wwPDB X-ray Structure Validation Summary Report (i)

Dec 1, 2022 – 04:12 PM JST

PDB ID	:	8GRB
Title	:	Crystal structure of a constitutively active mutant of the alpha beta heterodimer of human IDH3
Authors	:	Sun, P.; Chen, X.; Ding, J.
Deposited on	:	2022-09-01
Resolution	:	2.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

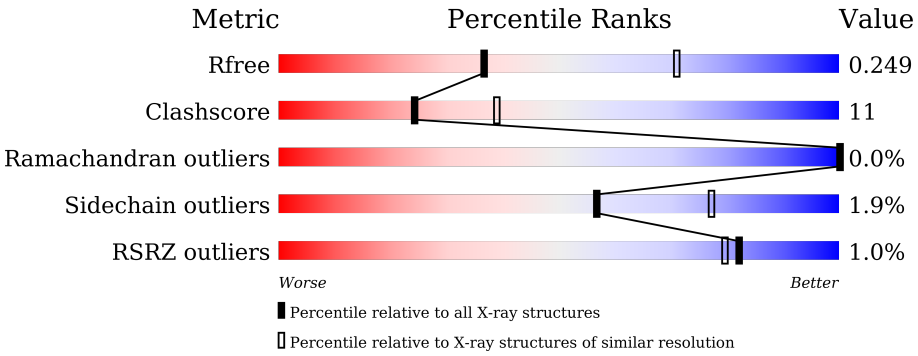
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.85 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 of 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	339	76% 23%
1	B	339	76% 21%
1	E	339	81% 18%
1	G	339	76% 22%
1	I	339	74% 24%
1	K	339	82% 17%

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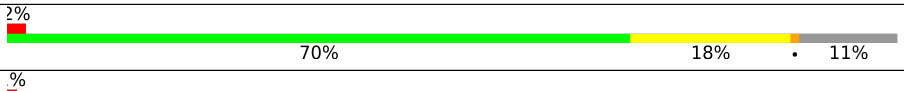
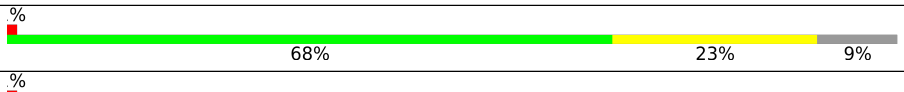
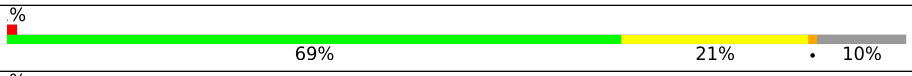
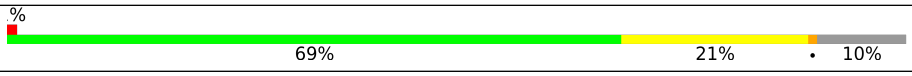
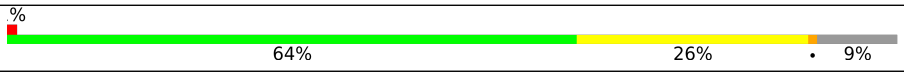
Mol	Chain	Length	Quality of chain
1	M	339	
1	O	339	
2	C	352	
2	D	352	
2	F	352	
2	H	352	
2	J	352	
2	L	352	
2	N	352	
2	P	352	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 39053 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 Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	333	Total	C	N	O	S	0	0	0
			2474	1553	421	478	22			
1	A	335	Total	C	N	O	S	0	0	0
			2502	1572	428	480	22			
1	E	337	Total	C	N	O	S	0	0	0
			2509	1575	429	483	22			
1	G	335	Total	C	N	O	S	0	0	0
			2483	1561	426	474	22			
1	I	333	Total	C	N	O	S	0	0	0
			2468	1549	421	476	22			
1	K	333	Total	C	N	O	S	0	0	0
			2472	1553	421	476	22			
1	M	335	Total	C	N	O	S	0	0	0
			2490	1565	425	478	22			
1	O	335	Total	C	N	O	S	0	0	0
			2491	1564	426	480	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	ALA	GLN	engineered mutation	UNP P50213
A	139	ALA	GLN	engineered mutation	UNP P50213
E	139	ALA	GLN	engineered mutation	UNP P50213
G	139	ALA	GLN	engineered mutation	UNP P50213
I	139	ALA	GLN	engineered mutation	UNP P50213
K	139	ALA	GLN	engineered mutation	UNP P50213
M	139	ALA	GLN	engineered mutation	UNP P50213
O	139	ALA	GLN	engineered mutation	UNP P50213

- Molecule 2 is a protein called Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	319	Total	C	N	O	S	0	0	0
			2413	1530	418	445	20			
2	D	319	Total	C	N	O	S	0	0	0
			2391	1509	414	448	20			
2	F	315	Total	C	N	O	S	0	0	0
			2383	1511	414	438	20			
2	H	319	Total	C	N	O	S	0	0	0
			2395	1512	416	447	20			
2	J	317	Total	C	N	O	S	0	0	0
			2406	1525	420	441	20			
2	L	317	Total	C	N	O	S	0	0	0
			2384	1508	416	440	20			
2	N	316	Total	C	N	O	S	0	0	0
			2391	1513	414	444	20			
2	P	320	Total	C	N	O	S	0	0	0
			2401	1516	416	449	20			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	341	GLU	-	expression tag	UNP O43837-2
C	342	ILE	-	expression tag	UNP O43837-2
C	343	CYS	-	expression tag	UNP O43837-2
C	344	ARG	-	expression tag	UNP O43837-2
C	345	ARG	-	expression tag	UNP O43837-2
C	346	VAL	-	expression tag	UNP O43837-2
C	347	LYS	-	expression tag	UNP O43837-2
C	348	ASP	-	expression tag	UNP O43837-2
C	349	LEU	-	expression tag	UNP O43837-2
C	350	ASP	-	expression tag	UNP O43837-2
C	351	GLU	-	expression tag	UNP O43837-2
C	352	ASN	-	expression tag	UNP O43837-2
D	341	GLU	-	expression tag	UNP O43837-2
D	342	ILE	-	expression tag	UNP O43837-2
D	343	CYS	-	expression tag	UNP O43837-2
D	344	ARG	-	expression tag	UNP O43837-2
D	345	ARG	-	expression tag	UNP O43837-2
D	346	VAL	-	expression tag	UNP O43837-2
D	347	LYS	-	expression tag	UNP O43837-2
D	348	ASP	-	expression tag	UNP O43837-2
D	349	LEU	-	expression tag	UNP O43837-2
D	350	ASP	-	expression tag	UNP O43837-2
D	351	GLU	-	expression tag	UNP O43837-2
D	352	ASN	-	expression tag	UNP O43837-2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	341	GLU	-	expression tag	UNP O43837-2
F	342	ILE	-	expression tag	UNP O43837-2
F	343	CYS	-	expression tag	UNP O43837-2
F	344	ARG	-	expression tag	UNP O43837-2
F	345	ARG	-	expression tag	UNP O43837-2
F	346	VAL	-	expression tag	UNP O43837-2
F	347	LYS	-	expression tag	UNP O43837-2
F	348	ASP	-	expression tag	UNP O43837-2
F	349	LEU	-	expression tag	UNP O43837-2
F	350	ASP	-	expression tag	UNP O43837-2
F	351	GLU	-	expression tag	UNP O43837-2
F	352	ASN	-	expression tag	UNP O43837-2
H	341	GLU	-	expression tag	UNP O43837-2
H	342	ILE	-	expression tag	UNP O43837-2
H	343	CYS	-	expression tag	UNP O43837-2
H	344	ARG	-	expression tag	UNP O43837-2
H	345	ARG	-	expression tag	UNP O43837-2
H	346	VAL	-	expression tag	UNP O43837-2
H	347	LYS	-	expression tag	UNP O43837-2
H	348	ASP	-	expression tag	UNP O43837-2
H	349	LEU	-	expression tag	UNP O43837-2
H	350	ASP	-	expression tag	UNP O43837-2
H	351	GLU	-	expression tag	UNP O43837-2
H	352	ASN	-	expression tag	UNP O43837-2
J	341	GLU	-	expression tag	UNP O43837-2
J	342	ILE	-	expression tag	UNP O43837-2
J	343	CYS	-	expression tag	UNP O43837-2
J	344	ARG	-	expression tag	UNP O43837-2
J	345	ARG	-	expression tag	UNP O43837-2
J	346	VAL	-	expression tag	UNP O43837-2
J	347	LYS	-	expression tag	UNP O43837-2
J	348	ASP	-	expression tag	UNP O43837-2
J	349	LEU	-	expression tag	UNP O43837-2
J	350	ASP	-	expression tag	UNP O43837-2
J	351	GLU	-	expression tag	UNP O43837-2
J	352	ASN	-	expression tag	UNP O43837-2
L	341	GLU	-	expression tag	UNP O43837-2
L	342	ILE	-	expression tag	UNP O43837-2
L	343	CYS	-	expression tag	UNP O43837-2
L	344	ARG	-	expression tag	UNP O43837-2
L	345	ARG	-	expression tag	UNP O43837-2
L	346	VAL	-	expression tag	UNP O43837-2

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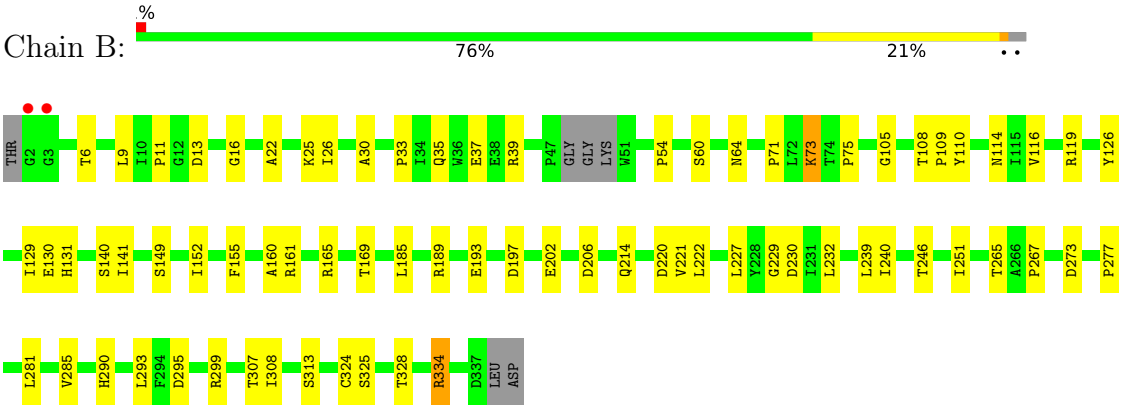
Chain	Residue	Modelled	Actual	Comment	Reference
L	347	LYS	-	expression tag	UNP O43837-2
L	348	ASP	-	expression tag	UNP O43837-2
L	349	LEU	-	expression tag	UNP O43837-2
L	350	ASP	-	expression tag	UNP O43837-2
L	351	GLU	-	expression tag	UNP O43837-2
L	352	ASN	-	expression tag	UNP O43837-2
N	341	GLU	-	expression tag	UNP O43837-2
N	342	ILE	-	expression tag	UNP O43837-2
N	343	CYS	-	expression tag	UNP O43837-2
N	344	ARG	-	expression tag	UNP O43837-2
N	345	ARG	-	expression tag	UNP O43837-2
N	346	VAL	-	expression tag	UNP O43837-2
N	347	LYS	-	expression tag	UNP O43837-2
N	348	ASP	-	expression tag	UNP O43837-2
N	349	LEU	-	expression tag	UNP O43837-2
N	350	ASP	-	expression tag	UNP O43837-2
N	351	GLU	-	expression tag	UNP O43837-2
N	352	ASN	-	expression tag	UNP O43837-2
P	341	GLU	-	expression tag	UNP O43837-2
P	342	ILE	-	expression tag	UNP O43837-2
P	343	CYS	-	expression tag	UNP O43837-2
P	344	ARG	-	expression tag	UNP O43837-2
P	345	ARG	-	expression tag	UNP O43837-2
P	346	VAL	-	expression tag	UNP O43837-2
P	347	LYS	-	expression tag	UNP O43837-2
P	348	ASP	-	expression tag	UNP O43837-2
P	349	LEU	-	expression tag	UNP O43837-2
P	350	ASP	-	expression tag	UNP O43837-2
P	351	GLU	-	expression tag	UNP O43837-2
P	352	ASN	-	expression tag	UNP O43837-2

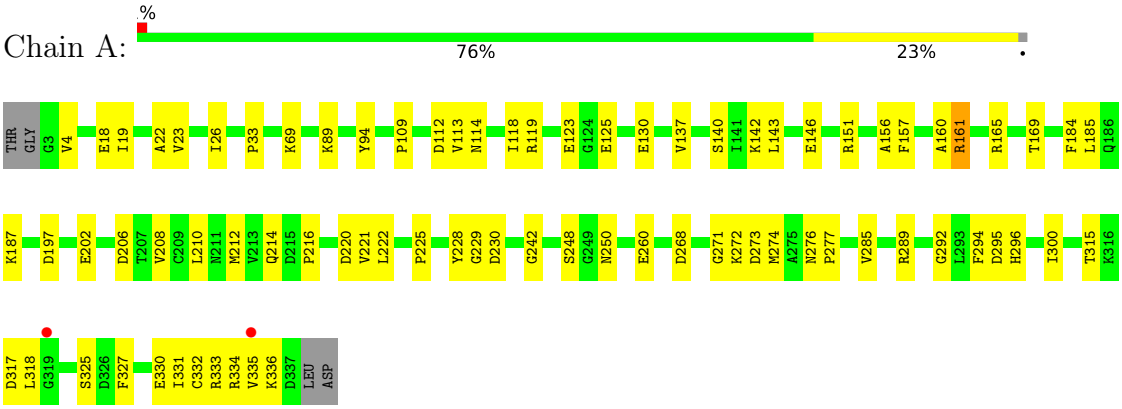
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

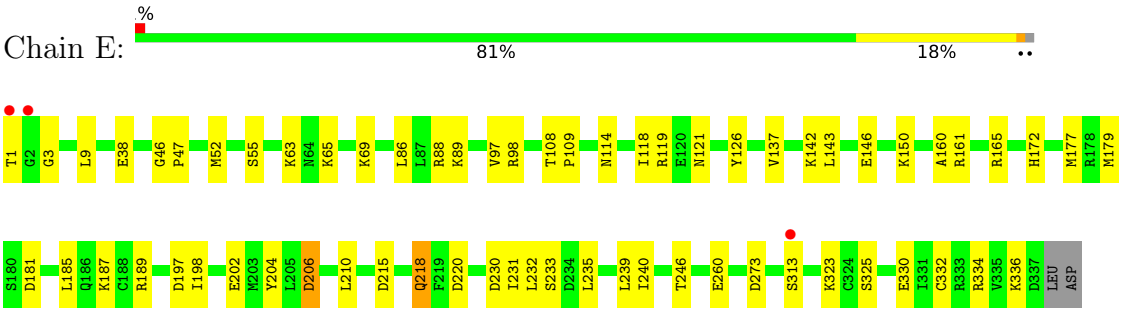
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial



• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

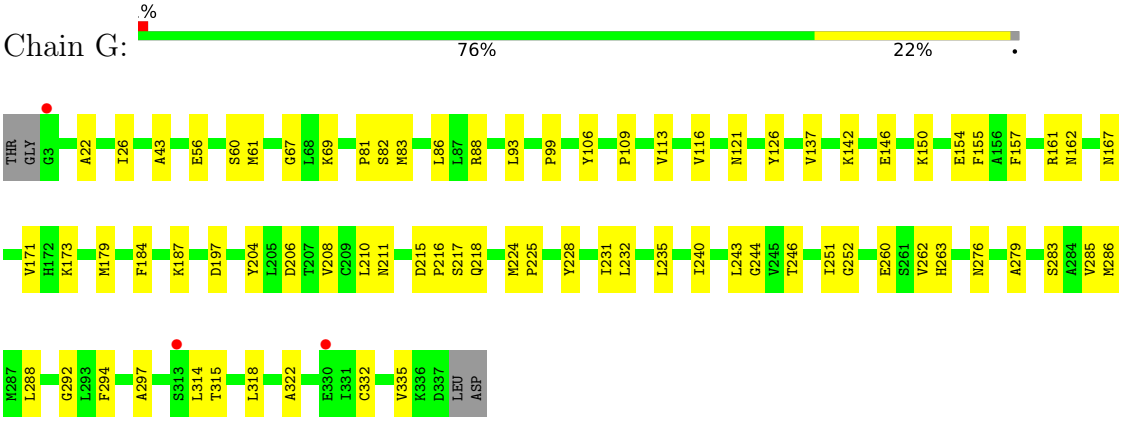


• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial



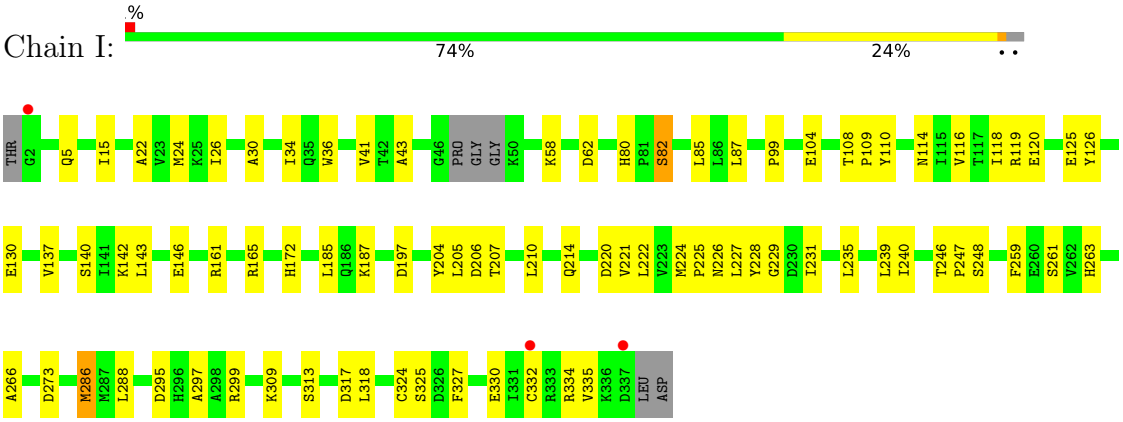
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain G:



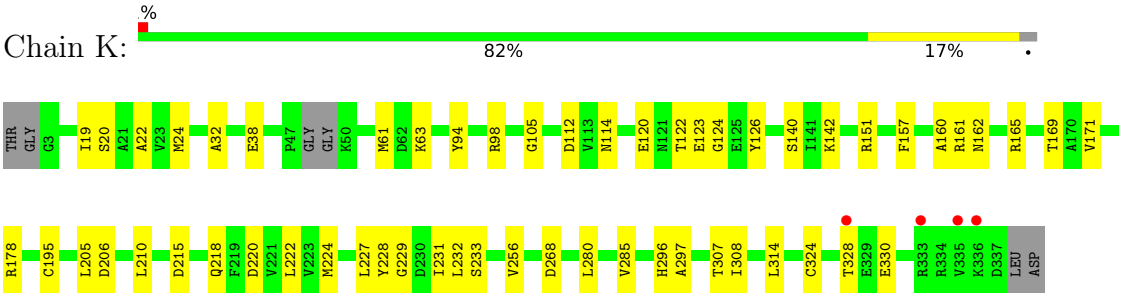
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain I:



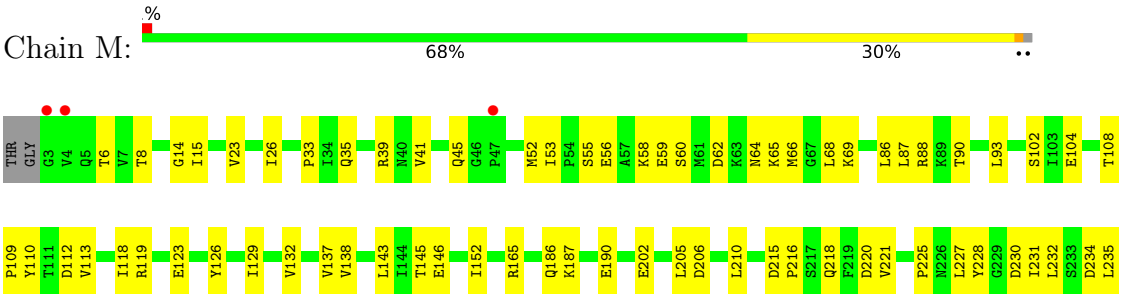
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

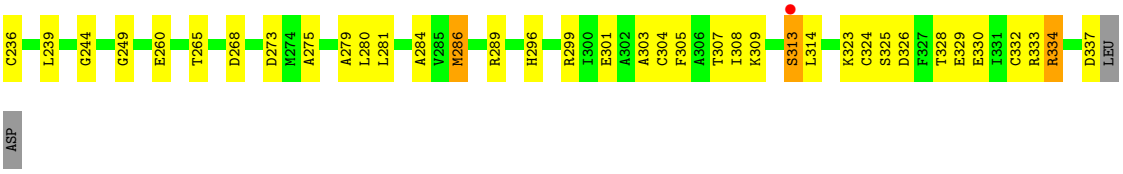
Chain K:



• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

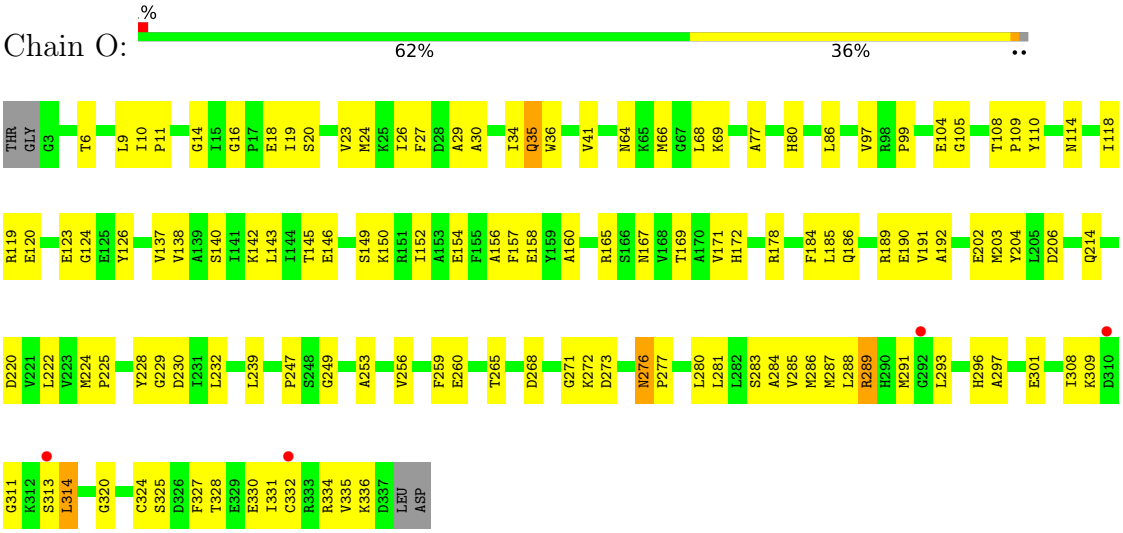
Chain M:





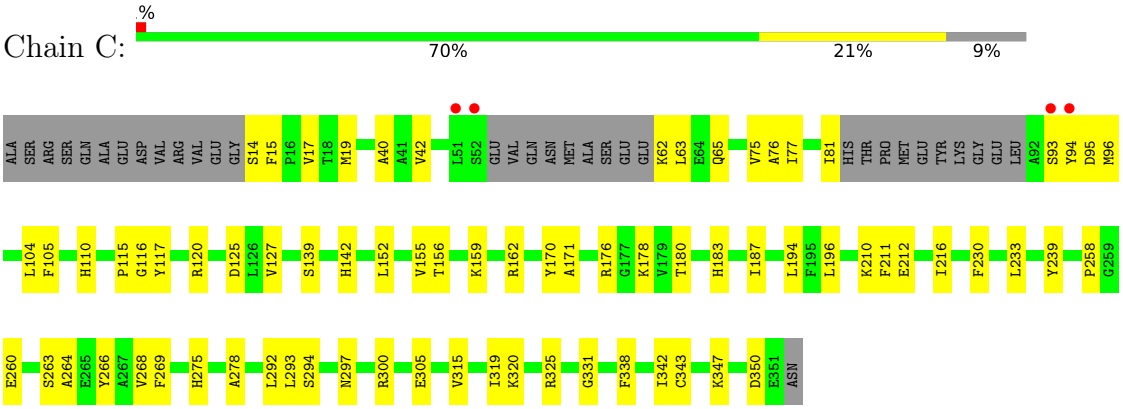
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain O:



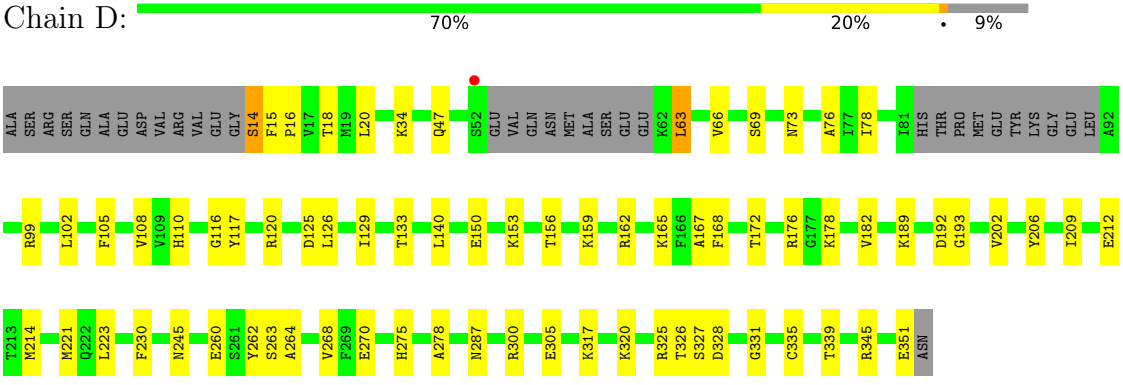
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain C:



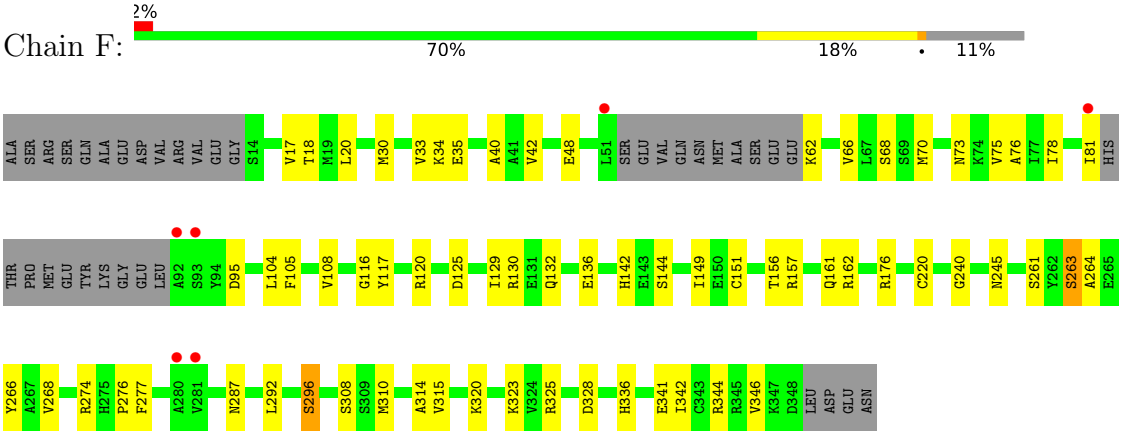
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain D:



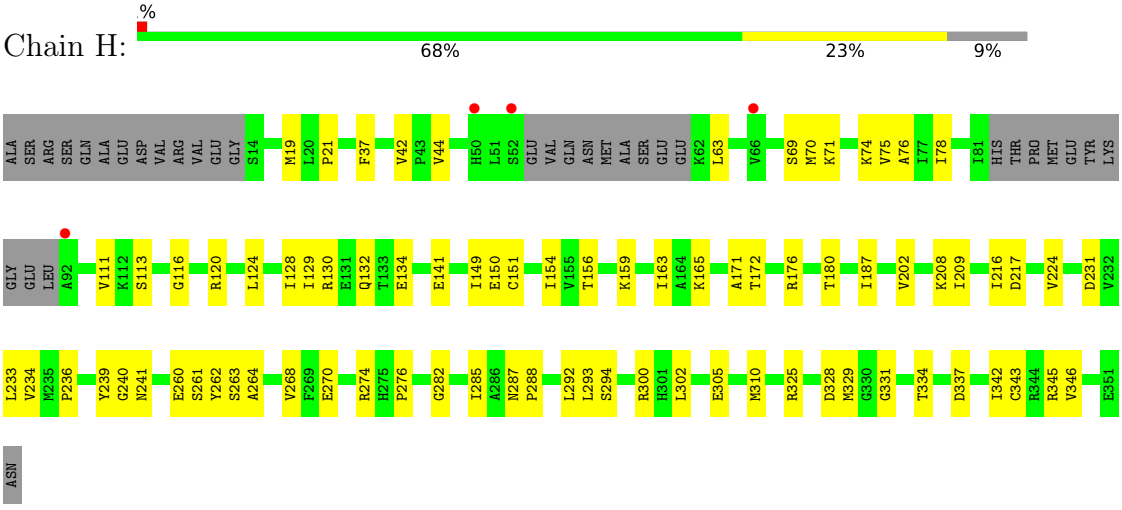
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain F:



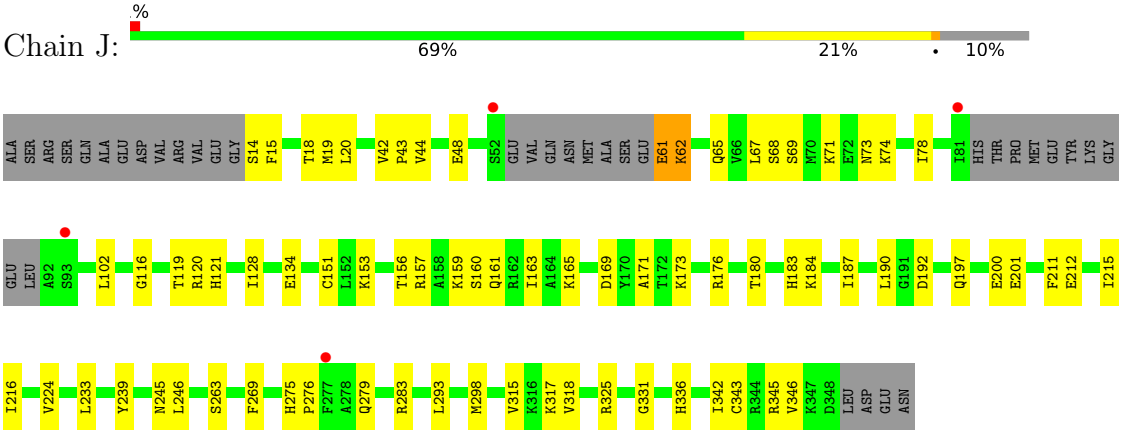
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain H:



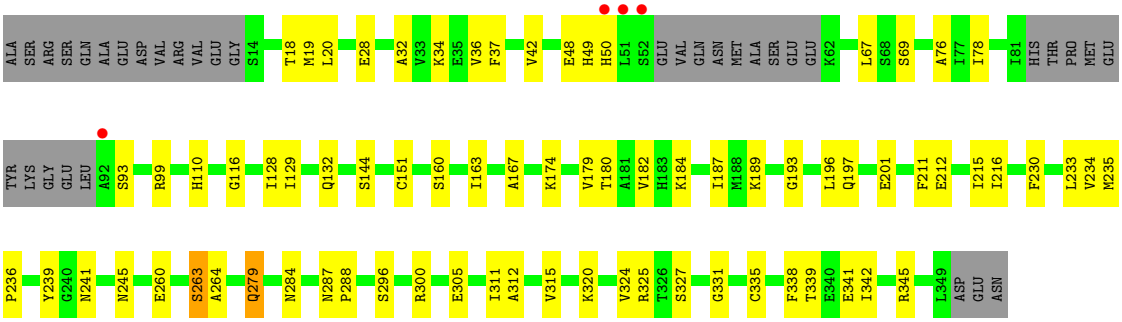
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain J:



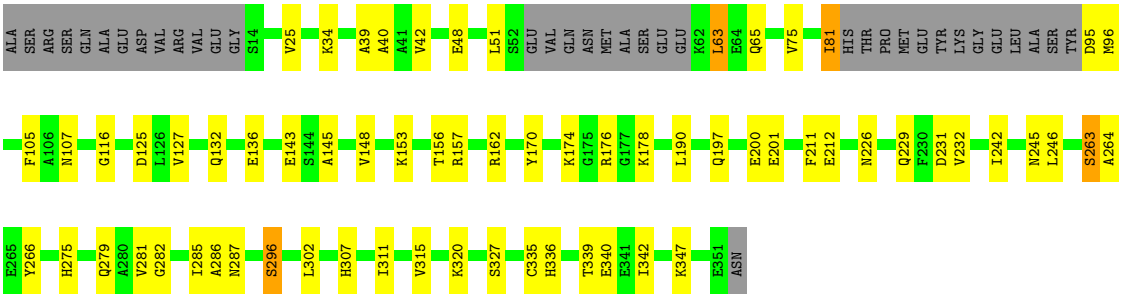
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain L:



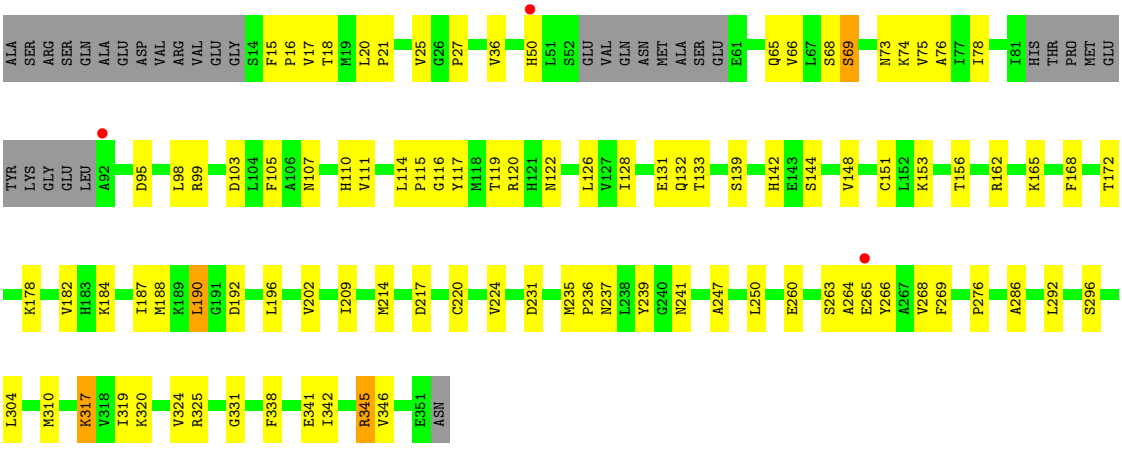
• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain N:



• Molecule 2: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.15Å 170.03Å 208.69Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	49.14 – 2.85 49.14 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.14-2.85) 99.7 (49.14-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.199 , 0.249 0.199 , 0.249	Depositor DCC
R_{free} test set	8371 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	39053	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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 (i)

5.1 Standard geometry (i)

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	0.45	0/2545	0.62	1/3448 (0.0%)
1	B	0.48	0/2514	0.63	1/3408 (0.0%)
1	E	0.46	0/2552	0.61	0/3459
1	G	0.45	0/2526	0.61	0/3426
1	I	0.49	0/2508	0.65	0/3400
1	K	0.48	0/2512	0.65	0/3406
1	M	0.52	0/2532	0.68	0/3432
1	O	0.54	0/2534	0.74	1/3437 (0.0%)
2	C	0.48	0/2454	0.64	0/3315
2	D	0.47	0/2430	0.64	0/3286
2	F	0.46	0/2424	0.67	1/3275 (0.0%)
2	H	0.44	0/2435	0.61	0/3292
2	J	0.47	0/2447	0.67	0/3304
2	L	0.47	0/2424	0.65	0/3275
2	N	0.48	0/2431	0.67	2/3286 (0.1%)
2	P	0.47	0/2442	0.63	1/3303 (0.0%)
All	All	0.48	0/39710	0.65	7/53752 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	323	LYS	CD-CE-NZ	-8.80	91.46	111.70
1	A	161	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	O	26	ILE	CG1-CB-CG2	-7.68	94.51	111.40
1	B	73	LYS	CA-CB-CG	6.63	127.99	113.40
2	N	63	LEU	CB-CG-CD1	6.33	121.76	111.00

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	2502	0	2479	53	0
1	B	2474	0	2429	58	0
1	E	2509	0	2481	52	0
1	G	2483	0	2447	56	0
1	I	2468	0	2419	64	0
1	K	2472	0	2426	48	0
1	M	2490	0	2461	83	0
1	O	2491	0	2450	92	0
2	C	2413	0	2389	48	1
2	D	2391	0	2337	45	0
2	F	2383	0	2361	49	1
2	H	2395	0	2345	54	0
2	J	2406	0	2397	61	0
2	L	2384	0	2352	56	0
2	N	2391	0	2364	49	0
2	P	2401	0	2336	69	0
All	All	39053	0	38473	850	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 11.

The worst 5 of 850 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:N:51:LEU:HD13	2:N:63:LEU:HD22	1.40	1.03
1:B:39:ARG:NE	1:B:60:SER:HB2	1.79	0.98
1:O:268:ASP:O	1:O:272:LYS:NZ	2.02	0.91
1:M:108:THR:HG21	1:M:239:LEU:O	1.69	0.91
1:K:224:MET:CE	1:K:229:GLY:HA2	2.02	0.89

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)
2:C:350:ASP:OD1	2:F:344:ARG:NH1[3_545]	2.03	0.17

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	333/339 (98%)	319 (96%)	14 (4%)	0	100	100
1	B	329/339 (97%)	308 (94%)	21 (6%)	0	100	100
1	E	335/339 (99%)	322 (96%)	13 (4%)	0	100	100
1	G	333/339 (98%)	310 (93%)	23 (7%)	0	100	100
1	I	329/339 (97%)	312 (95%)	17 (5%)	0	100	100
1	K	329/339 (97%)	310 (94%)	19 (6%)	0	100	100
1	M	333/339 (98%)	306 (92%)	26 (8%)	1 (0%)	41	61
1	O	333/339 (98%)	300 (90%)	33 (10%)	0	100	100
2	C	313/352 (89%)	294 (94%)	19 (6%)	0	100	100
2	D	313/352 (89%)	295 (94%)	18 (6%)	0	100	100
2	F	309/352 (88%)	289 (94%)	20 (6%)	0	100	100
2	H	313/352 (89%)	296 (95%)	17 (5%)	0	100	100
2	J	311/352 (88%)	286 (92%)	25 (8%)	0	100	100
2	L	311/352 (88%)	296 (95%)	15 (5%)	0	100	100
2	N	310/352 (88%)	293 (94%)	17 (6%)	0	100	100
2	P	314/352 (89%)	295 (94%)	19 (6%)	0	100	100
All	All	5148/5528 (93%)	4831 (94%)	316 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	109	PRO

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	266/276 (96%)	263 (99%)	3 (1%)	73	86
1	B	261/276 (95%)	257 (98%)	4 (2%)	65	82
1	E	266/276 (96%)	262 (98%)	4 (2%)	65	82
1	G	261/276 (95%)	256 (98%)	5 (2%)	57	77
1	I	259/276 (94%)	257 (99%)	2 (1%)	81	90
1	K	260/276 (94%)	259 (100%)	1 (0%)	91	95
1	M	263/276 (95%)	255 (97%)	8 (3%)	41	65
1	O	263/276 (95%)	253 (96%)	10 (4%)	33	59
2	C	252/296 (85%)	249 (99%)	3 (1%)	71	85
2	D	248/296 (84%)	242 (98%)	6 (2%)	49	72
2	F	249/296 (84%)	243 (98%)	6 (2%)	49	72
2	H	249/296 (84%)	245 (98%)	4 (2%)	62	81
2	J	253/296 (86%)	249 (98%)	4 (2%)	62	81
2	L	248/296 (84%)	243 (98%)	5 (2%)	55	76
2	N	252/296 (85%)	247 (98%)	5 (2%)	55	76
2	P	248/296 (84%)	242 (98%)	6 (2%)	49	72
All	All	4098/4576 (90%)	4022 (98%)	76 (2%)	57	77

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	263	SER
2	P	117	TYR
2	N	327	SER
1	O	178	ARG
2	P	345	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	35	GLN
2	P	107	ASN
2	P	132	GLN
2	P	50	HIS
1	K	40	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	335/339 (98%)	-0.31	2 (0%)	89	88	31, 46, 77, 91	0
1	B	333/339 (98%)	-0.31	2 (0%)	89	88	34, 50, 73, 112	0
1	E	337/339 (99%)	-0.34	3 (0%)	84	83	34, 45, 67, 95	0
1	G	335/339 (98%)	-0.20	3 (0%)	84	83	39, 55, 80, 94	0
1	I	333/339 (98%)	-0.35	3 (0%)	84	83	33, 46, 71, 96	0
1	K	333/339 (98%)	-0.27	4 (1%)	79	76	28, 45, 71, 87	0
1	M	335/339 (98%)	-0.24	4 (1%)	79	76	32, 51, 83, 97	0
1	O	335/339 (98%)	-0.08	4 (1%)	79	76	32, 59, 89, 101	0
2	C	319/352 (90%)	-0.39	4 (1%)	77	74	32, 47, 82, 98	0
2	D	319/352 (90%)	-0.36	1 (0%)	94	93	34, 49, 78, 96	0
2	F	315/352 (89%)	-0.34	6 (1%)	66	62	38, 51, 86, 102	0
2	H	319/352 (90%)	-0.33	4 (1%)	77	74	40, 52, 83, 99	0
2	J	317/352 (90%)	-0.38	4 (1%)	77	74	34, 47, 79, 98	0
2	L	317/352 (90%)	-0.32	4 (1%)	77	74	32, 48, 84, 121	0
2	N	316/352 (89%)	-0.41	0	100	100	34, 48, 76, 104	0
2	P	320/352 (90%)	-0.36	3 (0%)	84	83	36, 50, 80, 104	0
All	All	5218/5528 (94%)	-0.31	51 (0%)	82	79	28, 50, 80, 121	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	292	GLY	5.1
2	P	92	ALA	4.7
1	E	2	GLY	4.5
2	F	280	ALA	4.5
1	B	3	GLY	4.1

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.