Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 02:23 PM GMT

PDB ID	:	3XIN
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	:	1992-04-06
Resolution	:	2.30 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:

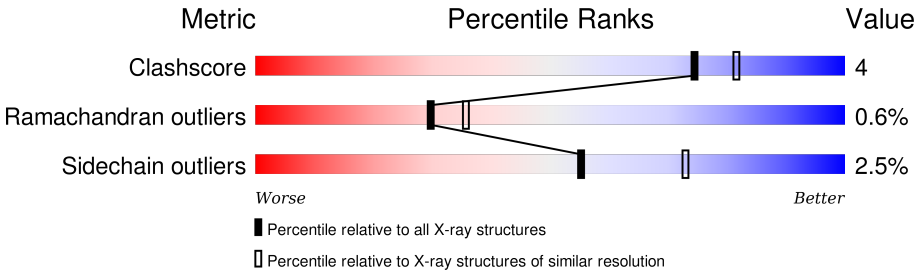
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	80% 18%
1	B	393	81% 16%
1	C	393	83% 15%
1	D	393	80% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13116 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	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			
1	B	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			
1	C	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			
1	D	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLN	GLU	CONFLICT	UNP P12851
B	181	GLN	GLU	CONFLICT	UNP P12851
C	181	GLN	GLU	CONFLICT	UNP P12851
D	181	GLN	GLU	CONFLICT	UNP P12851

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	229	Total	O	0	0
			229	229		
2	B	221	Total	O	0	0
			221	221		
2	C	238	Total	O	0	0
			238	238		
2	D	216	Total	O	0	0
			216	216		

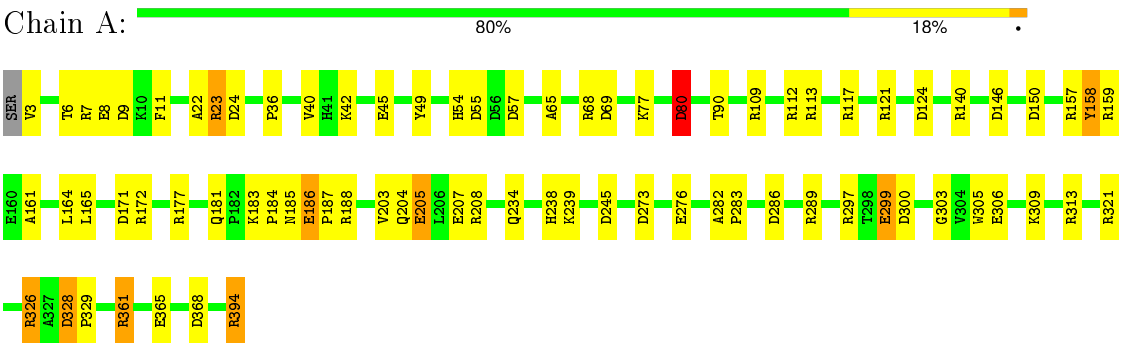
3 Residue-property plots (i)

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.

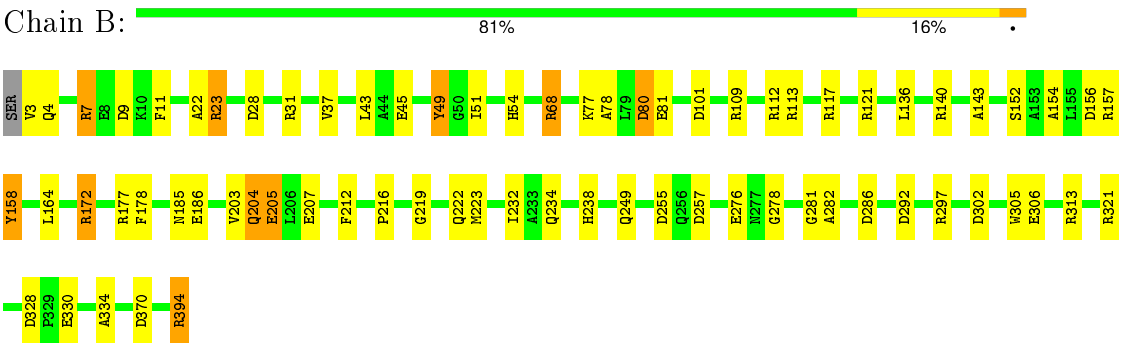
- Molecule 1: D-XYLOSE ISOMERASE

Chain A:



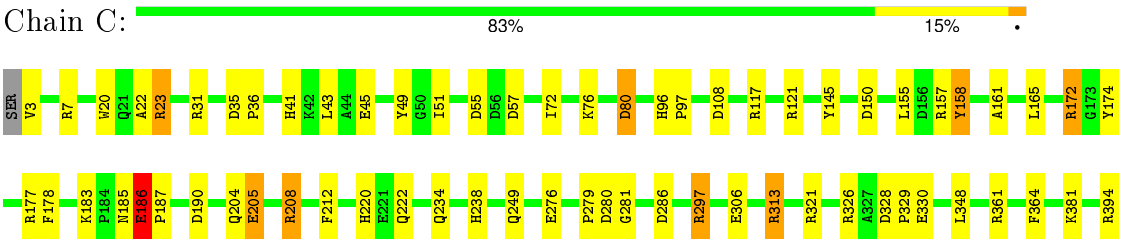
- Molecule 1: D-XYLOSE ISOMERASE

Chain B:



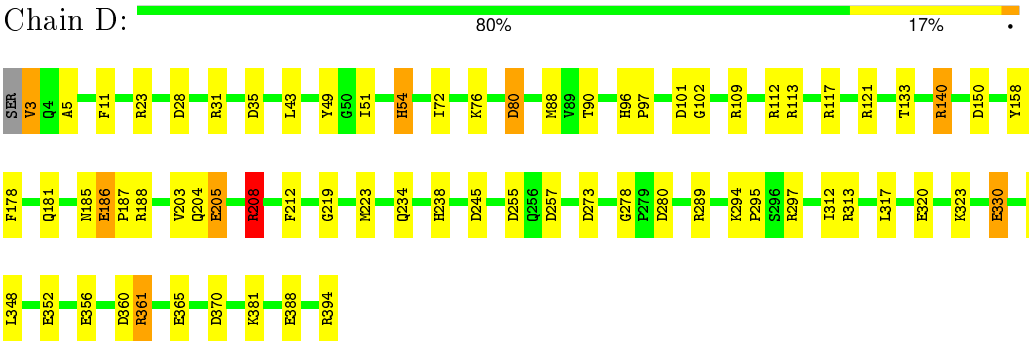
- Molecule 1: D-XYLOSE ISOMERASE

Chain C:



- Molecule 1: D-XYLOSE ISOMERASE

Chain D:


80%
17%
SER V3 Q4 A5 F11 R23 D28 R31 D35 L43 Y49 G50 I51 H54 I72 K76 D80 M88 V89 T90 H96 P97 D101 G102 R109 R112 R113 R117 R121 T133 R140 D150 Y158 R159 R172 R177
F178 Q181 N185 E186 P187 R188 V203 Q204 E205 R208 F212 G219 M223 Q234 H238 D245 D255 Q256 D257 D273 G278 P279 D280 R289 K294 P295 S296 R297 I312 R313 L317 E320 K323 E330 E333 E342 L343
I348 E352 E356 D360 R361 E365 D370 K381 E388 R394

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) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.153 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13116	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	0.80	0/3125	1.66	54/4233 (1.3%)
1	B	0.79	0/3125	1.68	54/4233 (1.3%)
1	C	0.80	0/3125	1.59	48/4233 (1.1%)
1	D	0.80	0/3125	1.62	46/4233 (1.1%)
All	All	0.80	0/12500	1.64	202/16932 (1.2%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	394	ARG	NE-CZ-NH2	-20.38	110.11	120.30
1	B	172	ARG	NE-CZ-NH1	19.30	129.95	120.30
1	B	117	ARG	NE-CZ-NH1	16.39	128.50	120.30
1	A	172	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	C	172	ARG	NE-CZ-NH1	15.30	127.95	120.30
1	C	172	ARG	NE-CZ-NH2	-15.23	112.69	120.30
1	C	117	ARG	NE-CZ-NH1	14.66	127.63	120.30
1	B	157	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	B	172	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	D	117	ARG	NE-CZ-NH1	12.77	126.69	120.30
1	D	313	ARG	NE-CZ-NH2	12.68	126.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	255	ASP	CB-CG-OD1	12.41	129.47	118.30
1	D	31	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	A	394	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	D	150	ASP	CB-CG-OD1	11.71	128.83	118.30
1	B	330	GLU	OE1-CD-OE2	11.69	137.33	123.30
1	B	177	ARG	NE-CZ-NH2	-11.57	114.51	120.30
1	C	23	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	A	361	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	D	121	ARG	NE-CZ-NH2	-11.01	114.79	120.30
1	A	117	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	117	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	A	80	ASP	CB-CG-OD1	-10.56	108.80	118.30
1	A	321	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	C	177	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	D	117	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	326	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	121	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	D	172	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	A	146	ASP	CB-CG-OD1	9.68	127.01	118.30
1	A	150	ASP	CB-CG-OD1	9.65	126.99	118.30
1	A	394	ARG	NH1-CZ-NH2	9.50	129.85	119.40
1	B	328	ASP	CB-CG-OD2	9.38	126.74	118.30
1	B	177	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	23	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	C	313	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	109	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	B	321	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	B	313	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	B	117	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	A	159	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	68	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	A	394	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	C	321	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	D	112	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	C	31	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	D	172	ARG	CD-NE-CZ	8.56	135.59	123.60
1	D	113	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	B	80	ASP	CB-CG-OD1	-8.52	110.63	118.30
1	A	124	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	172	ARG	CD-NE-CZ	8.43	135.41	123.60
1	A	188	ARG	CD-NE-CZ	8.40	135.36	123.60
1	A	299	GLU	OE1-CD-OE2	8.40	133.38	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	158	TYR	CB-CG-CD2	8.35	126.01	121.00
1	A	172	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	D	394	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	A	328	ASP	CB-CG-OD2	8.27	125.74	118.30
1	A	205	GLU	OE1-CD-OE2	-8.20	113.46	123.30
1	A	109	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	31	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	B	113	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	D	188	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	B	156	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	B	321	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	342	GLU	CG-CD-OE2	7.49	133.28	118.30
1	A	157	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	368	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	35	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	57	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	A	158	TYR	CB-CG-CD2	7.29	125.37	121.00
1	B	394	ARG	N-CA-CB	7.28	123.70	110.60
1	A	80	ASP	CA-CB-CG	-7.24	97.47	113.40
1	C	330	GLU	OE1-CD-OE2	7.23	131.97	123.30
1	C	321	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	55	ASP	CB-CG-OD1	7.20	124.78	118.30
1	B	140	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	D	330	GLU	OE1-CD-OE2	7.04	131.75	123.30
1	A	313	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	113	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	C	361	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	C	117	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	D	28	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	C	177	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	D	109	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	368	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	C	45	GLU	CA-CB-CG	6.64	128.01	113.40
1	C	208	ARG	CD-NE-CZ	-6.59	114.37	123.60
1	D	257	ASP	CB-CG-OD1	6.58	124.23	118.30
1	D	140	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	B	23	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	360	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	B	370	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	68	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	A	361	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	55	ASP	CB-CG-OD1	6.47	124.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	ARG	CA-CB-CG	6.44	127.56	113.40
1	C	286	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	113	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	300	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	205	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	D	31	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	188	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	157	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	C	190	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	276	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	B	286	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	326	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	C	306	GLU	CG-CD-OE1	6.29	130.89	118.30
1	A	273	ASP	CB-CG-OD1	6.28	123.96	118.30
1	B	394	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	276	GLU	CG-CD-OE2	6.26	130.82	118.30
1	D	342	GLU	OE1-CD-OE2	-6.26	115.78	123.30
1	B	109	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	292	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	394	ARG	NH1-CZ-NH2	6.22	126.24	119.40
1	C	80	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	C	108	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	320	GLU	CA-CB-CG	6.18	127.00	113.40
1	A	171	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	207	GLU	CA-CB-CG	6.17	126.98	113.40
1	D	150	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	255	ASP	CB-CG-OD1	6.15	123.84	118.30
1	D	361	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	302	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	B	158	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	7	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	300	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	121	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	150	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	361	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	302	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	23	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	172	ARG	CD-NE-CZ	-5.91	115.33	123.60
1	B	28	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	80	ASP	OD1-CG-OD2	5.88	134.48	123.30
1	A	205	GLU	CG-CD-OE2	5.88	130.05	118.30
1	B	255	ASP	CB-CG-OD2	-5.84	113.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	23	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	205	GLU	CG-CD-OE2	5.81	129.92	118.30
1	B	276	GLU	CG-CD-OE2	5.80	129.90	118.30
1	C	297	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	C	23	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	101	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	24	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	297	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	276	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	D	177	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	177	ARG	N-CA-CB	5.65	120.77	110.60
1	D	370	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	112	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	D	255	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	57	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	174	TYR	CB-CG-CD1	5.62	124.37	121.00
1	B	394	ARG	CD-NE-CZ	-5.61	115.75	123.60
1	D	205	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	C	394	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	D	159	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	257	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	145	TYR	CB-CG-CD2	5.51	124.31	121.00
1	C	394	ARG	CD-NE-CZ	-5.50	115.91	123.60
1	D	273	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	174	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	C	121	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	186	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	B	157	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
1	A	8	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	B	334	ALA	CB-CA-C	5.42	118.23	110.10
1	B	207	GLU	CG-CD-OE2	-5.39	107.51	118.30
1	D	205	GLU	CG-CD-OE2	5.39	129.08	118.30
1	A	289	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	313	ARG	N-CA-CB	5.38	120.29	110.60
1	A	140	ARG	CD-NE-CZ	5.36	131.10	123.60
1	C	7	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	121	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	321	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	330	GLU	CG-CD-OE2	-5.30	107.71	118.30
1	D	333	GLU	CG-CD-OE1	5.29	128.88	118.30
1	A	68	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	45	GLU	CA-CB-CG	5.26	124.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	113	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	155	LEU	CB-CA-C	5.25	120.18	110.20
1	C	297	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	D	80	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	B	204	GLN	OE1-CD-NE2	-5.23	109.88	121.90
1	A	112	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	305	TRP	CA-CB-CG	-5.20	103.81	113.70
1	B	394	ARG	CB-CA-C	-5.18	100.05	110.40
1	C	208	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	143	ALA	N-CA-CB	-5.16	102.88	110.10
1	B	7	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	156	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	281	GLY	N-CA-C	-5.15	100.23	113.10
1	D	54	HIS	N-CA-CB	5.13	119.83	110.60
1	B	205	GLU	CG-CD-OE2	5.12	128.53	118.30
1	B	54	HIS	N-CA-CB	5.10	119.77	110.60
1	C	158	TYR	CB-CG-CD2	5.08	124.05	121.00
1	C	150	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	289	ARG	N-CA-C	-5.05	97.38	111.00
1	D	54	HIS	N-CA-C	-5.03	97.42	111.00
1	D	388	GLU	CG-CD-OE1	-5.03	108.25	118.30
1	C	208	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	121	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	ARG	Sidechain
1	C	172	ARG	Sidechain
1	D	208	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	3053	0	2956	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3053	0	2956	28	0
1	C	3053	0	2956	23	0
1	D	3053	0	2956	30	0
2	A	229	0	0	1	0
2	B	221	0	0	0	0
2	C	238	0	0	1	0
2	D	216	0	0	4	0
All	All	13116	0	11824	96	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 4.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.59	1.18
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.61	1.15
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.15	1.11
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.17	0.92
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.86
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.22	0.82
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.82
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.68	0.75
1:D:208:ARG:NH1	1:D:208:ARG:HG2	1.92	0.71
1:B:3:VAL:HG12	1:B:4:GLN:H	1.57	0.69
1:D:3:VAL:HG23	2:D:591:HOH:O	1.96	0.65
1:A:204:GLN:HG2	2:A:546:HOH:O	1.99	0.63
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.80	0.62
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.83	0.61
1:A:36:PRO:O	1:A:40:VAL:HG23	2.02	0.59
1:B:77:LYS:O	1:B:80:ASP:HB2	2.01	0.59
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.86	0.58
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.85	0.58
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.87	0.57
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.09	0.57
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.85	0.56
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.89	0.56
1:A:238:HIS:O	1:A:239:LYS:HB2	2.06	0.54
1:B:7:ARG:HG2	1:B:49:TYR:HB2	1.88	0.54
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.42	0.54
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.44	0.53
1:C:72:ILE:O	1:C:76:LYS:HG3	2.10	0.52
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.74	0.52
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.92	0.52
1:B:216:PRO:HG2	1:B:232:ILE:HD11	1.93	0.50
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.50
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.93	0.50
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.93	0.49
1:C:41:HIS:HE1	2:C:517:HOH:O	1.95	0.49
1:B:152:SER:HB2	2:D:563:HOH:O	2.11	0.49
1:A:305:TRP:O	1:A:309:LYS:HG3	2.13	0.48
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.43	0.48
1:A:65:ALA:O	1:A:69:ASP:HB2	2.14	0.48
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.49	0.48
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.96	0.47
1:C:161:ALA:O	1:C:165:LEU:HG	2.15	0.46
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.50	0.46
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.51	0.46
1:A:186:GLU:HA	1:A:187:PRO:HA	1.79	0.46
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.97	0.46
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.31	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.97	0.46
1:B:216:PRO:HG2	1:B:232:ILE:CD1	2.46	0.45
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.79	0.45
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.98	0.45
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.52	0.44
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.00	0.44
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.99	0.44
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.53	0.44
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.17	0.44
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.54	0.43
1:B:203:VAL:HG22	1:B:212:PHE:HB3	2.00	0.43
1:B:278:GLY:CA	1:B:282:ALA:O	2.66	0.43
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.95	0.43
1:D:72:ILE:O	1:D:76:LYS:HG3	2.19	0.43
1:B:37:VAL:HG13	1:B:78:ALA:HB2	2.01	0.43
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.89	0.43
1:C:208:ARG:HD3	1:C:208:ARG:HH11	1.47	0.43
1:B:278:GLY:HA3	1:B:282:ALA:O	2.18	0.42
1:B:219:GLY:O	1:B:223:MET:HG3	2.19	0.42
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.85	0.42
1:D:330:GLU:OE1	2:D:604:HOH:O	2.21	0.42
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.86	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.88	0.42
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.55	0.42
1:A:6:THR:O	1:A:9:ASP:HB2	2.20	0.42
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.80	0.42
1:A:183:LYS:HG2	1:A:184:PRO:HD2	2.02	0.42
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.54	0.42
1:A:326:ARG:HD3	1:A:326:ARG:HA	1.92	0.41
1:D:219:GLY:O	1:D:223:MET:HG3	2.21	0.41
1:A:164:LEU:HD23	1:A:164:LEU:C	2.41	0.41
1:C:234:GLN:HE21	1:C:238:HIS:CE1	2.12	0.41
1:A:42:LYS:O	1:A:45:GLU:HB3	2.20	0.41
1:D:178:PHE:HB2	1:D:212:PHE:CD1	2.56	0.41
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.85	0.41
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.16	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:D:88:MET:HA	1:D:133:THR:O	2.21	0.41
1:A:299:GLU:HB3	1:A:303:GLY:HA3	2.01	0.41
1:D:181:GLN:NE2	1:D:245:ASP:OD2	2.53	0.41
1:A:77:LYS:O	1:A:80:ASP:CB	2.69	0.41
1:A:161:ALA:O	1:A:165:LEU:HG	2.21	0.40
1:A:181:GLN:NE2	1:A:245:ASP:OD2	2.54	0.40
1:D:317:LEU:HA	1:D:317:LEU:HD23	1.87	0.40
1:D:278:GLY:HA2	2:D:505:HOH:O	2.21	0.40
1:D:186:GLU:HA	1:D:187:PRO:HA	1.79	0.40
1:B:101:ASP:CG	1:B:101:ASP:O	2.59	0.40
1:C:186:GLU:HA	1:C:187:PRO:HA	1.92	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	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	46	57
1	B	390/393 (99%)	375 (96%)	13 (3%)	2 (0%)	34	41
1	C	390/393 (99%)	376 (96%)	10 (3%)	4 (1%)	19	21
1	D	390/393 (99%)	375 (96%)	13 (3%)	2 (0%)	34	41
All	All	1560/1572 (99%)	1502 (96%)	49 (3%)	9 (1%)	30	36

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
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%)	296 (97%)	10 (3%)	45	61
1	B	306/310 (99%)	300 (98%)	6 (2%)	63	79
1	C	306/310 (99%)	300 (98%)	6 (2%)	63	79
1	D	306/310 (99%)	298 (97%)	8 (3%)	54	71
All	All	1224/1240 (99%)	1194 (98%)	30 (2%)	55	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	49	TYR

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Mol	Chain	Res	Type
1	A	80	ASP
1	A	158	TYR
1	A	177	ARG
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	A	286	ASP
1	A	394	ARG
1	B	49	TYR
1	B	81	GLU
1	B	136	LEU
1	B	158	TYR
1	B	185	ASN
1	B	394	ARG
1	C	3	VAL
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	185	ASN
1	C	313	ARG
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	158	TYR
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	323	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	204	GLN
1	A	238	HIS
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

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Mol	Chain	Res	Type
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.