



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 2PC4 / pdb_00002pc4
Title : Crystal structure of fructose-bisphosphate aldolase from Plasmodium falciparum in complex with TRAP-tail determined at 2.4 angstrom resolution
Authors : Bosch, J.; Buscaglia, C.A.; Krumm, B.; Cardozo, T.; Nussenzweig, V.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2007-03-29
Resolution : 2.40 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
Xtriage (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

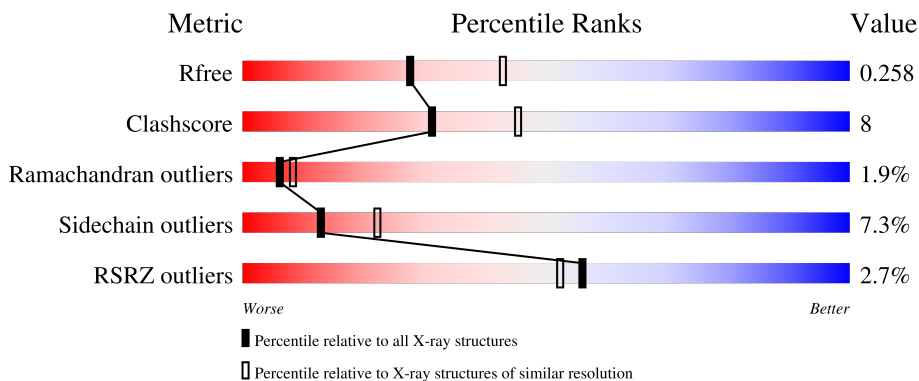
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	369	 2% 79% 15% . .
1	B	369	 4% 73% 18% . 5%
1	C	369	 3% 79% 17% . .
1	D	369	 1% 73% 19% . 5%
2	H	6	 33% 17% 50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11457 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2749	1741	476	522	10	0	1	0
1	B	351	2688	1702	466	510	10	0	2	0
1	C	365	2781	1757	484	530	10	0	1	0
1	D	351	2689	1702	467	510	10	0	2	0

- Molecule 2 is a protein called PbTRAP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	H	3	31	19	5	7	0	0	0

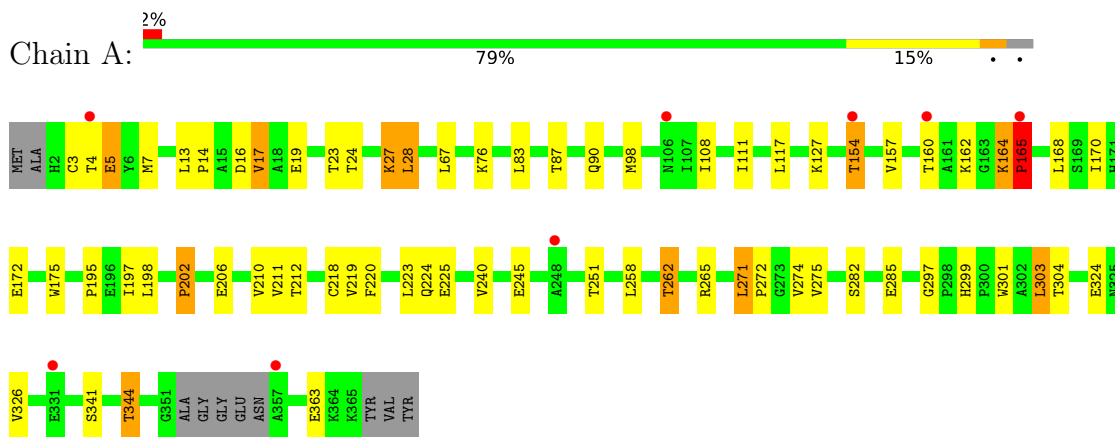
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total 127	O 127	0	0
3	B	131	Total 131	O 131	0	0
3	C	134	Total 134	O 134	0	0
3	D	125	Total 125	O 125	0	0
3	H	2	Total 2	O 2	0	0

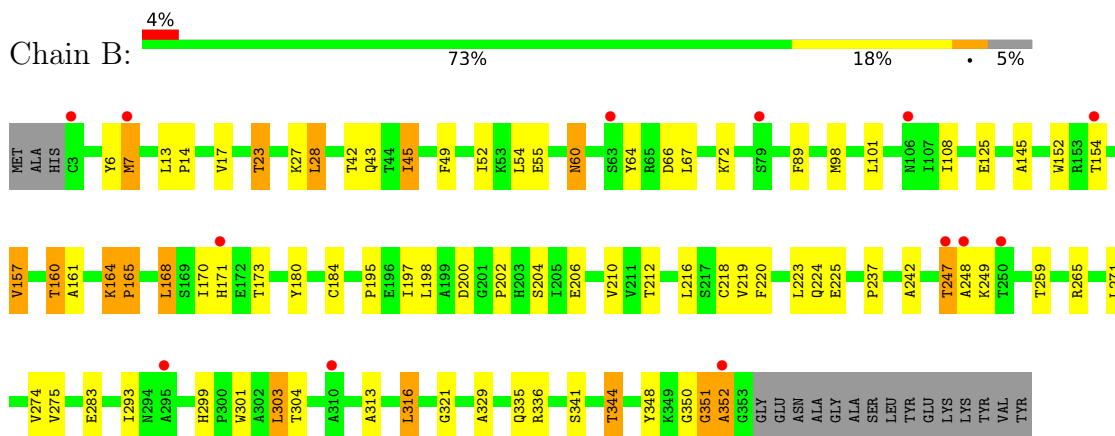
3 Residue-property plots [i](#)

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.

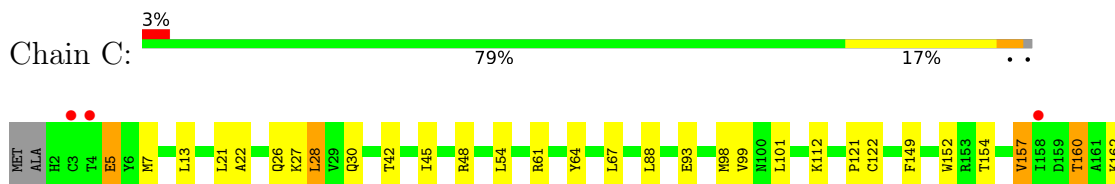
- Molecule 1: Fructose-bisphosphate aldolase

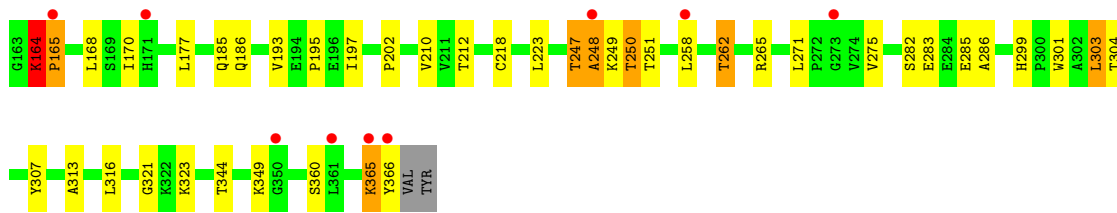


- Molecule 1: Fructose-bisphosphate aldolase

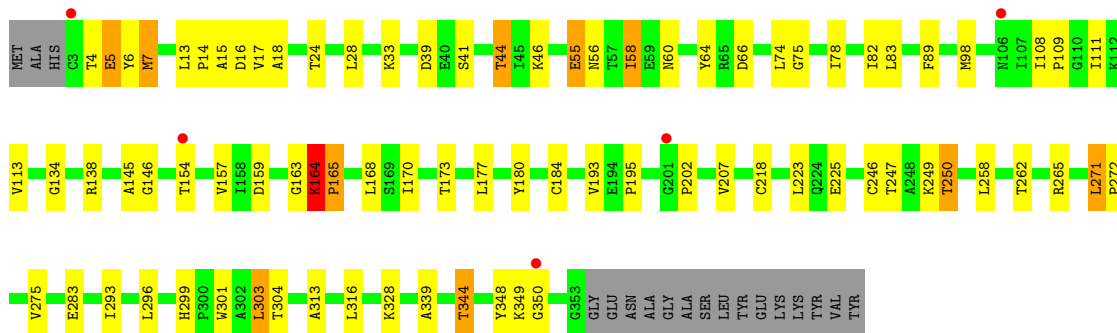
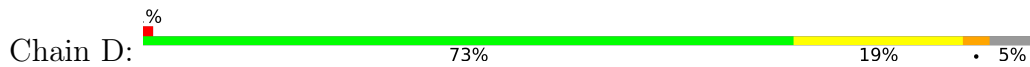


- Molecule 1: Fructose-bisphosphate aldolase

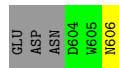
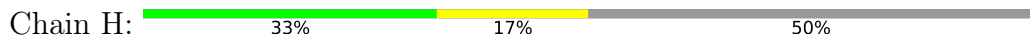




● Molecule 1: Fructose-bisphosphate aldolase



● Molecule 2: PbTRAP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.39Å 145.52Å 148.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.40 19.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.97-2.40) 94.5 (19.97-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.250 0.206 , 0.258	Depositor DCC
R_{free} test set	3164 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.750	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.010 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11457	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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	0.56	0/2798	0.81	3/3788 (0.1%)
1	B	0.55	0/2740	0.81	2/3713 (0.1%)
1	C	0.55	0/2831	0.81	3/3837 (0.1%)
1	D	0.54	0/2740	0.80	2/3712 (0.1%)
2	H	0.49	0/32	0.43	0/42
All	All	0.55	0/11141	0.81	10/15092 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	LYS	CA-C-N	8.82	130.86	119.84
1	C	164	LYS	C-N-CA	8.82	130.86	119.84
1	B	164	LYS	CA-C-N	8.68	130.68	119.84
1	B	164	LYS	C-N-CA	8.68	130.68	119.84
1	A	164	LYS	CA-C-N	7.99	129.83	119.84
1	A	164	LYS	C-N-CA	7.99	129.83	119.84
1	D	164	LYS	CA-C-N	-6.23	112.06	119.84
1	D	164	LYS	C-N-CA	-6.23	112.06	119.84
1	C	164	LYS	N-CA-C	5.29	121.49	109.81
1	A	165	PRO	N-CA-C	-5.12	101.92	112.47

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	LYS	Peptide
1	A	297	GLY	Peptide
1	A	363	GLU	Peptide
1	B	164	LYS	Peptide
1	C	164	LYS	Peptide
1	C	249	LYS	Peptide
1	D	164	LYS	Peptide

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	2749	0	2805	43	0
1	B	2688	0	2744	57	0
1	C	2781	0	2811	41	0
1	D	2689	0	2750	53	0
2	H	31	0	19	0	0
3	A	127	0	0	4	0
3	B	131	0	0	6	0
3	C	134	0	0	5	0
3	D	125	0	0	3	0
3	H	2	0	0	0	0
All	All	11457	0	11129	181	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 8.

All (181) 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:204:SER:HA	1:B:247:THR:HG21	1.26	1.10
1:D:157:VAL:O	1:D:165:PRO:HD3	1.51	1.10
1:C:258:LEU:O	1:C:262:THR:HG23	1.54	1.08
1:A:258:LEU:O	1:A:262:THR:HG23	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:O	1:B:165:PRO:CD	2.17	0.92
1:B:157:VAL:O	1:B:165:PRO:HD3	1.70	0.91
1:C:250:THR:HG21	3:C:401:HOH:O	1.77	0.84
1:D:262:THR:HG22	3:D:383:HOH:O	1.82	0.79
1:B:6:TYR:HA	1:C:160:THR:HG22	1.70	0.73
1:B:157:VAL:O	1:B:165:PRO:HD2	1.87	0.73
1:D:164:LYS:O	1:D:165:PRO:C	2.34	0.71
1:B:170:ILE:HG22	1:B:218:CYS:SG	2.32	0.69
1:D:275:VAL:HG12	1:D:304:THR:HG23	1.73	0.69
1:A:258:LEU:O	1:A:262:THR:CG2	2.42	0.68
1:A:90:GLN:HB3	1:A:98:MET:HE2	1.76	0.68
1:B:219:VAL:O	1:B:223:LEU:HD13	1.95	0.67
1:C:262:THR:HG22	3:C:388:HOH:O	1.94	0.67
1:C:157:VAL:O	1:C:164:LYS:O	2.13	0.67
1:D:299:HIS:CD2	1:D:303:LEU:HD22	2.30	0.66
1:B:242:ALA:HB1	1:B:247:THR:HG22	1.77	0.66
1:D:177:LEU:HD22	1:D:193:VAL:HG13	1.78	0.65
1:B:160:THR:HG23	1:C:5:GLU:O	1.97	0.64
1:A:23:THR:HG23	1:A:27:LYS:NZ	2.13	0.64
1:D:250:THR:O	1:D:250:THR:HG23	1.97	0.64
1:D:163:GLY:O	1:D:164:LYS:O	2.15	0.63
1:D:55:GLU:O	1:D:60:ASN:ND2	2.30	0.63
1:A:14:PRO:HB2	1:A:17:VAL:HG12	1.82	0.62
1:A:154:THR:HG22	3:A:370:HOH:O	1.99	0.62
1:A:165:PRO:HD2	1:D:6:TYR:CE1	2.35	0.62
1:B:23:THR:HG21	3:B:375:HOH:O	2.00	0.62
1:A:160:THR:HG21	1:D:4:THR:O	2.00	0.61
1:A:5:GLU:HB2	1:D:207:VAL:HG22	1.82	0.61
1:B:161:ALA:HB2	3:B:452:HOH:O	2.00	0.61
1:B:299:HIS:CD2	1:B:303:LEU:HD22	2.36	0.60
1:A:87:THR:HG23	1:A:98:MET:CE	2.32	0.60
1:A:157:VAL:HG22	1:A:198:LEU:HD12	1.82	0.60
1:B:351:GLY:O	1:B:352:ALA:CB	2.50	0.60
1:D:66:ASP:HA	1:D:98:MET:HE1	1.84	0.60
1:B:54:LEU:HD23	1:B:60:ASN:HD21	1.65	0.59
1:A:271:LEU:HD22	1:A:272:PRO:HD2	1.85	0.59
1:B:6:TYR:CE1	1:C:165:PRO:HD2	2.37	0.59
1:B:242:ALA:HB1	1:B:247:THR:CG2	2.33	0.58
1:B:154:THR:HG21	3:B:369:HOH:O	2.03	0.58
1:C:13:LEU:HD21	3:C:395:HOH:O	2.03	0.58
1:A:23:THR:HG23	1:A:27:LYS:HZ3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG22	1:A:218:CYS:SG	2.44	0.57
1:D:299:HIS:CG	1:D:303:LEU:HD22	2.40	0.57
1:B:275:VAL:HG12	1:B:304:THR:HG23	1.85	0.57
1:B:28:LEU:HD13	1:B:108:ILE:HD12	1.87	0.57
1:D:154:THR:HG21	3:D:369:HOH:O	2.05	0.56
1:B:66:ASP:HA	1:B:98:MET:HE1	1.87	0.56
1:A:299:HIS:CD2	1:A:303:LEU:HD22	2.41	0.56
1:C:64:TYR:CZ	1:C:316:LEU:HD13	2.40	0.56
1:B:54:LEU:HD21	1:B:321:GLY:HA3	1.87	0.55
1:C:54:LEU:HD22	1:C:321:GLY:HA3	1.89	0.55
1:B:168:LEU:HA	1:B:171[A]:HIS:CE1	2.42	0.55
1:D:33:LYS:HE2	1:D:75:GLY:O	2.07	0.54
1:D:41:SER:OG	1:D:44:THR:HG23	2.08	0.54
1:C:283:GLU:CD	1:C:313:ALA:HB3	2.32	0.54
1:A:87:THR:HG23	1:A:98:MET:HE1	1.89	0.54
1:A:162:LYS:C	1:B:7:MET:HG2	2.33	0.54
1:C:88:LEU:HD12	1:C:99:VAL:HG11	1.90	0.54
1:C:247:THR:O	1:C:248:ALA:HB2	2.07	0.54
3:A:489:HOH:O	1:B:7:MET:HE2	2.08	0.53
1:A:117:LEU:HD22	1:A:127:LYS:HB3	1.90	0.53
1:B:206:GLU:O	1:B:210:VAL:HG23	2.09	0.53
1:C:162:LYS:C	1:D:7:MET:HG2	2.33	0.52
3:B:373:HOH:O	1:C:210:VAL:HG21	2.10	0.52
1:D:271:LEU:HD22	1:D:272:PRO:HD2	1.92	0.52
1:C:48:ARG:HB3	1:C:316:LEU:HD21	1.91	0.51
1:A:157:VAL:CG2	1:A:198:LEU:HD12	2.39	0.51
1:B:98:MET:CE	1:B:101:LEU:HD12	2.40	0.51
1:A:13:LEU:HD11	3:A:403:HOH:O	2.10	0.51
1:C:28:LEU:HD21	1:C:149:PHE:CD1	2.46	0.51
1:C:152:TRP:CD1	1:C:177:LEU:HD23	2.47	0.50
1:A:282:SER:OG	1:A:285:GLU:HG2	2.11	0.50
1:B:299:HIS:CG	1:B:303:LEU:HD22	2.46	0.50
1:C:170:ILE:HG22	1:C:218:CYS:SG	2.51	0.50
1:B:52:ILE:HD12	1:B:54:LEU:HD13	1.93	0.50
1:D:74:LEU:HD11	1:D:78:ILE:HD12	1.94	0.50
1:C:67:LEU:C	1:C:67:LEU:HD23	2.37	0.50
1:C:42:THR:HG23	1:C:61:ARG:NH1	2.27	0.50
1:D:170:ILE:HG22	1:D:218:CYS:SG	2.52	0.50
1:C:365:LYS:O	1:C:366:TYR:CB	2.60	0.49
1:D:109:PRO:HG2	1:D:146:GLY:O	2.13	0.49
1:C:299:HIS:CD2	1:C:303:LEU:HD22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:THR:O	1:D:28:LEU:HD13	2.12	0.49
1:D:154:THR:OG1	1:D:173:THR:HG23	2.13	0.49
1:C:64:TYR:CE1	1:C:316:LEU:HD13	2.48	0.49
1:A:219:VAL:O	1:A:223:LEU:HD13	2.14	0.48
1:B:348:TYR:CZ	1:B:350:GLY:HA2	2.48	0.48
1:C:286:ALA:HB1	1:C:307:TYR:CE2	2.47	0.48
1:D:66:ASP:CA	1:D:98:MET:HE1	2.43	0.48
1:D:39:ASP:HB3	1:D:82:ILE:HG22	1.96	0.48
1:D:344:THR:CG2	3:D:370:HOH:O	2.62	0.48
1:B:23:THR:HG22	3:B:424:HOH:O	2.13	0.48
1:B:98:MET:HE3	1:B:101:LEU:HD12	1.96	0.48
1:D:258:LEU:O	1:D:262:THR:HG23	2.13	0.48
1:A:202:PRO:HD2	3:A:456:HOH:O	2.14	0.47
1:D:339:ALA:HB1	1:D:348:TYR:CE1	2.49	0.47
1:B:45:ILE:HD11	1:B:49:PHE:CZ	2.50	0.47
1:B:204:SER:HA	1:B:247:THR:CG2	2.19	0.47
1:D:293:ILE:HG22	1:D:303:LEU:HD23	1.96	0.47
1:C:275:VAL:HG12	1:C:304:THR:HG23	1.96	0.47
1:C:247:THR:O	1:C:248:ALA:CB	2.62	0.47
1:C:98:MET:HA	1:C:101:LEU:HD12	1.97	0.47
1:D:14:PRO:HB2	1:D:17:VAL:HG12	1.96	0.47
1:B:67:LEU:HD11	1:B:329:ALA:CB	2.45	0.46
1:C:22:ALA:O	1:C:26:GLN:HG2	2.16	0.46
1:C:27:LYS:HA	1:C:30:GLN:HG3	1.97	0.46
1:D:89:PHE:CE1	1:D:145:ALA:HB2	2.51	0.46
1:A:67:LEU:HD12	1:A:326:VAL:HG22	1.98	0.46
1:C:282:SER:OG	1:C:285:GLU:HG2	2.16	0.46
1:C:112:LYS:NZ	3:C:374:HOH:O	2.48	0.46
1:D:163:GLY:C	1:D:164:LYS:O	2.57	0.46
1:C:177:LEU:HD22	1:C:193:VAL:HG13	1.98	0.46
1:B:64:TYR:OH	1:B:316:LEU:HD22	2.16	0.46
1:D:164:LYS:HB3	1:D:165:PRO:CD	2.46	0.46
1:A:28:LEU:HD13	1:A:108:ILE:HD12	1.99	0.45
1:B:247:THR:HG23	1:B:247:THR:O	2.15	0.45
1:D:64:TYR:CE1	1:D:316:LEU:HD12	2.51	0.45
1:B:198:LEU:HB3	1:B:200:ASP:OD2	2.16	0.45
1:C:154:THR:HG21	3:C:371:HOH:O	2.16	0.45
1:B:220:PHE:O	1:B:224:GLN:HG2	2.17	0.45
1:B:64:TYR:OH	1:B:316:LEU:CD2	2.65	0.44
1:B:67:LEU:HD11	1:B:329:ALA:HB3	1.99	0.44
1:D:74:LEU:CD1	1:D:78:ILE:HD12	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:CE1	1:B:184:CYS:SG	3.10	0.44
1:B:283:GLU:OE2	1:B:313:ALA:HB3	2.18	0.44
1:A:83:LEU:O	1:A:111:ILE:HD12	2.18	0.44
1:C:197:ILE:CD1	1:C:212:THR:HA	2.48	0.44
1:D:28:LEU:HD12	1:D:108:ILE:HD12	1.99	0.44
1:A:275:VAL:HG12	1:A:304:THR:HG23	1.99	0.44
1:C:275:VAL:HG23	1:C:275:VAL:O	2.18	0.44
1:B:275:VAL:O	1:B:275:VAL:HG23	2.17	0.44
1:D:113:VAL:O	1:D:138[B]:ARG:NH2	2.51	0.44
1:A:240:VAL:HG21	1:A:262:THR:HG21	2.00	0.44
1:A:206:GLU:O	1:A:210:VAL:HG23	2.18	0.43
1:C:21:LEU:HD13	1:C:185:GLN:HG2	1.99	0.43
1:A:175:TRP:HH2	1:B:171[A]:HIS:CE1	2.36	0.43
1:A:197:ILE:CD1	1:A:212:THR:HA	2.49	0.43
1:B:237:PRO:HD3	1:B:274:VAL:HG13	2.00	0.43
1:A:160:THR:HG21	1:D:4:THR:HG23	2.01	0.43
1:A:67:LEU:C	1:A:67:LEU:HD23	2.44	0.43
1:A:220:PHE:O	1:A:224:GLN:HG2	2.19	0.43
1:A:341:SER:O	1:A:344:THR:HB	2.18	0.43
1:B:54:LEU:CD2	1:B:321:GLY:HA3	2.49	0.43
1:A:165:PRO:HG2	1:A:211:VAL:HG13	2.01	0.43
1:B:154:THR:OG1	1:B:173:THR:HG23	2.18	0.43
1:C:121:PRO:O	1:C:122:CYS:HB2	2.19	0.43
1:C:299:HIS:CG	1:C:303:LEU:HD22	2.53	0.43
1:D:159:ASP:HB3	1:D:164:LYS:HB2	2.01	0.43
1:A:274:VAL:HB	1:A:303:LEU:HD12	2.01	0.42
3:B:437:HOH:O	1:C:210:VAL:HG22	2.19	0.42
1:D:283:GLU:CD	1:D:313:ALA:HB3	2.44	0.42
1:B:14:PRO:HG2	1:B:17:VAL:HG22	2.00	0.42
1:A:275:VAL:O	1:A:275:VAL:HG23	2.19	0.42
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.91	0.42
1:C:45:ILE:HG21	1:C:61:ARG:HD3	2.01	0.42
1:B:64:TYR:CE1	1:B:316:LEU:HD13	2.55	0.42
1:B:259:THR:HB	1:B:293:ILE:CD1	2.50	0.42
1:A:160:THR:CG2	1:D:5:GLU:O	2.68	0.42
1:B:42:THR:HA	1:B:45:ILE:HG22	2.02	0.42
1:B:341:SER:O	1:B:344:THR:HB	2.20	0.42
1:D:46:LYS:HD2	1:D:56:ASN:HD22	1.85	0.41
1:A:24:THR:HG22	1:A:28:LEU:HD22	2.01	0.41
1:A:165:PRO:CD	1:D:6:TYR:CE1	3.03	0.41
1:D:14:PRO:O	1:D:15:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASP:H	1:D:164:LYS:HB2	1.84	0.41
1:A:299:HIS:CG	1:A:303:LEU:HD22	2.56	0.41
1:B:89:PHE:CE1	1:B:145:ALA:HB2	2.56	0.41
1:D:180:TYR:CE1	1:D:184:CYS:SG	3.14	0.41
1:A:160:THR:HG23	1:D:5:GLU:O	2.21	0.41
1:D:58:ILE:O	1:D:58:ILE:HD13	2.21	0.41
1:B:152:TRP:HB3	1:B:180:TYR:CE2	2.56	0.40
1:D:28:LEU:CD1	1:D:108:ILE:HD12	2.51	0.40
1:D:134:GLY:O	1:D:138[A]:ARG:HG3	2.21	0.40
1:D:13:LEU:HB2	1:D:18:ALA:HB2	2.03	0.40
1:B:197:ILE:CD1	1:B:212:THR:HA	2.51	0.40
1:B:351:GLY:O	1:B:352:ALA:HB3	2.22	0.40
1:D:83:LEU:O	1:D:111:ILE:HD12	2.21	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	356/369 (96%)	334 (94%)	18 (5%)	4 (1%)	11	18
1	B	351/369 (95%)	326 (93%)	17 (5%)	8 (2%)	5	6
1	C	364/369 (99%)	336 (92%)	22 (6%)	6 (2%)	7	11
1	D	351/369 (95%)	326 (93%)	16 (5%)	9 (3%)	4	4
2	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1423/1482 (96%)	1323 (93%)	73 (5%)	27 (2%)	6	8

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	THR

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Mol	Chain	Res	Type
1	B	165	PRO
1	B	247	THR
1	B	352	ALA
1	C	247	THR
1	C	248	ALA
1	C	365	LYS
1	D	164	LYS
1	D	349	LYS
1	A	165	PRO
1	C	165	PRO
1	D	165	PRO
1	B	351	GLY
1	D	246	CYS
1	B	248	ALA
1	D	250	THR
1	D	350	GLY
1	B	160	THR
1	C	202	PRO
1	D	296	LEU
1	B	195	PRO
1	D	195	PRO
1	A	195	PRO
1	B	202	PRO
1	C	195	PRO
1	A	202	PRO
1	D	202	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/298 (98%)	271 (92%)	22 (8%)	12	21
1	B	287/298 (96%)	264 (92%)	23 (8%)	11	19
1	C	293/298 (98%)	272 (93%)	21 (7%)	13	23
1	D	287/298 (96%)	269 (94%)	18 (6%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	3/6 (50%)	2 (67%)	1 (33%)	0	0
All	All	1163/1198 (97%)	1078 (93%)	85 (7%)	13	22

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	5	GLU
1	A	7	MET
1	A	16	ASP
1	A	17	VAL
1	A	19	GLU
1	A	27	LYS
1	A	28	LEU
1	A	76	LYS
1	A	154	THR
1	A	168	LEU
1	A	172	GLU
1	A	225	GLU
1	A	245	GLU
1	A	251	THR
1	A	262	THR
1	A	265	ARG
1	A	271	LEU
1	A	301	TRP
1	A	303	LEU
1	A	324	GLU
1	A	344	THR
1	B	7	MET
1	B	13	LEU
1	B	23	THR
1	B	27	LYS
1	B	28	LEU
1	B	43	GLN
1	B	45	ILE
1	B	55	GLU
1	B	60	ASN
1	B	72	LYS
1	B	125	GLU
1	B	157	VAL
1	B	168	LEU
1	B	225	GLU

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Mol	Chain	Res	Type
1	B	249	LYS
1	B	265	ARG
1	B	271	LEU
1	B	301	TRP
1	B	303	LEU
1	B	316	LEU
1	B	335	GLN
1	B	336	ARG
1	B	344	THR
1	C	5	GLU
1	C	7	MET
1	C	28	LEU
1	C	93	GLU
1	C	157	VAL
1	C	160	THR
1	C	164	LYS
1	C	168	LEU
1	C	186	GLN
1	C	223	LEU
1	C	250	THR
1	C	251	THR
1	C	262	THR
1	C	265	ARG
1	C	271	LEU
1	C	301	TRP
1	C	303	LEU
1	C	323	LYS
1	C	344	THR
1	C	349	LYS
1	C	360	SER
1	D	5	GLU
1	D	7	MET
1	D	16	ASP
1	D	44	THR
1	D	55	GLU
1	D	58	ILE
1	D	164	LYS
1	D	168	LEU
1	D	223	LEU
1	D	225	GLU
1	D	247	THR
1	D	249	LYS

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Mol	Chain	Res	Type
1	D	265	ARG
1	D	271	LEU
1	D	301	TRP
1	D	303	LEU
1	D	328	LYS
1	D	344	THR
2	H	606	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	GLN
1	B	203	HIS
1	B	226	ASN
1	C	213	GLN
1	C	317	ASN
1	D	56	ASN
1	D	213	GLN
1	D	226	ASN
1	D	281	GLN
1	D	289	ASN
1	D	320	GLN

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

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, 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	359/369 (97%)	0.35	8 (2%) 62 58	42, 66, 83, 111	1 (0%)
1	B	351/369 (95%)	0.57	13 (3%) 45 41	39, 66, 88, 97	2 (0%)
1	C	365/369 (98%)	0.46	12 (3%) 49 45	33, 66, 89, 105	1 (0%)
1	D	351/369 (95%)	0.29	5 (1%) 73 69	36, 65, 81, 95	2 (0%)
2	H	3/6 (50%)	0.98	0 100 100	51, 51, 53, 54	3 (100%)
All	All	1429/1482 (96%)	0.42	38 (2%) 56 52	33, 66, 86, 111	9 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	365	LYS	5.8
1	B	247	THR	4.9
1	C	366	TYR	4.8
1	B	154	THR	4.7
1	D	154	THR	4.5
1	C	171[A]	HIS	3.2
1	B	310	ALA	2.9
1	A	357	ALA	2.8
1	D	201	GLY	2.7
1	C	158	ILE	2.7
1	B	7	MET	2.6
1	A	248	ALA	2.6
1	B	248	ALA	2.5
1	C	248	ALA	2.5
1	D	350	GLY	2.4
1	A	4	THR	2.4
1	C	361	LEU	2.4
1	B	3	CYS	2.4
1	C	4	THR	2.3
1	B	63	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	2.3
1	B	79	SER	2.3
1	B	171[A]	HIS	2.3
1	B	106	ASN	2.2
1	C	3	CYS	2.2
1	C	165	PRO	2.2
1	A	165	PRO	2.2
1	C	258	LEU	2.1
1	C	273	GLY	2.1
1	A	154	THR	2.1
1	A	160	THR	2.1
1	B	250	THR	2.1
1	A	331	GLU	2.1
1	A	106	ASN	2.1
1	D	106	ASN	2.1
1	D	3	CYS	2.0
1	B	295	ALA	2.0
1	C	350	GLY	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.