Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:59 PM GMT

PDB ID	:	1DIE
Title	:	OBSERVATIONS OF REACTION INTERMEDIATES AND THE MECHANISM OF ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE
Authors	:	Collyer, C.A.; Viehmann, H.; Goldberg, J.D.; Blow, D.M.
Deposited on	:	1992-06-04
Resolution	:	2.50 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:

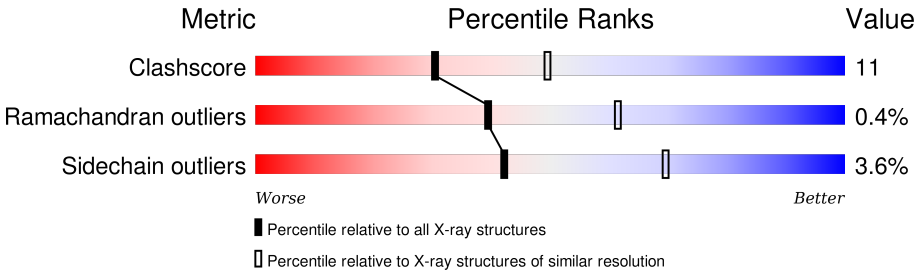
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	394	63% 31% 5% •
1	B	394	63% 31% 5% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6659 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.

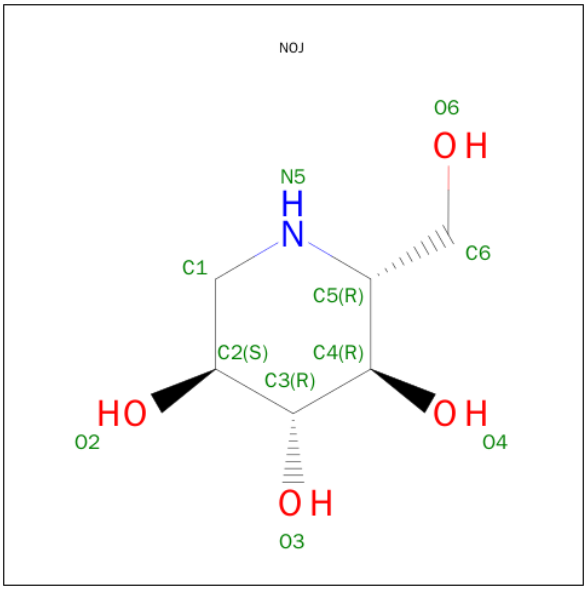
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3026	1919	521	577	9			
1	B	393	Total	C	N	O	S	0	0	0
			3026	1919	521	577	9			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-DEOXYNOJIRIMYCIN (three-letter code: NOJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	291	Total	O	0	0
			291	291		
4	B	290	Total	O	0	0
			290	290		

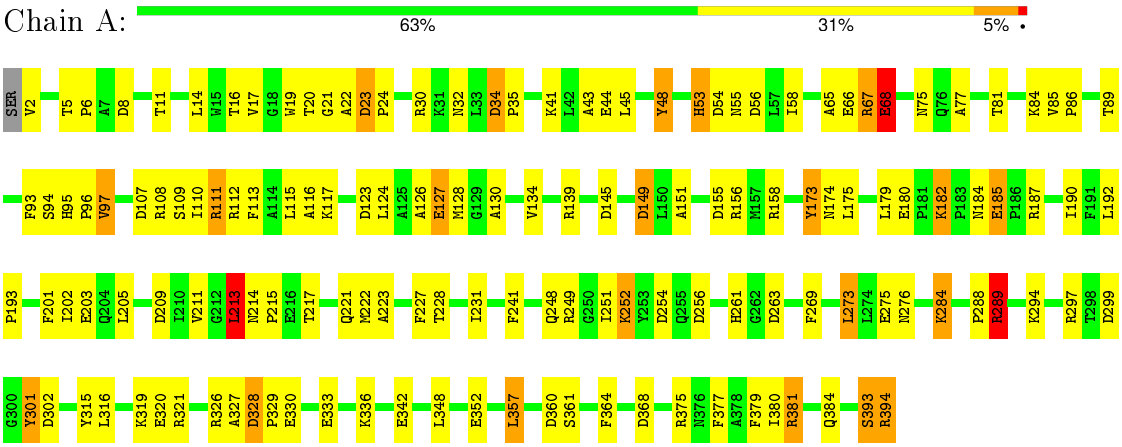
3 Residue-property plots (i)

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.

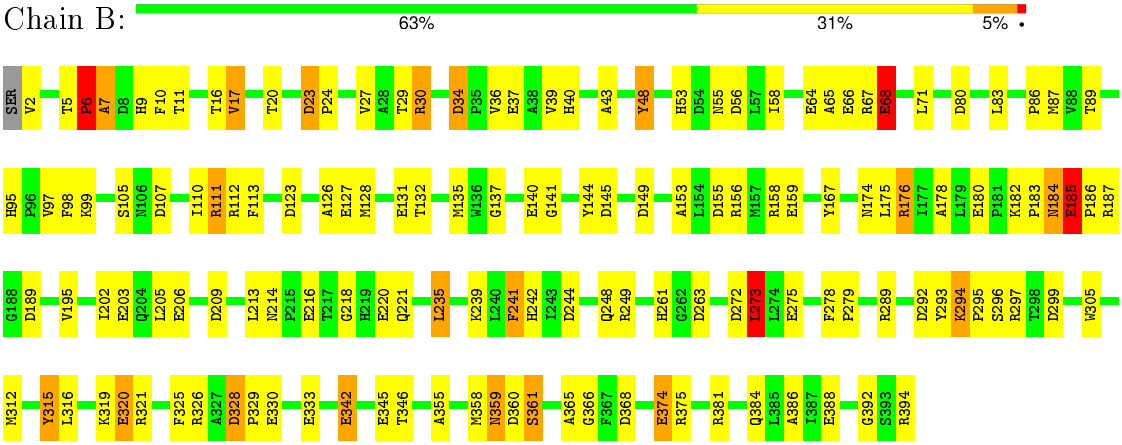
- Molecule 1: D-XYLOSE ISOMERASE

Chain A:



- Molecule 1: D-XYLOSE ISOMERASE

Chain B:



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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.60Å 105.60Å 153.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6659	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NOJ

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	1.15	0/3100	2.11	116/4201 (2.8%)
1	B	1.15	1/3100 (0.0%)	2.08	95/4201 (2.3%)
All	All	1.15	1/6200 (0.0%)	2.10	211/8402 (2.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	GLU	CD-OE1	-5.64	1.19	1.25

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	ARG	NE-CZ-NH2	-19.63	110.49	120.30
1	B	381	ARG	NE-CZ-NH2	-19.31	110.65	120.30
1	B	375	ARG	NE-CZ-NH2	-18.86	110.87	120.30
1	B	321	ARG	NE-CZ-NH2	-16.19	112.21	120.30
1	A	111	ARG	NE-CZ-NH1	15.84	128.22	120.30
1	A	289	ARG	NE-CZ-NH1	15.49	128.04	120.30
1	B	34	ASP	CB-CG-OD1	15.33	132.09	118.30
1	A	256	ASP	CB-CG-OD1	15.25	132.02	118.30
1	B	360	ASP	CB-CG-OD2	15.15	131.93	118.30
1	B	249	ARG	NE-CZ-NH1	14.79	127.69	120.30
1	A	381	ARG	NE-CZ-NH1	14.19	127.40	120.30
1	B	144	TYR	CB-CG-CD1	-13.84	112.70	121.00
1	B	289	ARG	CD-NE-CZ	12.99	141.79	123.60
1	A	149	ASP	CB-CG-OD1	12.91	129.92	118.30
1	A	381	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	B	244	ASP	CB-CG-OD1	12.44	129.49	118.30
1	B	381	ARG	NE-CZ-NH1	12.29	126.45	120.30
1	A	375	ARG	NE-CZ-NH1	12.05	126.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	ARG	NE-CZ-NH1	12.02	126.31	120.30
1	A	67	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	B	111	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	108	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	B	30	ARG	NE-CZ-NH2	-11.39	114.60	120.30
1	B	328	ASP	CB-CG-OD1	11.07	128.26	118.30
1	A	209	ASP	CB-CG-OD1	11.06	128.25	118.30
1	B	144	TYR	CB-CG-CD2	10.82	127.49	121.00
1	B	394	ARG	CD-NE-CZ	10.69	138.56	123.60
1	B	127	GLU	CA-CB-CG	10.52	136.55	113.40
1	A	326	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	297	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	113	PHE	CB-CG-CD2	-10.04	113.77	120.80
1	A	139	ARG	NE-CZ-NH2	10.05	125.32	120.30
1	A	67	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	B	30	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	B	249	ARG	CD-NE-CZ	9.87	137.41	123.60
1	A	302	ASP	CB-CG-OD2	9.86	127.18	118.30
1	B	112	ARG	NE-CZ-NH2	9.81	125.21	120.30
1	A	269	PHE	CB-CG-CD1	-9.76	113.97	120.80
1	B	187	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	A	256	ASP	CB-CG-OD2	-9.42	109.83	118.30
1	B	299	ASP	CB-CG-OD1	9.31	126.68	118.30
1	B	34	ASP	CB-CG-OD2	-9.29	109.94	118.30
1	B	68	GLU	CA-CB-CG	8.88	132.93	113.40
1	A	54	ASP	CB-CG-OD1	8.76	126.19	118.30
1	B	273	LEU	CA-CB-CG	8.65	135.20	115.30
1	B	244	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	A	156	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	B	123	ASP	CB-CG-OD2	8.13	125.62	118.30
1	B	359	ASN	CA-CB-CG	8.08	131.17	113.40
1	A	127	GLU	CA-CB-CG	8.00	130.99	113.40
1	B	149	ASP	CB-CG-OD1	7.99	125.49	118.30
1	B	176	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	158	ARG	CD-NE-CZ	7.94	134.72	123.60
1	A	289	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	375	ARG	NH1-CZ-NH2	7.93	128.13	119.40
1	A	375	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	175	LEU	O-C-N	7.81	135.20	122.70
1	A	23	ASP	CB-CG-OD1	7.77	125.30	118.30
1	B	187	ARG	CD-NE-CZ	7.74	134.44	123.60
1	B	241	PHE	CB-CG-CD2	-7.73	115.39	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	213	LEU	CA-CB-CG	7.72	133.06	115.30
1	A	368	ASP	CB-CG-OD2	7.64	125.18	118.30
1	B	30	ARG	CD-NE-CZ	7.56	134.19	123.60
1	A	182	LYS	CD-CE-NZ	7.53	129.02	111.70
1	A	43	ALA	CB-CA-C	7.48	121.32	110.10
1	B	315	TYR	CB-CG-CD1	7.42	125.45	121.00
1	A	394	ARG	CD-NE-CZ	7.40	133.96	123.60
1	A	66	GLU	CG-CD-OE2	7.33	132.95	118.30
1	A	65	ALA	CB-CA-C	7.32	121.07	110.10
1	A	158	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	187	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	113	PHE	CB-CG-CD1	7.20	125.84	120.80
1	B	156	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	7	ALA	N-CA-CB	6.99	119.88	110.10
1	B	23	ASP	CB-CA-C	6.93	124.27	110.40
1	A	249	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	B	358	MET	CG-SD-CE	6.84	111.15	100.20
1	B	155	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	B	155	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	269	PHE	CB-CG-CD2	6.83	125.58	120.80
1	A	203	GLU	CG-CD-OE2	6.77	131.84	118.30
1	A	115	LEU	CB-CA-C	6.75	123.02	110.20
1	A	34	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	326	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	213	LEU	CA-CB-CG	6.57	130.41	115.30
1	B	68	GLU	CB-CG-CD	6.56	131.91	114.20
1	A	330	GLU	OE1-CD-OE2	6.55	131.16	123.30
1	A	320	GLU	CA-CB-CG	6.54	127.80	113.40
1	A	139	ARG	NH1-CZ-NH2	-6.52	112.23	119.40
1	B	107	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	299	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	276	ASN	CA-C-O	-6.45	106.55	120.10
1	B	272	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	203	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	B	135	MET	CG-SD-CE	6.42	110.48	100.20
1	A	321	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	128	MET	CG-SD-CE	6.36	110.37	100.20
1	A	44	GLU	CA-CB-CG	6.35	127.37	113.40
1	B	37	GLU	CB-CG-CD	6.31	131.23	114.20
1	A	328	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	48	TYR	CB-CG-CD2	6.26	124.75	121.00
1	A	241	PHE	CB-CG-CD1	6.24	125.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	333	GLU	CA-CB-CG	6.21	127.06	113.40
1	A	21	GLY	N-CA-C	6.17	128.54	113.10
1	A	209	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	B	209	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	394	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	98	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	B	345	GLU	CA-CB-CG	6.12	126.87	113.40
1	A	330	GLU	CG-CD-OE2	-6.10	106.09	118.30
1	A	352	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	A	107	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	145	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	113	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	A	22	ALA	CB-CA-C	6.01	119.11	110.10
1	A	151	ALA	CB-CA-C	6.00	119.10	110.10
1	B	144	TYR	CG-CD2-CE2	-5.99	116.51	121.30
1	A	379	PHE	CA-CB-CG	5.98	128.26	113.90
1	B	56	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	173	TYR	CB-CG-CD1	5.94	124.56	121.00
1	B	346	THR	CA-CB-OG1	-5.93	96.54	109.00
1	A	97	VAL	CG1-CB-CG2	-5.89	101.47	110.90
1	A	187	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	342	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	A	352	GLU	CG-CD-OE2	5.86	130.03	118.30
1	A	201	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	B	216	GLU	CG-CD-OE1	5.86	130.02	118.30
1	A	112	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	254	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	249	ARG	CD-NE-CZ	5.85	131.79	123.60
1	B	360	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	B	368	ASP	CB-CG-OD1	5.84	123.55	118.30
1	B	330	GLU	CG-CD-OE1	-5.83	106.65	118.30
1	A	252	LYS	CB-CG-CD	5.75	126.56	111.60
1	B	289	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	B	48	TYR	N-CA-CB	-5.73	100.28	110.60
1	B	80	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	263	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	301	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	B	203	GLU	CG-CD-OE2	5.66	129.62	118.30
1	B	321	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	149	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	333	GLU	CG-CD-OE1	5.58	129.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	PHE	CA-C-O	-5.57	108.40	120.10
1	B	273	LEU	CB-CG-CD1	5.57	120.46	111.00
1	A	342	GLU	CG-CD-OE2	-5.57	107.17	118.30
1	B	320	GLU	CG-CD-OE1	-5.56	107.17	118.30
1	B	180	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	A	320	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	B	392	GLY	C-N-CA	5.54	135.54	121.70
1	B	374	GLU	CA-CB-CG	5.54	125.58	113.40
1	B	326	ARG	CD-NE-CZ	5.53	131.34	123.60
1	B	368	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	263	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	53	HIS	N-CA-CB	5.51	120.51	110.60
1	B	27	VAL	CA-CB-CG1	-5.50	102.65	110.90
1	B	206	GLU	CA-CB-CG	5.48	125.45	113.40
1	A	66	GLU	CG-CD-OE1	-5.43	107.43	118.30
1	A	173	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	297	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	155	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	A	149	ASP	N-CA-C	-5.39	96.44	111.00
1	A	320	GLU	CG-CD-OE2	5.38	129.06	118.30
1	A	93	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	B	110	ILE	CB-CG1-CD1	5.35	128.89	113.90
1	A	23	ASP	CB-CA-C	5.35	121.10	110.40
1	A	377	PHE	CA-C-N	5.35	128.96	117.20
1	B	272	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	A	68	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	B	368	ASP	OD1-CG-OD2	-5.33	113.17	123.30
1	A	211	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	228	THR	O-C-N	-5.32	114.19	122.70
1	B	316	LEU	CB-CA-C	5.32	120.31	110.20
1	A	156	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	359	ASN	N-CA-CB	-5.30	101.06	110.60
1	A	134	VAL	CA-CB-CG1	5.29	118.84	110.90
1	A	326	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	156	ARG	CB-CG-CD	5.28	125.33	111.60
1	A	112	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	145	ASP	CA-C-N	5.25	126.70	116.20
1	A	357	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	393	SER	N-CA-CB	-5.25	102.63	110.50
1	B	305	TRP	CB-CA-C	5.24	120.87	110.40
1	A	223	ALA	C-N-CA	5.22	133.26	122.30
1	B	294	LYS	CB-CG-CD	-5.21	98.05	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	342	GLU	CG-CD-OE1	5.20	128.70	118.30
1	A	288	PRO	O-C-N	5.19	131.00	122.70
1	A	34	ASP	OD1-CG-OD2	-5.17	113.47	123.30
1	A	297	ARG	CG-CD-NE	5.14	122.60	111.80
1	B	178	ALA	O-C-N	-5.13	114.49	122.70
1	A	174	ASN	CB-CA-C	5.13	120.65	110.40
1	A	126	ALA	CB-CA-C	5.12	117.78	110.10
1	A	327	ALA	CB-CA-C	5.12	117.78	110.10
1	B	167	TYR	CB-CG-CD1	5.11	124.06	121.00
1	B	27	VAL	CA-CB-CG2	5.11	118.56	110.90
1	A	56	ASP	N-CA-CB	5.10	119.78	110.60
1	B	126	ALA	CB-CA-C	5.08	117.72	110.10
1	A	109	SER	CB-CA-C	5.08	119.75	110.10
1	B	297	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	357	LEU	CB-CG-CD2	-5.07	102.37	111.00
1	B	37	GLU	OE1-CD-OE2	-5.07	117.21	123.30
1	B	34	ASP	CA-CB-CG	5.07	124.55	113.40
1	A	394	ARG	CA-CB-CG	5.04	124.50	113.40
1	A	117	LYS	CD-CE-NZ	5.04	123.29	111.70
1	B	67	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	179	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	185	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	B	159	GLU	CG-CD-OE1	5.02	128.34	118.30
1	A	316	LEU	CB-CA-C	5.01	119.72	110.20
1	B	153	ALA	CB-CA-C	5.00	117.60	110.10

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	3026	0	2888	62	1
1	B	3026	0	2887	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	12	2	0
3	B	11	0	12	1	0
4	A	291	0	0	20	4
4	B	290	0	0	19	3
All	All	6659	0	5799	130	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 (130) 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:374:GLU:HG2	4:B:402:HOH:O	1.25	1.33
1:A:5:THR:HB	4:A:563:HOH:O	1.38	1.20
1:B:374:GLU:CG	4:B:402:HOH:O	1.85	1.00
1:A:364:PHE:HB2	4:A:628:HOH:O	1.69	0.92
1:A:95:HIS:HD2	1:A:97:VAL:H	1.33	0.77
1:B:95:HIS:HD2	1:B:97:VAL:H	1.31	0.76
1:B:342:GLU:OE1	4:B:622:HOH:O	2.04	0.74
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.69	0.73
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.69	0.73
1:B:40:HIS:HE1	4:B:585:HOH:O	1.72	0.72
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.12	0.70
1:B:6:PRO:O	1:B:9:HIS:HD2	1.74	0.70
1:A:394:ARG:HD3	4:A:618:HOH:O	1.90	0.70
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.58	0.69
1:A:32:ASN:ND2	4:A:568:HOH:O	2.26	0.69
1:A:294:LYS:NZ	4:A:691:HOH:O	2.24	0.68
1:A:68:GLU:HG3	4:A:580:HOH:O	1.95	0.66
1:B:65:ALA:HA	1:B:68:GLU:HG3	1.78	0.66
1:A:20:THR:HG22	4:A:564:HOH:O	1.95	0.66
1:B:16:THR:OG1	1:B:17:VAL:N	2.29	0.64
1:B:292:ASP:OD2	3:B:400:NOJ:H3	1.96	0.64
1:B:9:HIS:HB2	4:B:580:HOH:O	1.96	0.63
1:B:333:GLU:CG	4:B:662:HOH:O	2.47	0.63
1:B:176:ARG:HB3	1:B:241:PHE:CE2	2.34	0.63
1:B:24:PRO:HA	4:B:582:HOH:O	1.98	0.63
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.80	0.63
1:B:374:GLU:HG3	4:B:402:HOH:O	1.75	0.62
1:B:6:PRO:O	1:B:9:HIS:CD2	2.53	0.62
1:B:333:GLU:HG3	4:B:662:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.82	0.60
1:A:95:HIS:CD2	1:A:97:VAL:H	2.15	0.60
1:B:361:SER:OG	1:B:365:ALA:HB3	2.02	0.59
1:A:202:ILE:O	1:A:205:LEU:HB2	2.04	0.58
1:A:68:GLU:OE1	4:A:585:HOH:O	2.17	0.58
1:A:301:TYR:HD2	4:A:527:HOH:O	1.86	0.58
1:A:252:LYS:HE3	4:B:406:HOH:O	2.03	0.58
1:A:217:THR:HA	1:A:227:PHE:CD1	2.39	0.57
1:A:284:LYS:HE3	4:A:520:HOH:O	2.04	0.57
1:A:75:ASN:ND2	4:A:587:HOH:O	2.35	0.57
1:B:64:GLU:CB	4:B:652:HOH:O	2.52	0.57
1:B:87:MET:HA	1:B:132:THR:O	2.06	0.56
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.70	0.55
1:B:55:ASN:HA	1:B:58:ILE:O	2.07	0.55
1:B:319:LYS:HD3	4:B:546:HOH:O	2.05	0.55
1:B:333:GLU:CB	4:B:662:HOH:O	2.54	0.55
1:B:40:HIS:CE1	4:B:585:HOH:O	2.52	0.55
1:B:235:LEU:HD12	1:B:273:LEU:HD11	1.89	0.54
1:A:252:LYS:CE	4:B:406:HOH:O	2.54	0.54
1:B:361:SER:O	1:B:366:GLY:N	2.32	0.54
1:A:68:GLU:CG	4:A:580:HOH:O	2.54	0.54
1:B:5:THR:O	1:B:7:ALA:N	2.41	0.53
1:A:273:LEU:HD23	4:A:521:HOH:O	2.08	0.53
1:B:333:GLU:HB2	4:B:662:HOH:O	2.09	0.53
1:B:95:HIS:CD2	1:B:97:VAL:HG12	2.44	0.53
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.91	0.52
1:A:89:THR:HG21	3:A:400:NOJ:H62	1.92	0.51
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.92	0.51
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.93	0.50
1:B:34:ASP:OD1	1:B:36:VAL:HB	2.11	0.50
1:A:55:ASN:HA	1:A:58:ILE:O	2.11	0.50
1:A:6:PRO:HD2	4:A:563:HOH:O	2.11	0.50
1:B:105:SER:O	1:B:111:ARG:HD3	2.10	0.50
1:B:182:LYS:HE2	1:B:184:ASN:O	2.11	0.50
1:A:20:THR:HB	1:A:30:ARG:O	2.11	0.50
1:B:43:ALA:HA	1:B:83:LEU:HD21	1.92	0.50
1:A:222:MET:O	1:A:251:ILE:HG23	2.12	0.49
1:A:2:VAL:HG12	1:A:2:VAL:O	2.12	0.49
1:B:66:GLU:HA	4:B:589:HOH:O	2.12	0.49
1:A:19:TRP:CE3	1:A:294:LYS:HB3	2.47	0.49
1:A:48:TYR:CZ	1:A:84:LYS:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:OG1	1:A:17:VAL:N	2.46	0.49
1:A:380:ILE:HD11	1:B:296:SER:HB2	1.95	0.49
1:A:217:THR:O	1:A:221:GLN:HG3	2.13	0.48
1:A:182:LYS:HD3	1:A:185:GLU:O	2.13	0.48
1:B:141:GLY:HA3	1:B:189:ASP:O	2.14	0.48
1:B:6:PRO:O	1:B:48:TYR:CD1	2.66	0.47
1:B:95:HIS:CD2	1:B:97:VAL:H	2.21	0.47
1:B:53:HIS:CD2	1:B:89:THR:HG23	2.49	0.47
1:B:355:ALA:O	1:B:359:ASN:HB3	2.14	0.47
1:A:328:ASP:OD2	4:A:618:HOH:O	2.20	0.47
1:A:124:LEU:HA	1:A:127:GLU:HG3	1.97	0.47
1:B:71:LEU:HD22	1:B:128:MET:CE	2.44	0.47
1:A:14:LEU:HD11	4:A:570:HOH:O	2.14	0.47
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.85	0.46
1:B:315:TYR:O	1:B:319:LYS:HB2	2.16	0.46
1:A:289:ARG:HD2	4:A:403:HOH:O	2.14	0.46
1:B:20:THR:HB	1:B:30:ARG:O	2.16	0.46
1:B:53:HIS:HA	1:B:89:THR:O	2.15	0.46
1:A:85:VAL:O	1:A:130:ALA:HA	2.16	0.46
1:A:348:LEU:HD23	1:A:357:LEU:HD22	1.97	0.46
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.78	0.45
1:A:329:PRO:HG3	4:A:664:HOH:O	2.16	0.45
1:B:10:PHE:CD2	1:B:312:MET:HG2	2.52	0.45
1:A:381:ARG:HG3	4:A:634:HOH:O	2.16	0.45
1:B:137:GLY:CA	1:B:140:GLU:HG2	2.47	0.45
1:A:58:ILE:HD13	1:A:67:ARG:HG3	1.99	0.45
1:B:158:ARG:HG3	1:B:205:LEU:HD23	1.98	0.45
1:B:2:VAL:HG12	1:B:2:VAL:O	2.17	0.45
1:B:9:HIS:CB	4:B:580:HOH:O	2.62	0.44
1:B:131:GLU:O	1:B:175:LEU:HA	2.18	0.44
1:A:95:HIS:CD2	1:A:96:PRO:HD2	2.53	0.44
1:B:176:ARG:HB3	1:B:241:PHE:HE2	1.80	0.44
1:A:5:THR:O	1:A:8:ASP:HB2	2.17	0.44
1:B:202:ILE:HG21	1:B:239:LYS:HE3	1.99	0.44
1:A:77:ALA:O	1:A:81:THR:HG23	2.18	0.44
1:B:176:ARG:HB2	4:B:471:HOH:O	2.18	0.43
1:A:34:ASP:HA	1:A:35:PRO:HD3	1.87	0.43
1:A:192:LEU:N	1:A:193:PRO:CD	2.81	0.43
1:A:261:HIS:NE2	1:B:384:GLN:NE2	2.65	0.43
1:A:384:GLN:NE2	1:B:261:HIS:NE2	2.66	0.43
1:A:180:GLU:HG3	1:A:214:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:HG2	1:A:315:TYR:CE2	2.54	0.42
1:B:328:ASP:HA	1:B:329:PRO:HD2	1.76	0.42
1:A:53:HIS:NE2	3:A:400:NOJ:N5	2.68	0.41
1:B:71:LEU:CD2	1:B:128:MET:CE	2.98	0.41
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.54	0.41
1:A:289:ARG:CD	4:A:403:HOH:O	2.68	0.41
1:A:215:PRO:HG2	1:A:231:ILE:HG22	2.02	0.41
1:A:110:ILE:O	1:A:111:ARG:C	2.58	0.41
1:B:20:THR:O	1:B:29:THR:N	2.48	0.41
1:B:218:GLY:HA2	1:B:248:GLN:HB2	2.02	0.41
1:A:182:LYS:O	1:A:190:ILE:HB	2.21	0.41
1:A:41:LYS:O	1:A:45:LEU:HG	2.21	0.40
1:A:202:ILE:CD1	1:A:213:LEU:HD23	2.51	0.40
1:A:123:ASP:OD1	1:A:173:TYR:OH	2.22	0.40
1:B:23:ASP:CB	1:B:24:PRO:HD2	2.48	0.40
1:B:185:GLU:HA	1:B:186:PRO:HA	1.85	0.40
1:B:325:PHE:CZ	1:B:386:ALA:HB2	2.56	0.40
1:B:182:LYS:HG2	1:B:183:PRO:HD2	2.03	0.40
1:B:214:ASN:OD1	1:B:242:HIS:ND1	2.45	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:A:116:ALA:CB	4:A:628:HOH:O[4_555]	1.44	0.76
4:B:529:HOH:O	4:B:609:HOH:O[4_555]	2.03	0.17
4:A:472:HOH:O	4:A:600:HOH:O[4_555]	2.05	0.15
4:A:552:HOH:O	4:B:679:HOH:O[4_555]	2.18	0.02
4:A:566:HOH:O	4:B:435:HOH:O[4_555]	2.19	0.01

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	391/394 (99%)	375 (96%)	15 (4%)	1 (0%)	46 68
1	B	391/394 (99%)	378 (97%)	11 (3%)	2 (0%)	34 55
All	All	782/788 (99%)	753 (96%)	26 (3%)	3 (0%)	39 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	PRO
1	A	185	GLU
1	B	185	GLU

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	305/310 (98%)	294 (96%)	11 (4%)	42 69
1	B	305/310 (98%)	294 (96%)	11 (4%)	42 69
All	All	610/620 (98%)	588 (96%)	22 (4%)	42 69

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	94	SER
1	A	149	ASP
1	A	184	ASN
1	A	213	LEU
1	A	273	LEU
1	A	284	LYS
1	A	289	ARG
1	A	336	LYS
1	A	361	SER
1	A	393	SER
1	B	6	PRO
1	B	17	VAL

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Mol	Chain	Res	Type
1	B	68	GLU
1	B	99	LYS
1	B	174	ASN
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	293	TYR
1	B	320	GLU
1	B	361	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	9	HIS
1	A	40	HIS
1	A	75	ASN
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	384	GLN
1	B	9	HIS
1	B	95	HIS
1	B	184	ASN
1	B	221	GLN
1	B	349	ASN
1	B	384	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NOJ	A	400	2	11,11,11	4.85	3 (27%)	11,15,15	2.02	6 (54%)
3	NOJ	B	400	2	11,11,11	4.65	3 (27%)	11,15,15	1.72	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NOJ	A	400	2	-	0/2/19/19	0/1/1/1
3	NOJ	B	400	2	-	0/2/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	NOJ	C5-N5	-13.81	1.33	1.47
3	B	400	NOJ	C5-N5	-13.11	1.33	1.47
3	A	400	NOJ	C1-N5	-7.25	1.35	1.47
3	B	400	NOJ	C1-N5	-6.86	1.36	1.47
3	B	400	NOJ	C1-C2	2.30	1.54	1.52
3	A	400	NOJ	O6-C6	2.77	1.54	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	NOJ	C2-C3-C4	-3.25	105.53	111.04
3	B	400	NOJ	C2-C3-C4	-2.80	106.28	111.04
3	A	400	NOJ	O6-C6-C5	-2.54	104.33	111.12
3	B	400	NOJ	O6-C6-C5	-2.17	105.33	111.12
3	A	400	NOJ	C1-C2-C3	-2.10	107.89	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	NOJ	O3-C3-C4	2.08	115.01	110.34
3	A	400	NOJ	O2-C2-C3	2.09	114.32	110.12
3	A	400	NOJ	O2-C2-C1	2.24	114.05	109.57
3	B	400	NOJ	O2-C2-C3	3.41	116.99	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NOJ	2	0
3	B	400	NOJ	1	0

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.