Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:35 PM GMT

PDB ID	:	1BHW
Title	:	LOW TEMPERATURE MIDDLE RESOLUTION STRUCTURE OF XYLOSE ISOMERASE FROM MASC DATA
Authors	:	Ramin, M.; Shepard, W.; Fourme, R.; Kahn, R.
Deposited on	:	1998-06-10
Resolution	:	4.10 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:

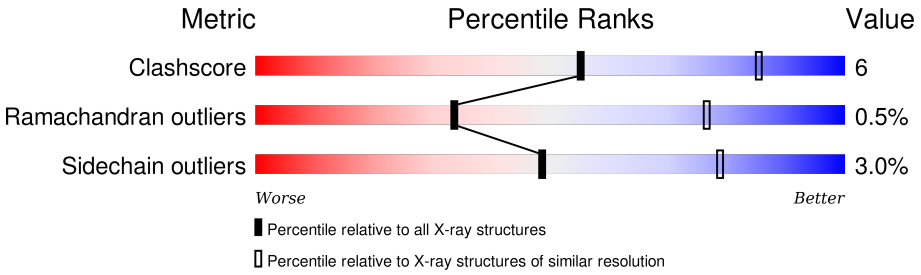
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 4.10 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	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)

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	76% 20%
1	B	393	77% 19%
1	C	393	79% 18%
1	D	393	76% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12248 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			
1	B	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			
1	C	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			
1	D	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ASN	HIS	CONFLICT	UNP P12851
B	220	ASN	HIS	CONFLICT	UNP P12851
C	220	ASN	HIS	CONFLICT	UNP P12851
D	220	ASN	HIS	CONFLICT	UNP P12851

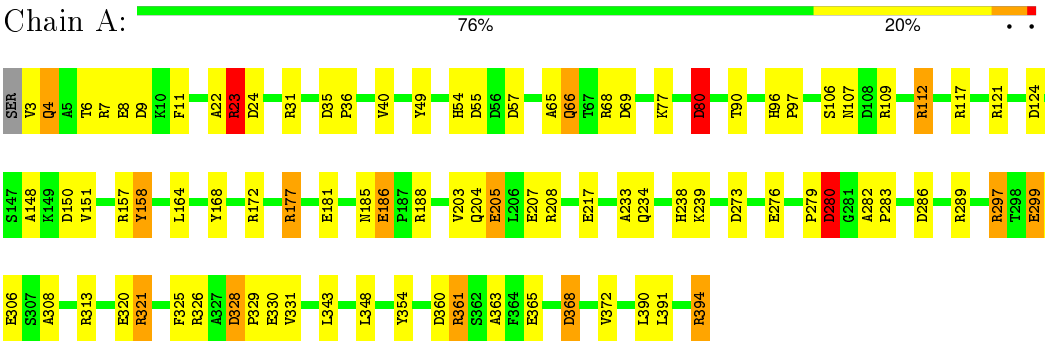
3 Residue-property plots (i)

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.

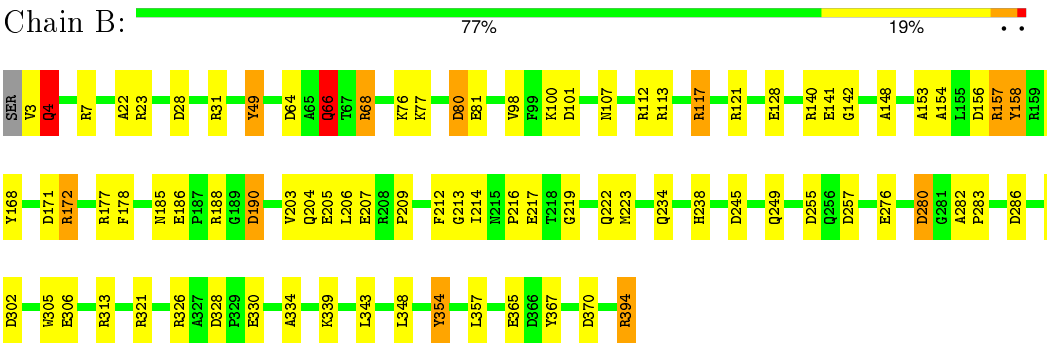
- Molecule 1: XYLOSE ISOMERASE

Chain A:



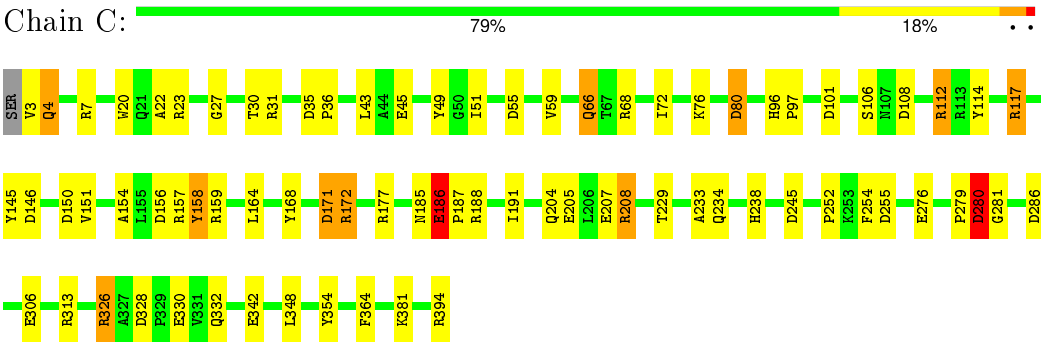
- Molecule 1: XYLOSE ISOMERASE

Chain B:



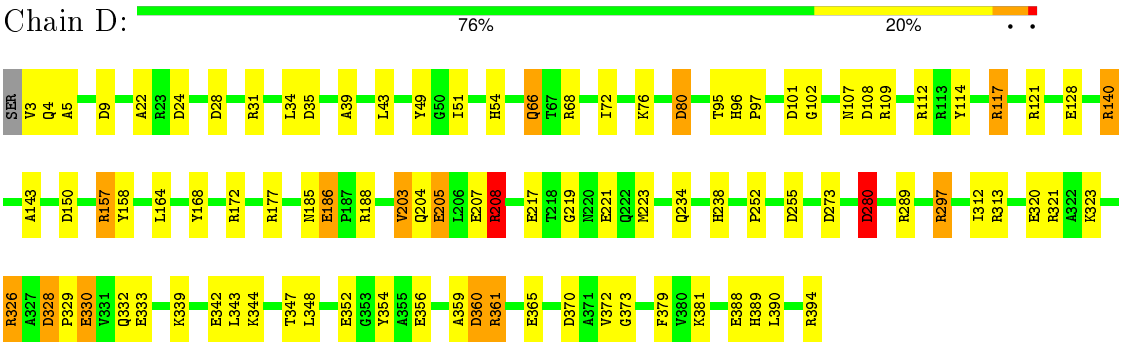
- Molecule 1: XYLOSE ISOMERASE

Chain C:



• Molecule 1: 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	141.91Å 141.91Å 227.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 4.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-4.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.315 , 0.321	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12248	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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	2.12	11/3133 (0.4%)	2.72	85/4243 (2.0%)
1	B	1.97	11/3133 (0.4%)	2.66	70/4243 (1.6%)
1	C	2.09	13/3133 (0.4%)	2.74	71/4243 (1.7%)
1	D	1.96	12/3133 (0.4%)	2.65	74/4243 (1.7%)
All	All	2.04	47/12532 (0.4%)	2.69	300/16972 (1.8%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4	GLN	CG-CD	-47.80	0.41	1.51
1	C	4	GLN	CG-CD	-46.65	0.43	1.51
1	A	66	GLN	CG-CD	-46.63	0.43	1.51
1	C	66	GLN	CG-CD	-46.63	0.43	1.51
1	A	4	GLN	CG-CD	-45.34	0.46	1.51
1	D	280	ASP	CB-CG	-42.30	0.62	1.51
1	C	66	GLN	CB-CG	-40.16	0.44	1.52
1	A	66	GLN	CB-CG	-39.45	0.46	1.52
1	B	4	GLN	CG-CD	-38.84	0.61	1.51
1	B	66	GLN	CG-CD	-38.84	0.61	1.51
1	D	66	GLN	CG-CD	-38.84	0.61	1.51
1	B	66	GLN	CB-CG	-38.67	0.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4	GLN	CB-CG	-38.29	0.49	1.52
1	A	280	ASP	CB-CG	-37.96	0.72	1.51
1	A	66	GLN	CD-OE1	-36.48	0.43	1.24
1	B	4	GLN	CD-OE1	-36.45	0.43	1.24
1	C	4	GLN	CD-OE1	-36.45	0.43	1.24
1	C	66	GLN	CD-OE1	-36.45	0.43	1.24
1	A	4	GLN	CD-OE1	-36.43	0.43	1.24
1	A	4	GLN	CB-CG	-36.12	0.55	1.52
1	B	4	GLN	CB-CG	-36.02	0.55	1.52
1	D	66	GLN	CB-CG	-33.92	0.60	1.52
1	B	66	GLN	CD-NE2	31.88	2.12	1.32
1	B	280	ASP	CB-CG	-30.45	0.87	1.51
1	C	4	GLN	CB-CG	-29.64	0.72	1.52
1	C	280	ASP	CB-CG	-29.49	0.89	1.51
1	D	280	ASP	CG-OD2	-23.23	0.71	1.25
1	B	280	ASP	CG-OD2	-21.70	0.75	1.25
1	D	66	GLN	CD-OE1	-18.46	0.83	1.24
1	D	66	GLN	CD-NE2	-18.39	0.86	1.32
1	A	66	GLN	CD-NE2	-18.34	0.86	1.32
1	B	4	GLN	CD-NE2	-18.32	0.87	1.32
1	C	4	GLN	CD-NE2	-18.30	0.87	1.32
1	A	4	GLN	CD-NE2	-18.27	0.87	1.32
1	C	280	ASP	CG-OD2	-18.27	0.83	1.25
1	C	280	ASP	CG-OD1	15.24	1.60	1.25
1	D	280	ASP	CG-OD1	13.21	1.55	1.25
1	C	66	GLN	CD-NE2	-11.75	1.03	1.32
1	D	328	ASP	C-N	-11.11	1.13	1.34
1	C	328	ASP	C-N	-10.06	1.15	1.34
1	D	4	GLN	CD-NE2	-9.66	1.08	1.32
1	B	66	GLN	CD-OE1	-7.93	1.06	1.24
1	D	4	GLN	CD-OE1	-7.89	1.06	1.24
1	A	328	ASP	C-N	-7.17	1.20	1.34
1	B	328	ASP	C-N	-7.01	1.21	1.34
1	A	280	ASP	CG-OD2	6.24	1.39	1.25
1	C	186	GLU	CD-OE2	-5.42	1.19	1.25

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	280	ASP	CB-CG-OD2	58.83	171.25	118.30
1	D	280	ASP	OD1-CG-OD2	-58.57	12.02	123.30
1	C	280	ASP	CB-CG-OD2	57.08	169.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	GLN	OE1-CD-NE2	-53.00	0.00	121.90
1	A	66	GLN	OE1-CD-NE2	-52.98	0.05	121.90
1	C	4	GLN	OE1-CD-NE2	-52.98	0.05	121.90
1	A	4	GLN	OE1-CD-NE2	-52.96	0.09	121.90
1	B	4	GLN	OE1-CD-NE2	-52.96	0.09	121.90
1	D	280	ASP	CB-CG-OD1	51.55	164.69	118.30
1	C	280	ASP	OD1-CG-OD2	-50.92	26.55	123.30
1	B	280	ASP	OD1-CG-OD2	-49.49	29.26	123.30
1	A	280	ASP	CA-CB-CG	-48.81	6.01	113.40
1	C	66	GLN	OE1-CD-NE2	-48.02	11.45	121.90
1	C	4	GLN	CA-CB-CG	-44.86	14.71	113.40
1	C	280	ASP	CA-CB-CG	-44.49	15.53	113.40
1	A	280	ASP	OD1-CG-OD2	-44.33	39.07	123.30
1	A	66	GLN	CA-CB-CG	-43.38	17.97	113.40
1	D	280	ASP	CA-CB-CG	-43.04	18.72	113.40
1	D	4	GLN	OE1-CD-NE2	-41.36	26.78	121.90
1	D	66	GLN	OE1-CD-NE2	-40.16	29.54	121.90
1	D	280	ASP	CB-CG-OD2	38.98	153.39	118.30
1	A	4	GLN	CA-CB-CG	-35.97	34.27	113.40
1	A	280	ASP	CB-CG-OD2	-35.23	86.59	118.30
1	B	66	GLN	CG-CD-OE1	-33.42	54.75	121.60
1	D	66	GLN	CA-CB-CG	-33.38	39.97	113.40
1	D	4	GLN	CA-CB-CG	-31.05	45.09	113.40
1	A	66	GLN	CG-CD-OE1	29.15	179.89	121.60
1	C	66	GLN	CG-CD-OE1	29.15	179.89	121.60
1	C	4	GLN	CG-CD-OE1	29.11	179.81	121.60
1	C	280	ASP	CB-CG-OD1	27.64	143.17	118.30
1	B	280	ASP	CB-CG-OD1	26.93	142.53	118.30
1	A	4	GLN	CG-CD-OE1	26.70	175.01	121.60
1	C	66	GLN	CA-CB-CG	-26.54	55.01	113.40
1	A	66	GLN	CG-CD-NE2	26.34	179.91	116.70
1	C	4	GLN	CG-CD-NE2	26.32	179.86	116.70
1	B	66	GLN	CG-CD-NE2	-25.81	54.75	116.70
1	B	66	GLN	CA-CB-CG	-25.13	58.11	113.40
1	B	4	GLN	CA-CB-CG	-25.01	58.38	113.40
1	B	280	ASP	CA-CB-CG	-24.53	59.43	113.40
1	D	4	GLN	CB-CG-CD	24.31	174.81	111.60
1	A	4	GLN	CG-CD-NE2	24.26	174.93	116.70
1	D	4	GLN	CG-CD-NE2	21.98	169.45	116.70
1	A	66	GLN	CB-CG-CD	21.64	167.86	111.60
1	C	66	GLN	CG-CD-NE2	21.58	168.50	116.70
1	A	4	GLN	CB-CG-CD	20.27	164.31	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	66	GLN	CB-CG-CD	20.17	164.04	111.60
1	B	117	ARG	NE-CZ-NH1	20.12	130.36	120.30
1	B	4	GLN	CG-CD-OE1	19.49	160.58	121.60
1	C	66	GLN	CB-CG-CD	19.05	161.14	111.60
1	B	4	GLN	CG-CD-NE2	18.25	160.50	116.70
1	B	172	ARG	NE-CZ-NH1	18.19	129.40	120.30
1	B	394	ARG	NE-CZ-NH2	-17.54	111.53	120.30
1	D	66	GLN	CG-CD-OE1	-15.76	90.08	121.60
1	B	157	ARG	NE-CZ-NH1	15.66	128.13	120.30
1	B	117	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	C	117	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	A	326	ARG	NE-CZ-NH1	14.35	127.47	120.30
1	B	172	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	C	172	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	A	172	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	D	117	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	B	66	GLN	CB-CG-CD	13.27	146.11	111.60
1	B	140	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	A	280	ASP	CB-CG-OD1	-13.21	106.42	118.30
1	D	4	GLN	CG-CD-OE1	12.84	147.28	121.60
1	D	150	ASP	CB-CG-OD1	12.73	129.75	118.30
1	A	361	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	D	328	ASP	O-C-N	12.29	144.44	121.10
1	C	172	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	D	140	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	A	394	ARG	NE-CZ-NH2	-12.01	114.30	120.30
1	D	255	ASP	CB-CG-OD2	-11.94	107.56	118.30
1	A	117	ARG	NE-CZ-NH1	11.55	126.07	120.30
1	C	177	ARG	NE-CZ-NH1	11.45	126.03	120.30
1	A	80	ASP	CB-CG-OD1	-11.44	108.00	118.30
1	A	321	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	B	321	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	D	313	ARG	NE-CZ-NH2	11.21	125.91	120.30
1	C	158	TYR	CB-CG-CD2	11.14	127.68	121.00
1	B	177	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	D	172	ARG	CD-NE-CZ	10.92	138.89	123.60
1	D	188	ARG	NE-CZ-NH2	10.92	125.76	120.30
1	B	113	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	B	68	ARG	NE-CZ-NH1	-10.73	114.94	120.30
1	B	157	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	328	ASP	CB-CG-OD2	10.44	127.69	118.30
1	A	205	GLU	OE1-CD-OE2	-10.09	111.19	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	255	ASP	CB-CG-OD1	9.94	127.25	118.30
1	C	188	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	B	158	TYR	CB-CG-CD2	9.84	126.90	121.00
1	B	330	GLU	OE1-CD-OE2	9.75	135.00	123.30
1	C	297	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	A	172	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	150	ASP	CB-CG-OD1	9.48	126.83	118.30
1	D	328	ASP	C-N-CD	9.46	148.27	128.40
1	A	326	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	7	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	D	117	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	146	ASP	CB-CG-OD1	9.19	126.57	118.30
1	B	286	ASP	CB-CG-OD1	9.18	126.56	118.30
1	D	328	ASP	CA-C-N	-9.12	91.58	117.10
1	D	35	ASP	CB-CG-OD1	8.99	126.39	118.30
1	A	313	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	172	ARG	CD-NE-CZ	8.95	136.13	123.60
1	D	326	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	A	117	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	188	ARG	CD-NE-CZ	8.81	135.94	123.60
1	D	330	GLU	OE1-CD-OE2	8.76	133.81	123.30
1	A	31	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	80	ASP	CA-CB-CG	-8.71	94.24	113.40
1	A	121	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	D	109	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	124	ASP	CB-CG-OD1	8.60	126.04	118.30
1	D	31	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	80	ASP	CB-CG-OD1	-8.51	110.64	118.30
1	B	31	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	C	117	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	158	TYR	CB-CG-CD2	8.34	126.00	121.00
1	B	113	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	B	80	ASP	CB-CG-OD1	-8.31	110.82	118.30
1	C	31	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	D	9	ASP	CB-CG-OD2	8.24	125.71	118.30
1	A	394	ARG	NH1-CZ-NH2	8.21	128.44	119.40
1	C	23	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	D	370	ASP	CB-CG-OD2	8.06	125.56	118.30
1	D	24	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	C	23	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	273	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	121	ARG	NE-CZ-NH2	-7.92	116.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	186	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	C	328	ASP	O-C-N	7.84	136.00	121.10
1	B	302	ASP	CB-CG-OD1	7.84	125.35	118.30
1	D	9	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	B	328	ASP	O-C-N	7.79	135.91	121.10
1	C	276	GLU	OE1-CD-OE2	-7.79	113.95	123.30
1	B	112	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	C	330	GLU	OE1-CD-OE2	7.68	132.52	123.30
1	C	313	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	D	112	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	156	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	A	300	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C	7	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	109	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	188	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	B	302	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	297	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	328	ASP	CB-CG-OD2	7.40	124.96	118.30
1	A	361	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	D	208	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	172	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	80	ASP	OD1-CG-OD2	7.35	137.26	123.30
1	D	394	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	158	TYR	CB-CG-CD1	-7.34	116.60	121.00
1	A	24	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	55	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	121	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	D	188	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	B	121	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	C	157	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	320	GLU	OE1-CD-OE2	-7.16	114.70	123.30
1	C	394	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	D	360	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	B	141	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	B	394	ARG	N-CA-CB	6.98	123.16	110.60
1	C	286	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	313	ARG	CD-NE-CZ	6.94	133.32	123.60
1	D	109	ARG	CD-NE-CZ	6.92	133.29	123.60
1	A	68	ARG	CD-NE-CZ	6.90	133.26	123.60
1	B	321	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	342	GLU	CG-CD-OE2	6.81	131.91	118.30
1	A	186	GLU	OE1-CD-OE2	-6.78	115.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	ASP	O-C-N	6.74	133.90	121.10
1	C	55	ASP	CB-CG-OD1	6.72	124.35	118.30
1	C	108	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	55	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	68	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	205	GLU	CG-CD-OE2	6.67	131.63	118.30
1	C	145	TYR	CB-CG-CD2	6.66	124.99	121.00
1	D	140	ARG	NH1-CZ-NH2	6.64	126.71	119.40
1	D	24	ASP	CB-CG-OD1	6.64	124.28	118.30
1	C	276	GLU	CG-CD-OE2	6.62	131.53	118.30
1	A	368	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	204	GLN	OE1-CD-NE2	-6.56	106.80	121.90
1	C	245	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	28	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	112	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	57	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	23	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	121	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	342	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	C	156	ASP	CB-CG-OD1	6.26	123.93	118.30
1	C	177	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	146	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	68	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	D	54	HIS	N-CA-CB	6.22	121.80	110.60
1	C	207	GLU	CG-CD-OE1	6.20	130.69	118.30
1	D	177	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	177	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	203	VAL	CA-CB-CG1	6.17	120.16	110.90
1	C	80	ASP	OD1-CG-OD2	6.17	135.03	123.30
1	D	205	GLU	CG-CD-OE2	6.16	130.62	118.30
1	C	101	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	297	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	394	ARG	CA-CB-CG	6.12	126.86	113.40
1	D	150	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	80	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	D	221	GLU	CG-CD-OE1	6.08	130.46	118.30
1	A	394	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	C	208	ARG	CD-NE-CZ	-6.04	115.14	123.60
1	D	205	GLU	OE1-CD-OE2	-6.03	116.06	123.30
1	C	150	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	255	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	23	ARG	NE-CZ-NH2	-5.96	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	157	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	159	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	C	289	ARG	CD-NE-CZ	5.90	131.86	123.60
1	D	207	GLU	CA-CB-CG	5.90	126.38	113.40
1	A	300	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	204	GLN	OE1-CD-NE2	-5.87	108.39	121.90
1	B	328	ASP	CA-C-N	-5.83	100.76	117.10
1	C	177	ARG	N-CA-CB	5.82	121.08	110.60
1	A	158	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	B	255	ASP	CB-CG-OD1	5.78	123.50	118.30
1	D	28	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	157	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	281	GLY	N-CA-C	-5.73	98.77	113.10
1	D	333	GLU	CG-CD-OE2	5.72	129.75	118.30
1	A	31	ARG	NH1-CZ-NH2	5.71	125.69	119.40
1	D	143	ALA	N-CA-CB	-5.69	102.13	110.10
1	A	299	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	C	207	GLU	CG-CD-OE2	-5.68	106.94	118.30
1	C	313	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
1	D	217	GLU	CG-CD-OE1	-5.65	106.99	118.30
1	A	289	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	172	ARG	CD-NE-CZ	-5.64	115.70	123.60
1	B	121	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	208	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	276	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	B	305	TRP	CA-CB-CG	-5.61	103.04	113.70
1	B	313	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	45	GLU	CA-CB-CG	5.61	125.73	113.40
1	B	188	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	326	ARG	CD-NE-CZ	5.57	131.40	123.60
1	D	361	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	C	326	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	C	158	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	B	190	ASP	N-CA-CB	5.51	120.52	110.60
1	C	328	ASP	CA-C-N	-5.48	101.75	117.10
1	B	112	ARG	CG-CD-NE	5.46	123.27	111.80
1	C	191	ILE	CA-CB-CG2	5.46	121.83	110.90
1	A	8	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	B	394	ARG	CD-NE-CZ	-5.45	115.97	123.60
1	A	217	GLU	CG-CD-OE2	5.45	129.20	118.30
1	D	361	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	229	THR	CA-CB-OG1	-5.44	97.58	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	GLU	CG-CD-OE1	5.44	129.18	118.30
1	B	334	ALA	CB-CA-C	5.43	118.24	110.10
1	A	146	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	365	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	D	108	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	112	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	207	GLU	CA-CB-CG	5.40	125.28	113.40
1	D	320	GLU	CA-CB-CG	5.38	125.24	113.40
1	C	306	GLU	CG-CD-OE1	5.37	129.03	118.30
1	D	289	ARG	CD-NE-CZ	5.36	131.11	123.60
1	B	394	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	D	388	GLU	CG-CD-OE2	5.35	129.00	118.30
1	B	370	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	394	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	D	273	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	177	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	112	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	C	255	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	313	ARG	N-CA-CB	-5.29	101.07	110.60
1	B	68	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	101	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	394	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	B	330	GLU	CG-CD-OE2	-5.26	107.77	118.30
1	B	354	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	321	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	145	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	B	292	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	B	207	GLU	CG-CD-OE1	5.20	128.71	118.30
1	B	276	GLU	CG-CD-OE2	5.20	128.70	118.30
1	A	68	ARG	NH1-CZ-NH2	-5.20	113.69	119.40
1	C	158	TYR	CA-CB-CG	5.20	123.27	113.40
1	B	207	GLU	CG-CD-OE2	-5.19	107.93	118.30
1	C	143	ALA	CB-CA-C	-5.19	102.32	110.10
1	D	297	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	57	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	257	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	128	GLU	CA-CB-CG	5.12	124.66	113.40
1	A	148	ALA	N-CA-CB	-5.09	102.97	110.10
1	A	8	GLU	CA-CB-CG	-5.09	102.20	113.40
1	A	308	ALA	CB-CA-C	5.08	117.72	110.10
1	A	128	GLU	CG-CD-OE1	-5.08	108.14	118.30
1	A	328	ASP	CA-C-N	-5.07	102.91	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	54	HIS	N-CA-C	-5.07	97.32	111.00
1	B	213	GLY	O-C-N	5.06	130.79	122.70
1	C	171	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	A	280	ASP	Sidechain
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	3062	0	2967	58	0
1	B	3062	0	2967	58	0
1	C	3062	0	2964	39	0
1	D	3062	0	2967	60	0
All	All	12248	0	11865	151	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 6.

All (151) 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:66:GLN:CD	1:A:66:GLN:C	1.97	1.22
1:A:66:GLN:HB2	1:A:66:GLN:CD	1.61	1.18
1:A:66:GLN:N	1:A:66:GLN:CD	1.99	1.15
1:A:66:GLN:CD	1:A:66:GLN:HB3	1.69	1.12
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.27	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLN:CD	1:A:66:GLN:CB	0.88	0.98
1:A:66:GLN:HE22	1:A:66:GLN:CD	1.49	0.92
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.18	0.92
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.51	0.91
1:A:66:GLN:CD	1:A:66:GLN:HE21	1.49	0.90
1:A:279:PRO:O	1:A:280:ASP:OD2	1.92	0.87
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.86
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.21	0.84
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.83
1:A:66:GLN:CD	1:A:66:GLN:CA	0.72	0.81
1:A:66:GLN:CD	1:A:66:GLN:NE2	0.87	0.81
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.62	0.79
1:B:354:TYR:CD1	1:D:168:TYR:HD1	2.07	0.73
1:A:66:GLN:HA	1:A:66:GLN:CD	1.11	0.73
1:D:326:ARG:O	1:D:332:GLN:NE2	2.24	0.70
1:A:66:GLN:HG2	1:A:66:GLN:CD	1.09	0.69
1:A:66:GLN:CD	1:A:66:GLN:HG3	1.09	0.69
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.76	0.67
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.78	0.66
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.79	0.66
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.80	0.65
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.78	0.64
1:B:164:LEU:HD12	1:D:348:LEU:CD1	2.24	0.63
1:A:36:PRO:O	1:A:40:VAL:HG23	1.97	0.63
1:B:354:TYR:CD1	1:D:168:TYR:CD1	2.86	0.62
1:B:154:ALA:CB	1:D:343:LEU:HD21	2.29	0.62
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.82	0.61
1:D:208:ARG:NH1	1:D:208:ARG:HG2	2.04	0.59
1:B:339:LYS:HB2	1:D:107:ASN:HB3	1.85	0.58
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.86	0.58
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.85	0.57
1:B:171:ASP:CB	1:D:354:TYR:OH	2.52	0.57
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.87	0.56
1:A:168:TYR:HD1	1:C:354:TYR:CD1	2.23	0.56
1:A:354:TYR:CD1	1:C:168:TYR:HD1	2.23	0.56
1:B:107:ASN:HB3	1:D:339:LYS:HB2	1.88	0.55
1:B:164:LEU:CD1	1:D:348:LEU:HD21	2.37	0.55
1:C:72:ILE:O	1:C:76:LYS:HG3	2.06	0.55
1:B:171:ASP:OD2	1:D:354:TYR:OH	2.25	0.55
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.87	0.55
1:A:391:LEU:HD22	1:D:390:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HB2	1:D:344:LYS:HG2	1.88	0.54
1:B:77:LYS:O	1:B:80:ASP:HB2	2.08	0.53
1:A:233:ALA:HB1	1:C:151:VAL:HB	1.91	0.53
1:D:328:ASP:OD1	1:D:330:GLU:N	2.33	0.53
1:B:98:VAL:HA	1:D:373:GLY:HA2	1.90	0.53
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.10	0.52
1:A:348:LEU:HD11	1:C:164:LEU:CD1	2.40	0.52
1:B:354:TYR:CE1	1:D:168:TYR:HD1	2.28	0.51
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.92	0.51
1:B:3:VAL:HG12	1:B:4:GLN:H	1.77	0.50
1:C:254:PHE:CD1	1:D:186:GLU:HB2	2.47	0.49
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.94	0.49
1:A:6:THR:O	1:A:9:ASP:HB2	2.13	0.49
1:A:360:ASP:O	1:C:117:ARG:NH1	2.46	0.49
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.95	0.49
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.78	0.49
1:C:326:ARG:O	1:C:332:GLN:NE2	2.45	0.48
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.48	0.48
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.48
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.95	0.48
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.95	0.48
1:C:27:GLY:HA2	1:D:95:THR:HA	1.94	0.48
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.49	0.48
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.94	0.48
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:B:160:GLU:CD	1:D:347:THR:H	2.18	0.47
1:B:171:ASP:HB2	1:D:354:TYR:OH	2.14	0.47
1:C:106:SER:O	1:C:112:ARG:HD3	2.15	0.47
1:D:321:ARG:HG2	1:D:389:HIS:O	2.15	0.47
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.74	0.47
1:A:204:GLN:HB2	1:C:204:GLN:OE1	2.15	0.46
1:B:168:TYR:HD1	1:D:354:TYR:CD1	2.34	0.46
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.95	0.46
1:C:208:ARG:HD3	1:C:208:ARG:HH11	1.50	0.46
1:A:343:LEU:HD21	1:C:154:ALA:HB2	1.98	0.46
1:A:238:HIS:O	1:A:239:LYS:HB2	2.15	0.46
1:A:348:LEU:HD11	1:C:164:LEU:HD12	1.97	0.46
1:C:252:PRO:HB2	1:D:252:PRO:HB2	1.97	0.46
1:B:348:LEU:HD11	1:D:164:LEU:HD12	1.98	0.45
1:B:154:ALA:HB2	1:D:343:LEU:CD2	2.41	0.45
1:A:368:ASP:O	1:A:372:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.97	0.45
1:B:154:ALA:CA	1:D:343:LEU:HD21	2.47	0.45
1:B:107:ASN:HB3	1:D:339:LYS:CB	2.46	0.45
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.92	0.45
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.13	0.44
1:A:77:LYS:O	1:A:80:ASP:CB	2.65	0.44
1:C:30:THR:HG22	1:D:97:PRO:HB3	1.99	0.44
1:A:363:ALA:O	1:C:114:TYR:HA	2.17	0.44
1:B:164:LEU:C	1:B:164:LEU:HD23	2.37	0.44
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.90	0.44
1:A:354:TYR:OH	1:C:171:ASP:CB	2.66	0.44
1:A:325:PHE:O	1:A:331:VAL:HG11	2.17	0.44
1:A:164:LEU:HD12	1:C:348:LEU:CD1	2.47	0.44
1:B:100:LYS:HE2	1:D:373:GLY:O	2.17	0.44
1:B:219:GLY:O	1:B:223:MET:HG3	2.17	0.44
1:A:151:VAL:HB	1:C:233:ALA:CB	2.48	0.44
1:B:148:ALA:HB1	1:D:379:PHE:CE1	2.53	0.43
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.84	0.43
1:A:391:LEU:HD22	1:D:390:LEU:O	2.17	0.43
1:B:357:LEU:O	1:D:117:ARG:HD3	2.19	0.43
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.99	0.43
1:A:321:ARG:HD3	1:A:390:LEU:HA	2.01	0.43
1:A:348:LEU:CD1	1:C:164:LEU:HD12	2.49	0.43
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.54	0.43
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.54	0.42
1:B:343:LEU:O	1:D:157:ARG:HD2	2.19	0.42
1:B:282:ALA:HB1	1:B:283:PRO:HD2	2.01	0.42
1:A:233:ALA:CB	1:C:151:VAL:HB	2.49	0.42
1:D:356:GLU:O	1:D:359:ALA:HB3	2.19	0.42
1:B:142:GLY:HA3	1:B:190:ASP:O	2.19	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.42
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.01	0.42
1:B:348:LEU:HD11	1:D:164:LEU:CD1	2.50	0.42
1:A:330:GLU:OE1	1:A:394:ARG:NH1	2.52	0.42
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.35	0.42
1:A:354:TYR:CG	1:C:168:TYR:HD1	2.37	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.89	0.42
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.46	0.42
1:D:22:ALA:HB1	1:D:297:ARG:HG3	2.02	0.42
1:C:186:GLU:HA	1:C:187:PRO:HA	1.91	0.41
1:B:206:LEU:O	1:B:209:PRO:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:VAL:HG21	1:C:68:ARG:HG3	2.02	0.41
1:B:148:ALA:HB1	1:D:379:PHE:CD1	2.55	0.41
1:B:64:ASP:OD2	1:B:66:GLN:CD	2.59	0.41
1:B:101:ASP:CG	1:B:101:ASP:O	2.58	0.41
1:B:367:TYR:CD2	1:D:114:TYR:CD1	3.09	0.41
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.86	0.41
1:D:72:ILE:O	1:D:76:LYS:HG3	2.21	0.41
1:D:219:GLY:O	1:D:223:MET:HG3	2.20	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:A:107:ASN:O	1:C:342:GLU:HB3	2.21	0.41
1:B:117:ARG:NH1	1:D:360:ASP:O	2.54	0.41
1:B:164:LEU:CD1	1:D:348:LEU:HD11	2.37	0.41
1:B:157:ARG:HG3	1:D:343:LEU:HD12	2.01	0.41
1:B:98:VAL:HG23	1:D:372:VAL:HB	2.02	0.41
1:A:151:VAL:HB	1:C:233:ALA:HB1	2.02	0.41
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.51	0.41
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.36	0.40
1:A:106:SER:O	1:A:112:ARG:HD3	2.21	0.40
1:A:164:LEU:HD23	1:A:164:LEU:C	2.41	0.40
1:B:214:ILE:HG13	1:B:216:PRO:HD3	2.04	0.40
1:B:339:LYS:CB	1:D:107:ASN:HB3	2.50	0.40
1:B:217:GLU:HA	1:B:245:ASP:O	2.22	0.40
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.54	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 82
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	46 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	19 65
1	D	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	34 76
All	All	1560/1572 (99%)	1504 (96%)	48 (3%)	8 (0%)	34 76

All (8) 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	D	186	GLU
1	D	280	ASP
1	C	364	PHE

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	309/310 (100%)	299 (97%)	10 (3%)	46 78
1	B	309/310 (100%)	301 (97%)	8 (3%)	54 81
1	C	309/310 (100%)	301 (97%)	8 (3%)	54 81
1	D	309/310 (100%)	298 (96%)	11 (4%)	42 76
All	All	1236/1240 (100%)	1199 (97%)	37 (3%)	48 79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	GLN
1	A	49	TYR
1	A	80	ASP

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Mol	Chain	Res	Type
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	B	4	GLN
1	B	49	TYR
1	B	66	GLN
1	B	81	GLU
1	B	158	TYR
1	B	185	ASN
1	B	280	ASP
1	B	394	ARG
1	C	3	VAL
1	C	4	GLN
1	C	49	TYR
1	C	66	GLN
1	C	80	ASP
1	C	158	TYR
1	C	185	ASN
1	C	280	ASP
1	D	3	VAL
1	D	49	TYR
1	D	66	GLN
1	D	80	ASP
1	D	158	TYR
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	280	ASP
1	D	323	LYS
1	D	329	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	66	GLN
1	A	185	ASN
1	A	222	GLN
1	A	238	HIS

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Mol	Chain	Res	Type
1	B	185	ASN
1	B	222	GLN
1	B	238	HIS
1	C	4	GLN
1	C	185	ASN
1	C	222	GLN
1	C	238	HIS
1	C	250	HIS
1	D	4	GLN
1	D	185	ASN
1	D	222	GLN
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.