Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 03:52 AM EDT

PDB ID	:	1F2J
Title	:	CRYSTAL STRUCTURE ANALYSIS OF ALDOLASE FROM T. BRUCEI
Authors	:	Chudzik, D.M.; Michels, P.A.; De Walque, S.; Hol, W.G.J.
Deposited on	:	2000-05-25
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 (i) 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 (i)) were used in the production of this report:

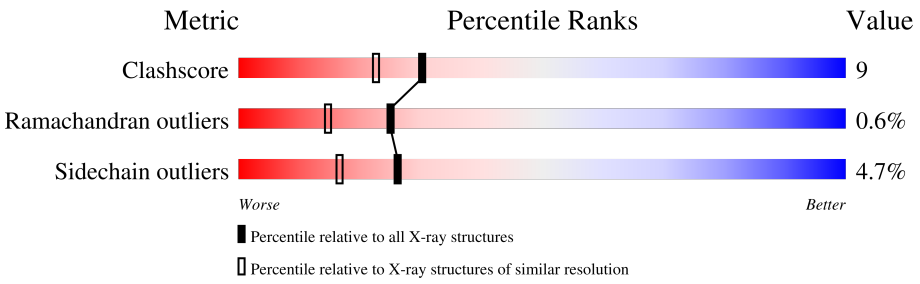
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	55% 29% 10% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2948 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, GLYCOSOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2707	1709	478	501	19	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	241	241	241	0	0

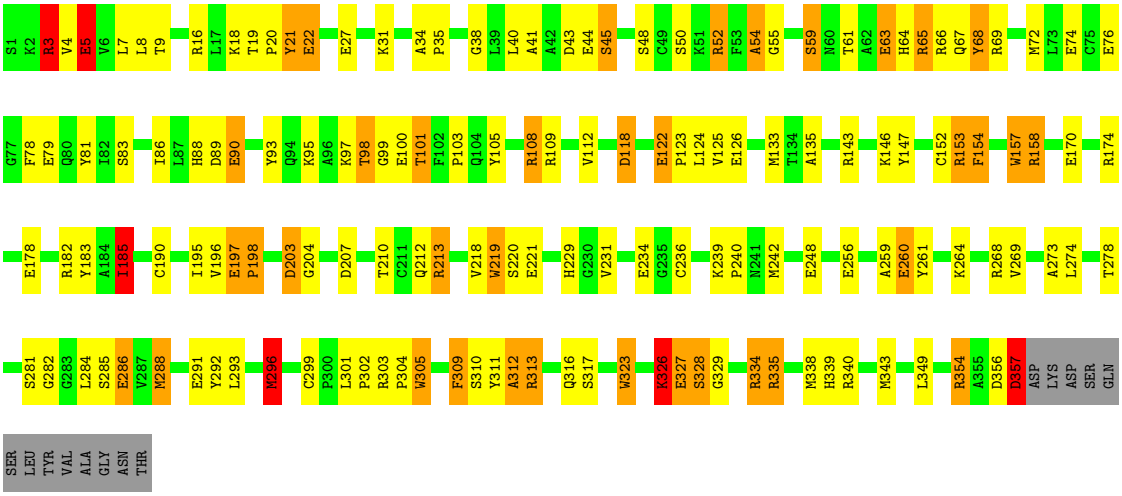
3 Residue-property plots (i)

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-BISPHOSPHATE ALDOLASE, GLYCOSOMAL

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	209.66Å 209.66Å 209.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.199 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2948	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.98	54/2762 (2.0%)	2.35	120/3745 (3.2%)

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	3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	GLU	CD-OE2	17.15	1.44	1.25
1	A	213	ARG	NE-CZ	14.48	1.51	1.33
1	A	178	GLU	CD-OE2	13.11	1.40	1.25
1	A	221	GLU	CD-OE2	12.90	1.39	1.25
1	A	126	GLU	CD-OE2	11.33	1.38	1.25
1	A	260	GLU	CD-OE2	11.30	1.38	1.25
1	A	327	GLU	CD-OE2	11.10	1.37	1.25
1	A	27	GLU	CD-OE2	11.04	1.37	1.25
1	A	313	ARG	CZ-NH2	9.88	1.45	1.33
1	A	44	GLU	CD-OE1	-9.03	1.15	1.25
1	A	5	GLU	CD-OE2	8.65	1.35	1.25
1	A	197	GLU	CD-OE2	8.57	1.35	1.25
1	A	281	SER	CB-OG	8.22	1.52	1.42
1	A	22	GLU	CD-OE1	-8.16	1.16	1.25
1	A	335	ARG	CZ-NH1	8.04	1.43	1.33
1	A	221	GLU	CD-OE1	7.95	1.34	1.25
1	A	281	SER	CA-CB	7.87	1.64	1.52
1	A	213	ARG	CD-NE	7.82	1.59	1.46
1	A	291	GLU	CD-OE2	7.62	1.34	1.25
1	A	213	ARG	CG-CD	7.47	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	GLU	CG-CD	-7.38	1.40	1.51
1	A	63	GLU	CD-OE2	7.27	1.33	1.25
1	A	286	GLU	CD-OE2	7.07	1.33	1.25
1	A	40	LEU	C-O	6.80	1.36	1.23
1	A	3	ARG	NE-CZ	6.66	1.41	1.33
1	A	90	GLU	CD-OE2	6.62	1.32	1.25
1	A	220	SER	CB-OG	-6.58	1.33	1.42
1	A	22	GLU	CG-CD	6.29	1.61	1.51
1	A	260	GLU	CG-CD	-6.25	1.42	1.51
1	A	356	ASP	CG-OD2	6.23	1.39	1.25
1	A	45	SER	CB-OG	6.22	1.50	1.42
1	A	313	ARG	CZ-NH1	6.10	1.41	1.33
1	A	174	ARG	CZ-NH2	6.10	1.41	1.33
1	A	248	GLU	CD-OE1	-6.08	1.19	1.25
1	A	338	MET	CG-SD	6.02	1.96	1.81
1	A	69	ARG	NE-CZ	6.01	1.40	1.33
1	A	170	GLU	CD-OE2	5.99	1.32	1.25
1	A	74	GLU	CD-OE2	5.93	1.32	1.25
1	A	100	GLU	CD-OE2	5.86	1.32	1.25
1	A	109	ARG	CZ-NH1	5.80	1.40	1.33
1	A	174	ARG	CZ-NH1	5.77	1.40	1.33
1	A	157	TRP	CD2-CE2	5.69	1.48	1.41
1	A	256	GLU	CG-CD	5.63	1.60	1.51
1	A	3	ARG	CZ-NH1	5.59	1.40	1.33
1	A	63	GLU	CD-OE1	5.46	1.31	1.25
1	A	323	TRP	CD2-CE2	5.32	1.47	1.41
1	A	323	TRP	CD1-NE1	5.27	1.47	1.38
1	A	99	GLY	CA-C	5.24	1.60	1.51
1	A	76	GLU	CD-OE1	-5.22	1.20	1.25
1	A	304	PRO	N-CD	5.17	1.55	1.47
1	A	264	LYS	CD-CE	5.14	1.64	1.51
1	A	236	CYS	CA-CB	5.10	1.65	1.53
1	A	22	GLU	CD-OE2	5.07	1.31	1.25
1	A	204	GLY	N-CA	5.07	1.53	1.46

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	ARG	NE-CZ-NH1	19.67	130.13	120.30
1	A	213	ARG	NE-CZ-NH2	16.96	128.78	120.30
1	A	109	ARG	NE-CZ-NH2	-16.72	111.94	120.30
1	A	3	ARG	NE-CZ-NH1	15.78	128.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	153	ARG	NE-CZ-NH2	14.63	127.62	120.30
1	A	16	ARG	NE-CZ-NH2	-14.43	113.08	120.30
1	A	143	ARG	NE-CZ-NH2	-14.41	113.10	120.30
1	A	221	GLU	OE1-CD-OE2	13.78	139.83	123.30
1	A	334	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	A	52	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	A	213	ARG	NH1-CZ-NH2	-12.74	105.39	119.40
1	A	213	ARG	CB-CG-CD	12.21	143.34	111.60
1	A	260	GLU	CB-CG-CD	-11.98	81.86	114.20
1	A	185	ILE	CA-CB-CG1	-11.70	88.78	111.00
1	A	203	ASP	CB-CG-OD1	11.69	128.82	118.30
1	A	66	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	A	59	SER	N-CA-CB	-11.18	93.72	110.50
1	A	268	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	207	ASP	CB-CG-OD1	10.90	128.11	118.30
1	A	203	ASP	CB-CG-OD2	-10.74	108.63	118.30
1	A	213	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	A	221	GLU	CG-CD-OE2	-10.50	97.30	118.30
1	A	89	ASP	CB-CG-OD1	10.43	127.68	118.30
1	A	335	ARG	NE-CZ-NH2	-10.01	115.29	120.30
1	A	147	TYR	CD1-CE1-CZ	-9.98	110.81	119.80
1	A	158	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	54	ALA	C-N-CA	-9.63	102.08	122.30
1	A	334	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	A	182	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	213	ARG	CD-NE-CZ	9.16	136.43	123.60
1	A	185	ILE	CA-CB-CG2	9.09	129.09	110.90
1	A	296	MET	CA-CB-CG	8.77	128.20	113.30
1	A	268	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	153	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	A	109	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	31	LYS	CB-CA-C	7.89	126.19	110.40
1	A	101	THR	CA-CB-CG2	-7.82	101.46	112.40
1	A	313	ARG	CD-NE-CZ	7.65	134.31	123.60
1	A	340	ARG	NE-CZ-NH1	-7.61	116.49	120.30
1	A	338	MET	CA-CB-CG	-7.40	100.71	113.30
1	A	212	GLN	N-CA-CB	-7.24	97.56	110.60
1	A	79	GLU	CG-CD-OE2	-7.18	103.93	118.30
1	A	133	MET	CG-SD-CE	7.07	111.50	100.20
1	A	147	TYR	CG-CD1-CE1	7.04	126.93	121.30
1	A	147	TYR	CG-CD2-CE2	-7.03	115.68	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	LYS	CB-CA-C	6.93	124.26	110.40
1	A	207	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	213	ARG	CB-CA-C	6.71	123.81	110.40
1	A	273	ALA	CB-CA-C	-6.69	100.07	110.10
1	A	5	GLU	CB-CG-CD	-6.66	96.22	114.20
1	A	356	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	288	MET	CA-CB-CG	6.63	124.58	113.30
1	A	98	THR	CA-CB-CG2	-6.63	103.12	112.40
1	A	105	TYR	CB-CG-CD2	6.62	124.97	121.00
1	A	354	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	135	ALA	N-CA-CB	-6.57	100.90	110.10
1	A	261	TYR	CG-CD2-CE2	6.48	126.49	121.30
1	A	72	MET	CA-CB-CG	-6.48	102.28	113.30
1	A	210	THR	CA-CB-CG2	-6.46	103.36	112.40
1	A	274	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	A	4	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	A	219	TRP	C-N-CA	-6.26	106.06	121.70
1	A	349	LEU	CA-CB-CG	-6.20	101.04	115.30
1	A	311	TYR	CG-CD1-CE1	-6.14	116.38	121.30
1	A	143	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	312	ALA	N-CA-CB	6.04	118.55	110.10
1	A	326	LYS	CD-CE-NZ	5.98	125.46	111.70
1	A	292	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	340	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	7	LEU	CA-CB-CG	-5.89	101.75	115.30
1	A	313	ARG	CB-CG-CD	5.89	126.92	111.60
1	A	309	PHE	CG-CD2-CE2	5.82	127.20	120.80
1	A	234	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	50	SER	N-CA-CB	5.78	119.16	110.50
1	A	260	GLU	CG-CD-OE1	-5.77	106.75	118.30
1	A	229	HIS	C-N-CA	-5.74	110.25	122.30
1	A	43	ASP	CB-CG-OD1	5.72	123.44	118.30
1	A	154	PHE	N-CA-CB	5.72	120.89	110.60
1	A	65	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	A	248	GLU	OE1-CD-OE2	-5.70	116.47	123.30
1	A	328	SER	N-CA-CB	-5.69	101.96	110.50
1	A	197	GLU	CA-CB-CG	-5.67	100.93	113.40
1	A	78	PHE	CB-CG-CD1	5.61	124.72	120.80
1	A	195	ILE	CA-CB-CG1	-5.60	100.36	111.00
1	A	61	THR	CA-CB-CG2	-5.60	104.56	112.40
1	A	261	TYR	CD1-CE1-CZ	5.59	124.83	119.80
1	A	9	THR	CA-CB-CG2	-5.57	104.60	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	LYS	CB-CG-CD	5.52	125.96	111.60
1	A	269	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	A	122	GLU	CB-CA-C	-5.48	99.44	110.40
1	A	152	CYS	CA-CB-SG	-5.48	104.14	114.00
1	A	81	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	A	261	TYR	CG-CD1-CE1	-5.44	116.95	121.30
1	A	112	VAL	CB-CA-C	-5.43	101.09	111.40
1	A	105	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	A	21	TYR	CZ-CE2-CD2	5.40	124.66	119.80
1	A	292	TYR	CB-CG-CD1	5.39	124.23	121.00
1	A	218	VAL	CA-CB-CG2	-5.32	102.92	110.90
1	A	190	CYS	CA-CB-SG	-5.31	104.45	114.00
1	A	311	TYR	CB-CG-CD2	-5.31	117.82	121.00
1	A	299	CYS	CB-CA-C	-5.30	99.80	110.40
1	A	8	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	296	MET	CG-SD-CE	-5.29	91.74	100.20
1	A	259	ALA	C-N-CA	-5.26	108.55	121.70
1	A	357	ASP	N-CA-CB	-5.26	101.14	110.60
1	A	313	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	68	TYR	CB-CG-CD1	5.24	124.14	121.00
1	A	311	TYR	CZ-CE2-CD2	-5.24	115.09	119.80
1	A	5	GLU	CG-CD-OE2	-5.18	107.95	118.30
1	A	95	LYS	CA-CB-CG	-5.15	102.07	113.40
1	A	242	MET	CA-CB-CG	-5.14	104.57	113.30
1	A	122	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	109	ARG	C-N-CA	-5.12	111.56	122.30
1	A	108	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	197	GLU	N-CA-CB	-5.08	101.45	110.60
1	A	83	SER	N-CA-CB	-5.06	102.92	110.50
1	A	63	GLU	CG-CD-OE2	-5.04	108.22	118.30
1	A	16	ARG	CD-NE-CZ	5.02	130.62	123.60
1	A	248	GLU	CG-CD-OE1	5.00	128.31	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASP	Sidechain
1	A	260	GLU	Sidechain
1	A	5	GLU	Sidechain

5.2 Too-close contacts (i)

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	2707	0	2668	50	0
2	A	241	0	0	1	1
All	All	2948	0	2668	50	1

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 (50) 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:A:285:SER:H	1:A:288:MET:HE3	1.30	0.94
1:A:88:HIS:HD2	1:A:90:GLU:H	1.24	0.84
1:A:88:HIS:CD2	1:A:90:GLU:H	1.97	0.81
1:A:63:GLU:HG3	1:A:67:GLN:NE2	1.97	0.78
1:A:284:LEU:HB3	1:A:288:MET:HG2	1.71	0.72
1:A:326:LYS:O	1:A:329:GLY:N	2.26	0.65
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.61	0.64
1:A:323:TRP:O	1:A:326:LYS:HE2	2.00	0.61
1:A:122:GLU:HB3	1:A:123:PRO:HD2	1.87	0.56
1:A:293:LEU:O	1:A:296:MET:HB2	2.06	0.56
1:A:19:THR:OG1	1:A:20:PRO:HD2	2.06	0.56
1:A:339:HIS:O	1:A:343:MET:HG2	2.06	0.55
1:A:339:HIS:HE1	1:A:357:ASP:OD1	1.90	0.55
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.88	0.54
1:A:88:HIS:HD2	1:A:90:GLU:N	2.01	0.54
1:A:286:GLU:OE2	1:A:317:SER:HB3	2.11	0.51
1:A:278:THR:HB	1:A:310:SER:HB2	1.94	0.50
1:A:63:GLU:HG3	1:A:67:GLN:HE22	1.73	0.49
1:A:97:LYS:HG3	1:A:98:THR:N	2.26	0.48
1:A:219:TRP:CZ2	1:A:240:PRO:HB2	2.49	0.48
1:A:196:VAL:O	1:A:198:PRO:HD3	2.14	0.47
1:A:54:ALA:O	1:A:55:GLY:C	2.50	0.47
1:A:197:GLU:HG3	1:A:239:LYS:O	2.15	0.47
1:A:101:THR:HB	1:A:103:PRO:HD2	1.97	0.46
1:A:59:SER:HB3	1:A:64:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HA	1:A:197:GLU:HB3	1.98	0.46
1:A:118:ASP:HA	1:A:157:TRP:CE3	2.51	0.45
1:A:52:ARG:HA	1:A:52:ARG:HD3	1.79	0.45
1:A:21:TYR:O	1:A:22:GLU:C	2.54	0.45
1:A:313:ARG:O	1:A:317:SER:HB2	2.17	0.45
1:A:93:TYR:OH	1:A:146:LYS:HE2	2.17	0.44
1:A:52:ARG:NH1	1:A:316:GLN:OE1	2.52	0.43
1:A:185:ILE:HD11	1:A:231:VAL:HA	2.00	0.43
1:A:334:ARG:O	1:A:335:ARG:C	2.56	0.42
1:A:41:ALA:HB3	1:A:312:ALA:HB2	2.01	0.42
1:A:86:ILE:HG12	1:A:154:PHE:HE1	1.84	0.42
1:A:108:ARG:NH1	1:A:108:ARG:HG2	2.34	0.42
1:A:301:LEU:HB3	1:A:302:PRO:CD	2.49	0.42
1:A:124:LEU:O	1:A:125:VAL:HB	2.20	0.41
1:A:65:ARG:O	1:A:68:TYR:HB3	2.20	0.41
1:A:34:ALA:HA	1:A:35:PRO:HD3	1.93	0.41
1:A:153:ARG:HD3	1:A:153:ARG:HA	1.82	0.41
1:A:122:GLU:HB3	1:A:123:PRO:CD	2.50	0.41
1:A:101:THR:CB	1:A:103:PRO:HD2	2.51	0.41
1:A:34:ALA:HA	2:A:575:HOH:O	2.21	0.41
1:A:38:GLY:HA3	1:A:309:PHE:CZ	2.56	0.41
1:A:45:SER:N	1:A:48:SER:OG	2.54	0.41
1:A:303:ARG:HA	1:A:305:TRP:CZ3	2.56	0.41
1:A:197:GLU:HA	1:A:239:LYS:O	2.22	0.40
1:A:339:HIS:CE1	1:A:357:ASP:OD1	2.73	0.40

All (1) 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)
2:A:593:HOH:O	2:A:593:HOH:O[38_556]	1.92	0.28

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%)	343 (97%)	10 (3%)	2 (1%)	25 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	A	282	GLY

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	276/302 (91%)	263 (95%)	13 (5%)	26 16

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	GLU
1	A	183	TYR
1	A	185	ILE
1	A	203	ASP
1	A	213	ARG
1	A	296	MET
1	A	305	TRP
1	A	326	LYS
1	A	327	GLU
1	A	328	SER
1	A	354	ARG
1	A	357	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	88	HIS
1	A	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.