Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 09:38 pm GMT

PDB ID	:	5M2E
Title	:	Apo structure of Pseudomonas aeruginosa Isocitrate Dehydrogenase, ICD.
Authors	:	Crousilles, A.; Welch, M.
Deposited on	:	2016-10-12
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 (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 (i)) were used in the production of this report:

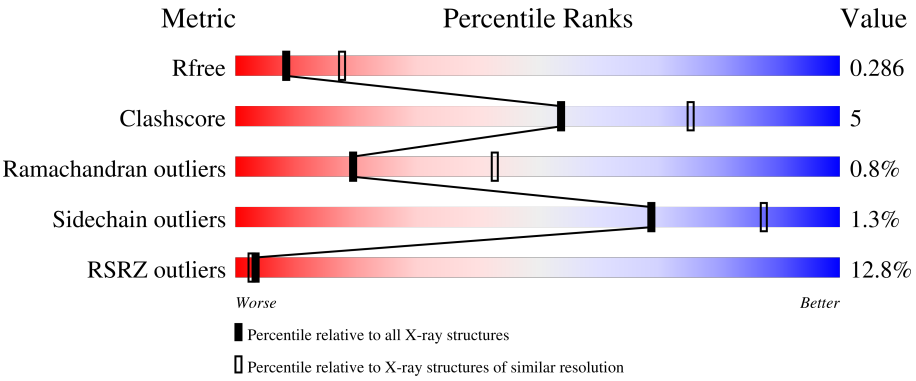
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	418	4% 91% 9%
1	B	418	11% 90% 9%
1	C	418	22% 81% 17%
1	D	418	14% 86% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25716 atoms, of which 12884 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 [NADP].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	0	0
			6420	2035	3221	535	610	19			
1	B	418	Total	C	H	N	O	S	0	0	0
			6420	2035	3221	535	610	19			
1	C	418	Total	C	H	N	O	S	0	0	0
			6420	2035	3221	535	610	19			
1	D	418	Total	C	H	N	O	S	0	0	0
			6420	2035	3221	535	610	19			

- Molecule 2 is water.

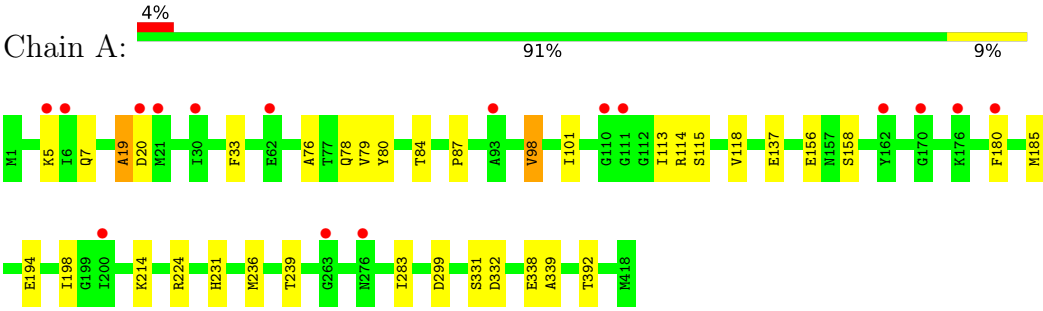
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	2	Total	O	0	0
			2	2		
2	C	13	Total	O	0	0
			13	13		
2	D	8	Total	O	0	0
			8	8		

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.

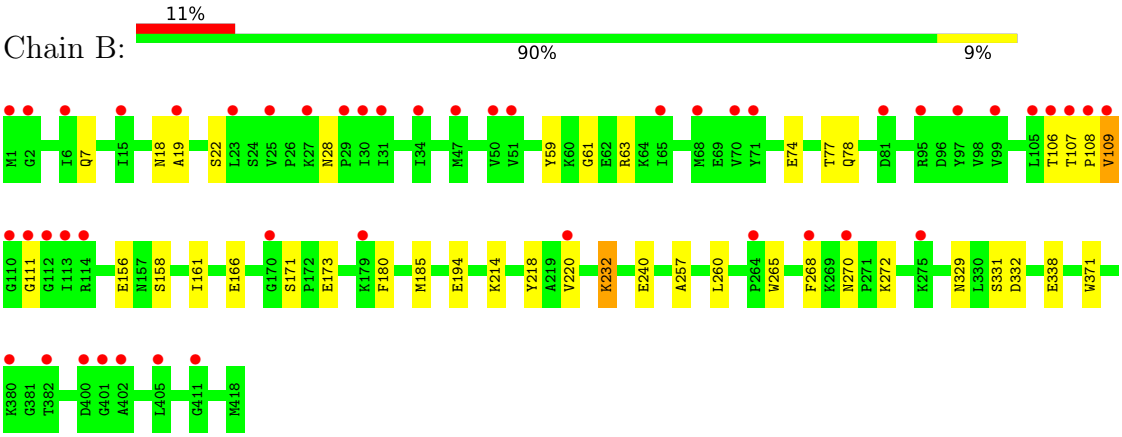
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain A:



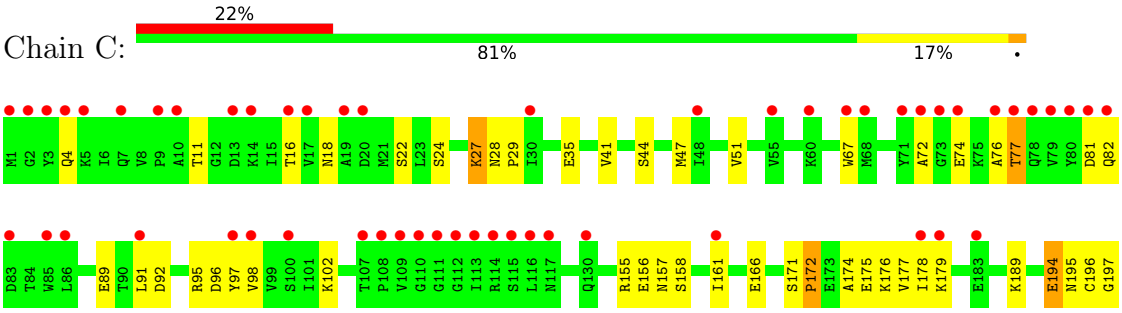
• Molecule 1: Isocitrate dehydrogenase [NADP]

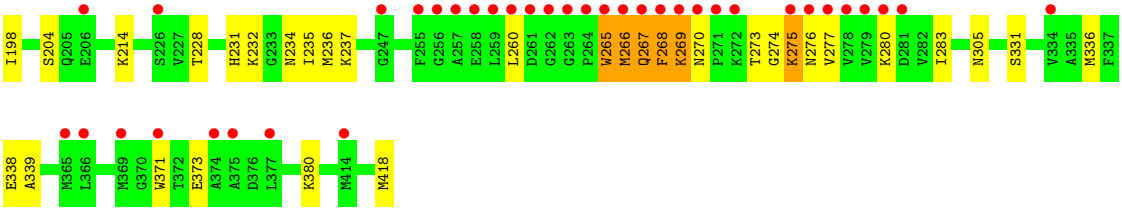
Chain B:



• Molecule 1: Isocitrate dehydrogenase [NADP]

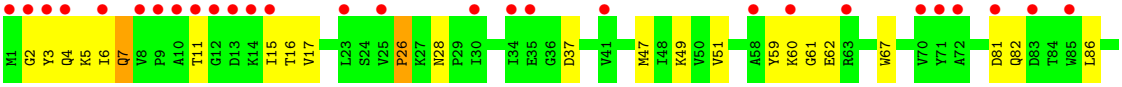
Chain C:

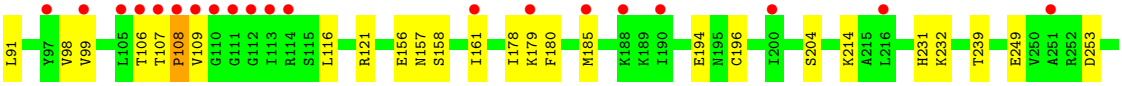


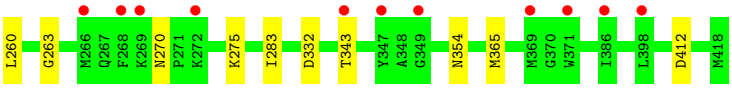


• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.88Å 95.55Å 104.02Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	47.78 – 2.70 47.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.78-2.70) 98.5 (47.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.10-2155	Depositor
R, R_{free}	0.245 , 0.284 0.247 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.7	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	0.92	EDS
Total number of atoms	25716	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

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	0.26	0/3260	0.45	0/4415
1	B	0.25	0/3260	0.44	0/4415
1	C	0.26	0/3260	0.47	0/4415
1	D	0.25	0/3260	0.44	0/4415
All	All	0.26	0/13040	0.45	0/17660

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	3199	3221	3221	26	0
1	B	3199	3221	3221	23	0
1	C	3199	3221	3221	59	0
1	D	3199	3221	3221	35	0
2	A	13	0	0	2	0
2	B	2	0	0	2	0
2	C	13	0	0	2	0
2	D	8	0	0	1	0
All	All	12832	12884	12884	137	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 5.

All (137) 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:5:LYS:NZ	1:A:79:VAL:O	1.92	1.02
1:A:114:ARG:O	1:A:114:ARG:NH1	2.04	0.91
1:D:7:GLN:N	1:D:7:GLN:OE1	2.10	0.85
1:C:274:GLY:O	1:C:276:ASN:N	2.11	0.83
1:D:11:THR:O	1:D:28:ASN:ND2	2.13	0.81
1:A:98:VAL:O	2:A:501:HOH:O	1.97	0.81
1:C:156:GLU:OE2	1:C:158:SER:OG	2.01	0.79
1:B:214:LYS:O	2:B:501:HOH:O	2.00	0.78
1:A:137:GLU:OE1	1:A:137:GLU:N	2.17	0.78
1:B:329:ASN:ND2	1:B:338:GLU:OE2	2.17	0.77
1:B:171:SER:OG	1:B:173:GLU:OE1	2.04	0.75
1:C:16:THR:OG1	1:C:24:SER:OG	2.04	0.75
1:D:354:ASN:O	2:D:501:HOH:O	2.06	0.74
1:C:267:GLN:NE2	1:C:276:ASN:OD1	2.21	0.73
1:B:218:TYR:N	2:B:501:HOH:O	2.22	0.73
1:B:74:GLU:O	1:B:77:THR:OG1	2.08	0.71
1:B:156:GLU:OE2	1:B:158:SER:OG	2.07	0.71
1:A:78:GLN:N	1:A:78:GLN:OE1	2.26	0.69
1:C:11:THR:O	1:C:28:ASN:ND2	2.27	0.67
1:B:18:ASN:OD1	1:B:22:SER:OG	2.13	0.66
1:B:194:GLU:OE1	1:B:194:GLU:N	2.30	0.65
1:A:76:ALA:O	1:A:80:TYR:N	2.27	0.64
1:D:260:LEU:O	1:D:263:GLY:N	2.30	0.60
1:D:16:THR:OG1	1:D:17:VAL:N	2.27	0.59
1:A:214:LYS:NZ	1:A:331:SER:O	2.35	0.59
1:C:172:PRO:HA	1:C:175:GLU:HB2	1.85	0.59
1:C:228:THR:OG1	2:C:501:HOH:O	2.17	0.58
1:D:249:GLU:O	1:D:253:ASP:N	2.37	0.57
1:B:220:VAL:O	1:B:270:ASN:ND2	2.37	0.57
1:A:156:GLU:OE2	1:A:158:SER:OG	2.20	0.57
1:A:80:TYR:CE2	1:A:87:PRO:HB3	2.40	0.56
1:C:102:LYS:HG3	1:C:338:GLU:HG3	1.87	0.56
1:C:234:ASN:O	1:C:237:LYS:NZ	2.39	0.55
1:C:338:GLU:HG2	1:C:339:ALA:N	2.22	0.55
1:C:81:ASP:OD1	1:C:82:GLN:N	2.39	0.54
1:D:270:ASN:ND2	1:D:275:LYS:O	2.38	0.54
1:C:194:GLU:OE1	1:C:195:ASN:N	2.40	0.54
1:D:194:GLU:N	1:D:194:GLU:OE1	2.41	0.54
1:C:27:LYS:HD2	1:C:27:LYS:N	2.23	0.54
1:D:121:ARG:NH1	1:D:157:ASN:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LYS:NZ	1:C:418:MET:O	2.42	0.53
1:C:172:PRO:O	1:C:176:LYS:N	2.41	0.52
1:D:15:ILE:HG21	1:D:26:PRO:HD3	1.91	0.52
1:A:392:THR:OG1	2:A:502:HOH:O	2.19	0.52
1:C:166:GLU:OE2	1:D:239:THR:N	2.44	0.51
1:C:175:GLU:HA	1:C:178:ILE:HG12	1.92	0.50
1:C:77:THR:O	1:C:77:THR:HG23	2.12	0.49
1:C:265:TRP:HB3	1:C:280:LYS:HG3	1.94	0.49
1:D:81:ASP:OD1	1:D:82:GLN:N	2.43	0.49
1:A:239:THR:N	1:B:166:GLU:OE2	2.45	0.49
1:D:156:GLU:OE2	1:D:158:SER:OG	2.20	0.49
1:D:6:ILE:HD12	1:D:6:ILE:N	2.27	0.49
1:C:92:ASP:OD1	1:C:95:ARG:NH2	2.46	0.49
1:C:267:GLN:HB2	1:C:277:VAL:O	2.13	0.49
1:C:47:MET:O	1:C:51:VAL:HG12	2.13	0.48
1:A:236:MET:SD	1:B:161:ILE:HG21	2.54	0.48
1:D:4:GLN:O	1:D:5:LYS:HB2	2.14	0.48
1:C:373:GLU:N	1:C:373:GLU:OE1	2.47	0.48
1:B:260:LEU:HD21	1:B:265:TRP:HB2	1.96	0.48
1:C:189:LYS:NZ	2:C:504:HOH:O	2.39	0.48
1:A:7:GLN:N	1:A:7:GLN:OE1	2.47	0.47
1:C:72:ALA:HA	1:C:76:ALA:HB2	1.96	0.47
1:D:2:GLY:O	1:D:4:GLN:N	2.47	0.47
1:D:180:PHE:CZ	1:D:185:MET:HE3	2.51	0.46
1:C:174:ALA:O	1:C:177:VAL:HG22	2.16	0.46
1:D:49:LYS:NZ	1:D:412:ASP:OD1	2.45	0.46
1:B:270:ASN:OD1	1:B:272:LYS:N	2.42	0.46
1:A:331:SER:OG	1:A:332:ASP:N	2.49	0.46
1:A:338:GLU:HG2	1:A:339:ALA:N	2.31	0.46
1:C:91:LEU:O	1:C:95:ARG:N	2.42	0.46
1:A:115:SER:O	1:A:118:VAL:HG12	2.16	0.45
1:C:267:GLN:OE1	1:C:269:LYS:NZ	2.31	0.45
1:C:51:VAL:HG11	1:C:67:TRP:CZ2	2.51	0.45
1:C:196:CYS:HA	1:D:204:SER:HA	1.97	0.45
1:C:214:LYS:NZ	1:C:331:SER:O	2.40	0.45
1:C:269:LYS:HE3	1:C:276:ASN:HA	1.99	0.45
1:C:268:PHE:C	1:C:268:PHE:CD1	2.90	0.45
1:C:157:ASN:HA	1:C:305:ASN:ND2	2.32	0.44
1:B:59:TYR:O	1:B:61:GLY:N	2.50	0.44
1:C:338:GLU:HG2	1:C:339:ALA:O	2.17	0.44
1:D:86:LEU:HG	1:D:91:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:HIS:O	1:C:283:ILE:HA	2.18	0.44
1:C:35:GLU:HG3	1:C:44:SER:HB2	1.98	0.44
1:C:268:PHE:C	1:C:268:PHE:HD1	2.21	0.44
1:C:74:GLU:HA	1:C:77:THR:HG22	2.00	0.43
1:D:59:TYR:O	1:D:62:GLU:N	2.46	0.43
1:C:102:LYS:HD3	1:C:336:MET:SD	2.59	0.43
1:D:47:MET:O	1:D:51:VAL:HG12	2.18	0.43
1:B:7:GLN:OE1	1:B:7:GLN:N	2.51	0.43
1:B:78:GLN:OE1	1:B:78:GLN:N	2.52	0.43
1:C:35:GLU:OE2	1:C:41:VAL:HA	2.19	0.43
1:A:80:TYR:HB3	1:A:84:THR:OG1	2.18	0.43
1:D:59:TYR:O	1:D:61:GLY:N	2.52	0.43
1:A:5:LYS:HD2	1:A:80:TYR:CE2	2.53	0.43
1:A:180:PHE:CZ	1:A:185:MET:HE3	2.54	0.42
1:C:18:ASN:O	1:C:22:SER:N	2.51	0.42
1:A:224:ARG:NH2	1:A:299:ASP:OD1	2.52	0.42
1:D:37:ASP:OD2	1:D:106:THR:OG1	2.34	0.42
1:C:171:SER:O	1:C:174:ALA:N	2.52	0.42
1:A:338:GLU:HG2	1:A:339:ALA:O	2.19	0.42
1:D:108:PRO:CG	1:D:116:LEU:HD12	2.49	0.42
1:C:232:LYS:HE3	1:C:235:ILE:HD12	2.02	0.42
1:D:98:VAL:HG23	1:D:99:VAL:HG23	2.02	0.41
1:C:178:ILE:HG13	1:C:179:LYS:N	2.34	0.41
1:D:107:THR:O	1:D:107:THR:HG23	2.19	0.41
1:D:106:THR:HG23	1:D:343:THR:HG21	2.02	0.41
1:C:4:GLN:HB2	1:C:89:GLU:OE1	2.20	0.41
1:C:371:TRP:HA	1:C:371:TRP:CE3	2.55	0.41
1:B:63:ARG:HD3	1:B:371:TRP:CE2	2.56	0.41
1:B:108:PRO:O	1:B:109:VAL:C	2.59	0.41
1:C:266:MET:HE2	1:C:266:MET:HB2	1.87	0.41
1:C:155:ARG:O	1:C:155:ARG:HG3	2.21	0.41
1:D:51:VAL:HG11	1:D:67:TRP:CZ2	2.56	0.41
1:D:178:ILE:HG13	1:D:179:LYS:N	2.34	0.41
1:C:4:GLN:CB	1:C:89:GLU:OE1	2.69	0.41
1:C:96:ASP:OD1	1:C:97:TYR:N	2.54	0.41
1:C:102:LYS:NZ	1:C:338:GLU:OE1	2.54	0.41
1:A:113:ILE:CG2	1:A:115:SER:O	2.69	0.40
1:B:106:THR:HG22	1:B:108:PRO:HD2	2.03	0.40
1:B:180:PHE:CZ	1:B:185:MET:HE3	2.56	0.40
1:C:204:SER:HA	1:D:196:CYS:HA	2.03	0.40
1:C:260:LEU:HB2	1:C:267:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:SER:OG	1:B:332:ASP:N	2.53	0.40
1:D:214:LYS:HE2	1:D:332:ASP:HA	2.03	0.40
1:A:33:PHE:HA	1:A:101:ILE:O	2.21	0.40
1:A:231:HIS:O	1:A:283:ILE:HA	2.21	0.40
1:B:232:LYS:N	1:B:240:GLU:OE1	2.46	0.40
1:B:257:ALA:HA	1:B:268:PHE:HB3	2.04	0.40
1:C:28:ASN:N	1:C:29:PRO:HD3	2.37	0.40
1:C:161:ILE:CD1	1:D:161:ILE:HD11	2.51	0.40
1:C:197:GLY:C	1:C:198:ILE:HD12	2.42	0.40
1:C:274:GLY:O	1:C:277:VAL:HG23	2.21	0.40
1:D:231:HIS:O	1:D:283:ILE:HA	2.21	0.40
1:A:19:ALA:O	1:A:20:ASP:HB2	2.21	0.40
1:A:188:LYS:O	1:A:189:LYS:HB2	2.21	0.40
1:C:270:ASN:HB3	1:C:274:GLY:N	2.37	0.40
1:D:99:VAL:CG1	1:D:365:MET:HG3	2.51	0.40

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	416/418 (100%)	392 (94%)	22 (5%)	2 (0%)	29	54
1	B	416/418 (100%)	387 (93%)	25 (6%)	4 (1%)	15	37
1	C	416/418 (100%)	386 (93%)	27 (6%)	3 (1%)	22	46
1	D	416/418 (100%)	385 (92%)	26 (6%)	5 (1%)	13	32
All	All	1664/1672 (100%)	1550 (93%)	100 (6%)	14 (1%)	19	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	273	THR
1	C	275	LYS
1	D	60	LYS
1	B	19	ALA
1	D	7	GLN
1	A	19	ALA
1	D	108	PRO
1	D	3	TYR
1	D	26	PRO
1	B	107	THR
1	B	109	VAL
1	B	111	GLY
1	C	98	VAL
1	A	98	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	339/339 (100%)	337 (99%)	2 (1%)	86 95
1	B	339/339 (100%)	337 (99%)	2 (1%)	86 95
1	C	339/339 (100%)	328 (97%)	11 (3%)	39 68
1	D	339/339 (100%)	337 (99%)	2 (1%)	86 95
All	All	1356/1356 (100%)	1339 (99%)	17 (1%)	69 87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	198	ILE
1	B	28	ASN
1	B	232	LYS
1	C	27	LYS
1	C	77	THR
1	C	172	PRO
1	C	194	GLU

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Mol	Chain	Res	Type
1	C	236	MET
1	C	265	TRP
1	C	266	MET
1	C	267	GLN
1	C	268	PHE
1	C	269	LYS
1	C	275	LYS
1	D	109	VAL
1	D	232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	418/418 (100%)	0.22	17 (4%) 37 36	39, 68, 137, 219	0
1	B	418/418 (100%)	0.83	47 (11%) 5 4	47, 93, 216, 513	0
1	C	418/418 (100%)	1.38	91 (21%) 0 0	49, 95, 534, 896	0
1	D	418/418 (100%)	0.85	59 (14%) 2 1	35, 100, 262, 697	0
All	All	1672/1672 (100%)	0.82	214 (12%) 3 3	35, 88, 237, 896	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	GLY	21.2
1	C	110	GLY	17.4
1	C	1	MET	17.4
1	D	111	GLY	16.9
1	D	114	ARG	14.6
1	B	111	GLY	13.8
1	B	107	THR	13.5
1	B	1	MET	13.4
1	C	111	GLY	12.6
1	B	108	PRO	11.8
1	C	266	MET	10.7
1	C	267	GLN	10.5
1	C	278	VAL	10.2
1	C	271	PRO	10.1
1	C	277	VAL	10.1
1	B	106	THR	10.0
1	C	265	TRP	10.0
1	C	263	GLY	9.4
1	C	76	ALA	8.5
1	C	261	ASP	8.5
1	D	2	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
1	C	279	VAL	8.2
1	C	113	ILE	8.1
1	B	112	GLY	7.9
1	C	4	GLN	7.8
1	C	268	PHE	7.7
1	C	280	LYS	7.6
1	C	112	GLY	7.5
1	D	110	GLY	7.2
1	D	3	TYR	7.2
1	D	108	PRO	7.0
1	B	109	VAL	6.9
1	C	109	VAL	6.9
1	C	264	PRO	6.8
1	C	80	TYR	6.7
1	D	23	LEU	6.7
1	C	258	GLU	6.7
1	A	110	GLY	6.6
1	D	4	GLN	6.6
1	B	2	GLY	6.5
1	B	114	ARG	6.4
1	C	77	THR	6.4
1	C	13	ASP	6.2
1	D	109	VAL	6.2
1	B	401	GLY	5.7
1	C	276	ASN	5.6
1	C	256	GLY	5.6
1	C	270	ASN	5.5
1	C	374	ALA	5.3
1	C	259	LEU	5.3
1	C	262	GLY	5.2
1	C	78	GLN	5.2
1	D	10	ALA	5.2
1	C	260	LEU	5.1
1	C	2	GLY	5.0
1	C	114	ARG	4.9
1	D	268	PHE	4.9
1	C	79	VAL	4.8
1	D	113	ILE	4.6
1	C	281	ASP	4.6
1	D	1	MET	4.6
1	A	111	GLY	4.5
1	C	30	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	110	GLY	4.4
1	C	107	THR	4.4
1	D	97	TYR	4.3
1	A	6	ILE	4.2
1	B	51	VAL	4.2
1	C	371	TRP	4.2
1	C	115	SER	4.2
1	D	9	PRO	4.1
1	D	71	TYR	4.1
1	C	183	GLU	4.1
1	B	31	ILE	4.0
1	C	179	LYS	4.0
1	D	81	ASP	4.0
1	D	72	ALA	3.9
1	C	20	ASP	3.9
1	C	98	VAL	3.8
1	D	8	VAL	3.8
1	C	269	LYS	3.8
1	C	366	LEU	3.7
1	D	70	VAL	3.7
1	B	95	ARG	3.7
1	D	35	GLU	3.7
1	D	63	ARG	3.7
1	D	349	GLY	3.6
1	D	12	GLY	3.6
1	C	67	TRP	3.5
1	B	411	GLY	3.5
1	C	72	ALA	3.5
1	C	81	ASP	3.5
1	C	257	ALA	3.4
1	B	400	ASP	3.4
1	B	380	LYS	3.4
1	D	13	ASP	3.4
1	B	34	ILE	3.4
1	B	70	VAL	3.4
1	D	14	LYS	3.4
1	B	268	PHE	3.4
1	A	93	ALA	3.4
1	A	200	ILE	3.3
1	A	176	LYS	3.3
1	B	19	ALA	3.2
1	B	65	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	15	ILE	3.2
1	D	369	MET	3.2
1	C	117	ASN	3.2
1	C	83	ASP	3.1
1	C	73	GLY	3.1
1	B	113	ILE	3.1
1	C	255	PHE	3.1
1	B	105	LEU	3.1
1	B	6	ILE	3.1
1	B	47	MET	3.1
1	C	91	LEU	3.0
1	D	34	ILE	3.0
1	C	55	VAL	3.0
1	C	85	TRP	3.0
1	C	334	VAL	3.0
1	C	108	PRO	3.0
1	D	371	TRP	3.0
1	C	60	LYS	3.0
1	D	6	ILE	2.9
1	D	11	THR	2.9
1	D	107	THR	2.9
1	C	272	LYS	2.9
1	C	375	ALA	2.9
1	D	200	ILE	2.8
1	C	178	ILE	2.8
1	D	105	LEU	2.8
1	C	14	LYS	2.7
1	C	116	LEU	2.7
1	B	264	PRO	2.7
1	B	97	TYR	2.7
1	C	7	GLN	2.7
1	C	3	TYR	2.7
1	C	226	SER	2.7
1	D	58	ALA	2.6
1	D	343	THR	2.6
1	D	216	LEU	2.6
1	B	68	MET	2.6
1	C	68	MET	2.6
1	B	179	LYS	2.6
1	D	99	VAL	2.6
1	D	41	VAL	2.6
1	B	405	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	190	ILE	2.5
1	C	71	TYR	2.5
1	B	29	PRO	2.5
1	D	30	ILE	2.5
1	D	60	LYS	2.5
1	C	100	SER	2.5
1	C	414	MET	2.5
1	C	74	GLU	2.5
1	A	30	ILE	2.4
1	A	180	PHE	2.4
1	C	97	TYR	2.4
1	B	170	GLY	2.4
1	D	185	MET	2.4
1	C	9	PRO	2.4
1	C	86	LEU	2.4
1	D	386	ILE	2.4
1	C	365	MET	2.4
1	A	276	ASN	2.4
1	C	5	LYS	2.3
1	C	161	ILE	2.3
1	B	270	ASN	2.3
1	A	170	GLY	2.3
1	D	398	LEU	2.3
1	B	275	LYS	2.3
1	B	81	ASP	2.3
1	C	206	GLU	2.2
1	B	15	ILE	2.2
1	C	275	LYS	2.2
1	D	188	LYS	2.2
1	D	269	LYS	2.2
1	C	130	GLN	2.2
1	D	25	VAL	2.2
1	A	62	GLU	2.2
1	B	30	ILE	2.2
1	C	82	GLN	2.2
1	D	83	ASP	2.2
1	D	179	LYS	2.2
1	B	71	TYR	2.2
1	B	382	THR	2.2
1	C	48	ILE	2.1
1	D	161	ILE	2.1
1	C	377	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	10	ALA	2.1
1	B	23	LEU	2.1
1	B	27	LYS	2.1
1	C	369	MET	2.1
1	A	187	VAL	2.1
1	A	5	LYS	2.1
1	B	50	VAL	2.1
1	B	99	VAL	2.1
1	B	220	VAL	2.1
1	C	247	GLY	2.1
1	D	272	LYS	2.1
1	D	85	TRP	2.1
1	A	20	ASP	2.1
1	D	347	TYR	2.1
1	D	251	ALA	2.1
1	C	19	ALA	2.1
1	B	25	VAL	2.1
1	C	17	VAL	2.1
1	D	106	THR	2.1
1	A	162	TYR	2.0
1	A	21	MET	2.0
1	A	263	GLY	2.0
1	C	16	THR	2.0
1	B	402	ALA	2.0
1	D	266	MET	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 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.