Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2016 – 12:01 AM GMT

PDB ID	:	7XIM
Title	:	PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES
Authors	:	Janin, J.
Deposited on	:	1992-04-03
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

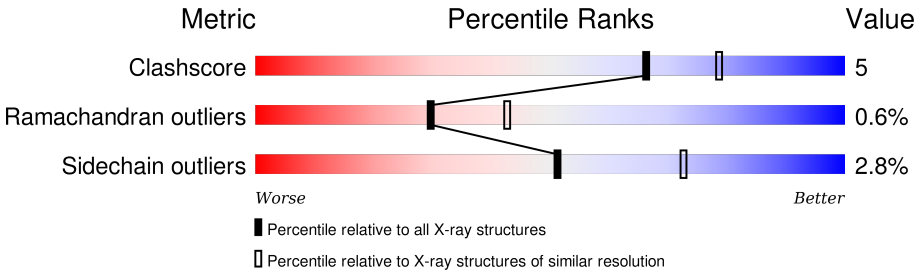
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 <=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	393	77% 19%
1	B	393	77% 19%
1	C	393	77% 18%
1	D	393	75% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13067 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 D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3045	1933	531	577	4			
1	B	390	Total	C	N	O	S	0	0	0
			3045	1933	531	577	4			
1	C	390	Total	C	N	O	S	0	0	0
			3041	1931	530	576	4			
1	D	390	Total	C	N	O	S	0	0	0
			3041	1931	530	576	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	222	Total	O	0	0
			222	222		
2	B	218	Total	O	0	0
			218	218		
2	C	235	Total	O	0	0
			235	235		
2	D	220	Total	O	0	0
			220	220		

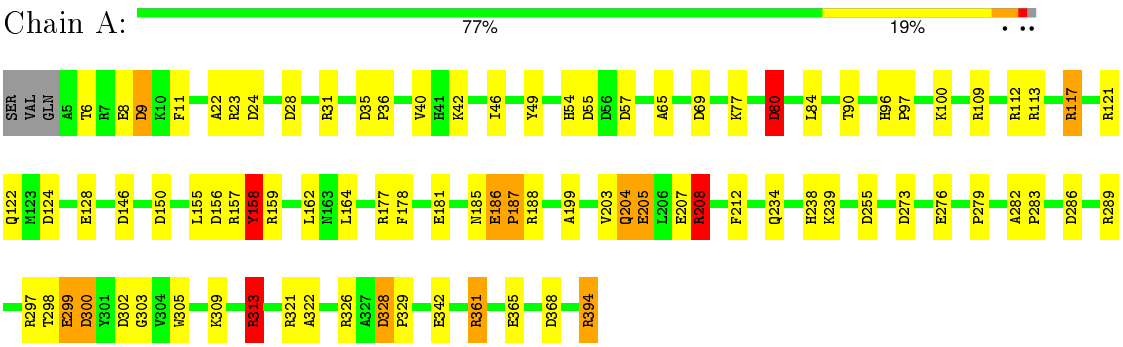
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

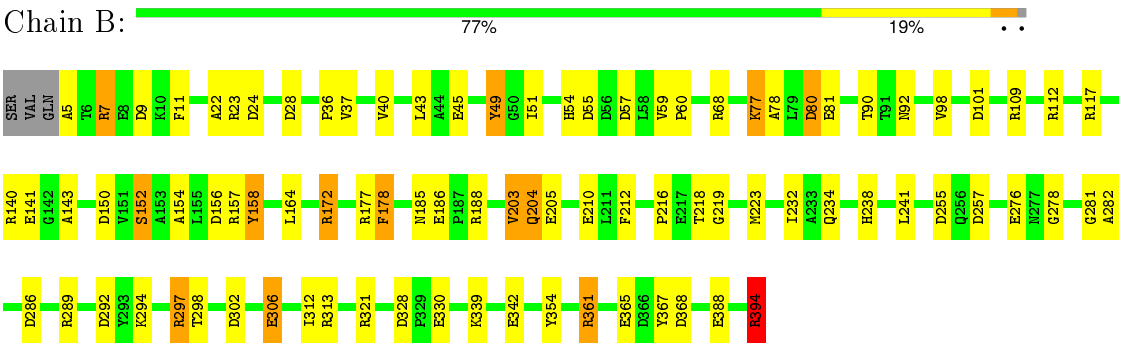
- Molecule 1: D-XYLOSE ISOMERASE

Chain A:



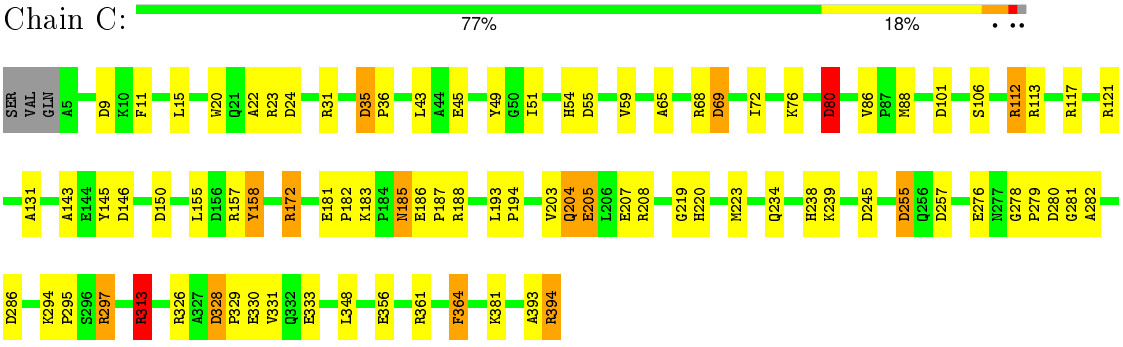
- Molecule 1: D-XYLOSE ISOMERASE

Chain B:



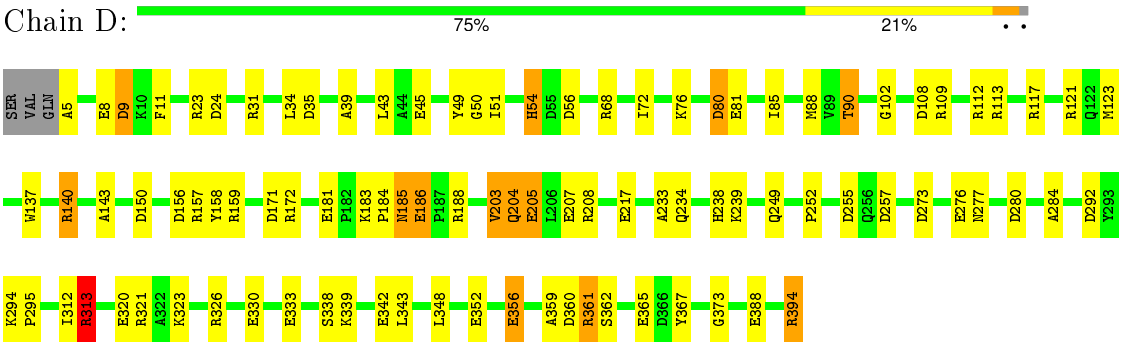
- Molecule 1: D-XYLOSE ISOMERASE

Chain C:



• Molecule 1: D-XYLOSE ISOMERASE

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13067	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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	0.86	0/3117	1.89	78/4221 (1.8%)
1	B	0.86	0/3117	1.82	69/4221 (1.6%)
1	C	0.86	0/3113	1.74	63/4216 (1.5%)
1	D	0.85	0/3113	1.80	77/4216 (1.8%)
All	All	0.86	0/12460	1.81	287/16874 (1.7%)

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	C	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	172	ARG	NE-CZ-NH1	25.60	133.10	120.30
1	B	157	ARG	NE-CZ-NH1	22.32	131.46	120.30
1	A	117	ARG	NE-CZ-NH1	21.63	131.12	120.30
1	B	394	ARG	NE-CZ-NH2	-20.19	110.20	120.30
1	C	172	ARG	NE-CZ-NH2	-19.74	110.43	120.30
1	B	117	ARG	NE-CZ-NH1	18.06	129.33	120.30
1	A	117	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	D	117	ARG	NE-CZ-NH1	15.22	127.91	120.30
1	A	177	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	C	361	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	B	321	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	D	113	ARG	NE-CZ-NH1	12.93	126.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	326	ARG	NE-CZ-NH2	12.73	126.67	120.30
1	D	361	ARG	NE-CZ-NH2	12.71	126.65	120.30
1	A	394	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	109	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	B	177	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	D	172	ARG	CD-NE-CZ	12.00	140.39	123.60
1	A	80	ASP	CB-CG-OD1	-11.74	107.73	118.30
1	B	321	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	57	ASP	CB-CG-OD2	11.47	128.62	118.30
1	B	117	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	A	113	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	A	113	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	B	330	GLU	OE1-CD-OE2	11.04	136.55	123.30
1	D	121	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	D	188	ARG	NE-CZ-NH2	10.98	125.79	120.30
1	A	394	ARG	CA-CB-CG	10.90	137.38	113.40
1	D	157	ARG	NE-CZ-NH2	10.87	125.73	120.30
1	D	150	ASP	CB-CG-OD1	10.67	127.91	118.30
1	A	177	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	C	394	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	B	23	ARG	CD-NE-CZ	10.44	138.22	123.60
1	D	330	GLU	OE1-CD-OE2	10.38	135.76	123.30
1	A	313	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	A	121	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	C	55	ASP	CB-CG-OD1	10.25	127.53	118.30
1	A	321	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	55	ASP	CB-CG-OD1	9.96	127.27	118.30
1	C	112	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	A	205	GLU	OE1-CD-OE2	-9.86	111.47	123.30
1	D	109	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	D	255	ASP	CB-CG-OD1	9.81	127.13	118.30
1	B	156	ASP	CB-CG-OD1	9.78	127.10	118.30
1	C	121	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	D	159	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	208	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	B	394	ARG	N-CA-CB	9.41	127.55	110.60
1	C	157	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	B	109	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	D	208	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	B	394	ARG	NH1-CZ-NH2	9.32	129.66	119.40
1	D	313	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	150	ASP	CB-CG-OD1	9.27	126.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	ARG	CD-NE-CZ	9.22	136.51	123.60
1	A	273	ASP	CB-CG-OD1	9.17	126.56	118.30
1	D	31	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	289	ARG	NE-CZ-NH1	-9.09	115.76	120.30
1	A	199	ALA	CB-CA-C	8.92	123.49	110.10
1	C	31	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	C	80	ASP	CB-CG-OD1	-8.91	110.28	118.30
1	B	157	ARG	NH1-CZ-NH2	-8.87	109.65	119.40
1	A	80	ASP	CA-CB-CG	-8.80	94.05	113.40
1	C	158	TYR	CB-CG-CD2	8.70	126.22	121.00
1	A	207	GLU	CG-CD-OE1	8.67	135.64	118.30
1	A	394	ARG	NH1-CZ-NH2	8.59	128.85	119.40
1	B	156	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	D	24	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	B	80	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	D	361	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	C	117	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	A	368	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	361	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	D	217	GLU	OE1-CD-OE2	8.08	132.99	123.30
1	A	157	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	181	GLU	OE1-CD-OE2	-8.05	113.64	123.30
1	B	143	ALA	N-CA-CB	-8.05	98.83	110.10
1	C	297	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	313	ARG	CG-CD-NE	7.99	128.58	111.80
1	C	35	ASP	CB-CG-OD2	7.86	125.37	118.30
1	B	55	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	9	ASP	CB-CG-OD2	7.84	125.36	118.30
1	A	361	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	255	ASP	CB-CG-OD1	7.74	125.26	118.30
1	A	328	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	299	GLU	OE1-CD-OE2	7.70	132.54	123.30
1	A	300	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	23	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	A	289	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	289	ARG	NH1-CZ-NH2	7.57	127.72	119.40
1	A	124	ASP	CB-CG-OD1	7.55	125.10	118.30
1	C	101	ASP	CB-CG-OD2	7.55	125.10	118.30
1	D	172	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	D	140	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	177	ARG	CD-NE-CZ	7.46	134.04	123.60
1	B	297	ARG	NE-CZ-NH2	-7.40	116.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	A	368	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	80	ASP	OD1-CG-OD2	7.27	137.11	123.30
1	B	286	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	204	GLN	OE1-CD-NE2	-7.22	105.30	121.90
1	D	321	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	C	188	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	88	MET	CA-CB-CG	7.12	125.41	113.30
1	D	255	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	117	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	112	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	68	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	31	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	B	112	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	C	328	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	207	GLU	CG-CD-OE2	-6.91	104.48	118.30
1	B	158	TYR	CB-CG-CD2	6.88	125.13	121.00
1	C	150	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	328	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	146	ASP	CB-CG-OD1	6.87	124.49	118.30
1	A	9	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	B	292	ASP	CB-CG-OD2	6.79	124.41	118.30
1	D	68	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	C	55	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	208	ARG	CD-NE-CZ	-6.69	114.23	123.60
1	C	326	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	D	112	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	367	TYR	O-C-N	6.57	133.22	122.70
1	A	326	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	207	GLU	CG-CD-OE2	-6.47	105.36	118.30
1	A	394	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	B	255	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	D	90	THR	CA-CB-CG2	6.40	121.36	112.40
1	D	121	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	45	GLU	OE1-CD-OE2	6.30	130.87	123.30
1	C	276	GLU	OE1-CD-OE2	-6.26	115.78	123.30
1	B	172	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	D	24	ASP	CB-CG-OD1	6.25	123.92	118.30
1	C	205	GLU	CG-CD-OE2	6.24	130.79	118.30
1	B	28	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	24	ASP	CB-CG-OD1	6.18	123.86	118.30
1	D	204	GLN	OE1-CD-NE2	-6.17	107.71	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	302	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	255	ASP	CB-CG-OD1	6.16	123.84	118.30
1	D	388	GLU	CG-CD-OE1	-6.16	105.98	118.30
1	C	245	ASP	CB-CG-OD1	6.14	123.82	118.30
1	B	257	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	55	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	276	GLU	CG-CD-OE2	6.13	130.56	118.30
1	D	273	ASP	CB-CG-OD2	6.13	123.81	118.30
1	C	145	TYR	CB-CG-CD2	6.13	124.68	121.00
1	D	342	GLU	CG-CD-OE2	6.11	130.52	118.30
1	D	80	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	D	108	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	112	ARG	CD-NE-CZ	6.08	132.12	123.60
1	D	356	GLU	CG-CD-OE2	6.08	130.47	118.30
1	A	322	ALA	CB-CA-C	6.08	119.22	110.10
1	D	117	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	D	249	GLN	CA-CB-CG	6.07	126.75	113.40
1	C	45	GLU	CA-CB-CG	6.06	126.73	113.40
1	D	292	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	146	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	C	394	ARG	CD-NE-CZ	-6.04	115.14	123.60
1	D	203	VAL	CA-CB-CG1	6.00	119.89	110.90
1	B	276	GLU	CG-CD-OE2	5.99	130.28	118.30
1	B	367	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	C	333	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	A	159	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	313	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
1	D	360	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	A	158	TYR	CB-CG-CD2	5.96	124.57	121.00
1	C	257	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	69	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	C	205	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	B	394	ARG	CD-NE-CZ	-5.95	115.27	123.60
1	D	80	ASP	CA-CB-CG	-5.93	100.35	113.40
1	A	255	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	361	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
1	A	276	GLU	CG-CD-OE2	5.90	130.10	118.30
1	D	35	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	188	ARG	CD-NE-CZ	5.87	131.82	123.60
1	C	313	ARG	CA-CB-CG	5.87	126.32	113.40
1	C	286	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	255	ASP	CB-CG-OD2	-5.86	113.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	326	ARG	CA-CB-CG	5.84	126.26	113.40
1	D	171	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	90	THR	CA-CB-OG1	-5.84	96.73	109.00
1	B	302	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	23	ARG	CD-NE-CZ	5.80	131.72	123.60
1	D	205	GLU	CG-CD-OE2	5.78	129.87	118.30
1	A	181	GLU	CG-CD-OE1	5.76	129.82	118.30
1	B	45	GLU	CA-CB-CG	5.76	126.07	113.40
1	D	156	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	8	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	D	56	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	54	HIS	N-CA-CB	5.71	120.87	110.60
1	C	113	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	207	GLU	CG-CD-OE1	5.68	129.65	118.30
1	C	204	GLN	OE1-CD-NE2	-5.67	108.86	121.90
1	A	394	ARG	CG-CD-NE	-5.66	99.91	111.80
1	A	298	THR	CA-CB-CG2	5.65	120.31	112.40
1	B	330	GLU	CG-CD-OE2	-5.62	107.06	118.30
1	C	150	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	81	GLU	CG-CD-OE1	-5.58	107.14	118.30
1	C	330	GLU	OE1-CD-OE2	5.58	129.99	123.30
1	B	112	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	326	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	313	ARG	CD-NE-CZ	5.56	131.38	123.60
1	C	207	GLU	CG-CD-OE1	5.55	129.39	118.30
1	B	354	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	128	GLU	CG-CD-OE1	-5.51	107.28	118.30
1	A	276	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	C	31	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	204	GLN	CB-CG-CD	5.47	125.81	111.60
1	D	205	GLU	OE1-CD-OE2	-5.46	116.74	123.30
1	D	140	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	B	77	LYS	O-C-N	5.42	131.38	122.70
1	D	313	ARG	CA-CB-CG	5.42	125.31	113.40
1	D	80	ASP	OD1-CG-OD2	5.40	133.56	123.30
1	C	313	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	188	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	C	203	VAL	N-CA-CB	-5.40	99.63	111.50
1	D	123	MET	CG-SD-CE	5.39	108.83	100.20
1	D	394	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	D	320	GLU	CA-CB-CG	5.36	125.18	113.40
1	B	7	ARG	NE-CZ-NH1	5.35	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	204	GLN	CG-CD-OE1	5.35	132.29	121.60
1	C	331	VAL	CB-CA-C	5.34	121.55	111.40
1	D	276	GLU	CG-CD-OE1	-5.34	107.62	118.30
1	D	181	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	A	155	LEU	CB-CA-C	5.32	120.30	110.20
1	D	233	ALA	N-CA-CB	5.32	117.54	110.10
1	B	57	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	80	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	284	ALA	CB-CA-C	5.29	118.04	110.10
1	B	150	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	178	PHE	O-C-N	5.28	131.14	122.70
1	B	218	THR	CA-CB-CG2	5.26	119.76	112.40
1	C	155	LEU	CB-CA-C	5.26	120.19	110.20
1	B	210	GLU	CA-CB-CG	5.25	124.94	113.40
1	B	141	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	C	356	GLU	OE1-CD-OE2	-5.24	117.02	123.30
1	C	54	HIS	N-CA-CB	5.24	120.02	110.60
1	C	281	GLY	CA-C-O	5.22	129.99	120.60
1	A	121	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	187	PRO	N-CA-C	5.21	125.64	112.10
1	B	152	SER	CB-CA-C	5.20	119.97	110.10
1	B	361	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	300	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	54	HIS	CB-CA-C	-5.17	100.06	110.40
1	D	68	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	D	333	GLU	CG-CD-OE2	5.15	128.60	118.30
1	C	80	ASP	N-CA-CB	-5.15	101.33	110.60
1	C	88	MET	CA-CB-CG	5.15	122.05	113.30
1	D	9	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	42	LYS	CB-CA-C	-5.15	100.11	110.40
1	A	156	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	54	HIS	N-CA-C	-5.14	97.11	111.00
1	A	394	ARG	CD-NE-CZ	-5.14	116.41	123.60
1	D	31	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	112	ARG	CG-CD-NE	5.13	122.58	111.80
1	A	28	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	B	204	GLN	CB-CG-CD	5.12	124.92	111.60
1	C	143	ALA	CB-CA-C	-5.10	102.45	110.10
1	A	342	GLU	CG-CD-OE2	5.10	128.50	118.30
1	D	143	ALA	O-C-N	5.09	130.85	122.70
1	A	321	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	204	GLN	CG-CD-OE1	5.08	131.77	121.60
1	B	306	GLU	CG-CD-OE1	-5.08	108.14	118.30
1	B	112	ARG	CG-CD-NE	5.07	122.45	111.80
1	B	368	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	152	SER	N-CA-CB	-5.06	102.91	110.50
1	D	313	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	393	ALA	N-CA-CB	5.05	117.17	110.10
1	D	342	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	C	187	PRO	N-CA-C	5.05	125.22	112.10
1	B	289	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	C	146	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	208	ARG	CG-CD-NE	-5.04	101.21	111.80
1	D	257	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	361	ARG	CA-CB-CG	-5.03	102.33	113.40
1	B	342	GLU	CG-CD-OE2	5.03	128.35	118.30
1	B	339	LYS	O-C-N	5.02	130.74	122.70
1	A	205	GLU	CG-CD-OE2	5.02	128.34	118.30
1	C	208	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	24	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	277	ASN	CB-CG-OD1	-5.01	111.57	121.60
1	B	388	GLU	CG-CD-OE2	5.01	128.32	118.30
1	B	54	HIS	N-CA-CB	5.00	119.61	110.60
1	C	281	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	172	ARG	Sidechain
1	C	313	ARG	Sidechain
1	D	313	ARG	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	3045	0	2949	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3045	0	2949	33	0
1	C	3041	0	2943	34	0
1	D	3041	0	2943	32	0
2	A	222	0	0	3	0
2	B	218	0	0	1	0
2	C	235	0	0	1	0
2	D	220	0	0	3	0
All	All	13067	0	11784	118	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 5.

All (118) 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:204:GLN:OE1	1:C:204:GLN:OE1	1.72	1.08
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.72	1.04
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.13	0.93
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.18	0.88
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.20	0.86
1:A:36:PRO:O	1:A:40:VAL:HG23	1.77	0.83
1:B:77:LYS:O	1:B:80:ASP:HB2	1.81	0.81
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.28	0.79
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.09	0.67
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.79	0.64
1:A:6:THR:O	1:A:9:ASP:HB2	1.97	0.64
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.79	0.64
1:D:72:ILE:O	1:D:76:LYS:HG3	1.97	0.63
1:D:34:LEU:HD21	1:D:39:ALA:HB2	1.80	0.63
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.82	0.63
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.06	0.61
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.84	0.61
1:A:204:GLN:HG2	2:A:545:HOH:O	2.00	0.60
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.01	0.60
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.84	0.60
1:D:394:ARG:HD2	2:D:606:HOH:O	2.05	0.56
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.89	0.55
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.89	0.54
1:A:204:GLN:HB3	2:A:544:HOH:O	2.06	0.54
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.37	0.54
1:C:24:ASP:O	1:D:23:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ARG:HG2	1:B:49:TYR:HB2	1.91	0.53
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.24	0.53
1:B:152:SER:HB2	2:D:567:HOH:O	2.08	0.52
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.91	0.52
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.91	0.52
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.45	0.51
1:C:183:LYS:HE2	1:C:185:ASN:O	2.11	0.51
1:A:77:LYS:O	1:A:80:ASP:CB	2.59	0.51
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.92	0.51
1:C:59:VAL:HG21	1:C:68:ARG:HG3	1.92	0.50
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.94	0.50
1:C:278:GLY:HA3	1:C:282:ALA:O	2.12	0.49
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.47	0.49
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.95	0.49
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.95	0.49
1:D:137:TRP:HB3	2:D:474:HOH:O	2.13	0.49
1:C:255:ASP:OD2	2:C:619:HOH:O	2.20	0.49
1:A:238:HIS:O	1:A:239:LYS:HB2	2.13	0.47
1:A:279:PRO:HG2	2:A:506:HOH:O	2.14	0.47
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.49	0.47
1:B:278:GLY:HA3	1:B:282:ALA:O	2.13	0.47
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.97	0.47
1:B:5:ALA:HB2	1:B:312:ILE:HG21	1.97	0.47
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.96	0.47
1:A:77:LYS:O	1:A:80:ASP:HB2	2.15	0.46
1:C:65:ALA:O	1:C:69:ASP:HB2	2.14	0.46
1:B:278:GLY:CA	1:B:282:ALA:O	2.63	0.46
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.96	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.98	0.46
1:A:305:TRP:O	1:A:309:LYS:HG3	2.15	0.46
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.98	0.46
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.16	0.46
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.82	0.45
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.98	0.45
1:C:394:ARG:HD3	1:C:394:ARG:HH11	1.45	0.45
1:A:117:ARG:HG3	1:C:364:PHE:HB2	1.97	0.45
1:B:92:ASN:C	1:B:92:ASN:OD1	2.54	0.44
1:A:186:GLU:HA	1:A:187:PRO:HA	1.68	0.44
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.52	0.44
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.74	0.44
1:C:72:ILE:O	1:C:76:LYS:HG3	2.18	0.44
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.51	0.44
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.53	0.44
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.63	0.44
1:D:238:HIS:O	1:D:239:LYS:HB2	2.17	0.43
1:B:98:VAL:HA	1:D:373:GLY:HA2	1.99	0.43
1:A:178:PHE:HB2	1:A:212:PHE:CD1	2.54	0.43
1:B:216:PRO:HG2	1:B:232:ILE:CD1	2.49	0.43
1:D:361:ARG:HH11	1:D:361:ARG:HD3	1.68	0.43
1:D:8:GLU:HG2	1:D:8:GLU:O	2.17	0.43
1:D:356:GLU:O	1:D:359:ALA:HB3	2.19	0.43
1:C:76:LYS:O	1:C:80:ASP:HB2	2.19	0.43
1:C:86:VAL:O	1:C:131:ALA:HA	2.19	0.43
1:B:294:LYS:HE2	2:B:583:HOH:O	2.19	0.43
1:B:241:LEU:HA	1:B:241:LEU:HD12	1.93	0.43
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.83	0.42
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.01	0.42
1:C:15:LEU:HD13	1:C:51:ILE:HD11	2.01	0.42
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.54	0.42
1:A:122:GLN:HG3	1:A:122:GLN:O	2.19	0.42
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.55	0.42
1:C:297:ARG:HH11	1:C:297:ARG:HD3	1.67	0.42
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.19	0.42
1:B:36:PRO:O	1:B:40:VAL:HG23	2.19	0.42
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.80	0.42
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.91	0.42
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.87	0.42
1:D:50:GLY:HA2	1:D:85:ILE:O	2.20	0.42
1:C:234:GLN:HE21	1:C:238:HIS:CE1	2.12	0.42
1:B:219:GLY:O	1:B:223:MET:HG3	2.20	0.42
1:D:338:SER:O	1:D:339:LYS:HB2	2.20	0.41
1:D:185:ASN:HD22	1:D:186:GLU:HB2	1.84	0.41
1:C:106:SER:O	1:C:112:ARG:HD3	2.20	0.41
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.33	0.41
1:A:100:LYS:HD2	1:B:298:THR:HA	2.03	0.41
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.56	0.41
1:C:278:GLY:CA	1:C:282:ALA:O	2.68	0.41
1:C:193:LEU:N	1:C:194:PRO:HD3	2.36	0.41
1:C:238:HIS:O	1:C:239:LYS:HB2	2.21	0.41
1:D:9:ASP:HB3	1:D:11:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.90	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
1:C:219:GLY:O	1:C:223:MET:HG3	2.21	0.41
1:A:300:ASP:OD1	1:A:302:ASP:HB2	2.20	0.41
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.03	0.40
1:D:183:LYS:HG2	1:D:184:PRO:HD2	2.03	0.40
1:A:158:TYR:O	1:A:162:LEU:HG	2.21	0.40
1:B:101:ASP:CG	1:B:101:ASP:O	2.59	0.40
1:B:203:VAL:HG22	1:B:212:PHE:HB3	2.03	0.40
1:B:59:VAL:HA	1:B:60:PRO:HD3	1.96	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	388/393 (99%)	376 (97%)	11 (3%)	1 (0%)	46	63
1	B	388/393 (99%)	375 (97%)	11 (3%)	2 (0%)	34	48
1	C	388/393 (99%)	372 (96%)	12 (3%)	4 (1%)	19	28
1	D	388/393 (99%)	373 (96%)	13 (3%)	2 (0%)	34	48
All	All	1552/1572 (99%)	1496 (96%)	47 (3%)	9 (1%)	30	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO

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Mol	Chain	Res	Type
1	C	364	PHE
1	D	186	GLU
1	D	280	ASP
1	B	281	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	306/310 (99%)	294 (96%)	12 (4%)	39	59
1	B	306/310 (99%)	298 (97%)	8 (3%)	54	74
1	C	305/310 (98%)	300 (98%)	5 (2%)	70	86
1	D	305/310 (98%)	296 (97%)	9 (3%)	48	70
All	All	1222/1240 (98%)	1188 (97%)	34 (3%)	51	72

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	46	ILE
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	158	TYR
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	A	286	ASP
1	A	313	ARG
1	A	394	ARG
1	B	49	TYR
1	B	81	GLU
1	B	158	TYR
1	B	172	ARG
1	B	185	ASN

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Mol	Chain	Res	Type
1	B	203	VAL
1	B	313	ARG
1	B	394	ARG
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	185	ASN
1	C	313	ARG
1	D	49	TYR
1	D	80	ASP
1	D	158	TYR
1	D	185	ASN
1	D	203	VAL
1	D	252	PRO
1	D	313	ARG
1	D	323	LYS
1	D	362	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	204	GLN
1	A	238	HIS
1	B	66	GLN
1	B	185	ASN
1	B	204	GLN
1	B	222	GLN
1	B	238	HIS
1	C	185	ASN
1	C	222	GLN
1	C	238	HIS
1	D	185	ASN
1	D	238	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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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