



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:20 PM EDT

PDB ID : 5ET7 / pdb_00005et7
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	:	4-5-2 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

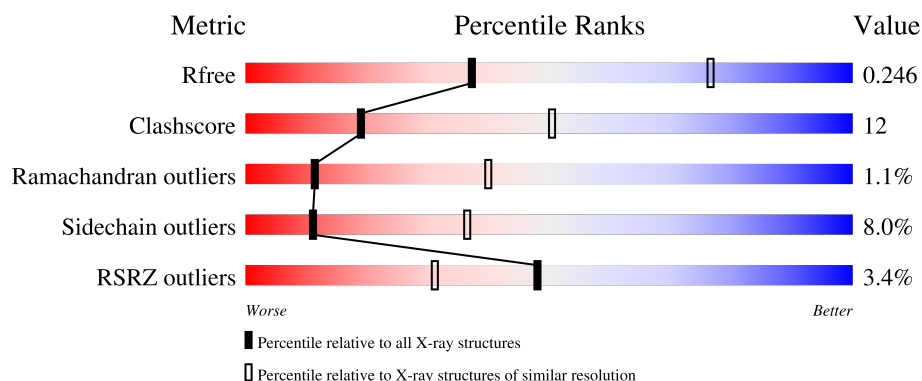
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 $\leq 5\%$. 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	338	2% 61% 21% • 15%
1	B	338	2% 57% 22% • 17%
1	C	338	3% 59% 19% • 18%
1	D	338	4% 54% 22% • • 19%

2 Entry composition

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			

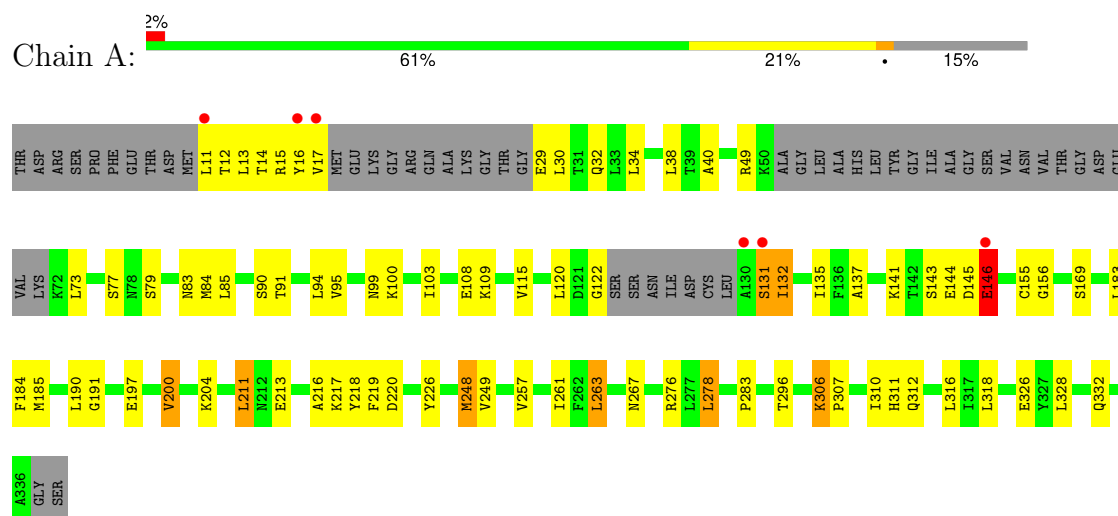
There are 4 discrepancies between the modelled and reference sequences:

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

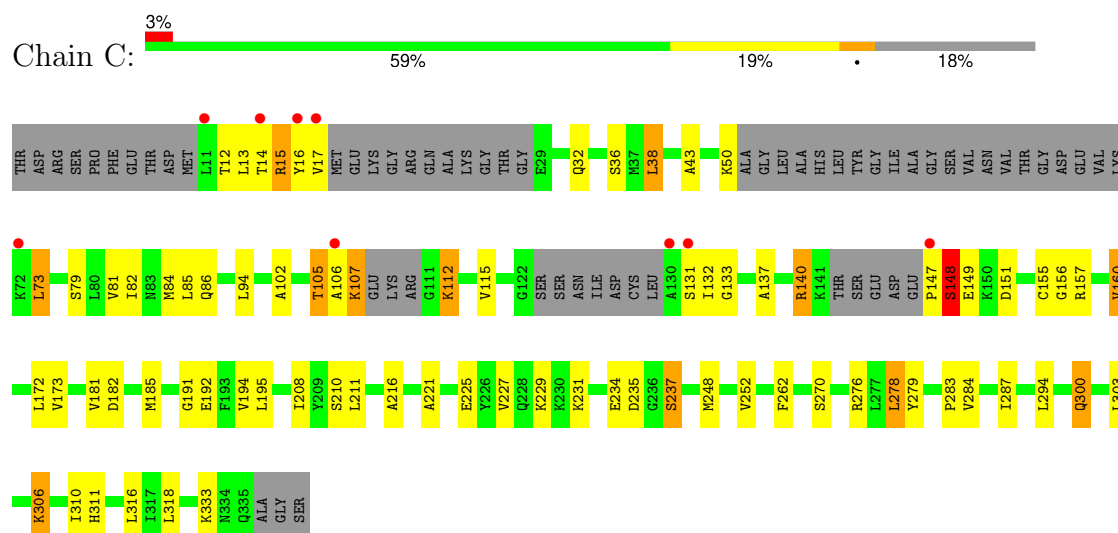
3 Residue-property plots

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

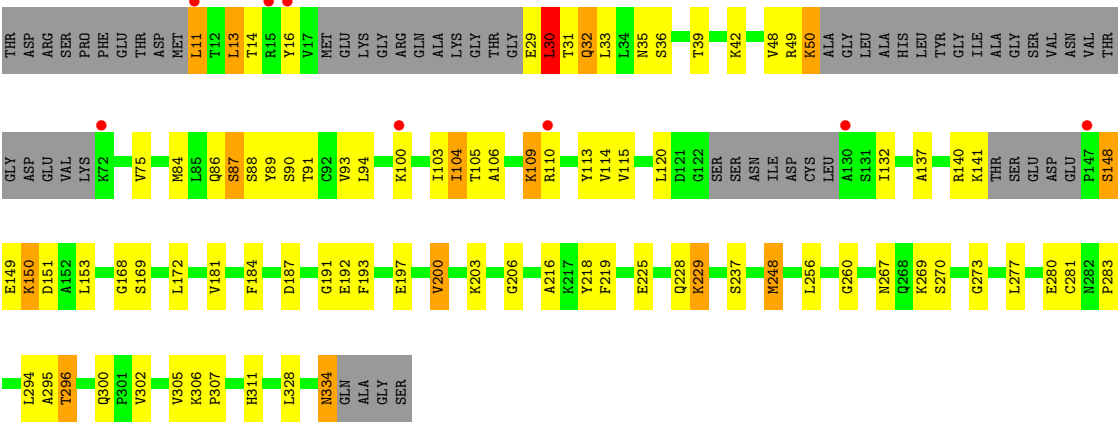


- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

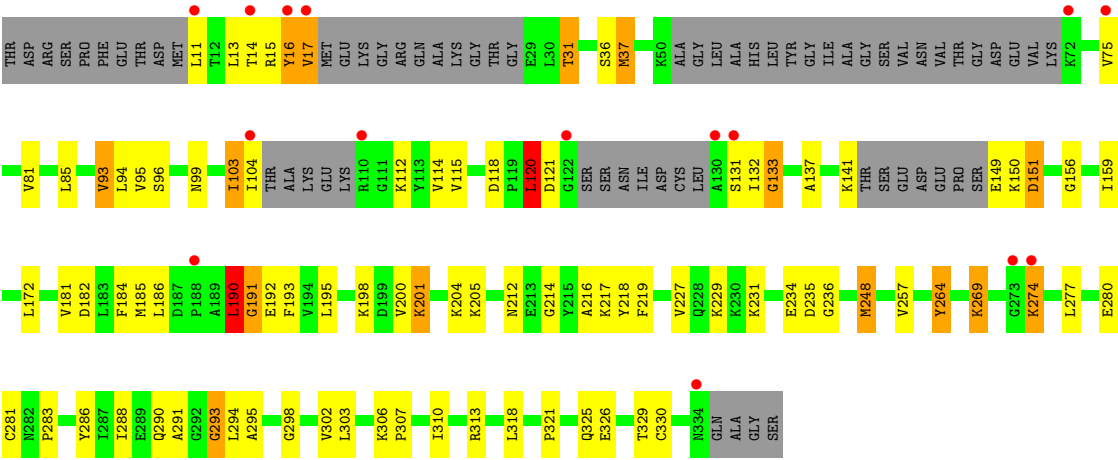


- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2





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



4 Data and refinement statistics

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 45.46 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.46-2.99) 99.4 (45.46-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.177 , 0.244 0.183 , 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 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

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	0.95	0/2239	1.23	8/3027 (0.3%)
1	B	0.78	0/2185	1.11	6/2951 (0.2%)
1	C	1.00	3/2164 (0.1%)	1.23	10/2923 (0.3%)
1	D	0.81	0/2131	1.18	13/2878 (0.5%)
All	All	0.89	3/8719 (0.0%)	1.19	37/11779 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	CYS	CB-SG	-7.15	1.57	1.81
1	C	221	ALA	CA-CB	-6.42	1.43	1.53
1	C	105	THR	CA-C	5.54	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LEU	N-CA-C	-12.38	99.15	114.75
1	A	257	VAL	N-CA-C	8.36	119.14	110.62
1	B	187	ASP	CA-C-N	-8.08	111.31	120.04
1	B	187	ASP	C-N-CA	-8.08	111.31	120.04
1	C	131	SER	N-CA-C	7.87	121.93	110.28
1	A	146	GLU	CA-C-N	-7.79	110.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	GLU	C-N-CA	-7.79	110.11	119.84
1	C	73	LEU	N-CA-C	-7.34	104.58	113.97
1	A	131	SER	N-CA-C	6.92	125.55	110.80
1	A	156	GLY	N-CA-C	6.55	121.67	114.40
1	D	298	GLY	N-CA-C	-6.30	105.82	114.64
1	D	120	LEU	CA-C-N	-6.14	114.60	122.77
1	D	120	LEU	C-N-CA	-6.14	114.60	122.77
1	C	132	ILE	CB-CA-C	-6.10	101.29	111.29
1	A	30	LEU	N-CA-C	-6.09	104.56	112.23
1	D	151	ASP	N-CA-C	-6.08	105.70	112.57
1	C	112	LYS	N-CA-C	6.07	120.89	112.45
1	D	236	GLY	N-CA-C	-6.04	106.98	115.32
1	C	148	SER	N-CA-C	5.96	119.69	108.65
1	D	264	TYR	CA-C-N	5.94	127.34	120.98
1	D	264	TYR	C-N-CA	5.94	127.34	120.98
1	C	133	GLY	N-CA-C	5.90	121.87	110.66
1	C	160	VAL	N-CA-C	-5.90	107.12	111.90
1	C	106	ALA	N-CA-C	5.81	119.59	111.74
1	D	133	GLY	N-CA-C	5.78	120.91	111.27
1	D	112	LYS	N-CA-C	5.55	120.21	113.38
1	B	148	SER	N-CA-C	5.45	118.74	108.65
1	C	300	GLN	CA-CB-CG	5.38	124.85	114.10
1	D	190	LEU	N-CA-C	-5.33	99.44	110.80
1	A	306	LYS	CA-C-N	5.32	125.08	119.76
1	A	306	LYS	C-N-CA	5.32	125.08	119.76
1	D	132	ILE	N-CA-C	5.30	114.99	108.53
1	D	257	VAL	N-CA-C	5.16	115.38	110.53
1	B	30	LEU	CA-C-O	5.08	124.26	118.47
1	B	39	THR	N-CA-C	-5.08	106.25	112.90
1	C	208	ILE	N-CA-C	5.05	115.39	108.12
1	D	293	GLY	N-CA-C	-5.02	106.76	112.79

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

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	46	0
1	B	2152	0	2216	66	0
1	C	2132	0	2191	50	0
1	D	2100	0	2158	55	0
All	All	8589	0	8822	205	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 12.

All (205) 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: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:248:MET:HE1	1:B:280:GLU:HB3	1.65	0.79
1:B:137:ALA:HB2	1:B:283:PRO:HG3	1.64	0.78
1:C:148:SER:OG	1:C:149:GLU:N	2.10	0.74
1:B:87:SER:C	1:B:89:TYR:H	1.96	0.74
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: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
1:A:73:LEU:HD23	1:A:120:LEU:HD21	1.77	0.67
1:D:15:ARG:HD2	1:D:15:ARG:C	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:141:LYS:HD2	1:B:151:ASP:CG	2.25	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:C:279:TYR:OH	1:C:311:HIS:ND1	2.32	0.60
1:B:11:LEU:N	1:B:16:TYR:HH	2.00	0.60
1:B:89:TYR:C	1:B:109:LYS:HE3	2.26	0.60
1:B:109:LYS:HD2	1:B:109:LYS:C	2.25	0.60
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:A:15:ARG:HH22	1:B:84:MET:HE3	1.68	0.58
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: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: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
1:B:87:SER:C	1:B:89:TYR:N	2.64	0.55
1:D:288:ILE:HG13	1:D:318:LEU:HD13	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:248:MET:HE2	1:C:284:VAL:HG11	1.91	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:B:48:VAL:C	1:B:50:LYS:H	2.18	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: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: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:B:248:MET:HE1	1:B:280:GLU:CB	2.41	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
1:D:15:ARG:O	1:D:17:VAL:N	2.45	0.49
1:C:14:THR:OG1	1:C:192:GLU:OE1	2.30	0.48
1:C:149:GLU:C	1:C:151:ASP:H	2.21	0.48
1:D:218:TYR:CE1	1:D:269:LYS:HE3	2.47	0.48
1:D:103:ILE:C	1:D:104:ILE:HD13	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:149:GLU:C	1:B:151:ASP:H	2.23	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: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:D:248:MET:HE1	1:D:280:GLU:HB3	1.98	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:D:185:MET:HE3	1:D:185:MET:HB2	1.78	0.45
1:C:157:ARG:HG2	1:C:303:LEU:O	2.15	0.45
1:B:109:LYS:HZ3	1:B:109:LYS:HG3	1.65	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:A:248:MET:HE3	1:A:248:MET:HB2	1.80	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ALA:HB2	1:C:283:PRO:HG3	1.99	0.44
1:B:295:ALA:C	1:B:302:VAL:HG23	2.42	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:B:248:MET:HE3	1:B:248:MET:HB3	1.79	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:D:212:ASN:C	1:D:214:GLY:H	2.26	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: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:328:LEU:HD23	1:B:328:LEU:HA	1.82	0.42
1:B:91:THR:HG21	1:B:94:LEU:HD21	2.02	0.42
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:A:29:GLU:HA	1:A:32:GLN:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:ALA:C	1:D:302:VAL:HG23	2.46	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: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

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	279/338 (82%)	266 (95%)	11 (4%)	2 (1%)	18	50
1	B	270/338 (80%)	246 (91%)	21 (8%)	3 (1%)	11	40
1	C	266/338 (79%)	247 (93%)	18 (7%)	1 (0%)	30	62
1	D	261/338 (77%)	234 (90%)	21 (8%)	6 (2%)	5	23
All	All	1076/1352 (80%)	993 (92%)	71 (7%)	12 (1%)	11	40

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 ⓘ

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%)	223 (93%)	17 (7%)	13	41
1	B	234/279 (84%)	215 (92%)	19 (8%)	11	36
1	C	232/279 (83%)	212 (91%)	20 (9%)	10	34
1	D	228/279 (82%)	209 (92%)	19 (8%)	10	35
All	All	934/1116 (84%)	859 (92%)	75 (8%)	11	36

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	17	VAL
1	A	49	ARG
1	A	77	SER
1	A	90	SER
1	A	108	GLU
1	A	109	LYS
1	A	132	ILE
1	A	169	SER
1	A	185	MET

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Mol	Chain	Res	Type
1	A	200	VAL
1	A	204	LYS
1	A	211	LEU
1	A	217	LYS
1	A	248	MET
1	A	263	LEU
1	A	278	LEU
1	C	15	ARG
1	C	17	VAL
1	C	36	SER
1	C	38	LEU
1	C	50	LYS
1	C	73	LEU
1	C	79	SER
1	C	84	MET
1	C	105	THR
1	C	107	LYS
1	C	140	ARG
1	C	148	SER
1	C	185	MET
1	C	211	LEU
1	C	234	GLU
1	C	237	SER
1	C	270	SER
1	C	278	LEU
1	C	300	GLN
1	C	306	LYS
1	B	11	LEU
1	B	13	LEU
1	B	30	LEU
1	B	32	GLN
1	B	50	LYS
1	B	75	VAL
1	B	104	ILE
1	B	109	LYS
1	B	132	ILE
1	B	169	SER
1	B	200	VAL
1	B	203	LYS
1	B	228	GLN
1	B	229	LYS
1	B	248	MET

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Mol	Chain	Res	Type
1	B	267	ASN
1	B	296	THR
1	B	306	LYS
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	75	VAL
1	D	93	VAL
1	D	96	SER
1	D	103	ILE
1	D	131	SER
1	D	172	LEU
1	D	201	LYS
1	D	204	LYS
1	D	205	LYS
1	D	234	GLU
1	D	248	MET
1	D	269	LYS
1	D	274	LYS
1	D	325	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	GLN
1	C	86	GLN
1	C	179	GLN
1	B	83	ASN
1	B	267	ASN
1	B	300	GLN
1	D	267	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	287/338 (84%)	-0.34	6 (2%)	63 44	35, 58, 105, 171	0
1	B	280/338 (82%)	-0.05	8 (2%)	53 35	52, 81, 120, 169	0
1	C	278/338 (82%)	-0.26	9 (3%)	50 33	31, 57, 105, 132	0
1	D	273/338 (80%)	0.10	15 (5%)	30 18	58, 86, 123, 149	0
All	All	1118/1352 (82%)	-0.14	38 (3%)	48 31	31, 72, 116, 171	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	PRO	5.2
1	C	147	PRO	4.9
1	C	130	ALA	4.8
1	D	131	SER	4.6
1	A	11	LEU	4.5
1	C	106	ALA	3.7
1	C	14	THR	3.7
1	C	17	VAL	3.6
1	D	14	THR	3.6
1	B	130	ALA	3.5
1	C	72	LYS	3.4
1	B	16	TYR	3.2
1	A	17	VAL	3.2
1	D	334	ASN	3.1
1	B	11	LEU	3.1
1	D	122	GLY	3.0
1	C	11	LEU	3.0
1	D	11	LEU	3.0
1	A	16	TYR	2.9
1	D	75	VAL	2.9
1	C	131	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	2.7
1	D	273	GLY	2.6
1	D	110	ARG	2.5
1	C	16	TYR	2.5
1	A	131	SER	2.5
1	D	188	PRO	2.4
1	D	17	VAL	2.4
1	D	130	ALA	2.4
1	B	15	ARG	2.3
1	D	104	ILE	2.3
1	B	110	ARG	2.2
1	D	16	TYR	2.2
1	D	72	LYS	2.1
1	B	72	LYS	2.0
1	A	146	GLU	2.0
1	B	100	LYS	2.0
1	D	274	LYS	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.