



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:18 PM UTC

PDB ID : 3FFS / pdb_00003ffs
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

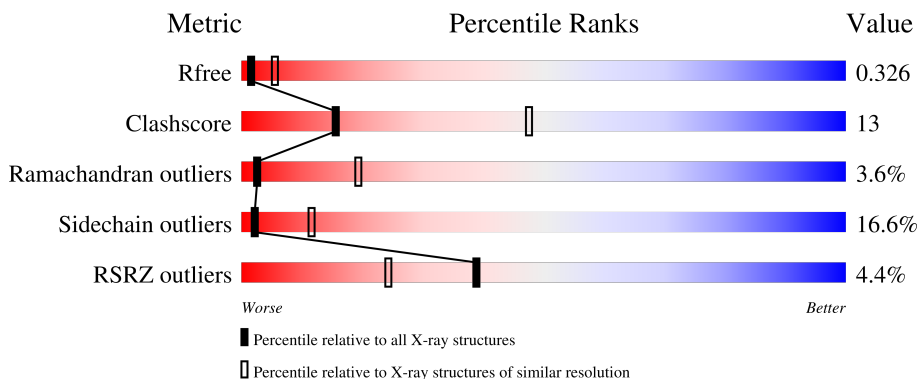
1 Overall quality at a glance i

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	 3% 51% 20% 5% 25%
1	B	400	 2% 51% 21% 5% 24%
1	C	400	 2% 46% 24% 5% 26%
1	D	400	 6% 47% 22% 6% 25%

2 Entry composition

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

4 Data and refinement statistics

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 48.34 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.34-3.19) 99.4 (48.34-3.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 3.19Å)	Xtrriage
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	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.73	0/2206	1.05	4/2976 (0.1%)
1	B	0.74	2/2211 (0.1%)	1.06	5/2994 (0.2%)
1	C	0.78	0/2155	1.08	11/2909 (0.4%)
1	D	0.81	2/2060 (0.1%)	1.05	7/2803 (0.2%)
All	All	0.77	4/8632 (0.0%)	1.06	27/11682 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	SER	C-N	-7.15	1.24	1.33
1	B	164	SER	C-O	5.76	1.31	1.23
1	D	55	GLU	CA-C	5.55	1.55	1.52
1	D	290	LEU	C-O	5.42	1.31	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	SER	CA-C-N	8.27	130.17	119.84
1	D	284	SER	C-N-CA	8.27	130.17	119.84
1	C	205	GLY	N-CA-C	8.16	122.31	113.58
1	C	284	SER	CA-C-N	7.51	129.22	119.84
1	C	284	SER	C-N-CA	7.51	129.22	119.84
1	C	204	ASN	N-CA-C	6.78	118.10	108.54
1	D	247	ILE	N-CA-C	6.52	114.00	107.55
1	B	185	ILE	N-CA-C	6.46	122.79	109.34
1	B	164	SER	CA-C-O	-6.31	114.06	121.44
1	C	141	ILE	CA-C-O	-6.08	115.37	121.45
1	C	18	VAL	CA-C-N	6.00	127.33	119.84
1	C	18	VAL	C-N-CA	6.00	127.33	119.84
1	B	247	ILE	N-CA-C	5.94	112.96	107.56
1	C	18	VAL	N-CA-C	5.91	113.92	107.60
1	A	231	GLN	N-CA-C	5.60	117.06	111.07
1	B	89	ASN	N-CA-C	5.60	116.43	108.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	GLN	N-CA-C	5.58	117.05	111.07
1	D	270	SER	N-CA-C	-5.57	106.61	113.41
1	A	189	VAL	N-CA-C	5.49	116.02	108.12
1	D	54	THR	N-CA-C	5.44	118.33	107.62
1	D	191	ASN	N-CA-C	5.40	118.27	110.28
1	A	295	VAL	N-CA-C	5.21	115.59	107.99
1	A	53	VAL	N-CA-C	5.17	116.34	111.48
1	C	371	SER	N-CA-C	5.12	116.98	108.02
1	D	169	SER	N-CA-C	5.04	115.02	108.07
1	B	364	ILE	N-CA-C	-5.02	105.53	111.00
1	C	187	VAL	N-CA-C	5.01	115.34	108.12

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	53	0
1	B	2190	0	2189	67	0
1	C	2140	0	2157	63	0
1	D	2043	0	1945	58	0
All	All	8561	0	8550	229	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 13.

All (229) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:SER:HA	1:D:273:MET:HE2	1.57	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:179:ILE:HG23	1:C:183:MET:HE2	1.70	0.74
1:D:62:MET:CE	1:D:341:MET:HE2	2.18	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:62:MET:HE2	1:D:341:MET:HE2	1.69	0.73
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:D:204:ASN:N	1:D:204:ASN:ND2	2.38	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
1:B:334:ARG:HD2	1:B:334:ARG:C	2.24	0.62
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ1	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:B:334:ARG:C	1:B:334:ARG:HH11	2.10	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:21:TYR:C	1:B:21:TYR:CD2	2.80	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: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: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
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:C:372:SER:HB3	1:D:6:ILE:CD1	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:356:MET:HE1	1:C:364:ILE:HG12	1.91	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:A:61:GLY:C	1:A:341:MET:HE1	2.37	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:C:245:PHE:C	1:C:247:ILE:H	2.20	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:D:56:HIS:C	1:D:58:MET:H	2.21	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

Continued on next page...

Continued from previous page...

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:D:243:SER:C	1:D:245:PHE:N	2.71	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:A:75:MET:HE1	1:A:83:GLU:HG3	1.95	0.47
1:C:85:LEU:O	1:C:89:ASN:HB2	2.15	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:D:62:MET:HE3	1:D:341:MET:HE2	1.95	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:B:243:SER:C	1:B:245:PHE:H	2.23	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:356:MET:HE1	1:D:364:ILE:HG13	1.98	0.45
1:B:21:TYR:C	1:B:21:TYR:HD2	2.24	0.45
1:C:35:LEU:HD11	1:C:188:ILE:HD11	1.98	0.45
1:D:243:SER:C	1:D:245:PHE:H	2.24	0.45
1:D:357:GLY:O	1:D:358:TYR:C	2.58	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:D:62:MET:HE2	1:D:341:MET:CE	2.45	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:D:61:GLY:C	1:D:341:MET:HE1	2.42	0.45
1:C:46:ILE:HD11	1:C:250:ILE:CG2	2.47	0.44
1:A:130:ASP:C	1:A:132:LYS:H	2.24	0.44
1:D:56:HIS:C	1:D:58:MET:N	2.75	0.44
1:A:209:ILE:O	1:A:209:ILE:HG12	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:HG13	1:B:43:ILE:O	2.17	0.44
1:A:239:SER:O	1:A:240:SER:C	2.60	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:D:131:ASN:C	1:D:133:GLY:H	2.26	0.43
1:D:377:THR:O	1:D:378:THR:C	2.61	0.43
1:B:142:GLY:O	1:B:143:VAL:C	2.61	0.43
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.18	0.43
1:B:23:GLU:HG2	1:C:170:LEU:HB2	1.99	0.43
1:C:46:ILE:HG13	1:C:273:MET:HE3	2.01	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:C:153:VAL:HG21	1:C:183:MET:HE3	2.01	0.43
1:D:203:GLU:C	1:D:205:GLY:H	2.27	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:B:15:ILE:CG2	1:B:16:LEU:N	2.83	0.42
1:D:64:ARG:HD3	1:D:64:ARG:C	2.45	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: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: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:D:174:ARG:C	1:D:176:LEU:N	2.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:32:GLU:HG2	1:B:42:LYS:HA	2.03	0.41
1:C:88:LYS:HE2	1:C:130:ASP:OD1	2.20	0.40
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:C:47:SER:N	1:C:62:MET:HE2	2.37	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:C:65:LEU:HD12	1:C:341:MET:HE1	2.03	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

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%)	9 39
1	B	295/400 (74%)	262 (89%)	25 (8%)	8 (3%)	4 25
1	C	286/400 (72%)	231 (81%)	43 (15%)	12 (4%)	2 16
1	D	287/400 (72%)	223 (78%)	46 (16%)	18 (6%)	1 8
All	All	1159/1600 (72%)	978 (84%)	139 (12%)	42 (4%)	2 19

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
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%)	191 (82%)	42 (18%)	2	9
1	B	230/334 (69%)	195 (85%)	35 (15%)	3	14
1	C	224/334 (67%)	189 (84%)	35 (16%)	2	13
1	D	194/334 (58%)	160 (82%)	34 (18%)	2	10
All	All	881/1336 (66%)	735 (83%)	146 (17%)	2	11

All (146) 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	141	ILE
1	A	143	VAL
1	A	146	ILE
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	213	ILE
1	A	223	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	ILE
1	A	233	THR
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
1	A	341	MET
1	A	354	SER
1	A	359	LEU
1	A	364	ILE
1	A	366	GLU
1	A	372	SER
1	A	374	VAL
1	B	5	ASN
1	B	11	THR
1	B	25	LEU
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	71	ILE
1	B	76	ASP
1	B	137	VAL
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	195	GLU
1	B	198	THR
1	B	200	GLU
1	B	203	GLU
1	B	209	ILE
1	B	239	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	243	SER
1	B	249	ILE
1	B	258	SER
1	B	277	ILE
1	B	287	GLU
1	B	288	LYS
1	B	290	LEU
1	B	334	ARG
1	B	352	LEU
1	B	359	LEU
1	B	366	GLU
1	C	5	ASN
1	C	6	ILE
1	C	11	THR
1	C	13	GLU
1	C	15	ILE
1	C	25	LEU
1	C	29	VAL
1	C	35	LEU
1	C	38	ASN
1	C	41	LEU
1	C	46	ILE
1	C	55	GLU
1	C	73	LYS
1	C	85	LEU
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	183	MET
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	249	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	334	ARG
1	C	349	VAL
1	C	354	SER
1	C	371	SER
1	D	15	ILE
1	D	24	VAL
1	D	25	LEU
1	D	46	ILE
1	D	47	SER
1	D	55	GLU
1	D	64	ARG
1	D	71	ILE
1	D	73	LYS
1	D	89	ASN
1	D	91	ILE
1	D	129	LEU
1	D	161	VAL
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	249	ILE
1	D	257	TYR
1	D	276	SER
1	D	277	ILE
1	D	291	ILE
1	D	293	ASP
1	D	341	MET
1	D	348	LEU
1	D	349	VAL
1	D	352	LEU
1	D	356	MET
1	D	366	GLU
1	D	372	SER
1	D	377	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	131	ASN
1	A	184	ASN
1	B	20	ASN
1	B	82	ASN
1	B	168	HIS
1	B	171	ASN
1	B	231	GLN
1	C	56	HIS
1	C	74	ASN
1	C	191	ASN
1	C	204	ASN
1	C	231	GLN
1	D	89	ASN
1	D	166	HIS
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 oligosaccharides 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%)	0.43	12 (3%) 42 26	24, 50, 65, 82	0
1	B	303/400 (75%)	0.37	8 (2%) 57 37	25, 53, 72, 81	0
1	C	298/400 (74%)	0.45	10 (3%) 48 30	26, 55, 68, 81	0
1	D	299/400 (74%)	0.77	23 (7%) 19 13	25, 56, 73, 83	0
All	All	1201/1600 (75%)	0.51	53 (4%) 39 24	24, 54, 70, 83	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	GLY	4.9
1	C	379	SER	4.8
1	C	91	ILE	4.7
1	A	91	ILE	4.7
1	C	225	ALA	3.9
1	D	91	ILE	3.8
1	A	225	ALA	3.5
1	D	291	ILE	3.3
1	D	160	ILE	3.3
1	D	151	LEU	3.2
1	A	261	ILE	3.0
1	D	130	ASP	2.9
1	B	183	MET	2.9
1	D	163	ASP	2.8
1	D	80	GLN	2.8
1	D	223	ILE	2.8
1	D	90	TRP	2.7
1	D	189	VAL	2.7
1	B	67	GLY	2.7
1	A	379	SER	2.7
1	C	365	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	223	ILE	2.5
1	D	183	MET	2.5
1	B	189	VAL	2.5
1	D	206	ALA	2.5
1	B	228	GLY	2.3
1	D	147	GLU	2.3
1	A	226	GLY	2.3
1	C	183	MET	2.3
1	A	256	ARG	2.3
1	D	76	ASP	2.2
1	A	298	TYR	2.2
1	D	149	ALA	2.2
1	D	124	TYR	2.2
1	D	159	VAL	2.2
1	B	92	SER	2.2
1	C	46	ILE	2.2
1	C	57	LEU	2.2
1	B	143	VAL	2.1
1	A	146	ILE	2.1
1	B	131	ASN	2.1
1	C	213	ILE	2.1
1	D	186	ASP	2.1
1	A	190	GLY	2.1
1	D	43	ILE	2.1
1	C	371	SER	2.0
1	A	123	ALA	2.0
1	D	142	GLY	2.0
1	D	236	GLU	2.0
1	D	287	GLU	2.0
1	B	223	ILE	2.0
1	A	163	ASP	2.0
1	A	355	CYS	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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.