



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 PM UTC

PDB ID : 1ZAH / pdb_00001zah
Title : Fructose-1,6-bisphosphate aldolase from rabbit muscle
Authors : St-Jean, M.; Lafrance-Vanasse, J.; Liotard, B.; Sygusch, J.
Deposited on : 2005-04-06
Resolution : 1.80 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

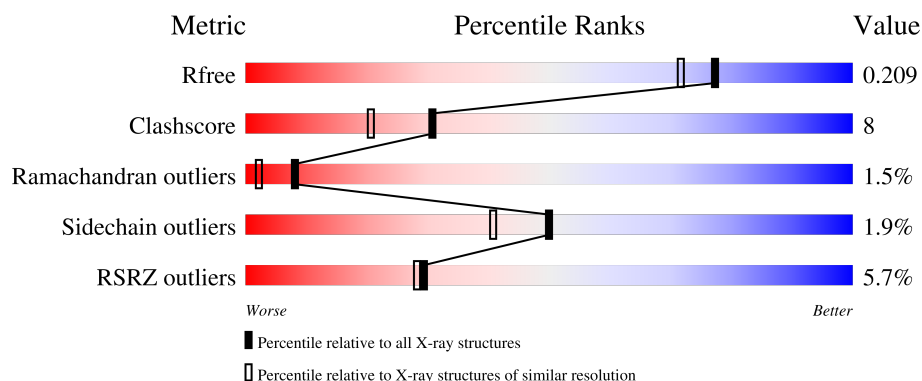
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	363	5% 83% 16% .
1	B	363	6% 78% 21% .
1	C	363	6% 82% 17% .
1	D	363	6% 78% 21% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13459 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	B	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	C	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	D	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			

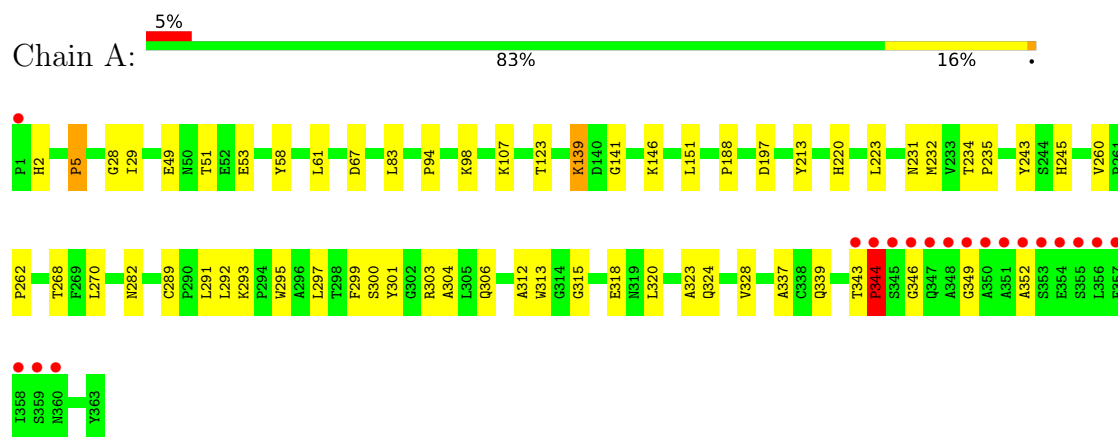
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	604	Total	O	0	0
			604	604		
2	B	604	Total	O	0	0
			604	604		
2	C	601	Total	O	0	0
			601	601		
2	D	618	Total	O	0	0
			618	618		

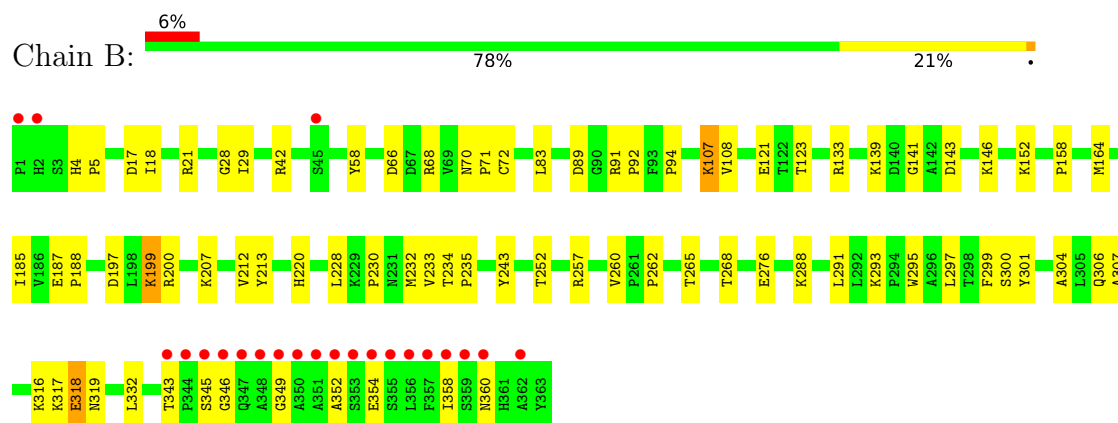
3 Residue-property plots

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.

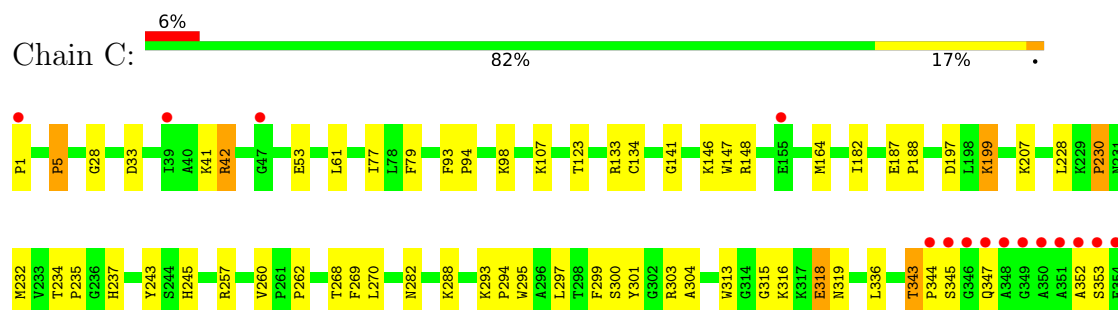
• Molecule 1: Fructose-bisphosphate aldolase A



• Molecule 1: Fructose-bisphosphate aldolase A

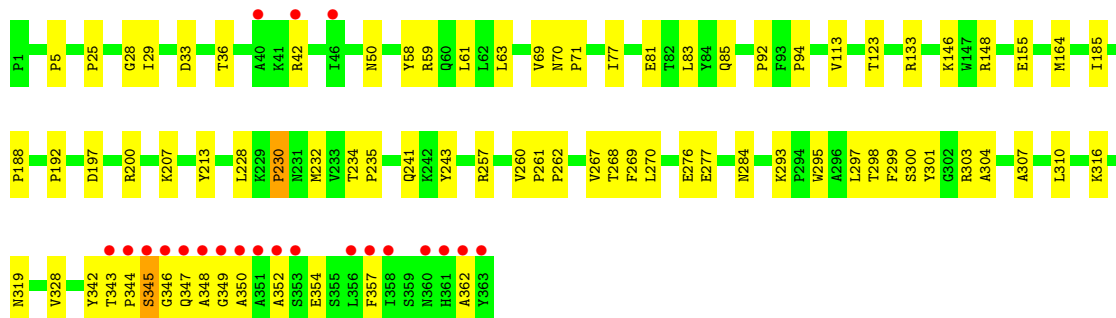
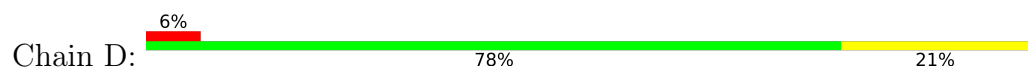


• Molecule 1: Fructose-bisphosphate aldolase A





- Molecule 1: Fructose-bisphosphate aldolase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.10Å 102.92Å 84.66Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-1.80) 95.1 (50.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.167 , 0.205 0.170 , 0.209	Depositor DCC
R_{free} test set	6370 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13459	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	0.37	0/2812	0.94	12/3810 (0.3%)
1	B	0.36	0/2812	0.89	8/3810 (0.2%)
1	C	0.36	0/2812	0.91	10/3810 (0.3%)
1	D	0.35	0/2812	0.87	7/3810 (0.2%)
All	All	0.36	0/11248	0.90	37/15240 (0.2%)

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	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	THR	CA-C-N	9.86	132.16	119.84
1	A	343	THR	C-N-CA	9.86	132.16	119.84
1	A	232	MET	N-CA-C	-8.31	99.33	110.55
1	D	260	VAL	N-CA-C	8.20	115.02	107.56
1	B	260	VAL	N-CA-C	7.98	114.82	107.56
1	D	232	MET	N-CA-C	-7.97	99.79	110.55
1	C	260	VAL	N-CA-C	7.40	114.30	107.56
1	C	232	MET	N-CA-C	-7.35	100.83	110.53
1	A	260	VAL	N-CA-C	7.14	114.06	107.56
1	C	123	THR	N-CA-C	-6.77	99.57	109.18
1	B	232	MET	N-CA-C	-6.66	101.57	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	THR	N-CA-C	-6.53	99.91	109.18
1	D	123	THR	N-CA-C	-6.46	100.01	109.18
1	A	141	GLY	N-CA-C	6.39	122.42	114.37
1	B	123	THR	N-CA-C	-6.30	100.23	109.18
1	A	270	LEU	N-CA-C	-6.26	100.37	110.32
1	C	270	LEU	N-CA-C	-6.08	100.65	110.32
1	A	289	CYS	CA-C-N	5.71	125.83	119.32
1	A	289	CYS	C-N-CA	5.71	125.83	119.32
1	C	141	GLY	N-CA-C	5.66	122.57	114.64
1	C	79	PHE	N-CA-C	-5.49	102.40	110.52
1	C	343	THR	CA-C-N	-5.48	114.45	119.82
1	C	343	THR	C-N-CA	-5.48	114.45	119.82
1	A	231	ASN	N-CA-C	-5.43	103.22	110.55
1	D	270	LEU	N-CA-C	-5.36	101.80	110.32
1	A	344	PRO	N-CA-C	5.35	123.49	112.47
1	D	113	VAL	N-CA-C	-5.26	104.88	109.19
1	B	4	HIS	CA-C-N	5.21	126.35	119.84
1	B	4	HIS	C-N-CA	5.21	126.35	119.84
1	B	360	ASN	N-CA-C	-5.20	106.91	113.20
1	B	265	THR	N-CA-C	5.15	116.89	111.28
1	A	223	LEU	N-CA-C	5.14	116.88	111.28
1	C	148	ARG	N-CA-C	5.11	116.85	108.52
1	D	148	ARG	N-CA-C	5.09	117.26	109.07
1	B	141	GLY	N-CA-C	5.09	121.76	114.64
1	D	269	PHE	N-CA-C	5.01	117.50	110.23
1	C	269	PHE	N-CA-C	5.00	117.48	110.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	TYR	Sidechain
1	B	213	TYR	Sidechain
1	D	213	TYR	Sidechain

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	2758	0	2776	36	0
1	B	2758	0	2776	55	0
1	C	2758	0	2776	45	0
1	D	2758	0	2776	56	0
2	A	604	0	0	8	0
2	B	604	0	0	12	0
2	C	601	0	0	10	0
2	D	618	0	0	14	0
All	All	13459	0	11104	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (184) 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:146:LYS:HE2	2:D:367:HOH:O	1.84	0.78
1:D:284:ASN:ND2	1:D:342:TYR:H	1.85	0.74
1:A:146:LYS:HE2	2:A:368:HOH:O	1.88	0.71
1:C:199:LYS:HG3	2:C:527:HOH:O	1.92	0.69
1:A:344:PRO:HD3	2:A:892:HOH:O	1.92	0.69
1:A:303:ARG:HB2	2:A:900:HOH:O	1.94	0.67
1:B:291:LEU:O	1:B:293:LYS:HD3	1.95	0.66
1:D:36:THR:HG22	1:D:50:ASN:HD21	1.62	0.64
1:C:146:LYS:C	1:C:146:LYS:HD3	2.24	0.63
1:D:345:SER:O	1:D:347:GLN:N	2.31	0.63
1:B:146:LYS:HE2	2:B:367:HOH:O	1.99	0.62
1:D:36:THR:HG21	2:D:630:HOH:O	1.98	0.62
1:B:220:HIS:HD2	1:C:207:LYS:NZ	1.98	0.62
1:A:344:PRO:HG2	2:A:934:HOH:O	2.00	0.60
1:B:70:ASN:HB2	1:B:71:PRO:HD3	1.82	0.60
1:D:42:ARG:HD2	1:D:303:ARG:HH11	1.67	0.59
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.38	0.59
1:B:146:LYS:C	1:B:146:LYS:HD3	2.28	0.59
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.85	0.59
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.83	0.59
1:C:41:LYS:HB3	2:C:634:HOH:O	2.02	0.59
1:C:1:PRO:HA	2:C:905:HOH:O	2.03	0.58
1:D:133:ARG:HD2	2:D:797:HOH:O	2.01	0.58
1:B:343:THR:HG21	1:B:349:GLY:HA2	1.85	0.58
1:D:345:SER:HA	2:D:916:HOH:O	2.03	0.57
1:B:318:GLU:H	1:B:318:GLU:CD	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.34	0.57
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.87	0.56
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.88	0.56
1:A:292:LEU:HD21	2:A:625:HOH:O	2.05	0.56
1:A:146:LYS:NZ	2:A:367:HOH:O	2.39	0.56
1:C:146:LYS:HE2	2:C:367:HOH:O	2.06	0.56
1:C:313:TRP:CE2	1:C:315:GLY:HA2	2.41	0.56
1:A:301:TYR:HB3	1:A:304:ALA:HB3	1.89	0.55
1:A:220:HIS:HD2	1:D:207:LYS:NZ	2.04	0.55
1:C:293:LYS:HD2	1:C:297:LEU:HD12	1.86	0.55
1:C:245:HIS:HD2	1:C:282:ASN:OD1	1.89	0.55
1:C:318:GLU:H	1:C:318:GLU:CD	2.13	0.55
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.88	0.54
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.89	0.54
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.07	0.54
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.89	0.54
1:D:146:LYS:HD3	1:D:146:LYS:C	2.32	0.54
1:D:350:ALA:O	1:D:354:GLU:HG3	2.08	0.53
1:B:316:LYS:HB2	1:B:319:ASN:ND2	2.23	0.53
1:B:108:VAL:O	1:B:133:ARG:NH2	2.41	0.53
1:B:316:LYS:HE3	2:B:683:HOH:O	2.09	0.53
1:B:207:LYS:NZ	2:B:829:HOH:O	2.42	0.52
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.45	0.52
1:B:200:ARG:HG3	1:B:200:ARG:HH11	1.74	0.52
1:B:92:PRO:HB2	1:B:94:PRO:HD2	1.92	0.52
1:B:220:HIS:HD2	1:C:207:LYS:HZ1	1.57	0.52
1:B:316:LYS:HB3	1:B:318:GLU:OE2	2.10	0.52
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.10	0.52
1:D:284:ASN:HD21	1:D:342:TYR:H	1.54	0.52
1:B:164:MET:C	1:B:164:MET:SD	2.93	0.51
1:B:66:ASP:OD1	1:B:68:ARG:HB2	2.10	0.51
1:A:2:HIS:HE1	1:D:155:GLU:O	1.92	0.51
1:A:98:LYS:NZ	2:A:836:HOH:O	2.42	0.51
1:A:146:LYS:HD3	1:A:146:LYS:C	2.34	0.51
1:D:146:LYS:NZ	2:D:368:HOH:O	2.43	0.51
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.35	0.51
1:D:61:LEU:C	1:D:61:LEU:HD23	2.36	0.51
1:D:301:TYR:HB3	1:D:304:ALA:HB3	1.92	0.50
1:D:92:PRO:HB3	2:D:866:HOH:O	2.12	0.50
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.12	0.50
1:C:303:ARG:HB3	2:C:855:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:CYS:HB3	1:C:182:ILE:HD12	1.92	0.50
1:D:36:THR:CG2	1:D:50:ASN:HD21	2.25	0.50
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.27	0.49
1:D:185:ILE:HD13	2:D:787:HOH:O	2.11	0.49
1:B:72:CYS:SG	1:B:332:LEU:HD23	2.52	0.49
1:C:343:THR:C	1:C:345:SER:N	2.68	0.49
1:B:18:ILE:HD13	1:B:143:ASP:HB3	1.94	0.49
1:B:301:TYR:HB3	1:B:304:ALA:HB3	1.93	0.49
1:C:42:ARG:HE	1:C:42:ARG:HA	1.77	0.49
1:D:83:LEU:HD12	1:D:94:PRO:HG3	1.95	0.49
1:A:139:LYS:HB2	1:A:139:LYS:NZ	2.28	0.49
1:A:146:LYS:HG2	2:A:364:HOH:O	2.11	0.49
1:D:164:MET:C	1:D:164:MET:SD	2.96	0.49
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.48	0.49
1:B:139:LYS:HE3	2:B:689:HOH:O	2.12	0.49
1:C:234:THR:HB	1:C:235:PRO:HD2	1.93	0.49
1:D:241:GLN:NE2	2:D:816:HOH:O	2.46	0.48
1:A:292:LEU:HD23	1:A:292:LEU:C	2.38	0.48
1:A:291:LEU:O	1:A:293:LYS:HD3	2.14	0.48
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.95	0.48
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.96	0.48
1:B:107:LYS:HG3	1:B:146:LYS:HD2	1.95	0.48
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.96	0.48
1:A:324:GLN:O	1:A:328:VAL:HG23	2.14	0.48
1:B:343:THR:CG2	1:B:349:GLY:HA2	2.45	0.47
1:A:107:LYS:HG3	1:A:146:LYS:HD2	1.96	0.47
1:C:93:PHE:N	1:C:94:PRO:HD2	2.29	0.47
1:A:61:LEU:C	1:A:61:LEU:HD23	2.40	0.47
1:D:277:GLU:OE2	1:D:344:PRO:HB3	2.15	0.47
1:C:164:MET:SD	1:C:164:MET:C	2.98	0.47
1:B:199:LYS:HD3	2:B:704:HOH:O	2.14	0.46
1:A:313:TRP:CZ2	1:A:315:GLY:HA2	2.51	0.46
1:C:107:LYS:HG3	1:C:146:LYS:HD2	1.96	0.46
1:C:245:HIS:HE1	2:C:757:HOH:O	1.98	0.46
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.98	0.46
1:D:25:PRO:HG2	2:D:886:HOH:O	2.15	0.46
1:B:58:TYR:OH	1:B:306:GLN:HB3	2.15	0.46
1:B:288:LYS:NZ	1:B:352:ALA:HA	2.30	0.46
1:B:317:LYS:HG2	2:B:932:HOH:O	2.15	0.46
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.51	0.46
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HB	1:A:300:SER:HB2	1.98	0.45
1:D:303:ARG:HD2	2:D:729:HOH:O	2.16	0.45
1:B:28:GLY:HA3	1:B:299:PHE:CE1	2.51	0.45
1:B:262:PRO:CG	1:C:294:PRO:HG3	2.46	0.45
1:B:199:LYS:HE3	2:B:828:HOH:O	2.16	0.45
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.98	0.45
1:B:316:LYS:HB2	1:B:319:ASN:HD22	1.81	0.45
1:C:343:THR:C	1:C:345:SER:H	2.25	0.45
1:D:293:LYS:HD2	1:D:297:LEU:HD12	1.99	0.45
1:D:319:ASN:HA	2:D:553:HOH:O	2.17	0.45
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.98	0.45
1:B:146:LYS:NZ	2:B:368:HOH:O	2.50	0.44
1:B:257:ARG:HA	1:C:262:PRO:HG2	1.98	0.44
1:C:146:LYS:HD3	1:C:147:TRP:N	2.32	0.44
1:C:268:THR:HB	1:C:300:SER:HB2	2.00	0.44
1:A:320:LEU:O	1:A:324:GLN:HG3	2.18	0.44
1:D:146:LYS:HG2	2:D:366:HOH:O	2.15	0.44
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.17	0.44
1:B:268:THR:HB	1:B:300:SER:HB2	1.98	0.44
1:D:268:THR:HB	1:D:300:SER:HB2	2.00	0.44
1:A:151:LEU:HD22	1:A:151:LEU:N	2.32	0.44
1:A:234:THR:HB	1:A:235:PRO:HD2	2.00	0.44
1:C:146:LYS:HE3	1:C:187:GLU:OE1	2.17	0.44
1:D:42:ARG:HD2	1:D:303:ARG:NH1	2.31	0.44
1:B:121:GLU:OE2	1:B:158:PRO:HA	2.18	0.44
1:C:237:HIS:HD2	2:C:618:HOH:O	2.00	0.44
1:A:29:ILE:HB	1:A:300:SER:HA	2.00	0.43
1:B:233:VAL:CG2	1:B:252:THR:HA	2.49	0.43
1:D:348:ALA:HB1	1:D:352:ALA:CB	2.49	0.43
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.53	0.43
1:D:69:VAL:CG1	1:D:328:VAL:HG22	2.49	0.43
1:D:192:PRO:HG2	1:D:357:PHE:HE2	1.83	0.43
1:B:17:ASP:O	1:B:21:ARG:HG3	2.18	0.43
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.54	0.43
1:B:234:THR:HB	1:B:235:PRO:HD2	2.00	0.43
1:D:58:TYR:O	1:D:61:LEU:HB3	2.19	0.43
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.54	0.42
1:C:42:ARG:HD2	2:C:464:HOH:O	2.18	0.42
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.92	0.42
1:A:58:TYR:OH	1:A:306:GLN:HB3	2.20	0.42
1:D:200:ARG:HH11	1:D:200:ARG:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LYS:HD2	2:C:854:HOH:O	2.18	0.42
1:C:61:LEU:C	1:C:61:LEU:HD23	2.44	0.42
1:A:337:ALA:C	1:A:339:GLN:H	2.26	0.42
1:A:312:ALA:HB3	1:A:323:ALA:HA	2.02	0.42
1:B:293:LYS:HB2	1:B:293:LYS:HE2	1.81	0.42
1:C:146:LYS:C	1:C:146:LYS:CD	2.93	0.42
1:D:29:ILE:HB	1:D:300:SER:HA	2.00	0.42
1:D:298:THR:OG1	1:D:299:PHE:N	2.53	0.42
1:C:336:LEU:HD11	1:C:347:GLN:NE2	2.35	0.42
1:B:262:PRO:HD2	1:C:257:ARG:O	2.20	0.41
1:B:146:LYS:HE3	1:B:187:GLU:OE1	2.20	0.41
1:A:262:PRO:HD2	1:D:257:ARG:O	2.21	0.41
1:B:152:LYS:HE2	2:B:607:HOH:O	2.21	0.41
1:B:318:GLU:HG3	2:B:913:HOH:O	2.20	0.41
1:D:234:THR:HB	1:D:235:PRO:HD2	2.02	0.41
1:B:212:VAL:HG13	2:B:770:HOH:O	2.20	0.41
1:C:133:ARG:HD3	2:C:412:HOH:O	2.20	0.41
1:B:343:THR:C	1:B:345:SER:H	2.28	0.41
1:B:29:ILE:HB	1:B:300:SER:HA	2.03	0.41
1:B:89:ASP:OD2	1:B:91:ARG:HD3	2.21	0.41
1:B:276:GLU:CD	1:B:307:ALA:HB3	2.46	0.41
1:C:94:PRO:O	1:C:98:LYS:HG3	2.21	0.41
1:C:288:LYS:NZ	1:C:352:ALA:HB1	2.35	0.41
1:D:59:ARG:O	1:D:63:LEU:HG	2.21	0.41
1:D:81:GLU:O	1:D:85:GLN:HG3	2.20	0.41
1:D:347:GLN:HG3	2:D:723:HOH:O	2.20	0.41
1:D:310:LEU:C	1:D:310:LEU:HD13	2.46	0.41
1:D:316:LYS:HB2	1:D:319:ASN:OD1	2.20	0.41
1:D:344:PRO:O	1:D:345:SER:HB3	2.21	0.40
1:D:347:GLN:O	1:D:348:ALA:HB3	2.21	0.40
1:B:200:ARG:HG3	1:B:200:ARG:NH1	2.36	0.40
1:D:276:GLU:HG3	2:D:540:HOH:O	2.21	0.40
1:A:139:LYS:NZ	1:A:139:LYS:CB	2.84	0.40
1:C:134:CYS:CB	1:C:182:ILE:HD12	2.51	0.40
1:B:185:ILE:HD13	2:B:875:HOH:O	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	361/363 (99%)	335 (93%)	19 (5%)	7 (2%)	6	1
1	B	361/363 (99%)	338 (94%)	18 (5%)	5 (1%)	9	2
1	C	361/363 (99%)	342 (95%)	15 (4%)	4 (1%)	11	3
1	D	361/363 (99%)	341 (94%)	14 (4%)	6 (2%)	7	2
All	All	1444/1452 (99%)	1356 (94%)	66 (5%)	22 (2%)	8	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	346	GLY
1	A	346	GLY
1	A	349	GLY
1	D	349	GLY
1	A	5	PRO
1	B	188	PRO
1	C	353	SER
1	D	345	SER
1	A	67	ASP
1	A	188	PRO
1	A	344	PRO
1	A	352	ALA
1	B	5	PRO
1	B	354	GLU
1	C	5	PRO
1	C	188	PRO
1	D	362	ALA
1	B	358	ILE
1	C	356	LEU
1	D	5	PRO
1	D	188	PRO
1	B	346	GLY

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	291/291 (100%)	285 (98%)	6 (2%)	47	36
1	B	291/291 (100%)	286 (98%)	5 (2%)	53	45
1	C	291/291 (100%)	283 (97%)	8 (3%)	39	27
1	D	291/291 (100%)	288 (99%)	3 (1%)	68	64
All	All	1164/1164 (100%)	1142 (98%)	22 (2%)	50	41

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	53	GLU
1	A	139	LYS
1	A	295	TRP
1	A	318	GLU
1	A	344	PRO
1	B	42	ARG
1	B	107	LYS
1	B	199	LYS
1	B	295	TRP
1	B	318	GLU
1	C	5	PRO
1	C	42	ARG
1	C	53	GLU
1	C	199	LYS
1	C	230	PRO
1	C	295	TRP
1	C	318	GLU
1	C	344	PRO
1	D	230	PRO
1	D	295	TRP
1	D	343	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	54	ASN
1	A	119	ASN
1	A	156	HIS
1	A	180	ASN
1	A	220	HIS
1	A	241	GLN
1	A	245	HIS
1	A	319	ASN
1	B	2	HIS
1	B	4	HIS
1	B	95	GLN
1	B	119	ASN
1	B	136	GLN
1	B	220	HIS
1	B	237	HIS
1	B	324	GLN
1	B	347	GLN
1	C	4	HIS
1	C	136	GLN
1	C	241	GLN
1	C	245	HIS
1	C	339	GLN
1	C	347	GLN
1	C	360	ASN
1	D	50	ASN
1	D	54	ASN
1	D	237	HIS
1	D	241	GLN
1	D	284	ASN
1	D	306	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 [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	363/363 (100%)	-0.11	19 (5%)	33	31	10, 19, 41, 67	15 (4%)
1	B	363/363 (100%)	0.01	22 (6%)	27	25	10, 19, 47, 68	15 (4%)
1	C	363/363 (100%)	-0.04	21 (5%)	29	27	10, 19, 43, 70	15 (4%)
1	D	363/363 (100%)	0.09	21 (5%)	29	27	11, 23, 63, 92	3 (0%)
All	All	1452/1452 (100%)	-0.01	83 (5%)	29	28	10, 20, 48, 92	48 (3%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	ALA	8.1
1	C	351	ALA	7.9
1	C	350	ALA	7.7
1	A	356	LEU	7.7
1	B	357	PHE	7.7
1	B	358	ILE	7.5
1	C	345	SER	7.4
1	B	356	LEU	7.1
1	C	346	GLY	7.1
1	C	352	ALA	6.9
1	C	349	GLY	6.6
1	B	349	GLY	6.2
1	A	357	PHE	6.2
1	B	350	ALA	5.8
1	D	363	TYR	5.4
1	D	362	ALA	5.3
1	B	359	SER	5.3
1	C	359	SER	5.3
1	C	357	PHE	5.3
1	A	348	ALA	5.2
1	A	359	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	352	ALA	5.1
1	A	358	ILE	5.0
1	A	351	ALA	4.9
1	C	355	SER	4.8
1	B	352	ALA	4.8
1	B	348	ALA	4.7
1	B	353	SER	4.7
1	C	358	ILE	4.7
1	A	350	ALA	4.6
1	D	348	ALA	4.6
1	B	347	GLN	4.5
1	C	356	LEU	4.5
1	C	347	GLN	4.5
1	B	351	ALA	4.4
1	D	356	LEU	4.3
1	A	344	PRO	4.3
1	A	355	SER	4.2
1	D	361	HIS	3.9
1	D	352	ALA	3.9
1	D	358	ILE	3.9
1	D	357	PHE	3.9
1	D	350	ALA	3.8
1	A	353	SER	3.8
1	A	345	SER	3.7
1	D	346	GLY	3.7
1	A	346	GLY	3.6
1	D	353	SER	3.6
1	C	353	SER	3.6
1	D	344	PRO	3.5
1	A	354	GLU	3.3
1	C	344	PRO	3.3
1	B	346	GLY	3.3
1	C	1	PRO	3.2
1	A	349	GLY	3.2
1	B	354	GLU	3.1
1	C	354	GLU	3.0
1	A	1	PRO	3.0
1	B	345	SER	2.9
1	D	351	ALA	2.9
1	D	349	GLY	2.9
1	D	360	ASN	2.9
1	B	360	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	355	SER	2.7
1	D	42	ARG	2.6
1	A	347	GLN	2.6
1	A	360	ASN	2.6
1	C	360	ASN	2.5
1	D	347	GLN	2.4
1	D	345	SER	2.4
1	B	1	PRO	2.4
1	C	47	GLY	2.4
1	A	343	THR	2.4
1	D	46	ILE	2.4
1	B	344	PRO	2.3
1	D	343	THR	2.3
1	D	40	ALA	2.3
1	B	343	THR	2.3
1	B	362	ALA	2.2
1	C	39	ILE	2.0
1	C	155	GLU	2.0
1	B	2	HIS	2.0
1	B	45	SER	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.