Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 03:00 AM EDT

PDB ID	:	3FFS
Title	:	The Crystal Structure of Cryptosporidium parvum Inosine-5'-Monophosphate Dehydrogenase
Authors	:	Riera, T.V.; D'Aquino, J.A.; Lu, J.; Petsko, G.A.; Hedstrom, L.
Deposited on	:	2008-12-04
Resolution	:	3.19 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 (1)) were used in the production of this report:

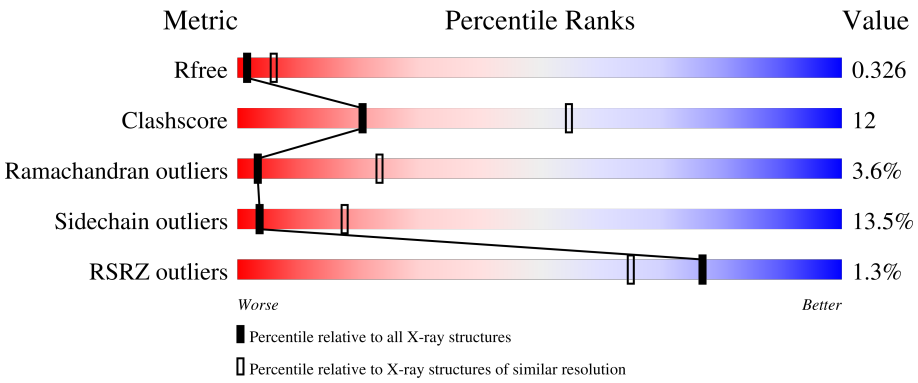
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	400	54% 18% • 25%
1	B	400	53% 19% • 24%
1	C	400	% 49% 21% • 26%
1	D	400	3% 50% 20% • 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8561 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 Inosine-5-monophosphate dehydrogenase.

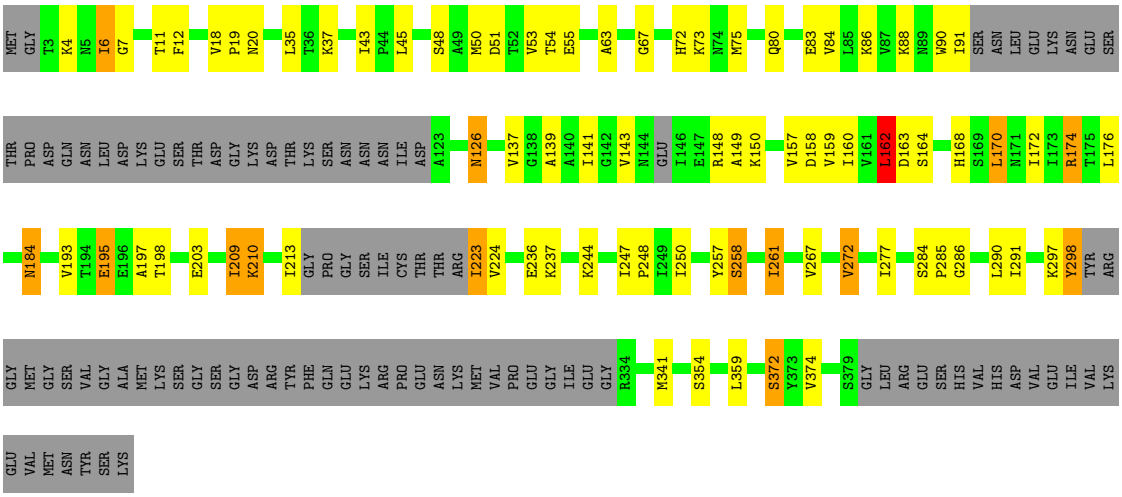
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2188	1388	371	418	11	0	0	0
1	B	303	2190	1383	364	433	10	0	0	0
1	C	298	2140	1348	363	418	11	0	0	0
1	D	299	2043	1290	346	397	10	0	0	0

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.

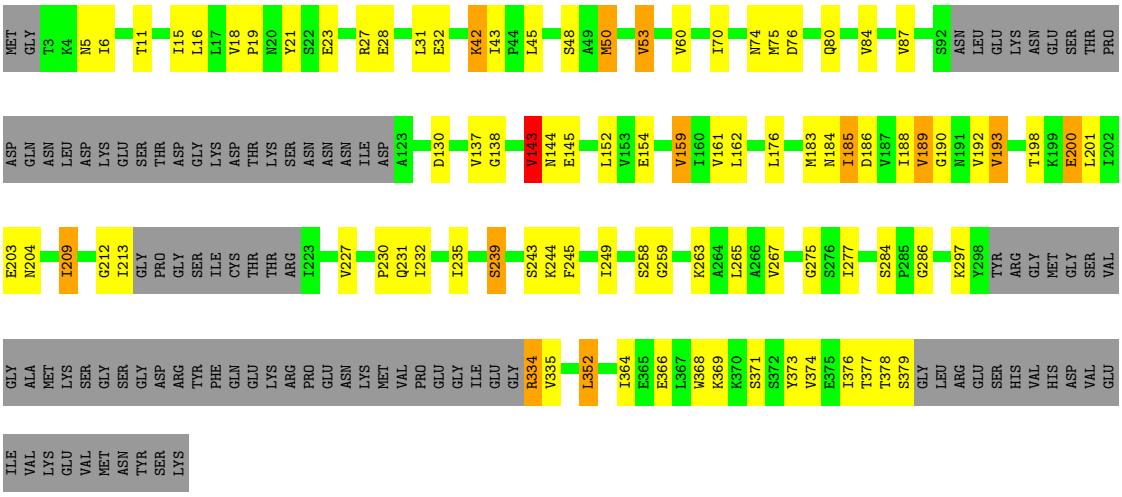
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain A: 54% 18% • 25%



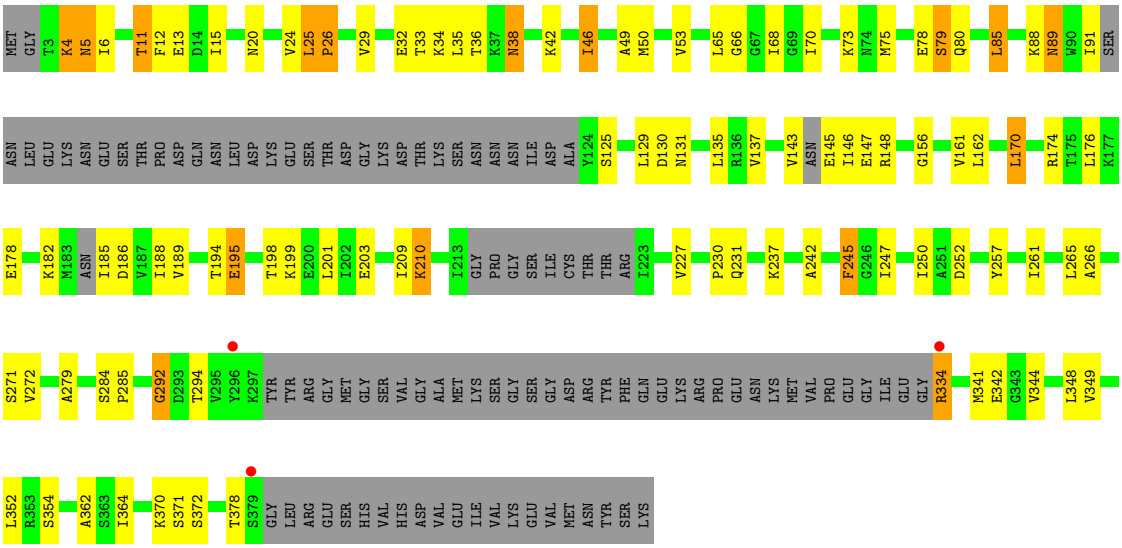
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain B: 53% 19% • 24%



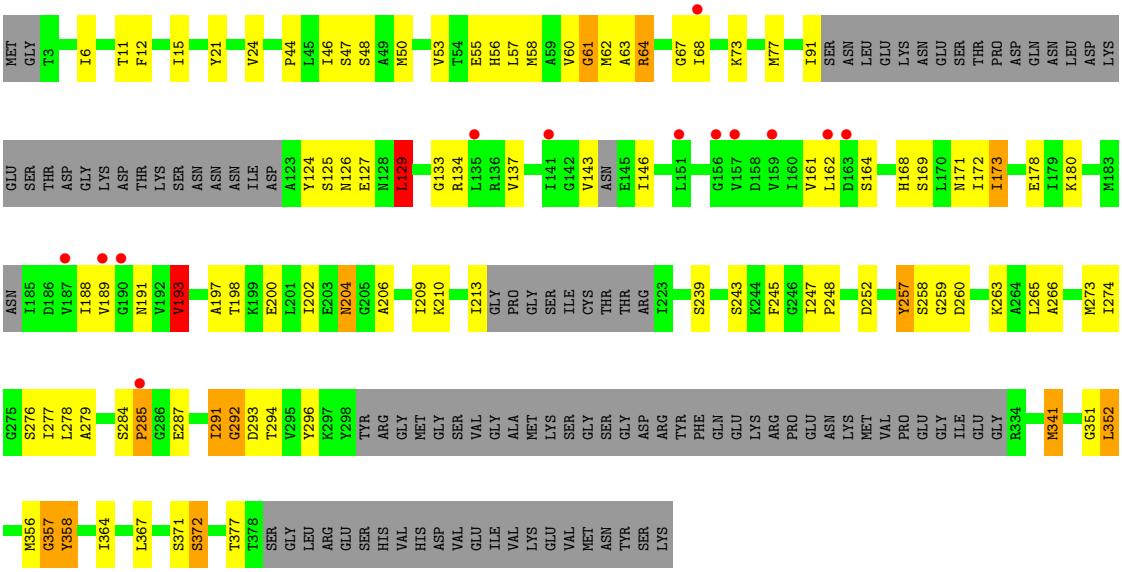
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain C:



- Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.07Å 153.32Å 98.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 3.19 48.32 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.34-3.19) 99.1 (48.32-3.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.269 , 0.328 0.272 , 0.326	Depositor DCC
R_{free} test set	1536 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	74.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.4	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	0.87	EDS
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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	0.52	0/2206	0.71	1/2976 (0.0%)
1	B	0.52	0/2211	0.71	0/2994
1	C	0.54	0/2155	0.70	0/2909
1	D	0.56	0/2060	0.69	1/2803 (0.0%)
All	All	0.54	0/8632	0.70	2/11682 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	LEU	CA-CB-CG	6.58	130.44	115.30
1	D	129	LEU	CA-CB-CG	5.26	127.40	115.30

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	2188	0	2259	49	0
1	B	2190	0	2189	66	0
1	C	2140	0	2157	57	0
1	D	2043	0	1945	50	0
All	All	8561	0	8550	210	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 12.

All (210) 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:C:25:LEU:HD13	1:C:26:PRO:HD2	1.37	1.05
1:B:15:ILE:HD11	1:B:232:ILE:HG21	1.49	0.95
1:C:185:ILE:HG13	1:C:186:ASP:H	1.32	0.94
1:C:334:ARG:HH11	1:C:334:ARG:HG2	1.39	0.87
1:B:21:TYR:HE2	1:B:23:GLU:HG3	1.40	0.85
1:C:372:SER:HB3	1:D:6:ILE:HD11	1.59	0.84
1:D:204:ASN:N	1:D:204:ASN:HD22	1.71	0.84
1:B:70:ILE:HD13	1:B:161:VAL:HG21	1.60	0.82
1:D:169:SER:OG	1:D:172:ILE:HD13	1.81	0.80
1:C:334:ARG:HH11	1:C:334:ARG:CG	1.93	0.80
1:A:297:LYS:O	1:A:298:TYR:HB2	1.82	0.77
1:D:50:MET:HB2	1:D:53:VAL:HG12	1.66	0.77
1:C:284:SER:HB2	1:C:285:PRO:HD2	1.67	0.77
1:A:170:LEU:HD11	1:A:174:ARG:HH11	1.50	0.75
1:C:185:ILE:HG13	1:C:186:ASP:N	2.02	0.74
1:A:170:LEU:HD11	1:A:174:ARG:NH1	2.02	0.74
1:C:46:ILE:HG22	1:C:68:ILE:HG22	1.70	0.73
1:B:16:LEU:HB2	1:B:376:ILE:HD11	1.70	0.73
1:B:212:GLY:O	1:B:213:ILE:HG13	1.88	0.73
1:D:204:ASN:N	1:D:204:ASN:ND2	2.38	0.72
1:B:11:THR:HG23	1:B:230:PRO:HB3	1.70	0.71
1:D:146:ILE:HD11	1:D:178:GLU:HB3	1.72	0.70
1:D:63:ALA:HA	1:D:67:GLY:O	1.90	0.70
1:A:141:ILE:HD11	1:A:149:ALA:HB2	1.73	0.70
1:A:18:VAL:HB	1:A:372:SER:HB3	1.73	0.69
1:B:235:ILE:O	1:B:239:SER:HB3	1.93	0.69
1:B:231:GLN:HE21	1:B:231:GLN:HA	1.58	0.69
1:C:143:VAL:O	1:C:145:GLU:N	2.26	0.68
1:A:141:ILE:CD1	1:A:149:ALA:HB2	2.22	0.68
1:C:189:VAL:HG11	1:C:201:LEU:HD22	1.76	0.67
1:C:210:LYS:HG2	1:C:252:ASP:HB2	1.77	0.67
1:A:11:THR:HG22	1:A:12:PHE:N	2.11	0.66
1:A:170:LEU:CD1	1:A:174:ARG:HH11	2.08	0.65
1:B:162:LEU:O	1:B:190:GLY:HA2	1.96	0.65
1:C:11:THR:HG22	1:C:230:PRO:HB3	1.78	0.65
1:B:192:VAL:HG11	1:B:201:LEU:HD12	1.80	0.64
1:A:50:MET:HB2	1:A:53:VAL:HG22	1.80	0.63
1:C:261:ILE:HG23	1:C:272:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:HG2	1:A:237:LYS:HB3	1.82	0.62
1:C:33:THR:HB	1:C:364:ILE:HD12	1.82	0.61
1:A:141:ILE:HG22	1:A:162:LEU:HA	1.81	0.61
1:D:259:GLY:O	1:D:263:LYS:HE3	2.01	0.61
1:B:263:LYS:O	1:B:267:VAL:HG23	2.00	0.61
1:B:371:SER:HB2	1:C:4:LYS:HZ2	1.65	0.61
1:B:371:SER:HB2	1:C:4:LYS:NZ	2.16	0.61
1:D:61:GLY:HA2	1:D:64:ARG:HD2	1.82	0.61
1:A:258:SER:O	1:A:261:ILE:HG22	2.01	0.60
1:B:231:GLN:HA	1:B:231:GLN:NE2	2.15	0.60
1:B:297:LYS:O	1:B:334:ARG:HA	2.00	0.60
1:D:202:ILE:HA	1:D:206:ALA:HB3	1.83	0.60
1:C:50:MET:HB2	1:C:53:VAL:HG12	1.84	0.60
1:D:258:SER:HB3	1:D:351:GLY:HA3	1.83	0.59
1:C:70:ILE:HG12	1:C:161:VAL:HG21	1.84	0.59
1:D:143:VAL:HG21	1:D:172:ILE:HG13	1.84	0.59
1:D:169:SER:OG	1:D:172:ILE:CD1	2.50	0.59
1:B:138:GLY:HA3	1:B:159:VAL:HG23	1.86	0.58
1:C:334:ARG:HH11	1:C:334:ARG:CB	2.17	0.58
1:B:15:ILE:HG23	1:B:373:TYR:HB2	1.85	0.58
1:D:204:ASN:ND2	1:D:204:ASN:H	2.02	0.58
1:C:12:PHE:CZ	1:C:231:GLN:HG2	2.39	0.58
1:A:11:THR:CG2	1:A:12:PHE:N	2.66	0.57
1:B:70:ILE:HA	1:B:138:GLY:O	2.04	0.57
1:B:334:ARG:HD2	1:B:334:ARG:C	2.24	0.57
1:C:46:ILE:HD11	1:C:250:ILE:HG23	1.86	0.57
1:A:261:ILE:HG12	1:A:272:VAL:HG11	1.85	0.57
1:D:146:ILE:CD1	1:D:178:GLU:HB3	2.35	0.57
1:D:161:VAL:HG13	1:D:188:ILE:HB	1.85	0.57
1:B:43:ILE:HD12	1:B:45:LEU:HD12	1.86	0.57
1:D:169:SER:O	1:D:173:ILE:HB	2.06	0.56
1:A:84:VAL:HG23	1:A:137:VAL:HG11	1.86	0.56
1:C:199:LYS:O	1:C:203:GLU:HB2	2.06	0.56
1:A:51:ASP:HA	1:A:72:HIS:CD2	2.40	0.56
1:B:334:ARG:C	1:B:334:ARG:HH11	2.10	0.55
1:C:334:ARG:HH11	1:C:334:ARG:HB3	1.70	0.55
1:B:87:VAL:HB	1:B:137:VAL:HG21	1.88	0.55
1:D:162:LEU:HB2	1:D:189:VAL:HA	1.89	0.55
1:A:80:GLN:O	1:A:84:VAL:HG12	2.07	0.54
1:A:75:MET:O	1:A:148:ARG:NH1	2.34	0.54
1:B:21:TYR:CE2	1:B:23:GLU:HG3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:HIS:CE1	1:D:21:TYR:HB2	2.43	0.54
1:C:38:ASN:ND2	1:C:186:ASP:OD2	2.39	0.53
1:B:21:TYR:C	1:B:21:TYR:CD2	2.80	0.53
1:C:372:SER:HB3	1:D:6:ILE:CD1	2.35	0.53
1:B:75:MET:SD	1:B:80:GLN:HB2	2.48	0.53
1:C:334:ARG:HG2	1:C:334:ARG:NH1	2.10	0.53
1:B:16:LEU:HD22	1:B:376:ILE:CD1	2.39	0.53
1:B:192:VAL:HG11	1:B:201:LEU:CD1	2.39	0.52
1:B:189:VAL:CB	1:B:209:ILE:HA	2.39	0.52
1:B:31:LEU:HD22	1:B:352:LEU:HD13	1.91	0.52
1:B:15:ILE:HG22	1:B:16:LEU:N	2.23	0.52
1:C:265:LEU:HD12	1:C:352:LEU:HD21	1.92	0.52
1:C:344:VAL:O	1:C:348:LEU:HG	2.10	0.52
1:D:44:PRO:HG3	1:D:364:ILE:HD11	1.91	0.52
1:B:200:GLU:O	1:B:204:ASN:ND2	2.43	0.52
1:B:48:SER:HB3	1:B:50:MET:HG3	1.91	0.51
1:B:16:LEU:HD22	1:B:376:ILE:HD11	1.93	0.51
1:D:284:SER:HB2	1:D:285:PRO:HD2	1.93	0.51
1:A:193:VAL:HG22	1:A:213:ILE:HG13	1.93	0.51
1:D:266:ALA:HA	1:D:367:LEU:HG	1.93	0.51
1:D:274:ILE:HG23	1:D:277:ILE:HG23	1.93	0.51
1:C:33:THR:OG1	1:C:34:LYS:N	2.44	0.50
1:D:129:LEU:HD12	1:D:134:ARG:O	2.12	0.50
1:D:291:ILE:O	1:D:292:GLY:O	2.30	0.50
1:D:193:VAL:HG22	1:D:213:ILE:HD12	1.94	0.50
1:C:49:ALA:HB2	1:C:70:ILE:HG22	1.93	0.50
1:A:51:ASP:O	1:A:285:PRO:HG2	2.11	0.49
1:D:191:ASN:HA	1:D:210:LYS:O	2.12	0.49
1:A:80:GLN:NE2	1:A:139:ALA:HB1	2.28	0.49
1:B:15:ILE:HD12	1:B:232:ILE:HG13	1.93	0.49
1:B:53:VAL:HA	1:B:284:SER:HB2	1.94	0.49
1:D:64:ARG:HA	1:D:127:GLU:HA	1.95	0.49
1:A:162:LEU:HD11	1:A:172:ILE:HG23	1.94	0.49
1:B:377:THR:O	1:B:379:SER:N	2.43	0.49
1:B:183:MET:O	1:B:185:ILE:HG22	2.13	0.48
1:C:334:ARG:HB3	1:C:334:ARG:NH1	2.27	0.48
1:A:11:THR:CG2	1:A:12:PHE:H	2.26	0.48
1:C:24:VAL:HG11	1:C:362:ALA:HB2	1.95	0.48
1:A:19:PRO:HG3	1:B:227:VAL:CG1	2.43	0.48
1:B:373:TYR:CZ	1:C:5:ASN:HB3	2.48	0.48
1:C:75:MET:HB2	1:C:79:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG23	1:A:137:VAL:CG1	2.44	0.48
1:C:189:VAL:HG11	1:C:201:LEU:CD2	2.43	0.48
1:B:143:VAL:HG23	1:B:145:GLU:HG3	1.94	0.48
1:B:162:LEU:O	1:B:190:GLY:CA	2.62	0.48
1:A:141:ILE:CG2	1:A:162:LEU:HA	2.44	0.47
1:D:173:ILE:HD11	1:D:200:GLU:HG3	1.95	0.47
1:B:185:ILE:HG13	1:B:186:ASP:H	1.78	0.47
1:D:294:THR:HG1	1:D:296:TYR:HE1	1.62	0.47
1:C:85:LEU:O	1:C:89:ASN:HB2	2.15	0.47
1:D:48:SER:HA	1:D:273:MET:CE	2.45	0.47
1:A:88:LYS:NZ	1:A:158:ASP:OD1	2.44	0.47
1:A:53:VAL:HG23	1:A:54:THR:N	2.31	0.46
1:A:73:LYS:O	1:A:148:ARG:NH2	2.48	0.46
1:A:86:LYS:O	1:A:90:TRP:HD1	1.99	0.46
1:A:210:LYS:HB3	1:A:250:ILE:HB	1.97	0.46
1:B:15:ILE:CD1	1:B:232:ILE:HG13	2.46	0.46
1:B:185:ILE:HG13	1:B:186:ASP:N	2.31	0.46
1:A:6:ILE:HG13	1:A:7:GLY:H	1.81	0.46
1:C:88:LYS:NZ	1:C:156:GLY:O	2.28	0.46
1:A:141:ILE:HD12	1:A:149:ALA:HB2	1.95	0.45
1:C:261:ILE:HG23	1:C:272:VAL:CG1	2.45	0.45
1:D:198:THR:HG22	1:D:209:ILE:HD13	1.98	0.45
1:B:286:GLY:HA3	1:B:297:LYS:HE3	1.98	0.45
1:B:373:TYR:CE2	1:C:5:ASN:HB3	2.51	0.45
1:D:62:MET:HE3	1:D:341:MET:HE2	1.99	0.45
1:C:35:LEU:HD11	1:C:188:ILE:HD11	1.98	0.45
1:B:231:GLN:HE21	1:B:231:GLN:CA	2.23	0.45
1:C:80:GLN:OE1	1:C:148:ARG:NH2	2.49	0.45
1:B:259:GLY:O	1:B:263:LYS:HG3	2.17	0.45
1:C:250:ILE:HA	1:C:271:SER:O	2.17	0.45
1:C:46:ILE:HD11	1:C:250:ILE:CG2	2.47	0.44
1:C:245:PHE:C	1:C:247:ILE:H	2.20	0.44
1:A:209:ILE:HG12	1:A:209:ILE:O	2.17	0.44
1:D:56:HIS:C	1:D:58:MET:H	2.21	0.44
1:B:43:ILE:HG13	1:B:43:ILE:O	2.17	0.44
1:D:257:TYR:O	1:D:260:ASP:HB2	2.18	0.44
1:D:247:ILE:HA	1:D:248:PRO:HD2	1.90	0.44
1:A:286:GLY:HA3	1:A:297:LYS:HG2	1.99	0.43
1:C:292:GLY:O	1:C:294:THR:N	2.47	0.43
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.18	0.43
1:D:243:SER:C	1:D:245:PHE:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLU:HG2	1:C:170:LEU:HB2	1.99	0.43
1:C:195:GLU:OE2	1:C:237:LYS:HE3	2.18	0.43
1:D:277:ILE:HG13	1:D:277:ILE:O	2.18	0.43
1:C:20:ASN:ND2	1:C:370:LYS:O	2.52	0.43
1:D:202:ILE:HA	1:D:206:ALA:H	1.84	0.43
1:B:373:TYR:CE2	1:C:5:ASN:CB	3.01	0.43
1:D:252:ASP:HA	1:D:273:MET:HB3	2.00	0.43
1:C:185:ILE:CG1	1:C:186:ASP:H	2.18	0.43
1:A:126:ASN:HD22	1:A:126:ASN:HA	1.64	0.42
1:A:267:VAL:HG12	1:A:267:VAL:O	2.18	0.42
1:B:21:TYR:HE2	1:B:23:GLU:CG	2.22	0.42
1:A:168:HIS:HB2	1:A:197:ALA:HB1	2.00	0.42
1:C:42:LYS:HB2	1:C:66:GLY:CA	2.49	0.42
1:D:168:HIS:CD2	1:D:197:ALA:HA	2.54	0.42
1:A:18:VAL:HG21	1:B:6:ILE:HD11	2.01	0.42
1:A:63:ALA:HA	1:A:67:GLY:O	2.18	0.42
1:A:223:ILE:HG13	1:A:224:VAL:N	2.34	0.42
1:D:48:SER:HA	1:D:273:MET:HE2	2.00	0.42
1:B:15:ILE:CG2	1:B:16:LEU:N	2.83	0.42
1:B:161:VAL:HG22	1:B:188:ILE:HG13	2.02	0.42
1:D:274:ILE:HG22	1:D:278:LEU:HD12	2.00	0.42
1:D:357:GLY:O	1:D:358:TYR:C	2.58	0.42
1:A:35:LEU:HD21	1:A:159:VAL:HG11	2.01	0.42
1:A:43:ILE:HD12	1:A:45:LEU:HD12	2.03	0.41
1:A:261:ILE:HG12	1:A:272:VAL:CG1	2.48	0.41
1:B:84:VAL:HG21	1:B:152:LEU:HD22	2.02	0.41
1:B:243:SER:C	1:B:245:PHE:H	2.23	0.41
1:B:265:LEU:HD13	1:B:364:ILE:HD12	2.02	0.41
1:B:334:ARG:NH1	1:B:335:VAL:HA	2.35	0.41
1:B:130:ASP:OD1	1:B:130:ASP:N	2.48	0.41
1:C:36:THR:O	1:C:38:ASN:N	2.54	0.41
1:A:141:ILE:HG22	1:A:162:LEU:CA	2.50	0.41
1:D:68:ILE:HD11	1:D:137:VAL:O	2.21	0.41
1:A:55:GLU:HB3	1:A:83:GLU:OE1	2.21	0.41
1:B:243:SER:O	1:B:244:LYS:CB	2.69	0.41
1:B:374:VAL:HG12	1:C:6:ILE:HG13	2.03	0.41
1:C:146:ILE:HD11	1:C:178:GLU:HB3	2.03	0.41
1:D:62:MET:HE2	1:D:341:MET:HE1	2.02	0.41
1:B:32:GLU:HG2	1:B:42:LYS:HA	2.03	0.41
1:B:21:TYR:C	1:B:21:TYR:HD2	2.24	0.40
1:C:88:LYS:HE2	1:C:130:ASP:OD1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LEU:HD12	1:D:352:LEU:HD21	2.04	0.40
1:A:247:ILE:HA	1:A:248:PRO:HD3	1.82	0.40
1:D:11:THR:OG1	1:D:12:PHE:N	2.54	0.40
1:B:18:VAL:HA	1:B:19:PRO:HD3	1.91	0.40
1:B:364:ILE:HG22	1:B:368:TRP:NE1	2.37	0.40
1:A:184:ASN:H	1:A:184:ASN:HD22	1.68	0.40
1:C:65:LEU:HD11	1:C:342:GLU:HG2	2.03	0.40
1:D:243:SER:C	1:D:245:PHE:H	2.24	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	291/400 (73%)	262 (90%)	25 (9%)	4 (1%)	11	46
1	B	295/400 (74%)	262 (89%)	25 (8%)	8 (3%)	5	30
1	C	286/400 (72%)	231 (81%)	43 (15%)	12 (4%)	3	20
1	D	287/400 (72%)	223 (78%)	46 (16%)	18 (6%)	1	10
All	All	1159/1600 (72%)	978 (84%)	139 (12%)	42 (4%)	3	23

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	B	143	VAL
1	B	184	ASN
1	B	185	ILE
1	B	378	THR
1	C	32	GLU
1	D	60	VAL

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Mol	Chain	Res	Type
1	D	125	SER
1	D	292	GLY
1	D	371	SER
1	B	74	ASN
1	B	189	VAL
1	C	4	LYS
1	C	89	ASN
1	C	242	ALA
1	C	266	ALA
1	C	292	GLY
1	C	378	THR
1	D	61	GLY
1	D	77	MET
1	D	126	ASN
1	D	291	ILE
1	D	358	TYR
1	A	6	ILE
1	C	131	ASN
1	C	135	LEU
1	C	182	LYS
1	D	279	ALA
1	D	287	GLU
1	A	48	SER
1	B	275	GLY
1	C	279	ALA
1	D	133	GLY
1	C	26	PRO
1	D	57	LEU
1	D	124	TYR
1	D	372	SER
1	D	357	GLY
1	A	291	ILE
1	B	193	VAL
1	D	285	PRO
1	D	193	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	233/334 (70%)	197 (84%)	36 (16%)	2 12
1	B	230/334 (69%)	204 (89%)	26 (11%)	6 25
1	C	224/334 (67%)	191 (85%)	33 (15%)	3 14
1	D	194/334 (58%)	170 (88%)	24 (12%)	4 21
All	All	881/1336 (66%)	762 (86%)	119 (14%)	4 18

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	20	ASN
1	A	37	LYS
1	A	91	ILE
1	A	126	ASN
1	A	143	VAL
1	A	150	LYS
1	A	157	VAL
1	A	160	ILE
1	A	162	LEU
1	A	163	ASP
1	A	164	SER
1	A	170	LEU
1	A	174	ARG
1	A	176	LEU
1	A	184	ASN
1	A	195	GLU
1	A	198	THR
1	A	203	GLU
1	A	209	ILE
1	A	210	LYS
1	A	223	ILE
1	A	236	GLU
1	A	257	TYR
1	A	258	SER
1	A	261	ILE
1	A	272	VAL
1	A	277	ILE
1	A	284	SER
1	A	290	LEU
1	A	298	TYR

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Mol	Chain	Res	Type
1	A	341	MET
1	A	354	SER
1	A	359	LEU
1	A	372	SER
1	A	374	VAL
1	B	5	ASN
1	B	27	ARG
1	B	28	GLU
1	B	42	LYS
1	B	50	MET
1	B	53	VAL
1	B	60	VAL
1	B	76	ASP
1	B	143	VAL
1	B	144	ASN
1	B	154	GLU
1	B	159	VAL
1	B	176	LEU
1	B	193	VAL
1	B	198	THR
1	B	200	GLU
1	B	203	GLU
1	B	209	ILE
1	B	239	SER
1	B	249	ILE
1	B	258	SER
1	B	277	ILE
1	B	334	ARG
1	B	352	LEU
1	B	366	GLU
1	B	369	LYS
1	C	5	ASN
1	C	11	THR
1	C	13	GLU
1	C	15	ILE
1	C	25	LEU
1	C	29	VAL
1	C	38	ASN
1	C	46	ILE
1	C	73	LYS
1	C	79	SER
1	C	85	LEU

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Mol	Chain	Res	Type
1	C	91	ILE
1	C	125	SER
1	C	129	LEU
1	C	137	VAL
1	C	147	GLU
1	C	162	LEU
1	C	170	LEU
1	C	174	ARG
1	C	176	LEU
1	C	194	THR
1	C	195	GLU
1	C	198	THR
1	C	209	ILE
1	C	210	LYS
1	C	227	VAL
1	C	245	PHE
1	C	257	TYR
1	C	334	ARG
1	C	341	MET
1	C	349	VAL
1	C	354	SER
1	C	371	SER
1	D	15	ILE
1	D	24	VAL
1	D	46	ILE
1	D	47	SER
1	D	55	GLU
1	D	64	ARG
1	D	73	LYS
1	D	91	ILE
1	D	129	LEU
1	D	164	SER
1	D	171	ASN
1	D	173	ILE
1	D	180	LYS
1	D	193	VAL
1	D	204	ASN
1	D	239	SER
1	D	257	TYR
1	D	276	SER
1	D	293	ASP
1	D	341	MET

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Mol	Chain	Res	Type
1	D	352	LEU
1	D	356	MET
1	D	372	SER
1	D	377	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	128	ASN
1	A	184	ASN
1	B	171	ASN
1	B	231	GLN
1	C	5	ASN
1	C	204	ASN
1	C	231	GLN
1	D	89	ASN
1	D	204	ASN

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	301/400 (75%)	-0.05	0 100 100	24, 50, 65, 82	0
1	B	303/400 (75%)	-0.10	0 100 100	25, 53, 72, 81	0
1	C	298/400 (74%)	0.00	3 (1%) 82 72	26, 55, 68, 81	0
1	D	299/400 (74%)	0.28	13 (4%) 35 22	25, 56, 73, 83	0
All	All	1201/1600 (75%)	0.03	16 (1%) 77 65	24, 54, 70, 83	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	GLY	4.6
1	D	189	VAL	3.9
1	D	187	VAL	3.4
1	D	163	ASP	2.8
1	D	162	LEU	2.8
1	C	379	SER	2.7
1	D	151	LEU	2.6
1	D	68	ILE	2.5
1	D	135	LEU	2.4
1	D	159	VAL	2.3
1	D	141	ILE	2.3
1	D	157	VAL	2.3
1	C	334	ARG	2.3
1	D	156	GLY	2.2
1	C	296	TYR	2.0
1	D	285	PRO	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.