Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:45 pm BST

PDB ID	:	3PFN
Title	:	Crystal Structure of human NAD kinase
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Deposited on	:	2010-10-28
Resolution	:	2.70 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:

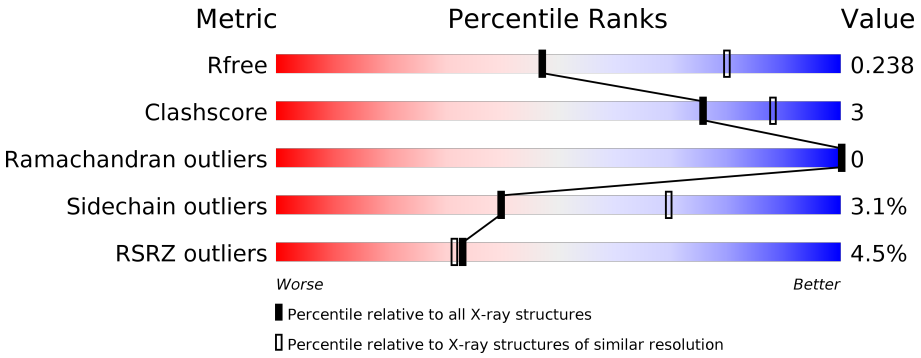
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. 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 <=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	365	3% 81% 8% • 10%
1	B	365	5% 82% 7% 10%
1	C	365	3% 81% 7% 12%
1	D	365	5% 78% 9% 13%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	11	-	-	-	X
2	UNX	A	5	-	-	-	X
2	UNX	B	56	-	-	-	X
2	UNX	D	62	-	-	-	X
2	UNX	D	9	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9218 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 NAD kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	Se	0	0	0
			2388	1528	400	444	8	8			
1	B	327	Total	C	N	O	S	Se	0	0	0
			2330	1496	384	434	8	8			
1	C	321	Total	C	N	O	S	Se	0	0	0
			2222	1426	370	411	7	8			
1	D	317	Total	C	N	O	S	Se	0	0	0
			2216	1426	368	406	8	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	MSE	-	EXPRESSION TAG	UNP O95544
A	262	LYS	ASN	VARIANT	UNP O95544
A	427	HIS	-	EXPRESSION TAG	UNP O95544
A	428	HIS	-	EXPRESSION TAG	UNP O95544
A	429	HIS	-	EXPRESSION TAG	UNP O95544
A	430	HIS	-	EXPRESSION TAG	UNP O95544
A	431	HIS	-	EXPRESSION TAG	UNP O95544
B	67	MSE	-	EXPRESSION TAG	UNP O95544
B	262	LYS	ASN	VARIANT	UNP O95544
B	427	HIS	-	EXPRESSION TAG	UNP O95544
B	428	HIS	-	EXPRESSION TAG	UNP O95544
B	429	HIS	-	EXPRESSION TAG	UNP O95544
B	430	HIS	-	EXPRESSION TAG	UNP O95544
B	431	HIS	-	EXPRESSION TAG	UNP O95544
C	67	MSE	-	EXPRESSION TAG	UNP O95544
C	262	LYS	ASN	VARIANT	UNP O95544
C	427	HIS	-	EXPRESSION TAG	UNP O95544
C	428	HIS	-	EXPRESSION TAG	UNP O95544
C	429	HIS	-	EXPRESSION TAG	UNP O95544
C	430	HIS	-	EXPRESSION TAG	UNP O95544
C	431	HIS	-	EXPRESSION TAG	UNP O95544

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Chain	Residue	Modelled	Actual	Comment	Reference
D	67	MSE	-	EXPRESSION TAG	UNP O95544
D	262	LYS	ASN	VARIANT	UNP O95544
D	427	HIS	-	EXPRESSION TAG	UNP O95544
D	428	HIS	-	EXPRESSION TAG	UNP O95544
D	429	HIS	-	EXPRESSION TAG	UNP O95544
D	430	HIS	-	EXPRESSION TAG	UNP O95544
D	431	HIS	-	EXPRESSION TAG	UNP O95544

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

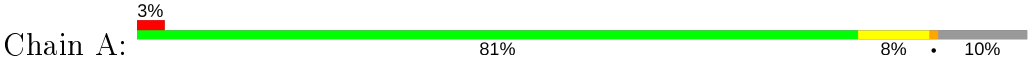
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	20	Total X 20 20	0	0
2	A	21	Total X 21 21	0	0
2	D	7	Total X 7 7	0	0
2	C	14	Total X 14 14	0	0

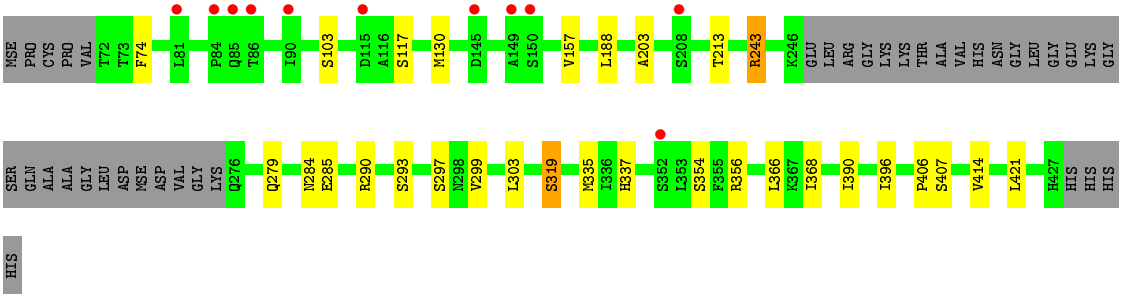
3 Residue-property plots (i)

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: NAD kinase

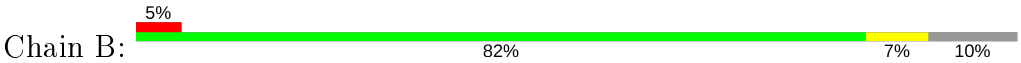
Chain A:

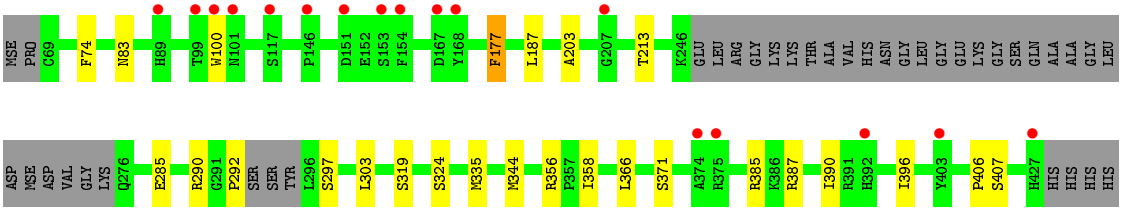




- Molecule 1: NAD kinase

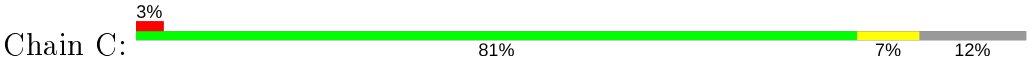
Chain B:

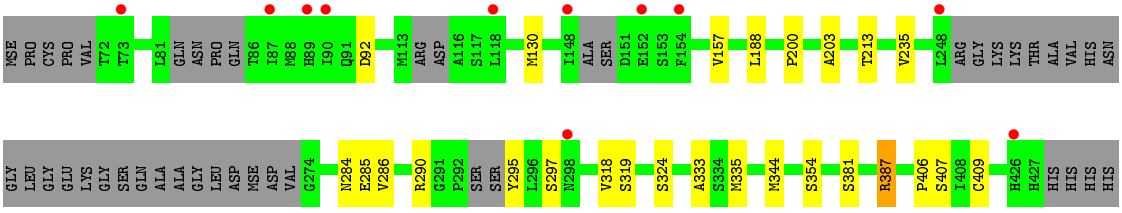




- Molecule 1: NAD kinase

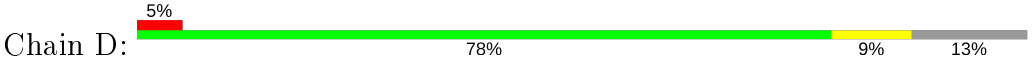
Chain C:

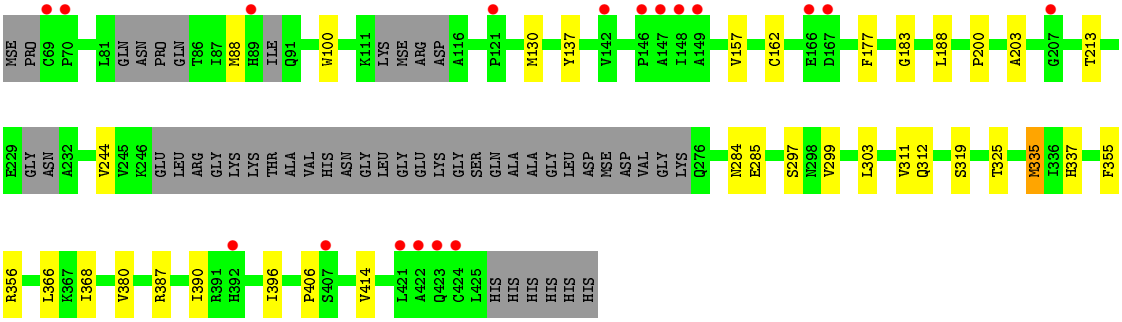




- Molecule 1: NAD kinase

Chain D:




MSE PRO C69 P70 L81 GLN ASN PRO GLN T86 I87 M88 H89 ILE Q91 W100 K111 LYS MSE ARG ASP A116 P121 M130 Y137 V142 P146 A147 I148 A149 V157 C162 E166 D167 F177 G183 L188 P200 A203 G207 T213
E229 GLY ASN A232 V244 V245 K246 GLU LEU ARG GLY LYS LYS THR ALA VAL HIS ASN GLY LEU GLY GLU LYS GLY SER GLN ALA ALA GLY LEU ASP MSE ASP VAL GLY LYS Q276 N284 E285 S297 N298 V299 L303 V311 Q312 S319 T325 M335 I336 H337 F355
R356 L366 K367 I368 V380 R387 I390 R391 H392 I396 P406 S407 V414 L421 A422 Q423 C424 L425 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.09Å 133.59Å 162.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 2.70 29.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.84-2.70) 98.4 (29.81-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.68Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.209 , 0.236 0.216 , 0.238	Depositor DCC
R_{free} test set	2107 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9218	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UNX

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	0.49	0/2433	0.67	0/3310
1	B	0.49	0/2373	0.68	0/3237
1	C	0.48	0/2260	0.67	0/3085
1	D	0.46	0/2256	0.67	0/3082
All	All	0.48	0/9322	0.67	0/12714

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	2388	0	2262	18	0
1	B	2330	0	2159	14	0
1	C	2222	0	1965	13	0
1	D	2216	0	2001	20	0
2	A	21	0	0	1	0
2	B	20	0	0	0	0
2	C	14	0	0	0	0
2	D	7	0	0	0	0
All	All	9218	0	8387	54	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 3.

All (54) 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:A:188:LEU:HD21	1:A:284:ASN:ND2	2.00	0.77
1:B:290:ARG:HB3	1:B:297:SER:HB3	1.79	0.64
1:C:188:LEU:HD21	1:C:284:ASN:ND2	2.12	0.64
1:A:319:SER:OG	2:A:8:UNX:UNK	1.79	0.63
1:B:390:ILE:HG13	1:B:396:ILE:HD11	1.79	0.63
1:D:244:VAL:HG22	1:D:396:ILE:HD13	1.83	0.59
1:A:390:ILE:HG13	1:A:396:ILE:HD11	1.85	0.59
1:C:290:ARG:HB3	1:C:297:SER:HB3	1.85	0.57
1:B:100:TRP:HH2	1:B:177:PHE:HB3	1.70	0.56
1:A:356:ARG:NH2	1:B:335:MSE:HG3	2.21	0.56
1:D:188:LEU:HD21	1:D:284:ASN:ND2	2.20	0.55
1:D:390:ILE:HD11	1:D:396:ILE:HD11	1.87	0.54
1:B:324:SER:HB3	1:B:344:MSE:SE	2.58	0.54
1:B:292:PRO:HB3	1:C:387:ARG:HD3	1.90	0.54
1:A:299:VAL:HG13	1:A:368:ILE:HG23	1.93	0.51
1:C:324:SER:HB3	1:C:344:MSE:SE	2.60	0.51
1:A:130:MSE:SE	1:A:157:VAL:HG13	2.60	0.51
1:C:335:MSE:HG3	1:D:356:ARG:HH12	1.76	0.50
1:D:203:ALA:HB1	1:D:213:THR:HG22	1.92	0.50
1:C:235:VAL:HG23	1:C:409:CYS:SG	2.52	0.49
1:C:335:MSE:HG3	1:D:356:ARG:NH1	2.28	0.49
1:D:130:MSE:SE	1:D:157:VAL:HG13	2.63	0.48
1:A:203:ALA:HB1	1:A:213:THR:HG22	1.94	0.48
1:C:203:ALA:HB1	1:C:213:THR:HG22	1.96	0.48
1:B:203:ALA:HB1	1:B:213:THR:HG22	1.96	0.47
1:D:100:TRP:HH2	1:D:177:PHE:HB2	1.79	0.47
1:A:335:MSE:HG3	1:B:356:ARG:NH2	2.30	0.46
1:A:303:LEU:HD23	1:A:366:LEU:HG	1.98	0.46
1:D:380:VAL:HG21	1:D:396:ILE:HD12	1.98	0.46
1:A:356:ARG:HH22	1:B:335:MSE:HG3	1.81	0.45
1:C:130:MSE:SE	1:C:157:VAL:HG13	2.66	0.45
1:D:299:VAL:HG13	1:D:368:ILE:HG23	1.97	0.45
1:A:406:PRO:HG3	1:B:74:PHE:CD1	2.51	0.45
1:D:183:GLY:HA2	1:D:213:THR:HG21	1.98	0.45
1:D:200:PRO:HA	1:D:406:PRO:HG2	2.00	0.44
1:A:421:LEU:HD11	1:B:358:ILE:HD11	2.00	0.44
1:D:311:VAL:HG22	1:D:355:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:SER:O	1:D:312:GLN:HA	2.18	0.43
1:A:290:ARG:HB3	1:A:297:SER:HB3	2.00	0.43
1:A:243:ARG:HG3	1:A:279:GLN:HG3	2.00	0.43
1:C:200:PRO:HA	1:C:406:PRO:HG2	2.00	0.42
1:A:74:PHE:CD1	1:B:406:PRO:HG3	2.53	0.42
1:D:137:TYR:HA	1:D:162:CYS:O	2.20	0.42
1:A:337:HIS:HE2	1:A:414:VAL:HA	1.84	0.42
1:D:390:ILE:CD1	1:D:396:ILE:HD11	2.50	0.42
1:C:286:VAL:HG13	1:C:318:VAL:HB	2.02	0.42
1:D:337:HIS:HE2	1:D:414:VAL:HA	1.85	0.41
1:C:92:ASP:HA	1:D:88:MSE:SE	2.71	0.41
1:B:303:LEU:HD23	1:B:366:LEU:HG	2.02	0.41
1:A:356:ARG:NH1	1:B:324:SER:O	2.54	0.41
1:D:325:THR:HG22	1:D:335:MSE:HE2	2.03	0.41
1:C:333:ALA:HB1	1:C:344:MSE:CE	2.51	0.41
1:A:290:ARG:NH1	1:A:293:SER:O	2.53	0.41
1:D:303:LEU:HD23	1:D:366:LEU:HG	2.03	0.41

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	323/365 (88%)	311 (96%)	12 (4%)	0	100	100
1	B	321/365 (88%)	310 (97%)	11 (3%)	0	100	100
1	C	309/365 (85%)	299 (97%)	10 (3%)	0	100	100
1	D	305/365 (84%)	295 (97%)	10 (3%)	0	100	100
All	All	1258/1460 (86%)	1215 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/305 (80%)	238 (97%)	7 (3%)	42	71
1	B	229/305 (75%)	220 (96%)	9 (4%)	32	61
1	C	201/305 (66%)	194 (96%)	7 (4%)	36	65
1	D	207/305 (68%)	203 (98%)	4 (2%)	57	82
All	All	882/1220 (72%)	855 (97%)	27 (3%)	40	69

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	SER
1	A	117	SER
1	A	243	ARG
1	A	285	GLU
1	A	319	SER
1	A	354	SER
1	A	407	SER
1	B	83	ASN
1	B	177	PHE
1	B	187	LEU
1	B	285	GLU
1	B	319	SER
1	B	371	SER
1	B	385	ARG
1	B	387	ARG
1	B	407	SER
1	C	285	GLU
1	C	295	TYR
1	C	319	SER
1	C	354	SER
1	C	381	SER
1	C	387	ARG
1	C	407	SER
1	D	285	GLU

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Mol	Chain	Res	Type
1	D	319	SER
1	D	335	MSE
1	D	387	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	284	ASN
1	C	231	ASN
1	C	284	ASN
1	D	219	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 62 ligands modelled in this entry, 62 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 95^{th} 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	318/365 (87%)	-0.12	11 (3%)	44	44	25, 52, 85, 103	0
1	B	318/365 (87%)	0.05	17 (5%)	26	25	26, 56, 97, 119	0
1	C	312/365 (85%)	-0.02	11 (3%)	44	44	24, 57, 97, 123	0
1	D	309/365 (84%)	0.25	18 (5%)	23	22	33, 66, 99, 111	0
All	All	1257/1460 (86%)	0.04	57 (4%)	33	31	24, 57, 96, 123	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	ALA	5.2
1	D	89	HIS	4.8
1	D	167	ASP	4.8
1	C	89	HIS	4.6
1	B	151	ASP	4.1
1	A	84	PRO	3.7
1	D	147	ALA	3.7
1	A	86	THR	3.7
1	D	69	CYS	3.4
1	C	87	ILE	3.3
1	B	375	ARG	3.2
1	B	154	PHE	3.1
1	D	207	GLY	3.1
1	A	149	ALA	3.1
1	B	100	TRP	3.1
1	B	168	TYR	3.0
1	C	90	ILE	2.9
1	A	150	SER	2.9
1	A	115	ASP	2.9
1	B	146	PRO	2.9
1	B	99	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	423	GLN	2.7
1	B	117	SER	2.7
1	C	118	LEU	2.7
1	A	85	GLN	2.7
1	B	207	GLY	2.6
1	D	142	VAL	2.6
1	C	248	LEU	2.5
1	B	101	ASN	2.4
1	B	374	ALA	2.4
1	D	424	CYS	2.4
1	B	392	HIS	2.4
1	C	298	ASN	2.4
1	D	149	ALA	2.4
1	D	146	PRO	2.3
1	B	153	SER	2.3
1	C	152	GLU	2.3
1	C	73	THR	2.3
1	D	421	LEU	2.2
1	D	70	PRO	2.2
1	C	154	PHE	2.2
1	D	148	ILE	2.2
1	A	208	SER	2.2
1	B	89	HIS	2.2
1	C	148	ILE	2.2
1	B	427	HIS	2.2
1	D	392	HIS	2.2
1	A	145	ASP	2.2
1	C	426	HIS	2.1
1	B	167	ASP	2.1
1	D	407	SER	2.1
1	A	81	LEU	2.1
1	A	90	ILE	2.1
1	D	121	PRO	2.0
1	B	403	TYR	2.0
1	D	166	GLU	2.0
1	A	352	SER	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, 95^{th} 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(Å^2)	Q<0.9
2	UNX	D	58	1/1	0.65	0.34	30,30,30,30	0
2	UNX	A	5	1/1	0.67	0.43	30,30,30,30	0
2	UNX	B	56	1/1	0.68	0.45	30,30,30,30	0
2	UNX	B	60	1/1	0.68	0.40	30,30,30,30	0
2	UNX	D	62	1/1	0.68	0.47	30,30,30,30	0
2	UNX	A	2	1/1	0.72	0.40	30,30,30,30	0
2	UNX	A	11	1/1	0.73	0.44	30,30,30,30	0
2	UNX	A	54	1/1	0.76	0.27	30,30,30,30	0
2	UNX	B	26	1/1	0.79	0.31	30,30,30,30	0
2	UNX	B	29	1/1	0.79	0.28	30,30,30,30	0
2	UNX	D	9	1/1	0.79	0.72	30,30,30,30	0
2	UNX	A	3	1/1	0.79	0.22	30,30,30,30	0
2	UNX	B	18	1/1	0.80	0.32	30,30,30,30	0
2	UNX	B	22	1/1	0.80	0.31	30,30,30,30	0
2	UNX	A	36	1/1	0.81	0.17	30,30,30,30	0
2	UNX	B	38	1/1	0.82	0.20	30,30,30,30	0
2	UNX	B	19	1/1	0.82	0.29	30,30,30,30	0
2	UNX	A	43	1/1	0.83	0.34	30,30,30,30	0
2	UNX	C	61	1/1	0.83	0.33	30,30,30,30	0
2	UNX	A	40	1/1	0.83	0.29	30,30,30,30	0
2	UNX	C	53	1/1	0.84	0.28	30,30,30,30	0
2	UNX	C	47	1/1	0.84	0.36	30,30,30,30	0
2	UNX	C	27	1/1	0.84	0.46	30,30,30,30	0
2	UNX	B	17	1/1	0.85	0.37	30,30,30,30	0
2	UNX	A	4	1/1	0.85	0.27	30,30,30,30	0
2	UNX	B	23	1/1	0.86	0.31	30,30,30,30	0
2	UNX	B	57	1/1	0.87	0.31	30,30,30,30	0
2	UNX	A	28	1/1	0.87	0.31	30,30,30,30	0
2	UNX	B	45	1/1	0.87	0.24	30,30,30,30	0
2	UNX	D	41	1/1	0.88	0.20	30,30,30,30	0
2	UNX	B	15	1/1	0.88	0.17	30,30,30,30	0
2	UNX	C	34	1/1	0.88	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UNX	A	7	1/1	0.88	0.39	30,30,30,30	0
2	UNX	B	20	1/1	0.89	0.30	30,30,30,30	0
2	UNX	C	31	1/1	0.90	0.29	30,30,30,30	0
2	UNX	C	35	1/1	0.90	0.23	30,30,30,30	0
2	UNX	A	8	1/1	0.90	0.25	30,30,30,30	0
2	UNX	B	50	1/1	0.91	0.30	30,30,30,30	0
2	UNX	D	59	1/1	0.91	0.23	30,30,30,30	0
2	UNX	D	48	1/1	0.91	0.33	30,30,30,30	0
2	UNX	A	16	1/1	0.91	0.40	30,30,30,30	0
2	UNX	A	42	1/1	0.91	0.24	30,30,30,30	0
2	UNX	C	55	1/1	0.92	0.20	30,30,30,30	0
2	UNX	B	21	1/1	0.92	0.26	30,30,30,30	0
2	UNX	A	1	1/1	0.92	0.20	30,30,30,30	0
2	UNX	C	46	1/1	0.92	0.23	30,30,30,30	0
2	UNX	C	32	1/1	0.92	0.48	30,30,30,30	0
2	UNX	C	39	1/1	0.93	0.23	30,30,30,30	0
2	UNX	B	24	1/1	0.93	0.23	30,30,30,30	0
2	UNX	A	14	1/1	0.93	0.33	30,30,30,30	0
2	UNX	A	51	1/1	0.93	0.33	30,30,30,30	0
2	UNX	D	37	1/1	0.93	0.23	30,30,30,30	0
2	UNX	A	13	1/1	0.94	0.20	30,30,30,30	0
2	UNX	B	49	1/1	0.94	0.18	30,30,30,30	0
2	UNX	A	6	1/1	0.95	0.17	30,30,30,30	0
2	UNX	C	30	1/1	0.95	0.25	30,30,30,30	0
2	UNX	B	25	1/1	0.95	0.18	30,30,30,30	0
2	UNX	A	10	1/1	0.96	0.09	30,30,30,30	0
2	UNX	C	33	1/1	0.96	0.12	30,30,30,30	0
2	UNX	C	52	1/1	0.96	0.18	30,30,30,30	0
2	UNX	A	44	1/1	0.97	0.16	30,30,30,30	0
2	UNX	B	12	1/1	0.97	0.25	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.