Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 10:55 PM EDT

PDB ID	:	2EPH
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

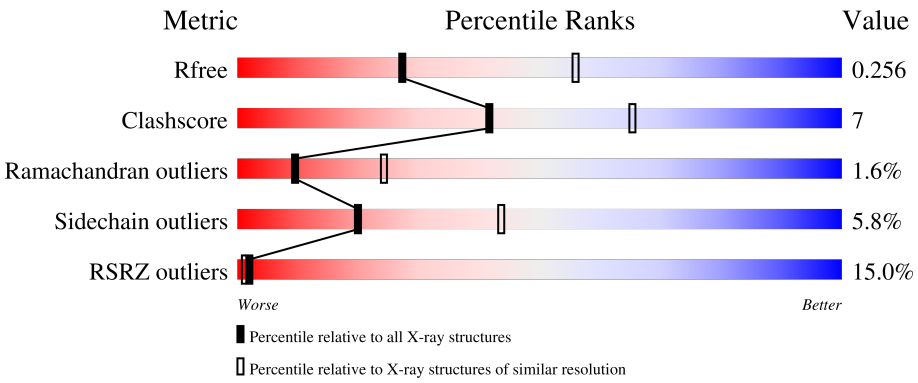
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	12% 77% 19% • •
1	B	369	20% 74% 18% • 5%
1	C	369	14% 81% 15% • •
1	D	369	12% 79% 13% • 5%
2	H	6	50% 50%

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.

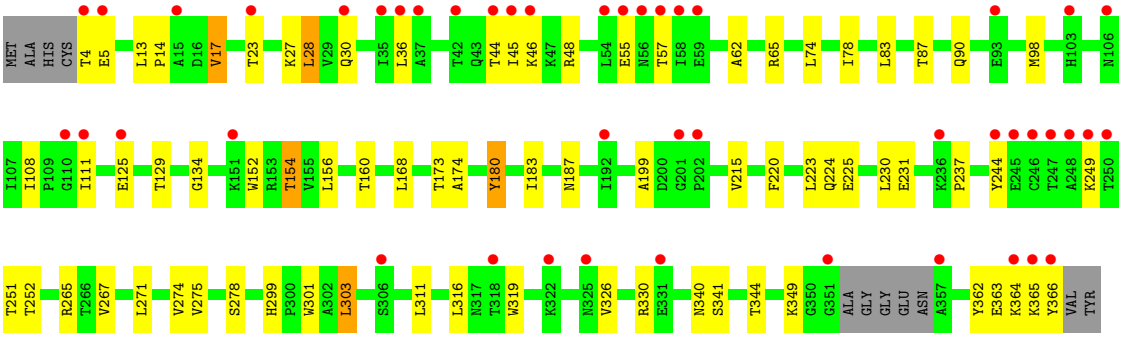
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	77	77	77	0	0
3	B	83	83	83	0	0
3	C	87	87	87	0	0
3	D	88	88	88	0	0
3	H	1	1	1	0	0

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.

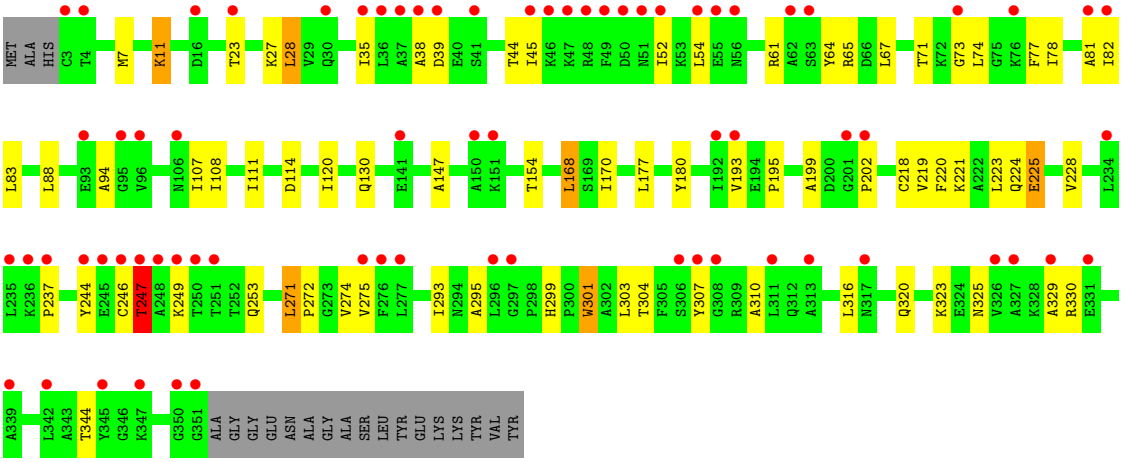
• Molecule 1: Fructose-bisphosphate aldolase

Chain A:



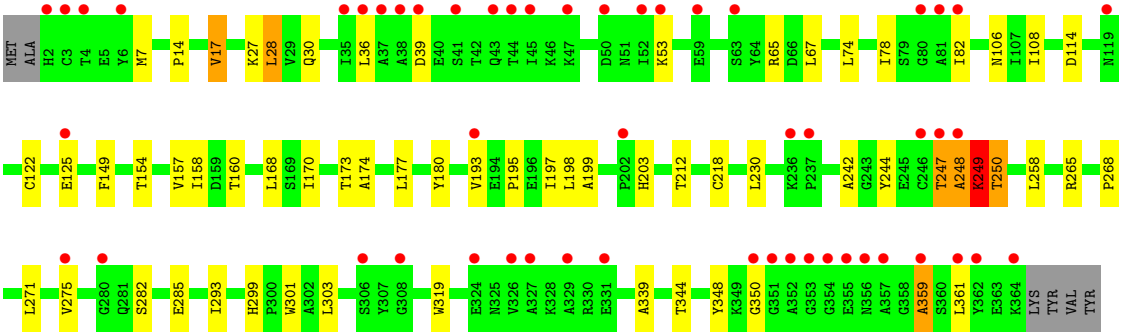
• Molecule 1: Fructose-bisphosphate aldolase

Chain B:



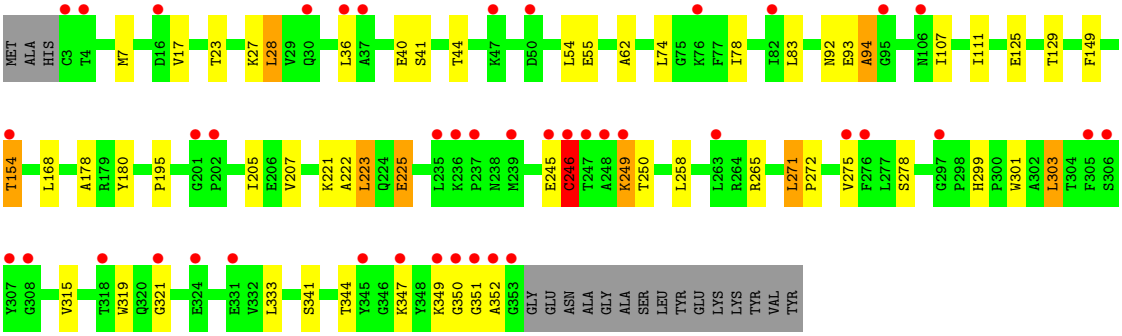
• Molecule 1: Fructose-bisphosphate aldolase

Chain C:



• Molecule 1: Fructose-bisphosphate aldolase

Chain D:



• Molecule 2: PbTRAP

Chain H:

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 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
$< I/\sigma(I) >$ [1]	2.65 (at 2.68Å)	Xtriage
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	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.41	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(^{o})	Ideal(^{o})
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 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	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

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 7.

All (154) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:C:275:VAL:HG23	1:C:275:VAL:O	2.03	0.58
1:D:36:LEU:HB2	1:D:78:ILE:HD13	1.85	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:67:LEU:C	1:C:67:LEU:HD23	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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%)	19	43
1	B	348/369 (94%)	326 (94%)	17 (5%)	5 (1%)	11	28
1	C	362/369 (98%)	335 (92%)	19 (5%)	8 (2%)	6	17
1	D	350/369 (95%)	327 (93%)	17 (5%)	6 (2%)	9	23
2	H	1/6 (17%)	0	1 (100%)	0	100	100
All	All	1415/1482 (96%)	1321 (93%)	72 (5%)	22 (2%)	9	24

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%)	271 (93%)	20 (7%)	15	35
1	B	286/298 (96%)	272 (95%)	14 (5%)	25	52
1	C	294/298 (99%)	278 (95%)	16 (5%)	22	47
1	D	286/298 (96%)	269 (94%)	17 (6%)	19	43
2	H	3/6 (50%)	3 (100%)	0	100	100
All	All	1160/1198 (97%)	1093 (94%)	67 (6%)	20	43

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	180	TYR
1	C	249	LYS
1	C	258	LEU
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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	358/369 (97%)	0.80	46 (12%)	3	3	58, 70, 92, 129	0
1	B	349/369 (94%)	1.23	72 (20%)	1	0	59, 70, 92, 100	0
1	C	363/369 (98%)	0.97	52 (14%)	2	1	56, 70, 90, 100	0
1	D	351/369 (95%)	0.82	43 (12%)	4	3	54, 69, 86, 93	0
2	H	3/6 (50%)	1.29	0	100	100	63, 63, 65, 68	3 (100%)
All	All	1424/1482 (96%)	0.96	213 (14%)	2	1	54, 70, 90, 129	3 (0%)

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	CYS	15.4
1	D	351	GLY	13.1
1	D	350	GLY	12.1
1	C	353	GLY	11.6
1	C	356	ASN	11.3
1	C	354	GLY	10.9
1	B	351	GLY	9.9
1	C	355	GLU	9.7
1	C	2	HIS	9.4
1	A	366	TYR	9.1
1	B	247	THR	8.7
1	B	46	LYS	8.2
1	C	352	ALA	8.0
1	D	3	CYS	7.7
1	D	352	ALA	7.7
1	C	248	ALA	7.4
1	B	47	LYS	7.3
1	D	249	LYS	7.2
1	A	248	ALA	6.9
1	C	3	CYS	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	246	CYS	6.5
1	B	52	ILE	6.5
1	B	63	SER	6.5
1	C	247	THR	6.4
1	C	82	ILE	6.3
1	C	362	TYR	5.9
1	B	106	ASN	5.8
1	D	247	THR	5.8
1	C	351	GLY	5.8
1	B	306	SER	5.7
1	B	82	ILE	5.5
1	C	4	THR	5.3
1	B	202	PRO	5.3
1	A	44	THR	4.8
1	B	37	ALA	4.6
1	B	55	GLU	4.6
1	C	331	GLU	4.5
1	A	35	ILE	4.5
1	B	35	ILE	4.5
1	B	50	ASP	4.5
1	A	364	LYS	4.5
1	A	106	ASN	4.4
1	A	202	PRO	4.4
1	D	202	PRO	4.4
1	A	351	GLY	4.3
1	B	4	THR	4.3
1	B	248	ALA	4.2
1	B	250	THR	4.2
1	D	276	PHE	4.2
1	B	342	LEU	4.1
1	A	357	ALA	4.1
1	C	125	GLU	4.0
1	B	236	LYS	4.0
1	A	37	ALA	4.0
1	A	365	LYS	4.0
1	C	306	SER	3.9
1	B	192	ILE	3.9
1	A	125	GLU	3.9
1	B	45	ILE	3.9
1	D	201	GLY	3.8
1	B	93	GLU	3.8
1	B	23	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	35	ILE	3.7
1	B	96	VAL	3.7
1	D	246	CYS	3.7
1	A	58	ILE	3.7
1	C	37	ALA	3.6
1	B	249	LYS	3.6
1	C	327	ALA	3.6
1	B	326	VAL	3.6
1	B	331	GLU	3.6
1	C	324	GLU	3.6
1	B	62	ALA	3.6
1	B	54	LEU	3.6
1	D	82	ILE	3.6
1	B	311	LEU	3.6
1	D	106	ASN	3.6
1	A	201	GLY	3.5
1	D	353	GLY	3.5
1	A	56	ASN	3.5
1	D	297	GLY	3.5
1	B	73	GLY	3.4
1	B	151	LYS	3.4
1	B	81	ALA	3.4
1	C	59	GLU	3.4
1	D	248	ALA	3.4
1	B	95	GLY	3.4
1	D	30	GLN	3.4
1	C	53	LYS	3.3
1	D	318	THR	3.3
1	B	36	LEU	3.3
1	C	43	GLN	3.3
1	D	349	LYS	3.3
1	A	42	THR	3.3
1	B	48	ARG	3.2
1	A	249	LYS	3.2
1	D	324	GLU	3.1
1	A	247	THR	3.1
1	B	38	ALA	3.1
1	A	4	THR	3.1
1	B	297	GLY	3.1
1	B	245	GLU	3.1
1	B	16	ASP	3.1
1	C	36	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	251	THR	3.0
1	D	239	MET	3.0
1	B	150	ALA	3.0
1	B	313	ALA	3.0
1	C	38	ALA	3.0
1	C	359	ALA	3.0
1	B	308	GLY	3.0
1	C	119	ASN	3.0
1	B	277	LEU	3.0
1	A	30	GLN	2.9
1	C	280	GLY	2.9
1	A	36	LEU	2.9
1	B	235	LEU	2.9
1	A	103	HIS	2.9
1	A	246	CYS	2.9
1	D	321	GLY	2.8
1	A	5	GLU	2.8
1	B	39	ASP	2.8
1	B	350	GLY	2.8
1	B	275	VAL	2.8
1	C	329	ALA	2.8
1	D	37	ALA	2.8
1	D	245	GLU	2.7
1	C	50	ASP	2.7
1	C	357	ALA	2.7
1	B	201	GLY	2.7
1	C	80	GLY	2.7
1	A	45	ILE	2.7
1	D	47	LYS	2.7
1	D	306	SER	2.7
1	B	237	PRO	2.7
1	A	244	TYR	2.7
1	D	331	GLU	2.7
1	C	52	ILE	2.7
1	C	63	SER	2.6
1	A	55	GLU	2.6
1	D	307	TYR	2.6
1	A	46	LYS	2.6
1	A	322	LYS	2.6
1	A	331	GLU	2.6
1	B	51	ASN	2.6
1	B	244	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	236	LYS	2.6
1	B	76	LYS	2.6
1	A	54	LEU	2.6
1	D	16	ASP	2.6
1	C	246	CYS	2.6
1	D	347	LYS	2.5
1	B	141[A]	GLU	2.5
1	B	56	ASN	2.5
1	B	317	ASN	2.5
1	A	57	THR	2.5
1	D	36	LEU	2.5
1	D	275	VAL	2.5
1	D	237	PRO	2.5
1	A	110	GLY	2.5
1	C	81	ALA	2.5
1	A	245	GLU	2.5
1	D	4	THR	2.5
1	A	111	ILE	2.5
1	A	23	THR	2.5
1	C	45	ILE	2.5
1	C	350	GLY	2.4
1	D	95	GLY	2.4
1	D	305	PHE	2.4
1	B	307	TYR	2.4
1	D	154	THR	2.4
1	D	50	ASP	2.4
1	B	49	PHE	2.4
1	D	263	LEU	2.4
1	C	275	VAL	2.4
1	A	250	THR	2.4
1	A	318	THR	2.4
1	D	236	LYS	2.4
1	C	44	THR	2.4
1	D	76	LYS	2.3
1	B	234	LEU	2.3
1	C	361	LEU	2.3
1	D	308	GLY	2.3
1	C	202	PRO	2.3
1	C	41	SER	2.3
1	B	30	GLN	2.3
1	B	276	PHE	2.3
1	C	47	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	235	LEU	2.3
1	B	296	LEU	2.3
1	A	325	ASN	2.3
1	B	193	VAL	2.3
1	C	6	TYR	2.2
1	D	345	TYR	2.2
1	C	193	VAL	2.2
1	B	329	ALA	2.2
1	A	306	SER	2.2
1	A	93	GLU	2.2
1	B	41	SER	2.2
1	A	151	LYS	2.1
1	B	327	ALA	2.1
1	A	59	GLU	2.1
1	C	326	VAL	2.1
1	C	237	PRO	2.1
1	B	347	LYS	2.1
1	C	236	LYS	2.1
1	C	364	LYS	2.1
1	B	339	ALA	2.1
1	C	308	GLY	2.1
1	A	192	ILE	2.1
1	A	15	ALA	2.1
1	B	345	TYR	2.0
1	C	39	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.