



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:25 AM UTC

PDB ID : 2EPH / pdb_00002eph
Title : Crystal structure of fructose-bisphosphate aldolase from Plasmodium falciparum in complex with TRAP-tail determined at 2.7 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 : 2007-03-30
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

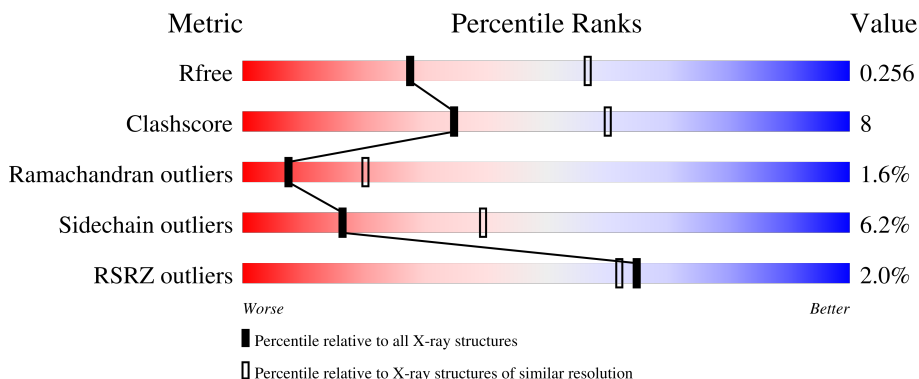
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% (poor fit), 77% (0 outliers), 18% (1 outlier), 3% (2 outliers), 2% (3+ outliers)
1	B	369	 2% (poor fit), 73% (0 outliers), 19% (1 outlier), 5% (2 outliers)
1	C	369	 2% (poor fit), 80% (0 outliers), 16% (1 outlier), 2% (2 outliers), 2% (3+ outliers)
1	D	369	 0% (poor fit), 78% (0 outliers), 14% (1 outlier), 5% (2 outliers)
2	H	6	 33% (poor fit), 50% (0 outliers), 17% (1 outlier)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11239 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.

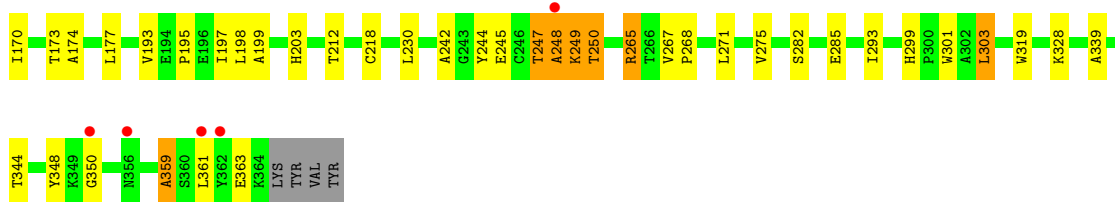
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2742	1739	473	521	9	0	0	0
1	B	349	2675	1694	462	509	10	0	1	0
1	C	363	2771	1753	480	528	10	0	1	0
1	D	351	2684	1700	465	509	10	0	1	0

- Molecule 2 is a protein called PbTRAP.

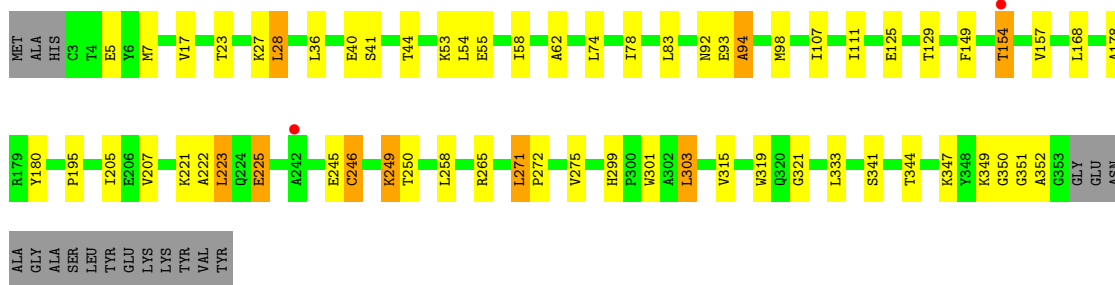
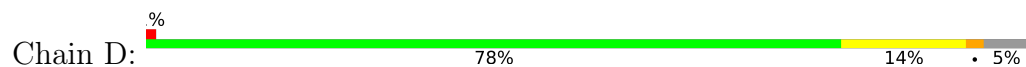
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	H	3	31	19	5	7	0	0	0

- Molecule 3 is water.

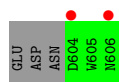
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total 77	O 77	0	0
3	B	83	Total 83	O 83	0	0
3	C	87	Total 87	O 87	0	0
3	D	88	Total 88	O 88	0	0
3	H	1	Total 1	O 1	0	0



- Molecule 1: Fructose-bisphosphate aldolase



- Molecule 2: PbTRAP



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.02Å 146.16Å 148.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.70 19.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-2.70) 97.7 (19.97-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.250 0.199 , 0.256	Depositor DCC
R_{free} test set	2150 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtrriage
Anisotropy	0.904	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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	0.54	0/2788	0.78	1/3775 (0.0%)
1	B	0.51	0/2723	0.75	0/3690
1	C	0.54	0/2821	0.76	2/3822 (0.1%)
1	D	0.54	0/2732	0.77	0/3701
2	H	0.38	0/32	0.47	0/42
All	All	0.53	0/11096	0.76	3/15030 (0.0%)

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	1
1	C	1	0
All	All	1	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	ALA	N-CA-C	7.08	125.87	110.80
1	A	364	LYS	N-CA-C	5.32	122.13	110.80
1	C	267	VAL	N-CA-C	5.12	112.62	107.55

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	359	ALA	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	GLU	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	2742	0	2797	47	0
1	B	2675	0	2730	54	0
1	C	2771	0	2820	37	0
1	D	2684	0	2745	33	0
2	H	31	0	19	0	0
3	A	77	0	0	6	0
3	B	83	0	0	16	0
3	C	87	0	0	3	0
3	D	88	0	0	6	0
3	H	1	0	0	0	0
All	All	11239	0	11111	166	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 (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:HB2	3:A:376:HOH:O	1.05	1.19
1:D:78:ILE:HG22	3:D:389:HOH:O	1.47	1.12
1:B:78:ILE:HG23	3:B:438:HOH:O	1.46	1.10
1:C:174:ALA:HB2	3:C:415:HOH:O	1.61	0.98
1:B:228:VAL:HG21	3:B:439:HOH:O	1.63	0.97
1:A:129:THR:OG1	1:A:154:THR:HG22	1.71	0.90
1:B:299:HIS:CD2	1:B:303:LEU:HD22	2.08	0.89
1:B:23:THR:HG22	1:B:27:LYS:HE2	1.54	0.88
1:C:74:LEU:HD11	1:C:78:ILE:HD12	1.63	0.80
1:A:129:THR:OG1	1:A:154:THR:CG2	2.33	0.77
1:A:299:HIS:CD2	1:A:303:LEU:HD22	2.20	0.76
1:B:295:ALA:HB2	3:B:429:HOH:O	1.89	0.73
1:C:122:CYS:SG	3:C:436:HOH:O	2.45	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:MET:HE2	1:C:101:LEU:HD12	1.71	0.72
1:B:28:LEU:HD13	1:B:108:ILE:HD12	1.73	0.70
1:A:87:THR:HG23	1:A:98:MET:CE	2.21	0.70
1:B:88:LEU:HD11	3:B:390:HOH:O	1.91	0.69
1:D:349:LYS:O	1:D:351:GLY:N	2.27	0.65
1:D:98:MET:HA	1:D:98:MET:HE2	1.78	0.65
1:A:36:LEU:HB2	1:A:78:ILE:HD13	1.79	0.64
1:B:73:GLY:O	3:B:369:HOH:O	2.15	0.63
1:A:156:LEU:HD11	1:A:173:THR:HG21	1.80	0.63
1:C:299:HIS:CD2	1:C:303:LEU:HD22	2.34	0.62
1:A:160:THR:HG21	3:D:400:HOH:O	1.98	0.62
1:C:39:ASP:HB3	1:C:82:ILE:HG22	1.82	0.62
1:D:23:THR:HG22	1:D:27:LYS:HE2	1.81	0.61
1:C:247:THR:O	1:C:248:ALA:HB2	1.99	0.61
1:A:134:GLY:H	1:B:130:GLN:HE22	1.49	0.60
1:B:67:LEU:C	1:B:67:LEU:HD23	2.26	0.60
1:A:90:GLN:HB3	1:A:98:MET:HE2	1.83	0.60
1:A:87:THR:HG23	1:A:98:MET:HE3	1.83	0.60
1:B:202:PRO:O	1:B:247:THR:HG23	2.03	0.59
1:D:36:LEU:HB2	1:D:78:ILE:HD13	1.85	0.58
1:C:275:VAL:HG23	1:C:275:VAL:O	2.03	0.58
1:D:250:THR:O	1:D:250:THR:HG23	2.04	0.57
1:D:40:GLU:HB3	1:D:44:THR:HG23	1.86	0.57
1:A:275:VAL:O	1:A:275:VAL:HG23	2.05	0.57
1:B:64:TYR:OH	1:B:316:LEU:HD21	2.05	0.57
1:B:199:ALA:HB3	1:B:244:TYR:CZ	2.40	0.56
1:B:154:THR:HG21	3:B:377:HOH:O	2.06	0.56
1:B:28:LEU:CD1	1:B:108:ILE:HD12	2.34	0.56
1:C:28:LEU:HD13	1:C:108:ILE:HD12	1.89	0.55
1:D:154:THR:HG21	3:D:370:HOH:O	2.05	0.55
1:D:275:VAL:HG23	1:D:275:VAL:O	2.06	0.55
1:A:299:HIS:CG	1:A:303:LEU:HD22	2.41	0.55
1:D:74:LEU:HD11	1:D:78:ILE:HD12	1.89	0.55
1:B:38:ALA:HB3	3:B:406:HOH:O	2.07	0.55
1:C:247:THR:HG21	1:C:249:LYS:HE3	1.89	0.55
1:B:275:VAL:O	1:B:275:VAL:HG23	2.07	0.54
1:A:74:LEU:HD11	1:A:78:ILE:HD12	1.90	0.54
1:A:251:THR:HG22	1:A:252:THR:H	1.72	0.54
1:C:28:LEU:HD21	1:C:149:PHE:CD1	2.43	0.54
1:C:199:ALA:HB3	1:C:244:TYR:CZ	2.43	0.54
1:B:170:ILE:HG22	1:B:218:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:O	1:B:329:ALA:N	2.34	0.54
1:C:36:LEU:HB2	1:C:78:ILE:HD13	1.91	0.53
1:C:66:ASP:HA	1:C:98:MET:HE1	1.90	0.53
1:B:98:MET:HA	1:B:98:MET:HE2	1.90	0.53
1:C:67:LEU:C	1:C:67:LEU:HD23	2.33	0.53
1:A:14:PRO:HG2	1:A:17:VAL:HG13	1.91	0.52
1:D:249:LYS:O	1:D:250:THR:HG22	2.08	0.52
1:D:315:VAL:HG21	1:D:333:LEU:HD13	1.90	0.52
1:A:267:VAL:N	3:A:442:HOH:O	2.42	0.52
1:A:199:ALA:HB3	1:A:244:TYR:CZ	2.44	0.52
1:B:301:TRP:CE3	1:B:303:LEU:HD11	2.44	0.52
1:A:220:PHE:O	1:A:224:GLN:HG2	2.10	0.52
1:C:92:ASN:HB3	1:C:98:MET:HE3	1.92	0.52
1:B:329:ALA:HA	3:B:410:HOH:O	2.08	0.52
1:B:202:PRO:O	1:B:247:THR:CG2	2.57	0.52
1:B:74:LEU:HD23	1:B:107:ILE:HD11	1.92	0.51
1:A:28:LEU:HD13	1:A:108:ILE:HD12	1.92	0.51
1:D:62:ALA:HB3	1:D:93:GLU:OE2	2.11	0.51
1:D:92:ASN:OD1	1:D:94:ALA:HB3	2.10	0.51
1:B:83:LEU:O	1:B:111:ILE:HD12	2.10	0.51
1:B:147:ALA:N	3:B:390:HOH:O	2.41	0.51
1:C:157[B]:VAL:HG12	1:C:198:LEU:HD12	1.92	0.51
1:D:222:ALA:HB2	3:D:447:HOH:O	2.11	0.50
1:A:156:LEU:HD22	1:A:215:VAL:HG21	1.94	0.50
1:B:301:TRP:HE3	1:B:303:LEU:HD11	1.77	0.49
1:C:170:ILE:HG22	1:C:218:CYS:SG	2.53	0.49
1:B:221:LYS:NZ	1:B:225:GLU:OE2	2.34	0.49
1:B:52:ILE:HD12	1:B:320:GLN:HA	1.94	0.49
1:B:246:CYS:O	1:B:247:THR:HG23	2.12	0.49
1:B:11:LYS:HB3	1:B:11:LYS:NZ	2.27	0.48
1:B:344:THR:HG22	3:B:387:HOH:O	2.11	0.48
1:B:223:LEU:HG	3:B:439:HOH:O	2.12	0.48
1:D:299:HIS:CD2	1:D:303:LEU:HD22	2.48	0.48
1:D:83:LEU:O	1:D:111:ILE:HD12	2.14	0.48
1:D:341:SER:O	1:D:344:THR:HB	2.14	0.48
1:A:4:THR:HG22	3:A:397:HOH:O	2.14	0.48
1:B:177:LEU:HD22	1:B:193:VAL:HG13	1.95	0.48
1:B:220:PHE:O	1:B:224:GLN:HG2	2.13	0.47
1:A:249:LYS:NZ	3:A:434:HOH:O	2.46	0.47
1:B:271:LEU:HD22	1:B:272:PRO:HD2	1.97	0.47
1:D:221:LYS:NZ	1:D:225:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:CD1	1:C:212:THR:HA	2.45	0.47
1:D:107:ILE:HG23	3:D:389:HOH:O	2.15	0.47
1:B:219:VAL:O	1:B:223:LEU:HD13	2.15	0.46
1:A:326:VAL:O	1:A:330:ARG:HG2	2.15	0.46
1:D:271:LEU:HD22	1:D:272:PRO:HD2	1.97	0.46
1:B:71:THR:HG23	1:B:330:ARG:HB3	1.97	0.46
1:C:282:SER:OG	1:C:285:GLU:HG2	2.16	0.46
1:D:54:LEU:HD13	1:D:321:GLY:HA3	1.98	0.46
1:A:83:LEU:O	1:A:111:ILE:HD12	2.15	0.46
1:C:66:ASP:CA	1:C:98:MET:HE1	2.45	0.46
1:A:5:GLU:HB2	1:D:207:VAL:HG22	1.98	0.46
1:B:45:ILE:HD13	1:B:61:ARG:HD2	1.98	0.46
1:A:223:LEU:HD23	1:A:230:LEU:HD21	1.97	0.45
1:A:316:LEU:HD22	3:A:407:HOH:O	2.17	0.45
1:A:199:ALA:HB3	1:A:244:TYR:CE2	2.51	0.45
1:C:74:LEU:CD1	1:C:78:ILE:HD12	2.42	0.45
1:C:247:THR:O	1:C:248:ALA:CB	2.62	0.45
1:C:230:LEU:HD13	1:C:268:PRO:HG2	1.99	0.45
1:B:77:PHE:N	3:B:369:HOH:O	2.49	0.44
1:B:64:TYR:OH	1:B:316:LEU:CD2	2.64	0.44
1:D:28:LEU:HD21	1:D:149:PHE:CG	2.52	0.44
1:B:81:ALA:HB1	3:B:406:HOH:O	2.17	0.44
1:A:87:THR:HG23	1:A:98:MET:HE1	1.96	0.44
1:D:41:SER:OG	1:D:44:THR:HG22	2.18	0.44
1:A:311:LEU:HD21	1:A:340:ASN:HD22	1.82	0.44
1:A:13:LEU:HG	1:A:17:VAL:CG2	2.48	0.44
1:A:162:LYS:C	1:B:7:MET:HG2	2.43	0.44
1:A:231:GLU:OE2	1:D:265:ARG:HD3	2.18	0.43
1:C:339:ALA:HB1	1:C:348:TYR:CE1	2.53	0.43
1:D:205:ILE:HG23	1:D:258:LEU:HD13	1.99	0.43
1:A:55:GLU:HG3	1:A:57:THR:HG23	1.99	0.43
1:C:27:LYS:HA	1:C:30:GLN:HG3	2.00	0.43
1:D:249:LYS:NZ	1:D:249:LYS:HA	2.34	0.43
1:A:4:THR:OG1	1:A:7:MET:HE2	2.18	0.43
1:C:158:ILE:HD12	1:C:203:HIS:CE1	2.53	0.43
1:B:120:ILE:HG21	1:B:168:LEU:HD13	1.99	0.43
1:B:293:ILE:CG2	1:B:303:LEU:HD23	2.49	0.43
1:D:129:THR:OG1	1:D:154:THR:HG22	2.18	0.43
1:D:245:GLU:O	1:D:246:CYS:SG	2.77	0.43
1:B:88:LEU:HD21	3:B:390:HOH:O	2.17	0.42
1:A:183:ILE:O	1:A:187:ASN:ND2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:HA	1:B:98:MET:HE1	2.01	0.42
1:C:28:LEU:HD12	1:C:28:LEU:HA	1.88	0.42
1:C:293:ILE:CG2	1:C:303:LEU:HD23	2.49	0.42
1:D:178:ALA:HA	1:D:223:LEU:HD12	2.02	0.42
1:C:249:LYS:CD	1:C:250:THR:H	2.32	0.42
1:D:315:VAL:HG23	3:D:415:HOH:O	2.19	0.42
1:A:237:PRO:HD3	1:A:274:VAL:HG13	2.01	0.42
1:C:28:LEU:HD21	1:C:149:PHE:CG	2.55	0.42
1:C:106:ASN:ND2	3:C:450:HOH:O	2.53	0.42
1:A:23:THR:HG22	1:A:27:LYS:HE2	2.02	0.41
1:B:237:PRO:HD3	1:B:274:VAL:HG13	2.02	0.41
1:B:307:TYR:HB3	1:B:310:ALA:HB3	2.01	0.41
1:A:341:SER:O	1:A:344:THR:HB	2.20	0.41
1:C:242:ALA:CB	1:C:250:THR:HG21	2.50	0.41
1:A:299:HIS:CD2	1:A:303:LEU:CD2	2.98	0.41
1:B:39:ASP:HB3	1:B:82:ILE:HG22	2.01	0.41
1:A:27:LYS:HA	1:A:30:GLN:HG3	2.02	0.41
1:A:129:THR:OG1	1:A:154:THR:HG23	2.19	0.41
1:A:162:LYS:HG2	1:B:7:MET:HE2	2.03	0.41
1:C:177:LEU:HB3	1:C:193:VAL:HG13	2.01	0.41
1:B:35:ILE:HA	3:B:438:HOH:O	2.21	0.41
1:B:92:ASN:HB3	1:B:98:MET:HE3	2.02	0.41
1:A:156:LEU:HD22	1:A:215:VAL:CG2	2.51	0.40
3:A:409:HOH:O	1:D:207:VAL:HG21	2.19	0.40
1:B:275:VAL:HG12	1:B:304:THR:HG23	2.03	0.40
1:C:14:PRO:HG2	1:C:17:VAL:HG13	2.04	0.40
1:A:62:ALA:HB2	1:A:90:GLN:NE2	2.37	0.40
1:C:154:THR:CB	1:C:173:THR:HG23	2.52	0.40
1:A:152:TRP:HB3	1:A:180:TYR:CE2	2.56	0.40
3:B:450:HOH:O	1:C:265:ARG:HD2	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	354/369 (96%)	333 (94%)	18 (5%)	3 (1%)	16	37
1	B	348/369 (94%)	326 (94%)	17 (5%)	5 (1%)	9	23
1	C	362/369 (98%)	335 (92%)	19 (5%)	8 (2%)	5	14
1	D	350/369 (95%)	327 (93%)	17 (5%)	6 (2%)	7	19
2	H	1/6 (17%)	0	1 (100%)	0	100	100
All	All	1415/1482 (96%)	1321 (93%)	72 (5%)	22 (2%)	7	20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	ALA
1	C	248	ALA
1	C	250	THR
1	C	359	ALA
1	D	94	ALA
1	D	350	GLY
1	A	364	LYS
1	B	54	LEU
1	B	249	LYS
1	D	352	ALA
1	B	247	THR
1	C	249	LYS
1	D	246	CYS
1	C	247	THR
1	A	319	TRP
1	A	365	LYS
1	C	319	TRP
1	D	195	PRO
1	D	319	TRP
1	C	195	PRO
1	C	350	GLY
1	B	195	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	291/298 (98%)	273 (94%)	18 (6%)	16	39
1	B	286/298 (96%)	269 (94%)	17 (6%)	18	42
1	C	294/298 (99%)	276 (94%)	18 (6%)	17	40
1	D	286/298 (96%)	267 (93%)	19 (7%)	15	36
2	H	3/6 (50%)	3 (100%)	0	100	100
All	All	1160/1198 (97%)	1088 (94%)	72 (6%)	16	39

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	28	LEU
1	A	44	THR
1	A	45	ILE
1	A	99	VAL
1	A	112	LYS
1	A	125	GLU
1	A	154	THR
1	A	168	LEU
1	A	180	TYR
1	A	225	GLU
1	A	265	ARG
1	A	271	LEU
1	A	278	SER
1	A	301	TRP
1	A	303	LEU
1	A	323	LYS
1	A	344	THR
1	B	7	MET
1	B	11	LYS
1	B	28	LEU
1	B	44	THR
1	B	47	LYS
1	B	78	ILE
1	B	125	GLU
1	B	130	GLN
1	B	157	VAL
1	B	168	LEU

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Mol	Chain	Res	Type
1	B	180	TYR
1	B	225	GLU
1	B	247	THR
1	B	253	GLN
1	B	271	LEU
1	B	301	TRP
1	B	323	LYS
1	C	7	MET
1	C	17	VAL
1	C	28	LEU
1	C	53	LYS
1	C	98	MET
1	C	114	ASP
1	C	125	GLU
1	C	160	THR
1	C	168	LEU
1	C	245	GLU
1	C	265	ARG
1	C	271	LEU
1	C	301	TRP
1	C	303	LEU
1	C	328	LYS
1	C	344	THR
1	C	361	LEU
1	C	363	GLU
1	D	5	GLU
1	D	7	MET
1	D	17	VAL
1	D	28	LEU
1	D	53	LYS
1	D	55	GLU
1	D	58	ILE
1	D	125	GLU
1	D	154	THR
1	D	157	VAL
1	D	168	LEU
1	D	180	TYR
1	D	223	LEU
1	D	225	GLU
1	D	249	LYS
1	D	271	LEU
1	D	301	TRP

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Mol	Chain	Res	Type
1	D	303	LEU
1	D	347	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	60	ASN
1	A	106	ASN
1	A	119	ASN
1	A	130	GLN
1	A	186	GLN
1	A	226	ASN
1	A	317	ASN
1	A	320	GLN
1	A	325	ASN
1	A	340	ASN
1	B	8	ASN
1	B	30	GLN
1	B	104	ASN
1	B	130	GLN
1	B	186	GLN
1	B	203	HIS
1	B	294	ASN
1	C	30	GLN
1	C	56	ASN
1	C	60	ASN
1	C	130	GLN
1	C	203	HIS
1	C	213	GLN
1	C	312	GLN
1	D	26	GLN
1	D	51	ASN
1	D	203	HIS
2	H	606	ASN

5.3.3 RNA

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	358/369 (97%)	0.14	7 (1%) 65 62	58, 70, 92, 129	0
1	B	349/369 (94%)	0.28	9 (2%) 57 54	40, 70, 92, 100	1 (0%)
1	C	363/369 (98%)	0.22	8 (2%) 62 59	40, 70, 90, 100	1 (0%)
1	D	351/369 (95%)	0.02	2 (0%) 85 85	39, 69, 86, 93	1 (0%)
2	H	3/6 (50%)	2.03	2 (66%) 0 0	38, 38, 41, 42	3 (100%)
All	All	1424/1482 (96%)	0.17	28 (1%) 65 62	38, 70, 90, 129	6 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	TYR	6.1
1	B	154	THR	3.7
1	B	3	CYS	3.0
1	C	248	ALA	3.0
1	B	350	GLY	2.9
1	A	267	VAL	2.9
2	H	606	ASN	2.8
1	A	365	LYS	2.7
1	D	154	THR	2.7
1	A	248	ALA	2.7
1	D	242	ALA	2.7
1	C	362	TYR	2.6
1	B	248	ALA	2.5
1	A	357	ALA	2.5
1	B	202	PRO	2.4
1	B	106	ASN	2.3
1	A	349	LYS	2.3
1	C	154	THR	2.2
1	B	273	GLY	2.2
1	C	361	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	35	ILE	2.2
1	C	356	ASN	2.1
1	C	104	ASN	2.1
2	H	604	ASP	2.1
1	B	247	THR	2.1
1	A	106	ASN	2.0
1	C	350	GLY	2.0
1	B	93	GLU	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.