231:ASN:H	0.97	1.10

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	336/339 (99%)	234 (70%)	75 (22%)	27 (8%)	1	8
1	B	336/339 (99%)	231 (69%)	70 (21%)	35 (10%)	0	4
1	G	336/339 (99%)	220 (66%)	74 (22%)	42 (12%)	0	2
1	H	336/339 (99%)	222 (66%)	82 (24%)	32 (10%)	1	5
2	C	20/25 (80%)	12 (60%)	6 (30%)	2 (10%)	1	4
2	D	21/25 (84%)	15 (71%)	3 (14%)	3 (14%)	0	1
2	I	20/25 (80%)	14 (70%)	5 (25%)	1 (5%)	2	17
2	J	21/25 (84%)	13 (62%)	5 (24%)	3 (14%)	0	1
All	All	1426/1456 (98%)	961 (67%)	320 (22%)	145 (10%)	1	4

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	105	ALA
1	A	146	ASP
1	A	155	CYS
1	A	206	VAL

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	284/284 (100%)	213 (75%)	71 (25%)	1	2
1	B	284/284 (100%)	208 (73%)	76 (27%)	0	2
1	G	284/284 (100%)	208 (73%)	76 (27%)	0	2
1	H	284/284 (100%)	223 (78%)	61 (22%)	1	5
2	C	19/22 (86%)	16 (84%)	3 (16%)	3	14
2	D	20/22 (91%)	17 (85%)	3 (15%)	3	16
2	I	19/22 (86%)	17 (90%)	2 (10%)	8	31
2	J	20/22 (91%)	18 (90%)	2 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1214/1224 (99%)	920 (76%)	294 (24%)	1 3

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	THR
1	G	56	PHE
1	H	221	LEU
1	B	256	ILE
2	C	69	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
2	C	64	ASN
1	H	241	ASN
1	B	269	GLN
1	G	45	HIS

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](#)

4 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	340	-	41,48,48	0.96	2 (4%)	43,73,73	1.71	7 (16%)
3	NAD	B	340	-	41,48,48	1.04	3 (7%)	43,73,73	1.84	6 (13%)
3	NAD	G	340	-	41,48,48	1.01	4 (9%)	43,73,73	2.20	5 (11%)
3	NAD	H	340	-	41,48,48	0.99	3 (7%)	43,73,73	1.53	3 (6%)

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	340	-	-	0/22/62/62	0/5/5/5
3	NAD	B	340	-	-	0/22/62/62	0/5/5/5
3	NAD	G	340	-	-	0/22/62/62	0/5/5/5
3	NAD	H	340	-	-	0/22/62/62	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	340	NAD	C3N-C7N	-2.93	1.46	1.50
3	G	340	NAD	C8A-N7A	-2.30	1.30	1.34
3	B	340	NAD	C8A-N7A	-2.27	1.30	1.34
3	H	340	NAD	C8A-N7A	-2.15	1.30	1.34
3	G	340	NAD	O4B-C1B	2.14	1.44	1.41

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	340	NAD	C4D-O4D-C1D	-9.32	99.84	109.77
3	H	340	NAD	N3A-C2A-N1A	-7.81	122.05	128.86
3	B	340	NAD	C4D-O4D-C1D	-7.06	102.25	109.77
3	B	340	NAD	N3A-C2A-N1A	-6.35	123.33	128.86
3	A	340	NAD	N3A-C2A-N1A	-5.91	123.71	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	340	NAD	18	0
3	B	340	NAD	20	0
3	G	340	NAD	30	0
3	H	340	NAD	17	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.56	0 100 100	2, 20, 39, 58	0
1	B	338/339 (99%)	-0.49	1 (0%) 93 93	6, 25, 44, 68	0
1	G	338/339 (99%)	-0.53	1 (0%) 93 93	4, 22, 41, 69	0
1	H	338/339 (99%)	-0.45	0 100 100	5, 27, 52, 66	0
2	C	22/25 (88%)	-0.11	1 (4%) 34 32	10, 28, 49, 67	0
2	D	23/25 (92%)	0.24	1 (4%) 36 34	26, 46, 67, 95	0
2	I	22/25 (88%)	-0.33	0 100 100	9, 25, 51, 54	0
2	J	23/25 (92%)	0.01	2 (8%) 11 10	17, 40, 70, 86	0
All	All	1442/1456 (99%)	-0.48	6 (0%) 92 92	2, 24, 48, 95	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	THR	6.0
2	J	53	THR	2.9
2	C	55	PRO	2.2
2	J	63	GLU	2.2
1	G	338	ALA	2.1

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
3	NAD	G	340	44/44	0.95	0.17	0.12	9,15,26,34	0
3	NAD	B	340	44/44	0.94	0.19	0.02	10,25,43,45	0
3	NAD	A	340	44/44	0.95	0.16	-0.20	10,17,29,33	0
3	NAD	H	340	44/44	0.96	0.14	-0.85	10,23,30,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.