



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:58 am BST

PDB ID : 1ZAH
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 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	:	2.11
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)	:	2.11

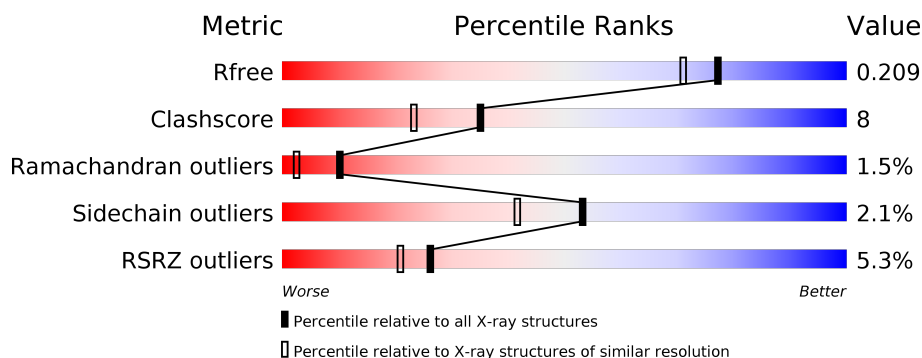
1 Overall quality at a glance ⓘ

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 on 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	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
1	B	363	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>19%</div> </div> </div>
1	C	363	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> </div>
1	D	363	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>19%</div> </div> </div>

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			

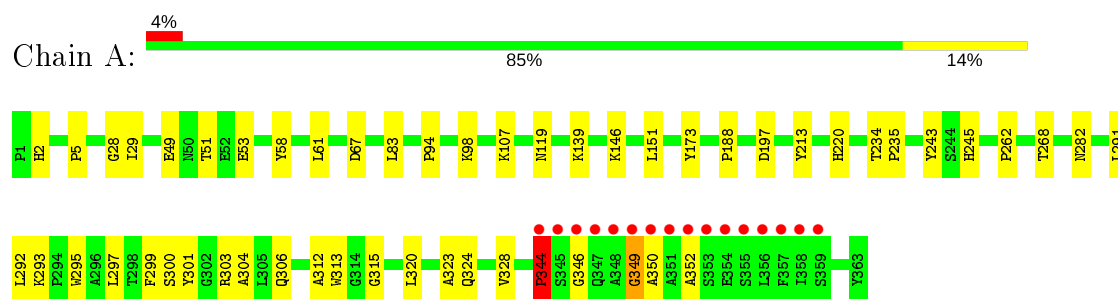
- Molecule 2 is water.

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		

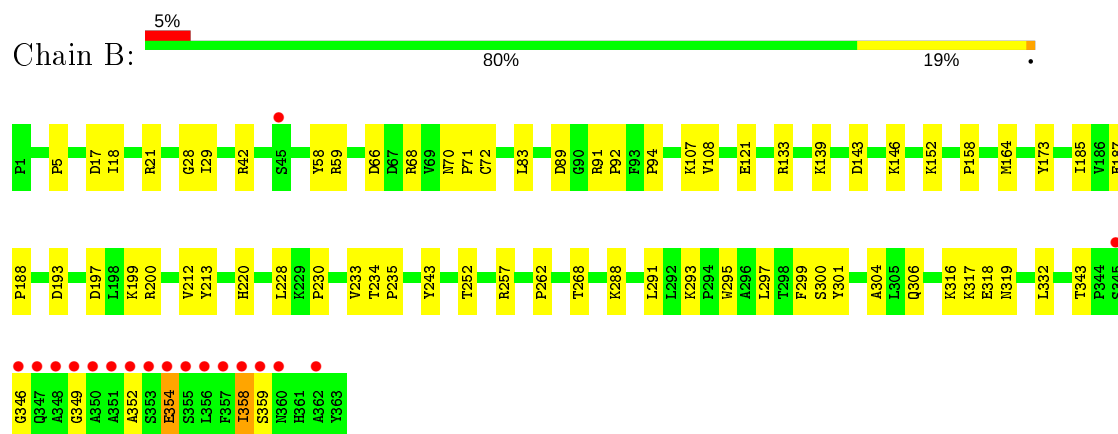
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

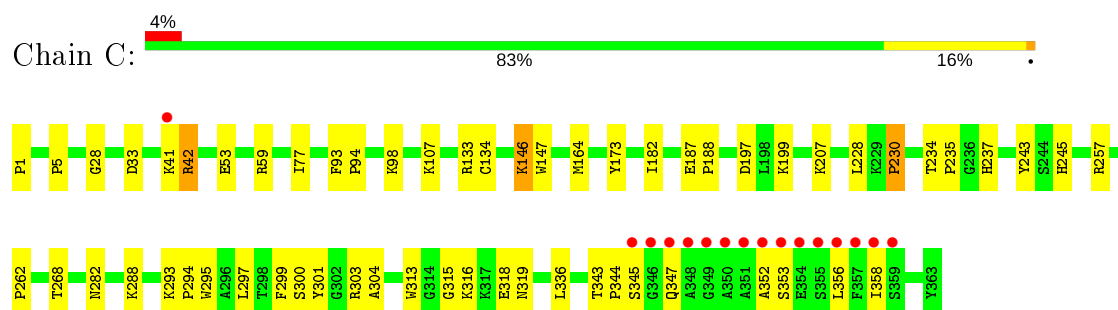
• Molecule 1: Fructose-bisphosphate aldolase A



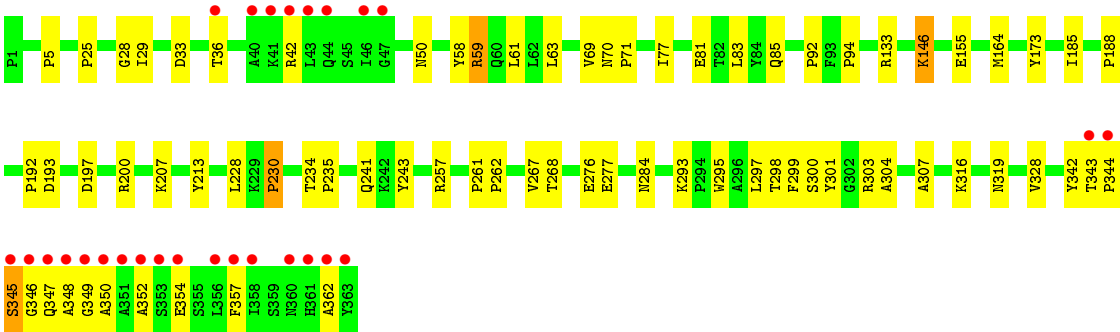
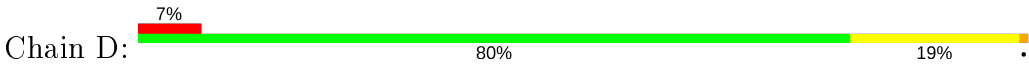
• Molecule 1: Fructose-bisphosphate aldolase A



• 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 43.85 – 1.79	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-1.80) 94.5 (43.85-1.79)	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)	0.34 , 64.8	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	0.30	0/2812	0.60	0/3810
1	B	0.30	0/2812	0.58	0/3810
1	C	0.30	0/2812	0.58	0/3810
1	D	0.28	0/2812	0.57	0/3810
All	All	0.29	0/11248	0.58	0/15240

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.

There are no bond angle outliers.

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	43	0
1	D	2758	0	2776	55	0
2	A	604	0	0	8	0
2	B	604	0	0	11	0
2	C	601	0	0	10	0
2	D	618	0	0	14	0
All	All	13459	0	11104	181	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 (181) 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:B:358:ILE:HG22	1:B:359:SER:H	1.56	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: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: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:146:LYS:C	1:C:146:LYS:HD3	2.24	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:146:LYS:C	1:B:146:LYS:HD3	2.28	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: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:200:ARG:HG3	1:B:200:ARG:HH11	1.74	0.52
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.45	0.52
1:B:316:LYS:HB3	1:B:318:GLU:OE2	2.10	0.52
1:B:92:PRO:HB2	1:B:94:PRO:HD2	1.92	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:66:ASP:OD1	1:B:68:ARG:HB2	2.10	0.51
1:C:318:GLU:H	1:C:318:GLU:CD	2.13	0.51
1:A:98:LYS:NZ	2:A:836:HOH:O	2.42	0.51
1:A:2:HIS:HE1	1:D:155:GLU:O	1.92	0.51
1:B:318:GLU:H	1:B:318:GLU:CD	2.12	0.51
1:D:146:LYS:NZ	2:D:368:HOH:O	2.43	0.51
1:B:220:HIS:HD2	1:C:207:LYS:HZ1	1.58	0.50
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
1:C:134:CYS:HB3	1:C:182:ILE:HD12	1.92	0.50
1:A:146:LYS:NZ	2:A:367:HOH:O	2.39	0.50
1:D:36:THR:CG2	1:D:50:ASN:HD21	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:C:42:ARG:HE	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: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: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:146:LYS:HD3	1:D:146:LYS:C	2.32	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:A:146:LYS:HD3	1:A:146:LYS:C	2.34	0.47
1:B:343:THR:CG2	1:B:349:GLY:HA2	2.45	0.47
1:C:93:PHE:N	1:C:94:PRO:HD2	2.29	0.47
1:A:107:LYS:HG3	1:A:146:LYS:HD2	1.96	0.47
1:B:164:MET:C	1:B:164:MET:SD	2.93	0.47
1:D:277:GLU:OE2	1:D:344:PRO:HB3	2.15	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:A:349:GLY:O	1:A:350:ALA:HB3	2.15	0.46
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.35	0.46
1:D:61:LEU:HD23	1:D:61:LEU:C	2.36	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:C:358:ILE:HD12	1:C:358:ILE:C	2.36	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:N	2.68	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:164:MET:SD	1:D:164:MET:C	2.96	0.44
1:D:268:THR:HB	1:D:300:SER:HB2	2.00	0.44
1:A:151:LEU:N	1:A:151:LEU:HD22	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:292:LEU:C	1:A:292:LEU:HD23	2.38	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:41:LYS:HD2	2:C:854:HOH:O	2.18	0.42
1:A:61:LEU:HD23	1:A:61:LEU:C	2.40	0.42
1:B:358:ILE:HG22	1:B:359:SER:N	2.31	0.42
1:C:164:MET:SD	1:C:164:MET:C	2.98	0.42
1:A:312:ALA:HB3	1:A:323:ALA:HA	2.02	0.42
1:B:293:LYS:HE2	1:B:293:LYS:HB2	1.81	0.42
1:D:298:THR:OG1	1:D:299:PHE:N	2.53	0.42
1:D:29:ILE:HB	1:D:300:SER:HA	2.00	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:B:354:GLU:OE1	1:B:354:GLU:HA	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: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:D:81:GLU:O	1:D:85:GLN:HG3	2.20	0.41
1:C:288:LYS:NZ	1:C:352:ALA:HB1	2.35	0.41
1:C:94:PRO:O	1:C:98:LYS:HG3	2.21	0.41
1:D:347:GLN:HG3	2:D:723:HOH:O	2.20	0.41
1:D:59:ARG:O	1:D:63:LEU:HG	2.21	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:CB	1:A:139:LYS:NZ	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%)	8	1
1	B	361/363 (99%)	338 (94%)	18 (5%)	5 (1%)	11	3
1	C	361/363 (99%)	342 (95%)	15 (4%)	4 (1%)	14	4
1	D	361/363 (99%)	341 (94%)	14 (4%)	6 (2%)	9	2
All	All	1444/1452 (99%)	1356 (94%)	66 (5%)	22 (2%)	10	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%)	286 (98%)	5 (2%)	60	51
1	B	291/291 (100%)	286 (98%)	5 (2%)	60	51
1	C	291/291 (100%)	283 (97%)	8 (3%)	44	31
1	D	291/291 (100%)	284 (98%)	7 (2%)	49	36
All	All	1164/1164 (100%)	1139 (98%)	25 (2%)	53	42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	119	ASN
1	A	173	TYR
1	A	295	TRP
1	A	344	PRO
1	B	42	ARG
1	B	59	ARG
1	B	173	TYR
1	B	193	ASP
1	B	295	TRP
1	C	42	ARG
1	C	53	GLU
1	C	59	ARG
1	C	146	LYS
1	C	173	TYR
1	C	230	PRO
1	C	295	TRP
1	C	344	PRO
1	D	59	ARG
1	D	146	LYS
1	D	173	TYR
1	D	193	ASP
1	D	230	PRO
1	D	295	TRP
1	D	343	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	119	ASN
1	A	180	ASN
1	A	220	HIS
1	A	241	GLN
1	A	245	HIS
1	A	319	ASN
1	B	95	GLN
1	B	119	ASN
1	B	136	GLN
1	B	156	HIS
1	B	220	HIS
1	B	319	ASN
1	B	347	GLN
1	C	241	GLN
1	C	245	HIS
1	C	319	ASN
1	C	347	GLN
1	D	50	ASN
1	D	54	ASN
1	D	180	ASN
1	D	241	GLN
1	D	284	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.13	16 (4%)	34	28	10, 19, 44, 101	15 (4%)
1	B	363/363 (100%)	0.46	18 (4%)	28	23	10, 19, 50, 105	15 (4%)
1	C	363/363 (100%)	0.45	16 (4%)	34	28	10, 19, 47, 104	15 (4%)
1	D	363/363 (100%)	0.22	27 (7%)	14	11	11, 23, 70, 104	3 (0%)
All	All	1452/1452 (100%)	0.32	77 (5%)	26	21	10, 20, 60, 105	48 (3%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	GLY	35.7
1	B	348	ALA	35.6
1	B	349	GLY	33.3
1	C	352	ALA	32.6
1	C	351	ALA	30.9
1	B	350	ALA	24.4
1	B	356	LEU	24.3
1	A	355	SER	23.0
1	C	356	LEU	21.8
1	C	353	SER	21.1
1	B	351	ALA	21.0
1	D	362	ALA	19.7
1	C	350	ALA	19.7
1	D	363	TYR	18.5
1	C	348	ALA	18.1
1	C	358	ILE	17.7
1	A	348	ALA	17.2
1	B	346	GLY	16.7
1	C	357	PHE	16.5
1	A	356	LEU	16.5
1	A	357	PHE	16.5

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Mol	Chain	Res	Type	RSRZ
1	A	351	ALA	15.3
1	B	353	SER	15.3
1	B	355	SER	15.2
1	B	358	ILE	14.9
1	A	350	ALA	14.5
1	B	347	GLN	14.2
1	A	353	SER	13.2
1	A	352	ALA	13.2
1	B	357	PHE	12.9
1	C	355	SER	12.3
1	A	358	ILE	11.6
1	C	347	GLN	11.1
1	A	354	GLU	10.9
1	A	349	GLY	10.7
1	B	352	ALA	10.0
1	B	345	SER	9.9
1	D	361	HIS	9.7
1	A	346	GLY	8.9
1	A	347	GLN	8.6
1	C	354	GLU	8.5
1	C	345	SER	8.2
1	B	359	SER	7.7
1	D	345	SER	7.4
1	C	346	GLY	7.4
1	B	354	GLU	7.3
1	D	348	ALA	7.0
1	A	359	SER	6.5
1	A	345	SER	5.7
1	D	350	ALA	4.9
1	D	346	GLY	4.7
1	D	347	GLN	4.7
1	C	359	SER	4.6
1	D	349	GLY	4.4
1	D	344	PRO	3.6
1	A	344	PRO	3.6
1	D	42	ARG	3.5
1	D	343	THR	3.3
1	D	352	ALA	3.3
1	D	358	ILE	3.2
1	D	353	SER	3.1
1	D	46	ILE	3.1
1	D	40	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	45	SER	2.9
1	B	360	ASN	2.9
1	D	41	LYS	2.9
1	B	362	ALA	2.7
1	D	36	THR	2.7
1	D	354	GLU	2.6
1	D	360	ASN	2.5
1	D	351	ALA	2.5
1	D	44	GLN	2.5
1	C	41	LYS	2.4
1	D	356	LEU	2.4
1	D	43	LEU	2.3
1	D	357	PHE	2.2
1	D	47	GLY	2.1

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 carbohydrates 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.