



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:46 PM UTC

PDB ID : 1FBA / pdb_00001fba
Title : THE CRYSTAL STRUCTURE OF FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE FROM DROSOPHILA MELANOGASTER AT 2.5 ANGSTROMS RESOLUTION
Authors : Piontek, K.; Hester, G.; Brenner-Holzach, O.
Deposited on : 1992-06-08
Resolution : 1.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

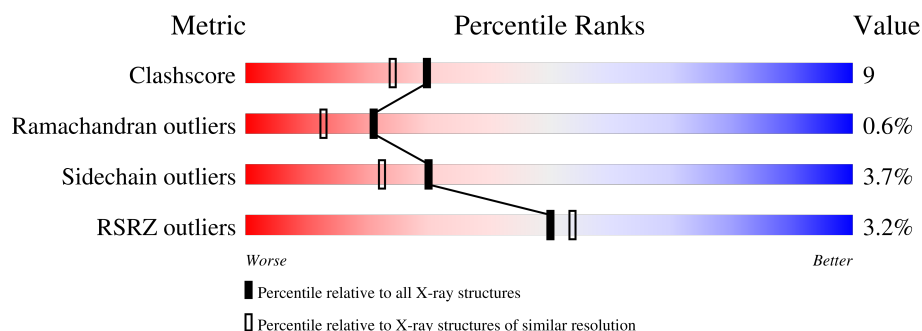
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	361	2% 83% 15% .
1	B	361	2% 85% 13% ..
1	C	361	4% 78% 19% ..
1	D	361	4% 83% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12796 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-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2745	1728	480	531	6			
1	B	361	Total	C	N	O	S	0	0	0
			2745	1728	480	531	6			
1	C	361	Total	C	N	O	S	0	0	0
			2745	1728	480	531	6			
1	D	361	Total	C	N	O	S	0	0	0
			2745	1728	480	531	6			

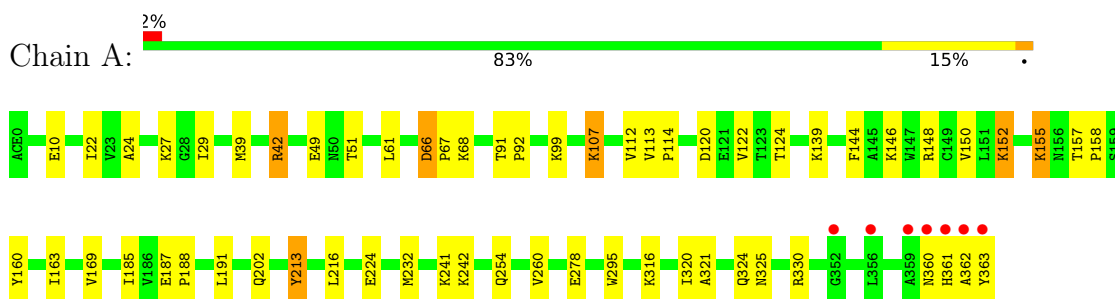
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	456	Total	O	0	0
			456	456		
2	B	477	Total	O	0	0
			477	477		
2	C	404	Total	O	0	0
			404	404		
2	D	479	Total	O	0	0
			479	479		

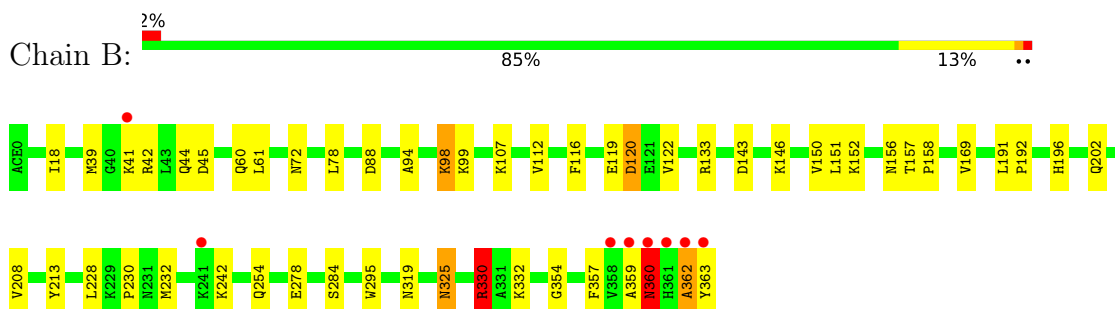
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

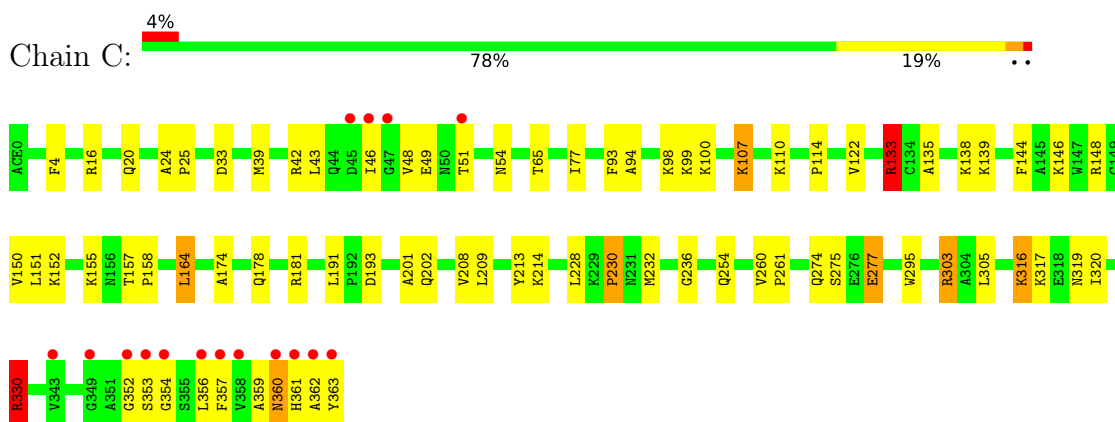
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE



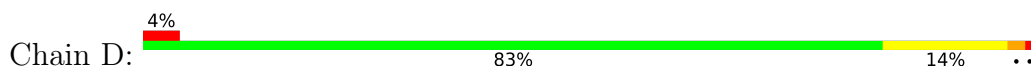
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

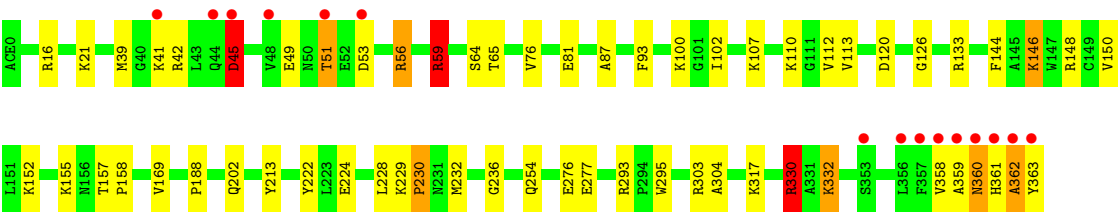


• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.60Å 116.80Å 151.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90 8.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.90) 93.8 (8.00-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 1.97Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12796	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	0.98	0/2789	1.38	11/3779 (0.3%)
1	B	1.00	0/2789	1.40	10/3779 (0.3%)
1	C	0.93	0/2789	1.42	14/3779 (0.4%)
1	D	0.98	0/2789	1.42	11/3779 (0.3%)
All	All	0.97	0/11156	1.41	46/15116 (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	1
1	C	0	1
1	D	0	3
All	All	0	5

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	ARG	CD-NE-CZ	10.88	139.63	124.40
1	D	45	ASP	CA-CB-CG	10.62	123.22	112.60
1	C	133	ARG	CD-NE-CZ	7.97	135.55	124.40
1	C	193	ASP	CA-CB-CG	7.82	120.42	112.60
1	C	330	ARG	CD-NE-CZ	7.80	135.32	124.40
1	A	224	GLU	CB-CG-CD	7.67	125.63	112.60
1	A	66	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	325	ASN	CA-CB-CG	-7.49	105.11	112.60
1	B	45	ASP	CA-CB-CG	6.73	119.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	GLU	CB-CG-CD	6.59	123.80	112.60
1	D	93	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	144	PHE	CA-CB-CG	6.16	119.96	113.80
1	B	354	GLY	N-CA-C	-6.13	104.17	112.57
1	C	277	GLU	CA-CB-CG	6.13	126.37	114.10
1	C	144	PHE	CA-CB-CG	6.04	119.84	113.80
1	D	144	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	213	TYR	CA-CB-CG	-5.92	103.25	113.90
1	A	187	GLU	CB-CG-CD	5.83	122.51	112.60
1	B	325	ASN	OD1-CG-ND2	5.72	128.32	122.60
1	A	330	ARG	CD-NE-CZ	5.61	132.25	124.40
1	B	330	ARG	CG-CD-NE	5.59	124.29	112.00
1	D	59	ARG	CD-NE-CZ	5.57	132.20	124.40
1	B	213	TYR	CA-CB-CG	-5.57	103.88	113.90
1	C	93	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	232	MET	N-CA-C	-5.43	103.22	110.55
1	C	214	LYS	N-CA-C	-5.40	105.47	111.36
1	D	213	TYR	CA-CB-CG	-5.37	104.23	113.90
1	D	113	VAL	O-C-N	5.36	125.07	121.69
1	C	232	MET	N-CA-C	-5.33	103.50	110.53
1	B	232	MET	N-CA-C	-5.30	103.02	110.50
1	A	330	ARG	CG-CD-NE	5.26	123.58	112.00
1	C	133	ARG	CG-CD-NE	5.20	123.44	112.00
1	D	232	MET	N-CA-C	-5.18	103.70	110.53
1	A	124	THR	CA-CB-OG1	-5.17	101.84	109.60
1	C	4	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	319	ASN	CA-CB-CG	5.16	117.75	112.60
1	A	113	VAL	O-C-N	5.15	124.93	121.69
1	C	236	GLY	CA-C-N	5.14	127.88	120.38
1	C	236	GLY	C-N-CA	5.14	127.88	120.38
1	D	330	ARG	CG-CD-NE	5.13	123.29	112.00
1	B	196	HIS	CA-CB-CG	-5.12	108.68	113.80
1	D	236	GLY	CA-C-N	5.06	127.57	120.28
1	D	236	GLY	C-N-CA	5.06	127.57	120.28
1	A	260	VAL	N-CA-C	5.04	112.55	107.55
1	C	213	TYR	CA-CB-CG	-5.04	104.84	113.90
1	B	330	ARG	CB-CG-CD	5.01	122.82	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ARG	Sidechain
1	C	133	ARG	Sidechain
1	D	293	ARG	Sidechain
1	D	330	ARG	Sidechain
1	D	56	ARG	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	2745	0	2769	43	0
1	B	2745	0	2769	39	0
1	C	2745	0	2769	60	0
1	D	2745	0	2769	47	0
2	A	456	0	0	10	0
2	B	477	0	0	7	0
2	C	404	0	0	9	0
2	D	479	0	0	13	0
All	All	12796	0	11076	188	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 9.

All (188) 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:B:122:VAL:HG21	1:B:362:ALA:HB1	1.37	1.02
1:B:330:ARG:HD2	2:B:615:HOH:O	1.64	0.98
1:D:359:ALA:O	1:D:360:ASN:HB2	1.69	0.92
1:A:325:ASN:HB3	2:A:550:HOH:O	1.68	0.92
1:C:152:LYS:HE2	1:C:362:ALA:HB3	1.55	0.88
1:C:359:ALA:O	1:C:360:ASN:HB2	1.75	0.87
1:D:152:LYS:HE2	1:D:362:ALA:HB3	1.61	0.82
1:C:164:LEU:C	1:C:164:LEU:HD23	2.04	0.82
1:B:112:VAL:HG21	1:B:362:ALA:HA	1.62	0.82
1:A:152:LYS:NZ	1:A:362:ALA:HB3	1.95	0.81
1:C:191:LEU:HD22	1:C:361:HIS:CD2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ARG:HH22	1:D:361:HIS:CG	1.97	0.81
1:A:160:TYR:HA	2:A:708:HOH:O	1.79	0.81
1:B:94:ALA:O	1:B:98:LYS:HG2	1.80	0.80
1:A:114:PRO:HB3	1:A:363:TYR:CE1	2.19	0.78
1:D:362:ALA:O	1:D:363:TYR:HB2	1.84	0.77
1:B:122:VAL:CG2	1:B:362:ALA:HB1	2.13	0.76
1:D:112:VAL:HG21	1:D:362:ALA:HA	1.67	0.75
1:A:241:LYS:HE3	2:A:690:HOH:O	1.85	0.75
1:C:46:ILE:HG13	1:C:48:VAL:HG23	1.69	0.73
1:B:152:LYS:NZ	1:B:362:ALA:O	2.22	0.73
1:C:191:LEU:HD13	1:C:361:HIS:HD2	1.55	0.72
1:B:120:ASP:OD2	1:B:363:TYR:CD2	2.43	0.71
1:B:120:ASP:OD2	1:B:363:TYR:HD2	1.74	0.70
1:D:330:ARG:HD2	2:D:604:HOH:O	1.89	0.70
1:C:146:LYS:HE2	2:C:1050:HOH:O	1.93	0.69
1:D:148:ARG:NH2	1:D:361:HIS:ND1	2.40	0.69
1:C:362:ALA:O	1:C:363:TYR:HB2	1.92	0.68
1:C:191:LEU:HD13	1:C:361:HIS:CD2	2.29	0.68
1:C:152:LYS:CE	1:C:362:ALA:HB3	2.24	0.67
1:C:51:THR:HG23	1:C:54:ASN:H	1.60	0.66
1:A:185:ILE:HD13	2:A:793:HOH:O	1.94	0.66
1:C:303:ARG:HH11	1:C:303:ARG:HB3	1.60	0.66
1:B:44:GLN:HB2	2:B:722:HOH:O	1.96	0.65
1:A:362:ALA:O	1:A:363:TYR:CD2	2.51	0.64
1:B:150:VAL:HG11	1:B:362:ALA:CB	2.28	0.63
1:A:39:MET:HE3	1:A:39:MET:HA	1.79	0.63
1:C:191:LEU:HD22	1:C:361:HIS:CG	2.34	0.62
1:A:362:ALA:O	1:A:363:TYR:HD2	1.82	0.62
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.81	0.62
1:D:21:LYS:HG3	2:D:459:HOH:O	1.99	0.62
1:A:148:ARG:NH2	1:A:361:HIS:ND1	2.47	0.62
1:A:163:ILE:HB	2:A:708:HOH:O	1.99	0.62
1:C:317:LYS:HD2	1:C:320:ILE:HD11	1.82	0.61
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.83	0.61
1:A:362:ALA:O	1:A:363:TYR:HB2	2.01	0.60
1:C:114:PRO:HB3	1:C:363:TYR:CE2	2.37	0.60
1:A:152:LYS:CE	1:A:362:ALA:HB3	2.32	0.59
1:B:242:LYS:HE2	1:B:278:GLU:OE2	2.02	0.58
1:A:148:ARG:HH22	1:A:361:HIS:CG	2.21	0.58
1:C:316:LYS:HE2	2:C:1273:HOH:O	2.03	0.58
1:D:152:LYS:HE2	1:D:362:ALA:CB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LYS:HE2	2:D:401:HOH:O	2.04	0.57
1:C:98:LYS:HE2	2:C:1205:HOH:O	2.04	0.57
1:C:164:LEU:C	1:C:164:LEU:CD2	2.74	0.57
1:B:146:LYS:HG2	2:B:538:HOH:O	2.05	0.57
1:A:152:LYS:HZ3	1:A:362:ALA:HB3	1.67	0.57
1:B:357:PHE:CE2	1:B:359:ALA:HB2	2.39	0.56
1:C:150:VAL:CG1	1:C:362:ALA:HB2	2.35	0.56
1:A:99:LYS:HB3	2:A:592:HOH:O	2.05	0.56
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.88	0.56
1:D:41:LYS:O	1:D:45:ASP:OD1	2.25	0.55
1:B:150:VAL:HG11	1:B:362:ALA:HB3	1.86	0.55
1:D:229:LYS:HD2	2:D:425:HOH:O	2.07	0.55
1:D:146:LYS:HE3	2:D:697:HOH:O	2.07	0.54
1:D:361:HIS:HD2	2:D:584:HOH:O	1.89	0.54
1:D:39:MET:HE3	1:D:42:ARG:HB2	1.90	0.54
1:C:361:HIS:CE1	2:C:1134:HOH:O	2.61	0.54
1:D:65:THR:O	1:D:100:LYS:NZ	2.39	0.53
1:A:362:ALA:O	1:A:363:TYR:CB	2.56	0.53
1:D:42:ARG:HA	1:D:45:ASP:OD1	2.09	0.53
1:C:274:GLN:O	1:C:356:LEU:HD12	2.09	0.53
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.90	0.53
1:B:357:PHE:CZ	1:B:359:ALA:HB2	2.43	0.52
1:C:94:ALA:O	1:C:98:LYS:HG3	2.09	0.52
1:B:41:LYS:HD2	2:B:712:HOH:O	2.09	0.52
1:A:150:VAL:CG1	1:A:191:LEU:HD11	2.40	0.52
1:C:148:ARG:HH22	1:C:361:HIS:HB3	1.74	0.52
1:C:122:VAL:HG13	1:C:363:TYR:CE1	2.45	0.51
1:C:303:ARG:HH11	1:C:303:ARG:CB	2.22	0.51
1:A:152:LYS:HE2	1:A:362:ALA:HB3	1.92	0.51
1:B:18:ILE:HD13	1:B:143:ASP:HB3	1.92	0.51
1:D:152:LYS:HB3	2:D:428:HOH:O	2.09	0.51
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.92	0.51
1:D:112:VAL:CG2	1:D:363:TYR:H	2.24	0.51
1:B:150:VAL:CG1	1:B:362:ALA:CB	2.89	0.51
1:B:202:GLN:HE22	1:B:254:GLN:HE21	1.59	0.50
1:C:202:GLN:HE22	1:C:254:GLN:HE21	1.58	0.50
1:A:242:LYS:HE3	1:A:278:GLU:OE2	2.11	0.50
1:C:201:ALA:HB1	2:C:1303:HOH:O	2.11	0.50
1:D:49:GLU:HG2	1:D:51:THR:HG22	1.91	0.50
1:D:150:VAL:CG1	1:D:362:ALA:HB2	2.42	0.50
1:B:116:PHE:HB2	2:B:373:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LYS:NZ	1:D:358:VAL:HG21	2.27	0.49
1:A:321:ALA:O	1:A:325:ASN:ND2	2.31	0.49
1:D:49:GLU:HG3	2:D:648:HOH:O	2.12	0.49
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.95	0.49
1:B:122:VAL:HG21	1:B:362:ALA:CB	2.26	0.49
1:A:107:LYS:HE3	2:A:565:HOH:O	2.13	0.48
1:A:320:ILE:O	1:A:324:GLN:HG3	2.13	0.48
1:C:303:ARG:HH11	1:C:303:ARG:CG	2.26	0.48
1:B:150:VAL:HG11	1:B:362:ALA:HB2	1.93	0.48
1:A:39:MET:HE3	1:A:42:ARG:HB2	1.96	0.48
1:A:146:LYS:HE3	2:A:566:HOH:O	2.13	0.47
1:A:146:LYS:HG3	2:A:566:HOH:O	2.13	0.47
1:A:114:PRO:HB3	1:A:363:TYR:CZ	2.49	0.47
1:C:110:LYS:HE3	2:C:1259:HOH:O	2.15	0.47
1:B:133:ARG:HD3	2:B:592:HOH:O	2.14	0.47
1:C:133:ARG:HG2	2:C:1120:HOH:O	2.14	0.47
1:D:362:ALA:O	1:D:363:TYR:CB	2.56	0.46
1:B:152:LYS:CE	1:B:362:ALA:O	2.63	0.46
1:A:155:LYS:HE2	1:C:155:LYS:HE2	1.98	0.46
1:C:275:SER:HB3	1:C:354:GLY:O	2.15	0.46
1:C:122:VAL:CG2	1:C:362:ALA:HB1	2.43	0.46
1:B:150:VAL:CG1	1:B:362:ALA:HB3	2.45	0.46
1:B:151:LEU:HD13	1:B:208:VAL:CG2	2.45	0.46
1:D:120:ASP:HA	1:D:363:TYR:OH	2.16	0.46
1:C:65:THR:O	1:C:100:LYS:NZ	2.48	0.46
1:D:317:LYS:HD2	2:D:702:HOH:O	2.15	0.46
1:D:112:VAL:HG21	1:D:363:TYR:H	1.80	0.45
1:C:151:LEU:HD13	1:C:208:VAL:CG2	2.46	0.45
1:D:222:TYR:CZ	1:D:224:GLU:HB2	2.52	0.45
1:B:72:ASN:HD21	1:B:332:LYS:HD2	1.81	0.45
1:B:359:ALA:O	1:B:360:ASN:HB2	2.15	0.45
1:C:316:LYS:HE3	1:C:319:ASN:OD1	2.17	0.45
1:A:22:ILE:HG21	1:A:29:ILE:HD11	1.98	0.45
1:C:317:LYS:CD	1:C:320:ILE:HD11	2.47	0.45
1:C:150:VAL:HG12	1:C:362:ALA:HB2	1.98	0.44
1:A:91:THR:HA	1:A:92:PRO:HD3	1.88	0.44
1:C:16:ARG:O	1:C:20:GLN:HG3	2.17	0.44
1:C:191:LEU:CD2	1:C:361:HIS:CG	3.00	0.44
1:C:305:LEU:HD23	1:C:330:ARG:HB3	1.99	0.44
1:A:139:LYS:HE3	1:A:139:LYS:HB2	1.81	0.44
1:B:60:GLN:OE1	1:B:88:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:HD3	2:D:691:HOH:O	2.17	0.44
1:C:49:GLU:O	1:C:54:ASN:ND2	2.51	0.44
1:C:51:THR:HG22	1:C:54:ASN:CG	2.43	0.44
1:D:64:SER:HB3	2:D:663:HOH:O	2.18	0.44
1:D:202:GLN:HE22	1:D:254:GLN:HE21	1.65	0.44
1:D:76:VAL:HG23	1:D:102:ILE:HG21	2.00	0.44
1:A:66:ASP:HA	1:A:67:PRO:HD2	1.80	0.43
1:B:157:THR:HA	1:B:158:PRO:C	2.43	0.43
1:A:122:VAL:CG2	1:A:362:ALA:HB1	2.49	0.43
1:C:107:LYS:HG3	1:C:146:LYS:HD2	1.99	0.43
1:D:359:ALA:O	1:D:360:ASN:CB	2.52	0.43
1:D:332:LYS:HA	1:D:332:LYS:HD2	1.76	0.43
1:B:152:LYS:HD2	2:B:589:HOH:O	2.18	0.43
1:B:94:ALA:O	1:B:98:LYS:CG	2.57	0.43
1:D:361:HIS:CD2	2:D:584:HOH:O	2.67	0.43
1:D:59:ARG:CG	1:D:59:ARG:HH11	2.32	0.42
1:A:10:GLU:H	1:A:10:GLU:CD	2.28	0.42
1:B:152:LYS:HE2	1:B:362:ALA:O	2.18	0.42
1:B:150:VAL:CG1	1:B:362:ALA:HB2	2.49	0.42
1:D:330:ARG:HD2	1:D:330:ARG:HH11	1.67	0.42
1:C:157:THR:HA	1:C:158:PRO:C	2.44	0.42
1:A:61:LEU:C	1:A:61:LEU:HD23	2.44	0.42
1:C:122:VAL:HG21	1:C:362:ALA:HB1	2.02	0.42
1:C:39:MET:O	1:C:43:LEU:HG	2.20	0.42
1:C:352:GLY:HA3	2:C:1080:HOH:O	2.20	0.42
1:A:112:VAL:HG21	1:A:362:ALA:HA	2.00	0.42
1:A:68:LYS:HE2	2:A:600:HOH:O	2.20	0.41
1:D:146:LYS:CE	2:D:697:HOH:O	2.66	0.41
1:B:119:GLU:OE1	1:B:156:ASN:HB2	2.20	0.41
1:C:150:VAL:HG11	1:C:362:ALA:HB2	2.01	0.41
1:C:174:ALA:O	1:C:178:GLN:HG3	2.19	0.41
1:D:42:ARG:CZ	1:D:303:ARG:HD2	2.51	0.41
1:D:150:VAL:HG11	1:D:362:ALA:HB2	2.02	0.41
1:A:24:ALA:HB3	1:A:27:LYS:HD2	2.02	0.41
1:B:39:MET:HE3	1:B:42:ARG:HB2	2.03	0.41
1:A:213:TYR:CE1	1:A:216:LEU:HD12	2.56	0.41
1:D:360:ASN:HB3	1:D:361:HIS:H	1.48	0.41
1:C:24:ALA:HA	1:C:25:PRO:HD3	1.89	0.40
1:D:157:THR:HA	1:D:158:PRO:C	2.46	0.40
1:A:148:ARG:HH22	1:A:361:HIS:CB	2.35	0.40
1:C:135:ALA:O	1:C:139:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ALA:O	1:C:363:TYR:CB	2.65	0.40
1:D:276:GLU:HG2	1:D:304:ALA:O	2.22	0.40
1:A:202:GLN:HE22	1:A:254:GLN:HE21	1.69	0.40
1:C:146:LYS:HG3	2:C:1181:HOH:O	2.21	0.40
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.98	0.40
1:C:357:PHE:CE2	1:C:359:ALA:HB2	2.57	0.40
1:D:49:GLU:HG2	1:D:51:THR:CG2	2.51	0.40
1:B:191:LEU:HA	1:B:192:PRO:HD3	1.97	0.40
1:A:157:THR:HA	1:A:158:PRO:C	2.46	0.40
1:B:61:LEU:C	1:B:61:LEU:HD23	2.47	0.40
1:C:122:VAL:HG13	1:C:363:TYR:CD1	2.57	0.40
1:C:138:LYS:HE2	1:C:181:ARG:HB2	2.02	0.40
1:D:56:ARG:HH21	1:D:87:ALA:C	2.30	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	359/361 (99%)	348 (97%)	9 (2%)	2 (1%)	21	13
1	B	359/361 (99%)	352 (98%)	5 (1%)	2 (1%)	21	13
1	C	359/361 (99%)	344 (96%)	13 (4%)	2 (1%)	21	13
1	D	359/361 (99%)	347 (97%)	9 (2%)	3 (1%)	16	8
All	All	1436/1444 (99%)	1391 (97%)	36 (2%)	9 (1%)	21	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ALA
1	C	360	ASN

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Mol	Chain	Res	Type
1	D	360	ASN
1	B	360	ASN
1	C	353	SER
1	A	360	ASN
1	D	362	ALA
1	A	188	PRO
1	D	188	PRO

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	287/287 (100%)	280 (98%)	7 (2%)	43	38
1	B	287/287 (100%)	276 (96%)	11 (4%)	29	21
1	C	287/287 (100%)	275 (96%)	12 (4%)	26	19
1	D	287/287 (100%)	274 (96%)	13 (4%)	24	17
All	All	1148/1148 (100%)	1105 (96%)	43 (4%)	30	22

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	120	ASP
1	A	152	LYS
1	A	155	LYS
1	A	169	VAL
1	A	295	TRP
1	A	316	LYS
1	B	78	LEU
1	B	98	LYS
1	B	99	LYS
1	B	107	LYS
1	B	120	ASP
1	B	169	VAL
1	B	284	SER

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Mol	Chain	Res	Type
1	B	295	TRP
1	B	325	ASN
1	B	330	ARG
1	B	360	ASN
1	C	42	ARG
1	C	99	LYS
1	C	107	LYS
1	C	133	ARG
1	C	164	LEU
1	C	209	LEU
1	C	230	PRO
1	C	277	GLU
1	C	295	TRP
1	C	303	ARG
1	C	316	LYS
1	C	330	ARG
1	D	45	ASP
1	D	51	THR
1	D	53	ASP
1	D	59	ARG
1	D	81	GLU
1	D	107	LYS
1	D	146	LYS
1	D	169	VAL
1	D	230	PRO
1	D	277	GLU
1	D	295	TRP
1	D	330	ARG
1	D	332	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	161	GLN
1	A	237	GLN
1	A	243	ASN
1	A	254	GLN
1	A	319	ASN
1	A	334	ASN
1	A	360	ASN
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	161	GLN
1	B	237	GLN
1	B	254	GLN
1	B	319	ASN
1	C	20	GLN
1	C	54	ASN
1	C	72	ASN
1	C	156	ASN
1	C	161	GLN
1	C	254	GLN
1	C	361	HIS
1	D	72	ASN
1	D	156	ASN
1	D	161	GLN
1	D	166	ASN
1	D	254	GLN
1	D	306	GLN
1	D	334	ASN

5.3.3 RNA [i](#)

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 ⓘ

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	360/361 (99%)	-0.33	7 (1%) 66 70	2, 11, 42, 79	0
1	B	360/361 (99%)	-0.36	8 (2%) 62 66	3, 12, 36, 89	0
1	C	360/361 (99%)	-0.07	16 (4%) 39 41	3, 16, 55, 86	0
1	D	360/361 (99%)	-0.33	15 (4%) 40 43	2, 11, 45, 86	0
All	All	1440/1444 (99%)	-0.27	46 (3%) 50 54	2, 13, 45, 89	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	361	HIS	6.2
1	B	363	TYR	6.1
1	D	363	TYR	5.7
1	A	360	ASN	5.0
1	C	363	TYR	4.7
1	D	362	ALA	4.6
1	B	361	HIS	4.5
1	C	361	HIS	4.4
1	A	363	TYR	4.4
1	A	361	HIS	4.2
1	B	359	ALA	4.2
1	D	360	ASN	4.1
1	A	362	ALA	4.0
1	D	41	LYS	4.0
1	A	359	ALA	3.9
1	D	359	ALA	3.6
1	B	358	VAL	3.6
1	B	360	ASN	3.5
1	C	360	ASN	3.5
1	C	45	ASP	3.3
1	C	349	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	3.0
1	D	48	VAL	2.9
1	D	45	ASP	2.8
1	A	352	GLY	2.8
1	C	356	LEU	2.7
1	C	343	VAL	2.6
1	C	51	THR	2.6
1	C	358	VAL	2.6
1	C	47	GLY	2.5
1	C	357	PHE	2.5
1	D	357	PHE	2.5
1	D	53	ASP	2.4
1	D	51	THR	2.4
1	C	362	ALA	2.4
1	C	353	SER	2.4
1	D	353	SER	2.3
1	D	44	GLN	2.3
1	D	358	VAL	2.3
1	C	46	ILE	2.2
1	B	41	LYS	2.2
1	C	352	GLY	2.2
1	A	356	LEU	2.2
1	D	356	LEU	2.1
1	B	241	LYS	2.1
1	C	354	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 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.