



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:14 PM GMT

PDB ID : 1EPX
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

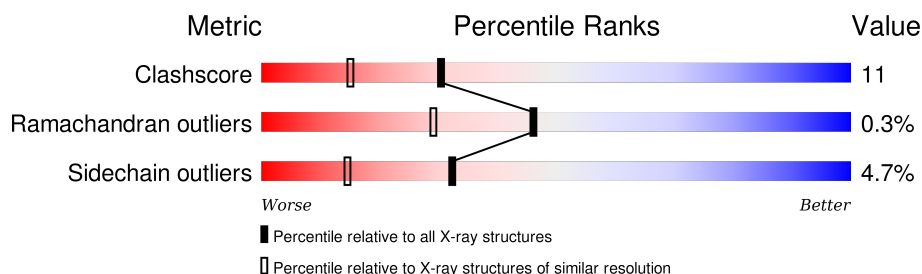
1 Overall quality at a glance

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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	 74% 19% . . .
1	B	370	 72% 20% . . .
1	C	370	 68% 23% 5% . .
1	D	370	 67% 24% 5% .

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		

Note EDS was not executed.

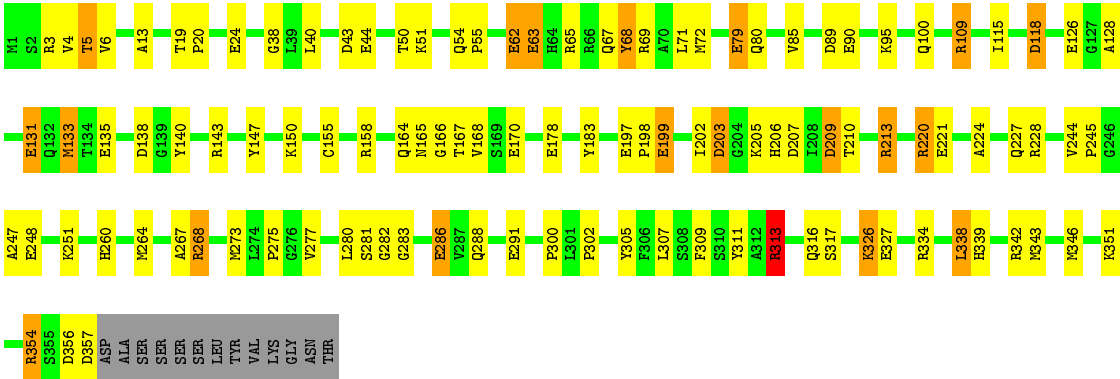
- Chain A:
-
- 74% 19%
- M1 S2 R3 V4 T5 Q10 Y14 T19 P20 E24 G38 L39 L40 D43 E44 E62 E63 E64 R65 R66 Q67 V68 R69 A70 L71 M72 E79 W85 D89 E90 N98 R109 I115 D118 E126 E131 Q132 M133 I134 E135 D138 E140 R143 Y147 C155 R158 E170 Y183 E197 P198 E199 D203 D209 E213 R220 E221 Q227 R228 E229 E234 V244 P245 E248 A267 R268 E289 A290 D291 E291 L280 S281 E282 E283 E286 V287 Q288 E291 P304 Y305 E306 L307

- Chain B:
-
- 72% 20%
- • •

- Chain C: 68% 23% 5% . .

SER
LEU
TYR
VAL
LYS
GLY
ASN
THR

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.80 Å 118.10 Å 159.60 Å 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	1.24	17/2749 (0.6%)	1.58	35/3730 (0.9%)
1	B	1.24	17/2749 (0.6%)	1.58	35/3730 (0.9%)
1	C	1.24	16/2749 (0.6%)	1.58	35/3730 (0.9%)
1	D	1.24	17/2749 (0.6%)	1.58	35/3730 (0.9%)
All	All	1.24	67/10996 (0.6%)	1.58	140/14920 (0.9%)

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	GLU	CD-OE1	-8.09	1.16	1.25
1	D	135	GLU	CD-OE1	-8.09	1.16	1.25
1	B	135	GLU	CD-OE1	-8.08	1.16	1.25
1	C	135	GLU	CD-OE1	-8.07	1.16	1.25
1	D	199	GLU	CD-OE2	7.97	1.34	1.25
1	A	199	GLU	CD-OE2	7.96	1.34	1.25
1	C	199	GLU	CD-OE2	7.95	1.34	1.25
1	B	199	GLU	CD-OE2	7.91	1.34	1.25
1	D	79	GLU	CD-OE2	7.83	1.34	1.25
1	C	79	GLU	CD-OE2	7.76	1.34	1.25
1	A	79	GLU	CD-OE2	7.75	1.34	1.25
1	B	79	GLU	CD-OE2	7.71	1.34	1.25
1	A	286	GLU	CD-OE2	6.78	1.33	1.25
1	C	286	GLU	CD-OE2	6.78	1.33	1.25
1	D	286	GLU	CD-OE2	6.77	1.33	1.25
1	B	286	GLU	CD-OE2	6.76	1.33	1.25
1	D	291	GLU	CD-OE2	6.59	1.32	1.25
1	A	291	GLU	CD-OE2	6.58	1.32	1.25
1	C	291	GLU	CD-OE2	6.57	1.32	1.25
1	D	62	GLU	CD-OE2	6.53	1.32	1.25
1	B	291	GLU	CD-OE2	6.52	1.32	1.25
1	C	62	GLU	CD-OE2	6.50	1.32	1.25
1	A	62	GLU	CD-OE2	6.47	1.32	1.25
1	D	24	GLU	CD-OE2	6.43	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	GLU	CD-OE2	6.43	1.32	1.25
1	B	62	GLU	CD-OE2	6.42	1.32	1.25
1	C	24	GLU	CD-OE2	6.41	1.32	1.25
1	A	24	GLU	CD-OE2	6.39	1.32	1.25
1	B	248	GLU	CD-OE2	6.27	1.32	1.25
1	D	248	GLU	CD-OE2	6.23	1.32	1.25
1	D	126	GLU	CD-OE2	6.22	1.32	1.25
1	C	248	GLU	CD-OE2	6.22	1.32	1.25
1	A	248	GLU	CD-OE2	6.21	1.32	1.25
1	B	126	GLU	CD-OE2	6.20	1.32	1.25
1	B	131	GLU	CD-OE2	6.18	1.32	1.25
1	A	126	GLU	CD-OE2	6.18	1.32	1.25
1	D	131	GLU	CD-OE2	6.18	1.32	1.25
1	A	131	GLU	CD-OE2	6.17	1.32	1.25
1	C	126	GLU	CD-OE2	6.17	1.32	1.25
1	D	197	GLU	CD-OE1	-6.15	1.18	1.25
1	A	197	GLU	CD-OE1	-6.13	1.19	1.25
1	B	197	GLU	CD-OE1	-6.13	1.19	1.25
1	C	197	GLU	CD-OE1	-6.13	1.19	1.25
1	C	131	GLU	CD-OE2	6.12	1.32	1.25
1	D	63	GLU	CD-OE2	5.99	1.32	1.25
1	C	63	GLU	CD-OE2	5.98	1.32	1.25
1	A	63	GLU	CD-OE2	5.94	1.32	1.25
1	B	63	GLU	CD-OE2	5.92	1.32	1.25
1	C	221	GLU	CD-OE2	5.73	1.31	1.25
1	A	221	GLU	CD-OE2	5.71	1.31	1.25
1	B	221	GLU	CD-OE2	5.71	1.31	1.25
1	D	221	GLU	CD-OE2	5.66	1.31	1.25
1	A	90	GLU	CD-OE2	5.49	1.31	1.25
1	C	327	GLU	CD-OE2	5.49	1.31	1.25
1	C	90	GLU	CD-OE2	5.48	1.31	1.25
1	D	90	GLU	CD-OE2	5.45	1.31	1.25
1	B	90	GLU	CD-OE2	5.44	1.31	1.25
1	A	327	GLU	CD-OE2	5.43	1.31	1.25
1	B	327	GLU	CD-OE2	5.42	1.31	1.25
1	D	327	GLU	CD-OE2	5.36	1.31	1.25
1	B	126	GLU	CD-OE1	-5.35	1.19	1.25
1	C	126	GLU	CD-OE1	-5.31	1.19	1.25
1	A	126	GLU	CD-OE1	-5.29	1.19	1.25
1	D	126	GLU	CD-OE1	-5.29	1.19	1.25
1	D	268	ARG	NE-CZ	5.07	1.39	1.33
1	A	268	ARG	NE-CZ	5.05	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	ARG	NE-CZ	5.03	1.39	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ARG	NE-CZ-NH1	28.54	134.57	120.30
1	A	268	ARG	NE-CZ-NH1	28.52	134.56	120.30
1	C	268	ARG	NE-CZ-NH1	28.52	134.56	120.30
1	D	268	ARG	NE-CZ-NH1	28.48	134.54	120.30
1	B	268	ARG	NE-CZ-NH2	-18.17	111.22	120.30
1	A	268	ARG	NE-CZ-NH2	-18.13	111.24	120.30
1	C	268	ARG	NE-CZ-NH2	-18.08	111.26	120.30
1	D	268	ARG	NE-CZ-NH2	-18.07	111.26	120.30
1	B	65	ARG	NE-CZ-NH2	-11.69	114.45	120.30
1	A	65	ARG	NE-CZ-NH2	-11.65	114.48	120.30
1	D	65	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	C	65	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	D	313	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	D	109	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	A	109	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	C	109	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	B	109	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	C	313	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	313	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	B	313	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	D	313	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	147	TYR	CB-CG-CD1	9.09	126.45	121.00
1	A	147	TYR	CB-CG-CD1	9.04	126.42	121.00
1	B	147	TYR	CB-CG-CD1	9.03	126.42	121.00
1	A	313	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	147	TYR	CB-CG-CD1	9.02	126.41	121.00
1	C	143	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	D	143	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	B	143	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	C	313	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	B	313	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	143	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	209	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	D	209	ASP	CB-CG-OD2	-8.87	110.31	118.30
1	C	209	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	B	209	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	B	213	ARG	NE-CZ-NH2	-8.75	115.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	213	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	D	213	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	118	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	D	118	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	B	118	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	C	118	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	D	147	TYR	CB-CG-CD2	-8.26	116.04	121.00
1	B	147	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	A	147	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	C	147	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	A	118	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	118	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	118	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	118	ASP	CB-CG-OD1	7.45	125.00	118.30
1	B	65	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	65	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	65	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	C	65	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	203	ASP	CB-CG-OD2	-7.21	111.82	118.30
1	A	203	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	203	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	D	109	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	203	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	109	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	109	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	109	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	158	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	133	MET	CG-SD-CE	7.03	111.45	100.20
1	A	133	MET	CG-SD-CE	7.02	111.43	100.20
1	B	133	MET	CG-SD-CE	7.02	111.43	100.20
1	D	133	MET	CG-SD-CE	7.00	111.41	100.20
1	A	158	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	158	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	354	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	C	158	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	354	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	354	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	C	354	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	268	ARG	CD-NE-CZ	6.50	132.70	123.60
1	D	268	ARG	CD-NE-CZ	6.47	132.66	123.60
1	A	268	ARG	CD-NE-CZ	6.46	132.65	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ARG	CD-NE-CZ	6.43	132.61	123.60
1	C	140	TYR	CB-CG-CD1	6.37	124.82	121.00
1	A	140	TYR	CB-CG-CD1	6.35	124.81	121.00
1	D	140	TYR	CB-CG-CD1	6.34	124.81	121.00
1	B	140	TYR	CB-CG-CD1	6.33	124.80	121.00
1	B	228	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	143	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	143	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	143	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	228	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	143	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	43	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	228	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	43	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	228	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	43	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	43	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	356	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	356	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	356	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	D	356	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	138	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	89	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	C	138	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	89	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	89	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	89	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	138	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	D	138	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	140	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	D	140	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	C	140	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	B	133	MET	CA-CB-CG	-5.63	103.73	113.30
1	C	288	GLN	CB-CA-C	-5.62	99.15	110.40
1	A	288	GLN	CB-CA-C	-5.62	99.17	110.40
1	A	133	MET	CA-CB-CG	-5.61	103.76	113.30
1	C	133	MET	CA-CB-CG	-5.61	103.76	113.30
1	D	133	MET	CA-CB-CG	-5.61	103.77	113.30
1	D	288	GLN	CB-CA-C	-5.61	99.19	110.40
1	A	140	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	B	288	GLN	CB-CA-C	-5.59	99.21	110.40
1	D	170	GLU	OE1-CD-OE2	-5.58	116.60	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	GLU	OE1-CD-OE2	-5.57	116.61	123.30
1	A	342	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	342	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	342	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	170	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	A	170	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	C	342	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	109	ARG	CD-NE-CZ	5.42	131.18	123.60
1	B	109	ARG	CD-NE-CZ	5.41	131.17	123.60
1	D	109	ARG	CD-NE-CZ	5.41	131.17	123.60
1	C	109	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	5	THR	CA-CB-CG2	-5.29	104.99	112.40
1	C	5	THR	CA-CB-CG2	-5.28	105.01	112.40
1	B	5	THR	CA-CB-CG2	-5.27	105.02	112.40
1	D	5	THR	CA-CB-CG2	-5.26	105.04	112.40
1	D	68	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	68	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	B	68	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	C	68	TYR	CB-CG-CD2	-5.16	117.91	121.00

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	53	1
1	B	2694	0	2628	59	1
1	C	2694	0	2628	91	3
1	D	2694	0	2628	96	3
2	A	329	0	0	4	0
2	B	291	0	0	10	0
2	C	376	0	0	36	1
2	D	359	0	0	32	1
All	All	12131	0	10512	233	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 11.

All (233) 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: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:C:346:MET:HE1	2:C:2068:HOH:O	1.83	0.77
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
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:346:MET:CE	2:C:2068:HOH:O	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:VAL:HB	1:D:307:LEU:HD23	1.76	0.67
1:A:273:MET:HE3	1:D:264:MET:HG3	1.77	0.67
1:D:300:PRO:O	2:D:1876:HOH:O	2.12	0.67
1:C:3:ARG:HA	1:D:6:VAL:O	1.95	0.67
1:A:272:ALA:HB3	1:D:267:ALA:HA	1.74	0.67
1:C:170:GLU:OE2	2:C:1830:HOH:O	2.13	0.67
1:C:80:GLN:CB	2:C:2066:HOH:O	2.43	0.67
1:A:229:HIS:ND1	1:C:126:GLU:OE2	2.19	0.67
1:C:351:LYS:CE	2:C:1099:HOH:O	2.25	0.67
1:B:277:VAL:HB	1:B:307:LEU:HD23	1.76	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:272:ALA:HB3	1:C:267:ALA:HA	1.79	0.65
1:B:20:PRO:HD2	2:B:1763:HOH:O	1.96	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:207:ASP:CG	2:D:1260:HOH:O	2.35	0.63
1:D:251:LYS:CB	2:D:1887:HOH:O	2.46	0.63
1:B:10:GLN:HE22	1:D:164:GLN:HB2	1.64	0.62
1:C:346:MET:HE3	1:C:351:LYS:HB2	1.82	0.62
1:B:346:MET:HE3	1:B:351:LYS:HB2	1.81	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:273:MET:HE3	1:C:264:MET:HG3	1.83	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	1.82	0.60
1:A:346:MET:HE3	1:A:351:LYS:HB2	1.82	0.60
1:C:351:LYS:CD	2:C:1099:HOH:O	2.50	0.59
1:A:10:GLN:CG	1:C:128:ALA:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HD2	1:D:227:GLN:HB3	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:339:HIS:HE1	1:D:357:ASP:OD1	1.87	0.57
1:D:178:GLU:HG2	2:D:1254:HOH:O	2.05	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: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:C:4:VAL:O	1:D:5:THR:HA	2.06	0.55
1:B:273:MET:CB	1:C:268:ARG:HG3	2.37	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:234:GLU:CD	1:D:268:ARG:HH11	2.10	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: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:A:19:THR:OG1	1:A:20:PRO:HD2	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:D:247:ALA:O	2:D:865:HOH:O	2.19	0.53
1:D:19:THR:OG1	1:D:20:PRO:HD2	2.08	0.53
1:C:346:MET:HE1	2:C:876:HOH:O	2.10	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:OE2	1:C:268:ARG:HD2	2.09	0.52
1:A:339:HIS:O	1:A:343:MET:HG2	2.10	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:HG2	1:D:268:ARG:HG3	1.93	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:C:207:ASP:CG	2:C:1931:HOH:O	2.51	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:A:273:MET:CE	1:D:264:MET:HG3	2.41	0.48
1:D:80:GLN:CB	2:D:1749:HOH:O	2.62	0.47
1:D:244:VAL:HB	1:D:245:PRO:HD2	1.97	0.47
1:C:72:MET:SD	1:C:316:GLN:HG2	2.55	0.47
1:B:304:PRO:HB2	1:C:302:PRO:HB3	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:C:5:THR:HA	1:D:4:VAL:O	2.15	0.46
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:272:ALA:N	1:C:267:ALA:O	2.49	0.46
1:B:14:TYR:CZ	1:C:166:GLY:O	2.69	0.46
1:B:10:GLN:NE2	1:D:164:GLN:HB2	2.28	0.46
1:B:234:GLU:CD	1:C:268:ARG:HH11	2.18	0.46
1:A:209:ASP:HB2	2:A:1151:HOH:O	2.16	0.46
1:D:72:MET:SD	1:D:316:GLN:HG2	2.55	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:C:204:GLY:HA3	2:C:969:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:SER:HB3	1:B:311:TYR:CD1	2.51	0.45
1:C:283:GLY:H	1:C:313:ARG:HH21	1.64	0.45
1:A:281:SER:HB3	1:A:311:TYR:CD1	2.51	0.45
1:B:346:MET:CE	1:B:351:LYS:HB2	2.47	0.45
1:A:283:GLY:H	1:A:313:ARG:HH21	1.64	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: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:B:68:TYR:O	1:B:71:LEU:HB3	2.18	0.44
1:C:346:MET:CE	1:C:351:LYS:HB2	2.47	0.43
1:C:216:GLU:HG2	2:C:1788:HOH:O	2.18	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
1:D:164:GLN:NE2	2:D:883:HOH:O	2.09	0.43
1:C:252:THR:CG2	2:C:1936:HOH:O	2.66	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:B:273:MET:CE	1:C:264:MET:HG3	2.47	0.43
1:A:3:ARG:NH2	1:D:165:ASN:OD1	2.52	0.43
1:A:199:GLU:HG3	1:A:280:LEU:HD21	2.01	0.43
1:A:115:ILE:O	1:A:155:CYS:HA	2.19	0.43
1:D:68:TYR:O	1:D:71:LEU:HB3	2.18	0.43
1:A:346:MET:CE	1:A:351:LYS:HB2	2.47	0.43
1:C:115:ILE:O	1:C:155:CYS:HA	2.19	0.43
1:D:346:MET:CE	1:D:351:LYS:HB2	2.47	0.43
1:B:34:THR:HA	1:B:35:PRO:HD3	1.88	0.43
1:D:115:ILE:O	1:D:155:CYS:HA	2.19	0.43
1:A:68:TYR:O	1:A:71:LEU:HB3	2.18	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:A:342:ARG:NE	2:A:1343:HOH:O	2.38	0.43
1:A:267:ALA:HB1	1:D:273:MET:N	2.34	0.43
1:A:63:GLU:HG3	1:A:67:GLN:NE2	2.34	0.42
1:C:68:TYR:O	1:C:71:LEU:HB3	2.18	0.42
1:D:63:GLU:HG3	1:D:67:GLN:NE2	2.34	0.42
1:B:115:ILE:O	1:B:155:CYS:HA	2.19	0.42
1:D:40:LEU:O	1:D:85:VAL:HA	2.20	0.42
1:B:283:GLY:H	1:B:313:ARG:HH21	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:O	1:C:85:VAL:HA	2.19	0.42
1:B:63:GLU:HG3	1:B:67:GLN:NE2	2.34	0.42
1:A:40:LEU:O	1:A:85:VAL:HA	2.20	0.42
1:D:38:GLY:HA3	1:D:309:PHE:CZ	2.54	0.42
1:B:267:ALA:HB1	1:C:273:MET:N	2.34	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:A:38:GLY:HA3	1:A:309:PHE:CZ	2.54	0.41
1:D:4:VAL:HG23	2:D:1607:HOH:O	2.19	0.41
1:B:38:GLY:HA3	1:B:309:PHE:CZ	2.54	0.41
1:D:79:GLU:H	1:D:79:GLU:CD	2.24	0.41
1:D:3:ARG:HH11	1:D:3:ARG:HD3	1.71	0.41
1:C:252:THR:HG22	2:C:1936:HOH:O	2.21	0.41
1:A:326:LYS:HE2	1:A:326:LYS:HB2	1.53	0.41
1:D:339:HIS:CE1	1:D:357:ASP:OD1	2.72	0.41
1:D:55:PRO:HA	2:D:2003:HOH:O	2.19	0.41
1:D:326:LYS:HB2	1:D:326:LYS:HE2	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:C:44:GLU:CD	1:C:44:GLU:H	2.24	0.41
1:A:44:GLU:H	1:A:44:GLU:CD	2.24	0.41
1:D:207:ASP:HB2	2:D:1260:HOH:O	2.20	0.40
1:B:79:GLU:H	1:B:79:GLU:CD	2.24	0.40
1:C:326:LYS:HB2	1:C:326:LYS:HE2	1.53	0.40
1:B:44:GLU:CD	1:B:44:GLU:H	2.24	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:D:44:GLU:CD	1:D:44:GLU:H	2.24	0.40
1:B:20:PRO:CD	2:B:1763:HOH:O	2.65	0.40
1:C:79:GLU:H	1:C:79:GLU:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	46	29
1	B	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	46	29
1	C	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	46	29
1	D	355/370 (96%)	346 (98%)	8 (2%)	1 (0%)	46	29
All	All	1420/1480 (96%)	1384 (98%)	32 (2%)	4 (0%)	46	29

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 [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	274/303 (90%)	261 (95%)	13 (5%)	32	14
1	B	274/303 (90%)	261 (95%)	13 (5%)	32	14
1	C	274/303 (90%)	261 (95%)	13 (5%)	32	14
1	D	274/303 (90%)	261 (95%)	13 (5%)	32	14
All	All	1096/1212 (90%)	1044 (95%)	52 (5%)	32	14

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	118	ASP
1	A	133	MET
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	118	ASP
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	118	ASP
1	C	133	MET
1	C	183	TYR
1	C	209	ASP
1	C	213	ARG
1	C	220	ARG

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

Some 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 ⓘ

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.