



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:19 AM UTC

PDB ID : 3DFN / pdb_00003dfn
Title : D33N mutant fructose-1,6-bisphosphate aldolase from rabbit muscle
Authors : St-Jean, M.; Sygusch, J.
Deposited on : 2008-06-12
Resolution : 1.86 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

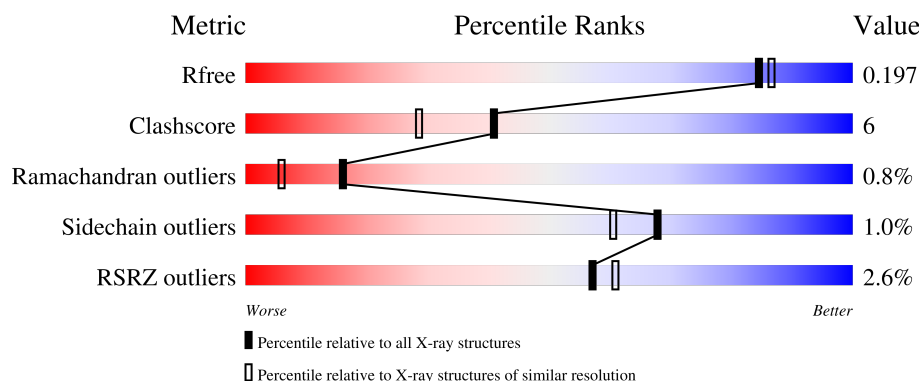
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	2% 79% 16% ..
1	B	363	2% 81% 15% ..
1	C	363	2% 81% 16% .
1	D	363	5% 81% 18% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13078 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	350	Total	C	N	O	S	0	1	0
			2682	1686	478	507	11			
1	B	350	Total	C	N	O	S	0	1	0
			2682	1686	478	507	11			
1	C	353	Total	C	N	O	S	0	1	0
			2700	1696	482	511	11			
1	D	361	Total	C	N	O	S	0	1	0
			2749	1727	490	521	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ASN	ASP	engineered mutation	UNP P00883
B	33	ASN	ASP	engineered mutation	UNP P00883
C	33	ASN	ASP	engineered mutation	UNP P00883
D	33	ASN	ASP	engineered mutation	UNP P00883

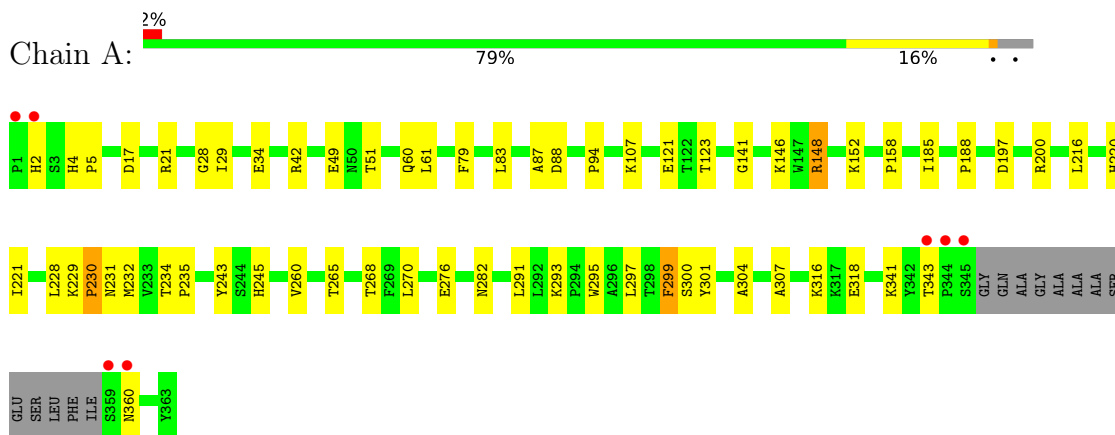
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	585	Total	O	0	3
			585	585		
2	B	556	Total	O	0	3
			556	556		
2	C	549	Total	O	0	3
			549	549		
2	D	575	Total	O	0	3
			575	575		

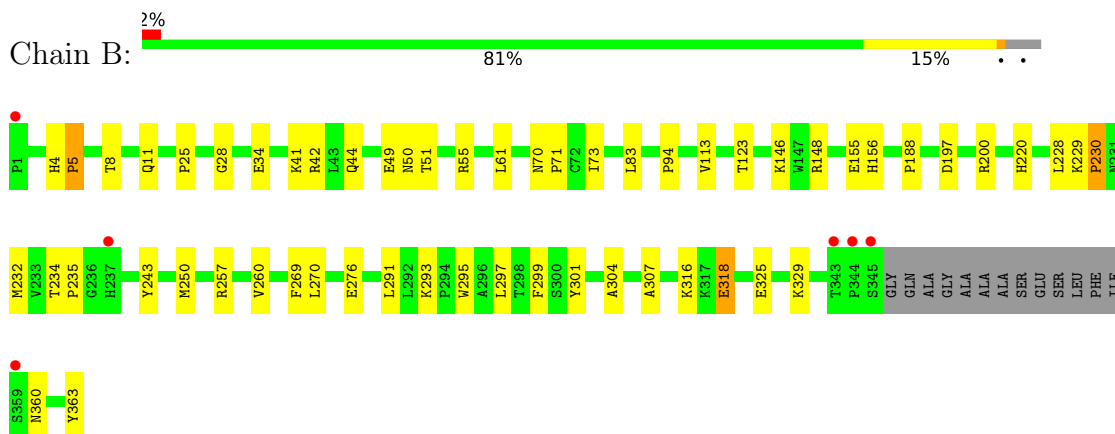
3 Residue-property plots

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.

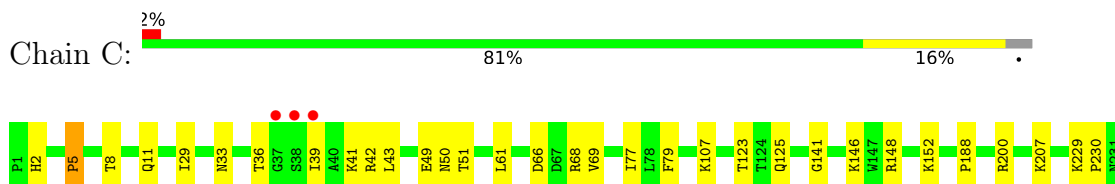
- Molecule 1: Fructose-bisphosphate aldolase A

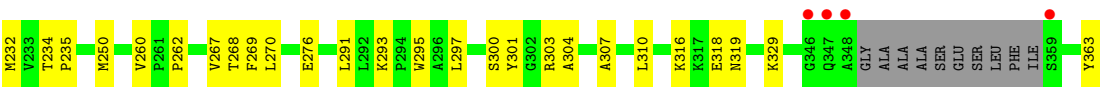


- Molecule 1: Fructose-bisphosphate aldolase A

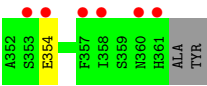
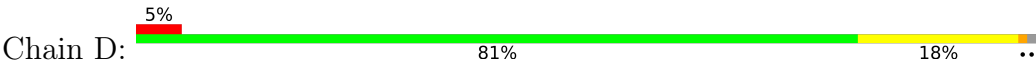


- Molecule 1: Fructose-bisphosphate aldolase A





● 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	84.25Å 103.87Å 84.88Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	44.07 – 1.86 44.07 – 1.86	Depositor EDS
% Data completeness (in resolution range)	81.9 (44.07-1.86) 91.0 (44.07-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.141 , 0.188 0.154 , 0.197	Depositor DCC
R_{free} test set	12159 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13078	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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	0.34	0/2734	0.88	12/3702 (0.3%)
1	B	0.34	0/2734	0.88	10/3702 (0.3%)
1	C	0.33	0/2752	0.86	8/3726 (0.2%)
1	D	0.34	0/2802	0.86	11/3796 (0.3%)
All	All	0.34	0/11022	0.87	41/14926 (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	D	0	1

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	260	VAL	N-CA-C	8.46	115.25	107.56
1	D	260	VAL	N-CA-C	7.22	114.13	107.56
1	A	232	MET	N-CA-C	-7.21	100.82	110.55
1	C	232	MET	N-CA-C	-7.05	101.03	110.55
1	B	260	VAL	N-CA-C	7.03	113.96	107.56
1	D	123	THR	N-CA-C	-7.02	99.21	109.18
1	D	232	MET	N-CA-C	-6.92	101.40	110.53
1	B	232	MET	N-CA-C	-6.82	101.34	110.55
1	A	260	VAL	N-CA-C	6.76	113.71	107.56
1	A	270	LEU	N-CA-C	-6.29	101.21	110.52
1	A	123	THR	N-CA-C	-6.03	100.62	109.18
1	B	73	ILE	N-CA-C	5.97	116.20	107.37
1	C	270	LEU	N-CA-C	-5.94	100.87	110.32
1	D	148	ARG	N-CA-C	5.90	118.14	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	LEU	N-CA-C	-5.72	101.22	110.32
1	C	79	PHE	N-CA-C	-5.70	102.09	110.52
1	B	123	THR	N-CA-C	-5.55	101.30	109.18
1	D	4	HIS	CA-C-N	5.54	126.77	119.84
1	D	4	HIS	C-N-CA	5.54	126.77	119.84
1	D	270	LEU	N-CA-C	-5.51	101.56	110.32
1	C	141	GLY	N-CA-C	5.47	122.30	114.64
1	A	79	PHE	N-CA-C	-5.46	102.44	110.52
1	A	265	THR	N-CA-C	5.41	117.18	111.28
1	D	289	CYS	CA-C-N	5.40	126.59	119.84
1	D	289	CYS	C-N-CA	5.40	126.59	119.84
1	C	269	PHE	N-CA-C	5.37	118.01	110.23
1	C	123	THR	N-CA-C	-5.30	101.65	109.18
1	A	4	HIS	CA-C-N	5.30	126.46	119.84
1	A	4	HIS	C-N-CA	5.30	126.46	119.84
1	B	269	PHE	N-CA-C	5.29	117.90	110.23
1	B	4	HIS	CA-C-N	5.27	126.42	119.84
1	B	4	HIS	C-N-CA	5.27	126.42	119.84
1	D	73	ILE	N-CA-C	5.22	115.09	107.37
1	C	148	ARG	N-CA-C	5.21	117.02	108.52
1	A	231	ASN	N-CA-C	-5.14	103.62	110.55
1	A	299	PHE	N-CA-C	5.13	117.93	109.72
1	B	113	VAL	N-CA-C	-5.12	104.99	109.19
1	D	269	PHE	N-CA-C	5.11	117.63	110.23
1	B	148	ARG	N-CA-C	5.09	116.81	108.52
1	A	141	GLY	N-CA-C	5.07	121.74	114.64
1	A	148	ARG	N-CA-C	5.07	116.78	108.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2682	0	2708	40	0
1	B	2682	0	2708	31	0
1	C	2700	0	2724	38	0
1	D	2749	0	2776	38	0
2	A	585	0	0	6	0
2	B	556	0	0	3	0
2	C	549	0	0	6	0
2	D	575	0	0	6	0
All	All	13078	0	10916	141	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 6.

All (141) 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:8:THR:H	1:C:11:GLN:HE21	1.19	0.86
1:A:60:GLN:NE2	1:A:88:ASP:H	1.80	0.79
1:D:107:LYS:HG3	1:D:146[B]:LYS:HD2	1.65	0.77
1:A:60:GLN:HE22	1:A:88:ASP:H	1.34	0.72
1:B:8:THR:H	1:B:11:GLN:HE21	1.36	0.70
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.74	0.70
1:C:293:LYS:HG2	1:C:297:LEU:HD11	1.74	0.68
1:D:316:LYS:HB2	1:D:319:ASN:ND2	2.11	0.66
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.79	0.64
1:C:291:LEU:O	1:C:293:LYS:HD3	1.98	0.63
1:C:125:GLN:HE22	1:D:129:GLY:H	1.47	0.62
1:D:284:ASN:ND2	1:D:342:TYR:H	1.97	0.62
1:B:291:LEU:O	1:B:293:LYS:HD3	1.98	0.62
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.82	0.62
1:A:60:GLN:HE21	1:A:87:ALA:HA	1.65	0.61
1:D:301:TYR:HB3	1:D:304:ALA:HB3	1.82	0.61
1:B:41:LYS:HA	1:B:44:GLN:HG2	1.83	0.61
1:D:316:LYS:HB2	1:D:319:ASN:HD22	1.65	0.61
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.82	0.60
1:B:34:GLU:HG2	1:B:42:ARG:HH12	1.67	0.60
1:B:70:ASN:HB2	1:B:71:PRO:HD3	1.83	0.59
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.84	0.59
1:A:146[B]:LYS:HD3	1:A:146[B]:LYS:C	2.29	0.57
1:C:49:GLU:HG2	1:C:51:THR:HG23	1.87	0.57
1:C:318:GLU:H	1:C:318:GLU:CD	2.13	0.57
1:A:60:GLN:NE2	1:A:88:ASP:N	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146[B]:LYS:C	1:C:146[B]:LYS:HD3	2.31	0.56
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.21	0.55
1:B:50:ASN:ND2	1:B:55:ARG:HH11	2.03	0.55
1:B:301:TYR:HB3	1:B:304:ALA:HB3	1.88	0.55
1:C:107:LYS:HG3	1:C:146[B]:LYS:HD2	1.89	0.54
1:A:301:TYR:HB3	1:A:304:ALA:HB3	1.91	0.53
1:A:341:LYS:HE3	2:A:471:HOH:O	2.09	0.53
1:B:200:ARG:HD2	2:C:988:HOH:O	2.08	0.53
1:C:39:ILE:HG12	1:C:43:LEU:HG	1.91	0.53
1:D:36:THR:HG23	1:D:50:ASN:HD21	1.73	0.53
1:B:360:ASN:HB2	2:B:769:HOH:O	2.08	0.52
1:A:60:GLN:HE22	1:A:88:ASP:N	2.03	0.52
1:A:2:HIS:HE1	1:D:155:GLU:O	1.93	0.52
1:D:36:THR:CG2	1:D:50:ASN:HD21	2.23	0.51
1:D:200:ARG:HH11	1:D:200:ARG:HG3	1.75	0.51
1:B:34:GLU:CD	1:B:42:ARG:HH22	2.19	0.51
1:C:42:ARG:HB3	1:C:310:LEU:HD21	1.91	0.51
1:A:276:GLU:CD	1:A:307:ALA:HB3	2.36	0.51
1:B:50:ASN:HD21	1:B:55:ARG:HD3	1.76	0.50
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.12	0.50
1:C:229:LYS:NZ	2:C:727[B]:HOH:O	2.40	0.50
1:D:61:LEU:C	1:D:61:LEU:HD23	2.36	0.50
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.93	0.50
1:B:220:HIS:HD2	1:C:207:LYS:NZ	2.10	0.50
1:C:152:LYS:HE2	2:C:1167:HOH:O	2.12	0.50
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.37	0.49
1:A:229:LYS:NZ	2:A:366[B]:HOH:O	2.41	0.49
1:D:345:SER:HB2	2:D:911:HOH:O	2.12	0.49
1:A:291:LEU:O	1:A:293:LYS:HD3	2.13	0.48
1:A:107:LYS:HG3	1:A:146[B]:LYS:HD2	1.94	0.48
1:C:77:ILE:HD13	1:C:146[A]:LYS:HD2	1.96	0.48
1:C:234:THR:HB	1:C:235:PRO:HD2	1.94	0.48
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.48	0.48
1:A:60:GLN:HE21	1:A:87:ALA:CA	2.27	0.47
1:A:61:LEU:C	1:A:61:LEU:HD23	2.40	0.47
1:B:146[B]:LYS:HD3	1:B:146[B]:LYS:C	2.39	0.47
1:A:220:HIS:HD2	1:D:207:LYS:NZ	2.13	0.47
1:B:51:THR:O	1:B:55:ARG:HG3	2.14	0.47
1:A:360:ASN:HB2	2:A:627:HOH:O	2.15	0.47
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.50	0.47
1:A:185:ILE:HD13	2:A:793:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ALA:O	1:D:354:GLU:HG3	2.15	0.46
1:D:277:GLU:O	1:D:281:ILE:HG13	2.16	0.46
1:B:257:ARG:HA	1:C:262:PRO:HG2	1.96	0.46
1:D:146[A]:LYS:HG3	2:D:814:HOH:O	2.16	0.46
1:D:291:LEU:O	1:D:293:LYS:HE2	2.15	0.46
1:B:234:THR:HB	1:B:235:PRO:HD2	1.97	0.46
1:B:318:GLU:H	1:B:318:GLU:CD	2.23	0.46
1:B:229:LYS:NZ	2:B:515[B]:HOH:O	2.47	0.46
1:A:29:ILE:HB	1:A:300:SER:HA	1.97	0.46
1:A:146[A]:LYS:NZ	1:A:229:LYS:NZ	2.64	0.46
1:C:329:LYS:HB3	2:C:1248:HOH:O	2.15	0.46
1:C:2:HIS:HD2	2:D:823:HOH:O	1.98	0.45
1:C:41:LYS:O	1:C:41:LYS:HD3	2.16	0.45
1:A:146[A]:LYS:HZ3	1:A:229:LYS:HZ2	1.62	0.45
1:C:36:THR:HG23	1:C:50:ASN:HD21	1.81	0.45
1:B:276:GLU:CD	1:B:307:ALA:HB3	2.41	0.45
1:C:42:ARG:NH2	1:C:303:ARG:HB3	2.31	0.45
2:C:767:HOH:O	1:D:164:MET:HE3	2.16	0.45
1:D:61:LEU:HG	1:D:320:LEU:HD12	1.99	0.45
1:D:66:ASP:OD1	1:D:68:ARG:HB2	2.17	0.45
1:D:229:LYS:NZ	2:D:366[B]:HOH:O	2.50	0.45
1:C:250:MET:HG2	1:C:363:TYR:CE2	2.52	0.44
1:C:276:GLU:CD	1:C:307:ALA:HB3	2.42	0.44
1:C:125:GLN:NE2	1:D:129:GLY:H	2.15	0.44
1:C:303:ARG:HG2	2:C:1163:HOH:O	2.17	0.44
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.99	0.44
1:C:39:ILE:O	1:C:43:LEU:HG	2.18	0.44
1:D:324:GLN:O	1:D:328:VAL:HG23	2.17	0.44
1:A:268:THR:HB	1:A:300:SER:HB2	2.00	0.44
1:C:61:LEU:C	1:C:61:LEU:HD23	2.43	0.43
1:D:146[B]:LYS:HD3	1:D:146[B]:LYS:C	2.42	0.43
1:A:216:LEU:HD22	1:A:221:ILE:HG13	2.01	0.43
1:C:200:ARG:HG3	1:C:200:ARG:HH11	1.82	0.43
1:D:325:GLU:O	1:D:329:LYS:HG3	2.19	0.43
1:D:351:ALA:HB3	2:D:433:HOH:O	2.19	0.43
1:D:146[A]:LYS:NZ	1:D:229:LYS:NZ	2.67	0.43
1:C:66:ASP:O	1:C:69:VAL:HG22	2.19	0.42
1:A:121:GLU:OE2	1:A:158:PRO:HA	2.20	0.42
1:B:325:GLU:O	1:B:329:LYS:HG3	2.19	0.42
1:C:66:ASP:OD1	1:C:68:ARG:HB2	2.20	0.42
1:A:343:THR:HG23	1:A:343:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:HE3	2:A:594:HOH:O	2.20	0.42
1:D:146[A]:LYS:HZ1	1:D:229:LYS:HZ3	1.68	0.42
1:D:228:LEU:HG	1:D:230:PRO:HD3	2.02	0.42
1:B:250:MET:HG2	1:B:363:TYR:CE2	2.55	0.41
1:C:268:THR:HB	1:C:300:SER:HB2	2.02	0.41
1:B:49:GLU:HG2	1:B:51:THR:HG23	2.01	0.41
1:B:316:LYS:HB3	1:B:318:GLU:OE2	2.21	0.41
1:C:36:THR:CG2	1:C:50:ASN:HD21	2.33	0.41
1:A:17:ASP:O	1:A:21:ARG:HG3	2.20	0.41
1:D:234:THR:HB	1:D:235:PRO:HD2	2.01	0.41
1:A:34:GLU:HG2	1:A:42:ARG:NH2	2.36	0.41
1:A:316:LYS:HB3	1:A:318:GLU:CD	2.45	0.41
1:D:51:THR:OG1	1:D:54:ASN:ND2	2.54	0.41
1:C:33:ASN:HB3	1:C:77:ILE:HG22	2.01	0.41
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.20	0.41
1:A:245:HIS:HD2	1:A:282:ASN:OD1	2.04	0.41
1:B:25:PRO:HD2	2:B:727:HOH:O	2.21	0.41
1:A:228:LEU:HG	1:A:230:PRO:HD3	2.02	0.41
1:A:146[B]:LYS:HE2	1:A:148:ARG:HB2	2.02	0.41
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.20	0.41
1:B:83:LEU:HD12	1:B:94:PRO:HG3	2.03	0.41
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.86	0.41
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.56	0.41
1:C:267:VAL:HB	1:C:297:LEU:HD23	2.02	0.41
1:C:293:LYS:HG2	1:C:297:LEU:CD1	2.47	0.41
1:D:83:LEU:HD12	1:D:94:PRO:HG3	2.03	0.41
1:D:185:ILE:HD13	2:D:822:HOH:O	2.21	0.41
1:B:155:GLU:HG2	1:B:156:HIS:CD2	2.56	0.40
1:D:268:THR:HB	1:D:300:SER:HB2	2.03	0.40
1:A:2:HIS:HD2	2:A:428:HOH:O	2.04	0.40
1:A:234:THR:HB	1:A:235:PRO:HD2	2.03	0.40
1:B:61:LEU:C	1:B:61:LEU:HD23	2.46	0.40
1:C:29:ILE:HB	1:C:300:SER:HA	2.04	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	347/363 (96%)	334 (96%)	11 (3%)	2 (1%)	21	10
1	B	347/363 (96%)	336 (97%)	9 (3%)	2 (1%)	21	10
1	C	350/363 (96%)	335 (96%)	13 (4%)	2 (1%)	21	10
1	D	360/363 (99%)	343 (95%)	12 (3%)	5 (1%)	9	2
All	All	1404/1452 (97%)	1348 (96%)	45 (3%)	11 (1%)	16	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	344	PRO
1	D	347	GLN
1	A	5	PRO
1	B	5	PRO
1	C	5	PRO
1	A	188	PRO
1	C	188	PRO
1	D	5	PRO
1	D	345	SER
1	B	188	PRO
1	D	188	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/291 (98%)	283 (99%)	2 (1%)	76	70
1	B	285/291 (98%)	281 (99%)	4 (1%)	59	49
1	C	286/291 (98%)	283 (99%)	3 (1%)	68	60
1	D	291/291 (100%)	289 (99%)	2 (1%)	76	70
All	All	1147/1164 (98%)	1136 (99%)	11 (1%)	68	60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	PRO
1	A	295	TRP
1	B	5	PRO
1	B	230	PRO
1	B	295	TRP
1	B	318	GLU
1	C	5	PRO
1	C	230	PRO
1	C	295	TRP
1	D	230	PRO
1	D	295	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	4	HIS
1	A	60	GLN
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	A	324	GLN
1	B	4	HIS
1	B	11	GLN
1	B	50	ASN
1	B	54	ASN
1	B	119	ASN
1	B	136	GLN

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Mol	Chain	Res	Type
1	B	156	HIS
1	B	179	GLN
1	B	220	HIS
1	B	241	GLN
1	B	287	ASN
1	B	306	GLN
1	C	11	GLN
1	C	50	ASN
1	C	54	ASN
1	C	125	GLN
1	C	136	GLN
1	C	241	GLN
1	C	339	GLN
1	C	360	ASN
1	C	361	HIS
1	D	4	HIS
1	D	50	ASN
1	D	54	ASN
1	D	95	GLN
1	D	156	HIS
1	D	237	HIS
1	D	241	GLN
1	D	284	ASN
1	D	319	ASN
1	D	347	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/363 (96%)	-0.42	7 (2%) 65 68	6, 13, 32, 53	3 (0%)
1	B	350/363 (96%)	-0.37	6 (1%) 69 73	5, 13, 34, 57	3 (0%)
1	C	353/363 (97%)	-0.27	7 (1%) 65 68	7, 15, 41, 66	3 (0%)
1	D	361/363 (99%)	-0.11	17 (4%) 36 39	6, 17, 55, 94	2 (0%)
All	All	1414/1452 (97%)	-0.29	37 (2%) 57 61	5, 14, 42, 94	11 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	ALA	9.6
1	C	359	SER	6.3
1	C	346	GLY	5.7
1	A	345	SER	5.5
1	A	359	SER	5.1
1	D	361	HIS	5.0
1	D	348	ALA	4.9
1	B	359	SER	4.9
1	B	1	PRO	4.2
1	B	345	SER	4.1
1	D	349	GLY	3.7
1	A	1	PRO	3.7
1	D	353	SER	3.3
1	D	350	ALA	3.3
1	D	1	PRO	3.1
1	D	351	ALA	3.0
1	D	346	GLY	2.9
1	D	358	ILE	2.9
1	D	345	SER	2.8
1	D	357	PHE	2.7
1	A	344	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	347	GLN	2.7
1	D	46	ILE	2.6
1	B	344	PRO	2.5
1	D	360	ASN	2.5
1	C	38	SER	2.5
1	D	38	SER	2.5
1	C	39	ILE	2.4
1	A	343	THR	2.4
1	B	343	THR	2.2
1	A	2	HIS	2.1
1	B	237	HIS	2.1
1	D	354	GLU	2.1
1	C	37	GLY	2.1
1	A	360	ASN	2.1
1	D	36	THR	2.0
1	D	347	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 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.