Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:32 AM GMT

PDB ID	:	2DHT
Title	:	Crystal structure of isocitrate dehydrogenase from Sulfolobus tokodaii strain7
Authors	:	Kondo, H.; Murakami, M.; Ihara, K.; Suzuki, S.; Kouyama, T.
Deposited on	:	2006-03-25
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

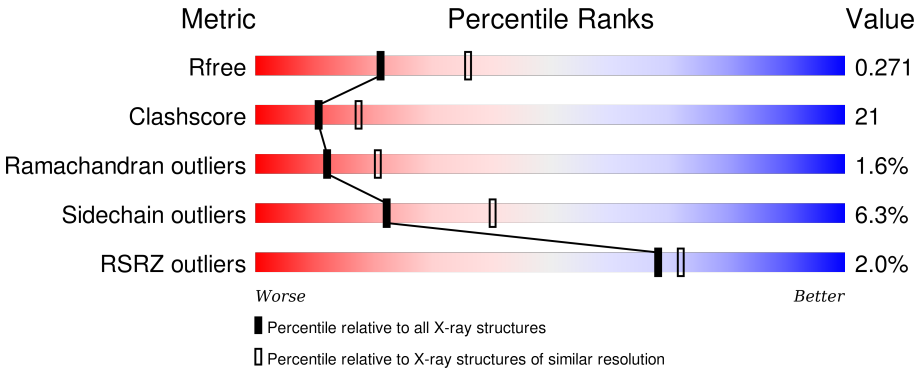
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

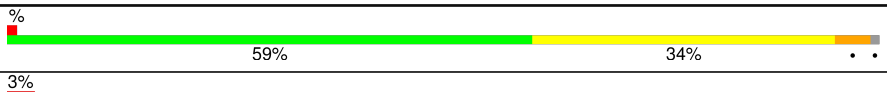
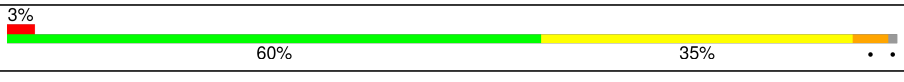
The reported resolution of this entry is 2.50 Å.

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	409	
1	B	409	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6484 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 409aa long hypothetical NADP-dependent isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3223	2063	545	600	15			
1	B	403	Total	C	N	O	S	0	0	0
			3223	2063	545	600	15			

- Molecule 2 is water.

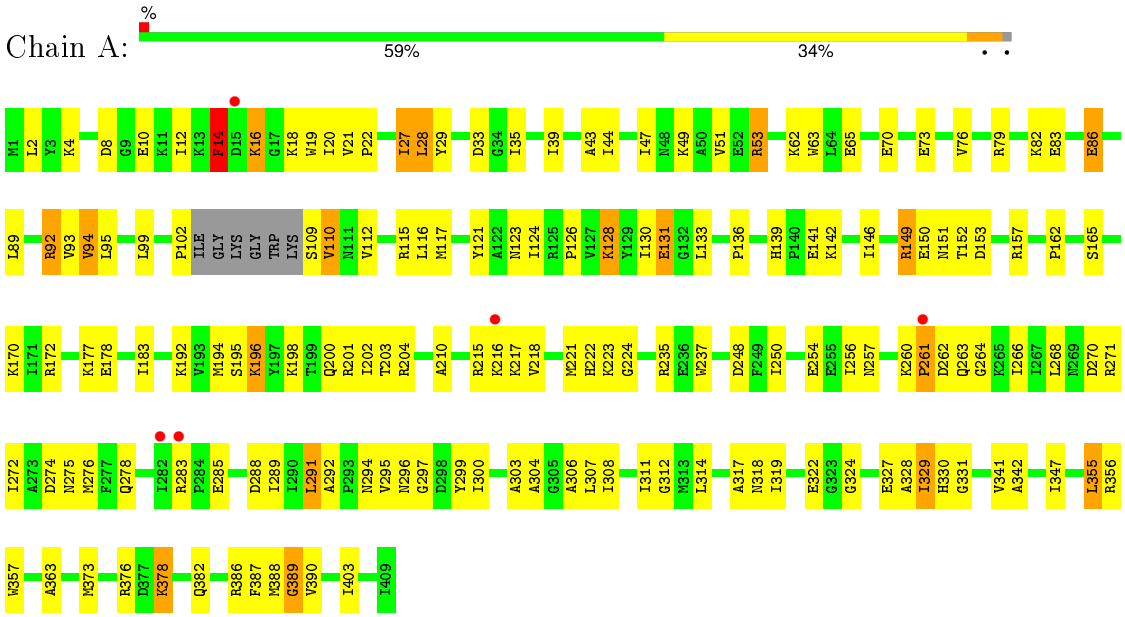
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	20	Total	O	0	0
			20	20		

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 errors 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.

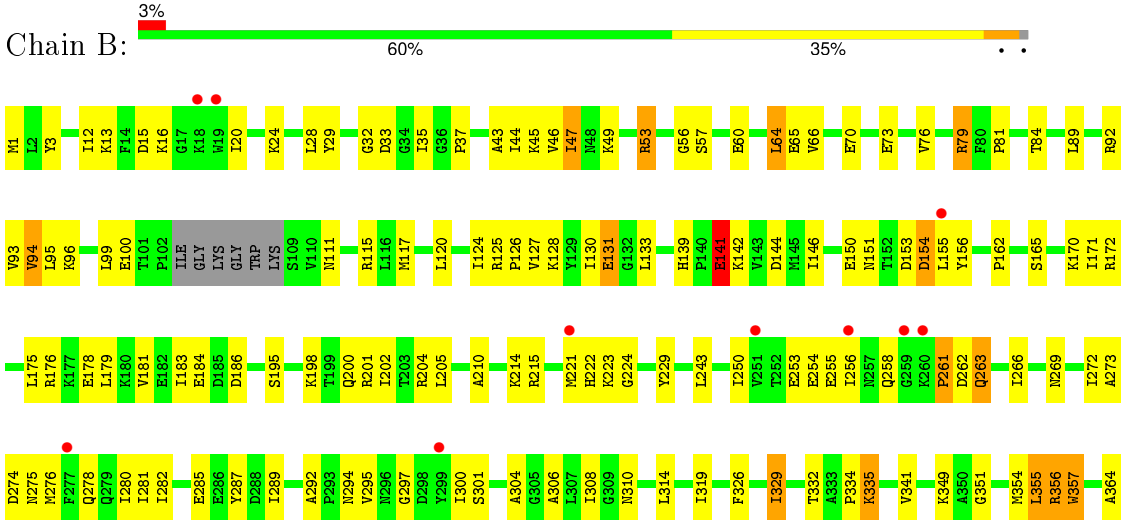
- Molecule 1: 409aa long hypothetical NADP-dependent isocitrate dehydrogenase

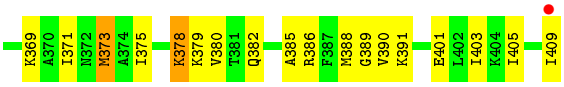
Chain A:



- Molecule 1: 409aa long hypothetical NADP-dependent isocitrate dehydrogenase

Chain B:




K369
A370
T371
N372
M373
A374
T375
K378
K379
V380
T381
Q382
A385
R386
F387
M388
G389
V390
K391
E401
L402
I403
K404
T405
I409

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.98Å 88.09Å 76.22Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 53.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-2.50) 98.5 (53.69-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.272 0.240 , 0.271	Depositor DCC
R_{free} test set	1474 reflections (4.43%)	DCC
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
Estimated twinning fraction	0.010 for l,k,-h 0.086 for h,-k,-l 0.022 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 33455 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6484	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.42	0/3279	0.68	2/4410 (0.0%)
1	B	0.39	0/3279	0.65	1/4410 (0.0%)
All	All	0.40	0/6558	0.66	3/8820 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	389	GLY	N-CA-C	6.73	129.93	113.10
1	A	92	ARG	N-CA-C	5.53	125.93	111.00
1	B	95	LEU	N-CA-C	-5.26	96.81	111.00

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	3223	0	3299	149	0
1	B	3223	0	3299	136	0
2	A	18	0	0	3	0
2	B	20	0	0	1	0
All	All	6484	0	6598	277	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 21.

All (277) 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:B:47:ILE:HD13	1:B:355:LEU:HD21	1.45	0.97
1:B:49:LYS:HG3	1:B:403:ILE:HG23	1.46	0.97
1:A:49:LYS:HG3	1:A:403:ILE:HG23	1.63	0.79
1:A:295:VAL:HG12	2:A:506:HOH:O	1.83	0.79
1:B:198:LYS:HA	1:B:201:ARG:HD2	1.65	0.79
1:A:223:LYS:HE3	1:A:274:ASP:HB3	1.65	0.78
1:A:8:ASP:HB3	1:A:62:LYS:NZ	1.99	0.77
1:A:297:GLY:HA2	1:A:300:ILE:HG22	1.65	0.77
1:A:222:HIS:HD2	1:A:224:GLY:H	1.30	0.77
1:B:162:PRO:HG2	1:B:165:SER:HB3	1.65	0.76
1:B:378:LYS:HG3	1:B:388:MET:HE3	1.66	0.76
1:A:14:PHE:HB3	1:A:19:TRP:HA	1.70	0.74
1:A:172:ARG:HG2	1:A:183:ILE:HD12	1.69	0.74
1:A:341:VAL:HG13	1:A:382:GLN:HG2	1.68	0.74
1:A:153:ASP:H	1:A:294:ASN:HD22	1.34	0.74
1:B:47:ILE:CD1	1:B:355:LEU:HD21	2.18	0.73
1:B:349:LYS:HE2	1:B:371:ILE:HD13	1.70	0.73
1:B:130:ILE:HD11	1:B:133:LEU:HG	1.71	0.73
1:B:221:MET:HB3	1:B:292:ALA:HB2	1.70	0.72
1:A:123:ASN:ND2	1:A:149:ARG:HH21	1.88	0.71
1:A:221:MET:HB3	1:A:292:ALA:HB2	1.72	0.71
1:A:8:ASP:HB3	1:A:62:LYS:HZ1	1.54	0.71
1:A:196:LYS:HB3	1:B:186:ASP:HB2	1.72	0.70
1:A:124:ILE:HD13	1:A:319:ILE:HD13	1.73	0.70
1:A:123:ASN:HD22	1:A:149:ARG:HH21	1.40	0.69
1:B:250:ILE:HG22	1:B:266:ILE:HB	1.75	0.67
1:A:27:ILE:HD12	1:A:93:VAL:HG23	1.76	0.67
1:B:341:VAL:HG13	1:B:382:GLN:HG2	1.77	0.67
1:A:308:ILE:HD11	1:A:314:LEU:HD21	1.75	0.66
1:A:222:HIS:CD2	1:A:224:GLY:H	2.13	0.66
1:B:222:HIS:HD2	1:B:224:GLY:H	1.44	0.66
1:B:351:GLY:O	1:B:355:LEU:HD22	1.96	0.66
1:B:382:GLN:O	1:B:386:ARG:HG3	1.96	0.65
1:B:142:LYS:HG2	1:B:285:GLU:HB3	1.77	0.65
1:B:195:SER:HB3	1:B:198:LYS:HB2	1.80	0.64
1:B:53:ARG:HE	1:B:409:ILE:HG13	1.62	0.64
1:A:304:ALA:HA	1:A:307:LEU:HD13	1.79	0.63
1:A:128:LYS:HE3	1:A:128:LYS:H	1.63	0.63
1:B:297:GLY:HA2	1:B:300:ILE:HG22	1.80	0.63
1:A:295:VAL:HG11	2:B:508:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LYS:HD2	1:B:335:LYS:H	1.64	0.62
1:A:149:ARG:HG3	1:A:297:GLY:HA3	1.81	0.62
1:A:2:LEU:H	1:A:2:LEU:HD23	1.65	0.62
1:B:263:GLN:H	1:B:263:GLN:NE2	1.98	0.62
1:B:45:LYS:HG2	1:B:403:ILE:HD11	1.83	0.61
1:B:111:ASN:HB3	1:B:115:ARG:HH21	1.66	0.61
1:A:329:ILE:HD13	1:A:329:ILE:O	2.01	0.61
1:A:33:ASP:OD2	1:A:70:GLU:HG2	2.01	0.61
1:A:16:LYS:N	1:A:16:LYS:HD2	2.16	0.61
1:A:123:ASN:HD22	1:A:149:ARG:NH2	1.98	0.60
1:B:308:ILE:HG13	1:B:308:ILE:O	2.01	0.60
1:B:20:ILE:HG13	1:B:20:ILE:O	2.00	0.60
1:B:3:TYR:CE2	1:B:66:VAL:HA	2.37	0.60
1:B:329:ILE:O	1:B:329:ILE:HD13	2.01	0.60
1:B:146:ILE:HG23	1:B:289:ILE:HG12	1.84	0.59
1:B:81:PRO:HG2	1:B:84:THR:OG1	2.02	0.59
1:B:266:ILE:HD12	1:B:266:ILE:H	1.68	0.59
1:B:256:ILE:HA	1:B:261:PRO:HA	1.84	0.58
1:B:154:ASP:HB3	1:B:295:VAL:HG23	1.86	0.58
1:B:33:ASP:OD1	1:B:70:GLU:HG2	2.04	0.58
1:B:222:HIS:CD2	1:B:224:GLY:H	2.20	0.58
1:B:125:ARG:NH2	1:B:125:ARG:HB3	2.20	0.57
1:B:28:LEU:HB3	1:B:94:VAL:HG13	1.86	0.57
1:A:126:PRO:HB3	1:A:146:ILE:HD13	1.86	0.57
1:B:29:TYR:CZ	1:B:65:GLU:HB2	2.39	0.57
1:B:243:LEU:HD12	1:B:250:ILE:HD11	1.87	0.57
1:A:272:ILE:N	1:A:272:ILE:HD12	2.19	0.57
1:B:198:LYS:O	1:B:201:ARG:HG2	2.06	0.56
1:A:124:ILE:CG2	1:A:146:ILE:HD11	2.35	0.56
1:A:150:GLU:OE1	1:A:153:ASP:HB2	2.05	0.56
1:A:314:LEU:O	1:A:329:ILE:HG22	2.06	0.56
1:A:210:ALA:HA	1:A:215:ARG:HB2	1.88	0.56
1:A:124:ILE:HG23	1:A:146:ILE:HD11	1.87	0.56
1:A:256:ILE:HG13	1:A:257:ASN:H	1.70	0.55
1:A:200:GLN:O	1:A:204:ARG:HG3	2.06	0.55
1:A:195:SER:HB3	1:A:198:LYS:HB2	1.88	0.55
1:A:14:PHE:HZ	1:A:92:ARG:HB2	1.72	0.55
1:A:82:LYS:O	1:A:86:GLU:HG2	2.06	0.55
1:B:314:LEU:O	1:B:329:ILE:HG22	2.07	0.55
1:B:125:ARG:HB3	1:B:125:ARG:HH21	1.71	0.55
1:A:27:ILE:HD12	1:A:93:VAL:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:HA	1:A:86:GLU:HG3	1.87	0.55
1:A:146:ILE:HG23	1:A:289:ILE:HA	1.88	0.55
1:A:136:PRO:HG3	1:B:282:ILE:HG22	1.89	0.55
1:A:126:PRO:HA	1:A:146:ILE:HA	1.89	0.54
1:A:2:LEU:N	1:A:2:LEU:HD23	2.23	0.54
1:B:154:ASP:HB2	1:B:294:ASN:HB3	1.90	0.54
1:B:183:ILE:HG22	1:B:184:GLU:O	2.07	0.54
1:B:130:ILE:HD12	1:B:375:ILE:HG12	1.89	0.54
1:B:223:LYS:NZ	1:B:274:ASP:HB3	2.24	0.53
1:B:12:ILE:HD12	1:B:93:VAL:HG21	1.90	0.53
1:A:314:LEU:HB2	1:A:329:ILE:CG2	2.37	0.53
1:B:35:ILE:HG12	1:B:332:THR:O	2.09	0.53
1:B:276:MET:O	1:B:280:ILE:HG23	2.08	0.53
1:A:250:ILE:HG22	1:A:266:ILE:HB	1.91	0.53
1:B:390:VAL:HG22	1:B:391:LYS:N	2.23	0.53
1:B:142:LYS:CG	1:B:285:GLU:HB3	2.39	0.53
1:A:89:LEU:HG	1:A:117:MET:HE2	1.90	0.53
1:B:297:GLY:HA2	1:B:300:ILE:CG2	2.39	0.52
1:A:73:GLU:OE1	1:A:79:ARG:HD3	2.10	0.52
1:A:10:GLU:HB2	1:A:22:PRO:HG2	1.91	0.52
1:A:28:LEU:CB	1:A:94:VAL:HG13	2.39	0.52
1:B:278:GLN:O	1:B:282:ILE:HG12	2.09	0.52
1:A:306:ALA:HB2	1:B:278:GLN:HG2	1.90	0.52
1:B:133:LEU:HD13	1:B:310:ASN:HD22	1.75	0.51
1:B:369:LYS:HD3	1:B:369:LYS:C	2.30	0.51
1:A:272:ILE:H	1:A:272:ILE:HD12	1.74	0.51
1:A:299:TYR:HE1	1:B:273:ALA:HB1	1.76	0.51
1:A:378:LYS:N	1:A:378:LYS:HD2	2.25	0.51
1:B:356:ARG:HD2	1:B:364:ALA:HB1	1.91	0.51
1:A:172:ARG:HA	1:A:183:ILE:HD11	1.92	0.51
1:B:13:LYS:HB2	1:B:20:ILE:HD11	1.93	0.51
1:A:128:LYS:HE2	2:A:530:HOH:O	2.10	0.51
1:B:47:ILE:HD12	1:B:47:ILE:O	2.11	0.51
1:A:18:LYS:O	1:A:19:TRP:HB2	2.11	0.51
1:A:142:LYS:HB3	1:A:285:GLU:HB3	1.93	0.51
1:A:177:LYS:HE3	1:A:178:GLU:OE2	2.11	0.50
1:B:150:GLU:HG3	1:B:153:ASP:HB2	1.93	0.50
1:A:99:LEU:HD13	1:A:110:VAL:HG21	1.93	0.50
1:A:115:ARG:HD3	1:A:151:ASN:HD21	1.77	0.50
1:A:218:VAL:O	1:A:268:LEU:HD12	2.11	0.50
1:A:14:PHE:CD1	1:A:322:GLU:HB2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE1	1:B:79:ARG:HB3	2.11	0.50
1:B:326:PHE:CE2	1:B:354:MET:HG3	2.46	0.50
1:A:297:GLY:HA2	1:A:300:ILE:CG2	2.40	0.50
1:A:12:ILE:HD12	1:A:93:VAL:HG21	1.94	0.50
1:A:99:LEU:HD13	1:A:110:VAL:CG2	2.41	0.50
1:B:32:GLY:HA2	1:B:99:LEU:CD2	2.42	0.50
1:B:300:ILE:HG23	1:B:301:SER:N	2.26	0.50
1:A:256:ILE:HG13	1:A:257:ASN:N	2.25	0.50
1:B:329:ILE:HG23	1:B:329:ILE:O	2.10	0.50
1:A:373:MET:HA	1:A:376:ARG:HG2	1.94	0.50
1:B:255:GLU:HA	1:B:258:GLN:HE21	1.77	0.49
1:B:200:GLN:O	1:B:204:ARG:HG3	2.11	0.49
1:A:4:LYS:N	1:A:4:LYS:HD3	2.27	0.49
1:B:349:LYS:HE2	1:B:371:ILE:CD1	2.41	0.49
1:B:133:LEU:HD13	1:B:310:ASN:ND2	2.27	0.49
1:A:266:ILE:H	1:A:266:ILE:HD12	1.78	0.49
1:A:76:VAL:HG12	1:A:76:VAL:O	2.12	0.49
1:A:16:LYS:HD2	1:A:16:LYS:H	1.77	0.49
1:B:356:ARG:HH21	1:B:356:ARG:HG3	1.77	0.49
1:B:280:ILE:HG22	1:B:287:TYR:CE2	2.47	0.49
1:A:20:ILE:N	1:A:20:ILE:HD12	2.28	0.49
1:B:379:LYS:HB3	1:B:401:GLU:HG2	1.95	0.49
1:A:261:PRO:HG2	1:A:262:ASP:H	1.77	0.48
1:A:139:HIS:CD2	1:A:141:GLU:HB2	2.48	0.48
1:A:261:PRO:HB2	1:A:263:GLN:OE1	2.13	0.48
1:A:121:TYR:CE1	1:A:201:ARG:HG3	2.49	0.48
1:A:2:LEU:CD2	1:A:83:GLU:HG2	2.44	0.48
1:B:124:ILE:N	1:B:124:ILE:HD12	2.29	0.48
1:B:45:LYS:HG2	1:B:403:ILE:CD1	2.43	0.48
1:B:319:ILE:HG12	1:B:357:TRP:CE2	2.49	0.48
1:B:150:GLU:N	1:B:202:ILE:HD12	2.28	0.48
1:B:378:LYS:N	1:B:378:LYS:HD2	2.28	0.48
1:A:162:PRO:HA	1:B:229:TYR:HB3	1.95	0.48
1:A:47:ILE:O	1:A:51:VAL:HG23	2.14	0.48
1:B:115:ARG:HA	1:B:120:LEU:HD12	1.95	0.48
1:A:44:ILE:HA	1:A:47:ILE:HG22	1.95	0.48
1:B:280:ILE:HG13	1:B:281:ILE:N	2.29	0.47
1:A:124:ILE:N	1:A:124:ILE:HD12	2.28	0.47
1:A:192:LYS:HD2	1:B:155:LEU:HD11	1.96	0.47
1:B:155:LEU:HD23	1:B:155:LEU:H	1.79	0.47
1:B:156:TYR:CE2	1:B:295:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:O	1:B:37:PRO:HD3	2.14	0.47
1:B:380:VAL:HG23	1:B:385:ALA:HB2	1.97	0.47
1:A:130:ILE:HD12	1:A:133:LEU:HD11	1.97	0.47
1:A:327:GLU:HG2	2:A:511:HOH:O	2.14	0.47
1:B:128:LYS:HD3	1:B:144:ASP:CG	2.35	0.47
1:A:2:LEU:H	1:A:2:LEU:CD2	2.27	0.47
1:B:32:GLY:HA2	1:B:99:LEU:HD21	1.96	0.47
1:A:43:ALA:O	1:A:47:ILE:HG22	2.15	0.47
1:A:271:ARG:HB2	1:A:276:MET:HE1	1.97	0.47
1:A:162:PRO:HG2	1:A:165:SER:HB3	1.96	0.47
1:B:378:LYS:HA	1:B:388:MET:HE3	1.97	0.47
1:A:378:LYS:HB3	1:A:390:VAL:HG21	1.95	0.47
1:A:8:ASP:HB3	1:A:62:LYS:HZ2	1.78	0.46
1:A:341:VAL:CG1	1:A:382:GLN:HG2	2.41	0.46
1:A:304:ALA:C	1:A:306:ALA:H	2.19	0.46
1:B:332:THR:OG1	1:B:334:PRO:HD3	2.16	0.46
1:A:328:ALA:HB2	1:A:347:ILE:N	2.30	0.46
1:A:330:HIS:HD2	1:A:331:GLY:O	1.99	0.46
1:B:272:ILE:HG13	1:B:275:ASN:ND2	2.31	0.46
1:B:223:LYS:HZ3	1:B:274:ASP:HB3	1.81	0.46
1:B:43:ALA:O	1:B:46:VAL:HG22	2.16	0.46
1:A:306:ALA:CB	1:B:278:GLN:HA	2.46	0.46
1:B:401:GLU:O	1:B:405:ILE:HG13	2.16	0.46
1:A:271:ARG:HB2	1:A:276:MET:CE	2.46	0.46
1:A:274:ASP:OD1	1:A:275:ASN:N	2.49	0.45
1:A:311:ILE:HD12	1:A:314:LEU:HD12	1.98	0.45
1:B:253:GLU:HB2	1:B:269:ASN:HB3	1.98	0.45
1:A:79:ARG:HH11	1:A:102:PRO:HD3	1.81	0.45
1:B:15:ASP:OD1	1:B:16:LYS:HD3	2.17	0.45
1:B:390:VAL:HG22	1:B:391:LYS:H	1.82	0.45
1:A:130:ILE:HB	1:A:133:LEU:HG	1.98	0.45
1:B:139:HIS:HA	1:B:141:GLU:OE2	2.17	0.45
1:B:53:ARG:HE	1:B:409:ILE:CG1	2.26	0.45
1:B:127:VAL:HG13	1:B:127:VAL:O	2.17	0.45
1:A:217:LYS:O	1:A:288:ASP:HB3	2.16	0.45
1:B:178:GLU:C	1:B:179:LEU:HD22	2.37	0.45
1:A:29:TYR:CZ	1:A:65:GLU:HB2	2.51	0.45
1:A:28:LEU:HB3	1:A:94:VAL:HG13	1.97	0.45
1:B:254:GLU:O	1:B:258:GLN:HB2	2.17	0.45
1:A:153:ASP:O	1:A:157:ARG:HD2	2.17	0.44
1:B:150:GLU:CA	1:B:202:ILE:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HE1	1:A:270:ASP:HB2	1.82	0.44
1:A:235:ARG:NH1	1:A:235:ARG:HB3	2.33	0.44
1:B:172:ARG:O	1:B:176:ARG:HG3	2.18	0.44
1:B:378:LYS:HA	1:B:388:MET:CE	2.47	0.44
1:B:130:ILE:CD1	1:B:375:ILE:HG12	2.47	0.44
1:B:256:ILE:C	1:B:258:GLN:H	2.21	0.44
1:A:150:GLU:CA	1:A:202:ILE:HD12	2.47	0.44
1:A:250:ILE:HA	1:A:266:ILE:O	2.17	0.44
1:B:141:GLU:CD	1:B:141:GLU:H	2.20	0.44
1:A:222:HIS:CE1	1:A:270:ASP:HB2	2.53	0.44
1:B:171:ILE:O	1:B:175:LEU:HG	2.17	0.44
1:A:311:ILE:HG23	1:A:312:GLY:N	2.32	0.43
1:B:127:VAL:HG11	1:B:304:ALA:HB1	2.01	0.43
1:A:130:ILE:O	1:A:131:GLU:HB2	2.17	0.43
1:B:96:LYS:O	1:B:96:LYS:HG3	2.18	0.43
1:B:124:ILE:HG22	1:B:126:PRO:HD3	1.99	0.43
1:A:29:TYR:HA	1:A:95:LEU:O	2.18	0.43
1:A:35:ILE:HG21	1:A:342:ALA:HB2	2.01	0.43
1:B:214:LYS:HD2	1:B:214:LYS:HA	1.88	0.43
1:A:221:MET:HB2	1:A:276:MET:SD	2.59	0.43
1:A:329:ILE:HG23	1:A:329:ILE:O	2.19	0.43
1:A:35:ILE:O	1:A:39:ILE:HG12	2.18	0.43
1:B:44:ILE:HA	1:B:47:ILE:CG2	2.49	0.43
1:A:260:LYS:HA	1:A:261:PRO:HD2	1.85	0.42
1:B:13:LYS:HB2	1:B:20:ILE:CG1	2.50	0.42
1:A:196:LYS:HE2	1:A:237:TRP:CD1	2.54	0.42
1:A:378:LYS:HG3	1:A:388:MET:SD	2.58	0.42
1:B:150:GLU:CG	1:B:153:ASP:HB2	2.49	0.42
1:A:314:LEU:HB2	1:A:329:ILE:HG21	2.02	0.42
1:A:262:ASP:C	1:A:264:GLY:H	2.23	0.42
1:A:14:PHE:CD1	1:A:14:PHE:N	2.85	0.42
1:A:136:PRO:HD2	1:A:307:LEU:O	2.20	0.42
1:B:155:LEU:HD23	1:B:295:VAL:HG21	2.00	0.42
1:B:89:LEU:HD21	1:B:117:MET:HE2	2.01	0.42
1:B:154:ASP:CB	1:B:295:VAL:HG23	2.49	0.42
1:A:79:ARG:NH1	1:A:102:PRO:HD3	2.35	0.42
1:A:93:VAL:HA	1:A:324:GLY:O	2.19	0.42
1:A:355:LEU:HG	1:A:363:ALA:HB3	2.01	0.42
1:A:386:ARG:NH1	1:A:386:ARG:HB2	2.34	0.42
1:A:203:THR:HA	1:A:291:LEU:HD11	2.01	0.42
1:B:201:ARG:HG2	1:B:202:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:O	1:A:200:GLN:HG3	2.19	0.42
1:B:44:ILE:HA	1:B:47:ILE:HG22	2.02	0.42
1:B:24:LYS:HA	1:B:60:GLU:O	2.20	0.41
1:B:64:LEU:HD22	1:B:65:GLU:N	2.34	0.41
1:A:222:HIS:HD2	1:A:224:GLY:N	2.06	0.41
1:A:21:VAL:HA	1:A:22:PRO:HD3	1.90	0.41
1:A:53:ARG:O	1:A:53:ARG:HD3	2.20	0.41
1:B:43:ALA:O	1:B:47:ILE:HG22	2.19	0.41
1:A:202:ILE:HG12	1:A:202:ILE:O	2.21	0.41
1:B:130:ILE:O	1:B:130:ILE:HG13	2.20	0.41
1:B:124:ILE:HG12	1:B:357:TRP:CH2	2.56	0.41
1:A:283:ARG:HG3	1:A:283:ARG:HH21	1.86	0.41
1:B:341:VAL:CG1	1:B:382:GLN:HG2	2.49	0.41
1:B:409:ILE:H	1:B:409:ILE:HG13	1.70	0.41
1:A:254:GLU:O	1:A:254:GLU:HG2	2.21	0.41
1:A:109:SER:O	1:A:112:VAL:HG12	2.21	0.41
1:A:27:ILE:HG23	1:A:63:TRP:CE3	2.56	0.41
1:A:303:ALA:O	1:A:306:ALA:HB3	2.21	0.41
1:B:126:PRO:HA	1:B:146:ILE:HA	2.03	0.41
1:A:44:ILE:HA	1:A:47:ILE:CG2	2.50	0.41
1:A:150:GLU:HA	1:A:202:ILE:HD12	2.01	0.40
1:A:317:ALA:HB1	1:A:319:ILE:CD1	2.51	0.40
1:A:295:VAL:HG13	1:A:296:ASN:N	2.36	0.40
1:B:115:ARG:HG2	1:B:120:LEU:HB2	2.04	0.40
1:A:89:LEU:HG	1:A:117:MET:CE	2.51	0.40
1:B:369:LYS:HZ1	1:B:373:MET:CG	2.35	0.40
1:B:76:VAL:HG12	1:B:76:VAL:O	2.19	0.40
1:A:356:ARG:HH11	1:A:356:ARG:HG2	1.86	0.40
1:A:278:GLN:HA	1:B:306:ALA:HB2	2.03	0.40
1:B:179:LEU:HB3	1:B:181:VAL:HG23	2.03	0.40
1:A:386:ARG:HH12	1:A:387:PHE:HE1	1.67	0.40
1:B:210:ALA:HA	1:B:215:ARG:HB2	2.02	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	399/409 (98%)	359 (90%)	35 (9%)	5 (1%)	15 26
1	B	399/409 (98%)	358 (90%)	33 (8%)	8 (2%)	9 15
All	All	798/818 (98%)	717 (90%)	68 (8%)	13 (2%)	12 21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	PRO
1	A	131	GLU
1	A	261	PRO
1	A	389	GLY
1	B	56	GLY
1	B	131	GLU
1	B	141	GLU
1	B	154	ASP
1	B	389	GLY
1	A	14	PHE
1	A	152	THR
1	B	57	SER
1	B	262	ASP

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	339/343 (99%)	317 (94%)	22 (6%)	21 39
1	B	339/343 (99%)	318 (94%)	21 (6%)	23 41
All	All	678/686 (99%)	635 (94%)	43 (6%)	22 40

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	16	LYS
1	A	27	ILE
1	A	28	LEU
1	A	53	ARG
1	A	86	GLU
1	A	94	VAL
1	A	110	VAL
1	A	116	LEU
1	A	128	LYS
1	A	149	ARG
1	A	170	LYS
1	A	194	MET
1	A	196	LYS
1	A	216	LYS
1	A	248	ASP
1	A	291	LEU
1	A	318	ASN
1	A	329	ILE
1	A	355	LEU
1	A	357	TRP
1	A	378	LYS
1	B	1	MET
1	B	47	ILE
1	B	53	ARG
1	B	64	LEU
1	B	79	ARG
1	B	92	ARG
1	B	94	VAL
1	B	100	GLU
1	B	131	GLU
1	B	141	GLU
1	B	151	ASN
1	B	170	LYS
1	B	205	LEU
1	B	263	GLN
1	B	329	ILE
1	B	335	LYS
1	B	355	LEU
1	B	356	ARG
1	B	357	TRP
1	B	373	MET
1	B	378	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	123	ASN
1	A	139	HIS
1	A	151	ASN
1	A	222	HIS
1	A	275	ASN
1	A	279	GLN
1	A	294	ASN
1	A	310	ASN
1	A	330	HIS
1	B	41	ASN
1	B	85	GLN
1	B	111	ASN
1	B	151	ASN
1	B	208	GLN
1	B	213	HIS
1	B	222	HIS
1	B	258	GLN
1	B	263	GLN
1	B	310	ASN
1	B	318	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

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	403/409 (98%)	0.13	5 (1%)	81	83	25, 48, 80, 112	0
1	B	403/409 (98%)	0.25	11 (2%)	58	62	30, 56, 87, 118	0
All	All	806/818 (98%)	0.19	16 (1%)	68	72	25, 52, 85, 118	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	PHE	3.7
1	B	256	ILE	3.6
1	B	155	LEU	3.5
1	B	259	GLY	3.4
1	B	299	TYR	3.1
1	B	251	VAL	2.8
1	B	260	LYS	2.7
1	B	409	ILE	2.6
1	A	216	LYS	2.6
1	B	18	LYS	2.3
1	B	221	MET	2.3
1	A	261	PRO	2.3
1	A	282	ILE	2.3
1	A	15	ASP	2.1
1	A	283	ARG	2.1
1	B	19	TRP	2.0

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

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.