Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 09:11 AM EDT

PDB ID	:	5ET7
Title	:	Human muscle fructose-1,6-bisphosphatase in inactive T-state
Authors	:	Barciszewski, J.; Wisniewski, J.; Kolodziejczyk, R.; Dzugaj, A.; Jaskolski, M.; Rakus, D.
Deposited on	:	2015-11-17
Resolution	:	2.99 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:

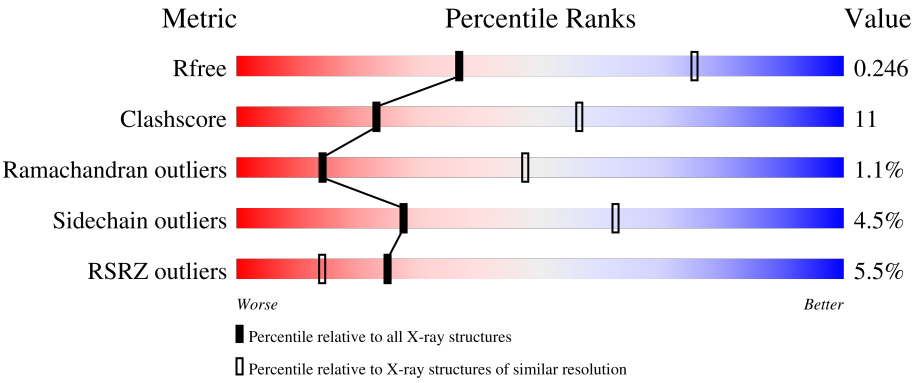
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	338	3% 63% 21% 15%
1	B	338	6% 59% 21% 17%
1	C	338	2% 62% 19% 18%
1	D	338	7% 58% 20% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8589 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-1,6-bisphosphatase isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2205	1410	363	423	9			
1	C	278	Total	C	N	O	S	0	0	0
			2132	1369	350	404	9			
1	B	280	Total	C	N	O	S	0	0	0
			2152	1381	355	407	9			
1	D	273	Total	C	N	O	S	0	0	0
			2100	1349	346	396	9			

There are 4 discrepancies between the modelled and reference sequences:

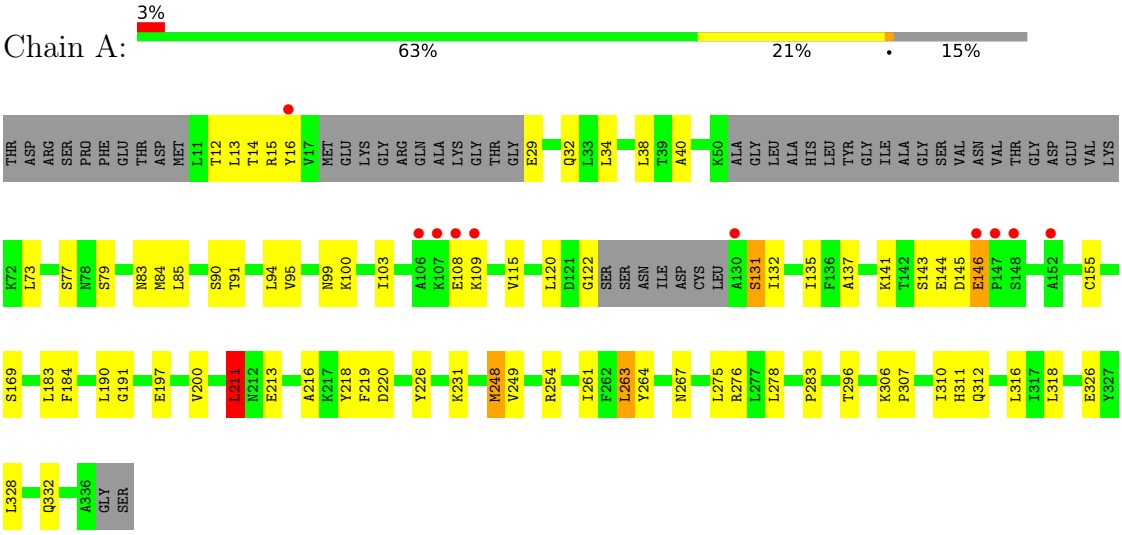
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	VAL	variant	UNP O00757
C	85	LEU	VAL	variant	UNP O00757
B	85	LEU	VAL	variant	UNP O00757
D	85	LEU	VAL	variant	UNP O00757

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.

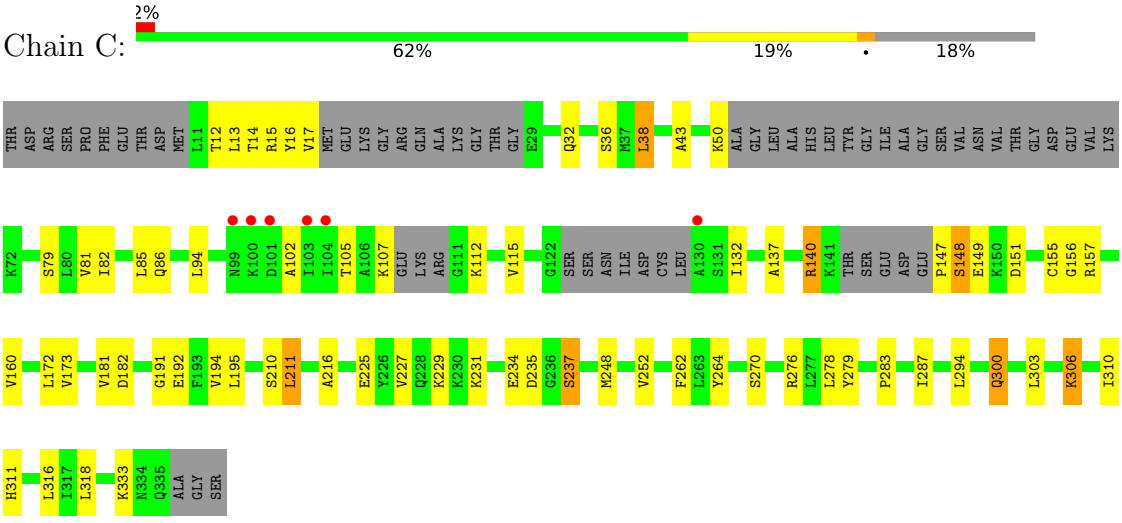
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain A:



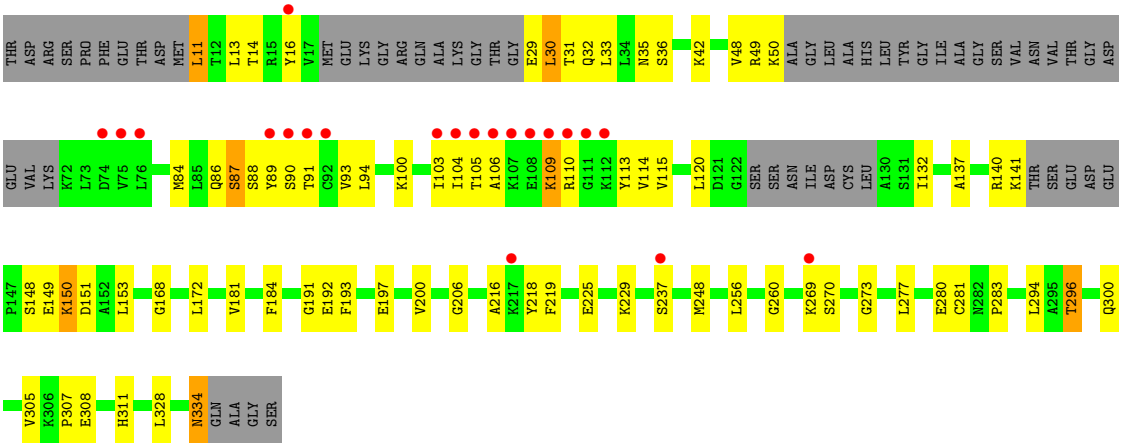
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain C:



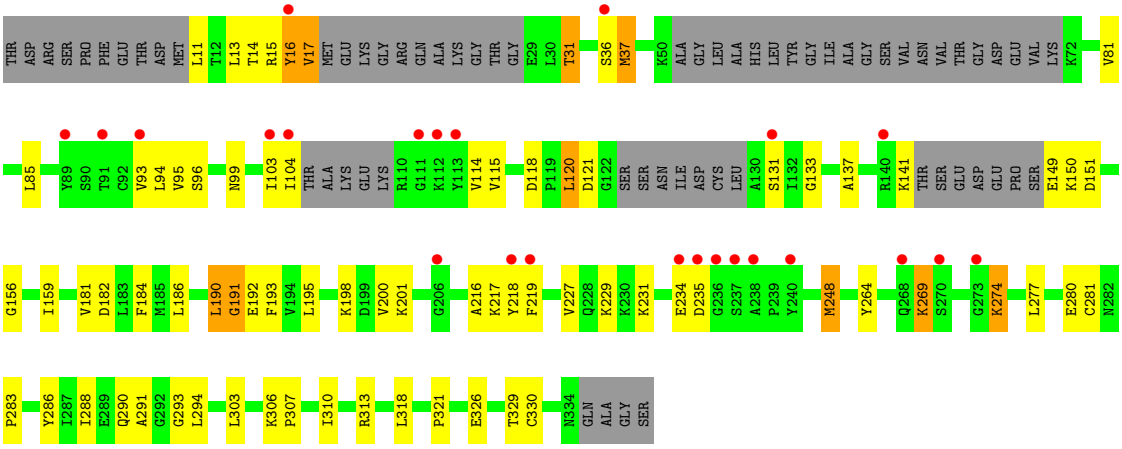
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain B:



• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	218.51Å 234.80Å 71.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.46 – 2.99 45.91 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.46-2.99) 99.5 (45.91-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.177 , 0.244 0.180 , 0.246	Depositor DCC
R_{free} test set	1000 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8589	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

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	0.77	0/2239	0.88	4/3027 (0.1%)
1	B	0.63	0/2185	0.77	0/2951
1	C	0.85	1/2164 (0.0%)	0.90	4/2923 (0.1%)
1	D	0.64	0/2131	0.82	0/2878
All	All	0.73	1/8719 (0.0%)	0.85	8/11779 (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	2
1	B	0	1
1	C	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	CYS	CB-SG	-14.46	1.57	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	C	211	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	C	211	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	131	SER	N-CA-C	5.39	125.55	111.00
1	C	300	GLN	CA-CB-CG	5.21	124.85	113.40
1	C	132	ILE	CB-CA-C	-5.15	101.29	111.60
1	A	254	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	231	LYS	CD-CE-NZ	-5.04	100.10	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	GLU	Peptide
1	A	16	TYR	Peptide
1	B	300	GLN	Peptide
1	C	147	PRO	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	2205	0	2257	45	0
1	B	2152	0	2216	64	0
1	C	2132	0	2191	50	0
1	D	2100	0	2158	52	0
All	All	8589	0	8822	199	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 11.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:SER:OG	1:C:149:GLU:N	2.10	0.84
1:D:293:GLY:HA2	1:D:321:PRO:HD3	1.61	0.83
1:B:29:GLU:HB3	1:B:31:THR:HG22	1.61	0.82
1:B:137:ALA:HB2	1:B:283:PRO:HG3	1.64	0.78
1:D:274:LYS:O	1:D:313:ARG:HD3	1.87	0.73
1:D:217:LYS:HD3	1:D:218:TYR:CE1	2.26	0.70
1:D:190:LEU:O	1:D:192:GLU:N	2.24	0.70
1:C:32:GLN:HE21	1:D:15:ARG:HD3	1.56	0.70
1:C:276:ARG:HH11	1:C:311:HIS:HB3	1.57	0.69
1:B:87:SER:C	1:B:89:TYR:H	1.96	0.69
1:A:40:ALA:HB2	1:A:84:MET:HG3	1.74	0.68
1:C:16:TYR:OH	1:C:182:ASP:OD2	2.08	0.68
1:B:90:SER:N	1:B:109:LYS:HE3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:MET:HE1	1:B:280:GLU:HB3	1.76	0.67
1:A:73:LEU:HD23	1:A:120:LEU:HD21	1.77	0.67
1:A:100:LYS:HD2	1:A:100:LYS:H	1.60	0.66
1:B:181:VAL:HB	1:B:200:VAL:HG22	1.77	0.66
1:A:122:GLY:HA3	1:A:132:ILE:HG22	1.78	0.65
1:B:11:LEU:N	1:B:16:TYR:HH	1.95	0.65
1:D:103:ILE:HG22	1:D:104:ILE:H	1.62	0.64
1:B:197:GLU:HG2	1:B:200:VAL:HG12	1.80	0.64
1:D:17:VAL:HG23	1:D:31:THR:HG23	1.80	0.64
1:A:29:GLU:HA	1:A:32:GLN:HE22	1.63	0.64
1:A:15:ARG:HH22	1:B:84:MET:HE3	1.63	0.63
1:D:15:ARG:HD2	1:D:15:ARG:C	2.20	0.63
1:D:264:TYR:CE2	1:D:274:LYS:HB2	2.34	0.63
1:A:13:LEU:HG	1:A:184:PHE:CE2	2.35	0.62
1:A:137:ALA:HB2	1:A:283:PRO:HG3	1.81	0.61
1:A:95:VAL:HG11	1:A:278:LEU:HD23	1.82	0.61
1:B:87:SER:O	1:B:89:TYR:N	2.31	0.61
1:B:148:SER:OG	1:B:149:GLU:N	2.19	0.60
1:D:201:LYS:HA	1:D:291:ALA:HB1	1.84	0.60
1:A:29:GLU:HA	1:A:32:GLN:NE2	2.17	0.60
1:A:276:ARG:NH1	1:A:311:HIS:O	2.34	0.60
1:B:49:ARG:NH2	1:B:168:GLY:O	2.35	0.59
1:D:37:MET:HB2	1:D:85:LEU:HD21	1.85	0.59
1:C:156:GLY:HA3	1:C:303:LEU:HD22	1.84	0.59
1:D:156:GLY:HA3	1:D:303:LEU:HD22	1.85	0.58
1:A:103:ILE:HD12	1:A:103:ILE:H	1.67	0.57
1:B:109:LYS:HD2	1:B:110:ARG:N	2.19	0.57
1:C:316:LEU:HD11	1:C:318:LEU:HD23	1.85	0.57
1:A:190:LEU:O	1:B:42:LYS:HD2	2.05	0.57
1:B:30:LEU:HB2	1:B:113:TYR:CE2	2.40	0.57
1:B:141:LYS:HD2	1:B:151:ASP:CG	2.25	0.57
1:D:227:VAL:HG12	1:D:231:LYS:HE3	1.87	0.56
1:D:13:LEU:HD13	1:D:184:PHE:CZ	2.41	0.56
1:C:112:LYS:O	1:C:112:LYS:HD2	2.04	0.56
1:D:216:ALA:HA	1:D:219:PHE:CE2	2.41	0.56
1:B:35:ASN:OD1	1:B:36:SER:N	2.38	0.56
1:B:109:LYS:HD2	1:B:109:LYS:C	2.25	0.56
1:B:150:LYS:HA	1:B:153:LEU:HD13	1.87	0.55
1:B:33:LEU:HB2	1:B:90:SER:HB2	1.87	0.55
1:D:229:LYS:NZ	1:D:330:CYS:SG	2.69	0.55
1:C:94:LEU:HD22	1:C:115:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ILE:HG13	1:D:318:LEU:HD13	1.86	0.55
1:B:89:TYR:C	1:B:109:LYS:HE3	2.26	0.55
1:D:95:VAL:HG11	1:D:310:ILE:HG21	1.87	0.55
1:A:332:GLN:HG3	1:C:294:LEU:HD21	1.87	0.54
1:B:100:LYS:HA	1:B:311:HIS:NE2	2.23	0.54
1:D:141:LYS:NZ	1:D:149:GLU:OE2	2.40	0.54
1:A:155:CYS:HB3	1:A:306:LYS:HG3	1.89	0.54
1:A:15:ARG:HE	1:B:88:SER:HA	1.72	0.54
1:C:276:ARG:NH1	1:C:311:HIS:HB3	2.23	0.53
1:A:94:LEU:HD22	1:A:115:VAL:HB	1.90	0.53
1:D:264:TYR:OH	1:D:274:LYS:HG2	2.09	0.53
1:C:140:ARG:HG2	1:C:160:VAL:CG2	2.38	0.53
1:D:190:LEU:HD23	1:D:192:GLU:HB2	1.91	0.53
1:C:43:ALA:HB2	1:D:190:LEU:HD12	1.91	0.53
1:B:104:ILE:HD12	1:B:106:ALA:HB2	1.90	0.52
1:A:191:GLY:HA3	1:B:191:GLY:HA3	1.91	0.52
1:C:32:GLN:NE2	1:D:15:ARG:HD3	2.24	0.52
1:D:186:LEU:HB2	1:D:193:PHE:CE1	2.45	0.52
1:C:235:ASP:HB2	1:C:237:SER:OG	2.09	0.52
1:C:191:GLY:HA3	1:D:191:GLY:HA3	1.91	0.51
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.93	0.51
1:A:218:TYR:O	1:A:267:ASN:HB2	2.11	0.51
1:D:93:VAL:HB	1:D:114:VAL:HG13	1.92	0.51
1:C:13:LEU:HD21	1:C:38:LEU:HG	1.92	0.51
1:D:277:LEU:HA	1:D:281:CYS:HB2	1.91	0.51
1:B:172:LEU:HD12	1:B:184:PHE:O	2.11	0.51
1:A:141:LYS:HE2	1:A:143:SER:O	2.12	0.50
1:C:279:TYR:OH	1:C:311:HIS:ND1	2.32	0.50
1:B:87:SER:C	1:B:89:TYR:N	2.64	0.50
1:B:13:LEU:HD13	1:B:184:PHE:CZ	2.46	0.50
1:D:159:ILE:HB	1:D:286:TYR:CE1	2.46	0.50
1:C:81:VAL:O	1:C:85:LEU:HG	2.10	0.50
1:D:16:TYR:OH	1:D:182:ASP:OD2	2.20	0.50
1:D:286:TYR:O	1:D:290:GLN:HG3	2.11	0.50
1:A:248:MET:HE3	1:A:275:LEU:HD13	1.94	0.50
1:C:112:LYS:HZ1	1:C:140:ARG:HA	1.77	0.50
1:B:93:VAL:HB	1:B:114:VAL:HG22	1.94	0.49
1:B:30:LEU:HD12	1:B:33:LEU:HD23	1.93	0.49
1:D:181:VAL:O	1:D:200:VAL:HG12	2.12	0.49
1:D:15:ARG:HD2	1:D:15:ARG:O	2.13	0.49
1:A:145:ASP:OD1	1:A:146:GLU:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ARG:O	1:D:17:VAL:N	2.45	0.49
1:D:218:TYR:CE1	1:D:269:LYS:HE3	2.47	0.48
1:C:112:LYS:HZ1	1:C:140:ARG:CA	2.25	0.48
1:C:102:ALA:HB3	1:C:149:GLU:HG3	1.95	0.48
1:A:12:THR:HG22	1:A:15:ARG:NH1	2.29	0.48
1:A:316:LEU:HD11	1:A:318:LEU:HD23	1.96	0.47
1:B:140:ARG:HG2	1:B:141:LYS:H	1.78	0.47
1:C:107:LYS:O	1:C:107:LYS:HG3	2.15	0.47
1:C:172:LEU:HD23	1:C:173:VAL:N	2.30	0.47
1:B:48:VAL:C	1:B:50:LYS:H	2.18	0.47
1:B:94:LEU:HD22	1:B:115:VAL:HB	1.96	0.47
1:D:294:LEU:HD12	1:D:321:PRO:HA	1.97	0.47
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.79	0.47
1:B:86:GLN:HG2	1:B:105:THR:HB	1.96	0.47
1:B:216:ALA:HA	1:B:219:PHE:CD2	2.49	0.47
1:B:89:TYR:HA	1:B:109:LYS:HE3	1.98	0.46
1:A:135:ILE:HD11	1:A:249:VAL:HG22	1.97	0.46
1:C:306:LYS:HB3	1:C:306:LYS:HE3	1.65	0.46
1:B:305:VAL:O	1:B:307:PRO:HD3	2.16	0.46
1:D:248:MET:HE1	1:D:280:GLU:HB3	1.97	0.46
1:A:261:ILE:HG12	1:A:263:LEU:CD2	2.46	0.46
1:D:137:ALA:HB2	1:D:283:PRO:HG3	1.97	0.46
1:A:197:GLU:HG2	1:A:200:VAL:HG12	1.96	0.46
1:A:220:ASP:OD1	1:A:220:ASP:N	2.49	0.46
1:A:332:GLN:HG3	1:C:294:LEU:CD2	2.46	0.46
1:C:248:MET:O	1:C:252:VAL:HG23	2.16	0.46
1:A:13:LEU:HD13	1:A:38:LEU:HD13	1.98	0.46
1:C:181:VAL:HG21	1:C:287:ILE:HG23	1.97	0.46
1:B:334:ASN:N	1:B:334:ASN:OD1	2.49	0.46
1:D:118:ASP:OD2	1:D:121:ASP:HB3	2.16	0.46
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.52	0.45
1:C:157:ARG:HG2	1:C:303:LEU:O	2.15	0.45
1:C:210:SER:HB3	1:C:262:PHE:HA	1.99	0.45
1:B:32:GLN:O	1:B:36:SER:HB2	2.16	0.45
1:C:12:THR:HG22	1:C:13:LEU:N	2.31	0.45
1:B:16:TYR:CD1	1:B:16:TYR:N	2.85	0.45
1:C:15:ARG:HD2	1:D:36:SER:HB2	1.99	0.44
1:C:149:GLU:O	1:C:149:GLU:HG2	2.17	0.44
1:B:91:THR:O	1:B:109:LYS:NZ	2.50	0.44
1:B:225:GLU:O	1:B:229:LYS:HG3	2.17	0.44
1:C:278:LEU:HD22	1:C:310:ILE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LYS:HB3	1:C:229:LYS:HE3	1.58	0.44
1:B:206:GLY:HA3	1:B:260:GLY:HA2	2.00	0.44
1:A:183:LEU:HG	1:A:200:VAL:HG11	1.99	0.44
1:C:137:ALA:HB2	1:C:283:PRO:HG3	1.99	0.44
1:C:149:GLU:C	1:C:151:ASP:H	2.21	0.44
1:A:79:SER:O	1:A:83:ASN:ND2	2.48	0.44
1:B:13:LEU:HB2	1:B:193:PHE:HB2	1.99	0.44
1:D:99:ASN:ND2	1:D:103:ILE:HD11	2.33	0.44
1:D:120:LEU:HA	1:D:133:GLY:O	2.17	0.44
1:A:14:THR:HG22	1:B:35:ASN:ND2	2.33	0.43
1:C:102:ALA:CB	1:C:149:GLU:HG3	2.47	0.43
1:D:103:ILE:C	1:D:104:ILE:HD13	2.38	0.43
1:C:194:VAL:HG12	1:C:195:LEU:O	2.17	0.43
1:A:278:LEU:HD22	1:A:310:ILE:HA	1.99	0.43
1:B:120:LEU:HD12	1:B:120:LEU:HA	1.88	0.43
1:C:156:GLY:HA3	1:C:303:LEU:CD2	2.48	0.43
1:B:148:SER:HG	1:B:149:GLU:H	1.61	0.43
1:D:217:LYS:HD3	1:D:218:TYR:CZ	2.53	0.43
1:C:235:ASP:OD1	1:C:235:ASP:N	2.52	0.43
1:C:227:VAL:CG1	1:C:231:LYS:HE3	2.49	0.43
1:B:50:LYS:HE2	1:B:50:LYS:HB3	1.50	0.43
1:B:200:VAL:HG21	1:B:256:LEU:HD21	2.01	0.43
1:D:288:ILE:HA	1:D:288:ILE:HD13	1.78	0.42
1:A:13:LEU:HG	1:A:184:PHE:CD2	2.54	0.42
1:A:211:LEU:HD13	1:A:213:GLU:HG3	2.01	0.42
1:D:151:ASP:OD1	1:D:151:ASP:N	2.35	0.42
1:C:13:LEU:CD2	1:C:38:LEU:HG	2.50	0.42
1:B:94:LEU:HB2	1:B:103:ILE:HB	2.02	0.42
1:D:195:LEU:HD21	1:D:198:LYS:HB2	2.01	0.42
1:B:141:LYS:HD2	1:B:151:ASP:OD2	2.19	0.42
1:D:81:VAL:O	1:D:85:LEU:HB2	2.19	0.42
1:A:99:ASN:ND2	1:A:103:ILE:HD11	2.35	0.42
1:A:306:LYS:HA	1:A:307:PRO:HD3	1.72	0.42
1:C:14:THR:OG1	1:C:192:GLU:OE1	2.30	0.42
1:C:227:VAL:HG12	1:C:231:LYS:HE3	2.01	0.42
1:B:16:TYR:N	1:B:16:TYR:HD1	2.18	0.42
1:B:216:ALA:HA	1:B:219:PHE:CE2	2.55	0.42
1:B:248:MET:CE	1:B:280:GLU:HB3	2.46	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.82	0.42
1:B:149:GLU:C	1:B:151:ASP:H	2.23	0.42
1:B:91:THR:HG21	1:B:94:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:THR:HG21	1:B:328:LEU:HD21	2.02	0.42
1:B:218:TYR:CE2	1:B:269:LYS:HE3	2.56	0.41
1:C:287:ILE:HD13	1:C:287:ILE:HA	1.83	0.41
1:D:94:LEU:HD22	1:D:115:VAL:HB	2.01	0.41
1:C:107:LYS:O	1:C:107:LYS:CG	2.68	0.41
1:C:225:GLU:OE2	1:C:333:LYS:HD2	2.21	0.41
1:C:294:LEU:HD23	1:C:294:LEU:HA	1.81	0.41
1:B:30:LEU:HB2	1:B:113:TYR:CZ	2.55	0.41
1:B:270:SER:O	1:B:273:GLY:N	2.53	0.41
1:D:99:ASN:HD22	1:D:103:ILE:HD11	1.85	0.41
1:D:306:LYS:HA	1:D:307:PRO:HD3	1.88	0.41
1:A:100:LYS:O	1:A:310:ILE:HD11	2.21	0.41
1:C:248:MET:HE2	1:C:252:VAL:HG21	2.02	0.41
1:A:226:TYR:CE1	1:A:326:GLU:HG2	2.57	0.40
1:A:307:PRO:HA	1:A:312:GLN:OE1	2.20	0.40
1:C:82:ILE:O	1:C:86:GLN:HG3	2.21	0.40
1:B:14:THR:OG1	1:B:192:GLU:OE1	2.39	0.40
1:D:326:GLU:O	1:D:329:THR:HB	2.20	0.40
1:A:85:LEU:HB3	1:A:91:THR:HG21	2.03	0.40
1:A:296:THR:HG21	1:A:328:LEU:HD21	2.03	0.40
1:D:294:LEU:HA	1:D:294:LEU:HD23	1.86	0.40
1:B:294:LEU:HA	1:B:294:LEU:HD23	1.92	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	279/338 (82%)	266 (95%)	11 (4%)	2 (1%)	22	58
1	B	270/338 (80%)	246 (91%)	21 (8%)	3 (1%)	14	47
1	C	266/338 (79%)	247 (93%)	18 (7%)	1 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	261/338 (77%)	234 (90%)	21 (8%)	6 (2%)	6 28
All	All	1076/1352 (80%)	993 (92%)	71 (7%)	12 (1%)	14 47

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	D	150	LYS
1	D	190	LEU
1	D	235	ASP
1	B	87	SER
1	D	16	TYR
1	D	191	GLY
1	A	131	SER
1	B	150	LYS
1	B	237	SER
1	D	120	LEU
1	C	216	ALA

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	240/279 (86%)	231 (96%)	9 (4%)	33 67
1	B	234/279 (84%)	227 (97%)	7 (3%)	41 73
1	C	232/279 (83%)	217 (94%)	15 (6%)	17 48
1	D	228/279 (82%)	217 (95%)	11 (5%)	25 60
All	All	934/1116 (84%)	892 (96%)	42 (4%)	27 62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	90	SER

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Mol	Chain	Res	Type
1	A	108	GLU
1	A	109	LYS
1	A	169	SER
1	A	211	LEU
1	A	248	MET
1	A	263	LEU
1	A	264	TYR
1	C	17	VAL
1	C	36	SER
1	C	38	LEU
1	C	50	LYS
1	C	79	SER
1	C	105	THR
1	C	140	ARG
1	C	148	SER
1	C	211	LEU
1	C	234	GLU
1	C	237	SER
1	C	264	TYR
1	C	270	SER
1	C	300	GLN
1	C	306	LYS
1	B	11	LEU
1	B	30	LEU
1	B	109	LYS
1	B	132	ILE
1	B	296	THR
1	B	308	GLU
1	B	334	ASN
1	D	11	LEU
1	D	14	THR
1	D	17	VAL
1	D	31	THR
1	D	37	MET
1	D	96	SER
1	D	131	SER
1	D	234	GLU
1	D	248	MET
1	D	269	LYS
1	D	274	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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^{th} 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	287/338 (84%)	-0.07	10 (3%) 44 26	35, 58, 105, 171	0
1	B	280/338 (82%)	0.15	21 (7%) 14 7	52, 81, 120, 169	0
1	C	278/338 (82%)	-0.13	6 (2%) 62 42	31, 57, 105, 132	0
1	D	273/338 (80%)	0.20	24 (8%) 10 5	58, 86, 123, 149	0
All	All	1118/1352 (82%)	0.04	61 (5%) 25 14	31, 72, 116, 171	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	4.8
1	B	108	GLU	3.9
1	A	16	TYR	3.9
1	D	270	SER	3.8
1	B	105	THR	3.8
1	B	110	ARG	3.6
1	D	112	LYS	3.6
1	D	273	GLY	3.5
1	D	219	PHE	3.4
1	D	89	TYR	3.4
1	A	108	GLU	3.4
1	B	106	ALA	3.3
1	B	109	LYS	3.3
1	B	107	LYS	3.3
1	A	106	ALA	3.2
1	B	89	TYR	3.1
1	B	112	LYS	3.0
1	B	104	ILE	3.0
1	B	16	TYR	2.9
1	D	91	THR	2.9
1	C	100	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	103	ILE	2.9
1	A	130	ALA	2.9
1	A	109	LYS	2.9
1	D	131	SER	2.9
1	D	140	ARG	2.8
1	C	99	ASN	2.8
1	D	218	TYR	2.8
1	D	104	ILE	2.8
1	B	76	LEU	2.8
1	B	217	LYS	2.7
1	A	148	SER	2.6
1	C	130	ALA	2.6
1	D	235	ASP	2.5
1	B	111	GLY	2.5
1	A	147	PRO	2.5
1	B	91	THR	2.5
1	D	237	SER	2.4
1	D	234	GLU	2.4
1	D	206	GLY	2.4
1	B	90	SER	2.4
1	D	238	ALA	2.4
1	C	101	ASP	2.4
1	D	103	ILE	2.4
1	D	236	GLY	2.3
1	A	152	ALA	2.3
1	B	269	LYS	2.3
1	D	113	TYR	2.3
1	D	111	GLY	2.2
1	B	103	ILE	2.1
1	B	75	VAL	2.1
1	B	237	SER	2.1
1	D	16	TYR	2.1
1	D	36	SER	2.1
1	B	92	CYS	2.1
1	D	240	TYR	2.1
1	A	107	LYS	2.1
1	B	74	ASP	2.1
1	A	146	GLU	2.1
1	C	104	ILE	2.0
1	D	268	GLN	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.