



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 02:05 AM GMT

PDB ID : 2EPH  
Title : Crystal structure of fructose-bisphosphatealdolase 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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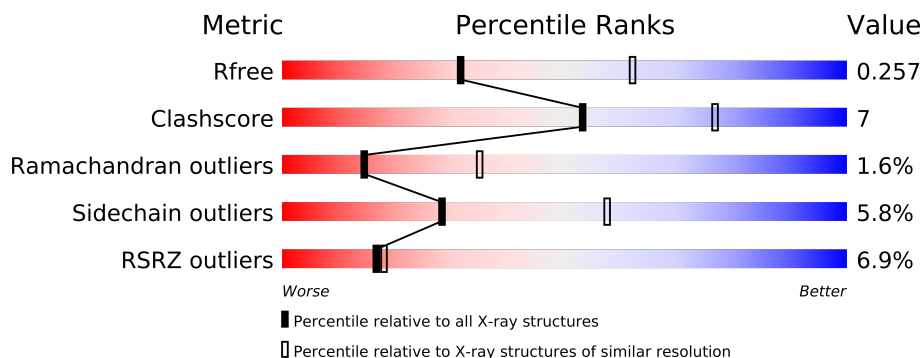
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	369	
1	B	369	
1	C	369	
1	D	369	
2	H	6	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11239 atoms, of which 0 are hydrogen and 0 are deuterium.

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-bisphosphatealdolase.

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

- Molecule 2 is a protein called PbTRAP.

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

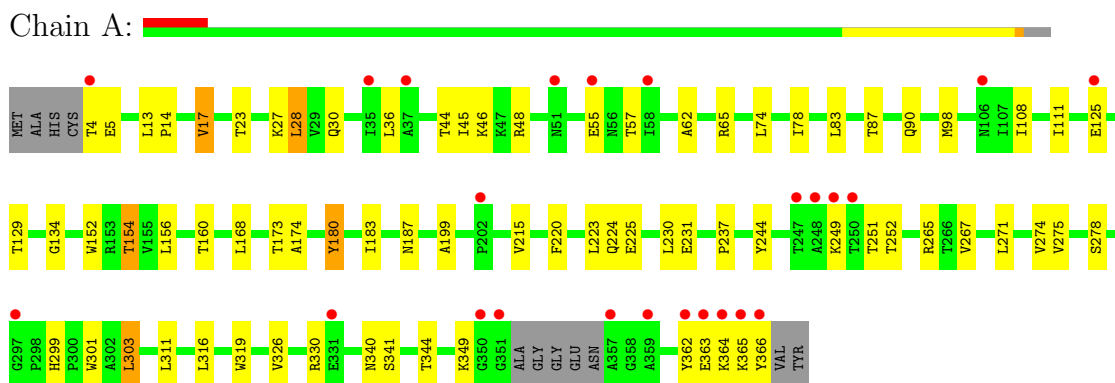
- Molecule 3 is water.

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

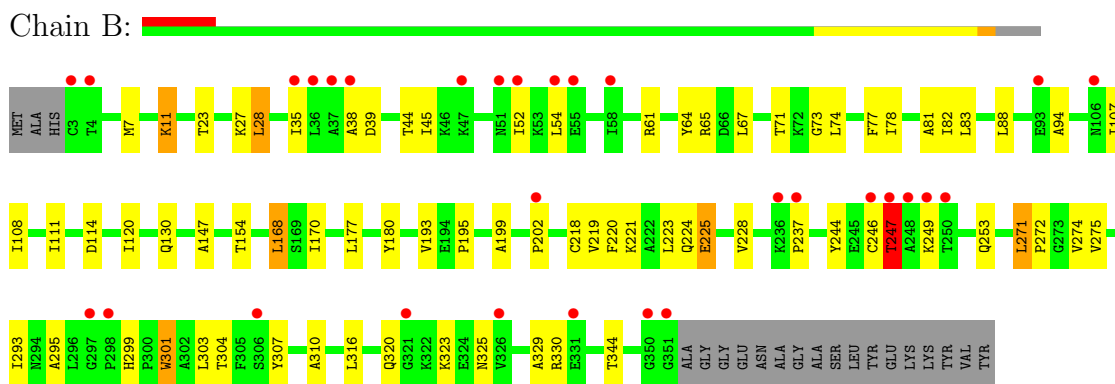
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

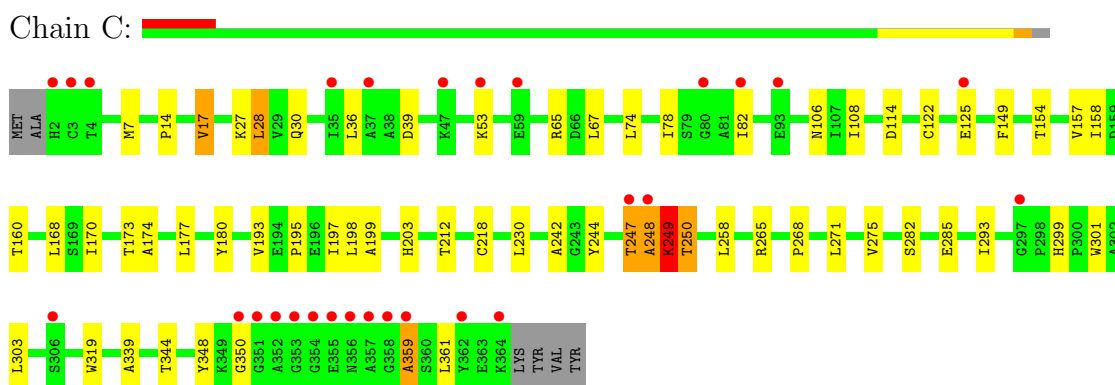
- Molecule 1: Fructose-bisphosphatealdolase



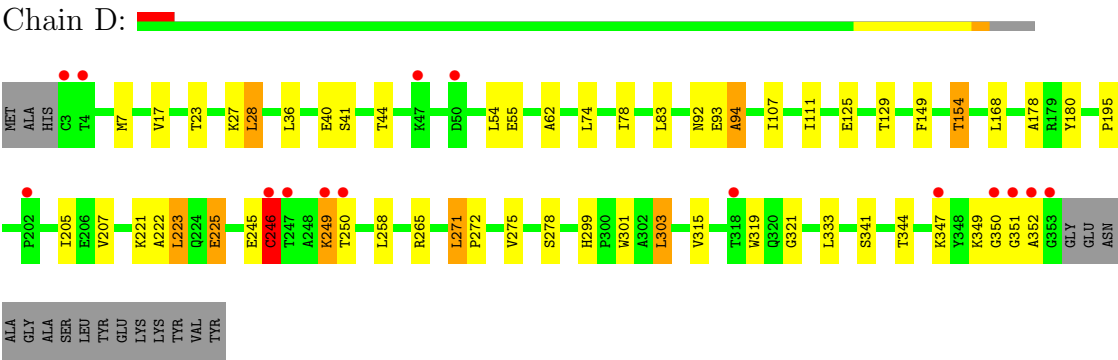
- Molecule 1: Fructose-bisphosphatealdolase



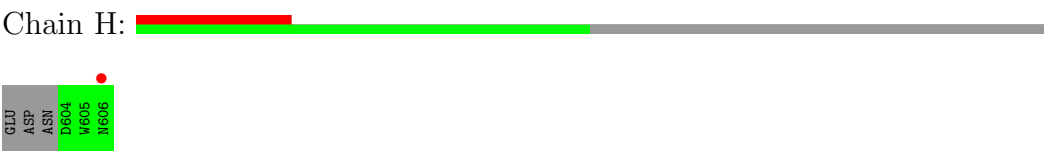
- Molecule 1: Fructose-bisphosphatealdolase



● Molecule 1: Fructose-bisphosphatealdolase



● Molecule 2: PbTRAP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.02Å 146.16Å 148.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.70 29.19 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-2.70) 97.7 (29.19-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.192 , 0.250 0.201 , 0.257	Depositor DCC
$R_{free}$ test set	2150 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 85.7	EDS
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 42686 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/2788	0.55	0/3775
1	B	0.40	0/2723	0.54	0/3690
1	C	0.41	0/2821	0.56	1/3822 (0.0%)
1	D	0.42	0/2732	0.56	0/3701
2	H	0.41	0/32	0.43	0/42
All	All	0.41	0/11096	0.55	1/15030 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	ALA	N-CA-C	5.51	125.87	111.00

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2742	0	2797	43	0
1	B	2675	0	2730	49	0
1	C	2771	0	2820	33	0
1	D	2684	0	2745	32	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	154	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:87:THR:HG23	1:A:98:MET:HE3	1.78	0.64
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: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:O	1:C:275:VAL:HG23	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:90:GLN:HB3	1:A:98:MET:HE2	1.87	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:67:LEU:C	1:B:67:LEU:HD23	2.26	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:D:74:LEU:HD11	1:D:78:ILE:HD12	1.89	0.55
1:A:299:HIS:CG	1:A:303:LEU:HD22	2.41	0.55
1:C:247:THR:HG21	1:C:249:LYS:HE3	1.89	0.55
1:B:38:ALA:HB3	3:B:406:HOH:O	2.07	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
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:D:249:LYS:O	1:D:250:THR:HG22	2.08	0.52
1:A:14:PRO:HG2	1:A:17:VAL:HG13	1.91	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:B:301:TRP:CE3	1:B:303:LEU:HD11	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:ALA:HB3	1:A:244:TYR:CZ	2.44	0.52
1:A:220:PHE:O	1:A:224:GLN:HG2	2.10	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:147:ALA:N	3:B:390:HOH:O	2.41	0.51
1:B:83:LEU:O	1:B:111:ILE:HD12	2.10	0.51
1:C:157[B]:VAL:HG12	1:C:198:LEU:HD12	1.92	0.51
1:D:221:LYS:NZ	1:D:225:GLU:OE2	2.32	0.50
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:246:CYS:O	1:B:247:THR:HG23	2.12	0.49
1:B:52:ILE:HD12	1:B:320:GLN:HA	1.94	0.49
1:B:11:LYS:NZ	1:B:11:LYS:HB3	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:C:67:LEU:HD23	1:C:67:LEU:C	2.33	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:B:177:LEU:HD22	1:B:193:VAL:HG13	1.95	0.48
1:A:4:THR:HG22	3:A:397:HOH:O	2.14	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:107:ILE:HG23	3:D:389:HOH:O	2.15	0.47
1:C:197:ILE:CD1	1:C:212:THR:HA	2.45	0.47
1:B:219:VAL:O	1:B:223:LEU:HD13	2.15	0.46
1:D:271:LEU:HD22	1:D:272:PRO:HD2	1.97	0.46
1:A:326:VAL:O	1:A:330:ARG:HG2	2.15	0.46
1:D:54:LEU:HD13	1:D:321:GLY:HA3	1.98	0.46
1:C:282:SER:OG	1:C:285:GLU:HG2	2.16	0.46
1:B:71:THR:HG23	1:B:330:ARG:HB3	1.97	0.46
1:A:83:LEU:O	1:A:111:ILE:HD12	2.15	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:199:ALA:HB3	1:A:244:TYR:CE2	2.51	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: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:231:GLU:OE2	1:D:265:ARG:HD3	2.18	0.43
1:D:205:ILE:HG23	1:D:258:LEU:HD13	1.99	0.43
1:C:339:ALA:HB1	1:C:348:TYR:CE1	2.53	0.43
1:D:249:LYS:NZ	1:D:249:LYS:HA	2.34	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: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
1:C:293:ILE:CG2	1:C:303:LEU:HD23	2.49	0.42
1:C:28:LEU:HA	1:C:28:LEU:HD12	1.88	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:C:28:LEU:HD21	1:C:149:PHE:CG	2.55	0.42
1:A:237:PRO:HD3	1:A:274:VAL:HG13	2.01	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:307:TYR:HB3	1:B:310:ALA:HB3	2.01	0.41
1:B:237:PRO:HD3	1:B:274:VAL:HG13	2.02	0.41
1:C:242:ALA:CB	1:C:250:THR:HG21	2.50	0.41
1:A:341:SER:O	1:A:344:THR:HB	2.20	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:129:THR:OG1	1:A:154:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:LYS:HA	1:A:30:GLN:HG3	2.02	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:A:156:LEU:HD22	1:A:215:VAL:CG2	2.51	0.40
1:B:275:VAL:HG12	1:B:304:THR:HG23	2.03	0.40
3:A:409:HOH:O	1:D:207:VAL:HG21	2.19	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

### 5.3.1 Protein backbone ⓘ

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%)	27	58
1	B	348/369 (94%)	326 (94%)	17 (5%)	5 (1%)	16	41
1	C	362/369 (98%)	335 (92%)	19 (5%)	8 (2%)	10	25
1	D	350/369 (95%)	327 (93%)	17 (5%)	6 (2%)	14	33
2	H	1/6 (17%)	0	1 (100%)	0	100	100
All	All	1415/1482 (96%)	1321 (93%)	72 (5%)	22 (2%)	14	35

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	271 (93%)	20 (7%)	22	48
1	B	286/298 (96%)	272 (95%)	14 (5%)	35	67
1	C	294/298 (99%)	278 (95%)	16 (5%)	31	61
1	D	286/298 (96%)	269 (94%)	17 (6%)	28	56
2	H	3/6 (50%)	3 (100%)	0	100	100
All	All	1160/1198 (97%)	1093 (94%)	67 (6%)	28	57

All (67) 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

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Mol	Chain	Res	Type
1	A	46	LYS
1	A	48	ARG
1	A	65	ARG
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	349	LYS
1	A	362	TYR
1	A	366	TYR
1	B	7	MET
1	B	11	LYS
1	B	28	LEU
1	B	44	THR
1	B	65	ARG
1	B	114	ASP
1	B	168	LEU
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	65	ARG
1	C	114	ASP
1	C	125	GLU
1	C	160	THR
1	C	168	LEU
1	C	180	TYR
1	C	249	LYS
1	C	258	LEU

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Mol	Chain	Res	Type
1	C	271	LEU
1	C	301	TRP
1	C	344	THR
1	C	361	LEU
1	D	7	MET
1	D	17	VAL
1	D	28	LEU
1	D	55	GLU
1	D	125	GLU
1	D	154	THR
1	D	168	LEU
1	D	180	TYR
1	D	223	LEU
1	D	225	GLU
1	D	246	CYS
1	D	249	LYS
1	D	271	LEU
1	D	278	SER
1	D	301	TRP
1	D	303	LEU
1	D	347	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	100	ASN
1	A	226	ASN
1	A	320	GLN
1	A	325	ASN
1	B	8	ASN
1	B	130	GLN
1	C	30	GLN
1	C	60	ASN
1	C	130	GLN
1	C	203	HIS
1	C	312	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	358/369 (97%)	0.15	24 (6%)	17 19	58, 70, 92, 129	0
1	B	349/369 (94%)	0.45	30 (8%)	11 11	59, 70, 92, 100	0
1	C	363/369 (98%)	0.28	28 (7%)	13 14	56, 70, 90, 100	0
1	D	351/369 (95%)	0.09	15 (4%)	34 38	55, 69, 86, 93	0
2	H	3/6 (50%)	1.41	1 (33%)	1 1	63, 63, 65, 68	3 (100%)
All	All	1424/1482 (96%)	0.25	98 (6%)	17 18	55, 70, 90, 129	3 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	GLY	12.2
1	C	354	GLY	10.9
1	B	3	CYS	10.7
1	C	356	ASN	10.2
1	A	366	TYR	8.7
1	C	353	GLY	8.7
1	D	351	GLY	8.1
1	D	350	GLY	7.8
1	C	355	GLU	7.4
1	D	3	CYS	7.4
1	C	248	ALA	7.4
1	D	353	GLY	7.3
1	B	248	ALA	6.8
1	D	249	LYS	6.5
1	D	352	ALA	6.4
1	A	351	GLY	6.3
1	C	352	ALA	6.2
1	C	351	GLY	6.0
1	B	247	THR	5.9
1	C	362	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	52	ILE	5.5
1	C	3	CYS	5.4
1	B	202	PRO	5.1
1	A	4	THR	4.7
1	A	357	ALA	4.6
1	D	247	THR	4.6
1	A	248	ALA	4.5
1	C	2	HIS	4.3
1	C	247	THR	4.1
1	C	4	THR	4.1
1	B	350	GLY	4.1
1	A	364	LYS	4.0
1	B	246	CYS	3.8
1	B	37	ALA	3.8
1	A	106	ASN	3.7
1	D	202	PRO	3.7
1	B	306	SER	3.7
1	B	250	THR	3.7
1	C	82	ILE	3.7
1	B	93	GLU	3.6
1	B	47	LYS	3.5
1	B	4	THR	3.5
1	A	247	THR	3.5
1	A	365	LYS	3.4
1	D	246	CYS	3.3
1	B	55	GLU	3.3
1	A	250	THR	3.3
1	A	350	GLY	3.3
1	D	4	THR	3.3
1	A	249	LYS	3.2
1	C	358	GLY	3.2
1	C	350	GLY	3.0
1	B	249	LYS	2.9
1	C	364	LYS	2.9
1	B	236	LYS	2.9
1	B	326	VAL	2.8
1	B	106	ASN	2.8
1	C	53	LYS	2.7
1	D	250	THR	2.7
1	A	55	GLU	2.6
1	C	357	ALA	2.6
1	C	93	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	359	ALA	2.6
1	B	54	LEU	2.5
1	A	362	TYR	2.5
1	B	237	PRO	2.5
1	A	35	ILE	2.5
1	C	80	GLY	2.5
1	A	331	GLU	2.5
1	C	37	ALA	2.5
1	B	297	GLY	2.4
1	A	51	ASN	2.4
1	A	297	GLY	2.3
1	D	318	THR	2.3
1	A	125	GLU	2.3
1	B	321	GLY	2.3
1	B	331	GLU	2.3
2	H	606	ASN	2.3
1	B	51	ASN	2.2
1	B	298	PRO	2.2
1	D	347	LYS	2.2
1	C	297	GLY	2.2
1	D	50	ASP	2.2
1	B	36	LEU	2.2
1	A	359	ALA	2.2
1	B	35	ILE	2.2
1	A	202	PRO	2.2
1	C	306	SER	2.2
1	C	47	LYS	2.2
1	C	59	GLU	2.1
1	C	125	GLU	2.1
1	A	37	ALA	2.1
1	B	58	ILE	2.1
1	B	38	ALA	2.1
1	D	47	LYS	2.1
1	A	58	ILE	2.1
1	C	35	ILE	2.1
1	A	363	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.