



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:18 PM UTC

PDB ID : 1EPX / pdb_00001epx
Title : CRYSTAL STRUCTURE ANALYSIS OF ALDOLASE FROM L. MEXI-
CANA
Authors : Chudzik, D.M.; Michels, P.A.; de Walque, S.; Hol, W.G.J.
Deposited on : 2000-03-29
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

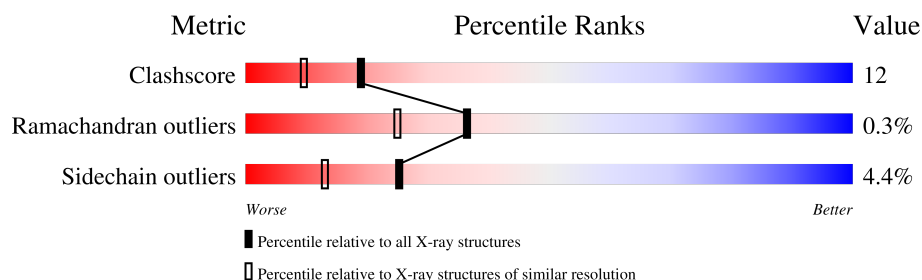
1 Overall quality at a glance

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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	 74% 19% . . .
1	B	370	 73% 20% . . .
1	C	370	 68% 25% . .
1	D	370	 66% 27% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12131 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	357	Total	C	N	O	S	0	0	0
			2694	1695	477	504	18			
1	B	357	Total	C	N	O	S	0	0	0
			2694	1695	477	504	18			
1	C	357	Total	C	N	O	S	0	0	0
			2694	1695	477	504	18			
1	D	357	Total	C	N	O	S	0	0	0
			2694	1695	477	504	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	329	Total	O	0	0
			329	329		
2	B	291	Total	O	0	0
			291	291		
2	C	376	Total	O	0	0
			376	376		
2	D	359	Total	O	0	0
			359	359		

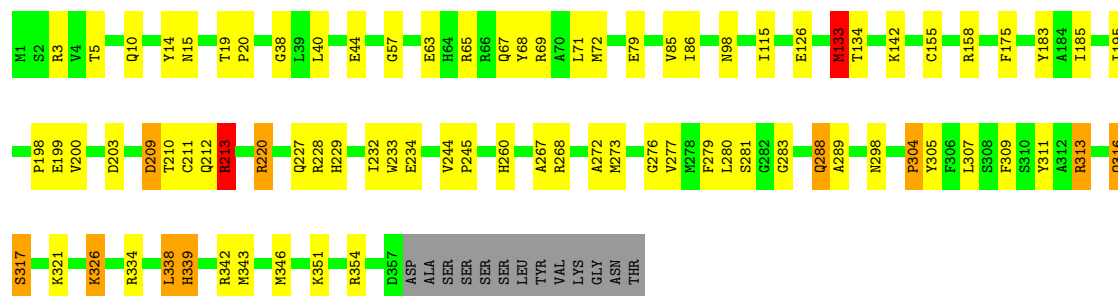
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

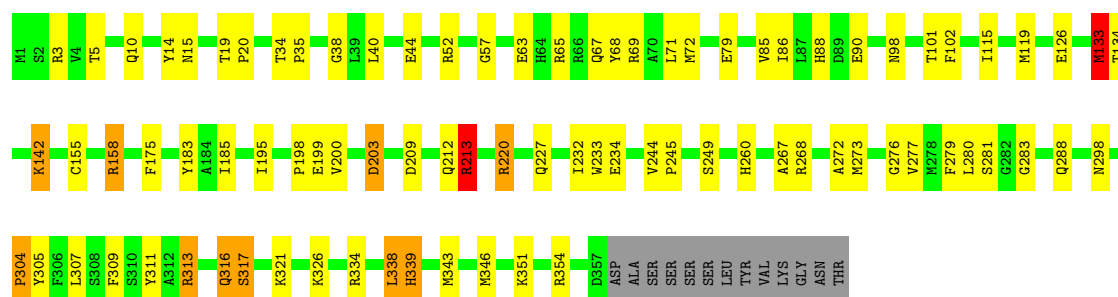
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE

Chain A: 



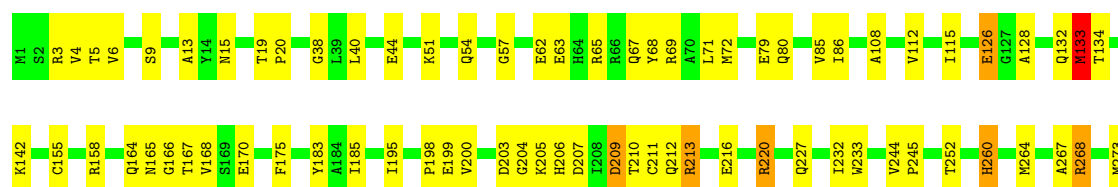
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE

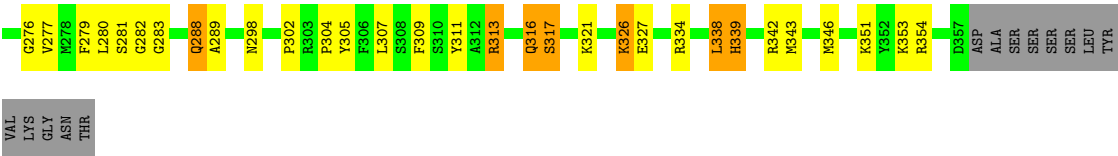
Chain B: 



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE

Chain C: 





● Molecule 1: FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.80Å 118.10Å 159.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	92.5 (20.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.161 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12131	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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	1.52	7/2749 (0.3%)	1.69	27/3730 (0.7%)
1	B	1.52	7/2749 (0.3%)	1.69	27/3730 (0.7%)
1	C	1.52	7/2749 (0.3%)	1.69	27/3730 (0.7%)
1	D	1.52	8/2749 (0.3%)	1.69	27/3730 (0.7%)
All	All	1.52	29/10996 (0.3%)	1.69	108/14920 (0.7%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	268	ARG	NE-CZ	6.00	1.39	1.33
1	A	268	ARG	NE-CZ	5.97	1.39	1.33
1	B	268	ARG	NE-CZ	5.94	1.39	1.33
1	C	268	ARG	NE-CZ	5.90	1.39	1.33
1	C	158	ARG	N-CA	-5.59	1.39	1.46
1	A	158	ARG	N-CA	-5.58	1.39	1.46
1	B	158	ARG	N-CA	-5.54	1.39	1.46
1	D	158	ARG	N-CA	-5.53	1.39	1.46
1	C	185	ILE	CA-CB	5.48	1.60	1.54
1	C	212	GLN	C-N	-5.48	1.26	1.33
1	D	185	ILE	CA-CB	5.46	1.60	1.54
1	B	212	GLN	C-N	-5.46	1.26	1.33
1	B	185	ILE	CA-CB	5.45	1.60	1.54
1	A	185	ILE	CA-CB	5.45	1.60	1.54
1	A	212	GLN	C-N	-5.44	1.26	1.33
1	D	212	GLN	C-N	-5.43	1.26	1.33
1	B	232	ILE	CA-CB	-5.40	1.47	1.53
1	C	232	ILE	CA-CB	-5.36	1.47	1.53
1	A	232	ILE	CA-CB	-5.33	1.47	1.53
1	D	232	ILE	CA-CB	-5.31	1.47	1.53
1	C	175	PHE	C-O	-5.24	1.18	1.24
1	B	175	PHE	C-O	-5.22	1.18	1.24
1	A	175	PHE	C-O	-5.20	1.18	1.24
1	D	175	PHE	C-O	-5.18	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	ILE	CA-C	-5.05	1.47	1.52
1	A	86	ILE	CA-C	-5.05	1.47	1.52
1	D	86	ILE	CA-C	-5.04	1.47	1.52
1	B	86	ILE	CA-C	-5.01	1.47	1.52
1	D	203	ASP	CG-OD2	5.01	1.34	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ARG	NE-CZ-NH1	13.07	134.57	121.50
1	A	268	ARG	NE-CZ-NH1	13.06	134.56	121.50
1	C	268	ARG	NE-CZ-NH1	13.06	134.56	121.50
1	D	268	ARG	NE-CZ-NH1	13.04	134.54	121.50
1	B	268	ARG	NE-CZ-NH2	-8.87	111.22	119.20
1	A	268	ARG	NE-CZ-NH2	-8.85	111.24	119.20
1	C	268	ARG	NE-CZ-NH2	-8.82	111.26	119.20
1	D	268	ARG	NE-CZ-NH2	-8.82	111.26	119.20
1	B	316	GLN	N-CA-C	7.31	122.33	113.41
1	A	316	GLN	N-CA-C	7.30	122.32	113.41
1	C	316	GLN	N-CA-C	7.30	122.32	113.41
1	D	316	GLN	N-CA-C	7.27	122.28	113.41
1	C	298	ASN	N-CA-C	-7.24	102.23	113.02
1	A	298	ASN	N-CA-C	-7.22	102.27	113.02
1	D	298	ASN	N-CA-C	-7.22	102.27	113.02
1	B	298	ASN	N-CA-C	-7.20	102.30	113.02
1	C	288	GLN	CB-CA-C	-7.01	99.15	110.79
1	A	288	GLN	CB-CA-C	-7.00	99.17	110.79
1	D	288	GLN	CB-CA-C	-6.99	99.19	110.79
1	B	288	GLN	CB-CA-C	-6.97	99.21	110.79
1	B	57	GLY	O-C-N	6.51	127.79	122.51
1	A	57	GLY	O-C-N	6.47	127.75	122.51
1	D	57	GLY	O-C-N	6.45	127.73	122.51
1	C	57	GLY	O-C-N	6.44	127.73	122.51
1	C	279	PHE	N-CA-C	6.20	118.79	110.35
1	A	279	PHE	N-CA-C	6.19	118.77	110.35
1	B	279	PHE	N-CA-C	6.18	118.75	110.35
1	D	279	PHE	N-CA-C	6.17	118.75	110.35
1	C	339	HIS	CA-C-O	6.08	127.20	120.82
1	D	339	HIS	CA-C-O	6.06	127.19	120.82
1	C	276	GLY	CA-C-N	6.06	131.25	123.13
1	C	276	GLY	C-N-CA	6.06	131.25	123.13
1	A	339	HIS	CA-C-O	6.05	127.17	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	GLY	CA-C-N	6.05	131.24	123.13
1	B	276	GLY	C-N-CA	6.05	131.24	123.13
1	B	339	HIS	CA-C-O	6.04	127.16	120.82
1	A	276	GLY	CA-C-N	6.03	131.21	123.13
1	A	276	GLY	C-N-CA	6.03	131.21	123.13
1	B	15	ASN	N-CA-CB	-6.00	101.79	110.56
1	D	276	GLY	CA-C-N	6.00	131.16	123.13
1	D	276	GLY	C-N-CA	6.00	131.16	123.13
1	C	15	ASN	N-CA-CB	-5.98	101.83	110.56
1	A	15	ASN	N-CA-CB	-5.98	101.83	110.56
1	C	268	ARG	CD-NE-CZ	5.93	132.70	124.40
1	D	268	ARG	CD-NE-CZ	5.90	132.66	124.40
1	A	268	ARG	CD-NE-CZ	5.89	132.65	124.40
1	D	203	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	203	ASP	CA-CB-CG	-5.87	106.73	112.60
1	B	268	ARG	CD-NE-CZ	5.86	132.61	124.40
1	B	203	ASP	CA-CB-CG	-5.86	106.74	112.60
1	C	203	ASP	CA-CB-CG	-5.86	106.75	112.60
1	D	195	ILE	N-CA-C	-5.79	99.53	107.99
1	B	195	ILE	N-CA-C	-5.77	99.56	107.99
1	A	195	ILE	N-CA-C	-5.76	99.58	107.99
1	D	298	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	D	15	ASN	N-CA-CB	-5.73	101.85	110.73
1	C	195	ILE	N-CA-C	-5.72	99.63	107.99
1	B	298	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	298	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	C	298	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	D	260	HIS	CA-CB-CG	-5.64	108.16	113.80
1	A	260	HIS	CA-CB-CG	-5.63	108.17	113.80
1	B	260	HIS	CA-CB-CG	-5.62	108.18	113.80
1	C	260	HIS	CA-CB-CG	-5.59	108.21	113.80
1	D	304	PRO	CB-CA-C	-5.47	103.69	111.68
1	A	317	SER	N-CA-C	5.47	117.69	111.02
1	B	304	PRO	CB-CA-C	-5.46	103.71	111.68
1	B	317	SER	N-CA-C	5.46	117.68	111.02
1	A	304	PRO	CB-CA-C	-5.46	103.72	111.68
1	D	317	SER	N-CA-C	5.45	117.67	111.02
1	C	304	PRO	CB-CA-C	-5.44	103.74	111.68
1	B	126	GLU	N-CA-C	-5.44	101.04	109.14
1	C	317	SER	N-CA-C	5.44	117.65	111.02
1	D	126	GLU	N-CA-C	-5.43	101.05	109.14
1	A	126	GLU	N-CA-C	-5.41	101.08	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	GLU	N-CA-C	-5.40	101.09	109.14
1	B	65	ARG	NE-CZ-NH2	-5.27	114.45	119.20
1	A	65	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	C	142	LYS	N-CA-C	-5.24	105.46	111.07
1	A	142	LYS	N-CA-C	-5.24	105.46	111.07
1	D	65	ARG	NE-CZ-NH2	-5.23	114.49	119.20
1	D	142	LYS	N-CA-C	-5.22	105.48	111.07
1	B	142	LYS	N-CA-C	-5.21	105.50	111.07
1	C	65	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	133	MET	CA-CB-CG	-5.18	103.73	114.10
1	C	213	ARG	CB-CA-C	-5.18	102.72	110.90
1	A	213	ARG	CB-CA-C	-5.18	102.72	110.90
1	B	213	ARG	CB-CA-C	-5.18	102.72	110.90
1	C	133	MET	CA-CB-CG	-5.17	103.76	114.10
1	A	133	MET	CA-CB-CG	-5.17	103.76	114.10
1	D	213	ARG	CB-CA-C	-5.17	102.73	110.90
1	D	133	MET	CA-CB-CG	-5.17	103.77	114.10
1	B	268	ARG	CB-CG-CD	5.15	123.14	111.30
1	D	268	ARG	CB-CG-CD	5.14	123.13	111.30
1	A	268	ARG	CB-CG-CD	5.12	123.08	111.30
1	B	321	LYS	N-CA-CB	5.12	117.74	110.16
1	C	268	ARG	CB-CG-CD	5.11	123.06	111.30
1	C	321	LYS	N-CA-CB	5.11	117.72	110.16
1	B	200	VAL	N-CA-C	-5.10	100.42	108.23
1	D	200	VAL	N-CA-C	-5.10	100.42	108.23
1	A	321	LYS	N-CA-CB	5.09	117.69	110.16
1	D	233	TRP	O-C-N	5.08	127.51	122.12
1	C	200	VAL	N-CA-C	-5.08	100.46	108.23
1	A	200	VAL	N-CA-C	-5.07	100.47	108.23
1	D	321	LYS	N-CA-CB	5.07	117.67	110.16
1	C	233	TRP	O-C-N	5.07	127.50	122.12
1	A	233	TRP	O-C-N	5.06	127.48	122.12
1	B	233	TRP	O-C-N	5.05	127.47	122.12

There are no chirality outliers.

There are no planarity outliers.

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	2694	0	2628	59	1
1	B	2694	0	2628	64	1
1	C	2694	0	2628	94	3
1	D	2694	0	2628	102	3
2	A	329	0	0	4	0
2	B	291	0	0	10	0
2	C	376	0	0	34	1
2	D	359	0	0	33	1
All	All	12131	0	10512	251	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (251) 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:51:LYS:CB	2:D:1443:HOH:O	1.94	1.16
1:C:353:LYS:HE3	2:C:1042:HOH:O	1.51	1.11
1:D:50:THR:O	2:D:2072:HOH:O	1.72	1.04
1:C:346:MET:HE1	2:C:2068:HOH:O	1.55	1.03
1:A:227:GLN:HB3	1:D:220:ARG:HD2	1.47	0.95
1:D:205:LYS:O	2:D:1417:HOH:O	1.86	0.93
1:D:54:GLN:CB	2:D:1634:HOH:O	2.16	0.92
1:B:227:GLN:HB3	1:C:220:ARG:HD2	1.50	0.91
1:C:62:GLU:OE1	2:C:1979:HOH:O	1.88	0.90
1:A:14:TYR:OH	1:D:166:GLY:O	1.92	0.86
1:C:9:SER:HA	2:C:2155:HOH:O	1.76	0.85
1:B:88:HIS:HD2	1:B:90:GLU:H	1.25	0.84
1:D:167:THR:OG1	2:D:901:HOH:O	1.95	0.83
1:D:62:GLU:OE1	2:D:1114:HOH:O	1.97	0.81
1:D:79:GLU:OE1	2:D:1854:HOH:O	1.97	0.81
1:C:3:ARG:HB3	1:D:5:THR:CG2	2.12	0.80
1:B:14:TYR:OH	1:C:166:GLY:O	2.00	0.79
1:C:54:GLN:CB	2:C:982:HOH:O	2.30	0.78
1:B:10:GLN:CG	1:D:128:ALA:HB2	2.16	0.76
1:D:51:LYS:HA	2:D:1443:HOH:O	1.85	0.76
1:C:6:VAL:O	1:D:3:ARG:HA	1.87	0.75
1:D:168:VAL:O	2:D:1107:HOH:O	2.03	0.75
1:A:273:MET:N	1:D:267:ALA:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:THR:CG2	1:D:3:ARG:HB3	2.16	0.75
1:C:62:GLU:OE1	2:C:1567:HOH:O	2.05	0.74
1:A:227:GLN:HB3	1:D:220:ARG:CD	2.16	0.74
1:C:168:VAL:O	2:C:1116:HOH:O	2.06	0.74
1:B:227:GLN:HB3	1:C:220:ARG:CD	2.19	0.73
1:B:203:ASP:OD1	2:B:2138:HOH:O	2.07	0.72
1:C:132:GLN:NE2	2:C:895:HOH:O	2.06	0.72
1:D:227:GLN:HA	2:D:1958:HOH:O	1.90	0.71
1:B:249:SER:O	2:B:2197:HOH:O	2.09	0.70
1:C:282:GLY:O	2:C:1033:HOH:O	2.09	0.70
1:B:10:GLN:HG2	1:D:128:ALA:HB2	1.72	0.69
1:B:273:MET:N	1:C:267:ALA:O	2.23	0.69
1:C:3:ARG:HB3	1:D:5:THR:HG22	1.73	0.69
1:C:5:THR:HG22	1:D:3:ARG:HB3	1.73	0.68
1:C:210:THR:OG1	2:C:1651:HOH:O	2.11	0.68
1:C:351:LYS:HD2	2:C:2068:HOH:O	1.93	0.68
1:D:207:ASP:CG	2:D:1260:HOH:O	2.35	0.68
1:D:277:VAL:HB	1:D:307:LEU:HD23	1.76	0.67
1:D:300:PRO:O	2:D:1876:HOH:O	2.12	0.67
1:A:272:ALA:HB3	1:D:267:ALA:HA	1.74	0.67
1:C:3:ARG:HA	1:D:6:VAL:O	1.95	0.67
1:C:80:GLN:CB	2:C:2066:HOH:O	2.43	0.67
1:C:170:GLU:OE2	2:C:1830:HOH:O	2.13	0.67
1:A:229:HIS:ND1	1:C:126:GLU:OE2	2.19	0.67
1:B:277:VAL:HB	1:B:307:LEU:HD23	1.76	0.67
1:C:351:LYS:CE	2:C:1099:HOH:O	2.25	0.67
1:A:277:VAL:HB	1:A:307:LEU:HD23	1.76	0.67
1:C:351:LYS:NZ	2:C:1099:HOH:O	1.63	0.66
1:C:209:ASP:OD2	2:C:2085:HOH:O	2.13	0.66
1:C:277:VAL:HB	1:C:307:LEU:HD23	1.76	0.66
1:A:213:ARG:NH1	2:A:2170:HOH:O	2.28	0.66
1:D:203:ASP:OD1	2:D:2148:HOH:O	2.13	0.66
1:C:205:LYS:O	2:C:1514:HOH:O	2.14	0.65
1:D:286:GLU:OE1	2:D:2035:HOH:O	2.14	0.65
1:B:20:PRO:HD2	2:B:1763:HOH:O	1.96	0.65
1:B:272:ALA:HB3	1:C:267:ALA:HA	1.79	0.65
1:B:52:ARG:NH2	2:B:1967:HOH:O	2.26	0.65
1:C:167:THR:OG1	2:C:915:HOH:O	2.14	0.64
1:A:10:GLN:HE22	1:C:164:GLN:HB2	1.62	0.64
1:C:20:PRO:HD2	2:C:1286:HOH:O	1.96	0.64
1:D:251:LYS:CB	2:D:1887:HOH:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:HE22	1:D:164:GLN:HB2	1.64	0.62
1:B:10:GLN:HG3	1:D:128:ALA:HB2	1.80	0.62
1:A:273:MET:CB	1:D:268:ARG:HG3	2.30	0.61
1:B:220:ARG:HD2	1:C:227:GLN:HB3	1.83	0.61
1:B:88:HIS:CD2	1:B:90:GLU:H	2.13	0.60
1:D:346:MET:HE3	1:D:351:LYS:HB2	1.84	0.60
1:C:346:MET:HE3	1:C:351:LYS:HB2	1.84	0.60
1:A:346:MET:HE3	1:A:351:LYS:HB2	1.84	0.59
1:C:351:LYS:CD	2:C:1099:HOH:O	2.50	0.59
1:A:234:GLU:CD	1:D:268:ARG:HH11	2.10	0.59
1:A:10:GLN:CG	1:C:128:ALA:HB2	2.34	0.58
1:A:220:ARG:HD2	1:D:227:GLN:HB3	1.84	0.58
1:B:346:MET:HE3	1:B:351:LYS:HB2	1.84	0.58
1:A:213:ARG:HG3	1:D:13:ALA:O	2.04	0.58
1:B:213:ARG:HG3	1:C:13:ALA:O	2.04	0.58
1:C:206:HIS:HA	2:C:1118:HOH:O	2.04	0.58
1:B:5:THR:O	1:D:165:ASN:HB3	2.03	0.58
1:D:260:HIS:HA	2:D:963:HOH:O	2.04	0.57
1:D:178:GLU:HG2	2:D:1254:HOH:O	2.05	0.57
1:D:339:HIS:HE1	1:D:357:ASP:OD1	1.87	0.57
1:A:334:ARG:O	1:A:338:LEU:HD22	2.04	0.57
1:B:334:ARG:O	1:B:338:LEU:HD22	2.05	0.57
1:A:14:TYR:CE1	1:D:166:GLY:O	2.57	0.57
1:A:10:GLN:NE2	1:C:164:GLN:HB2	2.19	0.56
1:A:10:GLN:HG2	1:C:128:ALA:HB2	1.88	0.56
1:C:170:GLU:HB3	2:C:1927:HOH:O	2.05	0.56
1:D:334:ARG:O	1:D:338:LEU:HD22	2.05	0.56
1:A:273:MET:HE3	1:D:264:MET:HG3	1.86	0.56
1:C:334:ARG:O	1:C:338:LEU:HD22	2.05	0.56
1:D:206:HIS:HA	2:D:1083:HOH:O	2.05	0.56
1:A:283:GLY:H	1:A:313:ARG:NH2	2.04	0.56
1:C:283:GLY:H	1:C:313:ARG:NH2	2.04	0.55
1:B:283:GLY:H	1:B:313:ARG:NH2	2.04	0.55
1:C:353:LYS:HD2	2:C:1791:HOH:O	2.07	0.55
1:B:273:MET:CB	1:C:268:ARG:HG3	2.37	0.55
1:C:4:VAL:O	1:D:5:THR:HA	2.06	0.55
1:D:283:GLY:H	1:D:313:ARG:NH2	2.04	0.55
1:A:14:TYR:OH	1:D:210:THR:HG23	2.07	0.54
1:A:14:TYR:CZ	1:D:166:GLY:O	2.60	0.54
1:B:119:MET:HG3	2:B:1618:HOH:O	2.08	0.54
1:A:19:THR:OG1	1:A:20:PRO:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:TYR:OH	1:C:210:THR:HG23	2.07	0.54
1:C:260:HIS:HA	2:C:1008:HOH:O	2.08	0.54
1:C:19:THR:OG1	1:C:20:PRO:HD2	2.08	0.53
1:D:275:PRO:HB3	2:D:2083:HOH:O	2.09	0.53
1:C:351:LYS:HD2	2:C:1099:HOH:O	2.09	0.53
1:A:234:GLU:OE2	1:D:268:ARG:HD2	2.08	0.53
1:C:207:ASP:CG	2:C:1931:HOH:O	2.51	0.53
1:D:247:ALA:O	2:D:865:HOH:O	2.19	0.53
1:B:273:MET:HE3	1:C:264:MET:HG3	1.91	0.53
1:D:19:THR:OG1	1:D:20:PRO:HD2	2.08	0.53
1:B:339:HIS:O	1:B:343:MET:HG2	2.10	0.52
1:B:19:THR:OG1	1:B:20:PRO:HD2	2.08	0.52
1:C:112:VAL:HA	2:C:1797:HOH:O	2.09	0.52
1:A:339:HIS:O	1:A:343:MET:HG2	2.10	0.52
1:B:234:GLU:OE2	1:C:268:ARG:HD2	2.09	0.52
1:D:339:HIS:O	1:D:343:MET:HG2	2.10	0.51
1:C:339:HIS:O	1:C:343:MET:HG2	2.10	0.51
1:B:14:TYR:CE1	1:C:166:GLY:O	2.64	0.51
1:B:142:LYS:CB	2:B:1908:HOH:O	2.59	0.51
1:D:224:ALA:HB2	2:D:1142:HOH:O	2.11	0.51
1:A:273:MET:CE	1:D:264:MET:HG3	2.41	0.50
1:A:273:MET:HG2	1:D:268:ARG:HG3	1.93	0.50
1:B:234:GLU:CD	1:C:268:ARG:HH11	2.18	0.50
1:A:272:ALA:N	1:D:267:ALA:O	2.45	0.50
1:A:304:PRO:HB2	1:D:302:PRO:HB3	1.93	0.50
1:B:158:ARG:HD3	2:B:1674:HOH:O	2.11	0.49
1:B:88:HIS:HE1	2:B:1246:HOH:O	1.94	0.49
1:D:202:ILE:HA	2:D:931:HOH:O	2.13	0.49
1:A:234:GLU:OE2	1:D:268:ARG:NH1	2.38	0.49
1:A:5:THR:O	1:C:165:ASN:HB3	2.13	0.48
1:D:150:LYS:HE3	2:D:1473:HOH:O	2.11	0.48
1:D:245:PRO:HG3	2:D:1357:HOH:O	2.14	0.48
1:D:80:GLN:CB	2:D:1749:HOH:O	2.62	0.47
1:B:304:PRO:HB2	1:C:302:PRO:HB3	1.97	0.47
1:C:72:MET:SD	1:C:316:GLN:HG2	2.55	0.47
1:D:244:VAL:HB	1:D:245:PRO:HD2	1.97	0.47
1:B:244:VAL:HB	1:B:245:PRO:HD2	1.97	0.46
1:B:273:MET:HG2	1:C:268:ARG:HG3	1.97	0.46
1:D:133:MET:HE2	1:D:134:THR:C	2.40	0.46
1:C:5:THR:HA	1:D:4:VAL:O	2.15	0.46
1:C:133:MET:HE2	1:C:134:THR:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:VAL:HB	1:C:245:PRO:HD2	1.97	0.46
1:A:10:GLN:HG3	1:C:128:ALA:HB2	1.98	0.46
1:A:72:MET:SD	1:A:316:GLN:HG2	2.55	0.46
1:A:244:VAL:HB	1:A:245:PRO:HD2	1.97	0.46
1:A:228:ARG:NH2	2:A:1070:HOH:O	2.49	0.46
1:B:72:MET:SD	1:B:316:GLN:HG2	2.55	0.46
1:B:133:MET:HE2	1:B:134:THR:C	2.40	0.46
1:B:272:ALA:N	1:C:267:ALA:O	2.49	0.46
1:A:209:ASP:HB2	2:A:1151:HOH:O	2.16	0.46
1:B:10:GLN:NE2	1:D:164:GLN:HB2	2.28	0.46
1:B:14:TYR:CZ	1:C:166:GLY:O	2.69	0.46
1:D:72:MET:SD	1:D:316:GLN:HG2	2.55	0.46
1:A:44:GLU:CD	1:A:44:GLU:H	2.24	0.46
1:C:44:GLU:CD	1:C:44:GLU:H	2.24	0.46
2:B:2051:HOH:O	1:D:165:ASN:HA	2.16	0.45
1:D:283:GLY:H	1:D:313:ARG:HH21	1.64	0.45
1:A:133:MET:HE2	1:A:134:THR:C	2.40	0.45
1:B:44:GLU:H	1:B:44:GLU:CD	2.24	0.45
1:B:79:GLU:CD	1:B:79:GLU:H	2.24	0.45
1:B:281:SER:HB3	1:B:311:TYR:CD1	2.51	0.45
1:C:204:GLY:HA3	2:C:969:HOH:O	2.16	0.45
1:A:281:SER:HB3	1:A:311:TYR:CD1	2.51	0.45
1:C:79:GLU:H	1:C:79:GLU:CD	2.24	0.45
1:C:283:GLY:H	1:C:313:ARG:HH21	1.64	0.45
1:A:283:GLY:H	1:A:313:ARG:HH21	1.64	0.45
1:B:346:MET:CE	1:B:351:LYS:HB2	2.47	0.45
1:D:44:GLU:H	1:D:44:GLU:CD	2.24	0.45
1:D:281:SER:HB3	1:D:311:TYR:CD1	2.51	0.45
1:B:10:GLN:HG2	1:D:128:ALA:CB	2.45	0.45
1:C:281:SER:HB3	1:C:311:TYR:CD1	2.51	0.45
1:D:79:GLU:CD	1:D:79:GLU:H	2.24	0.45
1:A:227:GLN:CD	1:D:220:ARG:HG3	2.42	0.45
1:B:3:ARG:NH2	1:C:165:ASN:OD1	2.49	0.45
1:D:131:GLU:HG2	2:D:934:HOH:O	2.16	0.45
1:A:346:MET:CE	1:A:351:LYS:HB2	2.47	0.44
1:A:79:GLU:CD	1:A:79:GLU:H	2.24	0.44
1:B:68:TYR:O	1:B:71:LEU:HB3	2.18	0.44
1:C:216:GLU:HG2	2:C:1788:HOH:O	2.18	0.43
1:C:346:MET:CE	1:C:351:LYS:HB2	2.47	0.43
1:B:10:GLN:CG	1:D:128:ALA:CB	2.92	0.43
1:C:342:ARG:NE	2:C:1447:HOH:O	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:THR:CG2	2:C:1936:HOH:O	2.66	0.43
1:D:164:GLN:NE2	2:D:883:HOH:O	2.09	0.43
1:D:199:GLU:HG3	1:D:280:LEU:HD21	2.01	0.43
1:B:199:GLU:HG3	1:B:280:LEU:HD21	2.01	0.43
1:C:199:GLU:HG3	1:C:280:LEU:HD21	2.01	0.43
1:A:3:ARG:NH2	1:D:165:ASN:OD1	2.52	0.43
1:A:115:ILE:O	1:A:155:CYS:HA	2.19	0.43
1:A:199:GLU:HG3	1:A:280:LEU:HD21	2.01	0.43
1:B:273:MET:CE	1:C:264:MET:HG3	2.47	0.43
1:D:68:TYR:O	1:D:71:LEU:HB3	2.18	0.43
1:C:115:ILE:O	1:C:155:CYS:HA	2.19	0.43
1:A:68:TYR:O	1:A:71:LEU:HB3	2.18	0.43
1:A:267:ALA:HB1	1:D:273:MET:N	2.34	0.43
1:A:342:ARG:NE	2:A:1343:HOH:O	2.38	0.43
1:B:34:THR:HA	1:B:35:PRO:HD3	1.88	0.43
1:C:38:GLY:HA3	1:C:309:PHE:CZ	2.54	0.43
1:C:63:GLU:HG3	1:C:67:GLN:NE2	2.34	0.43
1:C:288:GLN:O	1:C:289:ALA:C	2.62	0.43
1:D:79:GLU:CD	2:D:1854:HOH:O	2.53	0.43
1:D:115:ILE:O	1:D:155:CYS:HA	2.19	0.43
1:D:346:MET:CE	1:D:351:LYS:HB2	2.47	0.43
1:A:63:GLU:HG3	1:A:67:GLN:NE2	2.34	0.42
1:B:115:ILE:O	1:B:155:CYS:HA	2.19	0.42
1:C:68:TYR:O	1:C:71:LEU:HB3	2.18	0.42
1:D:40:LEU:O	1:D:85:VAL:HA	2.20	0.42
1:D:63:GLU:HG3	1:D:67:GLN:NE2	2.34	0.42
1:B:63:GLU:HG3	1:B:67:GLN:NE2	2.34	0.42
1:B:283:GLY:H	1:B:313:ARG:HH21	1.64	0.42
1:C:40:LEU:O	1:C:85:VAL:HA	2.19	0.42
1:B:339:HIS:CE1	1:B:343:MET:HE3	2.55	0.42
1:A:40:LEU:O	1:A:85:VAL:HA	2.20	0.42
1:B:267:ALA:HB1	1:C:273:MET:N	2.34	0.42
1:D:38:GLY:HA3	1:D:309:PHE:CZ	2.54	0.42
1:D:282:GLY:O	2:D:1326:HOH:O	2.22	0.42
1:A:273:MET:CG	1:D:268:ARG:HG3	2.49	0.42
1:B:40:LEU:O	1:B:85:VAL:HA	2.19	0.42
1:C:327:GLU:OE1	2:C:1960:HOH:O	2.22	0.42
1:C:339:HIS:CE1	1:C:343:MET:HE3	2.55	0.42
1:A:38:GLY:HA3	1:A:309:PHE:CZ	2.54	0.41
1:A:288:GLN:O	1:A:289:ALA:C	2.62	0.41
1:B:38:GLY:HA3	1:B:309:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLN:CD	1:C:220:ARG:HG3	2.45	0.41
1:D:4:VAL:HG23	2:D:1607:HOH:O	2.19	0.41
1:B:101:THR:O	1:B:102:PHE:C	2.62	0.41
1:C:252:THR:HG22	2:C:1936:HOH:O	2.21	0.41
1:D:3:ARG:HH11	1:D:3:ARG:HD3	1.71	0.41
1:A:326:LYS:HE2	1:A:326:LYS:HB2	1.53	0.41
1:A:339:HIS:CE1	1:A:343:MET:HE3	2.55	0.41
1:D:101:THR:O	1:D:102:PHE:C	2.62	0.41
1:D:288:GLN:O	1:D:289:ALA:C	2.62	0.41
1:D:339:HIS:CE1	1:D:357:ASP:OD1	2.72	0.41
1:C:210:THR:O	1:C:211:CYS:C	2.62	0.41
1:D:55:PRO:HA	2:D:2003:HOH:O	2.19	0.41
1:D:326:LYS:HE2	1:D:326:LYS:HB2	1.52	0.41
1:A:273:MET:N	1:D:267:ALA:HB1	2.36	0.41
1:D:95:LYS:NZ	2:D:1403:HOH:O	2.25	0.41
1:A:210:THR:O	1:A:211:CYS:C	2.62	0.41
1:C:326:LYS:HE2	1:C:326:LYS:HB2	1.53	0.40
1:D:207:ASP:HB2	2:D:1260:HOH:O	2.20	0.40
1:B:346:MET:HE3	1:B:346:MET:HB3	1.84	0.40
1:D:210:THR:O	1:D:211:CYS:C	2.62	0.40
1:C:353:LYS:CD	2:C:1791:HOH:O	2.67	0.40
1:D:273:MET:O	1:D:273:MET:HG3	2.22	0.40
1:B:20:PRO:CD	2:B:1763:HOH:O	2.65	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:CB	2:D:1790:HOH:O[4_435]	2.02	0.18
1:A:98:ASN:O	1:D:62:GLU:OE2[1_455]	2.04	0.16
1:B:98:ASN:O	1:C:62:GLU:OE2[1_655]	2.06	0.14
1:C:108:ALA:O	1:D:109:ARG:NH2[2_345]	2.09	0.11
1:D:100:GLN:NE2	2:C:2073:HOH:O[2_344]	2.15	0.05

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	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	36	25
1	B	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	36	25
1	C	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	36	25
1	D	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	36	25
All	All	1420/1480 (96%)	1384 (98%)	32 (2%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	B	198	PRO
1	C	198	PRO
1	D	198	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	274/303 (90%)	262 (96%)	12 (4%)	25	13
1	B	274/303 (90%)	262 (96%)	12 (4%)	25	13
1	C	274/303 (90%)	262 (96%)	12 (4%)	25	13
1	D	274/303 (90%)	262 (96%)	12 (4%)	25	13
All	All	1096/1212 (90%)	1048 (96%)	48 (4%)	25	13

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	133	MET

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Mol	Chain	Res	Type
1	A	183	TYR
1	A	209	ASP
1	A	213	ARG
1	A	220	ARG
1	A	305	TYR
1	A	313	ARG
1	A	317	SER
1	A	326	LYS
1	A	338	LEU
1	A	354	ARG
1	B	69	ARG
1	B	133	MET
1	B	183	TYR
1	B	209	ASP
1	B	213	ARG
1	B	220	ARG
1	B	305	TYR
1	B	313	ARG
1	B	317	SER
1	B	326	LYS
1	B	338	LEU
1	B	354	ARG
1	C	69	ARG
1	C	133	MET
1	C	183	TYR
1	C	209	ASP
1	C	213	ARG
1	C	220	ARG
1	C	305	TYR
1	C	313	ARG
1	C	317	SER
1	C	326	LYS
1	C	338	LEU
1	C	354	ARG
1	D	69	ARG
1	D	133	MET
1	D	183	TYR
1	D	209	ASP
1	D	213	ARG
1	D	220	ARG
1	D	305	TYR
1	D	313	ARG

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Mol	Chain	Res	Type
1	D	317	SER
1	D	326	LYS
1	D	338	LEU
1	D	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	HIS
1	D	339	HIS

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.